



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 06:49 PM EST

PDB ID : 5B5E  
Title : Crystal structure analysis of Photosystem II complex  
Authors : Tanaka, A.; Fukushima, Y.; Kamiya, N.  
Deposited on : 2016-05-02  
Resolution : 1.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

**i**

## X-RAY DIFFRACTION

A.

Ramachandran outliers

electron density. The numeric value is given above the bar.

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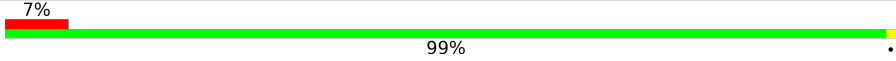

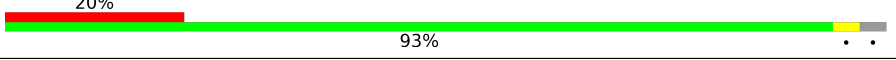

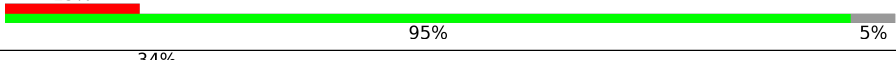
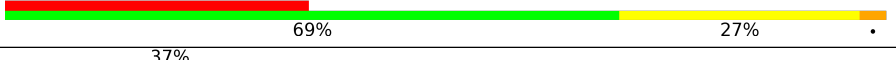

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Mol	Chain	Length	Quality of chain
4	D	342	
4	d	342	
5	E	83	
5	e	83	
6	F	44	
6	f	44	
7	H	65	
7	h	65	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	244	
13	o	244	
14	T	32	
14	t	32	
15	U	104	
15	u	104	
16	V	137	

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Mol	Chain	Length	Quality of chain
16	v	137	
17	Y	30	
17	y	30	
18	X	40	
18	x	40	
19	Z	62	
19	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	A	405	X	-	-	-
23	CLA	A	406	X	-	-	-
23	CLA	A	408	X	-	-	-
23	CLA	B	602	X	-	-	X
23	CLA	B	603	X	-	-	-
23	CLA	B	604	X	-	-	-
23	CLA	B	605	X	-	-	-
23	CLA	B	606	X	-	-	-
23	CLA	B	607	X	-	-	-
23	CLA	B	608	X	-	-	-
23	CLA	B	609	X	-	-	-
23	CLA	B	610	X	-	-	-
23	CLA	B	611	X	-	-	-
23	CLA	B	612	X	-	-	-
23	CLA	B	613	X	-	-	-
23	CLA	B	614	X	-	-	-
23	CLA	B	615	X	-	-	-
23	CLA	B	616	X	-	-	-
23	CLA	B	617	X	-	-	-
23	CLA	C	502	X	-	-	-
23	CLA	C	503	X	-	-	-
23	CLA	C	504	X	-	-	-
23	CLA	C	505	X	-	-	-
23	CLA	C	506	X	-	-	-
23	CLA	C	507	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	C	508	X	-	-	-
23	CLA	C	509	X	-	-	-
23	CLA	C	510	X	-	-	-
23	CLA	C	511	X	-	-	-
23	CLA	C	512	X	-	-	-
23	CLA	C	513	X	-	-	-
23	CLA	C	514	X	-	-	-
23	CLA	D	401	X	-	-	-
23	CLA	D	403	X	-	-	-
23	CLA	D	404	X	-	-	-
23	CLA	a	406	X	-	-	-
23	CLA	a	407	X	-	-	-
23	CLA	a	410	X	-	-	-
23	CLA	b	602	X	-	-	X
23	CLA	b	603	X	-	-	-
23	CLA	b	604	X	-	-	-
23	CLA	b	605	X	-	-	-
23	CLA	b	606	X	-	-	-
23	CLA	b	607	X	-	-	-
23	CLA	b	608	X	-	-	-
23	CLA	b	609	X	-	-	-
23	CLA	b	610	X	-	-	-
23	CLA	b	611	X	-	-	-
23	CLA	b	612	X	-	-	-
23	CLA	b	613	X	-	-	-
23	CLA	b	614	X	-	-	-
23	CLA	b	615	X	-	-	-
23	CLA	b	616	X	-	-	-
23	CLA	b	617	X	-	-	-
23	CLA	c	902	X	-	-	-
23	CLA	c	903	X	-	-	-
23	CLA	c	904	X	-	-	-
23	CLA	c	905	X	-	-	-
23	CLA	c	906	X	-	-	-
23	CLA	c	907	X	-	-	-
23	CLA	c	908	X	-	-	-
23	CLA	c	909	X	-	-	-
23	CLA	c	910	X	-	-	-
23	CLA	c	911	X	-	-	-
23	CLA	c	912	X	-	-	-
23	CLA	c	913	X	-	-	-
23	CLA	c	914	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CLA	d	401	X	-	-	-
23	CLA	d	403	X	-	-	-
23	CLA	d	404	X	-	-	-
25	BCR	B	619	-	-	-	X
25	BCR	D	405	-	-	-	X
25	BCR	T	101	-	-	-	X
25	BCR	d	405	-	-	-	X
26	SQD	A	415	-	-	-	X
26	SQD	B	621	-	-	-	X
26	SQD	L	102	-	-	-	X
26	SQD	a	417	-	-	-	X
27	PL9	A	411	-	-	-	X
27	PL9	a	414	-	-	-	X
28	LHG	A	412	-	-	-	X
28	LHG	E	101	-	-	-	X
28	LHG	K	101	-	-	-	X
28	LHG	d	402	-	-	-	X
28	LHG	d	408	-	-	-	X
28	LHG	e	101	-	-	-	X
29	UNL	A	414	-	-	-	X
29	UNL	A	417	-	-	-	X
29	UNL	B	629	-	-	-	X
29	UNL	B	632	-	-	-	X
29	UNL	D	413	-	-	-	X
29	UNL	E	102	-	-	-	X
29	UNL	E	103	-	-	-	X
29	UNL	I	103	-	-	-	X
29	UNL	J	103	-	-	-	X
29	UNL	J	104	-	-	-	X
29	UNL	J	105	-	-	-	X
29	UNL	T	102	-	-	-	X
29	UNL	U	201	-	-	-	X
29	UNL	X	101	-	-	-	X
29	UNL	Z	102	-	-	-	X
29	UNL	a	419	-	-	-	X
29	UNL	b	626	-	-	-	X
29	UNL	d	412	-	-	-	X
29	UNL	e	102	-	-	-	X
29	UNL	i	103	-	-	-	X
29	UNL	j	103	-	-	-	X
29	UNL	k	101	-	-	-	X
29	UNL	t	102	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	UNL	u	201	-	-	-	X
29	UNL	u	202	-	-	-	X
29	UNL	x	103	-	-	-	X
29	UNL	z	102	-	-	-	X
30	LMT	A	416	-	-	-	X
30	LMT	B	643	-	-	-	X
30	LMT	B	644	-	-	-	X
30	LMT	F	101	-	-	-	X
30	LMT	I	101	-	-	-	X
30	LMT	T	103	-	-	-	X
30	LMT	a	418	-	-	-	X
30	LMT	e	103	-	-	-	X
30	LMT	z	101	-	-	-	X
31	DMS	A	419	-	-	-	X
31	DMS	A	421	-	-	-	X
31	DMS	B	636	-	-	X	X
31	DMS	B	638	-	-	-	X
31	DMS	B	639	-	-	X	-
31	DMS	B	641	-	-	-	X
31	DMS	B	645	-	-	X	X
31	DMS	C	525	-	-	-	X
31	DMS	C	526	-	-	-	X
31	DMS	C	527	-	-	-	X
31	DMS	C	529	-	-	-	X
31	DMS	D	416	-	-	X	X
31	DMS	D	417	-	-	-	X
31	DMS	F	102	-	-	X	X
31	DMS	O	303	-	-	-	X
31	DMS	O	304	-	-	-	X
31	DMS	O	305	-	-	X	X
31	DMS	O	308	-	-	X	X
31	DMS	O	311	-	-	-	X
31	DMS	U	202	-	-	-	X
31	DMS	V	202	-	-	-	X
31	DMS	V	207	-	-	X	-
31	DMS	V	209	-	-	X	-
31	DMS	V	210	-	-	-	X
31	DMS	V	211	-	-	-	X
31	DMS	b	635	-	-	-	X
31	DMS	b	637	-	-	-	X
31	DMS	b	638	-	-	-	X
31	DMS	b	640	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	DMS	b	644	-	-	-	X
31	DMS	b	645	-	-	-	X
31	DMS	b	646	-	-	-	X
31	DMS	b	647	-	-	-	X
31	DMS	c	925	-	-	-	X
31	DMS	c	929	-	-	-	X
31	DMS	c	932	-	-	-	X
31	DMS	c	933	-	-	-	X
31	DMS	d	415	-	-	-	X
31	DMS	k	103	-	-	-	X
31	DMS	o	303	-	-	-	X
31	DMS	o	304	-	-	-	X
31	DMS	u	203	-	-	-	X
31	DMS	u	206	-	-	-	X
31	DMS	v	201	-	-	-	X
31	DMS	v	202	-	-	-	X
31	DMS	v	209	-	-	-	X
34	LMG	C	531	-	-	-	X
34	LMG	J	101	-	-	-	X
34	LMG	c	930	-	-	-	X
34	LMG	d	411	-	-	-	X
35	HTG	B	625	-	-	-	X
35	HTG	C	522	-	-	-	X
35	HTG	C	523	-	-	-	X
35	HTG	D	414	-	-	-	X
35	HTG	O	302	-	-	-	X
35	HTG	V	204	-	-	-	X
35	HTG	b	622	-	-	-	X
35	HTG	c	922	-	-	-	X
35	HTG	c	923	-	-	-	X
35	HTG	d	413	-	-	-	X
35	HTG	v	204	-	-	-	X
36	DGD	C	519	-	-	-	X
36	DGD	D	407	-	-	-	X
36	DGD	d	407	-	-	-	X
39	MG	j	102	-	-	-	X



## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 55401 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	1	0
			2622	1718	431	458	15			
1	a	334	Total	C	N	O	S	0	4	0
			2633	1727	431	460	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	see sequence details	UNP P51765
a	279	PRO	ARG	see sequence details	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	505	Total	C	N	O	S	0	4	0
			3992	2619	668	692	13			
2	b	501	Total	C	N	O	S	0	3	0
			3929	2582	653	681	13			

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	451	Total	C	N	O	S	0	4	0
			3511	2297	591	610	13			
3	c	455	Total	C	N	O	S	0	1	0
			3521	2305	589	614	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	19	ASN	-	see sequence details	UNP D0VWR7
C	20	SER	-	see sequence details	UNP D0VWR7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	ILE	-	see sequence details	UNP D0VWR7
C	22	PHE	-	see sequence details	UNP D0VWR7
c	19	ASN	-	see sequence details	UNP D0VWR7
c	20	SER	-	see sequence details	UNP D0VWR7
c	21	ILE	-	see sequence details	UNP D0VWR7
c	22	PHE	-	see sequence details	UNP D0VWR7

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	342	Total	C	N	O	S	0	2	0
			2733	1813	446	462	12			
4	d	342	Total	C	N	O	S	0	2	0
			2733	1813	446	462	12			

- Molecule 5 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	81	Total	C	N	O	0	0	0
			651	426	103	122			
5	e	79	Total	C	N	O	0	0	0
			637	419	101	117			

- Molecule 6 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			280	190	46	43	1			
6	f	32	Total	C	N	O	S	0	0	0
			255	173	43	38	1			

- Molecule 7 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	63	Total	C	N	O	S	0	2	0
			511	341	83	85	2			
7	h	63	Total	C	N	O	S	0	1	0
			506	338	83	83	2			

- Molecule 8 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			285	195	45	44	1			
8	i	38	Total	C	N	O	S	0	0	0
			303	205	48	49	1			

- Molecule 9 is a protein called Photosystem II reaction center protein J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	36	Total	C	N	O	S	0	0	0
			251	171	37	42	1			
9	j	40	Total	C	N	O	S	0	0	0
			285	190	44	49	2			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			293	204	43	46			
10	k	37	Total	C	N	O	0	0	0
			293	204	43	46			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	see sequence details	UNP P19054
K	39	TRP	VAL	see sequence details	UNP P19054
k	33	LEU	PHE	see sequence details	UNP P19054
k	39	TRP	VAL	see sequence details	UNP P19054

- Molecule 11 is a protein called Photosystem II reaction center protein L.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	1	0
			306	205	48	53			
11	l	36	Total	C	N	O	0	1	0
			297	200	47	50			

- Molecule 12 is a protein called Photosystem II reaction center protein M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	m	34	Total	C	N	O	S	0	1	0
			264	178	38	47	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	see sequence details	UNP P12312
m	8	LEU	PHE	see sequence details	UNP P12312

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	243	Total	C	N	O	S	0	2	0
			1861	1164	311	382	4			
13	o	243	Total	C	N	O	S	0	1	0
			1852	1159	310	379	4			

- Molecule 14 is a protein called Photosystem II reaction center protein T.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			256	180	36	38	2			
14	t	31	Total	C	N	O	S	0	0	0
			261	183	37	39	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	U	97	Total	C	N	O		0	0	0
			766	486	128	152				
15	u	97	Total	C	N	O		0	1	0
			776	493	129	154				

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	1	0
			1072	680	180	208	4			
16	v	137	Total	C	N	O	S	0	1	0
			1060	671	177	208	4			

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Y	29	Total	C	N	O	S	0	0	0
			210	137	37	33	3			
17	y	29	Total	C	N	O	S	0	0	0
			207	134	37	33	3			

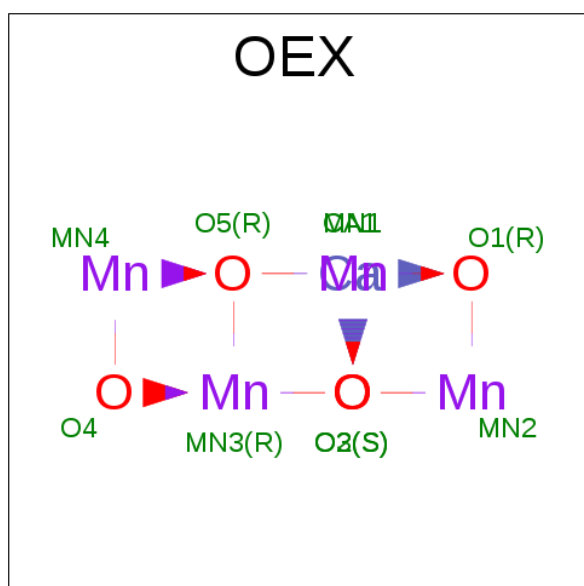
- Molecule 18 is a protein called Photosystem II reaction center protein X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	X	38	Total	C	N	O		0	1	0
			280	190	44	46				
18	x	38	Total	C	N	O		0	0	0
			275	185	44	46				

- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Z	62	Total	C	N	O	S	0	0	0
			468	320	71	75	2			
19	z	61	Total	C	N	O	S	0	0	0
			457	312	70	73	2			

- Molecule 20 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	a	1	Total	Ca	Mn	O	0	0
			10	1	4	5		

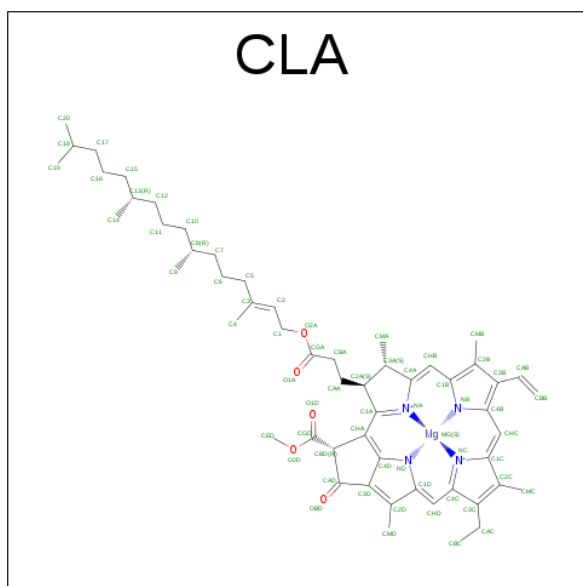
- Molecule 21 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	1	Total	Fe	0	0
			1	1		
21	a	1	Total	Fe	0	0
			1	1		

- Molecule 22 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	2	Total	Cl	0	0
			2	2		
22	a	2	Total	Cl	0	0
			2	2		

- Molecule 23 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	A	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	C	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	D	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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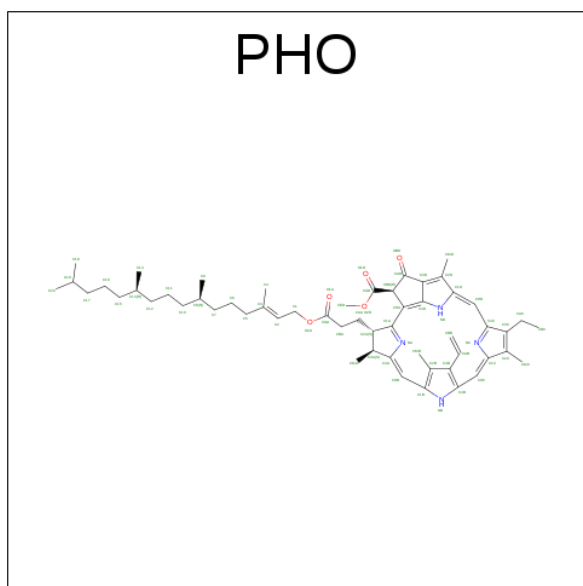
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
23	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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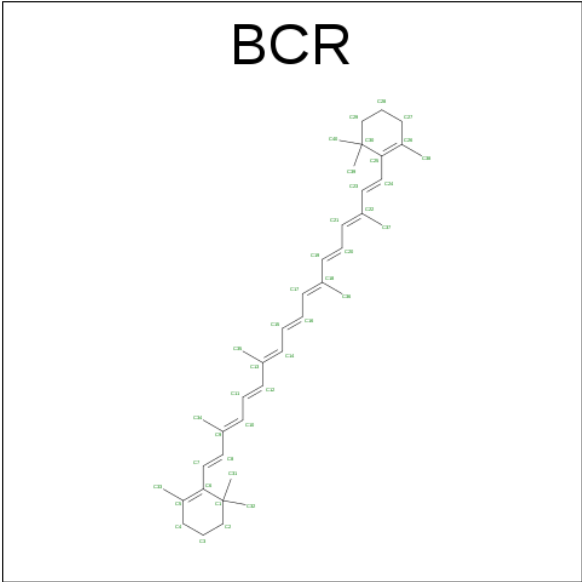
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
23	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 24 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			64	55	4	5		
24	D	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		
24	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 25 is BETA-CAROTENE (three-letter code: BCR) (formula:  $C_{40}H_{56}$ ).



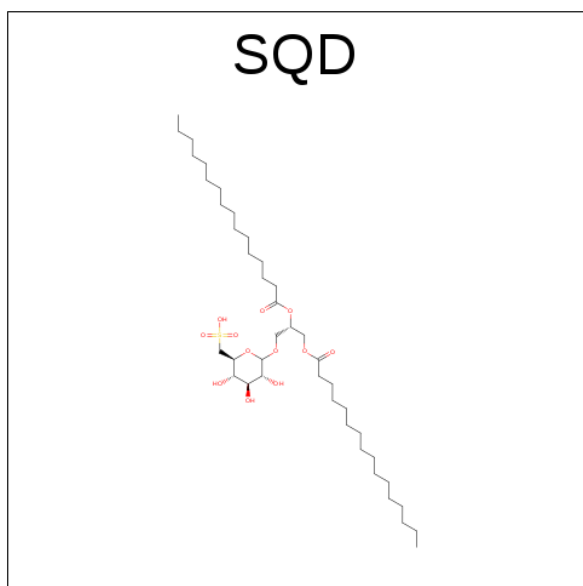
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	B	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	C	1	Total C 40 40	0	0
25	D	1	Total C 40 40	0	0
25	T	1	Total C 40 40	0	0
25	Y	1	Total C 40 40	0	0
25	a	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0
25	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	c	1	Total C 40 40	0	0
25	c	1	Total C 40 40	0	0
25	d	1	Total C 40 40	0	0
25	j	1	Total C 40 40	0	0
25	k	1	Total C 40 40	0	0
25	t	1	Total C 40 40	0	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



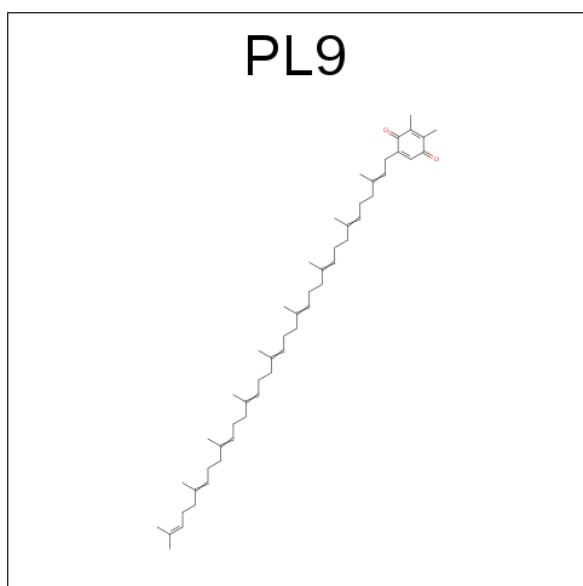
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	A	1	Total C O S 54 41 12 1	0	0
26	A	1	Total C O S 54 41 12 1	0	0
26	B	1	Total C O S 54 41 12 1	0	0
26	D	1	Total C O S 45 32 12 1	0	0
26	L	1	Total C O S 54 41 12 1	0	0

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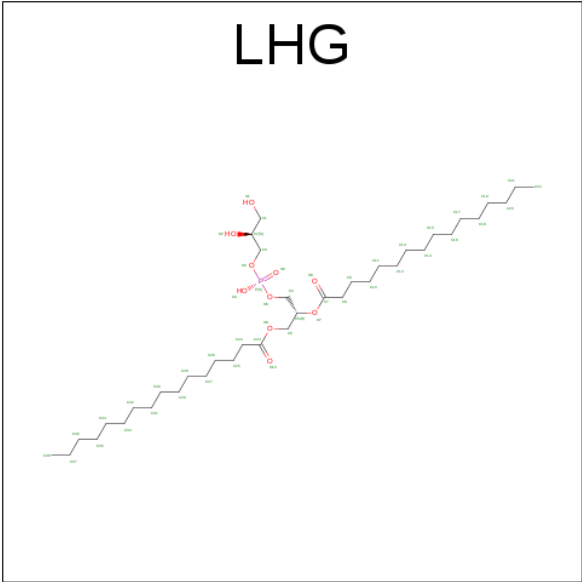
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	a	1	Total	C	O	S	0	0
			54	41	12	1		
26	x	1	Total	C	O	S	0	0
			41	28	12	1		

- Molecule 27 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total	C	O	0	0
			55	53	2		
27	D	1	Total	C	O	0	0
			55	53	2		
27	a	1	Total	C	O	0	0
			55	53	2		
27	d	1	Total	C	O	0	0
			55	53	2		

- Molecule 28 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula:  $C_{38}H_{75}O_{10}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	A	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			49	38	10	1		
28	D	1	Total	C	O	P	0	0
			46	35	10	1		
28	E	1	Total	C	O	P	0	0
			49	38	10	1		
28	K	1	Total	C	O	P	0	0
			44	35	8	1		
28	L	1	Total	C	O	P	0	0
			49	38	10	1		
28	a	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			44	33	10	1		
28	d	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			49	38	10	1		
28	d	1	Total	C	O	P	0	0
			46	35	10	1		
28	e	1	Total	C	O	P	0	0
			40	29	10	1		
28	l	1	Total	C	O	P	0	0
			49	38	10	1		

- Molecule 29 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

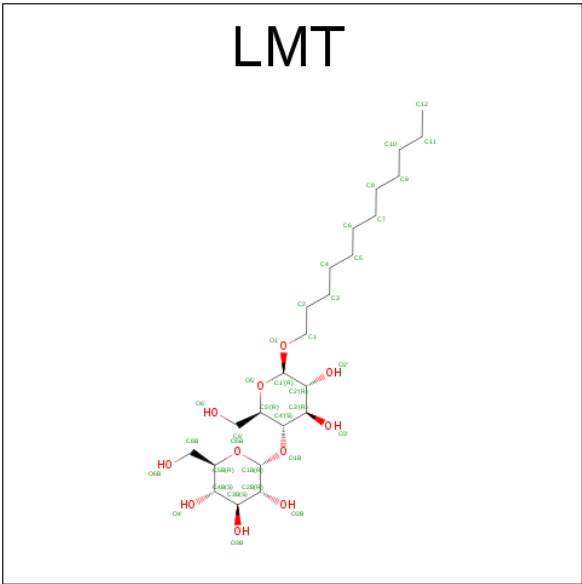
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	B	7	Total C 97 97	0	0
29	c	1	Total C 10 10	0	0
29	t	1	Total C 16 16	0	0
29	X	1	Total C 16 16	0	0
29	J	3	Total C 43 43	0	0
29	k	1	Total C 8 8	0	0
29	E	3	Total C 45 45	0	0
29	b	7	Total C 102 102	0	0
29	A	3	Total C 33 33	0	0
29	x	1	Total C 15 15	0	0
29	M	1	Total C 11 11	0	0
29	j	1	Total C 16 16	0	0
29	D	1	Total C 16 16	0	0
29	e	1	Total C 16 16	0	0
29	I	3	Total C 45 45	0	0
29	Z	2	Total C 23 23	0	0
29	a	2	Total C 16 16	0	0
29	U	1	Total C 14 14	0	0
29	m	1	Total C 11 11	0	0
29	d	2	Total C 27 27	0	0
29	H	1	Total C 14 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	i	4	Total	C	0	0
			64	64		
29	C	1	Total	C	0	0
			11	11		
29	z	1	Total	C	0	0
			13	13		
29	T	1	Total	C	0	0
			13	13		
29	u	2	Total	C	0	0
			27	27		

- Molecule 30 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	A	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			35	24	11		
30	B	1	Total	C	O	0	0
			24	18	6		
30	B	1	Total	C	O	0	0
			24	18	6		
30	F	1	Total	C	O	0	0
			35	24	11		
30	I	1	Total	C	O	0	0
			35	24	11		

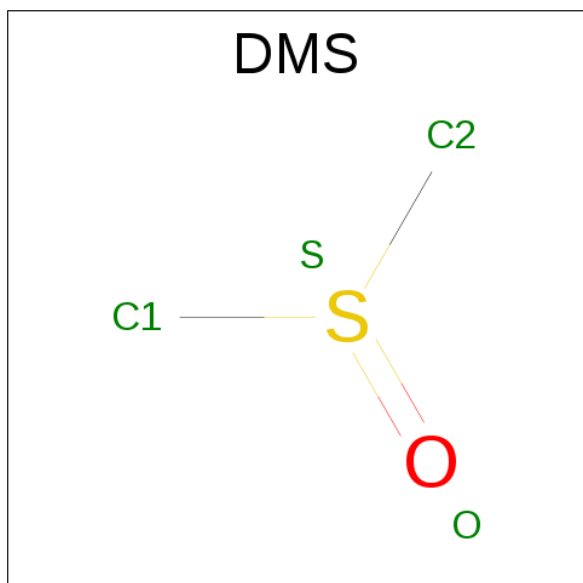
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	M	1	Total	C	O	0	0
			35	24	11		
30	T	1	Total	C	O	0	0
			24	18	6		
30	Z	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	a	1	Total	C	O	0	0
			35	24	11		
30	b	1	Total	C	O	0	0
			25	19	6		
30	e	1	Total	C	O	0	0
			25	19	6		
30	m	1	Total	C	O	0	0
			35	24	11		
30	m	1	Total	C	O	0	0
			35	24	11		
30	z	1	Total	C	O	0	0
			32	21	11		

- Molecule 31 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	A	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	B	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	C	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	D	1	Total 4	C 2	O 1	S 1	0	0
31	F	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	H	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	O	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0
31	U	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	V	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	a	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	b	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	c	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0

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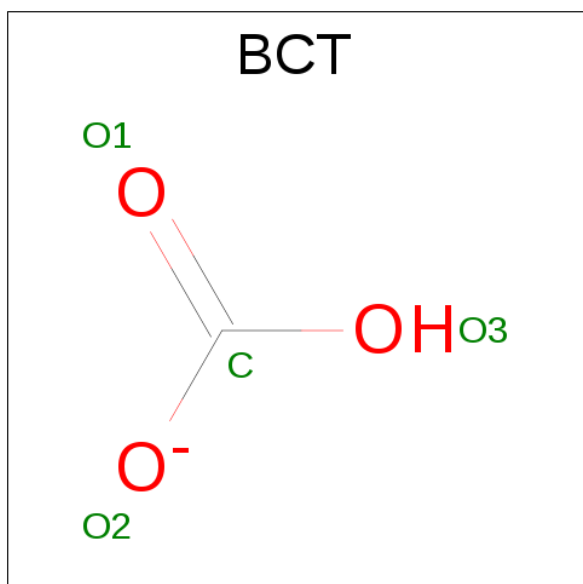
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	d	1	Total 4	C 2	O 1	S 1	0	0
31	e	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	h	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	i	1	Total 4	C 2	O 1	S 1	0	0
31	k	1	Total 4	C 2	O 1	S 1	0	0
31	l	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	o	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	u	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0
31	v	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		
31	v	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 32 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	A	1	Total	C	O	0	0
			4	1	3		
32	a	1	Total	C	O	0	0
			4	1	3		

- Molecule 33 is CALCIUM ION (three-letter code: CA) (formula: Ca).

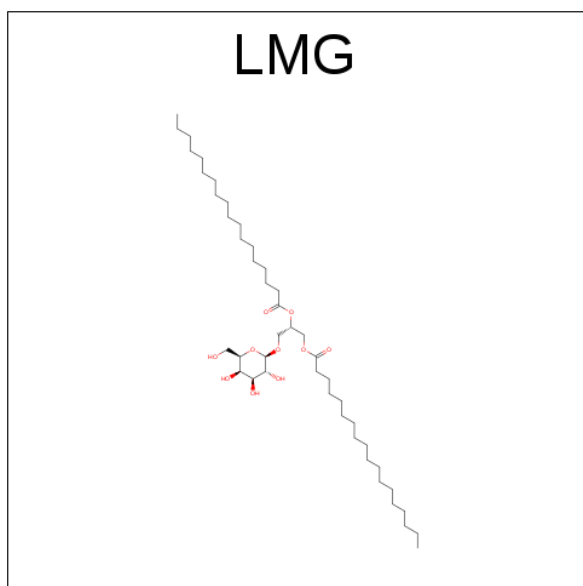
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	o	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	O	1	Total	Ca	0	0
			1	1		
33	B	1	Total	Ca	0	0
			1	1		
33	b	1	Total	Ca	0	0
			1	1		
33	c	1	Total	Ca	0	0
			1	1		

- Molecule 34 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	B	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	C	1	Total	C	O	0	0
			51	41	10		
34	D	1	Total	C	O	0	0
			51	41	10		
34	J	1	Total	C	O	0	0
			51	41	10		
34	a	1	Total	C	O	0	0
			51	41	10		

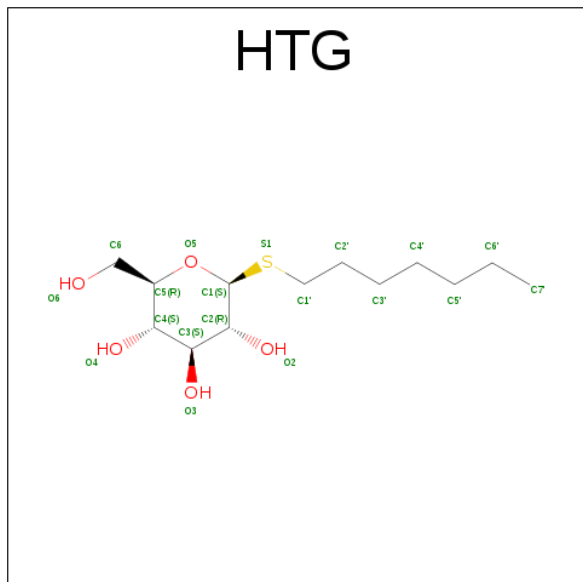
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	c	1	Total	C	O	0	0
			51	41	10		
34	c	1	Total	C	O	0	0
			51	41	10		
34	d	1	Total	C	O	0	0
			51	41	10		
34	j	1	Total	C	O	0	0
			51	41	10		
34	m	1	Total	C	O	0	0
			51	41	10		

- Molecule 35 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



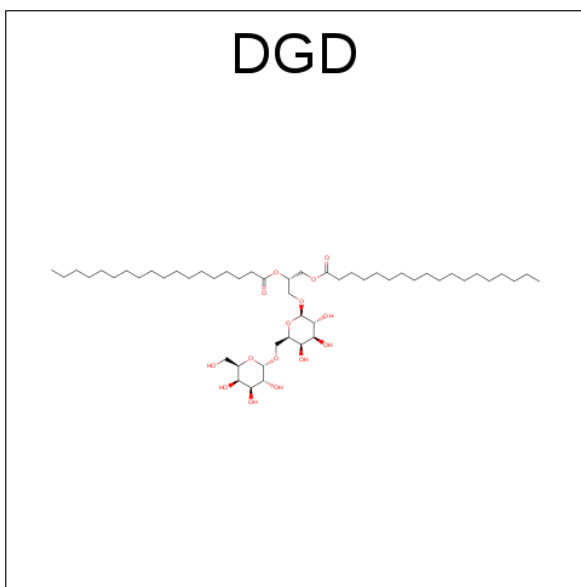
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	B	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	C	1	Total	C	O	S	0	0
			19	13	5	1		
35	D	1	Total	C	O	S	0	0
			19	13	5	1		
35	O	1	Total	C	O	S	0	0
			19	13	5	1		
35	V	1	Total	C	O	S	0	0
			14	8	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	b	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			19	13	5	1		
35	c	1	Total	C	O	S	0	0
			13	10	2	1		
35	d	1	Total	C	O	S	0	0
			19	13	5	1		
35	v	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 36 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: C<sub>51</sub>H<sub>96</sub>O<sub>15</sub>).



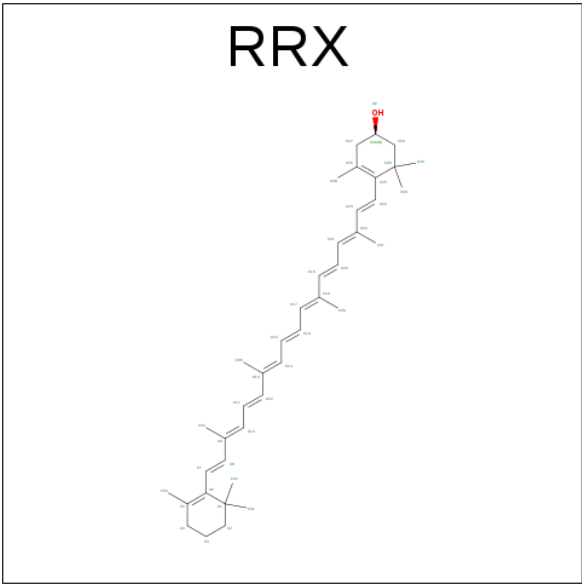
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	C	1	Total	C	O	0	0
			62	47	15		
36	D	1	Total	C	O	0	0
			50	41	9		
36	H	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	c	1	Total	C	O	0	0
			62	47	15		
36	d	1	Total	C	O	0	0
			50	41	9		
36	h	1	Total	C	O	0	0
			62	47	15		

- Molecule 37 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
37	V	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
37	e	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
37	v	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 38 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula: C<sub>40</sub>H<sub>56</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
38	H	1	Total	C	O	0	0
			41	40	1		
38	x	1	Total	C	O	0	0
			41	40	1		

- Molecule 39 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	J	1	Total	Mg	0	0
			1	1		
39	j	1	Total	Mg	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	176	Total	O	0	11
			187	187		
40	B	420	Total	O	0	17
			437	437		
40	C	286	Total	O	0	8
			294	294		
40	D	159	Total	O	0	7
			166	166		
40	E	44	Total	O	0	3
			47	47		
40	F	9	Total	O	0	0
			9	9		
40	H	54	Total	O	0	0
			54	54		
40	I	11	Total	O	0	2
			13	13		
40	J	16	Total	O	0	1
			17	17		
40	K	13	Total	O	0	1
			14	14		
40	L	23	Total	O	0	3
			26	26		
40	M	15	Total	O	0	2
			17	17		
40	O	251	Total	O	0	14
			265	265		
40	T	15	Total	O	0	1
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	U	123	Total 128	O 128	0	5
40	V	165	Total 169	O 169	0	4
40	Y	8	Total 8	O 8	0	0
40	X	14	Total 14	O 14	0	0
40	Z	8	Total 10	O 10	0	2
40	a	172	Total 175	O 175	0	3
40	b	405	Total 423	O 423	0	18
40	c	300	Total 320	O 320	0	20
40	d	177	Total 185	O 185	0	8
40	e	52	Total 56	O 56	0	4
40	f	9	Total 9	O 9	0	0
40	h	56	Total 57	O 57	0	1
40	i	12	Total 13	O 13	0	1
40	j	13	Total 13	O 13	0	0
40	k	14	Total 14	O 14	0	0
40	l	16	Total 19	O 19	0	3
40	m	14	Total 15	O 15	0	1
40	o	223	Total 240	O 240	0	17
40	t	19	Total 21	O 21	0	2
40	u	146	Total 157	O 157	0	11
40	v	147	Total 154	O 154	0	7

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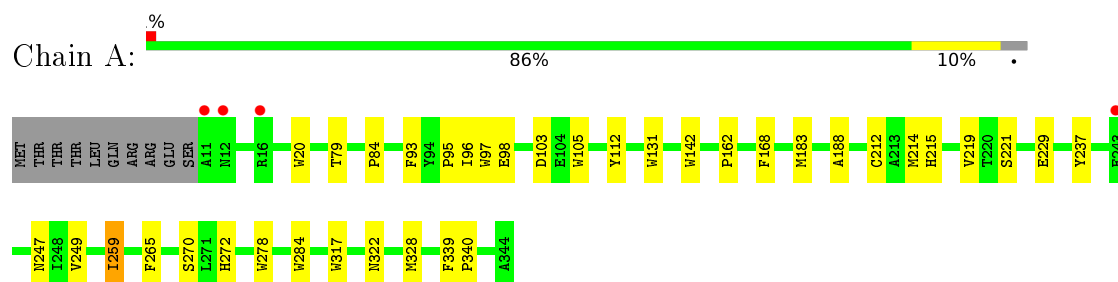
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	y	16	Total 16	O 16	0	0
40	x	18	Total 19	O 19	0	1
40	z	5	Total 5	O 5	0	0

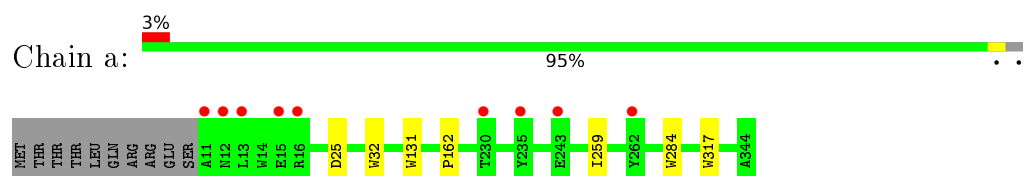
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

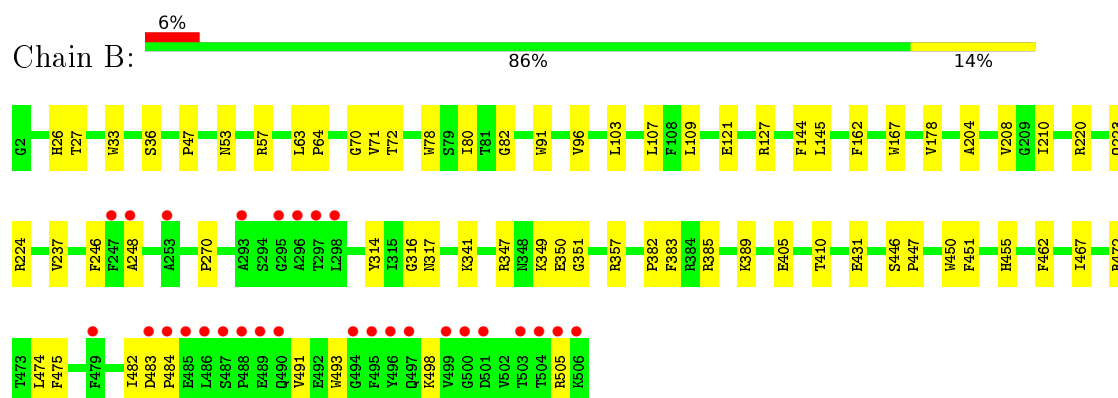
- Molecule 1: Photosystem II protein D1



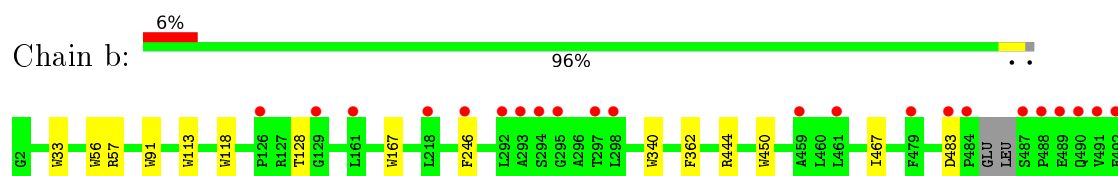
- Molecule 1: Photosystem II protein D1



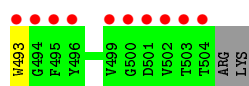
- Molecule 2: Photosystem II CP47 reaction center protein



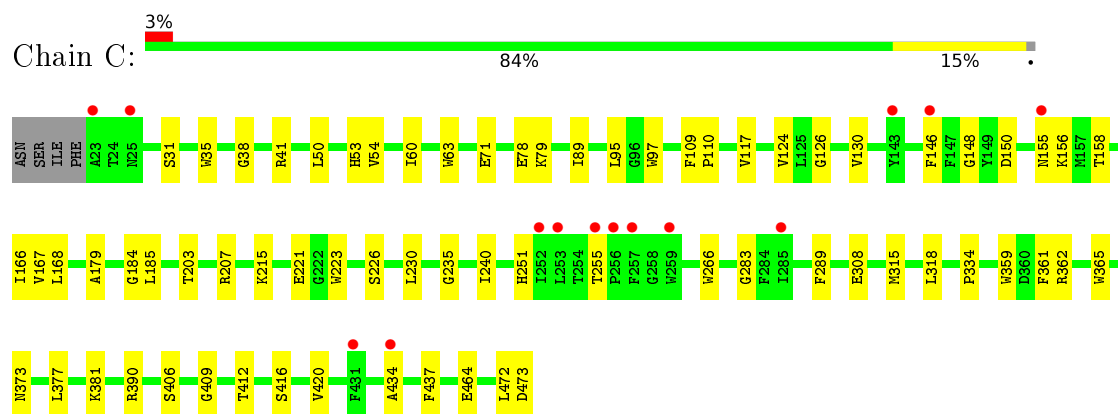
- Molecule 2: Photosystem II CP47 reaction center protein



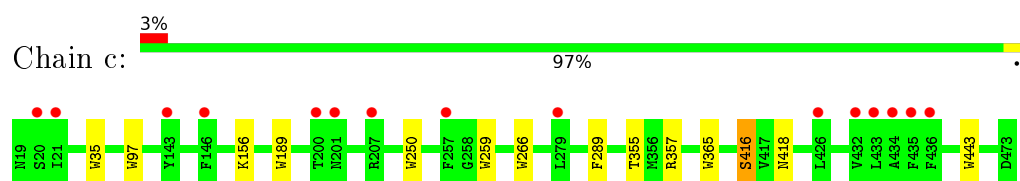




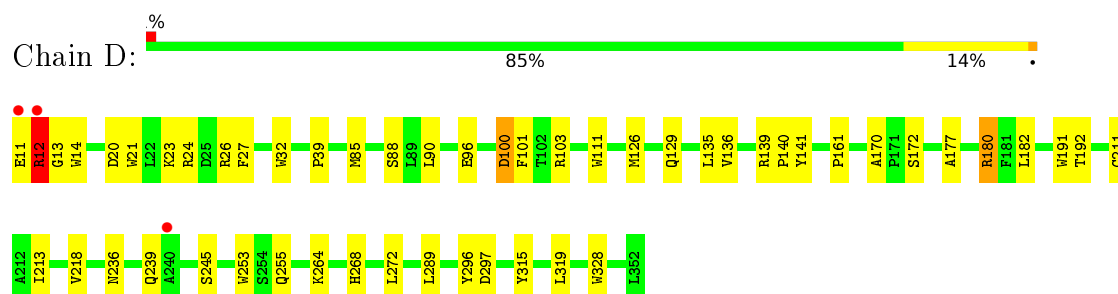
- Molecule 3: Photosystem II CP43 reaction center protein



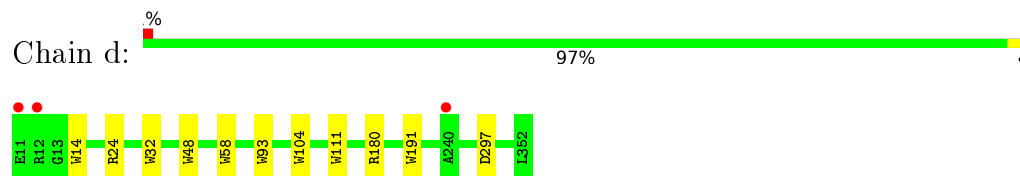
- Molecule 3: Photosystem II CP43 reaction center protein



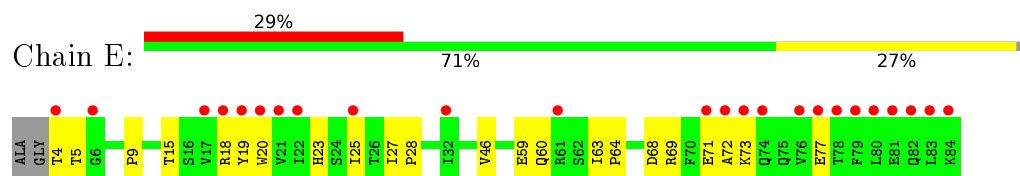
- Molecule 4: Photosystem II D2 protein



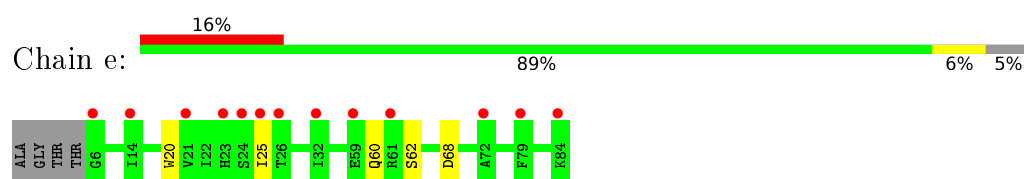
- Molecule 4: Photosystem II D2 protein



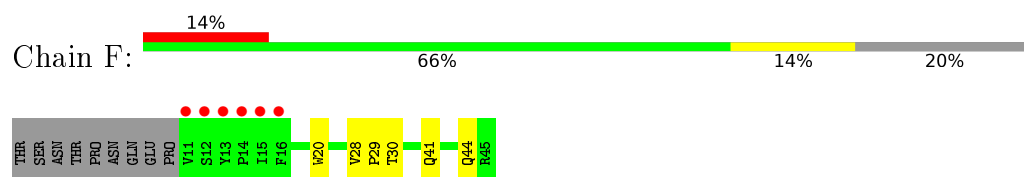
- Molecule 5: Cytochrome b559 subunit alpha



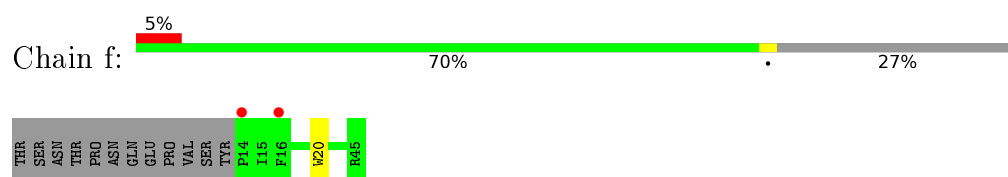
- Molecule 5: Cytochrome b559 subunit alpha



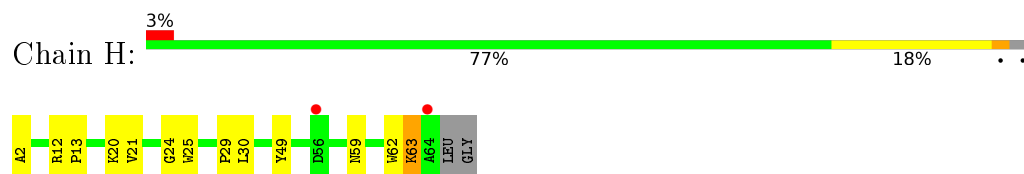
- Molecule 6: Cytochrome b559 subunit beta



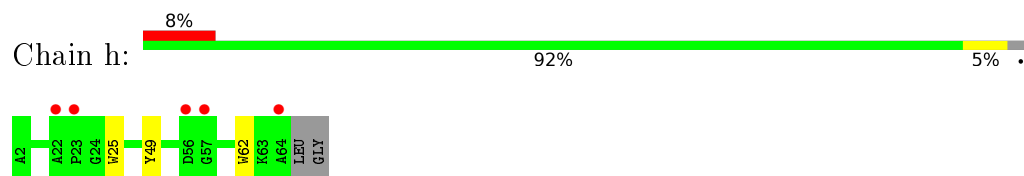
- Molecule 6: Cytochrome b559 subunit beta



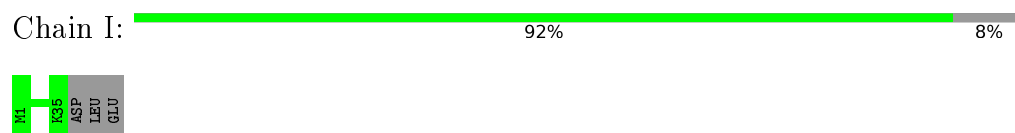
- Molecule 7: Photosystem II reaction center protein H



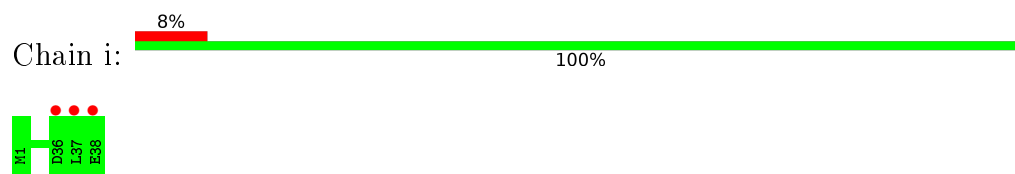
- Molecule 7: Photosystem II reaction center protein H



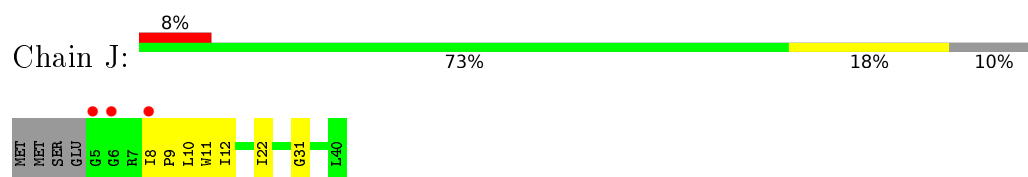
- Molecule 8: Photosystem II reaction center protein I



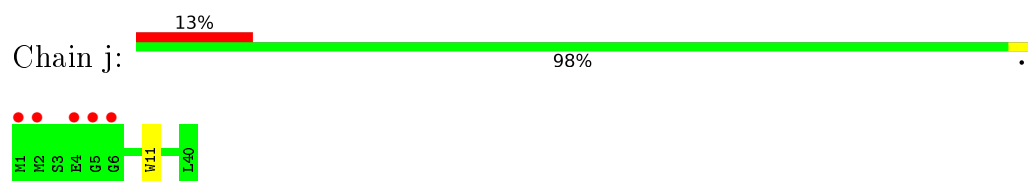
- Molecule 8: Photosystem II reaction center protein I



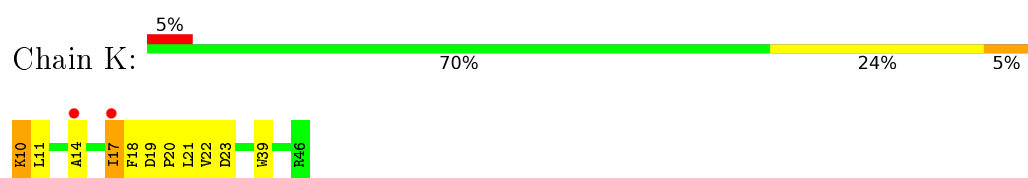
- Molecule 9: Photosystem II reaction center protein J



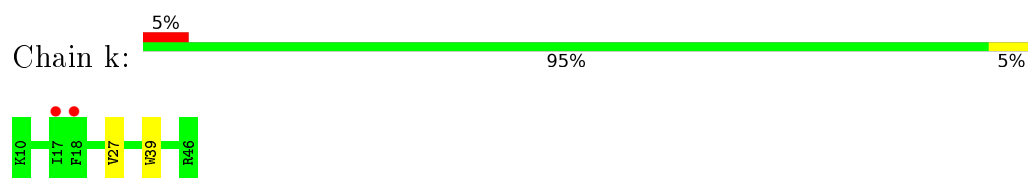
- Molecule 9: Photosystem II reaction center protein J



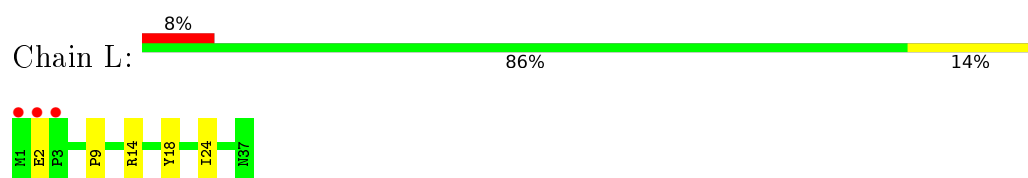
- Molecule 10: Photosystem II reaction center protein K



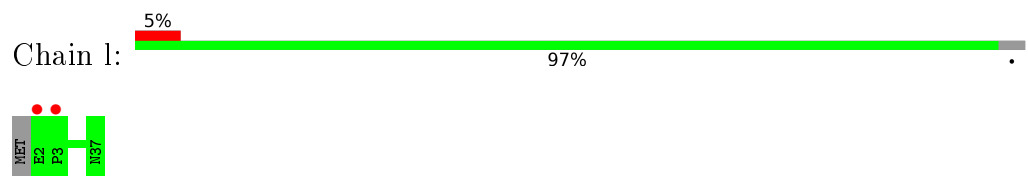
- Molecule 10: Photosystem II reaction center protein K



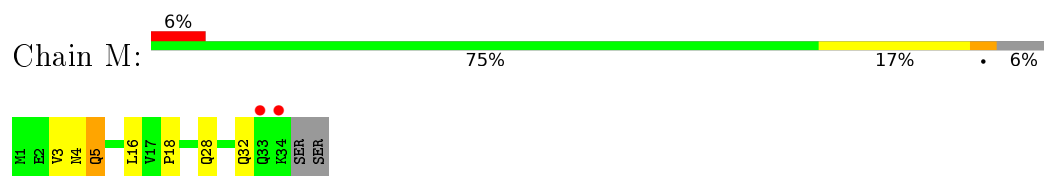
- Molecule 11: Photosystem II reaction center protein L



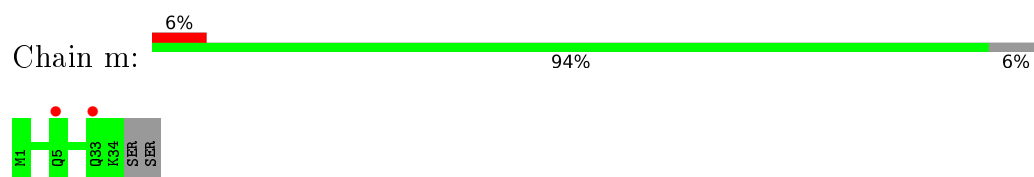
- Molecule 11: Photosystem II reaction center protein L



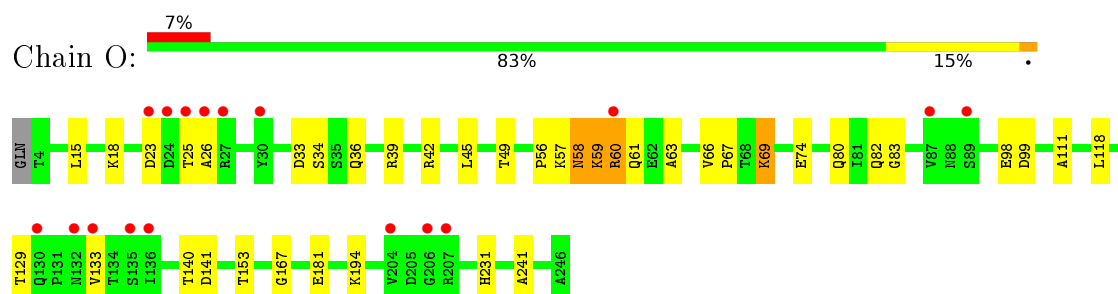
- Molecule 12: Photosystem II reaction center protein M



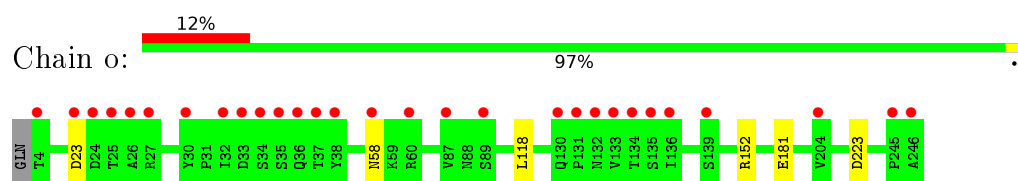
- Molecule 12: Photosystem II reaction center protein M



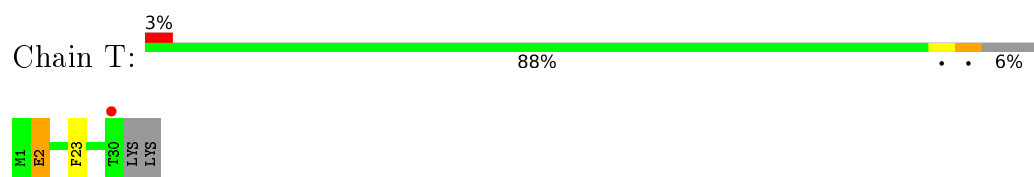
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



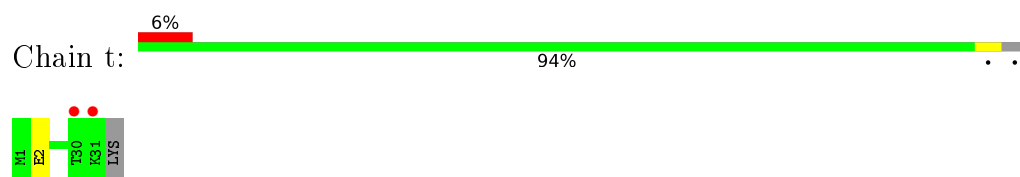
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



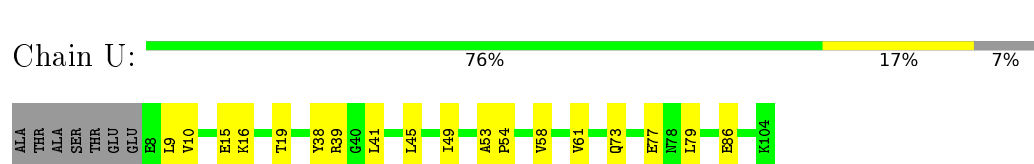
- Molecule 14: Photosystem II reaction center protein T



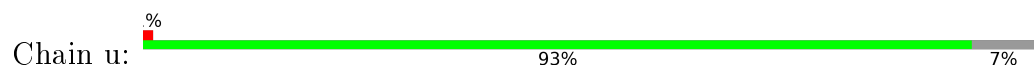
- Molecule 14: Photosystem II reaction center protein T

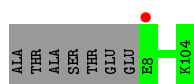


- Molecule 15: Photosystem II 12 kDa extrinsic protein



- Molecule 15: Photosystem II 12 kDa extrinsic protein





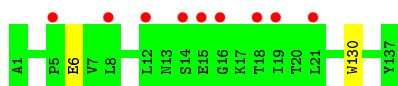
- Molecule 16: Cytochrome c-550

Chain V: 84% 15%



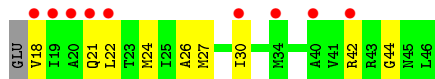
- Molecule 16: Cytochrome c-550

Chain v: 7% 99%



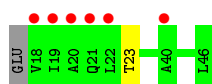
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain Y: 30% 67% 30%



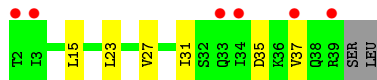
- Molecule 17: Photosystem II reaction center protein Ycf12

Chain y: 20% 93%



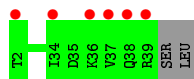
- Molecule 18: Photosystem II reaction center protein X

Chain X: 15% 80% 15% 5%



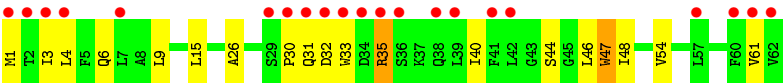
- Molecule 18: Photosystem II reaction center protein X

Chain x: 15% 95% 5%

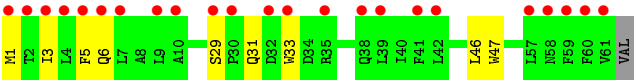
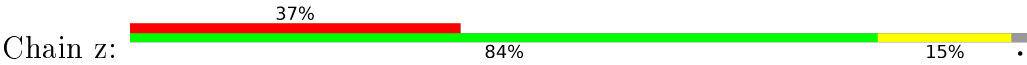


- Molecule 19: Photosystem II reaction center protein Z

Chain Z: 34% 69% 27%



● Molecule 19: Photosystem II reaction center protein Z



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	121.40Å 228.22Å 286.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 1.87 48.98 – 1.87	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.98-1.87) 99.8 (48.98-1.87)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.171 , 0.212 0.171 , 0.212	Depositor DCC
$R_{free}$ test set	32518 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.4	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 70.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	55401	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, HTG, MG, OEX, PHO, DGD, CL, CA, LMT, CLA, PL9, DMS, FE2, RRX, BCT, HEM, FME, UNL, LMG, BCR, SQD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.02	5/2710 (0.2%)	0.81	1/3696 (0.0%)
1	a	0.99	4/2730 (0.1%)	0.81	1/3723 (0.0%)
2	B	0.94	4/4144 (0.1%)	0.82	4/5647 (0.1%)
2	b	0.98	9/4076 (0.2%)	0.83	3/5558 (0.1%)
3	C	0.91	6/3633 (0.2%)	0.78	1/4945 (0.0%)
3	c	0.91	9/3638 (0.2%)	0.78	1/4953 (0.0%)
4	D	1.01	4/2834 (0.1%)	0.83	2/3861 (0.1%)
4	d	1.02	8/2834 (0.3%)	0.82	1/3861 (0.0%)
5	E	0.74	1/670 (0.1%)	0.71	0/917
5	e	0.71	1/656 (0.2%)	0.73	0/896
6	F	0.83	1/289 (0.3%)	0.64	0/394
6	f	0.83	1/262 (0.4%)	0.65	0/356
7	H	0.85	1/530 (0.2%)	0.78	0/722
7	h	0.89	2/522 (0.4%)	0.79	0/711
8	I	0.66	0/282	0.67	0/381
8	i	0.68	0/300	0.67	0/406
9	J	0.80	1/257 (0.4%)	0.63	0/349
9	j	0.84	1/291 (0.3%)	0.69	0/393
10	K	0.73	1/303 (0.3%)	0.70	0/416
10	k	0.77	1/303 (0.3%)	0.71	0/416
11	L	0.94	0/316	0.80	0/430
11	l	0.98	0/307	0.80	0/418
12	M	0.78	0/270	0.75	0/369
12	m	0.72	0/270	0.74	0/369
13	O	0.78	0/1898	0.83	0/2577
13	o	0.74	0/1886	0.83	2/2562 (0.1%)
14	T	0.83	0/255	0.79	0/346
14	t	0.82	0/260	0.74	0/353
15	U	0.82	0/777	0.84	2/1055 (0.2%)
15	u	0.80	0/790	0.82	0/1071
16	V	0.88	0/1096	0.83	1/1487 (0.1%)



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
16	v	0.78	1/1084 (0.1%)	0.76	0/1475
17	Y	0.54	0/211	0.71	0/282
17	y	0.51	0/208	0.63	0/278
18	X	0.61	0/286	0.73	0/387
18	x	0.60	0/278	0.71	0/376
19	Z	0.67	1/479 (0.2%)	0.67	0/656
19	z	0.63	2/468 (0.4%)	0.61	0/640
All	All	0.90	64/42403 (0.2%)	0.80	19/57732 (0.0%)

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	365	TRP	CD2-CE2	7.28	1.50	1.41
1	a	131	TRP	CD2-CE2	6.83	1.49	1.41
3	c	35	TRP	CD2-CE2	6.66	1.49	1.41
2	b	56	TRP	CD2-CE2	6.63	1.49	1.41
10	k	39	TRP	CD2-CE2	6.56	1.49	1.41
2	b	113	TRP	CD2-CE2	6.36	1.49	1.41
9	j	11	TRP	CD2-CE2	6.31	1.49	1.41
2	B	78	TRP	CD2-CE2	6.24	1.48	1.41
6	f	20	TRP	CD2-CE2	6.22	1.48	1.41
3	c	443	TRP	CD2-CE2	6.11	1.48	1.41
1	A	20	TRP	CD2-CE2	6.07	1.48	1.41
4	D	32	TRP	CD2-CE2	6.06	1.48	1.41
3	C	266	TRP	CD2-CE2	6.03	1.48	1.41
1	a	317	TRP	CD2-CE2	5.91	1.48	1.41
2	b	450	TRP	CD2-CE2	5.90	1.48	1.41
2	b	33	TRP	CD2-CE2	5.85	1.48	1.41
3	c	189	TRP	CD2-CE2	5.83	1.48	1.41
2	B	91	TRP	CD2-CE2	5.74	1.48	1.41
2	b	167	TRP	CD2-CE2	5.73	1.48	1.41
6	F	20	TRP	CD2-CE2	5.72	1.48	1.41
7	H	62	TRP	CD2-CE2	5.71	1.48	1.41
2	B	33	TRP	CD2-CE2	5.61	1.48	1.41
2	b	91	TRP	CD2-CE2	5.58	1.48	1.41
4	d	111	TRP	CD2-CE2	5.58	1.48	1.41
1	a	284	TRP	CD2-CE2	5.56	1.48	1.41
1	A	278	TRP	CD2-CE2	5.55	1.48	1.41
2	B	450	TRP	CD2-CE2	5.52	1.48	1.41
3	c	250	TRP	CD2-CE2	5.50	1.48	1.41
4	D	21	TRP	CD2-CE2	5.49	1.48	1.41
3	c	259	TRP	CD2-CE2	5.49	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	365	TRP	CD2-CE2	5.47	1.48	1.41
4	d	14	TRP	CD2-CE2	5.45	1.47	1.41
4	d	191	TRP	CD2-CE2	5.44	1.47	1.41
2	b	340	TRP	CD2-CE2	5.43	1.47	1.41
2	b	493	TRP	CD2-CE2	5.41	1.47	1.41
19	Z	47	TRP	CD2-CE2	5.41	1.47	1.41
3	C	63	TRP	CD2-CE2	5.40	1.47	1.41
9	J	11	TRP	CD2-CE2	5.40	1.47	1.41
7	h	62	TRP	CD2-CE2	5.39	1.47	1.41
1	a	32	TRP	CD2-CE2	5.36	1.47	1.41
4	d	104	TRP	CD2-CE2	5.34	1.47	1.41
1	A	142	TRP	CD2-CE2	5.33	1.47	1.41
4	d	32	TRP	CD2-CE2	5.33	1.47	1.41
16	v	130	TRP	CD2-CE2	5.33	1.47	1.41
5	E	20	TRP	CD2-CE2	5.31	1.47	1.41
3	C	359	TRP	CD2-CE2	5.29	1.47	1.41
10	K	39	TRP	CD2-CE2	5.29	1.47	1.41
3	c	365	TRP	CG-CD1	5.27	1.44	1.36
3	c	266	TRP	CD2-CE2	5.26	1.47	1.41
4	D	111	TRP	CD2-CE2	5.23	1.47	1.41
7	h	25	TRP	CD2-CE2	5.21	1.47	1.41
1	A	284	TRP	CD2-CE2	5.17	1.47	1.41
5	e	20	TRP	CD2-CE2	5.16	1.47	1.41
19	z	33	TRP	CD2-CE2	5.14	1.47	1.41
4	D	328	TRP	CD2-CE2	5.10	1.47	1.41
4	d	48	TRP	CD2-CE2	5.09	1.47	1.41
4	d	58	TRP	CD2-CE2	5.09	1.47	1.41
19	z	47	TRP	CD2-CE2	5.08	1.47	1.41
4	d	93	TRP	CD2-CE2	5.06	1.47	1.41
3	C	35	TRP	CD2-CE2	5.06	1.47	1.41
3	C	97	TRP	CD2-CE2	5.06	1.47	1.41
3	c	97	TRP	CD2-CE2	5.04	1.47	1.41
1	A	97	TRP	CD2-CE2	5.03	1.47	1.41
2	b	118	TRP	CD2-CE2	5.02	1.47	1.41

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	152	ARG	NE-CZ-NH2	-7.84	116.38	120.30
4	d	297	ASP	CB-CG-OD1	7.14	124.73	118.30
2	B	357	ARG	NE-CZ-NH2	-6.52	117.04	120.30
15	U	39	ARG	NE-CZ-NH2	-6.50	117.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	100	ASP	CB-CG-OD1	6.18	123.86	118.30
2	b	444	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	a	25	ASP	CB-CG-OD1	5.86	123.57	118.30
15	U	39	ARG	NE-CZ-NH1	5.82	123.21	120.30
16	V	99	ASP	CB-CG-OD1	5.63	123.37	118.30
13	o	223	ASP	CB-CG-OD1	5.50	123.25	118.30
4	D	297	ASP	CB-CG-OD1	5.46	123.22	118.30
2	B	57	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	131	TRP	CA-CB-CG	-5.45	103.35	113.70
2	B	57	ARG	NE-CZ-NH2	-5.34	117.63	120.30
2	b	444	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	B	474	LEU	CB-CG-CD1	-5.18	102.20	111.00
3	C	473	ASP	CB-CG-OD1	5.16	122.94	118.30
3	c	357	ARG	NE-CZ-NH1	-5.07	117.76	120.30
2	b	57	ARG	NE-CZ-NH2	-5.03	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2622	0	2519	33	0
1	a	2633	0	2540	0	0
2	B	3992	0	3848	71	0
2	b	3929	0	3774	0	0
3	C	3511	0	3440	51	0
3	c	3521	0	3439	0	0
4	D	2733	0	2647	54	0
4	d	2733	0	2647	0	0
5	E	651	0	626	17	0
5	e	637	0	617	0	0
6	F	280	0	284	3	0
6	f	255	0	263	0	0
7	H	511	0	535	10	0
7	h	506	0	531	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	I	285	0	305	0	0
8	i	303	0	313	0	0
9	J	251	0	257	4	0
9	j	285	0	293	0	0
10	K	293	0	305	9	0
10	k	293	0	305	0	0
11	L	306	0	320	5	0
11	l	297	0	311	0	0
12	M	264	0	283	7	0
12	m	264	0	283	0	0
13	O	1861	0	1825	40	0
13	o	1852	0	1812	0	0
14	T	256	0	256	2	0
14	t	261	0	258	0	0
15	U	766	0	758	15	0
15	u	776	0	775	0	0
16	V	1072	0	1086	26	0
16	v	1060	0	1053	0	0
17	Y	210	0	230	6	0
17	y	207	0	221	0	0
18	X	280	0	312	9	0
18	x	275	0	301	0	0
19	Z	468	0	492	20	0
19	z	457	0	471	0	0
20	A	10	0	0	0	0
20	a	10	0	0	0	0
21	A	1	0	0	0	0
21	a	1	0	0	0	0
22	A	2	0	0	0	0
22	a	2	0	0	0	0
23	A	195	0	216	12	0
23	B	1040	0	1152	55	0
23	C	845	0	936	38	0
23	D	195	0	216	12	0
23	a	195	0	216	0	0
23	b	1040	0	1152	0	0
23	c	845	0	936	0	0
23	d	195	0	216	0	0
24	A	64	0	74	2	0
24	D	64	0	74	3	0
24	a	128	0	148	0	0
25	A	40	0	56	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B	120	0	168	15	0
25	C	120	0	168	8	0
25	D	40	0	56	6	0
25	T	40	0	56	9	0
25	Y	40	0	56	1	0
25	a	40	0	56	0	0
25	b	120	0	168	0	0
25	c	80	0	112	0	0
25	d	40	0	56	0	0
25	j	40	0	56	0	0
25	k	40	0	56	0	0
25	t	40	0	56	0	0
26	A	108	0	155	11	0
26	B	54	0	78	4	0
26	D	45	0	57	2	0
26	L	54	0	78	3	0
26	a	108	0	156	0	0
26	x	41	0	49	0	0
27	A	55	0	80	12	0
27	D	55	0	80	0	0
27	a	55	0	80	0	0
27	d	55	0	80	0	0
28	A	49	0	74	1	0
28	D	144	0	213	8	0
28	E	49	0	74	7	0
28	K	44	0	67	0	0
28	L	49	0	74	1	0
28	a	49	0	74	0	0
28	d	188	0	274	0	0
28	e	40	0	53	0	0
28	l	49	0	74	0	0
29	A	33	0	0	1	0
29	B	97	0	0	1	0
29	C	11	0	0	0	0
29	D	16	0	0	0	0
29	E	45	0	0	0	0
29	H	14	0	0	0	0
29	I	45	0	0	0	0
29	J	43	0	0	1	0
29	M	11	0	0	0	0
29	T	13	0	0	0	0
29	U	14	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	X	16	0	0	0	0
29	Z	23	0	0	0	0
29	a	16	0	0	0	0
29	b	102	0	0	0	0
29	c	10	0	0	0	0
29	d	27	0	0	0	0
29	e	16	0	0	0	0
29	i	64	0	0	0	0
29	j	16	0	0	0	0
29	k	8	0	0	0	0
29	m	11	0	0	0	0
29	t	16	0	0	0	0
29	u	27	0	0	0	0
29	x	15	0	0	0	0
29	z	13	0	0	0	0
30	A	35	0	46	2	0
30	B	83	0	116	3	0
30	F	35	0	46	0	0
30	I	35	0	46	2	0
30	M	35	0	46	1	0
30	T	24	0	35	0	0
30	Z	35	0	46	7	0
30	a	70	0	92	0	0
30	b	25	0	35	0	0
30	e	25	0	35	0	0
30	m	70	0	92	0	0
30	z	32	0	33	0	0
31	A	24	0	36	4	0
31	B	48	0	72	26	0
31	C	28	0	42	3	0
31	D	12	0	18	7	0
31	F	4	0	6	6	0
31	H	8	0	12	6	0
31	O	36	0	54	20	0
31	U	12	0	18	4	0
31	V	36	0	54	14	0
31	a	16	0	24	0	0
31	b	60	0	90	0	0
31	c	48	0	72	0	0
31	d	20	0	30	0	0
31	e	4	0	6	0	0
31	h	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	i	8	0	12	0	0
31	k	4	0	6	0	0
31	l	4	0	6	0	0
31	o	12	0	18	0	0
31	u	16	0	24	0	0
31	v	32	0	48	0	0
32	A	4	0	0	0	0
32	a	4	0	0	0	0
33	B	1	0	0	0	0
33	O	1	0	0	0	0
33	b	1	0	0	0	0
33	c	1	0	0	0	0
33	o	1	0	0	0	0
34	B	51	0	72	2	0
34	C	153	0	216	4	0
34	D	51	0	72	5	0
34	J	51	0	72	3	0
34	a	51	0	72	0	0
34	c	102	0	144	0	0
34	d	51	0	72	0	0
34	j	51	0	72	0	0
34	m	51	0	72	0	0
35	B	95	0	130	1	0
35	C	57	0	78	1	0
35	D	19	0	26	3	0
35	O	19	0	26	2	0
35	V	14	0	13	2	0
35	b	76	0	104	0	0
35	c	51	0	70	0	0
35	d	19	0	26	0	0
35	v	19	0	26	0	0
36	C	186	0	246	2	0
36	D	50	0	69	10	0
36	H	62	0	82	0	0
36	c	186	0	246	0	0
36	d	50	0	69	0	0
36	h	62	0	82	0	0
37	E	43	0	30	1	0
37	V	43	0	30	0	0
37	e	43	0	30	0	0
37	v	43	0	30	0	0
38	H	41	0	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	x	41	0	56	0	0
39	J	1	0	0	0	0
39	j	1	0	0	0	0
40	A	187	0	0	6	0
40	B	437	0	0	15	0
40	C	294	0	0	4	0
40	D	166	0	0	5	0
40	E	47	0	0	0	0
40	F	9	0	0	0	0
40	H	54	0	0	2	0
40	I	13	0	0	0	0
40	J	17	0	0	3	0
40	K	14	0	0	1	0
40	L	26	0	0	1	0
40	M	17	0	0	1	0
40	O	265	0	0	17	0
40	T	16	0	0	0	0
40	U	128	0	0	5	0
40	V	169	0	0	9	0
40	X	14	0	0	0	0
40	Y	8	0	0	0	0
40	Z	10	0	0	2	0
40	a	175	0	0	0	0
40	b	423	0	0	0	0
40	c	320	0	0	0	0
40	d	185	0	0	0	0
40	e	56	0	0	0	0
40	f	9	0	0	0	0
40	h	57	0	0	0	0
40	i	13	0	0	0	0
40	j	13	0	0	0	0
40	k	14	0	0	0	0
40	l	19	0	0	0	0
40	m	15	0	0	0	0
40	o	240	0	0	0	0
40	t	21	0	0	0	0
40	u	157	0	0	0	0
40	v	154	0	0	0	0
40	x	19	0	0	0	0
40	y	16	0	0	0	0
40	z	5	0	0	0	0
All	All	55401	0	52590	528	0



The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (528) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347[B]:ARG:NH2	40:B:1034[B]:HOH:O	1.80	1.13
1:A:214:MET:HG2	27:A:411:PL9:H102	1.20	1.12
19:Z:35:ARG:HH11	19:Z:35:ARG:HG2	1.18	1.04
2:B:350:GLU:HG3	31:B:639:DMS:H11	1.38	1.04
16:V:90:GLU:HB2	31:V:209:DMS:H13	21.51	1.01
2:B:350:GLU:H	31:B:639:DMS:H12	1.24	0.99
26:A:410:SQD:H122	26:A:410:SQD:H162	1.44	0.95
31:B:636:DMS:H13	40:B:833:HOH:O	1.67	0.94
23:C:510:CLA:HBB1	23:C:510:CLA:HMB1	1.50	0.94
15:U:9:LEU:HA	31:U:204:DMS:S	2.08	0.94
23:D:404:CLA:HMB1	23:D:404:CLA:HBB1	1.93	0.93
16:V:90:GLU:HB2	31:V:209:DMS:C1	21.69	0.92
31:O:311:DMS:H12	40:O:573:HOH:O	1.73	0.87
2:B:350:GLU:H	31:B:639:DMS:C1	1.89	0.86
13:O:23:ASP:HB3	40:O:564:HOH:O	1.74	0.86
2:B:389:LYS:HE3	40:B:1009:HOH:O	1.75	0.85
13:O:82:GLN:NE2	40:O:402:HOH:O	2.08	0.85
2:B:472:ARG:HG2	31:D:416:DMS:H13	2.02	0.85
2:B:350:GLU:HG3	31:B:639:DMS:C1	2.07	0.85
5:E:9:PRO:HA	28:E:101:LHG:HC2	4.13	0.83
4:D:101:PHE:H	36:D:407:DGD:HA21	4.06	0.83
23:B:615:CLA:H18	34:B:622:LMG:H422	1.61	0.82
31:O:311:DMS:C1	40:O:573:HOH:O	2.27	0.82
23:B:614:CLA:HBB1	23:B:614:CLA:HMB1	1.62	0.81
13:O:74[B]:GLU:OE1	40:O:401:HOH:O	1.97	0.81
2:B:491:VAL:HG12	4:D:136:VAL:HG13	1.94	0.81
4:D:140:PRO:HD2	31:D:416:DMS:O	1.81	0.80
23:A:405:CLA:HBB1	23:A:405:CLA:HMB1	1.62	0.80
2:B:472:ARG:HG2	31:D:416:DMS:C1	2.18	0.79
4:D:103:ARG:HH21	5:E:77:GLU:HG3	1.47	0.79
4:D:135:LEU:HD23	34:D:412:LMG:HC5	1.66	0.78
31:B:636:DMS:H12	40:D:566:HOH:O	1.84	0.76
28:D:411:LHG:H141	28:D:411:LHG:C35	2.15	0.76
17:Y:26:ALA:O	17:Y:30:ILE:HG12	1.85	0.76
13:O:15:LEU:HD23	13:O:18:LYS:HD3	1.67	0.76
25:B:620:BCR:C8	25:B:620:BCR:H331	2.29	0.75
4:D:14:TRP:CD1	35:D:414:HTG:H61	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.69	0.74
19:Z:35:ARG:NH1	19:Z:35:ARG:HG2	1.94	0.74
23:B:616:CLA:HMB1	23:B:616:CLA:HBB1	1.68	0.73
30:B:644:LMT:H6E	40:B:914:HOH:O	1.87	0.73
23:B:612:CLA:HMB1	23:B:612:CLA:HBB1	1.71	0.73
23:B:603:CLA:HBB1	23:B:603:CLA:HMB1	2.37	0.72
1:A:98:GLU:OE1	40:A:654[B]:HOH:O	2.06	0.72
30:A:416:LMT:H6'1	40:A:650:HOH:O	1.90	0.72
1:A:183:MET:HA	23:A:405:CLA:HMD2	1.72	0.72
13:O:133:VAL:HG22	31:O:305:DMS:H21	1.72	0.71
23:A:406:CLA:HBB1	23:A:406:CLA:HMB1	2.02	0.71
13:O:33:ASP:HB3	13:O:36:GLN:HE21	6.87	0.70
2:B:467:ILE:HG13	4:D:126:MET:CE	2.63	0.69
2:B:347[A]:ARG:NH1	2:B:351:GLY:O	6.89	0.69
23:C:504:CLA:CHC	34:C:531:LMG:H241	2.22	0.68
1:A:183:MET:HA	23:A:406:CLA:HMD2	12.09	0.68
4:D:135:LEU:CD2	34:D:412:LMG:HC5	2.22	0.68
26:A:410:SQD:C12	26:A:410:SQD:H162	2.21	0.68
15:U:86:GLU:HG3	29:U:201:UNL:C14	2.23	0.68
23:C:507:CLA:H92	30:I:101:LMT:H111	1.74	0.68
31:B:646:DMS:H13	40:B:835:HOH:O	1.92	0.68
25:B:620:BCR:HC8	25:B:620:BCR:H331	2.14	0.68
31:H:101:DMS:H11	40:H:234:HOH:O	49.76	0.68
1:A:214:MET:HG2	27:A:411:PL9:C10	2.12	0.67
34:D:412:LMG:H352	35:D:414:HTG:H7'2	1.76	0.67
24:D:402:PHO:HBB1	24:D:402:PHO:HMB1	1.76	0.66
2:B:341:LYS:NZ	35:B:625:HTG:S1	2.62	0.66
5:E:15:THR:HB	9:J:8:ILE:O	1.96	0.65
23:C:513:CLA:H121	23:C:514:CLA:H142	1.78	0.65
25:T:101:BCR:HC8	25:T:101:BCR:H311	2.09	0.65
5:E:19:TYR:CE2	5:E:23:HIS:CE1	3.27	0.65
5:E:68:ASP:OD1	5:E:71:GLU:HB2	1.97	0.65
13:O:58:ASN:HD22	13:O:58:ASN:C	1.98	0.65
13:O:49[B]:THR:HG22	40:O:530:HOH:O	1.96	0.64
5:E:68:ASP:O	5:E:72:ALA:HB2	1.98	0.64
2:B:347[B]:ARG:HD2	31:B:645:DMS:C2	32.07	0.63
10:K:14:ALA:HB2	19:Z:61:VAL:HG12	1.80	0.63
23:C:507:CLA:HMC2	23:C:508:CLA:H102	1.80	0.63
31:O:304:DMS:H13	40:O:601:HOH:O	34.12	0.63
19:Z:1:MET:SD	19:Z:1:MET:N	4.27	0.63
31:F:102:DMS:C1	40:J:214:HOH:O	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:GLY:O	3:C:156:LYS:NZ	2.77	0.63
23:B:611:CLA:H203	23:B:611:CLA:H151	1.80	0.62
23:C:507:CLA:HMB1	23:C:507:CLA:HBB1	1.78	0.62
1:A:214:MET:CG	27:A:411:PL9:H102	2.13	0.62
23:B:617:CLA:HED2	23:B:617:CLA:H43	1.81	0.62
15:U:19:THR:HG21	40:U:358:HOH:O	27.68	0.62
2:B:467:ILE:HG13	4:D:126:MET:HE2	2.12	0.62
2:B:70:GLY:HA2	2:B:178:VAL:HG21	1.81	0.61
31:D:415:DMS:H12	40:D:575:HOH:O	2.00	0.61
4:D:13:GLY:HA3	35:D:414:HTG:H62	1.81	0.61
26:A:410:SQD:H381	9:J:22:ILE:HD11	1.82	0.61
13:O:133:VAL:HG13	31:O:305:DMS:H21	1.81	0.61
23:D:401:CLA:HMB1	23:D:401:CLA:HBB1	1.89	0.61
13:O:74[A]:GLU:OE1	40:O:403:HOH:O	2.16	0.61
40:B:749:HOH:O	13:O:57:LYS:HD2	41.98	0.61
16:V:55[A]:ARG:NH1	40:V:301:HOH:O	2.34	0.61
2:B:462:PHE:CE1	23:B:614:CLA:HMB3	2.49	0.61
4:D:24:ARG:HE	18:X:37:VAL:HG22	4.23	0.60
23:B:617:CLA:H142	25:B:620:BCR:H12C	3.66	0.60
13:O:133:VAL:HG22	31:O:305:DMS:C2	2.31	0.60
3:C:377:LEU:HG	3:C:381[A]:LYS:HE3	1.83	0.60
31:F:102:DMS:H12	40:J:214:HOH:O	2.01	0.60
7:H:12:ARG:HB3	7:H:13:PRO:HD3	2.27	0.60
7:H:2:ALA:N	40:H:201:HOH:O	2.35	0.59
15:U:10:VAL:H	31:U:204:DMS:C2	2.15	0.59
11:L:9:PRO:HA	30:M:101:LMT:H6D	16.84	0.59
2:B:446:SER:HB2	2:B:447:PRO:CD	2.32	0.59
31:A:421:DMS:H22	40:D:599:HOH:O	2.02	0.59
2:B:223[B]:GLN:OE1	7:H:21:VAL:HG21	2.78	0.59
10:K:21:LEU:HB2	17:Y:24:MET:HE2	5.92	0.59
1:A:237:TYR:CZ	4:D:264[B]:LYS:HG3	2.38	0.59
25:C:516:BCR:H331	25:C:516:BCR:C8	2.33	0.58
4:D:24:ARG:HD3	18:X:37:VAL:HG22	1.85	0.58
12:M:3:VAL:HG11	14:T:2:GLU:HG2	1.95	0.58
2:B:350:GLU:CG	31:B:639:DMS:C1	2.81	0.58
25:B:619:BCR:C8	25:B:619:BCR:H331	2.32	0.58
3:C:117:VAL:HG12	34:C:531:LMG:H211	1.85	0.58
2:B:103:LEU:HD21	23:B:606:CLA:HMC3	1.86	0.58
23:C:514:CLA:HMB1	23:C:514:CLA:HBB1	1.85	0.58
30:B:623:LMT:H22	34:D:412:LMG:HC91	1.85	0.58
23:C:506:CLA:HBB1	23:C:506:CLA:HMB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:K:23:ASP:OD2	17:Y:21:GLN:NE2	2.35	0.58
1:A:265:PHE:HE2	27:A:411:PL9:H122	1.68	0.58
2:B:467:ILE:HG13	4:D:126:MET:HE1	2.32	0.58
26:A:410:SQD:H291	23:C:509:CLA:H71	1.86	0.58
2:B:314:TYR:CE1	2:B:316:GLY:HA3	2.38	0.58
23:C:504:CLA:HBB1	23:C:504:CLA:HMB1	1.85	0.57
24:A:407:PHO:HMB1	24:A:407:PHO:HBB1	1.87	0.57
25:B:619:BCR:H382	25:T:101:BCR:H11C	46.56	0.57
31:F:102:DMS:C1	16:V:27:LEU:HD21	2.35	0.57
16:V:4:THR:HA	31:V:206:DMS:H22	5.43	0.57
2:B:220:ARG:HG3	7:H:20:LYS:HG2	1.87	0.56
15:U:58:VAL:HG12	15:U:79:LEU:HD22	2.53	0.56
15:U:73:GLN:O	15:U:77:GLU:HG3	2.04	0.56
3:C:60:ILE:HG22	23:C:504:CLA:HHD	1.88	0.56
16:V:90:GLU:CB	31:V:209:DMS:C1	21.43	0.56
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.56
2:B:350:GLU:N	31:B:636:DMS:C1	28.31	0.56
23:C:510:CLA:CBB	23:C:510:CLA:HMB1	2.32	0.55
23:D:404:CLA:H192	18:X:15[A]:LEU:HG	1.88	0.55
2:B:462:PHE:CZ	23:B:614:CLA:HMB3	2.69	0.55
31:C:529:DMS:H11	40:C:826:HOH:O	2.05	0.55
23:A:406:CLA:H152	27:A:411:PL9:H262	1.88	0.55
29:U:201:UNL:C14	40:U:413:HOH:O	2.55	0.55
23:A:406:CLA:HMD3	4:D:182:LEU:HD11	1.89	0.55
23:B:604:CLA:C4D	23:B:606:CLA:H43	2.36	0.55
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.89	0.55
1:A:215:HIS:HA	27:A:411:PL9:O1	2.05	0.55
2:B:248:ALA:HA	23:B:604:CLA:H42	1.98	0.55
23:B:615:CLA:H161	23:B:615:CLA:H111	2.29	0.55
31:C:526:DMS:H11	40:C:800:HOH:O	2.06	0.55
25:Y:101:BCR:HC8	25:Y:101:BCR:H321	1.89	0.54
19:Z:35:ARG:CG	19:Z:35:ARG:HH11	2.07	0.54
1:A:215:HIS:ND1	27:A:411:PL9:O1	2.35	0.54
23:B:617:CLA:H141	25:B:620:BCR:H10C	2.95	0.54
2:B:47:PRO:HG2	31:O:308:DMS:C2	53.06	0.54
23:B:609:CLA:HBB1	23:B:609:CLA:HMB1	1.88	0.54
4:D:85:MET:CE	4:D:96:GLU:HG2	2.64	0.54
26:A:410:SQD:H331	23:C:509:CLA:H202	1.88	0.54
13:O:58:ASN:ND2	40:O:403:HOH:O	35.94	0.54
23:B:616:CLA:H2	23:B:617:CLA:HBB2	2.16	0.54
3:C:150:ASP:OD1	40:C:601:HOH:O	2.18	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:B:621:SQD:H242	11:L:14:ARG:HD3	27.96	0.54
3:C:377:LEU:O	3:C:381[A]:LYS:HG3	2.08	0.54
25:D:405:BCR:HC22	36:D:407:DGD:HAF2	6.14	0.54
19:Z:9:LEU:HD13	19:Z:54:VAL:HG11	2.32	0.54
23:B:604:CLA:HMB1	23:B:604:CLA:HBB1	1.90	0.53
2:B:350:GLU:N	31:B:639:DMS:H12	2.08	0.53
25:T:101:BCR:HC8	25:T:101:BCR:H321	1.91	0.53
23:B:606:CLA:C14	23:B:611:CLA:HED2	2.38	0.53
31:B:645:DMS:H11	40:B:1107:HOH:O	2.08	0.53
26:A:410:SQD:H383	29:J:104:UNL:C16	2.39	0.53
2:B:82:GLY:O	31:B:641:DMS:S	2.66	0.53
4:D:192:THR:HG23	23:D:403:CLA:HBC2	2.13	0.53
25:D:405:BCR:H313	36:D:407:DGD:HAE1	1.91	0.52
31:U:202:DMS:H22	40:U:314:HOH:O	2.10	0.52
19:Z:15:LEU:HD22	19:Z:46:LEU:HD23	2.42	0.52
2:B:405:GLU:OE2	2:B:431:GLU:OE1	2.27	0.52
31:O:311:DMS:H11	40:O:477:HOH:O	2.10	0.52
4:D:100:ASP:HA	36:D:407:DGD:HA32	4.53	0.52
1:A:98:GLU:OE1	40:A:502:HOH:O	57.69	0.52
4:D:11:GLU:O	4:D:12:ARG:HB2	2.10	0.52
2:B:451:PHE:CE2	2:B:455:HIS:CE1	2.98	0.52
23:B:606:CLA:HHC	23:B:606:CLA:HBB1	1.91	0.52
26:A:415:SQD:H442	40:A:616[B]:HOH:O	2.10	0.52
13:O:231:HIS:HD2	31:O:304:DMS:O	12.55	0.52
23:B:602:CLA:H72	23:B:602:CLA:CGA	2.40	0.52
31:A:424:DMS:C1	35:O:302:HTG:H1'1	2.40	0.52
13:O:98:GLU:HG3	40:O:402:HOH:O	10.49	0.52
23:C:502:CLA:H42	23:C:503:CLA:HMD1	1.92	0.51
5:E:19:TYR:CD2	5:E:23:HIS:CE1	3.50	0.51
16:V:118:HIS:CE1	16:V:122:GLU:HG2	2.45	0.51
31:V:207:DMS:H22	40:V:405:HOH:O	2.10	0.51
10:K:14:ALA:CB	19:Z:61:VAL:HG12	2.41	0.51
19:Z:33:TRP:CZ2	30:Z:101:LMT:O3'	2.64	0.51
2:B:349:LYS:N	31:B:636:DMS:H13	27.72	0.51
34:B:622:LMG:O9	34:B:622:LMG:H132	2.10	0.51
2:B:27:THR:HG22	2:B:107:LEU:HD13	2.07	0.51
15:U:38:TYR:HB2	15:U:41:LEU:HD12	1.93	0.51
23:B:611:CLA:CBB	23:B:611:CLA:HHC	2.41	0.51
3:C:377:LEU:HB3	13:O:80:GLN:OE1	2.11	0.50
23:B:611:CLA:HBB1	23:B:611:CLA:HHC	1.98	0.50
23:B:615:CLA:C16	23:B:615:CLA:H111	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:42:ARG:O	13:O:241:ALA:HA	2.18	0.50
13:O:66:VAL:HB	13:O:67:PRO:HD2	1.93	0.50
19:Z:33:TRP:HZ2	30:Z:101:LMT:O3'	1.94	0.50
3:C:31:SER:CB	3:C:41:ARG:HG2	2.46	0.50
13:O:111:ALA:HB3	31:O:308:DMS:H12	1.93	0.50
16:V:4:THR:HG22	31:V:206:DMS:C2	4.25	0.50
23:C:512:CLA:HBB1	23:C:512:CLA:HMB1	1.92	0.50
15:U:86:GLU:HG2	40:U:373:HOH:O	22.90	0.50
23:B:605:CLA:H43	23:B:606:CLA:H2	1.93	0.50
23:B:616:CLA:H142	23:B:617:CLA:H201	7.20	0.50
3:C:117:VAL:CG1	34:C:531:LMG:H211	2.41	0.50
3:C:78:GLU:HB3	40:C:758[B]:HOH:O	2.11	0.50
1:A:221:SER:HB2	4:D:139:ARG:O	2.11	0.50
24:D:402:PHO:HHD	24:D:402:PHO:HBC2	1.94	0.50
15:U:45:LEU:O	15:U:49:ILE:HG13	2.12	0.50
23:C:510:CLA:CMB	23:C:510:CLA:HBB1	2.31	0.49
1:A:84:PRO:HA	1:A:112:TYR:CG	2.47	0.49
31:B:646:DMS:H22	40:B:1076:HOH:O	2.11	0.49
16:V:45:ILE:HD12	16:V:45:ILE:C	2.58	0.49
13:O:231:HIS:HE1	40:O:527:HOH:O	1.95	0.49
15:U:10:VAL:H	31:U:204:DMS:H21	1.76	0.49
23:A:405:CLA:CBD	23:D:401:CLA:HAC2	2.43	0.49
36:D:407:DGD:HB21	5:E:46:VAL:HG13	5.10	0.49
23:B:617:CLA:HMB1	23:B:617:CLA:HBB1	1.94	0.49
25:D:405:BCR:H331	25:D:405:BCR:C8	2.50	0.49
27:A:411:PL9:H502	4:D:39:PRO:HG3	1.93	0.49
6:F:41:GLN:OE1	9:J:31:GLY:HA3	2.26	0.49
4:D:236:ASN:O	4:D:239:GLN:HG2	2.40	0.49
19:Z:32:ASP:OD1	19:Z:35:ARG:HB3	5.26	0.49
28:D:409:LHG:O9	28:L:101:LHG:HC81	2.13	0.49
3:C:31:SER:HB2	3:C:41:ARG:HG2	2.02	0.49
23:C:508:CLA:HBB1	23:C:508:CLA:HMB1	1.95	0.49
31:A:424:DMS:H11	35:O:302:HTG:H1'1	1.95	0.49
31:F:102:DMS:H11	16:V:27:LEU:HD21	1.94	0.49
1:A:317:TRP:CZ3	4:D:180:ARG:HD2	2.49	0.48
3:C:373:ASN:HB3	40:O:470:HOH:O	31.92	0.48
23:C:514:CLA:HMC2	25:C:515:BCR:H372	1.96	0.48
5:E:18:ARG:NH1	37:E:105:HEM:O2A	4.95	0.48
23:A:405:CLA:CAD	23:D:401:CLA:HAC2	2.44	0.48
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.70	0.48
1:A:339:PHE:HB3	1:A:340:PRO:HD2	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:9:PRO:HD2	9:J:12:ILE:HD12	1.95	0.48
13:O:133:VAL:HG13	31:O:305:DMS:C2	2.44	0.48
19:Z:47:TRP:CE2	30:Z:101:LMT:H112	2.48	0.48
26:B:621:SQD:H1	26:B:621:SQD:H462	1.94	0.48
2:B:347[B]:ARG:HH11	31:B:645:DMS:C2	32.01	0.48
26:D:408:SQD:H461	18:X:31:ILE:HG21	1.96	0.48
2:B:47:PRO:HG2	31:O:308:DMS:H21	52.17	0.48
5:E:60:GLN:HB2	5:E:60:GLN:HE21	4.43	0.48
11:L:24[A]:ILE:CD1	12:M:18:PRO:HB2	2.70	0.48
23:B:611:CLA:OBD	23:B:611:CLA:H152	3.30	0.48
13:O:56:PRO:HD3	13:O:63:ALA:HB2	1.96	0.48
3:C:318:LEU:C	3:C:318:LEU:HD23	2.34	0.48
4:D:213:ILE:HD11	4:D:253:TRP:CH2	2.49	0.48
23:B:617:CLA:H142	29:B:634:UNL:C7	2.43	0.48
2:B:80:ILE:HD11	2:B:167:TRP:CZ3	2.48	0.48
3:C:179:ALA:O	3:C:184:GLY:HA2	2.25	0.48
10:K:17:ILE:HG23	10:K:18:PHE:CD2	4.83	0.48
2:B:121[B]:GLU:HG3	40:B:1025:HOH:O	2.13	0.47
3:C:406:SER:HA	3:C:420:VAL:HG23	1.95	0.47
40:A:538:HOH:O	31:V:207:DMS:C1	2.62	0.47
2:B:472:ARG:HG2	31:D:416:DMS:H12	1.96	0.47
36:D:407:DGD:HG11	36:D:407:DGD:O2D	2.15	0.47
15:U:16:LYS:HD2	40:U:358:HOH:O	27.83	0.47
31:F:102:DMS:H13	40:J:214:HOH:O	2.11	0.47
30:B:623:LMT:H3B	34:D:412:LMG:HC62	1.96	0.47
27:A:411:PL9:H152	28:E:101:LHG:H302	1.95	0.47
1:A:265:PHE:O	27:A:411:PL9:H531	2.15	0.47
4:D:264[B]:LYS:HE3	4:D:264[B]:LYS:HB3	1.86	0.47
4:D:191:TRP:CE3	4:D:289:LEU:HD11	2.54	0.47
4:D:85:MET:HE1	4:D:96:GLU:HG2	2.23	0.47
4:D:27:PHE:HE1	28:E:101:LHG:HC2	1.80	0.47
4:D:272:LEU:C	4:D:272:LEU:HD23	2.34	0.47
10:K:11:LEU:HD11	10:K:22:VAL:HG21	2.24	0.47
25:T:101:BCR:H382	25:T:101:BCR:C23	2.44	0.47
15:U:58:VAL:O	15:U:61:VAL:HG12	2.61	0.47
31:V:210:DMS:H13	40:V:328:HOH:O	5.79	0.47
2:B:224:ARG:HG3	7:H:25:TRP:CD2	2.50	0.47
23:A:408:CLA:H122	23:A:408:CLA:H162	1.58	0.47
13:O:23:ASP:OD1	13:O:23:ASP:N	3.12	0.47
15:U:86:GLU:H	29:U:201:UNL:C14	2.27	0.47
19:Z:61:VAL:HG13	40:Z:1605:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:605:CLA:HMD2	23:B:613:CLA:H203	2.16	0.47
36:D:407:DGD:HBN1	36:D:407:DGD:HB22	8.60	0.47
7:H:29:PRO:HD2	31:H:105:DMS:H21	1.96	0.47
3:C:126:GLY:O	3:C:130:VAL:HG23	2.58	0.47
3:C:381[B]:LYS:NZ	13:O:99:ASP:OD2	2.48	0.47
3:C:50:LEU:O	3:C:54:VAL:HG23	2.15	0.47
4:D:141:TYR:CZ	31:D:416:DMS:H22	3.86	0.47
4:D:161:PRO:HG3	4:D:170:ALA:HB2	2.25	0.47
3:C:38:GLY:HA3	23:C:512:CLA:HMD3	1.97	0.46
19:Z:3:ILE:HA	19:Z:6:GLN:HB2	3.36	0.46
12:M:16[B]:LEU:HD21	40:M:214:HOH:O	30.41	0.46
2:B:204:ALA:CB	23:B:603:CLA:HAB	2.46	0.46
12:M:28:GLN:O	12:M:32:GLN:HG3	2.16	0.46
23:D:403:CLA:HBC3	23:D:403:CLA:HHD	1.98	0.46
12:M:5:GLN:HG2	12:M:5:GLN:H	1.36	0.46
16:V:53:ASP:CG	16:V:55[B]:ARG:HG3	2.94	0.46
26:D:408:SQD:H242	18:X:31:ILE:HD13	1.98	0.46
2:B:72:THR:HG22	2:B:80:ILE:HD11	2.40	0.46
25:D:405:BCR:C38	34:J:101:LMG:H231	2.45	0.46
1:A:103:ASP:OD2	13:O:69:LYS:HE3	4.09	0.46
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.50	0.46
2:B:498:LYS:HD2	4:D:20:ASP:HA	1.98	0.46
2:B:162:PHE:O	23:B:607:CLA:HHD	2.23	0.46
23:B:606:CLA:HHC	23:B:606:CLA:CBB	2.45	0.46
26:B:621:SQD:H341	26:B:621:SQD:H311	1.64	0.46
3:C:437:PHE:CE1	23:C:511:CLA:HMB3	2.50	0.46
23:D:404:CLA:H161	23:D:404:CLA:H192	2.89	0.46
23:C:513:CLA:H101	23:C:514:CLA:H141	1.98	0.46
31:O:303:DMS:H22	40:O:416:HOH:O	2.15	0.46
3:C:409:GLY:HA2	31:V:202:DMS:S	2.56	0.46
3:C:390:ARG:HD3	16:V:100:ILE:HD12	2.06	0.46
31:V:207:DMS:H11	40:V:405:HOH:O	2.15	0.46
19:Z:26:ALA:HB3	19:Z:40:ILE:HD11	2.10	0.46
23:A:406:CLA:CBD	23:D:401:CLA:HAC2	14.69	0.46
23:B:614:CLA:H51	28:D:409:LHG:H351	1.97	0.46
31:B:646:DMS:H12	40:B:779:HOH:O	2.15	0.46
5:E:9:PRO:HA	28:E:101:LHG:C2	3.16	0.46
13:O:58:ASN:ND2	13:O:58:ASN:C	2.67	0.46
2:B:208:VAL:HG21	23:B:603:CLA:HMC1	1.99	0.45
25:B:620:BCR:C33	25:B:620:BCR:HC8	2.70	0.45
30:Z:101:LMT:H82	30:Z:101:LMT:H51	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:A:415:SQD:H272	2:B:109:LEU:HD13	59.80	0.45
23:B:617:CLA:C14	25:B:620:BCR:H12C	4.07	0.45
3:C:109:PHE:N	3:C:110:PRO:CD	3.01	0.45
28:E:101:LHG:H181	28:E:101:LHG:H212	4.37	0.45
5:E:63:ILE:HG23	5:E:64:PRO:HD2	2.09	0.45
13:O:33:ASP:CB	13:O:36:GLN:HE21	7.77	0.45
13:O:39:ARG:HB2	13:O:83:GLY:O	2.17	0.45
3:C:377:LEU:CB	13:O:80:GLN:OE1	2.64	0.45
25:T:101:BCR:H23C	25:T:101:BCR:H382	1.98	0.45
36:D:407:DGD:HA51	36:D:407:DGD:HA22	3.72	0.45
16:V:14:SER:HB2	35:V:204:HTG:O2	30.78	0.45
16:V:55[A]:ARG:NH1	40:V:306:HOH:O	33.35	0.45
30:Z:101:LMT:H1B	30:Z:101:LMT:H4B	2.15	0.45
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.58	0.45
23:B:617:CLA:H203	23:B:617:CLA:H122	7.46	0.45
25:B:619:BCR:H363	25:T:101:BCR:H19C	35.12	0.45
25:T:101:BCR:HC7	25:T:101:BCR:H331	1.61	0.45
2:B:63:LEU:N	2:B:64:PRO:HD2	2.31	0.45
23:C:505:CLA:H42	36:C:518:DGD:HB31	1.99	0.45
23:C:514:CLA:C4B	25:C:515:BCR:H383	2.46	0.45
17:Y:44:GLY:HA2	19:Z:30:PRO:HD3	2.38	0.45
1:A:247:ASN:HB3	2:B:482:ILE:HD11	2.39	0.45
1:A:249:VAL:HG12	2:B:491:VAL:CG2	2.47	0.45
25:B:620:BCR:H371	25:B:620:BCR:H24C	1.87	0.45
23:C:507:CLA:H151	23:C:507:CLA:H18	1.63	0.45
6:F:28:VAL:HB	6:F:29:PRO:HD3	2.10	0.45
26:L:102:SQD:H462	26:L:102:SQD:H1	1.99	0.45
13:O:59:LYS:O	13:O:60:ARG:CB	2.69	0.45
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.52	0.45
23:B:616:CLA:H2	23:B:617:CLA:CBB	2.65	0.45
23:C:509:CLA:HMB2	23:C:511:CLA:HBA1	1.99	0.45
4:D:141:TYR:CZ	31:D:416:DMS:C2	3.11	0.44
31:B:648:DMS:C2	11:L:2:GLU:HB2	2.47	0.44
23:B:617:CLA:H91	23:B:617:CLA:H112	3.52	0.44
23:C:511:CLA:HBC3	23:C:511:CLA:H192	2.00	0.44
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.98	0.44
28:D:410:LHG:H341	28:D:410:LHG:H302	5.70	0.44
11:L:18:TYR:OH	26:L:102:SQD:H242	2.18	0.44
3:C:334:PRO:HA	13:O:153:THR:OG1	2.21	0.44
2:B:475:PHE:CD2	4:D:140:PRO:HG3	2.53	0.44
23:B:603:CLA:CMB	23:B:603:CLA:HBB1	3.04	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:MET:HA	4:D:129:GLN:OE1	2.17	0.44
23:D:401:CLA:H203	23:D:401:CLA:H162	1.69	0.44
5:E:59:GLU:OE1	5:E:59:GLU:HA	2.40	0.44
13:O:111:ALA:HB3	31:O:308:DMS:C1	2.47	0.44
16:V:90:GLU:CB	31:V:209:DMS:H12	21.59	0.44
25:A:409:BCR:H331	25:A:409:BCR:C8	2.47	0.44
3:C:155[B]:ASN:OD1	3:C:255:THR:CB	2.66	0.44
3:C:362:ARG:HD3	31:C:525:DMS:O	2.17	0.44
16:V:86:GLN:NE2	40:V:302:HOH:O	24.53	0.44
2:B:26:HIS:HB2	23:B:613:CLA:HMB2	2.00	0.44
15:U:53:ALA:HB1	15:U:54:PRO:HA	2.22	0.44
25:A:409:BCR:H24C	25:A:409:BCR:H371	1.77	0.44
3:C:240:ILE:HA	3:C:240:ILE:HD13	2.00	0.44
4:D:24:ARG:NH1	40:D:610[B]:HOH:O	2.50	0.44
28:D:411:LHG:H322	28:D:411:LHG:H142	1.99	0.44
16:V:2:GLU:OE2	31:V:207:DMS:C1	2.66	0.44
1:A:162:PRO:HB3	1:A:168:PHE:HA	2.00	0.44
1:A:259:ILE:HD12	27:A:411:PL9:H253	2.00	0.44
2:B:144:PHE:CE2	2:B:210:ILE:HG23	2.60	0.44
4:D:23:LYS:HD3	4:D:135:LEU:HD21	2.56	0.44
31:B:639:DMS:H11	40:B:1013:HOH:O	2.18	0.43
25:C:530:BCR:H341	25:C:530:BCR:H11C	1.92	0.43
4:D:27:PHE:CD2	28:E:101:LHG:HC12	7.04	0.43
10:K:21:LEU:HD13	17:Y:24:MET:CE	5.24	0.43
16:V:129:LYS:HD2	40:V:410:HOH:O	2.18	0.43
16:V:4:THR:HG22	31:V:206:DMS:H22	4.90	0.43
16:V:72:LEU:O	16:V:76:MET:HG3	2.98	0.43
26:A:410:SQD:H122	26:A:410:SQD:C16	2.31	0.43
30:A:416:LMT:H123	29:A:417:UNL:C13	2.48	0.43
2:B:483:ASP:HA	2:B:484:PRO:HD3	2.12	0.43
23:B:602:CLA:H2	23:B:602:CLA:H72	4.61	0.43
31:O:303:DMS:H23	40:O:478:HOH:O	17.44	0.43
19:Z:47:TRP:CD2	30:Z:101:LMT:H112	2.54	0.43
3:C:464:GLU:OE2	4:D:245:SER:OG	2.25	0.43
13:O:129:THR:HA	13:O:141:ASP:O	2.20	0.43
35:V:204:HTG:H61	40:V:416:HOH:O	32.24	0.43
4:D:24:ARG:NH2	18:X:35:ASP:O	3.79	0.43
23:B:606:CLA:H41	23:B:606:CLA:H62	1.79	0.43
2:B:350:GLU:N	31:B:639:DMS:C1	2.69	0.43
23:C:504:CLA:H72	23:C:504:CLA:H112	1.77	0.43
40:L:208[B]:HOH:O	12:M:4:ASN:ND2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:79:PRO:HD3	16:V:94:SER:HB3	1.99	0.43
16:V:91:VAL:HG13	31:V:209:DMS:H12	22.45	0.43
28:A:412:LHG:H242	28:A:412:LHG:H111	2.00	0.43
31:B:641:DMS:C2	40:B:787:HOH:O	27.48	0.43
31:B:641:DMS:H22	40:B:896:HOH:O	26.87	0.43
3:C:203:THR:O	3:C:235:GLY:HA3	2.19	0.43
26:A:410:SQD:H142	28:D:411:LHG:C16	2.49	0.43
7:H:30:LEU:H	31:H:105:DMS:C2	2.30	0.43
2:B:493:TRP:HD1	5:E:5:THR:CG2	2.32	0.43
3:C:472:LEU:HD11	4:D:255:GLN:HG3	2.00	0.43
28:D:411:LHG:H322	28:D:411:LHG:C14	2.49	0.43
28:D:411:LHG:H331	28:D:411:LHG:H302	1.65	0.43
4:D:103:ARG:HG3	5:E:73:LYS:HG3	2.01	0.43
31:O:304:DMS:H11	40:O:532[B]:HOH:O	2.18	0.43
25:B:619:BCR:H361	25:B:619:BCR:H20C	1.85	0.43
23:C:507:CLA:H92	30:I:101:LMT:C11	2.45	0.43
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.72	0.43
10:K:19:ASP:HB2	10:K:20:PRO:HD3	2.01	0.43
26:L:102:SQD:H462	26:L:102:SQD:C1	2.48	0.43
13:O:194:LYS:HZ1	31:O:303:DMS:H22	1.84	0.43
1:A:188:ALA:HB2	1:A:328:MET:HB2	2.01	0.43
1:A:96:ILE:HD12	23:A:408:CLA:HMD1	2.01	0.43
3:C:167:VAL:HG13	23:C:513:CLA:H71	2.01	0.43
3:C:308:GLU:HB2	3:C:361:PHE:CE2	2.53	0.43
24:A:407:PHO:NC	24:A:407:PHO:ND	2.67	0.43
23:C:503:CLA:H193	35:C:521:HTG:H3'1	2.00	0.43
4:D:296:TYR:CE1	4:D:319:LEU:HD22	2.87	0.43
1:A:322:ASN:OD1	3:C:412:THR:HA	2.23	0.42
12:M:16[B]:LEU:HD23	12:M:16[B]:LEU:HA	3.36	0.42
16:V:129:LYS:CD	40:V:410:HOH:O	2.66	0.42
16:V:81:THR:CG2	16:V:86:GLN:HG3	2.49	0.42
1:A:249:VAL:HG12	2:B:491:VAL:HG23	2.16	0.42
25:C:515:BCR:H331	25:C:515:BCR:C8	2.48	0.42
7:H:59:ASN:ND2	7:H:63:LYS:O	2.53	0.42
15:U:10:VAL:HG11	15:U:15:GLU:OE2	2.34	0.42
31:F:102:DMS:H13	16:V:27:LEU:HD21	2.00	0.42
19:Z:3:ILE:CA	19:Z:6:GLN:HB2	3.93	0.42
26:B:621:SQD:H45	14:T:23:PHE:CD1	35.42	0.42
18:X:23:LEU:O	18:X:27:VAL:HG23	2.20	0.42
19:Z:44:SER:O	19:Z:48:ILE:HG13	3.11	0.42
1:A:265:PHE:HE2	27:A:411:PL9:C12	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:B:602:CLA:H91	23:B:602:CLA:H111	1.61	0.42
23:B:617:CLA:H92	23:B:617:CLA:H61	3.04	0.42
3:C:95:LEU:HD21	23:C:502:CLA:OBD	2.19	0.42
4:D:27:PHE:CE1	28:E:101:LHG:HC2	2.54	0.42
25:T:101:BCR:C38	25:T:101:BCR:C23	2.97	0.42
3:C:78:GLU:HG2	3:C:79:LYS:N	3.06	0.42
23:B:610:CLA:HMB2	23:B:611:CLA:C2B	2.50	0.42
3:C:53:HIS:CB	23:C:513:CLA:HMD1	2.49	0.42
2:B:410:THR:H	31:B:639:DMS:C2	20.69	0.42
2:B:36:SER:OG	25:B:619:BCR:H362	2.23	0.42
23:C:511:CLA:HBB1	23:C:511:CLA:HMB1	2.01	0.42
2:B:467:ILE:HD12	2:B:467:ILE:HA	2.39	0.42
25:B:618:BCR:H23C	25:B:618:BCR:H382	2.02	0.42
3:C:158:THR:O	3:C:251:HIS:HB3	2.19	0.42
34:C:501:LMG:H221	36:C:517:DGD:HAW1	2.01	0.42
4:D:24:ARG:HH22	18:X:35:ASP:CG	2.39	0.42
3:C:79:LYS:HD2	16:V:35:TYR:CE2	5.73	0.42
1:A:212:CYS:HB2	4:D:211:CYS:HB2	2.02	0.42
23:C:512:CLA:H191	30:Z:101:LMT:H122	2.01	0.42
1:A:270:SER:OG	26:A:410:SQD:H3	2.19	0.41
2:B:382:PRO:HG2	2:B:385:ARG:HD2	2.12	0.41
2:B:347[B]:ARG:HH11	31:B:645:DMS:H21	32.20	0.41
17:Y:18:VAL:O	17:Y:22:LEU:HD12	2.20	0.41
25:D:405:BCR:HC22	36:D:407:DGD:HA92	2.02	0.41
6:F:30:THR:HG21	34:J:101:LMG:H412	2.02	0.41
2:B:47:PRO:HG2	31:O:308:DMS:H23	53.22	0.41
2:B:145:LEU:HD11	23:B:616:CLA:HMB2	2.03	0.41
23:B:613:CLA:HBB1	23:B:613:CLA:HMB1	2.06	0.41
3:C:155[B]:ASN:OD1	3:C:255:THR:OG1	2.26	0.41
4:D:161:PRO:HB3	4:D:170:ALA:HB2	2.03	0.41
25:A:409:BCR:H351	25:A:409:BCR:H15C	1.96	0.41
31:A:422:DMS:H13	40:A:501:HOH:O	2.19	0.41
2:B:224:ARG:HG2	7:H:24:GLY:O	2.21	0.41
25:B:620:BCR:H20C	25:B:620:BCR:H361	1.93	0.41
13:O:140:THR:HG23	31:O:305:DMS:H22	2.02	0.41
2:B:237:VAL:HG12	23:B:613:CLA:HMD1	2.07	0.41
3:C:215:LYS:HB2	3:C:223:TRP:HA	2.02	0.41
3:C:71:GLU:HB3	3:C:89:ILE:HD12	2.64	0.41
1:A:79:THR:HG22	4:D:315:TYR:HB2	2.02	0.41
31:B:636:DMS:C1	40:D:553:HOH:O	2.68	0.41
19:Z:35:ARG:NH2	40:Z:1601:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:A:406:CLA:HBD	23:D:401:CLA:HAC2	14.51	0.41
13:O:61:GLN:HG2	13:O:61:GLN:O	2.21	0.41
18:X:23:LEU:HD23	18:X:23:LEU:HA	2.35	0.41
2:B:237:VAL:HG11	23:B:611:CLA:H201	2.39	0.41
23:B:617:CLA:H41	23:B:617:CLA:H72	2.02	0.41
23:C:503:CLA:HBD	23:C:504:CLA:H43	2.02	0.41
25:T:101:BCR:C8	25:T:101:BCR:H321	2.50	0.41
3:C:185:LEU:HB2	3:C:230:LEU:HD13	2.16	0.41
24:D:402:PHO:NC	24:D:402:PHO:ND	2.67	0.41
25:D:405:BCR:H383	34:J:101:LMG:H171	2.01	0.41
2:B:270:PRO:HG2	2:B:317:ASN:O	2.57	0.41
23:B:614:CLA:OBD	23:B:615:CLA:HHC	2.24	0.41
3:C:155[A]:ASN:H	3:C:155[A]:ASN:HD22	4.75	0.41
13:O:181:GLU:N	13:O:181:GLU:OE1	2.74	0.41
23:B:612:CLA:HMB2	23:B:614:CLA:HBA1	2.03	0.41
2:B:410:THR:H	31:B:639:DMS:H22	21.09	0.41
3:C:124:VAL:HB	25:C:515:BCR:H362	2.03	0.41
3:C:283:GLY:HA3	3:C:434:ALA:HB2	2.03	0.41
25:C:530:BCR:H24C	25:C:530:BCR:H371	1.71	0.41
4:D:85:MET:HE3	4:D:96:GLU:HG2	2.22	0.41
40:B:1104:HOH:O	31:H:101:DMS:H23	2.20	0.41
23:C:513:CLA:HBB1	23:C:513:CLA:HMB1	2.02	0.40
36:D:407:DGD:HG32	36:D:407:DGD:HD2	1.87	0.40
13:O:25:THR:HG23	40:O:564:HOH:O	2.19	0.40
13:O:133:VAL:CG2	31:O:305:DMS:H21	2.47	0.40
3:C:146:PHE:O	3:C:156:LYS:NZ	3.13	0.40
3:C:168:LEU:HA	3:C:168:LEU:HD23	2.02	0.40
23:D:403:CLA:CHD	23:D:403:CLA:HBC3	2.51	0.40
40:B:888:HOH:O	31:H:101:DMS:H21	59.39	0.40
10:K:10:LYS:N	40:K:204:HOH:O	48.34	0.40
2:B:498:LYS:HA	4:D:24:ARG:HA	2.29	0.40
23:B:615:CLA:H62	23:B:615:CLA:H41	2.09	0.40
3:C:437:PHE:CZ	23:C:511:CLA:HMB3	2.57	0.40
25:C:516:BCR:H15C	25:C:516:BCR:H351	1.91	0.40
7:H:30:LEU:H	31:H:105:DMS:H23	1.86	0.40
23:B:602:CLA:H162	23:B:602:CLA:H141	3.36	0.40
25:B:620:BCR:H383	25:B:620:BCR:C23	2.53	0.40
2:B:71:VAL:HG21	2:B:96:VAL:HG21	2.04	0.40
3:C:221:GLU:O	3:C:226:SER:HB3	2.20	0.40
3:C:166:ILE:HB	23:C:513:CLA:H203	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	325 (98%)	7 (2%)	1 (0%)	46	33
1	a	336/344 (98%)	330 (98%)	5 (2%)	1 (0%)	46	33
2	B	507/505 (100%)	497 (98%)	10 (2%)	0	100	100
2	b	500/505 (99%)	490 (98%)	10 (2%)	0	100	100
3	C	453/455 (100%)	440 (97%)	12 (3%)	1 (0%)	52	40
3	c	454/455 (100%)	441 (97%)	12 (3%)	1 (0%)	52	40
4	D	342/342 (100%)	333 (97%)	8 (2%)	1 (0%)	46	33
4	d	342/342 (100%)	333 (97%)	9 (3%)	0	100	100
5	E	79/83 (95%)	76 (96%)	3 (4%)	0	100	100
5	e	77/83 (93%)	76 (99%)	1 (1%)	0	100	100
6	F	33/44 (75%)	33 (100%)	0	0	100	100
6	f	30/44 (68%)	30 (100%)	0	0	100	100
7	H	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
7	h	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	I	33/38 (87%)	32 (97%)	1 (3%)	0	100	100
8	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
9	J	34/40 (85%)	33 (97%)	1 (3%)	0	100	100
9	j	38/40 (95%)	38 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
10	k	35/37 (95%)	35 (100%)	0	0	100	100
11	L	36/37 (97%)	36 (100%)	0	0	100	100
11	l	35/37 (95%)	35 (100%)	0	0	100	100
12	M	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
12	m	33/36 (92%)	32 (97%)	1 (3%)	0	100	100
13	O	243/244 (100%)	229 (94%)	11 (4%)	3 (1%)	16	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	o	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
14	T	28/32 (88%)	28 (100%)	0	0	100	100
14	t	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
15	U	95/104 (91%)	92 (97%)	3 (3%)	0	100	100
15	u	96/104 (92%)	93 (97%)	3 (3%)	0	100	100
16	V	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
16	v	136/137 (99%)	132 (97%)	4 (3%)	0	100	100
17	Y	27/30 (90%)	27 (100%)	0	0	100	100
17	y	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
18	X	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
18	x	36/40 (90%)	35 (97%)	1 (3%)	0	100	100
19	Z	60/62 (97%)	56 (93%)	3 (5%)	1 (2%)	11	2
19	z	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	5	0
All	All	5210/5350 (97%)	5059 (97%)	140 (3%)	11 (0%)	52	40

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	12	ARG
19	Z	31	GLN
3	c	416	SER
19	z	31	GLN
3	C	416	SER
19	z	3	ILE
13	O	26	ALA
13	O	59	LYS
13	O	60	ARG
1	A	259	ILE
1	a	259	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/279 (96%)	268 (100%)	1 (0%)	93	93
1	a	272/279 (98%)	271 (100%)	1 (0%)	93	93
2	B	403/403 (100%)	399 (99%)	4 (1%)	82	79
2	b	394/403 (98%)	389 (99%)	5 (1%)	76	71
3	C	355/356 (100%)	351 (99%)	4 (1%)	80	77
3	c	356/356 (100%)	351 (99%)	5 (1%)	74	69
4	D	278/277 (100%)	274 (99%)	4 (1%)	74	69
4	d	278/277 (100%)	276 (99%)	2 (1%)	88	87
5	E	70/72 (97%)	68 (97%)	2 (3%)	50	37
5	e	68/72 (94%)	64 (94%)	4 (6%)	24	11
6	F	28/38 (74%)	27 (96%)	1 (4%)	42	28
6	f	25/38 (66%)	25 (100%)	0	100	100
7	H	55/54 (102%)	53 (96%)	2 (4%)	42	28
7	h	54/54 (100%)	53 (98%)	1 (2%)	65	56
8	I	30/34 (88%)	30 (100%)	0	100	100
8	i	31/34 (91%)	31 (100%)	0	100	100
9	J	23/28 (82%)	22 (96%)	1 (4%)	35	21
9	j	27/28 (96%)	27 (100%)	0	100	100
10	K	30/30 (100%)	28 (93%)	2 (7%)	20	8
10	k	30/30 (100%)	29 (97%)	1 (3%)	45	31
11	L	35/35 (100%)	35 (100%)	0	100	100
11	l	34/35 (97%)	34 (100%)	0	100	100
12	M	30/33 (91%)	29 (97%)	1 (3%)	45	31
12	m	30/33 (91%)	30 (100%)	0	100	100
13	O	205/207 (99%)	200 (98%)	5 (2%)	57	46
13	o	203/207 (98%)	199 (98%)	4 (2%)	63	54
14	T	25/28 (89%)	24 (96%)	1 (4%)	38	24
14	t	25/28 (89%)	24 (96%)	1 (4%)	38	24
15	U	82/89 (92%)	82 (100%)	0	100	100
15	u	84/89 (94%)	84 (100%)	0	100	100
16	V	118/117 (101%)	115 (98%)	3 (2%)	55	44
16	v	115/117 (98%)	114 (99%)	1 (1%)	84	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	Y	20/23 (87%)	18 (90%)	2 (10%)	9	3
17	y	19/23 (83%)	18 (95%)	1 (5%)	28	14
18	X	30/33 (91%)	30 (100%)	0	100	100
18	x	29/33 (88%)	29 (100%)	0	100	100
19	Z	49/52 (94%)	47 (96%)	2 (4%)	37	23
19	z	46/52 (88%)	41 (89%)	5 (11%)	8	2
All	All	4255/4376 (97%)	4189 (98%)	66 (2%)	72	63

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	229	GLU
2	B	53	ASN
2	B	127	ARG
2	B	246	PHE
2	B	505	ARG
3	C	207[A]	ARG
3	C	207[B]	ARG
3	C	289	PHE
3	C	315	MET
4	D	12	ARG
4	D	26	ARG
4	D	90	LEU
4	D	180	ARG
5	E	4	THR
5	E	25	ILE
6	F	44	GLN
7	H	49	TYR
7	H	63	LYS
9	J	10	LEU
10	K	10	LYS
10	K	17	ILE
12	M	5	GLN
13	O	34	SER
13	O	45	LEU
13	O	58	ASN
13	O	69	LYS
13	O	118	LEU
14	T	2	GLU
16	V	30	LYS

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Mol	Chain	Res	Type
16	V	86	GLN
16	V	122	GLU
17	Y	27	MET
17	Y	42	ARG
19	Z	4	LEU
19	Z	35	ARG
1	a	162	PRO
2	b	128	THR
2	b	246	PHE
2	b	362	PHE
2	b	467	ILE
2	b	483	ASP
3	c	156	LYS
3	c	289	PHE
3	c	355	THR
3	c	416	SER
3	c	418	ASN
4	d	24	ARG
4	d	180	ARG
5	e	25	ILE
5	e	60	GLN
5	e	62	SER
5	e	68	ASP
7	h	49	TYR
10	k	27	VAL
13	o	23	ASP
13	o	58	ASN
13	o	118	LEU
13	o	181	GLU
14	t	2	GLU
16	v	6	GLU
17	y	23	THR
19	z	1	MET
19	z	5	PHE
19	z	6	GLN
19	z	29	SER
19	z	46	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN

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Mol	Chain	Res	Type
2	B	179	GLN
2	B	331	ASN
13	O	82	GLN
16	V	34	GLN
1	a	315	ASN
2	b	53	ASN
2	b	179	GLN
2	b	331	ASN
2	b	374	ASN
3	c	201	ASN
4	d	332	GLN
6	f	44	GLN
7	h	59	ASN
13	o	36	GLN
13	o	82	GLN
13	o	231	HIS
15	u	73	GLN
16	v	34	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
8	FME	I	1	8	8,9,10	0.73	0	5,9,11	1.32	1 (20%)
14	FME	T	1	14	8,9,10	0.48	0	5,9,11	2.00	2 (40%)
8	FME	i	1	8	8,9,10	0.68	0	5,9,11	1.95	2 (40%)
14	FME	t	1	14	8,9,10	0.63	0	5,9,11	1.82	2 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	I	1	8	-	0/6/9/11	0/0/0/0
14	FME	T	1	14	-	0/6/9/11	0/0/0/0
8	FME	i	1	8	-	0/6/9/11	0/0/0/0
14	FME	t	1	14	-	0/6/9/11	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	1	FME	O1-CN-N	-3.56	119.36	124.80
14	T	1	FME	O-C-CA	-2.72	118.27	125.69
14	t	1	FME	O-C-CA	-2.59	118.60	125.69
8	i	1	FME	O-C-CA	-2.26	119.50	125.69
8	I	1	FME	O1-CN-N	-2.13	121.54	124.80
14	t	1	FME	CE-SD-CG	2.28	108.28	100.36
14	T	1	FME	CE-SD-CG	2.56	109.25	100.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 366 ligands modelled in this entry, 53 are unknown and 13 are monoatomic - leaving 300 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
20	OEX	A	401	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
23	CLA	A	405	-	57,73,73	1.69	12 (21%)	61,113,113	2.26	21 (34%)
23	CLA	A	406	40	57,73,73	1.47	9 (15%)	61,113,113	2.26	19 (31%)
24	PHO	A	407	-	67,69,69	1.72	11 (16%)	86,99,99	2.03	24 (27%)
23	CLA	A	408	-	57,73,73	1.67	11 (19%)	61,113,113	2.15	20 (32%)
25	BCR	A	409	-	41,41,41	1.05	3 (7%)	56,56,56	1.44	10 (17%)
26	SQD	A	410	-	53,54,54	1.37	3 (5%)	62,65,65	2.32	17 (27%)
27	PL9	A	411	-	54,55,55	0.75	2 (3%)	68,69,69	1.68	15 (22%)
28	LHG	A	412	-	48,48,48	1.03	2 (4%)	49,54,54	1.00	4 (8%)
26	SQD	A	415	-	53,54,54	1.56	3 (5%)	62,65,65	2.32	12 (19%)
30	LMT	A	416	-	36,36,36	0.82	1 (2%)	47,47,47	1.26	6 (12%)
31	DMS	A	418	-	3,3,3	2.74	1 (33%)	3,3,3	0.59	0
31	DMS	A	419	-	3,3,3	2.75	1 (33%)	3,3,3	0.65	0
32	BCT	A	420	21	0,3,3	0.00	-	0,3,3	0.00	-
31	DMS	A	421	-	3,3,3	2.72	1 (33%)	3,3,3	0.74	0
31	DMS	A	422	-	3,3,3	2.68	1 (33%)	3,3,3	0.77	0
31	DMS	A	423	-	3,3,3	1.92	1 (33%)	3,3,3	0.61	0
31	DMS	A	424	-	3,3,3	2.76	1 (33%)	3,3,3	0.97	0
23	CLA	B	602	40	57,73,73	1.84	11 (19%)	61,113,113	2.22	15 (24%)
23	CLA	B	603	-	57,73,73	1.89	13 (22%)	61,113,113	2.02	19 (31%)
23	CLA	B	604	-	57,73,73	1.66	10 (17%)	61,113,113	2.70	21 (34%)
23	CLA	B	605	-	57,73,73	1.56	11 (19%)	61,113,113	2.03	18 (29%)
23	CLA	B	606	-	57,73,73	1.64	12 (21%)	61,113,113	2.04	17 (27%)
23	CLA	B	607	-	57,73,73	1.83	12 (21%)	61,113,113	2.13	18 (29%)
23	CLA	B	608	40	57,73,73	1.70	10 (17%)	61,113,113	2.14	18 (29%)
23	CLA	B	609	-	57,73,73	1.67	11 (19%)	61,113,113	2.02	16 (26%)
23	CLA	B	610	-	57,73,73	1.67	10 (17%)	61,113,113	2.22	16 (26%)
23	CLA	B	611	40	57,73,73	1.80	13 (22%)	61,113,113	2.13	16 (26%)
23	CLA	B	612	-	57,73,73	1.61	12 (21%)	61,113,113	2.05	15 (24%)
23	CLA	B	613	-	57,73,73	1.64	11 (19%)	61,113,113	2.20	23 (37%)
23	CLA	B	614	-	57,73,73	1.58	13 (22%)	61,113,113	1.95	16 (26%)
23	CLA	B	615	-	57,73,73	1.78	12 (21%)	61,113,113	2.09	17 (27%)
23	CLA	B	616	-	57,73,73	1.77	13 (22%)	61,113,113	1.91	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	B	617	-	57,73,73	1.76	12 (21%)	61,113,113	2.13	18 (29%)
25	BCR	B	618	-	41,41,41	1.05	2 (4%)	56,56,56	1.47	10 (17%)
25	BCR	B	619	-	41,41,41	1.06	2 (4%)	56,56,56	1.18	9 (16%)
25	BCR	B	620	-	41,41,41	0.99	1 (2%)	56,56,56	1.59	12 (21%)
26	SQD	B	621	-	53,54,54	1.30	4 (7%)	62,65,65	2.05	7 (11%)
34	LMG	B	622	-	51,51,55	0.96	3 (5%)	59,59,63	1.30	9 (15%)
30	LMT	B	623	-	36,36,36	0.57	0	47,47,47	1.08	3 (6%)
35	HTG	B	624	-	19,19,19	1.41	3 (15%)	22,24,24	1.80	4 (18%)
35	HTG	B	625	-	19,19,19	1.35	2 (10%)	22,24,24	2.16	8 (36%)
35	HTG	B	626	-	19,19,19	0.88	1 (5%)	22,24,24	2.08	1 (4%)
35	HTG	B	630	-	19,19,19	0.92	2 (10%)	22,24,24	1.60	2 (9%)
35	HTG	B	631	-	19,19,19	1.03	1 (5%)	22,24,24	1.44	2 (9%)
31	DMS	B	636	-	3,3,3	3.10	1 (33%)	3,3,3	0.72	0
31	DMS	B	637	-	3,3,3	2.27	1 (33%)	3,3,3	0.89	0
31	DMS	B	638	-	3,3,3	2.78	1 (33%)	3,3,3	0.92	0
31	DMS	B	639	-	3,3,3	2.77	1 (33%)	3,3,3	0.81	0
31	DMS	B	640	-	3,3,3	2.64	1 (33%)	3,3,3	0.70	0
31	DMS	B	641	-	3,3,3	2.83	1 (33%)	3,3,3	0.74	0
31	DMS	B	642	-	3,3,3	2.93	1 (33%)	3,3,3	1.17	0
30	LMT	B	643	-	24,24,36	0.38	0	29,29,47	0.93	2 (6%)
30	LMT	B	644	-	24,24,36	0.33	0	29,29,47	1.28	5 (17%)
31	DMS	B	645	-	3,3,3	2.81	1 (33%)	3,3,3	0.64	0
31	DMS	B	646	-	3,3,3	2.61	1 (33%)	3,3,3	0.65	0
31	DMS	B	647	-	3,3,3	2.73	1 (33%)	3,3,3	0.50	0
31	DMS	B	648	-	3,3,3	2.49	1 (33%)	3,3,3	0.96	0
31	DMS	B	649	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
34	LMG	C	501	-	51,51,55	0.92	2 (3%)	59,59,63	1.21	4 (6%)
23	CLA	C	502	-	57,73,73	1.70	11 (19%)	61,113,113	2.12	10 (16%)
23	CLA	C	503	-	57,73,73	1.84	11 (19%)	61,113,113	2.06	16 (26%)
23	CLA	C	504	-	57,73,73	1.97	12 (21%)	61,113,113	1.89	16 (26%)
23	CLA	C	505	40	57,73,73	1.72	11 (19%)	61,113,113	2.17	15 (24%)
23	CLA	C	506	-	57,73,73	1.89	13 (22%)	61,113,113	2.11	16 (26%)
23	CLA	C	507	-	57,73,73	1.87	12 (21%)	61,113,113	2.16	19 (31%)
23	CLA	C	508	40	57,73,73	1.89	12 (21%)	61,113,113	2.21	18 (29%)
23	CLA	C	509	-	57,73,73	1.97	12 (21%)	61,113,113	1.81	14 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	C	510	-	57,73,73	1.82	11 (19%)	61,113,113	2.18	19 (31%)
23	CLA	C	511	-	57,73,73	1.90	12 (21%)	61,113,113	2.08	16 (26%)
23	CLA	C	512	3	57,73,73	1.78	12 (21%)	61,113,113	1.95	16 (26%)
23	CLA	C	513	-	57,73,73	2.08	12 (21%)	61,113,113	1.91	16 (26%)
23	CLA	C	514	-	57,73,73	1.99	13 (22%)	61,113,113	1.90	15 (24%)
25	BCR	C	515	-	41,41,41	0.82	0	56,56,56	1.52	8 (14%)
25	BCR	C	516	-	41,41,41	0.99	0	56,56,56	1.38	7 (12%)
36	DGD	C	517	-	63,63,67	0.80	2 (3%)	77,77,81	1.24	9 (11%)
36	DGD	C	518	-	63,63,67	0.93	3 (4%)	77,77,81	1.11	5 (6%)
36	DGD	C	519	-	63,63,67	0.84	2 (3%)	77,77,81	1.13	6 (7%)
34	LMG	C	520	-	51,51,55	1.12	2 (3%)	59,59,63	1.36	9 (15%)
35	HTG	C	521	-	19,19,19	0.91	2 (10%)	22,24,24	2.26	1 (4%)
35	HTG	C	522	-	19,19,19	0.98	1 (5%)	22,24,24	2.31	3 (13%)
35	HTG	C	523	-	19,19,19	1.03	2 (10%)	22,24,24	2.33	1 (4%)
31	DMS	C	524	-	3,3,3	2.40	1 (33%)	3,3,3	0.88	0
31	DMS	C	525	-	3,3,3	2.63	1 (33%)	3,3,3	0.84	0
31	DMS	C	526	-	3,3,3	2.74	1 (33%)	3,3,3	0.53	0
31	DMS	C	527	-	3,3,3	2.57	1 (33%)	3,3,3	0.58	0
31	DMS	C	528	-	3,3,3	2.65	1 (33%)	3,3,3	0.64	0
31	DMS	C	529	-	3,3,3	2.56	1 (33%)	3,3,3	0.42	0
25	BCR	C	530	-	41,41,41	0.82	0	56,56,56	1.57	9 (16%)
34	LMG	C	531	-	51,51,55	1.00	2 (3%)	59,59,63	1.09	5 (8%)
31	DMS	C	533	-	3,3,3	2.67	1 (33%)	3,3,3	0.47	0
23	CLA	D	401	40	57,73,73	1.86	12 (21%)	61,113,113	2.29	21 (34%)
24	PHO	D	402	-	67,69,69	1.91	14 (20%)	86,99,99	1.86	20 (23%)
23	CLA	D	403	-	57,73,73	1.64	11 (19%)	61,113,113	2.52	20 (32%)
23	CLA	D	404	-	57,73,73	1.75	12 (21%)	61,113,113	1.80	18 (29%)
25	BCR	D	405	-	41,41,41	1.09	3 (7%)	56,56,56	2.00	13 (23%)
27	PL9	D	406	-	54,55,55	0.96	3 (5%)	68,69,69	1.61	13 (19%)
36	DGD	D	407	-	50,50,67	1.25	3 (6%)	58,58,81	1.85	8 (13%)
26	SQD	D	408	-	44,45,54	1.55	4 (9%)	53,56,65	2.59	12 (22%)
28	LHG	D	409	-	48,48,48	0.84	1 (2%)	49,54,54	1.29	6 (12%)
28	LHG	D	410	-	48,48,48	0.81	2 (4%)	49,54,54	1.13	3 (6%)
28	LHG	D	411	-	45,45,48	0.96	2 (4%)	46,51,54	1.03	3 (6%)
34	LMG	D	412	-	51,51,55	1.07	2 (3%)	59,59,63	1.43	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	HTG	D	414	-	19,19,19	0.88	1 (5%)	22,24,24	1.72	1 (4%)
31	DMS	D	415	-	3,3,3	2.75	1 (33%)	3,3,3	0.64	0
31	DMS	D	416	-	3,3,3	2.50	1 (33%)	3,3,3	0.84	0
31	DMS	D	417	-	3,3,3	3.00	1 (33%)	3,3,3	0.69	0
28	LHG	E	101	-	48,48,48	1.04	2 (4%)	49,54,54	1.21	5 (10%)
37	HEM	E	105	5,6	24,50,50	2.11	10 (41%)	16,82,82	2.49	6 (37%)
30	LMT	F	101	-	36,36,36	0.69	1 (2%)	47,47,47	1.22	5 (10%)
31	DMS	F	102	-	3,3,3	2.62	1 (33%)	3,3,3	0.23	0
31	DMS	H	101	-	3,3,3	2.78	1 (33%)	3,3,3	0.53	0
38	RRX	H	102	-	42,42,42	0.87	1 (2%)	57,58,58	1.57	9 (15%)
36	DGD	H	103	-	63,63,67	1.03	3 (4%)	77,77,81	1.32	7 (9%)
31	DMS	H	105	-	3,3,3	2.75	1 (33%)	3,3,3	0.60	0
30	LMT	I	101	-	36,36,36	0.72	1 (2%)	47,47,47	1.46	5 (10%)
34	LMG	J	101	39	51,51,55	0.91	2 (3%)	59,59,63	0.98	5 (8%)
28	LHG	K	101	-	43,43,48	1.06	2 (4%)	46,48,54	1.14	4 (8%)
28	LHG	L	101	-	48,48,48	0.94	3 (6%)	49,54,54	1.14	3 (6%)
26	SQD	L	102	-	53,54,54	1.46	3 (5%)	62,65,65	2.04	12 (19%)
30	LMT	M	101	-	36,36,36	0.62	0	47,47,47	0.98	2 (4%)
35	HTG	O	302	-	19,19,19	1.37	3 (15%)	22,24,24	1.56	4 (18%)
31	DMS	O	303	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
31	DMS	O	304	-	3,3,3	2.80	1 (33%)	3,3,3	0.78	0
31	DMS	O	305	-	3,3,3	2.66	1 (33%)	3,3,3	0.80	0
31	DMS	O	306	-	3,3,3	2.71	1 (33%)	3,3,3	0.50	0
31	DMS	O	307	-	3,3,3	2.75	1 (33%)	3,3,3	0.67	0
31	DMS	O	308	-	3,3,3	2.73	1 (33%)	3,3,3	0.62	0
31	DMS	O	309	-	3,3,3	2.88	1 (33%)	3,3,3	0.85	0
31	DMS	O	310	-	3,3,3	2.62	1 (33%)	3,3,3	0.64	0
31	DMS	O	311	-	3,3,3	2.65	1 (33%)	3,3,3	0.80	0
25	BCR	T	101	-	41,41,41	0.88	0	56,56,56	1.81	17 (30%)
30	LMT	T	103	-	24,24,36	0.49	0	29,29,47	1.35	4 (13%)
31	DMS	U	202	-	3,3,3	2.69	1 (33%)	3,3,3	1.47	1 (33%)
31	DMS	U	203	-	3,3,3	2.71	1 (33%)	3,3,3	0.45	0
31	DMS	U	204	-	3,3,3	2.89	1 (33%)	3,3,3	0.75	0
31	DMS	V	201	-	3,3,3	2.58	1 (33%)	3,3,3	0.68	0
31	DMS	V	202	-	3,3,3	2.66	1 (33%)	3,3,3	0.73	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	HEM	V	203	16	24,50,50	2.15	7 (29%)	16,82,82	1.98	4 (25%)
35	HTG	V	204	-	14,14,19	0.63	0	17,19,24	2.51	5 (29%)
31	DMS	V	205	-	3,3,3	2.64	1 (33%)	3,3,3	0.86	0
31	DMS	V	206	-	3,3,3	2.66	1 (33%)	3,3,3	0.69	0
31	DMS	V	207	-	3,3,3	2.85	1 (33%)	3,3,3	1.14	0
31	DMS	V	208	-	3,3,3	2.60	1 (33%)	3,3,3	0.37	0
31	DMS	V	209	-	3,3,3	2.53	1 (33%)	3,3,3	0.75	0
31	DMS	V	210	-	3,3,3	2.71	1 (33%)	3,3,3	0.47	0
31	DMS	V	211	-	3,3,3	2.98	1 (33%)	3,3,3	0.96	0
25	BCR	Y	101	-	41,41,41	0.83	0	56,56,56	1.69	14 (25%)
30	LMT	Z	101	-	36,36,36	0.67	1 (2%)	47,47,47	0.91	2 (4%)
31	DMS	a	401	-	3,3,3	2.71	1 (33%)	3,3,3	0.63	0
20	OEX	a	402	1,3,40	0,15,15	0.00	-	0,32,32	0.00	-
23	CLA	a	406	-	57,73,73	1.74	12 (21%)	61,113,113	2.32	22 (36%)
23	CLA	a	407	40	57,73,73	1.67	13 (22%)	61,113,113	2.39	16 (26%)
24	PHO	a	408	-	67,69,69	1.76	14 (20%)	86,99,99	1.76	20 (23%)
24	PHO	a	409	-	67,69,69	1.88	15 (22%)	86,99,99	1.98	23 (26%)
23	CLA	a	410	-	57,73,73	1.80	10 (17%)	61,113,113	2.28	22 (36%)
25	BCR	a	411	-	41,41,41	1.17	2 (4%)	56,56,56	1.35	5 (8%)
26	SQD	a	412	-	53,54,54	1.43	3 (5%)	62,65,65	2.64	12 (19%)
34	LMG	a	413	-	51,51,55	0.97	2 (3%)	59,59,63	1.14	4 (6%)
27	PL9	a	414	-	54,55,55	0.78	2 (3%)	68,69,69	1.73	18 (26%)
28	LHG	a	415	-	48,48,48	0.99	2 (4%)	49,54,54	1.09	3 (6%)
26	SQD	a	417	-	53,54,54	1.60	4 (7%)	62,65,65	1.45	7 (11%)
30	LMT	a	418	-	36,36,36	0.69	1 (2%)	47,47,47	1.30	5 (10%)
31	DMS	a	420	-	3,3,3	2.66	1 (33%)	3,3,3	0.32	0
31	DMS	a	421	-	3,3,3	2.68	1 (33%)	3,3,3	0.57	0
30	LMT	a	422	-	36,36,36	0.63	1 (2%)	47,47,47	1.02	3 (6%)
31	DMS	a	423	-	3,3,3	2.81	1 (33%)	3,3,3	0.74	0
32	BCT	a	424	21	0,3,3	0.00	-	0,3,3	0.00	-
23	CLA	b	602	40	57,73,73	1.94	13 (22%)	61,113,113	2.21	21 (34%)
23	CLA	b	603	-	57,73,73	1.72	13 (22%)	61,113,113	2.37	21 (34%)
23	CLA	b	604	-	57,73,73	1.65	11 (19%)	61,113,113	2.36	19 (31%)
23	CLA	b	605	-	57,73,73	1.68	11 (19%)	61,113,113	2.16	21 (34%)
23	CLA	b	606	-	57,73,73	1.52	11 (19%)	61,113,113	2.23	17 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	b	607	-	57,73,73	1.82	12 (21%)	61,113,113	1.91	13 (21%)
23	CLA	b	608	40	57,73,73	1.72	11 (19%)	61,113,113	2.07	18 (29%)
23	CLA	b	609	-	57,73,73	1.73	10 (17%)	61,113,113	2.23	22 (36%)
23	CLA	b	610	-	57,73,73	1.86	13 (22%)	61,113,113	1.91	16 (26%)
23	CLA	b	611	40	57,73,73	1.81	13 (22%)	61,113,113	1.79	16 (26%)
23	CLA	b	612	-	57,73,73	1.68	7 (12%)	61,113,113	1.89	16 (26%)
23	CLA	b	613	-	57,73,73	1.63	11 (19%)	61,113,113	2.25	16 (26%)
23	CLA	b	614	-	57,73,73	1.82	11 (19%)	61,113,113	1.97	15 (24%)
23	CLA	b	615	-	57,73,73	1.75	15 (26%)	61,113,113	1.80	17 (27%)
23	CLA	b	616	-	57,73,73	1.94	12 (21%)	61,113,113	2.18	19 (31%)
23	CLA	b	617	-	57,73,73	1.84	12 (21%)	61,113,113	2.11	22 (36%)
25	BCR	b	618	-	41,41,41	0.93	0	56,56,56	1.74	14 (25%)
25	BCR	b	619	-	41,41,41	1.01	1 (2%)	56,56,56	1.33	7 (12%)
25	BCR	b	620	-	41,41,41	0.89	2 (4%)	56,56,56	1.23	4 (7%)
30	LMT	b	621	-	25,25,36	0.60	1 (4%)	30,30,47	1.32	4 (13%)
35	HTG	b	622	-	19,19,19	1.26	2 (10%)	22,24,24	1.48	5 (22%)
35	HTG	b	623	-	19,19,19	1.05	1 (5%)	22,24,24	2.32	4 (18%)
35	HTG	b	627	-	19,19,19	1.15	2 (10%)	22,24,24	1.65	1 (4%)
35	HTG	b	628	-	19,19,19	0.84	1 (5%)	22,24,24	2.00	1 (4%)
31	DMS	b	633	-	3,3,3	1.83	1 (33%)	3,3,3	0.55	0
31	DMS	b	634	-	3,3,3	2.46	1 (33%)	3,3,3	0.88	0
31	DMS	b	635	-	3,3,3	2.72	1 (33%)	3,3,3	0.54	0
31	DMS	b	636	-	3,3,3	2.75	1 (33%)	3,3,3	0.48	0
31	DMS	b	637	-	3,3,3	2.68	1 (33%)	3,3,3	0.94	0
31	DMS	b	638	-	3,3,3	2.93	1 (33%)	3,3,3	0.98	0
31	DMS	b	639	-	3,3,3	2.77	1 (33%)	3,3,3	1.29	1 (33%)
31	DMS	b	640	-	3,3,3	2.70	1 (33%)	3,3,3	0.79	0
31	DMS	b	641	-	3,3,3	2.65	1 (33%)	3,3,3	0.70	0
31	DMS	b	642	-	3,3,3	2.71	1 (33%)	3,3,3	0.52	0
31	DMS	b	643	-	3,3,3	2.68	1 (33%)	3,3,3	0.55	0
31	DMS	b	644	-	3,3,3	2.79	1 (33%)	3,3,3	0.90	0
31	DMS	b	645	-	3,3,3	2.70	1 (33%)	3,3,3	0.44	0
31	DMS	b	646	-	3,3,3	2.75	1 (33%)	3,3,3	0.63	0
31	DMS	b	647	-	3,3,3	2.75	1 (33%)	3,3,3	0.64	0
23	CLA	c	902	-	57,73,73	1.72	12 (21%)	61,113,113	2.15	15 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	CLA	c	903	-	57,73,73	1.70	11 (19%)	61,113,113	2.14	22 (36%)
23	CLA	c	904	-	57,73,73	1.87	12 (21%)	61,113,113	1.91	17 (27%)
23	CLA	c	905	40	57,73,73	1.83	12 (21%)	61,113,113	1.91	16 (26%)
23	CLA	c	906	-	57,73,73	1.71	12 (21%)	61,113,113	2.00	17 (27%)
23	CLA	c	907	-	57,73,73	1.77	12 (21%)	61,113,113	1.94	16 (26%)
23	CLA	c	908	40	57,73,73	1.71	12 (21%)	61,113,113	1.98	15 (24%)
23	CLA	c	909	-	57,73,73	1.88	14 (24%)	61,113,113	1.63	11 (18%)
23	CLA	c	910	-	57,73,73	1.96	14 (24%)	61,113,113	2.14	18 (29%)
23	CLA	c	911	-	57,73,73	1.79	10 (17%)	61,113,113	2.03	15 (24%)
23	CLA	c	912	3	57,73,73	1.97	13 (22%)	61,113,113	1.89	14 (22%)
23	CLA	c	913	-	57,73,73	1.95	12 (21%)	61,113,113	2.05	15 (24%)
23	CLA	c	914	-	57,73,73	1.94	12 (21%)	61,113,113	2.01	17 (27%)
25	BCR	c	915	-	41,41,41	0.77	0	56,56,56	1.30	6 (10%)
25	BCR	c	916	-	41,41,41	0.81	0	56,56,56	1.57	11 (19%)
36	DGD	c	917	-	63,63,67	0.82	3 (4%)	77,77,81	1.26	8 (10%)
36	DGD	c	918	-	63,63,67	0.88	2 (3%)	77,77,81	1.18	9 (11%)
36	DGD	c	919	-	63,63,67	0.91	3 (4%)	77,77,81	1.25	10 (12%)
34	LMG	c	920	-	51,51,55	0.93	2 (3%)	59,59,63	1.32	7 (11%)
35	HTG	c	921	-	19,19,19	0.90	2 (10%)	22,24,24	1.72	2 (9%)
35	HTG	c	922	-	19,19,19	0.96	2 (10%)	22,24,24	2.16	3 (13%)
35	HTG	c	923	-	11,12,19	0.54	0	10,11,24	1.17	1 (10%)
31	DMS	c	924	-	3,3,3	2.37	1 (33%)	3,3,3	0.40	0
31	DMS	c	925	-	3,3,3	2.82	1 (33%)	3,3,3	0.77	0
31	DMS	c	926	-	3,3,3	2.62	1 (33%)	3,3,3	0.26	0
31	DMS	c	927	-	3,3,3	2.71	1 (33%)	3,3,3	1.16	0
31	DMS	c	928	-	3,3,3	2.65	1 (33%)	3,3,3	0.45	0
31	DMS	c	929	-	3,3,3	2.84	1 (33%)	3,3,3	0.63	0
34	LMG	c	930	-	51,51,55	1.05	3 (5%)	59,59,63	1.34	4 (6%)
31	DMS	c	932	-	3,3,3	2.65	1 (33%)	3,3,3	0.69	0
31	DMS	c	933	-	3,3,3	2.68	1 (33%)	3,3,3	0.85	0
31	DMS	c	934	-	3,3,3	2.70	1 (33%)	3,3,3	0.67	0
31	DMS	c	935	-	3,3,3	2.68	1 (33%)	3,3,3	0.69	0
31	DMS	c	936	-	3,3,3	2.74	1 (33%)	3,3,3	0.76	0
31	DMS	c	937	-	3,3,3	2.66	1 (33%)	3,3,3	0.56	0
23	CLA	d	401	40	57,73,73	1.59	10 (17%)	61,113,113	2.07	18 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
28	LHG	d	402	-	43,43,48	1.04	2 (4%)	44,49,54	1.00	4 (9%)
23	CLA	d	403	-	57,73,73	1.69	10 (17%)	61,113,113	2.18	19 (31%)
23	CLA	d	404	-	57,73,73	1.71	13 (22%)	61,113,113	2.20	18 (29%)
25	BCR	d	405	-	41,41,41	0.97	1 (2%)	56,56,56	1.93	19 (33%)
27	PL9	d	406	-	54,55,55	0.96	2 (3%)	68,69,69	1.65	12 (17%)
36	DGD	d	407	-	50,50,67	1.09	2 (4%)	58,58,81	1.26	6 (10%)
28	LHG	d	408	-	48,48,48	0.89	2 (4%)	49,54,54	1.29	3 (6%)
28	LHG	d	409	-	48,48,48	0.78	2 (4%)	49,54,54	1.27	9 (18%)
28	LHG	d	410	-	45,45,48	0.99	2 (4%)	46,51,54	1.02	3 (6%)
34	LMG	d	411	-	51,51,55	1.10	3 (5%)	59,59,63	1.34	8 (13%)
35	HTG	d	413	-	19,19,19	1.10	1 (5%)	22,24,24	2.60	3 (13%)
31	DMS	d	414	-	3,3,3	2.70	1 (33%)	3,3,3	0.70	0
31	DMS	d	415	-	3,3,3	2.66	1 (33%)	3,3,3	0.80	0
31	DMS	d	416	-	3,3,3	2.69	1 (33%)	3,3,3	0.52	0
31	DMS	d	418	-	3,3,3	2.75	1 (33%)	3,3,3	0.55	0
31	DMS	d	419	-	3,3,3	2.69	1 (33%)	3,3,3	0.65	0
28	LHG	e	101	-	39,39,48	1.13	2 (5%)	40,45,54	1.06	2 (5%)
30	LMT	e	103	-	25,25,36	0.68	1 (4%)	30,30,47	1.07	3 (10%)
31	DMS	e	104	-	3,3,3	2.68	1 (33%)	3,3,3	0.52	0
37	HEM	e	105	5,6	24,50,50	2.37	11 (45%)	16,82,82	2.49	9 (56%)
31	DMS	h	101	-	3,3,3	2.69	1 (33%)	3,3,3	1.24	0
36	DGD	h	102	-	63,63,67	0.90	3 (4%)	77,77,81	1.28	10 (12%)
31	DMS	h	103	-	3,3,3	2.65	1 (33%)	3,3,3	0.54	0
31	DMS	h	104	-	3,3,3	2.70	1 (33%)	3,3,3	0.52	0
31	DMS	h	105	-	3,3,3	2.75	1 (33%)	3,3,3	0.61	0
31	DMS	i	105	-	3,3,3	2.70	1 (33%)	3,3,3	0.83	0
31	DMS	i	106	-	3,3,3	2.74	1 (33%)	3,3,3	0.60	0
34	LMG	j	101	39	51,51,55	0.96	3 (5%)	59,59,63	1.17	7 (11%)
25	BCR	j	104	-	41,41,41	0.80	0	56,56,56	1.47	11 (19%)
25	BCR	k	102	-	41,41,41	1.00	1 (2%)	56,56,56	1.21	8 (14%)
31	DMS	k	103	-	3,3,3	2.66	1 (33%)	3,3,3	0.74	0
28	LHG	l	101	-	48,48,48	0.81	2 (4%)	49,54,54	1.04	2 (4%)
31	DMS	l	102	-	3,3,3	2.64	1 (33%)	3,3,3	0.43	0
34	LMG	m	102	-	51,51,55	0.93	2 (3%)	59,59,63	1.34	7 (11%)
30	LMT	m	103	-	36,36,36	0.60	1 (2%)	47,47,47	1.04	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	LMT	m	104	-	36,36,36	0.54	0	47,47,47	1.28	3 (6%)
31	DMS	o	301	-	3,3,3	2.14	1 (33%)	3,3,3	0.37	0
31	DMS	o	303	-	3,3,3	2.69	1 (33%)	3,3,3	0.94	0
31	DMS	o	304	-	3,3,3	2.76	1 (33%)	3,3,3	0.74	0
25	BCR	t	101	-	41,41,41	1.03	0	56,56,56	1.52	14 (25%)
31	DMS	u	203	-	3,3,3	2.58	1 (33%)	3,3,3	0.85	0
31	DMS	u	204	-	3,3,3	2.77	1 (33%)	3,3,3	0.78	0
31	DMS	u	205	-	3,3,3	2.63	1 (33%)	3,3,3	0.96	0
31	DMS	u	206	-	3,3,3	2.79	1 (33%)	3,3,3	0.57	0
31	DMS	v	201	-	3,3,3	2.43	1 (33%)	3,3,3	0.42	0
31	DMS	v	202	-	3,3,3	2.61	1 (33%)	3,3,3	0.29	0
37	HEM	v	203	16	24,50,50	2.40	7 (29%)	16,82,82	2.20	4 (25%)
35	HTG	v	204	-	19,19,19	0.85	1 (5%)	22,24,24	3.38	7 (31%)
31	DMS	v	205	-	3,3,3	2.65	1 (33%)	3,3,3	0.51	0
31	DMS	v	206	-	3,3,3	2.61	1 (33%)	3,3,3	0.73	0
31	DMS	v	207	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
31	DMS	v	208	-	3,3,3	2.73	1 (33%)	3,3,3	0.67	0
31	DMS	v	209	-	3,3,3	2.72	1 (33%)	3,3,3	0.64	0
31	DMS	v	210	-	3,3,3	2.68	1 (33%)	3,3,3	0.51	0
26	SQD	x	101	-	40,41,54	1.69	3 (7%)	49,52,65	1.56	9 (18%)
38	RRX	x	102	-	42,42,42	0.89	0	57,58,58	1.37	7 (12%)
30	LMT	z	101	-	32,32,36	0.62	1 (3%)	42,42,47	1.19	5 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	OEX	A	401	1,3,40	-	0/0/68/68	0/0/6/6
23	CLA	A	405	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	A	406	40	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	A	407	-	-	0/53/103/103	0/1/6/6
23	CLA	A	408	-	2/2/20/25	0/37/135/135	0/0/9/9
25	BCR	A	409	-	-	0/29/63/63	0/2/2/2
26	SQD	A	410	-	-	0/49/69/69	0/1/1/1
27	PL9	A	411	-	-	0/53/73/73	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	A	412	-	-	0/53/53/53	0/0/0/0
26	SQD	A	415	-	-	0/49/69/69	0/1/1/1
30	LMT	A	416	-	-	0/21/61/61	0/2/2/2
31	DMS	A	418	-	-	0/0/0/0	0/0/0/0
31	DMS	A	419	-	-	0/0/0/0	0/0/0/0
32	BCT	A	420	21	-	0/0/0/0	0/0/0/0
31	DMS	A	421	-	-	0/0/0/0	0/0/0/0
31	DMS	A	422	-	-	0/0/0/0	0/0/0/0
31	DMS	A	423	-	-	0/0/0/0	0/0/0/0
31	DMS	A	424	-	-	0/0/0/0	0/0/0/0
23	CLA	B	602	40	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	603	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	608	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	609	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	B	610	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	B	611	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	612	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	B	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	B	618	-	-	0/29/63/63	0/2/2/2
25	BCR	B	619	-	-	0/29/63/63	0/2/2/2
25	BCR	B	620	-	-	0/29/63/63	0/2/2/2
26	SQD	B	621	-	-	0/49/69/69	0/1/1/1
34	LMG	B	622	-	-	0/46/66/70	0/1/1/1
30	LMT	B	623	-	-	0/21/61/61	0/2/2/2
35	HTG	B	624	-	-	0/10/30/30	0/1/1/1
35	HTG	B	625	-	-	0/10/30/30	0/1/1/1
35	HTG	B	626	-	-	0/10/30/30	0/1/1/1
35	HTG	B	630	-	-	0/10/30/30	0/1/1/1
35	HTG	B	631	-	-	0/10/30/30	0/1/1/1
31	DMS	B	636	-	-	0/0/0/0	0/0/0/0
31	DMS	B	637	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	B	638	-	-	0/0/0/0	0/0/0/0
31	DMS	B	639	-	-	0/0/0/0	0/0/0/0
31	DMS	B	640	-	-	0/0/0/0	0/0/0/0
31	DMS	B	641	-	-	0/0/0/0	0/0/0/0
31	DMS	B	642	-	-	0/0/0/0	0/0/0/0
30	LMT	B	643	-	-	0/15/35/61	0/1/1/2
30	LMT	B	644	-	-	0/15/35/61	0/1/1/2
31	DMS	B	645	-	-	0/0/0/0	0/0/0/0
31	DMS	B	646	-	-	0/0/0/0	0/0/0/0
31	DMS	B	647	-	-	0/0/0/0	0/0/0/0
31	DMS	B	648	-	-	0/0/0/0	0/0/0/0
31	DMS	B	649	-	-	0/0/0/0	0/0/0/0
34	LMG	C	501	-	-	0/46/66/70	0/1/1/1
23	CLA	C	502	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	503	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	C	504	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	505	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	506	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	507	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	508	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	509	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	510	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	511	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	512	3	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	C	513	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	C	514	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	C	515	-	-	0/29/63/63	0/2/2/2
25	BCR	C	516	-	-	0/29/63/63	0/2/2/2
36	DGD	C	517	-	-	0/51/91/95	0/2/2/2
36	DGD	C	518	-	-	0/51/91/95	0/2/2/2
36	DGD	C	519	-	-	0/51/91/95	0/2/2/2
34	LMG	C	520	-	-	0/46/66/70	0/1/1/1
35	HTG	C	521	-	-	0/10/30/30	0/1/1/1
35	HTG	C	522	-	-	0/10/30/30	0/1/1/1
35	HTG	C	523	-	-	0/10/30/30	0/1/1/1
31	DMS	C	524	-	-	0/0/0/0	0/0/0/0
31	DMS	C	525	-	-	0/0/0/0	0/0/0/0
31	DMS	C	526	-	-	0/0/0/0	0/0/0/0
31	DMS	C	527	-	-	0/0/0/0	0/0/0/0
31	DMS	C	528	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	C	529	-	-	0/0/0/0	0/0/0/0
25	BCR	C	530	-	-	0/29/63/63	0/2/2/2
34	LMG	C	531	-	-	0/46/66/70	0/1/1/1
31	DMS	C	533	-	-	0/0/0/0	0/0/0/0
23	CLA	D	401	40	1/1/20/25	0/37/135/135	0/0/9/9
24	PHO	D	402	-	-	0/53/103/103	0/1/6/6
23	CLA	D	403	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	D	404	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	D	405	-	-	0/29/63/63	0/2/2/2
27	PL9	D	406	-	-	0/53/73/73	0/1/1/1
36	DGD	D	407	-	-	0/44/64/95	0/1/1/2
26	SQD	D	408	-	-	0/40/60/69	0/1/1/1
28	LHG	D	409	-	-	0/53/53/53	0/0/0/0
28	LHG	D	410	-	-	0/53/53/53	0/0/0/0
28	LHG	D	411	-	-	0/50/50/53	0/0/0/0
34	LMG	D	412	-	-	0/46/66/70	0/1/1/1
35	HTG	D	414	-	-	0/10/30/30	0/1/1/1
31	DMS	D	415	-	-	0/0/0/0	0/0/0/0
31	DMS	D	416	-	-	0/0/0/0	0/0/0/0
31	DMS	D	417	-	-	0/0/0/0	0/0/0/0
28	LHG	E	101	-	-	0/53/53/53	0/0/0/0
37	HEM	E	105	5,6	-	0/6/54/54	0/0/8/8
30	LMT	F	101	-	-	0/21/61/61	0/2/2/2
31	DMS	F	102	-	-	0/0/0/0	0/0/0/0
31	DMS	H	101	-	-	0/0/0/0	0/0/0/0
38	RRX	H	102	-	-	0/29/65/65	0/2/2/2
36	DGD	H	103	-	-	0/51/91/95	0/2/2/2
31	DMS	H	105	-	-	0/0/0/0	0/0/0/0
30	LMT	I	101	-	-	0/21/61/61	0/2/2/2
34	LMG	J	101	39	-	0/46/66/70	0/1/1/1
28	LHG	K	101	-	-	0/45/45/53	0/0/0/0
28	LHG	L	101	-	-	0/53/53/53	0/0/0/0
26	SQD	L	102	-	-	1/49/69/69	0/1/1/1
30	LMT	M	101	-	-	0/21/61/61	0/2/2/2
35	HTG	O	302	-	-	0/10/30/30	0/1/1/1
31	DMS	O	303	-	-	0/0/0/0	0/0/0/0
31	DMS	O	304	-	-	0/0/0/0	0/0/0/0
31	DMS	O	305	-	-	0/0/0/0	0/0/0/0
31	DMS	O	306	-	-	0/0/0/0	0/0/0/0
31	DMS	O	307	-	-	0/0/0/0	0/0/0/0
31	DMS	O	308	-	-	0/0/0/0	0/0/0/0
31	DMS	O	309	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	O	310	-	-	0/0/0/0	0/0/0/0
31	DMS	O	311	-	-	0/0/0/0	0/0/0/0
25	BCR	T	101	-	-	0/29/63/63	0/2/2/2
30	LMT	T	103	-	-	0/15/35/61	0/1/1/2
31	DMS	U	202	-	-	0/0/0/0	0/0/0/0
31	DMS	U	203	-	-	0/0/0/0	0/0/0/0
31	DMS	U	204	-	-	0/0/0/0	0/0/0/0
31	DMS	V	201	-	-	0/0/0/0	0/0/0/0
31	DMS	V	202	-	-	0/0/0/0	0/0/0/0
37	HEM	V	203	16	-	0/6/54/54	0/0/8/8
35	HTG	V	204	-	-	0/5/25/30	0/1/1/1
31	DMS	V	205	-	-	0/0/0/0	0/0/0/0
31	DMS	V	206	-	-	0/0/0/0	0/0/0/0
31	DMS	V	207	-	-	0/0/0/0	0/0/0/0
31	DMS	V	208	-	-	0/0/0/0	0/0/0/0
31	DMS	V	209	-	-	0/0/0/0	0/0/0/0
31	DMS	V	210	-	-	0/0/0/0	0/0/0/0
31	DMS	V	211	-	-	0/0/0/0	0/0/0/0
25	BCR	Y	101	-	-	0/29/63/63	0/2/2/2
30	LMT	Z	101	-	-	0/21/61/61	0/2/2/2
31	DMS	a	401	-	-	0/0/0/0	0/0/0/0
20	OEX	a	402	1,3,40	-	0/0/68/68	0/0/6/6
23	CLA	a	406	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	a	407	40	2/2/20/25	0/37/135/135	0/0/9/9
24	PHO	a	408	-	-	0/53/103/103	0/1/6/6
24	PHO	a	409	-	-	0/53/103/103	0/1/6/6
23	CLA	a	410	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	a	411	-	-	0/29/63/63	0/2/2/2
26	SQD	a	412	-	-	0/49/69/69	0/1/1/1
34	LMG	a	413	-	-	0/46/66/70	0/1/1/1
27	PL9	a	414	-	-	0/53/73/73	0/1/1/1
28	LHG	a	415	-	-	0/53/53/53	0/0/0/0
26	SQD	a	417	-	-	0/49/69/69	0/1/1/1
30	LMT	a	418	-	-	0/21/61/61	0/2/2/2
31	DMS	a	420	-	-	0/0/0/0	0/0/0/0
31	DMS	a	421	-	-	0/0/0/0	0/0/0/0
30	LMT	a	422	-	-	0/21/61/61	0/2/2/2
31	DMS	a	423	-	-	0/0/0/0	0/0/0/0
32	BCT	a	424	21	-	0/0/0/0	0/0/0/0
23	CLA	b	602	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	603	-	3/3/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	b	604	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	605	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	606	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	607	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	608	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	609	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	610	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	b	611	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	612	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	b	613	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	614	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	615	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	616	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	b	617	-	3/3/20/25	0/37/135/135	0/0/9/9
25	BCR	b	618	-	-	0/29/63/63	0/2/2/2
25	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	BCR	b	620	-	-	0/29/63/63	0/2/2/2
30	LMT	b	621	-	-	0/17/37/61	0/1/1/2
35	HTG	b	622	-	-	0/10/30/30	0/1/1/1
35	HTG	b	623	-	-	0/10/30/30	0/1/1/1
35	HTG	b	627	-	-	0/10/30/30	0/1/1/1
35	HTG	b	628	-	-	0/10/30/30	0/1/1/1
31	DMS	b	633	-	-	0/0/0/0	0/0/0/0
31	DMS	b	634	-	-	0/0/0/0	0/0/0/0
31	DMS	b	635	-	-	0/0/0/0	0/0/0/0
31	DMS	b	636	-	-	0/0/0/0	0/0/0/0
31	DMS	b	637	-	-	0/0/0/0	0/0/0/0
31	DMS	b	638	-	-	0/0/0/0	0/0/0/0
31	DMS	b	639	-	-	0/0/0/0	0/0/0/0
31	DMS	b	640	-	-	0/0/0/0	0/0/0/0
31	DMS	b	641	-	-	0/0/0/0	0/0/0/0
31	DMS	b	642	-	-	0/0/0/0	0/0/0/0
31	DMS	b	643	-	-	0/0/0/0	0/0/0/0
31	DMS	b	644	-	-	0/0/0/0	0/0/0/0
31	DMS	b	645	-	-	0/0/0/0	0/0/0/0
31	DMS	b	646	-	-	0/0/0/0	0/0/0/0
31	DMS	b	647	-	-	0/0/0/0	0/0/0/0
23	CLA	c	902	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	903	-	2/2/20/25	0/37/135/135	0/0/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	c	904	-	1/1/20/25	0/37/135/135	0/0/9/9
23	CLA	c	905	40	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	906	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	907	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	908	40	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	909	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	910	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	911	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	912	3	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	c	913	-	3/3/20/25	0/37/135/135	0/0/9/9
23	CLA	c	914	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	c	915	-	-	0/29/63/63	0/2/2/2
25	BCR	c	916	-	-	0/29/63/63	0/2/2/2
36	DGD	c	917	-	-	0/51/91/95	0/2/2/2
36	DGD	c	918	-	-	0/51/91/95	0/2/2/2
36	DGD	c	919	-	-	0/51/91/95	0/2/2/2
34	LMG	c	920	-	-	0/46/66/70	0/1/1/1
35	HTG	c	921	-	-	0/10/30/30	0/1/1/1
35	HTG	c	922	-	-	0/10/30/30	0/1/1/1
35	HTG	c	923	-	-	0/8/10/30	0/0/0/1
31	DMS	c	924	-	-	0/0/0/0	0/0/0/0
31	DMS	c	925	-	-	0/0/0/0	0/0/0/0
31	DMS	c	926	-	-	0/0/0/0	0/0/0/0
31	DMS	c	927	-	-	0/0/0/0	0/0/0/0
31	DMS	c	928	-	-	0/0/0/0	0/0/0/0
31	DMS	c	929	-	-	0/0/0/0	0/0/0/0
34	LMG	c	930	-	-	0/46/66/70	0/1/1/1
31	DMS	c	932	-	-	0/0/0/0	0/0/0/0
31	DMS	c	933	-	-	0/0/0/0	0/0/0/0
31	DMS	c	934	-	-	0/0/0/0	0/0/0/0
31	DMS	c	935	-	-	0/0/0/0	0/0/0/0
31	DMS	c	936	-	-	0/0/0/0	0/0/0/0
31	DMS	c	937	-	-	0/0/0/0	0/0/0/0
23	CLA	d	401	40	1/1/20/25	0/37/135/135	0/0/9/9
28	LHG	d	402	-	-	0/48/48/53	0/0/0/0
23	CLA	d	403	-	2/2/20/25	0/37/135/135	0/0/9/9
23	CLA	d	404	-	1/1/20/25	0/37/135/135	0/0/9/9
25	BCR	d	405	-	-	0/29/63/63	0/2/2/2
27	PL9	d	406	-	-	0/53/73/73	0/1/1/1
36	DGD	d	407	-	-	0/44/64/95	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LHG	d	408	-	-	0/53/53/53	0/0/0/0
28	LHG	d	409	-	-	0/53/53/53	0/0/0/0
28	LHG	d	410	-	-	0/50/50/53	0/0/0/0
34	LMG	d	411	-	-	0/46/66/70	0/1/1/1
35	HTG	d	413	-	-	1/10/30/30	0/1/1/1
31	DMS	d	414	-	-	0/0/0/0	0/0/0/0
31	DMS	d	415	-	-	0/0/0/0	0/0/0/0
31	DMS	d	416	-	-	0/0/0/0	0/0/0/0
31	DMS	d	418	-	-	0/0/0/0	0/0/0/0
31	DMS	d	419	-	-	0/0/0/0	0/0/0/0
28	LHG	e	101	-	-	0/44/44/53	0/0/0/0
30	LMT	e	103	-	-	0/17/37/61	0/1/1/2
31	DMS	e	104	-	-	0/0/0/0	0/0/0/0
37	HEM	e	105	5,6	-	0/6/54/54	0/0/8/8
31	DMS	h	101	-	-	0/0/0/0	0/0/0/0
36	DGD	h	102	-	-	0/51/91/95	0/2/2/2
31	DMS	h	103	-	-	0/0/0/0	0/0/0/0
31	DMS	h	104	-	-	0/0/0/0	0/0/0/0
31	DMS	h	105	-	-	0/0/0/0	0/0/0/0
31	DMS	i	105	-	-	0/0/0/0	0/0/0/0
31	DMS	i	106	-	-	0/0/0/0	0/0/0/0
34	LMG	j	101	39	-	0/46/66/70	0/1/1/1
25	BCR	j	104	-	-	0/29/63/63	0/2/2/2
25	BCR	k	102	-	-	0/29/63/63	0/2/2/2
31	DMS	k	103	-	-	0/0/0/0	0/0/0/0
28	LHG	l	101	-	-	0/53/53/53	0/0/0/0
31	DMS	l	102	-	-	0/0/0/0	0/0/0/0
34	LMG	m	102	-	-	0/46/66/70	0/1/1/1
30	LMT	m	103	-	-	0/21/61/61	0/2/2/2
30	LMT	m	104	-	-	0/21/61/61	0/2/2/2
31	DMS	o	301	-	-	0/0/0/0	0/0/0/0
31	DMS	o	303	-	-	0/0/0/0	0/0/0/0
31	DMS	o	304	-	-	0/0/0/0	0/0/0/0
25	BCR	t	101	-	-	0/29/63/63	0/2/2/2
31	DMS	u	203	-	-	0/0/0/0	0/0/0/0
31	DMS	u	204	-	-	0/0/0/0	0/0/0/0
31	DMS	u	205	-	-	0/0/0/0	0/0/0/0
31	DMS	u	206	-	-	0/0/0/0	0/0/0/0
31	DMS	v	201	-	-	0/0/0/0	0/0/0/0
31	DMS	v	202	-	-	0/0/0/0	0/0/0/0
37	HEM	v	203	16	-	0/6/54/54	0/0/8/8
35	HTG	v	204	-	-	0/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	DMS	v	205	-	-	0/0/0/0	0/0/0/0
31	DMS	v	206	-	-	0/0/0/0	0/0/0/0
31	DMS	v	207	-	-	0/0/0/0	0/0/0/0
31	DMS	v	208	-	-	0/0/0/0	0/0/0/0
31	DMS	v	209	-	-	0/0/0/0	0/0/0/0
31	DMS	v	210	-	-	0/0/0/0	0/0/0/0
26	SQD	x	101	-	-	0/36/56/69	0/1/1/1
38	RRX	x	102	-	-	0/29/65/65	0/2/2/2
30	LMT	z	101	-	-	0/15/55/61	0/2/2/2

All (1197) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	415	SQD	C6-S	-9.11	1.66	1.77
26	a	417	SQD	C6-S	-9.06	1.66	1.77
26	a	412	SQD	C6-S	-8.43	1.67	1.77
26	x	101	SQD	C6-S	-7.70	1.68	1.77
26	L	102	SQD	C6-S	-7.66	1.68	1.77
26	A	410	SQD	C6-S	-7.41	1.68	1.77
26	D	408	SQD	C6-S	-6.92	1.69	1.77
26	B	621	SQD	C6-S	-6.25	1.70	1.77
35	B	624	HTG	C1'-S1	-4.79	1.74	1.81
23	c	911	CLA	C4C-NC	-4.44	1.31	1.37
24	a	409	PHO	C1A-NA	-4.42	1.28	1.37
37	e	105	HEM	C3B-C2B	-4.17	1.35	1.40
37	V	203	HEM	C3C-C2C	-4.11	1.35	1.40
23	B	615	CLA	C1C-NC	-4.08	1.31	1.37
37	e	105	HEM	C3C-C2C	-4.07	1.35	1.40
37	v	203	HEM	C3B-C2B	-3.90	1.35	1.40
35	O	302	HTG	C1'-S1	-3.86	1.76	1.81
24	D	402	PHO	C1A-NA	-3.82	1.29	1.37
35	b	627	HTG	C1'-S1	-3.82	1.76	1.81
37	E	105	HEM	C3B-C2B	-3.79	1.35	1.40
35	C	523	HTG	C1'-S1	-3.56	1.76	1.81
35	B	631	HTG	C1'-S1	-3.51	1.76	1.81
35	b	623	HTG	C1'-S1	-3.49	1.76	1.81
37	v	203	HEM	C3C-C2C	-3.49	1.35	1.40
35	d	413	HTG	C1'-S1	-3.37	1.76	1.81
24	A	407	PHO	C1A-NA	-3.18	1.30	1.37
35	B	630	HTG	C1'-S1	-3.16	1.77	1.81
24	D	402	PHO	C3D-C4D	-3.13	1.33	1.43
23	c	909	CLA	C1C-NC	-3.09	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	922	HTG	C1'-S1	-3.06	1.77	1.81
23	a	407	CLA	C4C-NC	-3.06	1.33	1.37
23	c	910	CLA	C1C-NC	-3.03	1.33	1.37
37	E	105	HEM	C3C-C2C	-2.95	1.36	1.40
35	b	627	HTG	C1-S1	-2.94	1.76	1.80
35	C	522	HTG	C1'-S1	-2.92	1.77	1.81
37	V	203	HEM	C3B-C2B	-2.87	1.36	1.40
35	v	204	HTG	C1'-S1	-2.86	1.77	1.81
23	B	611	CLA	C1C-NC	-2.81	1.33	1.37
36	c	919	DGD	O2G-C2G	-2.81	1.39	1.46
23	C	511	CLA	C1C-NC	-2.79	1.33	1.37
23	b	614	CLA	C1C-NC	-2.78	1.33	1.37
35	c	921	HTG	C1'-S1	-2.78	1.77	1.81
35	C	521	HTG	C1'-S1	-2.71	1.77	1.81
23	a	406	CLA	CMD-C2D	-2.70	1.45	1.51
35	B	626	HTG	C1'-S1	-2.69	1.77	1.81
23	c	905	CLA	C1C-NC	-2.67	1.33	1.37
23	A	408	CLA	C1C-NC	-2.67	1.33	1.37
35	D	414	HTG	C1'-S1	-2.66	1.77	1.81
23	B	613	CLA	C1D-ND	-2.65	1.31	1.37
23	C	502	CLA	C1C-NC	-2.65	1.33	1.37
23	b	609	CLA	C1D-ND	-2.63	1.31	1.37
24	a	408	PHO	C1A-NA	-2.63	1.31	1.37
23	C	509	CLA	C4C-NC	-2.61	1.33	1.37
23	c	907	CLA	C1C-NC	-2.61	1.33	1.37
23	b	615	CLA	C4C-NC	-2.56	1.33	1.37
23	b	616	CLA	C4C-NC	-2.56	1.33	1.37
35	C	521	HTG	C1-S1	-2.53	1.76	1.80
23	B	617	CLA	C1C-NC	-2.53	1.33	1.37
23	c	903	CLA	C4C-NC	-2.52	1.34	1.37
23	C	506	CLA	C1D-ND	-2.51	1.31	1.37
24	a	408	PHO	C1C-NC	-2.50	1.33	1.38
35	b	628	HTG	C1'-S1	-2.50	1.78	1.81
23	b	603	CLA	C1D-ND	-2.48	1.31	1.37
23	c	909	CLA	C4C-NC	-2.45	1.34	1.37
23	B	616	CLA	C1C-NC	-2.45	1.34	1.37
23	d	404	CLA	C1C-NC	-2.36	1.34	1.37
25	D	405	BCR	C30-C25	-2.33	1.50	1.53
23	b	611	CLA	C4C-NC	-2.33	1.34	1.37
24	A	407	PHO	C3D-C4D	-2.25	1.36	1.43
23	B	607	CLA	C4C-NC	-2.23	1.34	1.37
24	a	409	PHO	C3D-C4D	-2.22	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	c	922	HTG	C1-S1	-2.21	1.77	1.80
23	D	403	CLA	C4C-NC	-2.18	1.34	1.37
35	c	921	HTG	C1-S1	-2.17	1.77	1.80
35	C	523	HTG	C1-S1	-2.17	1.77	1.80
23	a	406	CLA	O2A-C1	-2.17	1.39	1.46
23	B	606	CLA	O2A-C1	-2.15	1.39	1.46
23	b	606	CLA	C1D-ND	-2.15	1.32	1.37
24	D	402	PHO	CHB-C4A	-2.14	1.34	1.40
23	C	512	CLA	C4C-NC	-2.14	1.34	1.37
23	B	612	CLA	C1D-ND	-2.13	1.32	1.37
34	B	622	LMG	O7-C8	-2.12	1.40	1.46
23	B	603	CLA	C4C-NC	-2.12	1.34	1.37
23	B	616	CLA	C4C-NC	-2.11	1.34	1.37
28	L	101	LHG	O7-C5	-2.10	1.41	1.46
23	c	908	CLA	C1C-NC	-2.10	1.34	1.37
23	d	403	CLA	C1D-ND	-2.09	1.32	1.37
23	c	906	CLA	C1D-ND	-2.09	1.32	1.37
23	b	615	CLA	C1C-NC	-2.09	1.34	1.37
25	b	620	BCR	C30-C25	-2.09	1.51	1.53
23	b	602	CLA	C1C-NC	-2.08	1.34	1.37
24	a	408	PHO	CHB-C4A	-2.05	1.34	1.40
36	C	518	DGD	O2G-C2G	-2.04	1.41	1.46
35	B	630	HTG	C1-S1	-2.03	1.77	1.80
23	c	910	CLA	C4C-NC	-2.02	1.34	1.37
25	B	618	BCR	C1-C6	-2.00	1.51	1.53
23	B	607	CLA	C1C-C2C	2.00	1.48	1.44
25	A	409	BCR	C23-C22	2.00	1.50	1.45
37	E	105	HEM	CMD-C2D	2.00	1.55	1.51
23	C	507	CLA	C1A-CHA	2.01	1.51	1.43
34	j	101	LMG	O1-C1	2.01	1.43	1.40
23	b	604	CLA	C4B-CHC	2.01	1.45	1.40
37	e	105	HEM	C1C-NC	2.01	1.39	1.36
23	C	505	CLA	C4C-C3C	2.02	1.48	1.45
23	b	610	CLA	C4C-C3C	2.02	1.48	1.45
23	c	903	CLA	C4B-CHC	2.02	1.45	1.40
23	d	401	CLA	C4B-CHC	2.03	1.45	1.40
25	B	619	BCR	C37-C22	2.03	1.54	1.50
23	B	605	CLA	C3D-C2D	2.03	1.44	1.40
23	C	504	CLA	C1B-CHB	2.03	1.45	1.40
30	a	418	LMT	O1'-C1'	2.04	1.43	1.40
23	C	505	CLA	C1B-CHB	2.04	1.45	1.40
23	c	914	CLA	C4C-C3C	2.04	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	a	410	CLA	C4B-CHC	2.04	1.45	1.40
23	B	609	CLA	C4B-CHC	2.04	1.45	1.40
25	B	619	BCR	C34-C9	2.05	1.54	1.50
37	E	105	HEM	CMB-C2B	2.05	1.56	1.51
23	c	909	CLA	C1C-C2C	2.05	1.48	1.44
30	F	101	LMT	O1'-C1'	2.06	1.43	1.40
37	E	105	HEM	CAD-C3D	2.06	1.54	1.52
30	b	621	LMT	O1'-C1'	2.07	1.43	1.40
23	C	514	CLA	CHB-C4A	2.07	1.36	1.33
23	C	505	CLA	CHB-C4A	2.07	1.36	1.33
25	d	405	BCR	C19-C18	2.07	1.50	1.45
26	a	417	SQD	O7-S	2.08	1.51	1.45
23	c	912	CLA	C3D-CAD	2.08	1.51	1.45
23	b	602	CLA	C4C-C3C	2.08	1.48	1.45
23	B	615	CLA	C4B-CHC	2.08	1.45	1.40
23	b	603	CLA	C4B-CHC	2.08	1.45	1.40
23	A	405	CLA	CAA-C2A	2.09	1.58	1.54
23	b	614	CLA	C1B-CHB	2.09	1.45	1.40
23	B	603	CLA	CHB-C4A	2.09	1.36	1.33
23	C	503	CLA	CHD-C4C	2.09	1.46	1.41
23	B	614	CLA	C4B-CHC	2.09	1.45	1.40
23	c	912	CLA	C1C-C2C	2.09	1.48	1.44
25	k	102	BCR	C19-C18	2.09	1.50	1.45
23	B	612	CLA	CHD-C4C	2.09	1.46	1.41
23	B	614	CLA	C1C-C2C	2.09	1.48	1.44
23	b	603	CLA	C3D-C2D	2.10	1.44	1.40
23	c	906	CLA	C1C-C2C	2.10	1.48	1.44
23	B	617	CLA	C4C-C3C	2.10	1.48	1.45
25	a	411	BCR	C5-C6	2.11	1.38	1.34
23	B	614	CLA	C3B-CAB	2.12	1.52	1.47
23	A	405	CLA	C3B-CAB	2.12	1.52	1.47
23	C	507	CLA	C4C-C3C	2.12	1.48	1.45
23	d	404	CLA	C1C-C2C	2.12	1.48	1.44
35	O	302	HTG	C1-S1	2.13	1.84	1.80
28	d	409	LHG	O8-C23	2.13	1.39	1.33
23	b	608	CLA	C4C-C3C	2.13	1.48	1.45
26	D	408	SQD	O6-C1	2.13	1.44	1.40
23	c	910	CLA	C4B-CHC	2.13	1.45	1.40
30	m	103	LMT	O1'-C1'	2.13	1.44	1.40
23	c	912	CLA	C4B-CHC	2.14	1.45	1.40
23	b	605	CLA	C1C-C2C	2.14	1.48	1.44
23	b	610	CLA	CHB-C4A	2.15	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	510	CLA	C4B-CHC	2.15	1.45	1.40
23	C	510	CLA	CHD-C4C	2.16	1.46	1.41
23	b	615	CLA	CHB-C4A	2.16	1.36	1.33
37	e	105	HEM	CAA-C2A	2.16	1.55	1.52
26	B	621	SQD	O6-C1	2.16	1.44	1.40
23	D	403	CLA	C4B-CHC	2.16	1.45	1.40
23	b	607	CLA	CHD-C4C	2.16	1.46	1.41
23	B	611	CLA	C1C-C2C	2.16	1.48	1.44
23	c	911	CLA	C4B-CHC	2.17	1.46	1.40
23	c	902	CLA	C1C-C2C	2.17	1.48	1.44
23	B	603	CLA	O2A-CGA	2.17	1.39	1.33
23	b	611	CLA	O2A-CGA	2.17	1.39	1.33
23	B	605	CLA	C4B-CHC	2.18	1.46	1.40
23	d	401	CLA	C1B-CHB	2.19	1.46	1.40
23	D	404	CLA	CHD-C4C	2.19	1.46	1.41
23	B	606	CLA	C1C-C2C	2.19	1.48	1.44
23	b	617	CLA	C4C-C3C	2.19	1.49	1.45
27	d	406	PL9	C6-C5	2.19	1.47	1.35
34	c	930	LMG	O1-C1	2.19	1.44	1.40
23	B	612	CLA	C4C-C3C	2.21	1.49	1.45
24	a	408	PHO	O2A-CGA	2.21	1.39	1.33
23	B	615	CLA	CHD-C4C	2.21	1.46	1.41
23	c	907	CLA	C1C-C2C	2.21	1.48	1.44
37	E	105	HEM	CMC-C2C	2.22	1.56	1.51
23	a	407	CLA	CHD-C4C	2.22	1.46	1.41
37	E	105	HEM	C4D-ND	2.23	1.39	1.36
23	C	504	CLA	C4C-C3C	2.23	1.49	1.45
23	A	406	CLA	CHB-C4A	2.24	1.36	1.33
23	c	907	CLA	C1B-CHB	2.24	1.46	1.40
27	A	411	PL9	C6-C5	2.25	1.48	1.35
23	b	607	CLA	C4C-C3C	2.26	1.49	1.45
23	D	404	CLA	C1C-C2C	2.26	1.49	1.44
23	c	904	CLA	OBD-CAD	2.26	1.25	1.22
23	B	606	CLA	C4C-C3C	2.27	1.49	1.45
23	c	907	CLA	CHD-C4C	2.27	1.46	1.41
27	D	406	PL9	C23-C24	2.28	1.38	1.32
23	C	502	CLA	C1B-CHB	2.28	1.46	1.40
25	D	405	BCR	C20-C21	2.29	1.50	1.43
23	B	614	CLA	CHD-C4C	2.29	1.46	1.41
23	C	503	CLA	C4C-C3C	2.29	1.49	1.45
35	b	622	HTG	C1-C2	2.30	1.57	1.53
24	D	402	PHO	CHD-C4C	2.31	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	904	CLA	C1C-C2C	2.31	1.49	1.44
23	D	403	CLA	C1B-CHB	2.31	1.46	1.40
27	d	406	PL9	C23-C24	2.31	1.38	1.32
27	D	406	PL9	C6-C5	2.31	1.48	1.35
23	B	614	CLA	O2D-CGD	2.32	1.39	1.33
23	D	401	CLA	C3D-C2D	2.32	1.45	1.40
27	a	414	PL9	C6-C5	2.32	1.48	1.35
23	b	610	CLA	CHD-C4C	2.32	1.46	1.41
23	B	604	CLA	CAA-C2A	2.32	1.58	1.54
23	c	905	CLA	C1C-C2C	2.32	1.49	1.44
25	B	620	BCR	C20-C21	2.32	1.50	1.43
37	V	203	HEM	CMC-C2C	2.33	1.56	1.51
24	a	409	PHO	CHD-C4C	2.33	1.46	1.40
37	v	203	HEM	CMC-C2C	2.33	1.56	1.51
23	C	514	CLA	C1C-C2C	2.34	1.49	1.44
23	b	604	CLA	C4C-C3C	2.34	1.49	1.45
23	B	606	CLA	O1D-CGD	2.34	1.27	1.21
23	a	407	CLA	C4B-CHC	2.35	1.46	1.40
23	d	401	CLA	C4C-C3C	2.35	1.49	1.45
23	B	612	CLA	C3B-C2B	2.35	1.43	1.40
23	b	606	CLA	CHB-C4A	2.35	1.36	1.33
23	C	510	CLA	C4C-C3C	2.35	1.49	1.45
36	c	917	DGD	O5D-C1E	2.35	1.44	1.40
23	b	602	CLA	C4B-CHC	2.36	1.46	1.40
23	b	610	CLA	C1C-C2C	2.36	1.49	1.44
23	B	617	CLA	C4B-CHC	2.36	1.46	1.40
25	A	409	BCR	C8-C9	2.36	1.51	1.45
38	H	102	RRX	C5-C6	2.37	1.38	1.34
23	b	604	CLA	O2A-CGA	2.37	1.40	1.33
23	A	408	CLA	OBD-CAD	2.37	1.25	1.22
34	d	411	LMG	O1-C1	2.37	1.44	1.40
23	d	404	CLA	C1B-CHB	2.38	1.46	1.40
23	d	404	CLA	CHD-C4C	2.38	1.46	1.41
37	e	105	HEM	CMA-C3A	2.39	1.56	1.51
23	B	607	CLA	C1B-CHB	2.39	1.46	1.40
23	B	604	CLA	C3D-C2D	2.40	1.45	1.40
23	b	607	CLA	C1C-C2C	2.40	1.49	1.44
23	C	505	CLA	OBD-CAD	2.40	1.25	1.22
24	a	409	PHO	C4D-ND	2.40	1.41	1.36
23	B	616	CLA	C4B-CHC	2.40	1.46	1.40
23	C	508	CLA	C1C-C2C	2.40	1.49	1.44
23	B	611	CLA	C1B-CHB	2.40	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	608	CLA	C4B-CHC	2.40	1.46	1.40
36	C	518	DGD	O2G-C1B	2.40	1.41	1.34
23	B	610	CLA	C4B-CHC	2.41	1.46	1.40
23	c	904	CLA	CHD-C4C	2.41	1.46	1.41
23	B	609	CLA	CHB-C4A	2.41	1.36	1.33
23	B	602	CLA	C1C-C2C	2.41	1.49	1.44
23	c	913	CLA	C1C-C2C	2.41	1.49	1.44
25	b	620	BCR	C26-C25	2.41	1.38	1.34
23	b	608	CLA	CHD-C4C	2.41	1.46	1.41
23	c	907	CLA	C4B-CHC	2.42	1.46	1.40
37	e	105	HEM	CMC-C2C	2.42	1.56	1.51
23	c	909	CLA	C4C-C3C	2.42	1.49	1.45
23	B	609	CLA	C3D-C2D	2.43	1.45	1.40
23	b	613	CLA	CHD-C4C	2.43	1.46	1.41
24	a	409	PHO	CHC-C4B	2.43	1.46	1.40
23	D	401	CLA	C4C-C3C	2.44	1.49	1.45
30	z	101	LMT	O1'-C1'	2.44	1.44	1.40
23	b	617	CLA	CHD-C4C	2.44	1.46	1.41
23	c	910	CLA	C4C-C3C	2.45	1.49	1.45
23	B	617	CLA	C1B-CHB	2.45	1.46	1.40
30	e	103	LMT	O1'-C1'	2.46	1.44	1.40
37	e	105	HEM	C4D-ND	2.46	1.40	1.36
35	B	624	HTG	C1-C2	2.46	1.58	1.53
37	v	203	HEM	C4D-ND	2.46	1.40	1.36
35	B	624	HTG	O5-C1	2.47	1.46	1.42
23	c	909	CLA	CHD-C4C	2.47	1.47	1.41
23	C	513	CLA	C1C-C2C	2.48	1.49	1.44
23	b	605	CLA	CHD-C4C	2.48	1.47	1.41
23	b	606	CLA	OBD-CAD	2.48	1.26	1.22
23	c	908	CLA	C3D-C2D	2.48	1.45	1.40
23	B	613	CLA	C3D-C2D	2.48	1.45	1.40
23	C	507	CLA	OBD-CAD	2.49	1.26	1.22
23	b	608	CLA	O2A-CGA	2.49	1.40	1.33
23	b	604	CLA	C3B-C2B	2.49	1.43	1.40
23	B	613	CLA	C4B-CHC	2.49	1.46	1.40
23	C	511	CLA	C4C-C3C	2.49	1.49	1.45
23	a	406	CLA	C3D-C2D	2.50	1.45	1.40
23	c	902	CLA	CHD-C4C	2.50	1.47	1.41
23	A	405	CLA	C1B-CHB	2.51	1.46	1.40
23	B	602	CLA	CHD-C4C	2.51	1.47	1.41
23	C	508	CLA	C4B-CHC	2.51	1.46	1.40
27	A	411	PL9	C2-C3	2.51	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	401	CLA	C1B-CHB	2.51	1.46	1.40
23	b	603	CLA	C1B-CHB	2.51	1.46	1.40
23	C	503	CLA	C4B-CHC	2.52	1.46	1.40
23	b	613	CLA	C4B-CHC	2.52	1.46	1.40
27	D	406	PL9	C2-C3	2.52	1.41	1.34
23	A	406	CLA	C1B-CHB	2.53	1.46	1.40
23	b	616	CLA	C4C-C3C	2.53	1.49	1.45
23	A	408	CLA	CHD-C4C	2.53	1.47	1.41
23	b	617	CLA	C1C-C2C	2.54	1.49	1.44
23	b	607	CLA	O2A-CGA	2.54	1.40	1.33
23	b	611	CLA	C3D-C2D	2.54	1.45	1.40
23	B	603	CLA	C4B-CHC	2.55	1.47	1.40
23	C	512	CLA	C4B-CHC	2.55	1.47	1.40
23	b	605	CLA	C4C-C3C	2.55	1.49	1.45
23	B	610	CLA	CHB-C4A	2.55	1.37	1.33
23	B	617	CLA	CHD-C4C	2.56	1.47	1.41
23	b	606	CLA	C4B-CHC	2.58	1.47	1.40
23	b	602	CLA	C1C-C2C	2.58	1.49	1.44
23	B	612	CLA	CHB-C4A	2.59	1.37	1.33
23	B	606	CLA	CHD-C4C	2.59	1.47	1.41
23	B	615	CLA	C3B-C2B	2.59	1.43	1.40
23	C	506	CLA	C1B-CHB	2.59	1.47	1.40
30	a	422	LMT	O1'-C1'	2.59	1.44	1.40
23	b	615	CLA	CHD-C4C	2.60	1.47	1.41
23	B	616	CLA	CHD-C4C	2.60	1.47	1.41
23	c	909	CLA	C4B-CHC	2.60	1.47	1.40
23	C	509	CLA	C1C-C2C	2.60	1.49	1.44
23	C	512	CLA	CHD-C4C	2.60	1.47	1.41
23	B	611	CLA	C4B-CHC	2.61	1.47	1.40
23	c	908	CLA	C1C-C2C	2.61	1.49	1.44
24	a	409	PHO	C3B-C4B	2.61	1.48	1.43
23	d	404	CLA	O2D-CGD	2.61	1.39	1.33
23	D	403	CLA	CHC-C1C	2.61	1.43	1.35
23	b	604	CLA	CHD-C4C	2.62	1.47	1.41
24	A	407	PHO	OBD-CAD	2.62	1.26	1.22
23	D	401	CLA	O2A-CGA	2.63	1.41	1.33
24	a	408	PHO	CHC-C4B	2.63	1.47	1.40
36	c	919	DGD	O2G-C1B	2.64	1.42	1.34
23	b	603	CLA	C3B-CAB	2.64	1.53	1.47
23	C	506	CLA	CHB-C4A	2.64	1.37	1.33
23	b	606	CLA	C3D-C2D	2.64	1.45	1.40
23	b	615	CLA	C1B-CHB	2.64	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	d	410	LHG	O7-C7	2.66	1.42	1.34
23	B	608	CLA	O2A-CGA	2.66	1.41	1.33
23	b	611	CLA	C4C-C3C	2.66	1.49	1.45
23	b	605	CLA	O2A-CGA	2.67	1.41	1.33
23	c	910	CLA	CHB-C4A	2.67	1.37	1.33
35	O	302	HTG	O5-C1	2.68	1.47	1.42
23	b	608	CLA	OBD-CAD	2.69	1.26	1.22
23	b	605	CLA	C1B-CHB	2.69	1.47	1.40
25	D	405	BCR	C12-C13	2.69	1.51	1.45
23	B	614	CLA	CHB-C4A	2.69	1.37	1.33
23	a	410	CLA	CHD-C4C	2.69	1.47	1.41
23	b	614	CLA	CHD-C4C	2.69	1.47	1.41
23	d	403	CLA	C3D-C2D	2.69	1.46	1.40
23	b	606	CLA	O2A-CGA	2.71	1.41	1.33
28	d	409	LHG	O7-C7	2.71	1.42	1.34
36	h	102	DGD	O1G-C1A	2.71	1.41	1.33
23	B	612	CLA	C3D-C2D	2.71	1.46	1.40
36	C	517	DGD	O2G-C1B	2.71	1.42	1.34
28	l	101	LHG	O7-C7	2.72	1.42	1.34
23	B	613	CLA	CHD-C4C	2.72	1.47	1.41
23	C	513	CLA	C4B-CHC	2.73	1.47	1.40
23	c	905	CLA	C4B-CHC	2.73	1.47	1.40
23	B	612	CLA	O2A-CGA	2.73	1.41	1.33
23	B	613	CLA	C1B-CHB	2.73	1.47	1.40
23	B	605	CLA	OBD-CAD	2.74	1.26	1.22
23	c	905	CLA	C1B-CHB	2.74	1.47	1.40
23	A	405	CLA	C3D-C2D	2.75	1.46	1.40
23	D	401	CLA	OBD-CAD	2.75	1.26	1.22
23	c	912	CLA	C4C-C3C	2.75	1.50	1.45
23	A	405	CLA	CHD-C4C	2.75	1.47	1.41
23	c	902	CLA	C4C-C3C	2.75	1.50	1.45
30	I	101	LMT	O1'-C1'	2.75	1.45	1.40
36	c	917	DGD	O2G-C1B	2.76	1.42	1.34
23	B	609	CLA	C1B-CHB	2.76	1.47	1.40
23	d	403	CLA	C4B-CHC	2.76	1.47	1.40
23	A	406	CLA	C3D-C2D	2.76	1.46	1.40
23	c	907	CLA	C3D-C2D	2.76	1.46	1.40
23	a	407	CLA	C4C-C3C	2.76	1.50	1.45
30	Z	101	LMT	O1'-C1'	2.76	1.45	1.40
23	B	614	CLA	OBD-CAD	2.76	1.26	1.22
23	b	604	CLA	C3D-C2D	2.76	1.46	1.40
25	B	618	BCR	C14-C13	2.77	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	CHD-C4C	2.77	1.47	1.41
23	b	602	CLA	CHD-C4C	2.78	1.47	1.41
23	b	611	CLA	CHD-C4C	2.78	1.47	1.41
23	a	407	CLA	C1B-CHB	2.78	1.47	1.40
23	c	911	CLA	C3D-C2D	2.79	1.46	1.40
23	c	913	CLA	CHD-C4C	2.81	1.47	1.41
23	B	602	CLA	C3D-C2D	2.81	1.46	1.40
23	B	605	CLA	CHB-C4A	2.81	1.37	1.33
23	b	605	CLA	CHB-C4A	2.81	1.37	1.33
24	A	407	PHO	O2A-CGA	2.81	1.41	1.33
23	c	914	CLA	CHD-C4C	2.81	1.47	1.41
23	b	609	CLA	CHD-C4C	2.82	1.47	1.41
27	a	414	PL9	C2-C3	2.83	1.42	1.34
25	b	619	BCR	C5-C6	2.83	1.39	1.34
23	B	605	CLA	C1B-CHB	2.83	1.47	1.40
23	c	902	CLA	C1B-CHB	2.83	1.47	1.40
23	b	606	CLA	C3B-C2B	2.84	1.44	1.40
23	B	604	CLA	OBD-CAD	2.84	1.26	1.22
23	d	403	CLA	O2D-CGD	2.84	1.40	1.33
23	A	405	CLA	O2A-CGA	2.84	1.41	1.33
23	c	904	CLA	C4C-C3C	2.84	1.50	1.45
23	c	906	CLA	O2D-CGD	2.85	1.40	1.33
31	b	633	DMS	O-S	2.85	1.69	1.50
23	b	608	CLA	C1B-CHB	2.85	1.47	1.40
23	c	909	CLA	C1B-CHB	2.86	1.47	1.40
23	d	401	CLA	O2A-CGA	2.86	1.41	1.33
23	B	602	CLA	C4B-CHC	2.86	1.47	1.40
23	B	610	CLA	C1B-CHB	2.86	1.47	1.40
23	c	904	CLA	O2A-CGA	2.86	1.41	1.33
37	e	105	HEM	CAD-C3D	2.86	1.56	1.52
23	B	605	CLA	CHD-C4C	2.87	1.47	1.41
23	c	910	CLA	CHD-C4C	2.87	1.47	1.41
23	d	401	CLA	CHB-C4A	2.87	1.37	1.33
23	A	406	CLA	O2D-CGD	2.87	1.40	1.33
23	b	603	CLA	C4C-C3C	2.87	1.50	1.45
23	C	506	CLA	C4C-C3C	2.87	1.50	1.45
23	B	614	CLA	C1B-CHB	2.87	1.47	1.40
23	D	401	CLA	O2D-CGD	2.88	1.40	1.33
23	c	912	CLA	CHD-C4C	2.89	1.48	1.41
23	C	508	CLA	C4C-C3C	2.89	1.50	1.45
23	a	406	CLA	O2D-CGD	2.89	1.40	1.33
30	A	416	LMT	O1'-C1'	2.89	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	409	BCR	C19-C18	2.89	1.52	1.45
23	c	904	CLA	C4B-CHC	2.89	1.47	1.40
23	B	607	CLA	O2A-CGA	2.89	1.41	1.33
23	b	609	CLA	C3D-C2D	2.89	1.46	1.40
23	B	602	CLA	C1B-CHB	2.90	1.47	1.40
23	a	407	CLA	OBD-CAD	2.90	1.26	1.22
23	c	914	CLA	C1C-C2C	2.90	1.50	1.44
23	B	604	CLA	C3B-C2B	2.90	1.44	1.40
23	b	616	CLA	O2A-CGA	2.90	1.42	1.33
28	d	408	LHG	O7-C7	2.91	1.42	1.34
36	h	102	DGD	O2G-C1B	2.91	1.42	1.34
23	C	513	CLA	CHD-C4C	2.91	1.48	1.41
23	B	606	CLA	C1B-CHB	2.91	1.48	1.40
23	c	906	CLA	C4B-CHC	2.91	1.48	1.40
23	c	913	CLA	C4B-CHC	2.92	1.48	1.40
23	c	913	CLA	C1B-CHB	2.92	1.48	1.40
35	B	625	HTG	O5-C1	2.92	1.47	1.42
23	B	616	CLA	O2A-CGA	2.92	1.42	1.33
23	C	504	CLA	C1C-C2C	2.92	1.50	1.44
23	C	507	CLA	C4B-CHC	2.93	1.48	1.40
23	C	514	CLA	C4C-C3C	2.93	1.50	1.45
23	C	511	CLA	C4B-CHC	2.93	1.48	1.40
23	b	613	CLA	C1B-CHB	2.93	1.48	1.40
23	C	508	CLA	C1B-CHB	2.93	1.48	1.40
23	A	405	CLA	C3C-C2C	2.93	1.43	1.36
23	c	902	CLA	O2A-CGA	2.93	1.42	1.33
23	A	408	CLA	C4C-C3C	2.93	1.50	1.45
23	A	405	CLA	C4B-CHC	2.94	1.48	1.40
23	C	512	CLA	C4C-C3C	2.94	1.50	1.45
24	a	409	PHO	OBD-CAD	2.95	1.27	1.22
23	b	615	CLA	C1C-C2C	2.95	1.50	1.44
23	C	513	CLA	C4C-C3C	2.95	1.50	1.45
23	b	611	CLA	C1B-CHB	2.95	1.48	1.40
23	C	502	CLA	OBD-CAD	2.95	1.26	1.22
23	b	604	CLA	C1B-CHB	2.96	1.48	1.40
24	A	407	PHO	CHD-C4C	2.96	1.47	1.40
23	c	914	CLA	C4B-CHC	2.97	1.48	1.40
23	C	514	CLA	C4B-CHC	2.97	1.48	1.40
23	C	509	CLA	C1B-CHB	2.97	1.48	1.40
23	B	608	CLA	O2D-CGD	2.97	1.40	1.33
23	b	613	CLA	CHB-C4A	2.98	1.37	1.33
23	b	604	CLA	OBD-CAD	2.98	1.26	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	519	DGD	O2G-C1B	2.98	1.43	1.34
23	a	406	CLA	CHB-C4A	2.98	1.37	1.33
23	c	908	CLA	O2D-CGD	2.99	1.40	1.33
24	a	408	PHO	O2D-CGD	2.99	1.40	1.33
24	A	407	PHO	O2D-CGD	2.99	1.40	1.33
23	B	614	CLA	C3B-C2B	3.00	1.44	1.40
23	C	510	CLA	C1B-CHB	3.01	1.48	1.40
24	a	409	PHO	C3D-C2D	3.01	1.47	1.38
23	B	616	CLA	C4C-C3C	3.01	1.50	1.45
23	a	406	CLA	C1B-CHB	3.02	1.48	1.40
23	B	604	CLA	CHD-C4C	3.02	1.48	1.41
23	C	509	CLA	C4C-C3C	3.02	1.50	1.45
23	D	404	CLA	OBD-CAD	3.02	1.26	1.22
23	c	908	CLA	CHD-C4C	3.02	1.48	1.41
23	B	609	CLA	CHD-C4C	3.02	1.48	1.41
23	D	404	CLA	C4C-C3C	3.04	1.50	1.45
23	B	608	CLA	C4B-CHC	3.04	1.48	1.40
23	B	605	CLA	O2D-CGD	3.04	1.41	1.33
23	B	616	CLA	C3D-C2D	3.04	1.46	1.40
23	A	406	CLA	O2A-CGA	3.04	1.42	1.33
23	b	603	CLA	CHD-C4C	3.04	1.48	1.41
23	b	610	CLA	C4B-CHC	3.05	1.48	1.40
23	D	404	CLA	C4B-CHC	3.05	1.48	1.40
23	A	408	CLA	C4B-CHC	3.05	1.48	1.40
23	a	410	CLA	C3D-C2D	3.05	1.46	1.40
24	D	402	PHO	C3D-C2D	3.05	1.47	1.38
23	c	908	CLA	C1B-CHB	3.05	1.48	1.40
23	C	503	CLA	OBD-CAD	3.05	1.26	1.22
23	d	404	CLA	C4B-CHC	3.06	1.48	1.40
23	b	611	CLA	C4B-CHC	3.06	1.48	1.40
23	b	613	CLA	O2A-CGA	3.07	1.42	1.33
36	c	918	DGD	O2G-C1B	3.07	1.43	1.34
23	C	506	CLA	C4B-CHC	3.08	1.48	1.40
23	c	903	CLA	CHD-C4C	3.08	1.48	1.41
23	b	617	CLA	C4B-CHC	3.08	1.48	1.40
23	c	903	CLA	C1B-CHB	3.08	1.48	1.40
23	b	603	CLA	O2D-CGD	3.08	1.41	1.33
23	B	611	CLA	CHD-C4C	3.09	1.48	1.41
23	B	617	CLA	OBD-CAD	3.09	1.27	1.22
23	B	615	CLA	C3D-C2D	3.09	1.46	1.40
23	B	616	CLA	C1B-CHB	3.09	1.48	1.40
36	D	407	DGD	O3G-C1D	3.09	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	906	CLA	C1B-CHB	3.10	1.48	1.40
23	B	613	CLA	C3B-C2B	3.10	1.44	1.40
23	C	507	CLA	CHD-C4C	3.10	1.48	1.41
23	a	407	CLA	O2A-CGA	3.10	1.42	1.33
23	b	615	CLA	OBD-CAD	3.11	1.27	1.22
23	C	511	CLA	C1B-CHB	3.11	1.48	1.40
23	B	609	CLA	OBD-CAD	3.11	1.27	1.22
23	B	605	CLA	O2A-CGA	3.12	1.42	1.33
23	B	612	CLA	C4B-CHC	3.12	1.48	1.40
23	C	502	CLA	CHD-C4C	3.12	1.48	1.41
23	b	616	CLA	C1B-CHB	3.12	1.48	1.40
23	b	613	CLA	O2D-CGD	3.12	1.41	1.33
23	b	609	CLA	O2A-CGA	3.12	1.42	1.33
23	C	502	CLA	C4B-CHC	3.12	1.48	1.40
23	c	906	CLA	CHD-C4C	3.12	1.48	1.41
23	a	407	CLA	CHB-C4A	3.13	1.37	1.33
23	C	509	CLA	C4B-CHC	3.13	1.48	1.40
23	b	606	CLA	O2D-CGD	3.13	1.41	1.33
28	D	410	LHG	O8-C23	3.13	1.42	1.33
23	B	604	CLA	O2A-CGA	3.14	1.42	1.33
23	D	404	CLA	C1B-CHB	3.14	1.48	1.40
23	B	607	CLA	C4C-C3C	3.14	1.50	1.45
31	A	423	DMS	O-S	3.15	1.71	1.50
23	b	602	CLA	C1B-CHB	3.15	1.48	1.40
23	B	610	CLA	O2A-CGA	3.15	1.42	1.33
23	B	603	CLA	C4C-C3C	3.15	1.50	1.45
36	H	103	DGD	O1G-C1A	3.16	1.42	1.33
23	c	911	CLA	C1B-CHB	3.16	1.48	1.40
23	D	403	CLA	O2D-CGD	3.17	1.41	1.33
23	B	604	CLA	C1B-CHB	3.17	1.48	1.40
23	D	401	CLA	C4B-CHC	3.17	1.48	1.40
37	V	203	HEM	C4C-NC	3.17	1.41	1.36
23	a	406	CLA	O2A-CGA	3.18	1.42	1.33
23	c	909	CLA	O2A-CGA	3.19	1.42	1.33
23	C	514	CLA	CHD-C4C	3.19	1.48	1.41
36	C	517	DGD	O1G-C1A	3.19	1.42	1.33
23	c	902	CLA	C3D-C2D	3.19	1.47	1.40
23	b	616	CLA	C3D-C2D	3.19	1.47	1.40
23	B	609	CLA	O2A-CGA	3.19	1.42	1.33
23	c	908	CLA	C4B-CHC	3.20	1.48	1.40
23	b	611	CLA	OBD-CAD	3.20	1.27	1.22
23	B	615	CLA	C4C-C3C	3.20	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	d	404	CLA	C3D-C2D	3.20	1.47	1.40
23	B	613	CLA	O2A-CGA	3.21	1.42	1.33
23	B	608	CLA	CHB-C4A	3.22	1.37	1.33
23	d	403	CLA	C1B-CHB	3.22	1.48	1.40
28	l	101	LHG	O8-C23	3.22	1.42	1.33
23	B	603	CLA	CHD-C4C	3.23	1.48	1.41
23	b	615	CLA	O2D-CGD	3.23	1.41	1.33
23	B	616	CLA	OBD-CAD	3.23	1.27	1.22
23	C	508	CLA	CHD-C4C	3.24	1.48	1.41
34	B	622	LMG	O7-C10	3.24	1.43	1.34
23	b	607	CLA	C1B-CHB	3.24	1.48	1.40
23	B	610	CLA	O2D-CGD	3.25	1.41	1.33
28	D	410	LHG	O7-C7	3.25	1.43	1.34
23	c	903	CLA	O2A-CGA	3.26	1.43	1.33
23	c	905	CLA	C4C-C3C	3.27	1.50	1.45
24	a	408	PHO	C3D-C2D	3.27	1.47	1.38
23	B	608	CLA	C1B-CHB	3.27	1.48	1.40
23	b	602	CLA	C3D-C2D	3.27	1.47	1.40
23	b	606	CLA	CHD-C4C	3.27	1.48	1.41
23	c	902	CLA	C4B-CHC	3.27	1.48	1.40
36	c	917	DGD	O1G-C1A	3.28	1.43	1.33
23	B	606	CLA	C3B-C2B	3.28	1.44	1.40
23	b	616	CLA	CHB-C4A	3.28	1.37	1.33
23	C	514	CLA	C1B-CHB	3.28	1.49	1.40
23	b	614	CLA	C3D-C2D	3.29	1.47	1.40
37	e	105	HEM	C3C-CAC	3.29	1.54	1.47
23	b	603	CLA	O2A-CGA	3.29	1.43	1.33
23	c	910	CLA	C1B-CHB	3.30	1.49	1.40
23	c	913	CLA	C4C-C3C	3.30	1.51	1.45
23	B	611	CLA	O2A-CGA	3.30	1.43	1.33
23	d	404	CLA	O2A-CGA	3.31	1.43	1.33
23	B	606	CLA	O2A-CGA	3.31	1.43	1.33
23	b	617	CLA	OBD-CAD	3.31	1.27	1.22
23	C	506	CLA	CHD-C4C	3.31	1.49	1.41
23	b	616	CLA	CHD-C4C	3.32	1.49	1.41
23	C	512	CLA	C1B-CHB	3.32	1.49	1.40
23	B	603	CLA	C1B-CHB	3.32	1.49	1.40
28	D	411	LHG	O7-C7	3.32	1.44	1.34
24	a	409	PHO	O2A-CGA	3.32	1.43	1.33
23	B	603	CLA	C3D-C2D	3.33	1.47	1.40
23	B	608	CLA	OBD-CAD	3.33	1.27	1.22
23	b	611	CLA	CHB-C4A	3.33	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	610	CLA	C3D-C2D	3.34	1.47	1.40
23	c	906	CLA	OBD-CAD	3.34	1.27	1.22
25	a	411	BCR	C26-C25	3.34	1.40	1.34
23	C	508	CLA	C3D-C2D	3.34	1.47	1.40
23	B	614	CLA	C4C-C3C	3.35	1.51	1.45
23	C	505	CLA	CHD-C4C	3.35	1.49	1.41
23	b	612	CLA	O2A-CGA	3.35	1.43	1.33
23	C	502	CLA	O2A-CGA	3.35	1.43	1.33
23	C	507	CLA	C3D-C2D	3.37	1.47	1.40
23	b	614	CLA	CHB-C4A	3.37	1.38	1.33
23	b	607	CLA	C3D-C2D	3.37	1.47	1.40
23	A	408	CLA	O2A-CGA	3.38	1.43	1.33
23	c	914	CLA	C3D-C2D	3.38	1.47	1.40
35	B	625	HTG	C1-S1	3.39	1.86	1.80
23	a	406	CLA	CHD-C4C	3.39	1.49	1.41
23	b	609	CLA	O2D-CGD	3.39	1.41	1.33
24	D	402	PHO	OBD-CAD	3.40	1.28	1.22
23	d	401	CLA	CHD-C4C	3.40	1.49	1.41
23	c	906	CLA	C3D-C2D	3.40	1.47	1.40
23	D	404	CLA	C3D-C2D	3.40	1.47	1.40
23	a	407	CLA	O2D-CGD	3.40	1.42	1.33
23	c	903	CLA	OBD-CAD	3.41	1.27	1.22
34	J	101	LMG	O8-C28	3.41	1.43	1.33
23	C	504	CLA	C3D-C2D	3.43	1.47	1.40
24	D	402	PHO	O2A-CGA	3.43	1.43	1.33
23	b	607	CLA	OBD-CAD	3.43	1.27	1.22
37	e	105	HEM	C3B-CAB	3.43	1.55	1.47
28	d	410	LHG	O8-C23	3.43	1.43	1.33
23	d	403	CLA	O2A-CGA	3.43	1.43	1.33
23	c	905	CLA	O2A-CGA	3.43	1.43	1.33
23	b	615	CLA	C3D-C2D	3.43	1.47	1.40
23	b	613	CLA	OBD-CAD	3.44	1.27	1.22
23	a	407	CLA	C3C-C2C	3.44	1.44	1.36
23	C	514	CLA	O2A-CGA	3.45	1.43	1.33
26	a	412	SQD	O47-C7	3.45	1.44	1.34
23	C	503	CLA	O2A-CGA	3.45	1.43	1.33
31	o	301	DMS	O-S	3.45	1.73	1.50
23	b	617	CLA	C1B-CHB	3.46	1.49	1.40
23	C	506	CLA	O2A-CGA	3.47	1.43	1.33
24	D	402	PHO	CHC-C4B	3.47	1.49	1.40
23	C	513	CLA	C1B-CHB	3.48	1.49	1.40
23	c	913	CLA	O2A-CGA	3.48	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	403	CLA	OBD-CAD	3.48	1.27	1.22
37	V	203	HEM	C3D-C2D	3.49	1.48	1.37
23	A	406	CLA	OBD-CAD	3.49	1.27	1.22
23	b	605	CLA	C3D-C2D	3.49	1.47	1.40
23	a	407	CLA	C3D-C2D	3.49	1.47	1.40
23	B	607	CLA	C3D-C2D	3.49	1.47	1.40
23	C	512	CLA	O2A-CGA	3.49	1.43	1.33
23	D	403	CLA	CHD-C4C	3.50	1.49	1.41
23	b	609	CLA	C1B-CHB	3.50	1.49	1.40
23	C	509	CLA	O2A-CGA	3.50	1.43	1.33
23	B	606	CLA	OBD-CAD	3.50	1.27	1.22
23	c	912	CLA	C1B-CHB	3.50	1.49	1.40
23	B	607	CLA	C4B-CHC	3.51	1.49	1.40
23	C	514	CLA	OBD-CAD	3.51	1.27	1.22
23	c	908	CLA	OBD-CAD	3.51	1.27	1.22
23	B	617	CLA	C3D-C2D	3.52	1.47	1.40
23	b	613	CLA	C3D-C2D	3.52	1.47	1.40
23	C	502	CLA	O2D-CGD	3.52	1.42	1.33
23	D	403	CLA	O2A-CGA	3.52	1.43	1.33
23	b	612	CLA	C3D-C2D	3.53	1.47	1.40
23	C	508	CLA	O2A-CGA	3.54	1.43	1.33
23	c	905	CLA	C3D-C2D	3.54	1.47	1.40
23	c	903	CLA	C3D-C2D	3.54	1.47	1.40
23	c	910	CLA	O2A-CGA	3.55	1.43	1.33
23	b	617	CLA	C3D-C2D	3.55	1.47	1.40
28	D	411	LHG	O8-C23	3.55	1.43	1.33
23	C	511	CLA	O2A-CGA	3.56	1.43	1.33
23	B	614	CLA	O2A-CGA	3.56	1.43	1.33
23	d	401	CLA	OBD-CAD	3.56	1.27	1.22
36	h	102	DGD	O5D-C1E	3.56	1.46	1.40
23	b	610	CLA	OBD-CAD	3.56	1.27	1.22
23	a	407	CLA	C3B-C2B	3.57	1.44	1.40
23	B	611	CLA	C3D-C2D	3.57	1.47	1.40
23	c	903	CLA	C3C-C2C	3.57	1.44	1.36
23	B	612	CLA	O2D-CGD	3.57	1.42	1.33
23	A	408	CLA	O2D-CGD	3.57	1.42	1.33
23	B	611	CLA	C4C-C3C	3.58	1.51	1.45
23	c	914	CLA	C1B-CHB	3.58	1.49	1.40
23	C	505	CLA	O2A-CGA	3.58	1.44	1.33
23	c	904	CLA	C1B-CHB	3.59	1.49	1.40
34	j	101	LMG	O7-C10	3.59	1.44	1.34
23	B	608	CLA	C3D-C2D	3.59	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	617	CLA	O2A-CGA	3.59	1.44	1.33
23	c	904	CLA	C3D-C2D	3.59	1.47	1.40
23	C	512	CLA	CHC-C1C	3.60	1.45	1.35
23	c	912	CLA	C3D-C2D	3.60	1.47	1.40
23	b	615	CLA	C4B-CHC	3.60	1.49	1.40
23	C	512	CLA	OBD-CAD	3.60	1.27	1.22
23	c	902	CLA	C3C-C2C	3.60	1.44	1.36
23	B	610	CLA	C3B-C2B	3.60	1.44	1.40
23	C	504	CLA	C4B-CHC	3.61	1.49	1.40
23	a	406	CLA	OBD-CAD	3.61	1.27	1.22
23	b	610	CLA	C1B-CHB	3.61	1.49	1.40
23	a	410	CLA	C1B-CHB	3.61	1.49	1.40
23	D	404	CLA	O2A-CGA	3.61	1.44	1.33
23	C	505	CLA	C3D-C2D	3.63	1.48	1.40
23	D	403	CLA	CHB-C4A	3.64	1.38	1.33
26	A	410	SQD	O48-C23	3.64	1.44	1.33
24	a	408	PHO	OBD-CAD	3.64	1.28	1.22
23	B	615	CLA	O2D-CGD	3.64	1.42	1.33
23	b	615	CLA	C3C-C2C	3.64	1.44	1.36
23	B	603	CLA	O2D-CGD	3.64	1.42	1.33
23	B	615	CLA	O2A-CGA	3.65	1.44	1.33
28	L	101	LHG	O8-C23	3.68	1.44	1.33
23	c	907	CLA	OBD-CAD	3.69	1.27	1.22
24	a	408	PHO	CHD-C1D	3.69	1.46	1.38
23	B	606	CLA	O2D-CGD	3.69	1.42	1.33
23	D	404	CLA	O2D-CGD	3.69	1.42	1.33
23	d	403	CLA	OBD-CAD	3.70	1.27	1.22
23	D	401	CLA	C3C-C2C	3.70	1.44	1.36
23	c	912	CLA	O2A-CGA	3.70	1.44	1.33
28	L	101	LHG	O7-C7	3.70	1.45	1.34
23	A	406	CLA	C3C-C2C	3.70	1.44	1.36
24	a	408	PHO	CHD-C4C	3.71	1.49	1.40
23	C	507	CLA	C1B-CHB	3.71	1.50	1.40
23	d	404	CLA	CHC-C1C	3.71	1.46	1.35
24	a	408	PHO	C3B-C2B	3.71	1.44	1.37
37	E	105	HEM	C3B-CAB	3.72	1.55	1.47
23	C	502	CLA	C3D-C2D	3.72	1.48	1.40
23	C	504	CLA	OBD-CAD	3.72	1.27	1.22
23	b	610	CLA	O2A-CGA	3.72	1.44	1.33
23	B	604	CLA	CHC-C1C	3.73	1.46	1.35
26	B	621	SQD	O48-C23	3.73	1.44	1.33
23	B	615	CLA	C1B-CHB	3.73	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	c	908	CLA	O2A-CGA	3.73	1.44	1.33
36	C	518	DGD	O1G-C1A	3.73	1.44	1.33
23	b	610	CLA	O2D-CGD	3.74	1.42	1.33
36	c	919	DGD	O1G-C1A	3.74	1.44	1.33
23	C	513	CLA	OBD-CAD	3.74	1.28	1.22
23	b	615	CLA	O2A-CGA	3.74	1.44	1.33
23	b	616	CLA	CHC-C1C	3.74	1.46	1.35
23	c	911	CLA	O2A-CGA	3.75	1.44	1.33
23	b	615	CLA	C3B-C2B	3.75	1.45	1.40
23	B	611	CLA	C3B-C2B	3.75	1.45	1.40
23	c	909	CLA	O2D-CGD	3.75	1.42	1.33
31	B	637	DMS	O-S	3.76	1.75	1.50
23	b	617	CLA	O2A-CGA	3.76	1.44	1.33
36	H	103	DGD	O5D-C1E	3.76	1.47	1.40
23	B	610	CLA	C3D-C2D	3.77	1.48	1.40
23	C	512	CLA	C3D-C2D	3.77	1.48	1.40
26	A	415	SQD	O47-C7	3.77	1.45	1.34
36	c	918	DGD	O1G-C1A	3.78	1.44	1.33
23	B	611	CLA	OBD-CAD	3.78	1.28	1.22
23	A	406	CLA	CHC-C1C	3.78	1.46	1.35
23	C	506	CLA	C3D-C2D	3.79	1.48	1.40
23	d	404	CLA	C4C-C3C	3.79	1.51	1.45
34	C	501	LMG	O8-C28	3.79	1.44	1.33
36	H	103	DGD	O2G-C1B	3.79	1.45	1.34
28	d	408	LHG	O8-C23	3.79	1.44	1.33
26	a	412	SQD	O48-C23	3.80	1.44	1.33
35	b	622	HTG	C1-S1	3.80	1.86	1.80
23	c	902	CLA	CHC-C1C	3.80	1.46	1.35
23	B	609	CLA	CHC-C1C	3.81	1.46	1.35
23	c	913	CLA	C3D-C2D	3.82	1.48	1.40
23	a	410	CLA	O2A-CGA	3.83	1.44	1.33
23	C	513	CLA	C3D-C2D	3.83	1.48	1.40
24	A	407	PHO	CHC-C1C	3.83	1.46	1.38
23	B	611	CLA	O2D-CGD	3.83	1.43	1.33
26	A	410	SQD	O47-C7	3.84	1.45	1.34
23	a	410	CLA	OBD-CAD	3.86	1.28	1.22
23	A	408	CLA	C1B-CHB	3.86	1.50	1.40
34	J	101	LMG	O7-C10	3.86	1.45	1.34
23	A	405	CLA	O2D-CGD	3.87	1.43	1.33
24	D	402	PHO	CHC-C1C	3.88	1.46	1.38
23	B	609	CLA	C3C-C2C	3.89	1.45	1.36
23	A	405	CLA	CHC-C1C	3.89	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	b	613	CLA	C3B-C2B	3.89	1.45	1.40
23	b	615	CLA	C4C-C3C	3.91	1.52	1.45
23	c	906	CLA	O2A-CGA	3.91	1.45	1.33
34	m	102	LMG	O7-C10	3.91	1.45	1.34
23	c	906	CLA	CHC-C1C	3.92	1.46	1.35
23	c	902	CLA	O2D-CGD	3.92	1.43	1.33
23	c	910	CLA	C3D-C2D	3.92	1.48	1.40
23	c	910	CLA	C3C-C2C	3.92	1.45	1.36
23	c	913	CLA	OBD-CAD	3.92	1.28	1.22
23	c	914	CLA	OBD-CAD	3.93	1.28	1.22
23	A	408	CLA	CHC-C1C	3.94	1.46	1.35
23	C	503	CLA	C3D-C2D	3.94	1.48	1.40
31	C	524	DMS	O-S	3.95	1.76	1.50
23	C	504	CLA	CHD-C4C	3.95	1.50	1.41
34	c	920	LMG	O7-C10	3.95	1.45	1.34
24	a	409	PHO	C3C-C2C	3.95	1.45	1.36
24	A	407	PHO	CHD-C1D	3.95	1.46	1.38
23	C	508	CLA	CHC-C1C	3.96	1.47	1.35
23	B	605	CLA	C3B-C2B	3.96	1.45	1.40
23	C	505	CLA	CHC-C1C	3.96	1.47	1.35
31	c	924	DMS	O-S	3.96	1.76	1.50
23	b	609	CLA	OBD-CAD	3.97	1.28	1.22
23	b	609	CLA	C3B-C2B	3.97	1.45	1.40
23	c	903	CLA	O2D-CGD	3.97	1.43	1.33
37	E	105	HEM	C3C-CAC	3.98	1.56	1.47
23	B	607	CLA	OBD-CAD	3.98	1.28	1.22
23	c	909	CLA	C3D-C2D	3.98	1.48	1.40
23	b	607	CLA	CHC-C1C	3.98	1.47	1.35
23	D	404	CLA	CHC-C1C	4.00	1.47	1.35
23	B	613	CLA	OBD-CAD	4.00	1.28	1.22
23	C	509	CLA	C3D-C2D	4.01	1.48	1.40
23	c	909	CLA	OBD-CAD	4.01	1.28	1.22
23	c	904	CLA	O2D-CGD	4.01	1.43	1.33
31	B	648	DMS	O-S	4.02	1.77	1.50
23	b	612	CLA	C1B-CHB	4.03	1.51	1.40
34	j	101	LMG	O8-C28	4.03	1.45	1.33
23	b	611	CLA	C3B-C2B	4.04	1.45	1.40
34	c	920	LMG	O8-C28	4.04	1.45	1.33
26	L	102	SQD	O48-C23	4.04	1.45	1.33
23	D	403	CLA	C3B-C2B	4.04	1.45	1.40
24	D	402	PHO	O2D-CGD	4.04	1.43	1.33
28	d	402	LHG	O7-C7	4.05	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	508	CLA	OBD-CAD	4.05	1.28	1.22
23	B	610	CLA	OBD-CAD	4.05	1.28	1.22
23	b	614	CLA	O2A-CGA	4.06	1.45	1.33
23	a	406	CLA	CHC-C1C	4.06	1.47	1.35
31	v	201	DMS	O-S	4.07	1.77	1.50
23	b	607	CLA	C4B-CHC	4.07	1.51	1.40
23	b	602	CLA	CHC-C1C	4.09	1.47	1.35
23	a	410	CLA	O2D-CGD	4.10	1.43	1.33
23	C	510	CLA	C3B-C2B	4.10	1.45	1.40
23	b	607	CLA	C3C-C2C	4.10	1.45	1.36
23	A	408	CLA	C3C-C2C	4.10	1.45	1.36
23	b	603	CLA	C3B-C2B	4.11	1.45	1.40
23	B	605	CLA	C3C-C2C	4.12	1.45	1.36
23	D	401	CLA	CHC-C1C	4.12	1.47	1.35
23	b	614	CLA	OBD-CAD	4.12	1.28	1.22
23	C	507	CLA	O2A-CGA	4.13	1.45	1.33
23	C	503	CLA	C1B-CHB	4.13	1.51	1.40
31	b	634	DMS	O-S	4.13	1.78	1.50
23	C	504	CLA	O2D-CGD	4.13	1.43	1.33
34	C	531	LMG	O8-C28	4.14	1.45	1.33
23	d	401	CLA	C3C-C2C	4.14	1.45	1.36
23	c	905	CLA	CHC-C1C	4.14	1.47	1.35
23	C	509	CLA	CHC-C1C	4.14	1.47	1.35
34	C	520	LMG	O7-C10	4.14	1.46	1.34
23	b	608	CLA	CHC-C1C	4.14	1.47	1.35
24	A	407	PHO	C3C-C2C	4.14	1.45	1.36
23	C	510	CLA	CHC-C1C	4.15	1.47	1.35
23	c	911	CLA	O2D-CGD	4.15	1.43	1.33
23	c	907	CLA	O2A-CGA	4.15	1.45	1.33
23	C	508	CLA	O2D-CGD	4.16	1.43	1.33
23	c	914	CLA	O2A-CGA	4.16	1.45	1.33
23	b	605	CLA	C3B-C2B	4.16	1.45	1.40
23	b	603	CLA	CHC-C1C	4.16	1.47	1.35
34	a	413	LMG	O7-C10	4.17	1.46	1.34
23	C	503	CLA	CHC-C1C	4.17	1.47	1.35
23	b	613	CLA	CHC-C1C	4.17	1.47	1.35
36	C	519	DGD	O1G-C1A	4.17	1.45	1.33
23	B	611	CLA	CHC-C1C	4.18	1.47	1.35
23	C	510	CLA	O2A-CGA	4.18	1.45	1.33
23	B	609	CLA	O2D-CGD	4.19	1.44	1.33
28	a	415	LHG	O7-C7	4.19	1.46	1.34
23	c	910	CLA	CHC-C1C	4.19	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	417	SQD	O47-C7	4.20	1.46	1.34
23	c	911	CLA	CHC-C1C	4.20	1.47	1.35
23	d	401	CLA	CHC-C1C	4.20	1.47	1.35
31	u	203	DMS	O-S	4.21	1.78	1.50
23	D	403	CLA	C3C-C2C	4.21	1.45	1.36
23	b	608	CLA	O2D-CGD	4.22	1.44	1.33
34	C	501	LMG	O7-C10	4.22	1.46	1.34
23	B	602	CLA	OBD-CAD	4.23	1.28	1.22
31	C	525	DMS	O-S	4.23	1.78	1.50
23	C	504	CLA	O2A-CGA	4.24	1.45	1.33
31	D	416	DMS	O-S	4.24	1.78	1.50
23	B	605	CLA	CHC-C1C	4.24	1.47	1.35
23	B	615	CLA	OBD-CAD	4.24	1.28	1.22
31	V	209	DMS	O-S	4.24	1.78	1.50
23	b	608	CLA	C3D-C2D	4.24	1.49	1.40
23	A	405	CLA	C4C-C3C	4.24	1.52	1.45
24	a	409	PHO	O2D-CGD	4.25	1.44	1.33
26	A	415	SQD	O48-C23	4.25	1.46	1.33
23	c	906	CLA	C3B-C2B	4.26	1.45	1.40
23	C	511	CLA	C3C-C2C	4.27	1.46	1.36
23	B	608	CLA	CHC-C1C	4.27	1.47	1.35
23	c	908	CLA	CHC-C1C	4.27	1.47	1.35
23	B	602	CLA	CHC-C1C	4.27	1.47	1.35
23	B	608	CLA	C3C-C2C	4.28	1.46	1.36
31	C	529	DMS	O-S	4.28	1.79	1.50
23	B	616	CLA	CHC-C1C	4.28	1.48	1.35
28	K	101	LHG	O8-C23	4.28	1.46	1.33
28	K	101	LHG	O7-C7	4.29	1.46	1.34
23	b	603	CLA	OBD-CAD	4.29	1.28	1.22
31	C	527	DMS	O-S	4.29	1.79	1.50
23	c	910	CLA	O2D-CGD	4.29	1.44	1.33
28	E	101	LHG	O7-C7	4.30	1.47	1.34
23	A	406	CLA	C3B-C2B	4.30	1.45	1.40
31	u	205	DMS	O-S	4.30	1.79	1.50
23	d	401	CLA	C3B-C2B	4.30	1.45	1.40
23	C	506	CLA	CHC-C1C	4.30	1.48	1.35
23	B	617	CLA	O2D-CGD	4.30	1.44	1.33
23	b	615	CLA	CHC-C1C	4.31	1.48	1.35
26	B	621	SQD	O47-C7	4.31	1.47	1.34
23	b	617	CLA	O2D-CGD	4.31	1.44	1.33
23	C	510	CLA	O2D-CGD	4.31	1.44	1.33
31	U	202	DMS	O-S	4.31	1.79	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	417	SQD	O48-C23	4.32	1.46	1.33
34	c	930	LMG	O8-C28	4.32	1.46	1.33
37	V	203	HEM	C3B-CAB	4.32	1.57	1.47
36	d	407	DGD	O1G-C1A	4.33	1.46	1.33
31	V	202	DMS	O-S	4.33	1.79	1.50
31	V	201	DMS	O-S	4.33	1.79	1.50
23	C	514	CLA	CHC-C1C	4.33	1.48	1.35
31	O	310	DMS	O-S	4.33	1.79	1.50
31	B	640	DMS	O-S	4.34	1.79	1.50
23	c	911	CLA	C3B-C2B	4.34	1.45	1.40
23	C	502	CLA	C3B-C2B	4.34	1.45	1.40
23	C	509	CLA	OBD-CAD	4.34	1.28	1.22
23	C	511	CLA	C3D-C2D	4.34	1.49	1.40
24	D	402	PHO	C3C-C2C	4.34	1.46	1.36
23	B	616	CLA	C3B-C2B	4.34	1.45	1.40
31	V	208	DMS	O-S	4.35	1.79	1.50
23	b	607	CLA	O2D-CGD	4.36	1.44	1.33
26	x	101	SQD	O48-C23	4.37	1.46	1.33
24	D	402	PHO	CHD-C1D	4.37	1.47	1.38
31	v	202	DMS	O-S	4.37	1.79	1.50
23	b	611	CLA	C3C-C2C	4.37	1.46	1.36
23	b	608	CLA	C3B-C2B	4.37	1.45	1.40
31	B	646	DMS	O-S	4.38	1.79	1.50
31	v	206	DMS	O-S	4.38	1.79	1.50
28	A	412	LHG	O7-C7	4.38	1.47	1.34
31	V	205	DMS	O-S	4.38	1.79	1.50
23	C	507	CLA	O2D-CGD	4.39	1.44	1.33
23	b	612	CLA	CHC-C1C	4.39	1.48	1.35
23	C	513	CLA	O2A-CGA	4.39	1.46	1.33
28	D	409	LHG	O8-C23	4.39	1.46	1.33
23	b	602	CLA	OBD-CAD	4.39	1.29	1.22
23	c	905	CLA	O2D-CGD	4.40	1.44	1.33
23	c	913	CLA	CHC-C1C	4.41	1.48	1.35
23	C	510	CLA	C3D-C2D	4.41	1.49	1.40
23	B	613	CLA	CHC-C1C	4.41	1.48	1.35
23	c	906	CLA	C3C-C2C	4.41	1.46	1.36
31	C	528	DMS	O-S	4.42	1.80	1.50
23	c	905	CLA	OBD-CAD	4.42	1.29	1.22
34	m	102	LMG	O8-C28	4.42	1.46	1.33
23	C	514	CLA	C3D-C2D	4.42	1.49	1.40
23	B	614	CLA	C3C-C2C	4.42	1.46	1.36
31	b	637	DMS	O-S	4.42	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	927	DMS	O-S	4.43	1.80	1.50
26	D	408	SQD	O48-C23	4.43	1.46	1.33
31	v	205	DMS	O-S	4.43	1.80	1.50
31	c	928	DMS	O-S	4.43	1.80	1.50
23	B	612	CLA	OBD-CAD	4.43	1.29	1.22
31	c	932	DMS	O-S	4.44	1.80	1.50
31	V	206	DMS	O-S	4.44	1.80	1.50
23	B	613	CLA	O2D-CGD	4.44	1.44	1.33
31	d	415	DMS	O-S	4.44	1.80	1.50
31	c	926	DMS	O-S	4.44	1.80	1.50
31	O	311	DMS	O-S	4.44	1.80	1.50
28	e	101	LHG	O7-C7	4.44	1.47	1.34
26	x	101	SQD	O47-C7	4.44	1.47	1.34
23	c	907	CLA	C3C-C2C	4.45	1.46	1.36
31	k	103	DMS	O-S	4.45	1.80	1.50
31	c	937	DMS	O-S	4.45	1.80	1.50
31	h	101	DMS	O-S	4.45	1.80	1.50
23	C	513	CLA	CHC-C1C	4.46	1.48	1.35
26	D	408	SQD	O47-C7	4.46	1.47	1.34
31	b	641	DMS	O-S	4.46	1.80	1.50
23	b	605	CLA	O2D-CGD	4.46	1.44	1.33
31	h	103	DMS	O-S	4.46	1.80	1.50
31	F	102	DMS	O-S	4.46	1.80	1.50
23	b	612	CLA	C3C-C2C	4.46	1.46	1.36
31	l	102	DMS	O-S	4.46	1.80	1.50
31	C	533	DMS	O-S	4.46	1.80	1.50
23	B	613	CLA	C3C-C2C	4.47	1.46	1.36
31	c	935	DMS	O-S	4.47	1.80	1.50
23	b	614	CLA	C3B-C2B	4.47	1.46	1.40
31	d	419	DMS	O-S	4.47	1.80	1.50
23	b	614	CLA	C3C-C2C	4.47	1.46	1.36
23	C	506	CLA	O2D-CGD	4.47	1.44	1.33
23	d	403	CLA	C3C-C2C	4.48	1.46	1.36
23	c	913	CLA	O2D-CGD	4.48	1.44	1.33
31	c	933	DMS	O-S	4.48	1.80	1.50
28	A	412	LHG	O8-C23	4.48	1.46	1.33
34	c	930	LMG	O7-C10	4.48	1.47	1.34
34	B	622	LMG	O8-C28	4.48	1.46	1.33
23	d	404	CLA	C3C-C2C	4.48	1.46	1.36
23	d	404	CLA	OBD-CAD	4.49	1.29	1.22
31	e	104	DMS	O-S	4.49	1.80	1.50
31	a	421	DMS	O-S	4.49	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	a	408	PHO	C3C-C2C	4.49	1.46	1.36
31	b	643	DMS	O-S	4.49	1.80	1.50
23	C	511	CLA	CHC-C1C	4.49	1.48	1.35
23	c	912	CLA	OBD-CAD	4.49	1.29	1.22
31	v	210	DMS	O-S	4.50	1.80	1.50
23	C	512	CLA	C3C-C2C	4.50	1.46	1.36
23	c	914	CLA	CHC-C1C	4.50	1.48	1.35
31	O	305	DMS	O-S	4.50	1.80	1.50
23	c	902	CLA	OBD-CAD	4.50	1.29	1.22
28	a	415	LHG	O8-C23	4.50	1.46	1.33
37	V	203	HEM	C3C-CAC	4.50	1.57	1.47
31	A	422	DMS	O-S	4.51	1.80	1.50
23	B	616	CLA	C3C-C2C	4.51	1.46	1.36
23	c	911	CLA	OBD-CAD	4.51	1.29	1.22
31	c	934	DMS	O-S	4.51	1.80	1.50
23	c	903	CLA	C3B-C2B	4.52	1.46	1.40
23	C	507	CLA	CHC-C1C	4.52	1.48	1.35
31	b	642	DMS	O-S	4.52	1.80	1.50
31	a	420	DMS	O-S	4.52	1.80	1.50
23	c	909	CLA	CHC-C1C	4.52	1.48	1.35
31	b	640	DMS	O-S	4.53	1.80	1.50
31	o	303	DMS	O-S	4.53	1.80	1.50
23	B	610	CLA	CHC-C1C	4.53	1.48	1.35
31	O	306	DMS	O-S	4.53	1.80	1.50
31	b	645	DMS	O-S	4.53	1.80	1.50
31	O	303	DMS	O-S	4.53	1.80	1.50
31	c	936	DMS	O-S	4.53	1.80	1.50
31	B	649	DMS	O-S	4.53	1.80	1.50
31	d	414	DMS	O-S	4.53	1.80	1.50
31	U	203	DMS	O-S	4.53	1.80	1.50
31	i	105	DMS	O-S	4.54	1.80	1.50
31	a	401	DMS	O-S	4.54	1.80	1.50
23	b	616	CLA	O2D-CGD	4.54	1.44	1.33
23	b	604	CLA	O2D-CGD	4.54	1.44	1.33
31	h	104	DMS	O-S	4.54	1.80	1.50
23	c	912	CLA	CHC-C1C	4.55	1.48	1.35
23	c	911	CLA	C3C-C2C	4.55	1.46	1.36
31	v	207	DMS	O-S	4.55	1.80	1.50
31	A	421	DMS	O-S	4.55	1.80	1.50
23	B	612	CLA	C3C-C2C	4.55	1.46	1.36
23	a	406	CLA	C3B-C2B	4.56	1.46	1.40
31	B	647	DMS	O-S	4.56	1.80	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	635	DMS	O-S	4.56	1.81	1.50
23	c	907	CLA	CHC-C1C	4.56	1.48	1.35
23	b	605	CLA	CHC-C1C	4.56	1.48	1.35
31	v	208	DMS	O-S	4.57	1.81	1.50
34	a	413	LMG	O8-C28	4.57	1.46	1.33
23	C	503	CLA	C3C-C2C	4.57	1.46	1.36
31	v	209	DMS	O-S	4.57	1.81	1.50
23	B	606	CLA	CHC-C1C	4.58	1.48	1.35
31	V	210	DMS	O-S	4.58	1.81	1.50
31	A	419	DMS	O-S	4.58	1.81	1.50
36	d	407	DGD	O2G-C1B	4.58	1.47	1.34
23	b	606	CLA	CHC-C1C	4.58	1.48	1.35
23	B	606	CLA	C3C-C2C	4.58	1.46	1.36
31	A	418	DMS	O-S	4.58	1.81	1.50
31	b	646	DMS	O-S	4.59	1.81	1.50
31	i	106	DMS	O-S	4.59	1.81	1.50
23	b	602	CLA	O2D-CGD	4.59	1.45	1.33
23	C	512	CLA	O2D-CGD	4.59	1.45	1.33
28	e	101	LHG	O8-C23	4.59	1.47	1.33
23	B	617	CLA	C3B-C2B	4.60	1.46	1.40
28	d	402	LHG	O8-C23	4.60	1.47	1.33
31	h	105	DMS	O-S	4.60	1.81	1.50
31	d	416	DMS	O-S	4.60	1.81	1.50
31	D	415	DMS	O-S	4.60	1.81	1.50
31	b	639	DMS	O-S	4.60	1.81	1.50
34	D	412	LMG	O7-C10	4.60	1.47	1.34
23	b	611	CLA	CHC-C1C	4.60	1.48	1.35
31	d	418	DMS	O-S	4.61	1.81	1.50
31	O	307	DMS	O-S	4.61	1.81	1.50
23	B	602	CLA	O2D-CGD	4.61	1.45	1.33
23	B	612	CLA	CHC-C1C	4.61	1.48	1.35
36	D	407	DGD	O2G-C1B	4.61	1.47	1.34
31	O	308	DMS	O-S	4.62	1.81	1.50
23	B	614	CLA	CHC-C1C	4.62	1.49	1.35
31	b	644	DMS	O-S	4.62	1.81	1.50
23	a	407	CLA	CHC-C1C	4.62	1.49	1.35
37	v	203	HEM	C3D-C2D	4.62	1.51	1.37
31	o	304	DMS	O-S	4.63	1.81	1.50
23	B	602	CLA	C3C-C2C	4.63	1.46	1.36
23	C	502	CLA	CHC-C1C	4.63	1.49	1.35
31	u	204	DMS	O-S	4.63	1.81	1.50
26	L	102	SQD	O47-C7	4.63	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	607	CLA	O2D-CGD	4.63	1.45	1.33
31	H	105	DMS	O-S	4.63	1.81	1.50
31	H	101	DMS	O-S	4.64	1.81	1.50
23	b	614	CLA	CHC-C1C	4.64	1.49	1.35
31	C	526	DMS	O-S	4.64	1.81	1.50
31	b	647	DMS	O-S	4.64	1.81	1.50
24	a	408	PHO	CHB-C1B	4.66	1.47	1.38
31	B	638	DMS	O-S	4.66	1.81	1.50
31	b	636	DMS	O-S	4.66	1.81	1.50
24	a	408	PHO	CHC-C1C	4.66	1.47	1.38
23	B	607	CLA	C3B-C2B	4.67	1.46	1.40
31	A	424	DMS	O-S	4.67	1.81	1.50
23	b	604	CLA	C3C-C2C	4.67	1.46	1.36
31	B	639	DMS	O-S	4.67	1.81	1.50
34	d	411	LMG	O7-C10	4.68	1.48	1.34
23	B	604	CLA	C3C-C2C	4.68	1.46	1.36
31	u	206	DMS	O-S	4.69	1.81	1.50
31	B	645	DMS	O-S	4.69	1.81	1.50
23	b	616	CLA	OBD-CAD	4.69	1.29	1.22
23	b	612	CLA	O2D-CGD	4.69	1.45	1.33
31	O	304	DMS	O-S	4.69	1.81	1.50
34	d	411	LMG	O8-C28	4.70	1.47	1.33
34	C	531	LMG	O7-C10	4.72	1.48	1.34
23	b	617	CLA	CHC-C1C	4.72	1.49	1.35
23	B	607	CLA	CHC-C1C	4.72	1.49	1.35
31	c	925	DMS	O-S	4.73	1.82	1.50
23	c	908	CLA	C3B-C2B	4.73	1.46	1.40
23	A	405	CLA	OBD-CAD	4.73	1.29	1.22
31	B	641	DMS	O-S	4.73	1.82	1.50
23	b	614	CLA	O2D-CGD	4.75	1.45	1.33
31	V	207	DMS	O-S	4.75	1.82	1.50
31	a	423	DMS	O-S	4.75	1.82	1.50
23	c	903	CLA	CHC-C1C	4.75	1.49	1.35
31	c	929	DMS	O-S	4.76	1.82	1.50
23	B	617	CLA	CHC-C1C	4.76	1.49	1.35
23	C	509	CLA	C3C-C2C	4.76	1.47	1.36
23	D	401	CLA	CHB-C4A	4.76	1.39	1.33
23	B	603	CLA	OBD-CAD	4.77	1.29	1.22
23	B	603	CLA	CHC-C1C	4.77	1.49	1.35
23	b	613	CLA	C3C-C2C	4.77	1.47	1.36
23	C	506	CLA	OBD-CAD	4.78	1.29	1.22
23	d	403	CLA	CHC-C1C	4.78	1.49	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	O2D-CGD	4.78	1.45	1.33
23	B	615	CLA	CHC-C1C	4.78	1.49	1.35
23	b	617	CLA	C3B-C2B	4.78	1.46	1.40
23	C	505	CLA	O2D-CGD	4.78	1.45	1.33
37	E	105	HEM	C3D-C2D	4.78	1.51	1.37
23	c	914	CLA	O2D-CGD	4.79	1.45	1.33
23	C	514	CLA	O2D-CGD	4.79	1.45	1.33
23	B	609	CLA	C3B-C2B	4.80	1.46	1.40
23	c	912	CLA	C3C-C2C	4.80	1.47	1.36
31	U	204	DMS	O-S	4.81	1.82	1.50
31	O	309	DMS	O-S	4.81	1.82	1.50
23	B	603	CLA	C3C-C2C	4.81	1.47	1.36
24	D	402	PHO	CHB-C1B	4.83	1.48	1.38
23	B	617	CLA	C3C-C2C	4.84	1.47	1.36
24	a	409	PHO	CHC-C1C	4.84	1.48	1.38
23	C	509	CLA	O2D-CGD	4.84	1.45	1.33
23	D	404	CLA	C3C-C2C	4.85	1.47	1.36
23	C	503	CLA	O2D-CGD	4.85	1.45	1.33
23	c	907	CLA	O2D-CGD	4.87	1.45	1.33
23	c	905	CLA	C3B-C2B	4.87	1.46	1.40
23	B	615	CLA	C3C-C2C	4.87	1.47	1.36
37	v	203	HEM	C3C-CAC	4.88	1.58	1.47
28	E	101	LHG	O8-C23	4.89	1.47	1.33
31	B	642	DMS	O-S	4.89	1.83	1.50
31	b	638	DMS	O-S	4.90	1.83	1.50
23	C	502	CLA	C3C-C2C	4.90	1.47	1.36
24	a	409	PHO	C3B-C2B	4.90	1.46	1.37
23	B	610	CLA	C3C-C2C	4.90	1.47	1.36
24	a	409	PHO	CHD-C1D	4.92	1.48	1.38
34	D	412	LMG	O8-C28	4.92	1.48	1.33
23	C	511	CLA	OBD-CAD	4.94	1.29	1.22
23	b	610	CLA	CHC-C1C	4.95	1.50	1.35
36	D	407	DGD	O1G-C1A	4.96	1.48	1.33
31	V	211	DMS	O-S	4.96	1.83	1.50
23	c	909	CLA	C3C-C2C	4.96	1.47	1.36
23	B	604	CLA	O2D-CGD	4.97	1.46	1.33
23	C	506	CLA	C3B-C2B	4.98	1.46	1.40
23	B	602	CLA	C3B-C2B	4.99	1.46	1.40
23	a	410	CLA	C3C-C2C	5.00	1.47	1.36
23	C	507	CLA	C3C-C2C	5.00	1.47	1.36
31	D	417	DMS	O-S	5.00	1.83	1.50
23	b	606	CLA	C3C-C2C	5.00	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	CHC-C1C	5.01	1.50	1.35
23	b	602	CLA	C3C-C2C	5.01	1.47	1.36
24	a	409	PHO	CHB-C1B	5.02	1.48	1.38
23	b	611	CLA	O2D-CGD	5.02	1.46	1.33
23	C	512	CLA	C3B-C2B	5.02	1.46	1.40
23	b	608	CLA	C3C-C2C	5.02	1.47	1.36
23	D	404	CLA	C3B-C2B	5.02	1.46	1.40
23	B	608	CLA	C3B-C2B	5.03	1.46	1.40
34	C	520	LMG	O8-C28	5.04	1.48	1.33
23	B	602	CLA	O2A-CGA	5.04	1.48	1.33
23	C	505	CLA	C3C-C2C	5.07	1.47	1.36
23	c	904	CLA	CHC-C1C	5.07	1.50	1.35
23	b	609	CLA	CHC-C1C	5.08	1.50	1.35
23	C	510	CLA	OBD-CAD	5.09	1.30	1.22
23	a	410	CLA	CHC-C1C	5.09	1.50	1.35
23	D	401	CLA	C3B-C2B	5.10	1.46	1.40
23	b	604	CLA	CHC-C1C	5.11	1.50	1.35
23	d	404	CLA	C3B-C2B	5.11	1.46	1.40
23	c	914	CLA	C3C-C2C	5.12	1.47	1.36
23	c	912	CLA	O2D-CGD	5.12	1.46	1.33
23	b	616	CLA	C3C-C2C	5.12	1.47	1.36
24	A	407	PHO	C3B-C2B	5.12	1.46	1.37
23	c	905	CLA	C3C-C2C	5.13	1.47	1.36
23	c	908	CLA	C3C-C2C	5.14	1.47	1.36
23	C	506	CLA	C3C-C2C	5.15	1.47	1.36
23	B	611	CLA	C3C-C2C	5.15	1.47	1.36
23	C	508	CLA	C3C-C2C	5.15	1.47	1.36
37	v	203	HEM	C3B-CAB	5.16	1.58	1.47
23	d	403	CLA	C3B-C2B	5.17	1.46	1.40
23	c	910	CLA	C3B-C2B	5.17	1.46	1.40
23	a	406	CLA	C3C-C2C	5.19	1.48	1.36
23	b	610	CLA	C3C-C2C	5.19	1.48	1.36
23	b	609	CLA	C3C-C2C	5.21	1.48	1.36
23	b	603	CLA	C3C-C2C	5.21	1.48	1.36
23	A	408	CLA	C3B-C2B	5.25	1.47	1.40
23	b	617	CLA	C3C-C2C	5.26	1.48	1.36
23	C	505	CLA	C3B-C2B	5.27	1.47	1.40
23	B	616	CLA	O2D-CGD	5.27	1.46	1.33
23	C	511	CLA	C3B-C2B	5.29	1.47	1.40
23	C	504	CLA	C3C-C2C	5.31	1.48	1.36
23	c	907	CLA	C3B-C2B	5.32	1.47	1.40
31	B	636	DMS	O-S	5.32	1.86	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	D	401	CLA	CHD-C4C	5.34	1.53	1.41
23	b	605	CLA	C3C-C2C	5.35	1.48	1.36
23	b	610	CLA	C3B-C2B	5.36	1.47	1.40
23	b	602	CLA	O2A-CGA	5.40	1.49	1.33
23	C	510	CLA	C3C-C2C	5.43	1.48	1.36
23	c	913	CLA	C3C-C2C	5.44	1.48	1.36
23	b	612	CLA	C3B-C2B	5.45	1.47	1.40
23	c	904	CLA	C3B-C2B	5.45	1.47	1.40
23	C	513	CLA	O2D-CGD	5.47	1.47	1.33
23	C	514	CLA	C3C-C2C	5.52	1.48	1.36
23	a	410	CLA	C3B-C2B	5.57	1.47	1.40
23	c	904	CLA	C3C-C2C	5.66	1.49	1.36
23	B	607	CLA	C3C-C2C	5.68	1.49	1.36
37	e	105	HEM	C3D-C2D	5.68	1.54	1.37
23	C	507	CLA	C3B-C2B	5.83	1.47	1.40
24	A	407	PHO	CHB-C1B	5.86	1.50	1.38
23	c	909	CLA	C3B-C2B	5.86	1.47	1.40
23	c	902	CLA	C3B-C2B	5.88	1.47	1.40
23	c	914	CLA	C3B-C2B	5.96	1.47	1.40
23	b	602	CLA	C3B-C2B	6.00	1.48	1.40
23	B	603	CLA	C3B-C2B	6.03	1.48	1.40
24	D	402	PHO	C3B-C2B	6.09	1.48	1.37
23	C	503	CLA	C3B-C2B	6.11	1.48	1.40
23	c	913	CLA	C3B-C2B	6.12	1.48	1.40
23	C	513	CLA	C3C-C2C	6.18	1.50	1.36
23	c	912	CLA	C3B-C2B	6.25	1.48	1.40
23	C	514	CLA	C3B-C2B	6.30	1.48	1.40
23	C	504	CLA	C3B-C2B	6.41	1.48	1.40
23	c	910	CLA	OBD-CAD	6.50	1.32	1.22
23	C	509	CLA	C3B-C2B	6.56	1.48	1.40
23	C	508	CLA	C3B-C2B	6.57	1.48	1.40
23	b	616	CLA	C3B-C2B	6.63	1.48	1.40
23	b	607	CLA	C3B-C2B	6.74	1.48	1.40
23	C	513	CLA	C3B-C2B	6.74	1.48	1.40

All (2025) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	E	105	HEM	CBD-CAD-C3D	-7.65	99.05	112.47
35	V	204	HTG	O5-C1-C2	-7.21	100.39	110.22
25	D	405	BCR	C7-C8-C9	-6.73	116.05	126.21
23	b	603	CLA	C3B-CAB-CBB	-6.62	113.08	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	511	CLA	CHD-C4C-C3C	-6.33	115.15	124.91
23	b	606	CLA	CHD-C4C-C3C	-6.31	115.18	124.91
26	A	415	SQD	C1-O5-C5	-6.15	101.68	113.74
23	B	602	CLA	CHD-C4C-C3C	-6.10	115.49	124.91
26	a	412	SQD	C1-O5-C5	-6.10	101.77	113.74
23	B	606	CLA	CHD-C4C-C3C	-6.09	115.52	124.91
23	c	911	CLA	CHD-C4C-C3C	-6.07	115.54	124.91
26	A	410	SQD	C1-C2-C3	-6.00	98.08	109.98
23	B	607	CLA	C4B-CHC-C1C	-6.00	117.41	129.34
23	B	615	CLA	CHD-C4C-C3C	-5.85	115.88	124.91
23	B	610	CLA	CHD-C4C-C3C	-5.83	115.91	124.91
23	b	613	CLA	CHD-C4C-C3C	-5.75	116.03	124.91
25	b	618	BCR	C7-C8-C9	-5.73	117.56	126.21
23	B	604	CLA	CHD-C4C-C3C	-5.72	116.08	124.91
23	B	615	CLA	O2D-CGD-O1D	-5.71	111.76	123.77
23	B	604	CLA	C1C-C2C-C3C	-5.70	100.60	106.93
23	c	914	CLA	CHD-C4C-C3C	-5.65	116.19	124.91
23	C	507	CLA	CHD-C4C-C3C	-5.64	116.21	124.91
37	v	203	HEM	CBD-CAD-C3D	-5.58	102.69	112.47
23	c	903	CLA	CHD-C4C-C3C	-5.53	116.38	124.91
23	C	502	CLA	O2D-CGD-O1D	-5.50	112.19	123.77
23	a	407	CLA	C1C-C2C-C3C	-5.49	100.85	106.93
37	e	105	HEM	CBA-CAA-C2A	-5.48	102.86	112.49
25	d	405	BCR	C24-C23-C22	-5.46	117.95	126.21
25	C	515	BCR	C38-C26-C25	-5.37	118.90	124.62
23	c	908	CLA	CHD-C4C-C3C	-5.31	116.72	124.91
23	C	505	CLA	C1C-C2C-C3C	-5.28	101.07	106.93
23	B	611	CLA	CHD-C4C-C3C	-5.27	116.77	124.91
26	D	408	SQD	C1-O5-C5	-5.23	103.48	113.74
35	v	204	HTG	O5-C1-C2	-5.20	103.12	110.22
25	c	916	BCR	C24-C23-C22	-5.18	118.39	126.21
23	D	403	CLA	C1C-C2C-C3C	-5.15	101.22	106.93
23	c	902	CLA	CHD-C4C-C3C	-5.14	116.98	124.91
25	C	530	BCR	C24-C23-C22	-5.13	118.45	126.21
23	B	607	CLA	CHD-C4C-C3C	-5.11	117.03	124.91
23	c	912	CLA	CHD-C4C-C3C	-5.07	117.08	124.91
26	D	408	SQD	C1-C2-C3	-5.06	99.94	109.98
25	T	101	BCR	C38-C26-C25	-5.03	119.26	124.62
23	c	906	CLA	CHD-C4C-C3C	-4.96	117.25	124.91
26	a	412	SQD	C1-C2-C3	-4.94	100.18	109.98
23	A	406	CLA	C1C-C2C-C3C	-4.93	101.46	106.93
24	A	407	PHO	C3D-C2D-C1D	-4.93	97.68	105.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	620	BCR	C38-C26-C25	-4.90	119.40	124.62
23	b	604	CLA	CHD-C4C-C3C	-4.89	117.36	124.91
23	c	907	CLA	CHD-C4C-C3C	-4.89	117.37	124.91
23	C	508	CLA	C1C-C2C-C3C	-4.88	101.51	106.93
23	B	608	CLA	C3B-CAB-CBB	-4.87	116.60	126.40
23	a	406	CLA	C4B-CHC-C1C	-4.87	119.66	129.34
23	c	913	CLA	CHD-C4C-C3C	-4.87	117.40	124.91
23	C	502	CLA	CHD-C4C-C3C	-4.85	117.43	124.91
23	b	617	CLA	O1D-CGD-CBD	-4.84	117.11	124.64
23	b	614	CLA	CHD-C4C-C3C	-4.83	117.45	124.91
24	a	408	PHO	C3D-C2D-C1D	-4.82	97.85	105.76
23	D	403	CLA	CHD-C4C-C3C	-4.82	117.48	124.91
23	C	511	CLA	C4B-CHC-C1C	-4.81	119.78	129.34
23	a	406	CLA	CHD-C4C-C3C	-4.80	117.51	124.91
23	a	410	CLA	CHD-C4C-C3C	-4.79	117.52	124.91
23	B	617	CLA	CHD-C4C-C3C	-4.79	117.52	124.91
25	D	405	BCR	C40-C30-C25	-4.78	103.04	110.33
25	Y	101	BCR	C33-C5-C6	-4.75	119.56	124.62
37	V	203	HEM	CBD-CAD-C3D	-4.69	104.23	112.47
23	b	607	CLA	CHD-C4C-C3C	-4.69	117.68	124.91
23	C	506	CLA	C1C-C2C-C3C	-4.68	101.74	106.93
37	e	105	HEM	CBD-CAD-C3D	-4.66	104.30	112.47
23	d	404	CLA	CHD-C4C-C3C	-4.65	117.73	124.91
23	A	405	CLA	C3B-CAB-CBB	-4.64	117.06	126.40
23	b	604	CLA	C1C-C2C-C3C	-4.63	101.80	106.93
36	C	517	DGD	O3G-C3G-C2G	-4.63	99.98	110.99
23	b	602	CLA	CHD-C4C-C3C	-4.62	117.78	124.91
25	D	405	BCR	C24-C23-C22	-4.62	119.23	126.21
23	C	504	CLA	CHD-C4C-C3C	-4.62	117.78	124.91
23	b	616	CLA	CHD-C4C-C3C	-4.61	117.79	124.91
23	d	404	CLA	C1C-C2C-C3C	-4.59	101.84	106.93
23	C	506	CLA	CHD-C4C-C3C	-4.57	117.86	124.91
23	a	406	CLA	C3B-CAB-CBB	-4.55	117.25	126.40
23	B	612	CLA	CHD-C4C-C3C	-4.53	117.92	124.91
23	B	608	CLA	C1C-C2C-C3C	-4.50	101.94	106.93
23	B	609	CLA	C3B-CAB-CBB	-4.50	117.35	126.40
25	C	516	BCR	C7-C8-C9	-4.50	119.41	126.21
23	C	504	CLA	C3B-CAB-CBB	-4.49	117.36	126.40
23	b	617	CLA	CHD-C4C-C3C	-4.49	117.98	124.91
34	m	102	LMG	C9-C8-C7	-4.48	101.64	112.08
23	c	902	CLA	C1C-C2C-C3C	-4.47	101.97	106.93
38	x	102	RRX	C33-C5-C6	-4.46	119.87	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C15-C14-C13	-4.46	120.74	127.22
23	c	904	CLA	CHD-C4C-C3C	-4.45	118.04	124.91
23	B	613	CLA	C4B-CHC-C1C	-4.45	120.50	129.34
26	A	410	SQD	C1-O5-C5	-4.44	105.03	113.74
23	C	510	CLA	C1C-C2C-C3C	-4.44	102.01	106.93
26	a	417	SQD	C1-O5-C5	-4.43	105.05	113.74
23	D	401	CLA	CHD-C4C-C3C	-4.41	118.11	124.91
37	v	203	HEM	C3B-CAB-CBB	-4.40	117.55	126.40
36	H	103	DGD	O1G-C1A-O1A	-4.37	112.04	123.51
23	C	510	CLA	C3B-CAB-CBB	-4.37	117.61	126.40
23	d	403	CLA	CHD-C4C-C3C	-4.36	118.18	124.91
23	b	614	CLA	C1C-C2C-C3C	-4.35	102.10	106.93
23	b	610	CLA	CHD-C4C-C3C	-4.33	118.22	124.91
23	B	617	CLA	C4B-CHC-C1C	-4.33	120.74	129.34
25	A	409	BCR	C38-C26-C25	-4.32	120.02	124.62
26	A	415	SQD	C1-C2-C3	-4.32	101.42	109.98
23	B	607	CLA	C1C-C2C-C3C	-4.32	102.14	106.93
23	B	602	CLA	O1D-CGD-CBD	-4.31	117.93	124.64
25	D	405	BCR	C38-C26-C25	-4.31	120.03	124.62
23	C	512	CLA	C1C-C2C-C3C	-4.31	102.16	106.93
23	b	604	CLA	O2D-CGD-O1D	-4.30	114.72	123.77
23	c	907	CLA	C1C-C2C-C3C	-4.29	102.17	106.93
23	b	616	CLA	C1C-C2C-C3C	-4.28	102.19	106.93
23	d	401	CLA	C1C-C2C-C3C	-4.27	102.20	106.93
23	C	514	CLA	C1C-C2C-C3C	-4.26	102.21	106.93
27	a	414	PL9	C37-C38-C39	-4.26	118.36	127.75
24	D	402	PHO	C3D-C2D-C1D	-4.26	98.78	105.76
23	b	605	CLA	C1C-C2C-C3C	-4.25	102.22	106.93
23	C	513	CLA	CHD-C4C-C3C	-4.24	118.36	124.91
23	d	404	CLA	C3B-CAB-CBB	-4.24	117.87	126.40
23	b	608	CLA	C4B-CHC-C1C	-4.24	120.92	129.34
23	B	603	CLA	C1C-C2C-C3C	-4.23	102.24	106.93
23	b	605	CLA	CHD-C4C-C3C	-4.23	118.39	124.91
23	C	504	CLA	C1C-C2C-C3C	-4.21	102.26	106.93
38	H	102	RRX	C24-C23-C22	-4.21	119.85	126.21
23	a	406	CLA	C1C-C2C-C3C	-4.20	102.27	106.93
23	b	603	CLA	C1C-C2C-C3C	-4.20	102.27	106.93
23	c	912	CLA	O2D-CGD-O1D	-4.20	114.93	123.77
38	H	102	RRX	C38-C26-C25	-4.20	120.15	124.62
23	B	613	CLA	C1C-C2C-C3C	-4.19	102.28	106.93
25	b	618	BCR	C33-C5-C6	-4.17	120.18	124.62
23	B	614	CLA	C4B-CHC-C1C	-4.17	121.06	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	508	CLA	C3B-CAB-CBB	-4.15	118.05	126.40
23	C	503	CLA	CHD-C4C-C3C	-4.15	118.50	124.91
23	d	403	CLA	O2D-CGD-O1D	-4.14	115.04	123.77
23	b	608	CLA	CHD-C4C-C3C	-4.11	118.56	124.91
23	D	401	CLA	C1C-C2C-C3C	-4.11	102.37	106.93
25	B	618	BCR	C7-C8-C9	-4.11	120.00	126.21
23	B	609	CLA	C1C-C2C-C3C	-4.11	102.38	106.93
24	A	407	PHO	C4D-ND-C1D	-4.11	99.47	106.99
23	b	612	CLA	CHD-C4C-C3C	-4.10	118.58	124.91
23	B	614	CLA	CHD-C4C-C3C	-4.10	118.59	124.91
23	A	405	CLA	C1D-CHD-C4C	-4.09	114.75	125.40
23	B	614	CLA	C3B-CAB-CBB	-4.09	118.18	126.40
23	c	909	CLA	C2A-C1A-CHA	-4.08	117.23	123.80
23	A	408	CLA	CHD-C4C-C3C	-4.06	118.65	124.91
23	c	912	CLA	C1C-C2C-C3C	-4.05	102.44	106.93
23	B	616	CLA	CHD-C4C-C3C	-4.05	118.66	124.91
23	c	910	CLA	CHD-C4C-C3C	-4.05	118.66	124.91
28	D	409	LHG	O8-C23-O10	-4.04	112.91	123.51
23	C	505	CLA	C3B-CAB-CBB	-4.04	118.27	126.40
23	a	406	CLA	C1D-CHD-C4C	-4.04	114.89	125.40
23	c	913	CLA	C1C-C2C-C3C	-4.04	102.45	106.93
23	b	605	CLA	C6-C5-C3	-4.04	105.52	112.76
23	B	608	CLA	CHD-C4C-C3C	-4.03	118.69	124.91
23	D	403	CLA	O2D-CGD-O1D	-4.03	115.28	123.77
23	b	609	CLA	C3B-CAB-CBB	-4.03	118.30	126.40
23	b	602	CLA	C1C-C2C-C3C	-4.02	102.47	106.93
23	A	408	CLA	C4B-CHC-C1C	-4.02	121.35	129.34
36	c	917	DGD	O5D-C6D-C5D	-4.01	102.01	109.14
23	B	602	CLA	C1C-C2C-C3C	-4.01	102.49	106.93
23	a	410	CLA	C3B-CAB-CBB	-4.00	118.34	126.40
23	b	609	CLA	CHD-C4C-C3C	-4.00	118.74	124.91
25	d	405	BCR	C38-C26-C25	-3.99	120.37	124.62
23	b	607	CLA	C4B-CHC-C1C	-3.99	121.42	129.34
25	a	411	BCR	C38-C26-C25	-3.98	120.38	124.62
23	a	406	CLA	C2A-C1A-CHA	-3.97	117.40	123.80
23	B	616	CLA	C1C-C2C-C3C	-3.97	102.53	106.93
25	t	101	BCR	C28-C27-C26	-3.96	107.30	113.87
23	B	610	CLA	C2A-C1A-CHA	-3.96	117.42	123.80
23	b	616	CLA	O2D-CGD-O1D	-3.96	115.44	123.77
23	B	611	CLA	O2D-CGD-O1D	-3.96	115.44	123.77
23	c	908	CLA	C1C-C2C-C3C	-3.95	102.55	106.93
25	Y	101	BCR	C38-C26-C25	-3.94	120.42	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	502	CLA	C3B-CAB-CBB	-3.94	118.48	126.40
24	a	409	PHO	C4C-C3C-C2C	-3.94	102.52	106.80
26	A	415	SQD	O7-S-C6	-3.94	104.15	106.92
23	C	503	CLA	C1C-C2C-C3C	-3.93	102.57	106.93
24	A	407	PHO	C1C-C2C-C3C	-3.93	101.89	106.43
23	B	616	CLA	C3B-CAB-CBB	-3.93	118.50	126.40
23	a	407	CLA	CHD-C4C-C3C	-3.92	118.87	124.91
23	C	505	CLA	CHD-C4C-C3C	-3.92	118.87	124.91
28	d	408	LHG	O8-C23-O10	-3.91	113.25	123.51
23	C	503	CLA	C4B-CHC-C1C	-3.91	121.56	129.34
23	b	607	CLA	C1C-C2C-C3C	-3.91	102.59	106.93
35	V	204	HTG	C1-C2-C3	-3.91	101.84	110.58
23	b	613	CLA	C4B-CHC-C1C	-3.91	121.58	129.34
23	d	401	CLA	CHD-C4C-C3C	-3.91	118.88	124.91
26	a	412	SQD	O5-C1-C2	-3.90	102.17	110.28
23	d	401	CLA	C3B-CAB-CBB	-3.89	118.57	126.40
23	B	607	CLA	O2D-CGD-O1D	-3.89	115.59	123.77
23	b	616	CLA	C2A-C1A-CHA	-3.88	117.54	123.80
23	b	609	CLA	C1C-C2C-C3C	-3.87	102.64	106.93
35	V	204	HTG	C1-O5-C5	-3.87	105.27	112.73
23	c	911	CLA	C1C-C2C-C3C	-3.87	102.64	106.93
37	V	203	HEM	C3B-CAB-CBB	-3.86	118.63	126.40
23	B	612	CLA	C4B-CHC-C1C	-3.86	121.66	129.34
23	B	609	CLA	CHD-C4C-C3C	-3.86	118.95	124.91
25	A	409	BCR	C7-C8-C9	-3.86	120.38	126.21
23	C	508	CLA	CHD-C4C-C3C	-3.86	118.96	124.91
23	B	611	CLA	CAA-CBA-CGA	-3.85	102.15	113.28
23	d	401	CLA	C4B-CHC-C1C	-3.85	121.69	129.34
27	d	406	PL9	C7-C8-C9	-3.84	120.16	126.70
23	d	403	CLA	C1C-C2C-C3C	-3.84	102.67	106.93
25	b	618	BCR	C24-C23-C22	-3.83	120.42	126.21
23	C	509	CLA	C1C-C2C-C3C	-3.83	102.68	106.93
23	c	902	CLA	O2D-CGD-O1D	-3.80	115.76	123.77
23	A	406	CLA	CHD-C4C-C3C	-3.80	119.05	124.91
23	B	605	CLA	O2D-CGD-O1D	-3.79	115.79	123.77
23	c	906	CLA	C3B-CAB-CBB	-3.79	118.78	126.40
23	b	610	CLA	C3B-CAB-CBB	-3.79	118.78	126.40
23	d	404	CLA	C4B-CHC-C1C	-3.79	121.82	129.34
26	B	621	SQD	C1-O5-C5	-3.78	106.33	113.74
25	d	405	BCR	C39-C30-C25	-3.77	104.57	110.33
23	c	908	CLA	C4B-CHC-C1C	-3.77	121.85	129.34
23	b	611	CLA	C1C-C2C-C3C	-3.76	102.76	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	615	CLA	O2D-CGD-O1D	-3.75	115.88	123.77
23	C	514	CLA	O2D-CGD-O1D	-3.75	115.88	123.77
23	c	913	CLA	C3B-CAB-CBB	-3.74	118.87	126.40
23	A	406	CLA	C4B-CHC-C1C	-3.74	121.91	129.34
23	c	906	CLA	C1C-C2C-C3C	-3.73	102.80	106.93
23	c	910	CLA	C1C-C2C-C3C	-3.72	102.81	106.93
27	d	406	PL9	O1-C4-C3	-3.72	116.04	120.71
30	m	104	LMT	C1'-O5'-C5'	-3.71	106.46	113.74
23	B	614	CLA	C1C-C2C-C3C	-3.70	102.83	106.93
23	C	502	CLA	C1C-C2C-C3C	-3.70	102.83	106.93
23	c	904	CLA	C3B-CAB-CBB	-3.70	118.97	126.40
23	d	404	CLA	C6-C5-C3	-3.69	106.14	112.76
23	C	510	CLA	CHD-C4C-C3C	-3.68	119.23	124.91
23	a	406	CLA	C5-C3-C2	-3.68	114.12	120.98
23	B	610	CLA	C4B-CHC-C1C	-3.68	122.03	129.34
24	a	408	PHO	C4C-C3C-C2C	-3.68	102.80	106.80
23	B	603	CLA	CHD-C4C-C3C	-3.67	119.24	124.91
24	a	409	PHO	C3D-C2D-C1D	-3.67	99.74	105.76
23	c	906	CLA	CBC-CAC-C3C	-3.66	101.25	112.38
23	c	905	CLA	C1C-C2C-C3C	-3.65	102.88	106.93
34	c	920	LMG	C8-O7-C10	-3.65	108.88	117.91
23	c	914	CLA	C3B-CAB-CBB	-3.65	119.05	126.40
24	D	402	PHO	C4C-C3C-C2C	-3.64	102.83	106.80
23	b	608	CLA	C1C-C2C-C3C	-3.64	102.89	106.93
23	B	605	CLA	CHD-C4C-C3C	-3.62	119.32	124.91
23	c	909	CLA	CHD-C4C-C3C	-3.62	119.32	124.91
23	C	509	CLA	C5-C3-C2	-3.62	114.24	120.98
23	B	612	CLA	C1C-C2C-C3C	-3.61	102.92	106.93
23	b	608	CLA	C3B-CAB-CBB	-3.61	119.14	126.40
23	d	403	CLA	C2A-C1A-CHA	-3.60	117.99	123.80
25	b	620	BCR	C24-C23-C22	-3.60	120.78	126.21
24	D	402	PHO	C4D-ND-C1D	-3.60	100.41	106.99
23	D	404	CLA	C1C-C2C-C3C	-3.59	102.95	106.93
23	B	604	CLA	C2A-C1A-CHA	-3.59	118.02	123.80
23	C	502	CLA	C2A-C1A-CHA	-3.58	118.02	123.80
23	b	603	CLA	CHD-C4C-C3C	-3.58	119.38	124.91
23	C	514	CLA	C2A-C1A-CHA	-3.58	118.02	123.80
24	a	408	PHO	C1C-C2C-C3C	-3.57	102.31	106.43
25	c	915	BCR	C7-C8-C9	-3.57	120.82	126.21
23	c	904	CLA	C1C-C2C-C3C	-3.57	102.98	106.93
23	a	406	CLA	O2D-CGD-O1D	-3.56	116.27	123.77
23	C	511	CLA	O1D-CGD-CBD	-3.56	119.10	124.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	907	CLA	C2A-C1A-CHA	-3.56	118.07	123.80
23	C	509	CLA	CHD-C4C-C3C	-3.53	119.46	124.91
23	c	910	CLA	C6-C5-C3	-3.53	106.43	112.76
24	a	409	PHO	C4D-ND-C1D	-3.53	100.53	106.99
23	b	602	CLA	O2D-CGD-O1D	-3.53	116.35	123.77
23	c	905	CLA	CHD-C4C-C3C	-3.53	119.47	124.91
23	b	610	CLA	C1C-C2C-C3C	-3.52	103.03	106.93
25	b	619	BCR	C38-C26-C25	-3.52	120.87	124.62
25	B	620	BCR	C33-C5-C6	-3.51	120.88	124.62
25	j	104	BCR	C38-C26-C25	-3.50	120.89	124.62
23	B	605	CLA	C1C-C2C-C3C	-3.50	103.05	106.93
23	b	616	CLA	C1D-CHD-C4C	-3.49	116.33	125.40
23	B	603	CLA	O2D-CGD-O1D	-3.48	116.43	123.77
25	C	530	BCR	C33-C5-C6	-3.48	120.91	124.62
23	B	615	CLA	C4B-CHC-C1C	-3.48	122.43	129.34
23	D	401	CLA	C3B-CAB-CBB	-3.47	119.42	126.40
23	C	507	CLA	C3B-CAB-CBB	-3.47	119.42	126.40
23	a	407	CLA	C4B-CHC-C1C	-3.46	122.46	129.34
23	C	507	CLA	C2A-C3A-C4A	-3.46	98.28	101.84
23	b	617	CLA	C4-C3-C2	-3.45	116.91	123.58
25	C	530	BCR	C38-C26-C25	-3.45	120.95	124.62
23	b	615	CLA	C2A-C1A-CHA	-3.44	118.25	123.80
23	c	903	CLA	OBD-CAD-C3D	-3.44	122.02	128.09
23	b	606	CLA	C1C-C2C-C3C	-3.44	103.12	106.93
23	c	909	CLA	C1C-C2C-C3C	-3.43	103.12	106.93
25	a	411	BCR	C24-C23-C22	-3.43	121.03	126.21
23	B	604	CLA	O1D-CGD-CBD	-3.43	119.30	124.64
23	A	408	CLA	C5-C3-C2	-3.43	114.59	120.98
38	H	102	RRX	C7-C8-C9	-3.43	121.03	126.21
23	b	617	CLA	O2D-CGD-O1D	-3.43	116.55	123.77
38	H	102	RRX	C10-C11-C12	-3.43	112.52	123.11
23	B	602	CLA	C3B-CAB-CBB	-3.43	119.51	126.40
23	B	610	CLA	C1C-C2C-C3C	-3.42	103.14	106.93
24	a	409	PHO	O2D-CGD-O1D	-3.42	116.57	123.77
23	C	508	CLA	O2D-CGD-O1D	-3.42	116.57	123.77
23	a	406	CLA	CHC-C1C-C2C	-3.41	116.85	126.31
23	A	405	CLA	C2A-C1A-CHA	-3.40	118.32	123.80
23	c	914	CLA	C1C-C2C-C3C	-3.40	103.16	106.93
23	C	510	CLA	C4B-CHC-C1C	-3.39	122.60	129.34
26	A	410	SQD	O9-S-O7	-3.39	104.38	113.96
23	c	913	CLA	CBA-CAA-C2A	-3.39	105.22	113.96
24	D	402	PHO	CBA-CAA-C2A	-3.39	105.22	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	607	CLA	O2D-CGD-O1D	-3.39	116.64	123.77
25	T	101	BCR	C23-C24-C25	-3.37	117.46	127.24
23	b	609	CLA	O2D-CGD-O1D	-3.36	116.70	123.77
23	B	613	CLA	CAC-C3C-C2C	-3.36	121.74	127.51
36	c	919	DGD	O3G-C3G-C2G	-3.36	103.00	110.99
23	D	404	CLA	C2A-C1A-CHA	-3.35	118.39	123.80
23	b	613	CLA	C1C-C2C-C3C	-3.35	103.22	106.93
23	b	615	CLA	O2A-CGA-O1A	-3.35	114.73	123.51
23	C	507	CLA	C1C-C2C-C3C	-3.35	103.22	106.93
23	C	509	CLA	O2D-CGD-O1D	-3.35	116.73	123.77
23	C	513	CLA	O1D-CGD-CBD	-3.34	119.45	124.64
23	B	613	CLA	C3B-CAB-CBB	-3.33	119.69	126.40
24	A	407	PHO	C4C-C3C-C2C	-3.33	103.17	106.80
23	c	913	CLA	O2D-CGD-O1D	-3.33	116.76	123.77
23	b	615	CLA	C1C-C2C-C3C	-3.33	103.24	106.93
23	b	611	CLA	CHD-C4C-C3C	-3.32	119.79	124.91
23	b	613	CLA	O2D-CGD-O1D	-3.31	116.80	123.77
23	B	611	CLA	C1D-CHD-C4C	-3.31	116.79	125.40
23	c	910	CLA	C4B-CHC-C1C	-3.30	122.78	129.34
23	B	605	CLA	C6-C5-C3	-3.30	106.84	112.76
23	b	609	CLA	O2A-CGA-O1A	-3.30	114.87	123.51
34	B	622	LMG	C9-C8-C7	-3.29	104.42	112.08
36	h	102	DGD	O1G-C1A-O1A	-3.28	114.91	123.51
34	D	412	LMG	C1-C2-C3	-3.28	103.47	109.98
27	D	406	PL9	C40-C39-C38	-3.28	117.23	123.58
23	A	405	CLA	CHD-C4C-C3C	-3.28	119.85	124.91
27	D	406	PL9	C36-C37-C38	-3.28	103.00	111.61
23	B	611	CLA	C4C-C3C-C2C	-3.28	101.70	106.94
23	c	902	CLA	C4B-CHC-C1C	-3.28	122.83	129.34
23	b	605	CLA	O2D-CGD-O1D	-3.27	116.88	123.77
25	j	104	BCR	C33-C5-C6	-3.27	121.14	124.62
26	B	621	SQD	O5-C5-C4	-3.27	103.43	109.67
23	b	603	CLA	C2A-C3A-C4A	-3.26	98.49	101.84
26	a	412	SQD	O9-S-O7	-3.26	104.75	113.96
25	C	515	BCR	C32-C1-C6	-3.26	105.36	110.33
23	b	612	CLA	C4B-CHC-C1C	-3.26	122.87	129.34
23	c	903	CLA	C1C-C2C-C3C	-3.25	103.32	106.93
38	x	102	RRX	C16-C17-C18	-3.25	122.49	127.22
23	A	408	CLA	C2A-C1A-CHA	-3.25	118.56	123.80
23	C	513	CLA	C1C-C2C-C3C	-3.25	103.33	106.93
23	D	404	CLA	CHD-C4C-C3C	-3.25	119.90	124.91
23	A	408	CLA	O2D-CGD-O1D	-3.24	116.95	123.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	101	BCR	C15-C16-C17	-3.23	116.27	123.23
23	B	609	CLA	O2D-CGD-O1D	-3.22	117.00	123.77
23	B	608	CLA	CBC-CAC-C3C	-3.22	102.61	112.38
26	D	408	SQD	C44-O6-C1	-3.22	107.09	113.81
25	b	618	BCR	C15-C16-C17	-3.21	116.30	123.23
36	C	517	DGD	O5D-C6D-C5D	-3.21	103.43	109.14
23	B	617	CLA	O2D-CGD-O1D	-3.20	117.04	123.77
23	C	514	CLA	CHD-C4C-C3C	-3.20	119.98	124.91
23	b	602	CLA	C5-C3-C2	-3.20	115.03	120.98
23	b	612	CLA	O2D-CGD-O1D	-3.19	117.05	123.77
34	c	920	LMG	O1-C7-C8	-3.18	103.42	110.99
30	m	104	LMT	O1'-C1-C2	-3.18	100.47	109.63
23	a	410	CLA	O2D-CGD-O1D	-3.18	117.08	123.77
25	T	101	BCR	C7-C8-C9	-3.18	121.41	126.21
23	C	512	CLA	CHD-C4C-C3C	-3.18	120.01	124.91
25	d	405	BCR	C15-C14-C13	-3.17	122.61	127.22
23	d	404	CLA	C2A-C1A-CHA	-3.17	118.69	123.80
23	c	911	CLA	C1D-CHD-C4C	-3.17	117.15	125.40
36	c	917	DGD	O3G-C3G-C2G	-3.17	103.45	110.99
25	B	620	BCR	C23-C24-C25	-3.17	118.04	127.24
23	b	605	CLA	C3B-CAB-CBB	-3.17	120.03	126.40
23	C	507	CLA	O2D-CGD-O1D	-3.16	117.12	123.77
23	c	903	CLA	C3B-CAB-CBB	-3.15	120.06	126.40
23	a	410	CLA	C4B-CHC-C1C	-3.15	123.09	129.34
23	c	903	CLA	O2D-CGD-O1D	-3.14	117.16	123.77
23	C	503	CLA	C16-C17-C18	-3.14	100.41	115.92
25	C	530	BCR	C11-C10-C9	-3.14	122.66	127.22
23	c	903	CLA	C1D-CHD-C4C	-3.13	117.25	125.40
23	b	602	CLA	C1D-CHD-C4C	-3.12	117.27	125.40
23	b	612	CLA	C1C-C2C-C3C	-3.12	103.47	106.93
23	B	614	CLA	C2A-C1A-CHA	-3.11	118.78	123.80
25	Y	101	BCR	C7-C8-C9	-3.11	121.51	126.21
27	D	406	PL9	C12-C13-C14	-3.11	120.89	127.75
23	D	401	CLA	C4B-CHC-C1C	-3.10	123.18	129.34
23	b	603	CLA	CMB-C2B-C1B	-3.09	123.05	128.31
23	C	508	CLA	CBC-CAC-C3C	-3.09	103.00	112.38
23	b	615	CLA	CHD-C4C-C3C	-3.08	120.15	124.91
38	x	102	RRX	C38-C26-C25	-3.08	121.34	124.62
23	b	604	CLA	C2A-C3A-C4A	-3.08	98.68	101.84
23	B	607	CLA	O2A-CGA-O1A	-3.08	115.45	123.51
37	E	105	HEM	C3B-CAB-CBB	-3.07	120.22	126.40
23	B	604	CLA	C3B-CAB-CBB	-3.07	120.22	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	405	BCR	C11-C10-C9	-3.07	122.76	127.22
24	A	407	PHO	O2D-CGD-O1D	-3.06	117.33	123.77
23	b	608	CLA	C2A-C1A-CHA	-3.06	118.87	123.80
23	b	603	CLA	C1D-CHD-C4C	-3.06	117.45	125.40
23	B	611	CLA	O2A-CGA-O1A	-3.05	115.51	123.51
25	C	516	BCR	C33-C5-C6	-3.05	121.37	124.62
23	B	606	CLA	C4B-CHC-C1C	-3.05	123.28	129.34
27	a	414	PL9	C37-C36-C34	-3.05	102.53	112.61
26	L	102	SQD	O5-C1-C2	-3.04	103.95	110.28
23	b	614	CLA	C3B-CAB-CBB	-3.04	120.28	126.40
34	j	101	LMG	C9-C8-C7	-3.04	105.00	112.08
23	D	401	CLA	C1D-CHD-C4C	-3.03	117.51	125.40
23	B	605	CLA	O2A-CGA-O1A	-3.03	115.57	123.51
28	L	101	LHG	C6-C5-C4	-3.03	105.03	112.08
23	b	606	CLA	C2A-C1A-CHA	-3.03	118.92	123.80
23	c	913	CLA	CBC-CAC-C3C	-3.02	103.20	112.38
25	t	101	BCR	C38-C26-C25	-3.02	121.40	124.62
25	C	515	BCR	C15-C14-C13	-3.02	122.83	127.22
25	c	915	BCR	C20-C21-C22	-3.02	122.83	127.22
23	c	914	CLA	C2A-C1A-CHA	-3.01	118.94	123.80
23	b	616	CLA	OBD-CAD-C3D	-3.01	122.77	128.09
23	c	902	CLA	C3B-CAB-CBB	-3.01	120.35	126.40
35	B	625	HTG	O2-C2-C3	-3.00	103.59	110.36
23	B	615	CLA	C4C-C3C-C2C	-3.00	102.14	106.94
36	D	407	DGD	O1G-C1A-O1A	-3.00	115.64	123.51
25	Y	101	BCR	C24-C23-C22	-3.00	121.68	126.21
23	A	408	CLA	C1C-C2C-C3C	-3.00	103.61	106.93
25	B	618	BCR	C33-C5-C6	-2.99	121.43	124.62
23	B	603	CLA	OBD-CAD-C3D	-2.99	122.80	128.09
23	c	908	CLA	CBC-CAC-C3C	-2.99	103.29	112.38
23	C	506	CLA	O2A-CGA-O1A	-2.99	115.66	123.51
36	C	518	DGD	O2G-C1B-O1B	-2.99	115.55	123.67
34	c	920	LMG	O3-C3-C4	-2.99	103.63	110.36
23	C	505	CLA	O2D-CGD-O1D	-2.98	117.49	123.77
23	b	614	CLA	C4B-CHC-C1C	-2.98	123.42	129.34
23	B	608	CLA	C2A-C1A-CHA	-2.98	119.00	123.80
25	D	405	BCR	C33-C5-C6	-2.97	121.45	124.62
23	A	405	CLA	OBD-CAD-C3D	-2.97	122.84	128.09
26	A	415	SQD	O6-C44-C45	-2.97	103.92	110.99
25	T	101	BCR	C12-C13-C14	-2.96	114.18	118.95
23	B	604	CLA	CHC-C1C-NC	-2.96	118.43	123.92
26	A	410	SQD	O47-C7-O49	-2.96	115.62	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	OBD-CAD-C3D	-2.95	122.87	128.09
25	A	409	BCR	C15-C16-C17	-2.95	116.86	123.23
25	a	411	BCR	C15-C16-C17	-2.95	116.87	123.23
24	a	408	PHO	CHD-C1D-ND	-2.95	119.32	124.67
36	C	518	DGD	C2G-O2G-C1B	-2.95	110.62	117.91
25	k	102	BCR	C7-C8-C9	-2.94	121.76	126.21
23	b	612	CLA	OBD-CAD-CBD	-2.94	121.50	125.94
23	C	513	CLA	C3B-CAB-CBB	-2.93	120.51	126.40
27	d	406	PL9	C40-C39-C38	-2.93	117.92	123.58
25	D	405	BCR	C28-C27-C26	-2.93	109.02	113.87
23	b	609	CLA	C1D-CHD-C4C	-2.92	117.80	125.40
23	D	403	CLA	C2A-C1A-CHA	-2.92	119.09	123.80
23	C	506	CLA	C3B-CAB-CBB	-2.92	120.53	126.40
23	b	611	CLA	O2D-CGD-O1D	-2.92	117.63	123.77
23	d	403	CLA	C4B-CHC-C1C	-2.92	123.55	129.34
23	b	616	CLA	C3B-CAB-CBB	-2.91	120.54	126.40
23	C	511	CLA	C1C-C2C-C3C	-2.91	103.70	106.93
24	a	408	PHO	O2D-CGD-O1D	-2.91	117.64	123.77
25	C	515	BCR	C33-C5-C6	-2.91	121.52	124.62
25	c	916	BCR	C7-C8-C9	-2.91	121.81	126.21
38	H	102	RRX	C40-C30-C25	-2.91	105.89	110.33
23	d	403	CLA	O2A-CGA-O1A	-2.90	115.90	123.51
23	B	617	CLA	C4C-C3C-C2C	-2.90	102.30	106.94
23	D	404	CLA	CBC-CAC-C3C	-2.90	103.57	112.38
23	B	613	CLA	CAA-CBA-CGA	-2.90	104.90	113.28
23	D	403	CLA	C1D-CHD-C4C	-2.90	117.86	125.40
23	C	508	CLA	OBD-CAD-C3D	-2.90	122.97	128.09
23	b	611	CLA	C6-C5-C3	-2.89	107.57	112.76
23	b	606	CLA	C5-C3-C2	-2.89	115.59	120.98
23	B	613	CLA	CHD-C4C-C3C	-2.89	120.45	124.91
23	B	606	CLA	C1C-C2C-C3C	-2.89	103.73	106.93
23	c	910	CLA	O2D-CGD-O1D	-2.89	117.69	123.77
23	D	404	CLA	O2A-CGA-O1A	-2.89	115.94	123.51
23	a	407	CLA	O2A-CGA-O1A	-2.88	115.95	123.51
23	C	512	CLA	C3B-CAB-CBB	-2.88	120.61	126.40
38	x	102	RRX	C24-C23-C22	-2.87	121.87	126.21
23	b	606	CLA	O2D-CGD-O1D	-2.87	117.72	123.77
23	d	401	CLA	O2D-CGD-O1D	-2.87	117.73	123.77
23	b	614	CLA	C2A-C1A-CHA	-2.86	119.19	123.80
23	c	905	CLA	C3B-CAB-CBB	-2.86	120.65	126.40
23	B	613	CLA	O2D-CGD-O1D	-2.86	117.75	123.77
28	d	409	LHG	O8-C23-O10	-2.86	116.02	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	CLA	CHC-C1C-C2C	-2.86	118.39	126.31
23	b	613	CLA	C2A-C1A-CHA	-2.85	119.20	123.80
23	c	909	CLA	C7-C6-C5	-2.85	104.74	113.16
23	B	606	CLA	C2A-C1A-CHA	-2.85	119.21	123.80
23	B	605	CLA	C4B-CHC-C1C	-2.84	123.69	129.34
36	c	919	DGD	O1G-C1G-C2G	-2.84	101.05	108.70
23	B	602	CLA	C2A-C1A-CHA	-2.83	119.23	123.80
34	C	520	LMG	O8-C28-O10	-2.83	116.09	123.51
23	B	615	CLA	O2A-CGA-O1A	-2.82	116.11	123.51
24	a	409	PHO	C3B-C2B-C1B	-2.82	100.09	106.36
27	D	406	PL9	C36-C34-C33	-2.82	115.73	120.98
23	C	514	CLA	C3B-CAB-CBB	-2.82	120.72	126.40
23	c	910	CLA	C3B-CAB-CBB	-2.82	120.73	126.40
23	c	903	CLA	C6-C5-C3	-2.82	107.71	112.76
23	a	407	CLA	C2A-C1A-CHA	-2.82	119.26	123.80
23	d	401	CLA	CBC-CAC-C3C	-2.81	103.83	112.38
25	b	619	BCR	C8-C7-C6	-2.81	119.08	127.24
27	A	411	PL9	C17-C18-C19	-2.81	121.54	127.75
23	B	602	CLA	O2D-CGD-O1D	-2.81	117.85	123.77
26	B	621	SQD	O9-S-O7	-2.81	106.02	113.96
25	Y	101	BCR	C21-C20-C19	-2.81	114.43	123.11
27	d	406	PL9	C31-C32-C33	-2.81	104.23	111.61
23	C	510	CLA	O2A-CGA-O1A	-2.81	116.15	123.51
23	B	617	CLA	C1C-C2C-C3C	-2.81	103.82	106.93
37	V	203	HEM	C3C-CAC-CBC	-2.80	120.76	126.40
23	b	604	CLA	C4B-CHC-C1C	-2.80	123.78	129.34
25	b	620	BCR	C7-C8-C9	-2.80	121.98	126.21
27	d	406	PL9	C36-C37-C38	-2.80	104.26	111.61
23	c	911	CLA	C2A-C1A-CHA	-2.80	119.29	123.80
23	C	509	CLA	C4B-CHC-C1C	-2.80	123.78	129.34
23	a	410	CLA	C1C-C2C-C3C	-2.79	103.84	106.93
24	A	407	PHO	CBA-CAA-C2A	-2.78	106.78	113.96
23	b	617	CLA	C1C-C2C-C3C	-2.78	103.84	106.93
25	B	620	BCR	C32-C1-C6	-2.78	106.09	110.33
23	B	611	CLA	C1C-C2C-C3C	-2.77	103.86	106.93
23	B	613	CLA	C2A-C1A-CHA	-2.77	119.33	123.80
23	b	604	CLA	O2A-CGA-O1A	-2.77	116.25	123.51
23	B	614	CLA	O2A-CGA-O1A	-2.76	116.27	123.51
23	b	615	CLA	C4B-CHC-C1C	-2.76	123.85	129.34
23	b	604	CLA	C3B-CAB-CBB	-2.76	120.85	126.40
25	A	409	BCR	C28-C27-C26	-2.76	109.30	113.87
26	A	410	SQD	O48-C23-O10	-2.75	116.29	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	D	406	PL9	C27-C28-C29	-2.75	121.68	127.75
23	B	610	CLA	O2D-CGD-O1D	-2.75	117.98	123.77
30	z	101	LMT	C1B-C2B-C3B	-2.74	104.55	109.98
23	B	617	CLA	C4-C3-C2	-2.74	118.28	123.58
38	H	102	RRX	C16-C17-C18	-2.74	123.24	127.22
23	b	615	CLA	CBC-CAC-C3C	-2.74	104.07	112.38
23	B	603	CLA	CBC-CAC-C3C	-2.73	104.08	112.38
36	C	517	DGD	O1G-C1A-O1A	-2.73	116.35	123.51
25	C	515	BCR	C11-C10-C9	-2.73	123.25	127.22
23	d	403	CLA	C3B-CAB-CBB	-2.73	120.92	126.40
34	C	520	LMG	O5-C6-C5	-2.72	102.21	111.30
23	D	401	CLA	CBC-CAC-C3C	-2.72	104.11	112.38
34	d	411	LMG	C8-O7-C10	-2.72	111.19	117.91
23	c	908	CLA	O2D-CGD-O1D	-2.71	118.06	123.77
36	c	918	DGD	O1G-C1A-O1A	-2.71	116.41	123.51
23	c	911	CLA	O2A-CGA-O1A	-2.71	116.41	123.51
36	c	919	DGD	C6B-C5B-C4B	-2.71	100.48	114.54
23	b	606	CLA	OBD-CAD-C3D	-2.71	123.31	128.09
23	a	410	CLA	OBD-CAD-C3D	-2.71	123.31	128.09
25	b	618	BCR	C28-C27-C26	-2.71	109.38	113.87
23	A	406	CLA	OBD-CAD-CBD	-2.70	121.86	125.94
28	d	409	LHG	O7-C7-O9	-2.70	116.31	123.67
23	a	407	CLA	CHC-C1C-C2C	-2.70	118.82	126.31
23	C	509	CLA	C2A-C1A-CHA	-2.70	119.44	123.80
24	a	409	PHO	CAA-C2A-C1A	-2.70	105.30	112.36
23	A	405	CLA	CHC-C1C-C2C	-2.70	118.83	126.31
26	D	408	SQD	O4-C4-C3	-2.70	104.27	110.36
27	d	406	PL9	C22-C23-C24	-2.70	121.80	127.75
23	C	513	CLA	OBD-CAD-C3D	-2.70	123.32	128.09
23	b	609	CLA	C6-C5-C3	-2.69	107.93	112.76
25	T	101	BCR	C20-C21-C22	-2.69	123.31	127.22
23	b	603	CLA	CHC-C1C-NC	-2.69	118.94	123.92
30	M	101	LMT	O1'-C1-C2	-2.69	101.89	109.63
25	B	620	BCR	C24-C23-C22	-2.69	122.14	126.21
23	b	611	CLA	O2A-CGA-O1A	-2.69	116.46	123.51
23	c	906	CLA	O2D-CGD-O1D	-2.69	118.11	123.77
25	k	102	BCR	C38-C26-C25	-2.69	121.76	124.62
25	d	405	BCR	C16-C15-C14	-2.68	117.45	123.23
23	C	505	CLA	C4B-CHC-C1C	-2.68	124.02	129.34
26	A	410	SQD	C45-O47-C7	-2.68	111.29	117.91
27	a	414	PL9	C7-C8-C9	-2.67	122.16	126.70
23	b	611	CLA	C1D-CHD-C4C	-2.67	118.46	125.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	402	PHO	C3B-C2B-C1B	-2.67	100.44	106.36
23	d	404	CLA	CBA-CAA-C2A	-2.66	107.09	113.96
34	c	920	LMG	O8-C28-O10	-2.66	116.53	123.51
23	d	403	CLA	C1D-CHD-C4C	-2.66	118.48	125.40
30	m	103	LMT	C1B-O1B-C4'	-2.66	110.93	118.00
27	a	414	PL9	C17-C18-C19	-2.66	121.89	127.75
23	a	406	CLA	O2A-CGA-O1A	-2.65	116.55	123.51
25	c	916	BCR	C16-C17-C18	-2.65	123.37	127.22
23	c	912	CLA	CBC-CAC-C3C	-2.65	104.34	112.38
36	c	918	DGD	O2G-C1B-O1B	-2.64	116.49	123.67
23	b	613	CLA	C3B-CAB-CBB	-2.64	121.09	126.40
30	I	101	LMT	C3'-C4'-C5'	-2.64	104.82	110.85
23	B	616	CLA	O2D-CGD-O1D	-2.64	118.22	123.77
23	b	604	CLA	C5-C3-C2	-2.63	116.07	120.98
23	c	903	CLA	C4B-CHC-C1C	-2.63	124.11	129.34
23	A	406	CLA	O2D-CGD-O1D	-2.63	118.23	123.77
23	C	505	CLA	OBD-CAD-C3D	-2.63	123.44	128.09
25	C	530	BCR	C7-C8-C9	-2.63	122.23	126.21
25	t	101	BCR	C33-C5-C6	-2.63	121.82	124.62
23	b	610	CLA	C4B-CHC-C1C	-2.63	124.11	129.34
23	B	617	CLA	C2A-C1A-CHA	-2.63	119.56	123.80
36	c	918	DGD	O3D-C3D-C2D	-2.63	104.44	110.36
36	H	103	DGD	O4D-C4D-C3D	-2.62	104.44	110.36
27	a	414	PL9	C42-C43-C44	-2.62	121.96	127.75
23	b	616	CLA	O1D-CGD-CBD	-2.62	120.56	124.64
23	C	511	CLA	O2A-CGA-O1A	-2.62	116.65	123.51
23	a	407	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
30	B	643	LMT	C1-O1'-C1'	-2.61	109.43	114.00
23	b	607	CLA	C2A-C1A-CHA	-2.61	119.59	123.80
23	b	608	CLA	O2D-CGD-O1D	-2.61	118.27	123.77
23	b	617	CLA	C2A-C1A-CHA	-2.61	119.59	123.80
23	B	610	CLA	C4C-C3C-C2C	-2.61	102.77	106.94
23	b	602	CLA	C2A-C1A-CHA	-2.61	119.59	123.80
23	a	410	CLA	C4C-C3C-C2C	-2.61	102.78	106.94
23	b	612	CLA	C2A-C1A-CHA	-2.60	119.60	123.80
23	C	503	CLA	C3B-CAB-CBB	-2.60	121.17	126.40
36	d	407	DGD	O1G-C1A-O1A	-2.60	116.70	123.51
23	B	604	CLA	O2A-CGA-O1A	-2.59	116.71	123.51
23	B	617	CLA	CBC-CAC-C3C	-2.59	104.50	112.38
23	b	602	CLA	OBD-CAD-C3D	-2.59	123.51	128.09
36	c	917	DGD	O1G-C1G-C2G	-2.59	101.70	108.70
25	C	516	BCR	C3-C4-C5	-2.59	109.57	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	102	SQD	O9-S-O7	-2.59	106.65	113.96
30	B	644	LMT	C1-O1'-C1'	-2.59	109.48	114.00
25	c	916	BCR	C32-C1-C6	-2.59	106.38	110.33
23	C	507	CLA	C1D-CHD-C4C	-2.58	118.69	125.40
27	A	411	PL9	C7-C8-C9	-2.58	122.31	126.70
23	B	608	CLA	CMB-C2B-C1B	-2.58	123.92	128.31
27	d	406	PL9	C15-C14-C13	-2.58	118.59	123.58
25	k	102	BCR	C3-C4-C5	-2.58	109.59	113.87
23	b	605	CLA	C1D-CHD-C4C	-2.58	118.70	125.40
23	b	610	CLA	O2D-CGD-O1D	-2.57	118.36	123.77
23	C	503	CLA	O2D-CGD-O1D	-2.57	118.36	123.77
35	B	624	HTG	O3-C3-C4	-2.57	104.57	110.36
24	A	407	PHO	C7-C6-C5	-2.57	105.59	113.16
25	Y	101	BCR	C39-C30-C25	-2.56	106.41	110.33
24	D	402	PHO	CHC-C1C-C2C	-2.56	119.57	125.52
23	C	506	CLA	C4B-CHC-C1C	-2.56	124.25	129.34
23	B	614	CLA	CBC-CAC-C3C	-2.56	104.60	112.38
23	A	405	CLA	C7-C6-C5	-2.56	105.61	113.16
23	C	514	CLA	CBC-CAC-C3C	-2.56	104.61	112.38
23	B	608	CLA	O2D-CGD-O1D	-2.56	118.39	123.77
30	a	418	LMT	C1B-O1B-C4'	-2.55	111.23	118.00
23	B	612	CLA	C3B-CAB-CBB	-2.55	121.27	126.40
25	C	530	BCR	C20-C21-C22	-2.55	123.52	127.22
25	B	619	BCR	C30-C25-C26	-2.54	119.10	122.50
23	B	612	CLA	C1D-CHD-C4C	-2.54	118.78	125.40
23	C	504	CLA	O2D-CGD-O1D	-2.54	118.42	123.77
37	v	203	HEM	CAD-CBD-CGD	-2.54	107.84	112.78
23	A	406	CLA	CAC-C3C-C2C	-2.54	123.14	127.51
23	c	907	CLA	O1D-CGD-CBD	-2.54	120.68	124.64
25	T	101	BCR	C33-C5-C6	-2.54	121.92	124.62
23	c	904	CLA	O2A-CGA-O1A	-2.54	116.85	123.51
24	a	408	PHO	C4D-ND-C1D	-2.54	102.34	106.99
23	b	613	CLA	C5-C3-C2	-2.54	116.25	120.98
23	b	603	CLA	OBD-CAD-C3D	-2.54	123.61	128.09
23	C	504	CLA	C5-C3-C2	-2.54	116.26	120.98
23	b	612	CLA	CBC-CAC-C3C	-2.54	104.68	112.38
23	c	905	CLA	C2A-C1A-CHA	-2.53	119.71	123.80
27	a	414	PL9	C22-C23-C24	-2.53	122.16	127.75
23	C	504	CLA	C1D-CHD-C4C	-2.53	118.82	125.40
30	B	644	LMT	C1'-C2'-C3'	-2.53	104.97	109.98
23	B	606	CLA	C4C-C3C-C2C	-2.53	102.90	106.94
36	C	517	DGD	CDB-CCB-CBB	-2.52	101.43	114.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	912	CLA	C3B-CAB-CBB	-2.52	121.32	126.40
23	B	604	CLA	C2A-C3A-C4A	-2.52	99.25	101.84
27	a	414	PL9	C27-C28-C29	-2.52	122.19	127.75
23	d	404	CLA	C6-C7-C8	-2.52	107.67	115.46
27	A	411	PL9	O2-C1-C2	-2.51	116.11	121.78
23	c	904	CLA	O2D-CGD-O1D	-2.51	118.48	123.77
26	A	415	SQD	O5-C1-C2	-2.51	105.06	110.28
24	A	407	PHO	C3B-C2B-C1B	-2.51	100.79	106.36
24	a	409	PHO	CHD-C1D-ND	-2.51	120.12	124.67
23	b	609	CLA	C5-C3-C2	-2.51	116.31	120.98
30	a	418	LMT	O2'-C2'-C3'	-2.50	104.71	110.36
23	B	612	CLA	CBC-CAC-C3C	-2.50	104.78	112.38
23	B	616	CLA	C1D-CHD-C4C	-2.50	118.89	125.40
25	D	405	BCR	C10-C11-C12	-2.50	115.39	123.11
23	d	401	CLA	OBD-CAD-C3D	-2.50	123.68	128.09
36	c	917	DGD	CDB-CCB-CBB	-2.50	101.58	114.54
25	b	620	BCR	C38-C26-C25	-2.49	121.97	124.62
23	D	403	CLA	CAA-CBA-CGA	-2.49	106.07	113.28
25	b	618	BCR	C23-C22-C21	-2.49	114.94	118.95
36	C	517	DGD	O5D-C1E-C2E	-2.49	104.93	108.00
23	A	408	CLA	CBA-CAA-C2A	-2.49	107.54	113.96
25	C	530	BCR	C39-C30-C25	-2.49	106.53	110.33
23	C	509	CLA	O2A-CGA-O1A	-2.49	116.99	123.51
23	b	603	CLA	C2A-C1A-CHA	-2.49	119.79	123.80
25	c	915	BCR	C11-C10-C9	-2.48	123.61	127.22
23	C	513	CLA	C4C-C3C-C2C	-2.48	102.97	106.94
25	B	619	BCR	C11-C10-C9	-2.48	123.61	127.22
27	d	406	PL9	C36-C34-C33	-2.48	116.36	120.98
23	b	610	CLA	CBC-CAC-C3C	-2.48	104.84	112.38
34	c	920	LMG	O5-C6-C5	-2.48	103.02	111.30
23	c	904	CLA	CBC-CAC-C3C	-2.47	104.86	112.38
25	c	915	BCR	C33-C5-C6	-2.47	121.99	124.62
34	m	102	LMG	C30-C29-C28	-2.47	103.92	113.57
36	C	517	DGD	C3D-C4D-C5D	-2.47	105.82	110.23
25	T	101	BCR	C21-C20-C19	-2.47	115.48	123.11
30	m	104	LMT	C3'-C4'-C5'	-2.47	105.20	110.85
36	c	919	DGD	O3G-C1D-C2D	-2.47	104.96	108.00
36	H	103	DGD	C2G-O2G-C1B	-2.47	111.81	117.91
26	x	101	SQD	O48-C23-O10	-2.47	117.04	123.51
23	A	408	CLA	O1D-CGD-CBD	-2.47	120.80	124.64
34	m	102	LMG	O7-C10-O9	-2.46	116.97	123.67
23	D	403	CLA	CBA-CAA-C2A	-2.46	107.62	113.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	908	CLA	O2A-CGA-O1A	-2.46	117.06	123.51
23	C	507	CLA	O1D-CGD-CBD	-2.46	120.81	124.64
25	D	405	BCR	C29-C28-C27	-2.46	105.20	111.42
25	c	916	BCR	C21-C20-C19	-2.45	115.53	123.11
24	D	402	PHO	C1C-C2C-C3C	-2.45	103.61	106.43
23	C	512	CLA	O2D-CGD-O1D	-2.45	118.61	123.77
25	j	104	BCR	C15-C14-C13	-2.45	123.66	127.22
25	A	409	BCR	C24-C23-C22	-2.44	122.52	126.21
23	D	404	CLA	C6-C7-C8	-2.43	107.92	115.46
24	A	407	PHO	C1C-NC-C4C	-2.43	101.87	106.50
23	A	405	CLA	C4C-C3C-C2C	-2.43	103.05	106.94
23	b	602	CLA	O1D-CGD-CBD	-2.43	120.85	124.64
28	A	412	LHG	O8-C23-O10	-2.43	117.14	123.51
23	C	510	CLA	O1D-CGD-CBD	-2.43	120.86	124.64
25	k	102	BCR	C11-C10-C9	-2.43	123.69	127.22
23	b	617	CLA	C4C-C3C-C2C	-2.43	103.06	106.94
23	B	605	CLA	C3B-CAB-CBB	-2.42	121.52	126.40
23	B	609	CLA	C1D-CHD-C4C	-2.42	119.10	125.40
25	a	411	BCR	C8-C7-C6	-2.42	120.23	127.24
23	B	603	CLA	C4B-CHC-C1C	-2.42	124.54	129.34
23	c	906	CLA	C11-C10-C8	-2.41	107.99	115.46
23	c	904	CLA	OBD-CAD-C3D	-2.41	123.82	128.09
23	C	507	CLA	C4C-C3C-C2C	-2.41	103.08	106.94
23	C	507	CLA	OBD-CAD-C3D	-2.41	123.82	128.09
23	C	504	CLA	C2A-C1A-CHA	-2.41	119.91	123.80
34	J	101	LMG	O8-C28-O10	-2.41	117.19	123.51
23	b	607	CLA	O2A-CGA-O1A	-2.41	117.19	123.51
23	b	613	CLA	C4C-C3C-C2C	-2.41	103.09	106.94
27	D	406	PL9	C31-C32-C33	-2.41	105.29	111.61
25	b	620	BCR	C23-C24-C25	-2.41	120.25	127.24
25	t	101	BCR	C7-C8-C9	-2.40	122.58	126.21
25	A	409	BCR	C10-C11-C12	-2.40	115.69	123.11
28	D	409	LHG	C11-C10-C9	-2.40	102.07	114.54
23	B	604	CLA	O2D-CGD-O1D	-2.40	118.72	123.77
30	B	644	LMT	C4'-C3'-C2'	-2.40	106.37	110.79
23	b	617	CLA	C4B-CHC-C1C	-2.40	124.58	129.34
23	c	903	CLA	C2A-C1A-CHA	-2.40	119.94	123.80
24	A	407	PHO	CHC-C1C-C2C	-2.40	119.97	125.52
23	c	903	CLA	C16-C15-C13	-2.39	108.05	115.46
23	B	609	CLA	C2A-C1A-CHA	-2.39	119.94	123.80
25	j	104	BCR	C40-C30-C25	-2.39	106.68	110.33
23	b	605	CLA	C4B-CHC-C1C	-2.39	124.59	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	401	CLA	C1D-CHD-C4C	-2.39	119.19	125.40
23	C	508	CLA	C11-C10-C8	-2.39	108.07	115.46
24	A	407	PHO	CHD-C1D-ND	-2.39	120.34	124.67
25	t	101	BCR	C2-C3-C4	-2.39	105.38	111.42
23	c	910	CLA	CAA-CBA-CGA	-2.39	106.38	113.28
23	b	616	CLA	C11-C10-C8	-2.38	108.08	115.46
34	a	413	LMG	O8-C28-O10	-2.38	117.26	123.51
23	b	607	CLA	C11-C10-C8	-2.38	108.09	115.46
36	c	919	DGD	O2G-C2G-C1G	-2.38	100.00	108.36
34	j	101	LMG	O2-C2-C1	-2.38	104.73	110.01
36	c	917	DGD	C6D-O5D-C1E	-2.38	108.84	113.81
36	C	519	DGD	C3G-C2G-C1G	-2.38	106.54	112.08
23	B	603	CLA	C2A-C3A-C4A	-2.38	99.40	101.84
25	d	405	BCR	C32-C1-C2	-2.37	100.41	108.75
23	c	903	CLA	C16-C17-C18	-2.37	104.19	115.92
26	A	415	SQD	O48-C23-O10	-2.37	117.29	123.51
23	b	610	CLA	C4C-C3C-C2C	-2.37	103.15	106.94
25	k	102	BCR	C24-C23-C22	-2.37	122.63	126.21
28	d	409	LHG	C34-C33-C32	-2.37	102.23	114.54
35	v	204	HTG	C1-C2-C3	-2.37	105.29	110.58
25	T	101	BCR	C3-C4-C5	-2.37	109.94	113.87
23	b	602	CLA	O1A-CGA-CBA	-2.37	114.70	123.76
34	B	622	LMG	C30-C29-C28	-2.37	104.34	113.57
25	C	515	BCR	C24-C23-C22	-2.36	122.64	126.21
28	l	101	LHG	O8-C23-O10	-2.36	117.31	123.51
25	c	916	BCR	C11-C10-C9	-2.36	123.78	127.22
25	B	618	BCR	C24-C23-C22	-2.36	122.64	126.21
26	A	410	SQD	O5-C1-C2	-2.36	105.37	110.28
25	B	620	BCR	C7-C8-C9	-2.36	122.64	126.21
23	d	403	CLA	C5-C3-C2	-2.36	116.59	120.98
23	c	911	CLA	C4C-C3C-C2C	-2.36	103.17	106.94
23	b	612	CLA	O2A-CGA-O1A	-2.36	117.33	123.51
36	c	917	DGD	O2G-C1B-O1B	-2.36	117.26	123.67
37	e	105	HEM	CMD-C2D-C1D	-2.35	124.31	128.31
23	b	617	CLA	CMB-C2B-C1B	-2.35	124.31	128.31
23	b	603	CLA	O2D-CGD-O1D	-2.35	118.83	123.77
24	a	409	PHO	CHB-C1B-C2B	-2.35	120.08	125.52
28	d	410	LHG	O7-C7-O9	-2.34	117.29	123.67
28	d	409	LHG	C32-C31-C30	-2.34	102.37	114.54
25	T	101	BCR	C40-C30-C25	-2.34	106.75	110.33
23	B	607	CLA	O1D-CGD-CBD	-2.34	120.99	124.64
24	a	409	PHO	C16-C15-C13	-2.34	108.21	115.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	414	PL9	C16-C14-C13	-2.34	116.62	120.98
27	D	406	PL9	C11-C9-C8	-2.34	116.62	120.98
23	C	503	CLA	CGD-CBD-CHA	-2.34	102.86	110.88
30	z	101	LMT	C1B-O1B-C4'	-2.34	111.78	118.00
23	c	914	CLA	C4C-C3C-C2C	-2.34	103.21	106.94
23	A	405	CLA	O2A-CGA-O1A	-2.34	117.39	123.51
25	Y	101	BCR	C15-C16-C17	-2.33	118.20	123.23
23	B	615	CLA	OBD-CAD-C3D	-2.33	123.97	128.09
35	B	625	HTG	O5-C1-C2	-2.33	107.04	110.22
37	e	105	HEM	C3B-CAB-CBB	-2.33	121.70	126.40
23	D	401	CLA	CBA-CAA-C2A	-2.33	107.94	113.96
23	c	903	CLA	O2A-CGA-O1A	-2.33	117.40	123.51
28	l	101	LHG	C6-C5-C4	-2.33	106.65	112.08
37	e	105	HEM	C3C-CAC-CBC	-2.33	121.72	126.40
25	C	516	BCR	C24-C23-C22	-2.33	122.69	126.21
23	b	606	CLA	C1D-CHD-C4C	-2.33	119.34	125.40
36	C	519	DGD	O3D-C3D-C2D	-2.33	105.11	110.36
34	B	622	LMG	O7-C10-O9	-2.32	117.35	123.67
37	V	203	HEM	CMA-C3A-C4A	-2.32	124.36	128.31
23	b	602	CLA	CBC-CAC-C3C	-2.32	105.33	112.38
23	C	511	CLA	C4C-C3C-C2C	-2.32	103.23	106.94
36	c	918	DGD	O5D-C1E-C2E	-2.32	105.15	108.00
23	A	406	CLA	C6-C5-C3	-2.32	108.61	112.76
23	A	405	CLA	C5-C3-C2	-2.32	116.67	120.98
34	D	412	LMG	O1-C7-C8	-2.31	105.48	110.99
23	D	401	CLA	OBD-CAD-C3D	-2.31	124.00	128.09
34	C	531	LMG	O8-C28-O10	-2.31	117.45	123.51
24	a	408	PHO	CHD-C4C-C3C	-2.31	119.97	124.57
23	D	403	CLA	C4B-CHC-C1C	-2.31	124.75	129.34
35	b	622	HTG	O2-C2-C3	-2.31	105.15	110.36
23	B	605	CLA	C4C-C3C-C2C	-2.30	103.25	106.94
25	A	409	BCR	C39-C30-C25	-2.30	106.81	110.33
28	D	410	LHG	O7-C7-O9	-2.30	117.41	123.67
25	t	101	BCR	C29-C28-C27	-2.30	105.59	111.42
25	j	104	BCR	C16-C15-C14	-2.30	118.27	123.23
25	d	405	BCR	C34-C9-C10	-2.30	119.54	122.89
23	B	607	CLA	C3B-CAB-CBB	-2.30	121.77	126.40
23	b	608	CLA	O2A-CGA-O1A	-2.30	117.49	123.51
23	B	604	CLA	C4B-CHC-C1C	-2.30	124.78	129.34
23	A	406	CLA	C2A-C1A-CHA	-2.29	120.10	123.80
26	D	408	SQD	O48-C23-O10	-2.29	117.50	123.51
23	c	905	CLA	C4B-CHC-C1C	-2.29	124.79	129.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	101	BCR	C10-C11-C12	-2.29	116.03	123.11
35	B	625	HTG	C3-C4-C5	-2.29	106.14	110.23
23	b	609	CLA	C11-C10-C8	-2.29	108.37	115.46
23	c	904	CLA	C4C-C3C-C2C	-2.28	103.29	106.94
25	B	619	BCR	C33-C5-C6	-2.28	122.19	124.62
23	b	603	CLA	CAA-CBA-CGA	-2.28	106.68	113.28
24	a	408	PHO	C7-C6-C5	-2.28	106.43	113.16
24	a	408	PHO	C3B-C2B-C1B	-2.28	101.30	106.36
23	b	605	CLA	OBD-CAD-C3D	-2.28	124.06	128.09
25	b	618	BCR	C32-C1-C6	-2.28	106.85	110.33
25	c	915	BCR	C28-C27-C26	-2.28	110.09	113.87
23	c	914	CLA	O2D-CGD-O1D	-2.28	118.98	123.77
23	B	609	CLA	C6-C5-C3	-2.27	108.68	112.76
23	c	910	CLA	C12-C11-C10	-2.27	101.96	113.04
23	c	906	CLA	O2A-CGA-O1A	-2.27	117.56	123.51
30	M	101	LMT	C1'-O5'-C5'	-2.27	109.30	113.74
23	B	602	CLA	C1D-CHD-C4C	-2.26	119.51	125.40
25	C	516	BCR	C38-C26-C25	-2.26	122.21	124.62
37	E	105	HEM	CBA-CAA-C2A	-2.26	108.51	112.49
25	B	619	BCR	C39-C30-C25	-2.26	106.88	110.33
27	a	414	PL9	C45-C44-C43	-2.26	119.20	123.58
35	b	623	HTG	C1-O5-C5	-2.26	108.36	112.73
25	d	405	BCR	C16-C17-C18	-2.26	123.94	127.22
38	x	102	RRX	C7-C8-C9	-2.26	122.80	126.21
25	a	411	BCR	C7-C8-C9	-2.26	122.80	126.21
36	C	519	DGD	C3D-C4D-C5D	-2.26	106.20	110.23
23	D	403	CLA	C14-C13-C15	-2.26	102.66	111.10
34	C	520	LMG	O1-C7-C8	-2.26	105.61	110.99
23	B	613	CLA	CBA-CAA-C2A	-2.26	108.14	113.96
34	d	411	LMG	O8-C28-O10	-2.26	117.59	123.51
30	b	621	LMT	C6'-C5'-C4'	-2.25	106.63	113.25
23	c	907	CLA	CBC-CAC-C3C	-2.25	105.54	112.38
23	c	908	CLA	C16-C17-C18	-2.25	104.81	115.92
25	k	102	BCR	C8-C7-C6	-2.24	120.74	127.24
23	B	603	CLA	C3B-CAB-CBB	-2.24	121.89	126.40
23	b	604	CLA	C2A-C1A-CHA	-2.24	120.19	123.80
23	B	610	CLA	CBC-CAC-C3C	-2.23	105.60	112.38
23	B	606	CLA	C4-C3-C2	-2.23	119.26	123.58
23	a	410	CLA	C2A-C1A-CHA	-2.23	120.20	123.80
25	b	619	BCR	C30-C25-C26	-2.23	119.52	122.50
23	B	613	CLA	C14-C13-C15	-2.23	102.78	111.10
23	C	510	CLA	C4-C3-C2	-2.23	119.27	123.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	622	LMG	O8-C28-O10	-2.23	117.68	123.51
36	H	103	DGD	O5E-C6E-C5E	-2.22	103.87	111.30
23	B	613	CLA	C4-C3-C2	-2.22	119.28	123.58
23	B	603	CLA	C16-C15-C13	-2.22	108.58	115.46
25	b	618	BCR	C23-C24-C25	-2.22	120.80	127.24
23	B	606	CLA	O2D-CGD-O1D	-2.22	119.10	123.77
34	C	501	LMG	O6-C1-C2	-2.22	105.67	110.28
25	c	916	BCR	C15-C14-C13	-2.22	124.00	127.22
37	E	105	HEM	CMA-C3A-C4A	-2.21	124.55	128.31
25	c	916	BCR	C27-C26-C25	-2.21	120.30	122.73
23	c	902	CLA	O1D-CGD-CBD	-2.21	121.20	124.64
23	a	410	CLA	CBC-CAC-C3C	-2.21	105.67	112.38
23	a	407	CLA	CBA-CAA-C2A	-2.21	108.27	113.96
34	m	102	LMG	O8-C28-O10	-2.21	117.72	123.51
30	z	101	LMT	C1B-O5B-C5B	-2.20	109.42	113.74
23	b	617	CLA	OBD-CAD-C3D	-2.20	124.19	128.09
23	b	614	CLA	O2D-CGD-O1D	-2.20	119.13	123.77
25	B	619	BCR	C8-C7-C6	-2.20	120.85	127.24
24	A	407	PHO	CHB-C1B-NB	-2.20	120.67	124.67
34	B	622	LMG	O1-C7-C8	-2.20	105.75	110.99
23	c	905	CLA	O2A-CGA-O1A	-2.20	117.74	123.51
26	L	102	SQD	O48-C23-O10	-2.20	117.75	123.51
23	D	401	CLA	O2D-CGD-O1D	-2.20	119.14	123.77
23	B	615	CLA	C1C-C2C-C3C	-2.20	104.50	106.93
23	c	904	CLA	CGD-CBD-CHA	-2.20	103.35	110.88
23	c	911	CLA	C4B-CHC-C1C	-2.19	124.98	129.34
34	j	101	LMG	C31-C30-C29	-2.19	105.18	113.30
23	b	605	CLA	CHC-C1C-C2C	-2.19	120.23	126.31
25	C	516	BCR	C15-C14-C13	-2.19	124.03	127.22
36	h	102	DGD	CDA-CCA-CBA	-2.19	103.16	114.54
25	A	409	BCR	C8-C7-C6	-2.19	120.88	127.24
25	c	916	BCR	C35-C13-C14	-2.19	119.70	122.89
25	B	620	BCR	C10-C11-C12	-2.19	116.35	123.11
23	C	506	CLA	O2D-CGD-O1D	-2.19	119.16	123.77
25	t	101	BCR	C7-C6-C5	-2.18	116.29	121.36
36	c	918	DGD	O4E-C4E-C3E	-2.18	105.43	110.36
28	a	415	LHG	O8-C23-O10	-2.18	117.78	123.51
25	d	405	BCR	C7-C8-C9	-2.18	122.91	126.21
25	C	515	BCR	C16-C17-C18	-2.18	124.05	127.22
23	c	909	CLA	C4C-C3C-C2C	-2.18	103.45	106.94
23	c	902	CLA	O2A-CGA-O1A	-2.18	117.80	123.51
23	d	404	CLA	CBC-CAC-C3C	-2.18	105.77	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	E	101	LHG	O8-C23-O10	-2.18	117.80	123.51
38	x	102	RRX	C16-C15-C14	-2.18	118.54	123.23
34	C	520	LMG	C9-C8-C7	-2.18	107.01	112.08
23	b	606	CLA	C4C-C3C-C2C	-2.18	103.46	106.94
23	b	614	CLA	O2A-CGA-O1A	-2.17	117.81	123.51
28	d	409	LHG	C13-C12-C11	-2.17	103.26	114.54
23	B	616	CLA	C4C-C3C-C2C	-2.17	103.47	106.94
25	B	618	BCR	C21-C20-C19	-2.17	116.41	123.11
23	c	914	CLA	C1D-CHD-C4C	-2.17	119.76	125.40
23	B	603	CLA	C1D-CHD-C4C	-2.17	119.76	125.40
28	E	101	LHG	O7-C7-O9	-2.17	117.77	123.67
27	A	411	PL9	C16-C14-C13	-2.17	116.94	120.98
23	d	404	CLA	O2D-CGD-O1D	-2.17	119.21	123.77
23	C	512	CLA	CBC-CAC-C3C	-2.16	105.81	112.38
23	C	510	CLA	O2D-CGD-O1D	-2.16	119.21	123.77
23	b	605	CLA	O2A-CGA-O1A	-2.16	117.84	123.51
23	B	616	CLA	CBC-CAC-C3C	-2.16	105.82	112.38
23	b	608	CLA	CBA-CAA-C2A	-2.16	108.39	113.96
25	B	620	BCR	C8-C7-C6	-2.16	120.98	127.24
23	C	502	CLA	C4C-C3C-C2C	-2.16	103.49	106.94
24	a	408	PHO	CHB-C1B-NB	-2.16	120.76	124.67
23	C	511	CLA	O2D-CGD-O1D	-2.16	119.23	123.77
26	a	417	SQD	O8-S-O9	-2.15	106.50	111.26
26	a	412	SQD	O47-C7-O49	-2.15	117.82	123.67
23	B	609	CLA	C4B-CHC-C1C	-2.15	125.07	129.34
24	a	409	PHO	CHD-C4C-C3C	-2.15	120.29	124.57
23	a	410	CLA	C2A-C3A-C4A	-2.15	99.63	101.84
36	h	102	DGD	O3G-C3G-C2G	-2.15	105.88	110.99
25	T	101	BCR	C28-C27-C26	-2.14	110.31	113.87
28	D	409	LHG	O7-C7-O9	-2.14	117.84	123.67
23	b	609	CLA	C4C-C3C-C2C	-2.14	103.51	106.94
25	T	101	BCR	C7-C6-C5	-2.14	116.39	121.36
36	C	517	DGD	O1G-C1G-C2G	-2.14	102.92	108.70
23	c	907	CLA	C4B-CHC-C1C	-2.14	125.09	129.34
30	b	621	LMT	C1-O1'-C1'	-2.14	110.26	114.00
34	C	531	LMG	C9-C8-C7	-2.14	107.10	112.08
23	b	605	CLA	CGD-CBD-CAD	-2.14	103.46	110.70
28	d	402	LHG	O8-C23-O10	-2.14	117.90	123.51
24	a	409	PHO	C11-C12-C13	-2.14	108.85	115.46
23	B	607	CLA	C4C-C3C-C2C	-2.14	103.52	106.94
35	v	204	HTG	O4-C4-C3	-2.14	105.54	110.36
23	c	908	CLA	C11-C12-C13	-2.13	108.86	115.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	L	102	SQD	O47-C7-O49	-2.13	117.87	123.67
23	d	401	CLA	C6-C7-C8	-2.13	108.86	115.46
34	C	520	LMG	O7-C10-O9	-2.13	117.87	123.67
24	D	402	PHO	C4-C3-C2	-2.13	119.45	123.58
26	A	410	SQD	O3-C3-C2	-2.13	105.56	110.36
25	b	618	BCR	C40-C30-C25	-2.13	107.08	110.33
37	e	105	HEM	CMA-C3A-C4A	-2.13	124.70	128.31
25	Y	101	BCR	C8-C9-C10	-2.13	115.53	118.95
23	A	405	CLA	C1C-C2C-C3C	-2.12	104.58	106.93
27	D	406	PL9	C22-C23-C24	-2.12	123.07	127.75
23	C	512	CLA	C1D-CHD-C4C	-2.12	119.88	125.40
25	A	409	BCR	C20-C19-C18	-2.12	120.12	126.34
23	b	612	CLA	C7-C6-C5	-2.12	106.91	113.16
38	x	102	RRX	O2-C28-C27	-2.12	104.90	109.69
36	c	918	DGD	C2G-O2G-C1B	-2.11	112.68	117.91
23	b	617	CLA	CBC-CAC-C3C	-2.11	105.96	112.38
23	A	406	CLA	CBC-CAC-C3C	-2.11	105.97	112.38
23	C	512	CLA	O2A-CGA-O1A	-2.11	117.98	123.51
23	C	503	CLA	CHC-C1C-C2C	-2.11	120.46	126.31
23	B	606	CLA	C1D-CHD-C4C	-2.11	119.91	125.40
23	C	502	CLA	CBC-CAC-C3C	-2.11	105.98	112.38
23	c	913	CLA	C2A-C1A-CHA	-2.11	120.40	123.80
23	b	608	CLA	CGD-CBD-CAD	-2.11	103.57	110.70
36	h	102	DGD	O2G-C1B-O1B	-2.10	117.94	123.67
25	b	619	BCR	C37-C22-C21	-2.10	119.83	122.89
23	c	912	CLA	O2A-CGA-O1A	-2.10	118.00	123.51
28	d	409	LHG	O2-C2-C3	-2.10	101.45	109.32
26	a	417	SQD	O6-C44-C45	-2.10	105.98	110.99
30	I	101	LMT	C2'-C3'-C4'	-2.10	104.99	109.63
23	A	408	CLA	C4C-C3C-C2C	-2.10	103.58	106.94
34	J	101	LMG	C9-C8-C7	-2.10	107.19	112.08
36	c	919	DGD	O1G-C1A-O1A	-2.10	118.00	123.51
25	t	101	BCR	C21-C20-C19	-2.10	116.62	123.11
23	B	605	CLA	CGD-CBD-CAD	-2.10	103.59	110.70
23	c	914	CLA	O2A-CGA-O1A	-2.10	118.01	123.51
23	b	615	CLA	OBD-CAD-C3D	-2.10	124.39	128.09
23	B	607	CLA	C2A-C1A-CHA	-2.10	120.42	123.80
25	b	618	BCR	C29-C28-C27	-2.10	106.12	111.42
25	C	530	BCR	C16-C17-C18	-2.09	124.18	127.22
23	A	406	CLA	CHC-C1C-C2C	-2.09	120.51	126.31
34	j	101	LMG	O1-C7-C8	-2.09	106.01	110.99
30	T	103	LMT	O6'-C6'-C5'	-2.09	104.32	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	618	BCR	C20-C21-C22	-2.09	124.19	127.22
23	b	609	CLA	CHC-C1C-C2C	-2.09	120.52	126.31
28	D	411	LHG	O8-C23-O10	-2.09	118.04	123.51
23	c	907	CLA	O2D-CGD-O1D	-2.09	119.38	123.77
23	C	509	CLA	OBD-CAD-CBD	-2.08	122.79	125.94
25	b	618	BCR	C8-C7-C6	-2.08	121.19	127.24
23	c	905	CLA	C5-C3-C2	-2.08	117.10	120.98
27	D	406	PL9	C16-C17-C18	-2.08	106.14	111.61
25	A	409	BCR	C33-C5-C6	-2.08	122.41	124.62
23	c	911	CLA	C4-C3-C2	-2.08	119.56	123.58
23	C	508	CLA	C4B-CHC-C1C	-2.08	125.21	129.34
23	B	612	CLA	O2A-CGA-O1A	-2.08	118.06	123.51
23	c	909	CLA	C4B-CHC-C1C	-2.08	125.21	129.34
25	t	101	BCR	C8-C9-C10	-2.08	115.61	118.95
25	Y	101	BCR	C2-C1-C6	-2.08	107.38	110.48
25	B	619	BCR	C28-C27-C26	-2.08	110.43	113.87
25	k	102	BCR	C34-C9-C10	-2.08	119.87	122.89
23	c	905	CLA	O2D-CGD-O1D	-2.08	119.40	123.77
23	B	614	CLA	C7-C6-C5	-2.07	107.04	113.16
36	c	919	DGD	CEA-CDA-CCA	-2.07	103.77	114.54
23	c	907	CLA	C1D-CHD-C4C	-2.07	120.00	125.40
35	O	302	HTG	O2-C2-C3	-2.07	105.69	110.36
38	H	102	RRX	C16-C15-C14	-2.07	118.76	123.23
25	t	101	BCR	C12-C13-C14	-2.07	115.62	118.95
28	d	409	LHG	O8-C6-C5	-2.07	103.12	108.70
23	d	404	CLA	C2A-C3A-C4A	-2.07	99.71	101.84
36	C	517	DGD	O2G-C1B-O1B	-2.07	118.04	123.67
26	a	412	SQD	C44-O6-C1	-2.07	109.50	113.81
23	c	906	CLA	C2A-C1A-CHA	-2.07	120.47	123.80
25	B	619	BCR	C29-C28-C27	-2.06	106.19	111.42
34	B	622	LMG	C18-C17-C16	-2.06	103.82	114.54
35	B	624	HTG	O2-C2-C3	-2.06	105.71	110.36
36	C	519	DGD	C4E-C3E-C2E	-2.06	106.99	110.79
23	C	514	CLA	O2A-CGA-O1A	-2.06	118.11	123.51
34	D	412	LMG	C8-O7-C10	-2.06	112.81	117.91
25	d	405	BCR	C15-C16-C17	-2.06	118.79	123.23
23	A	405	CLA	C16-C15-C13	-2.06	109.09	115.46
36	d	407	DGD	O2G-C1B-O1B	-2.06	118.07	123.67
23	a	410	CLA	O2A-CGA-O1A	-2.06	118.12	123.51
23	b	610	CLA	C2A-C1A-CHA	-2.06	120.48	123.80
25	j	104	BCR	C8-C9-C10	-2.05	115.64	118.95
23	B	616	CLA	C11-C10-C8	-2.05	109.11	115.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CBC-CAC-C3C	-2.05	106.14	112.38
34	B	622	LMG	C38-C37-C36	-2.05	103.88	114.54
28	D	410	LHG	C6-C5-C4	-2.05	107.30	112.08
23	C	512	CLA	OBD-CAD-C3D	-2.05	124.46	128.09
25	B	620	BCR	C16-C17-C18	-2.05	124.24	127.22
25	B	618	BCR	C16-C15-C14	-2.05	118.82	123.23
24	A	407	PHO	O2A-CGA-O1A	-2.05	118.15	123.51
24	a	409	PHO	C1C-C2C-C3C	-2.04	104.07	106.43
25	b	619	BCR	C15-C16-C17	-2.04	118.82	123.23
24	a	409	PHO	CBA-CAA-C2A	-2.04	108.69	113.96
28	K	101	LHG	O8-C23-O10	-2.04	118.15	123.51
23	b	602	CLA	C3B-CAB-CBB	-2.04	122.29	126.40
25	j	104	BCR	C10-C11-C12	-2.04	116.80	123.11
23	c	907	CLA	CGD-CBD-CAD	-2.04	103.79	110.70
23	B	608	CLA	C4B-CHC-C1C	-2.04	125.29	129.34
36	c	919	DGD	C3E-C4E-C5E	-2.04	106.59	110.23
23	d	401	CLA	CHC-C1C-C2C	-2.04	120.67	126.31
23	D	403	CLA	OBD-CAD-C3D	-2.04	124.49	128.09
23	A	408	CLA	C3B-CAB-CBB	-2.04	122.30	126.40
25	j	104	BCR	C15-C16-C17	-2.04	118.84	123.23
23	D	401	CLA	C5-C3-C2	-2.04	117.19	120.98
36	H	103	DGD	O4E-C4E-C3E	-2.03	105.77	110.36
25	b	618	BCR	C11-C10-C9	-2.03	124.27	127.22
23	b	616	CLA	C5-C3-C2	-2.03	117.19	120.98
27	A	411	PL9	C32-C33-C34	-2.03	123.27	127.75
23	b	611	CLA	C2A-C1A-CHA	-2.03	120.53	123.80
23	b	611	CLA	OBD-CAD-C3D	-2.03	124.51	128.09
23	D	404	CLA	O2D-CGD-O1D	-2.02	119.51	123.77
25	d	405	BCR	C10-C11-C12	-2.02	116.86	123.11
25	b	619	BCR	C8-C9-C10	-2.02	115.70	118.95
23	B	615	CLA	CHC-C1C-NC	-2.02	120.18	123.92
25	B	618	BCR	C34-C9-C10	-2.02	119.95	122.89
24	A	407	PHO	CBC-CAC-C3C	-2.02	106.25	112.38
34	J	101	LMG	O7-C10-O9	-2.02	118.19	123.67
23	b	608	CLA	C7-C6-C5	-2.02	107.21	113.16
23	B	617	CLA	O1D-CGD-CBD	-2.01	121.50	124.64
37	E	105	HEM	C3C-C4C-NC	-2.01	107.14	110.94
23	c	905	CLA	C4C-C3C-C2C	-2.01	103.73	106.94
23	B	605	CLA	CAA-C2A-C3A	-2.01	107.33	112.79
23	C	513	CLA	C2A-C1A-CHA	-2.01	120.56	123.80
23	D	401	CLA	CAC-C3C-C2C	-2.01	124.06	127.51
23	b	614	CLA	C7-C6-C5	-2.01	107.23	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	m	102	LMG	C1-O6-C5	-2.01	109.81	113.74
23	C	513	CLA	C1D-CHD-C4C	-2.00	120.18	125.40
23	C	503	CLA	O1D-CGD-CBD	-2.00	121.52	124.64
23	C	503	CLA	O2A-CGA-CBA	2.00	118.01	111.85
26	a	417	SQD	O48-C23-C24	2.00	118.01	111.85
23	a	406	CLA	C4A-NA-C1A	2.00	108.92	106.38
23	C	507	CLA	O2A-CGA-CBA	2.00	118.02	111.85
23	a	406	CLA	CMC-C2C-C3C	2.01	131.68	125.91
23	B	614	CLA	C3C-C4C-NC	2.01	112.24	110.21
23	B	615	CLA	CMB-C2B-C1B	2.01	131.73	128.31
26	A	410	SQD	O8-S-C6	2.01	109.16	104.99
23	b	603	CLA	C3B-C4B-NB	2.01	111.81	109.21
24	D	402	PHO	C4-C3-C5	2.01	118.43	115.37
23	B	606	CLA	CMB-C2B-C3B	2.01	129.02	125.09
24	A	407	PHO	C4D-C3D-CAD	2.01	109.33	105.61
23	b	614	CLA	CMD-C2D-C3D	2.01	129.02	125.09
25	T	101	BCR	C1-C6-C7	2.01	121.70	115.96
23	c	910	CLA	C3C-C4C-NC	2.02	112.25	110.21
27	A	411	PL9	C35-C34-C36	2.02	118.44	115.37
23	C	508	CLA	O2A-CGA-CBA	2.02	118.06	111.85
23	b	602	CLA	OBD-CAD-CBD	2.02	128.99	125.94
25	B	618	BCR	C24-C25-C26	2.02	126.06	121.36
23	c	910	CLA	CMB-C2B-C1B	2.02	131.76	128.31
25	B	618	BCR	C37-C22-C23	2.03	121.39	118.08
27	a	414	PL9	C30-C29-C31	2.03	118.46	115.37
25	b	618	BCR	C24-C25-C26	2.03	126.06	121.36
23	B	616	CLA	O2D-CGD-CBD	2.03	114.14	111.22
25	c	915	BCR	C37-C22-C23	2.03	121.40	118.08
36	C	518	DGD	O5D-C6D-C5D	2.04	112.77	109.14
23	b	609	CLA	O2A-CGA-CBA	2.04	118.12	111.85
34	j	101	LMG	C6-C5-C4	2.04	118.10	112.99
23	b	610	CLA	CMC-C2C-C1C	2.04	128.02	125.00
30	B	644	LMT	O1'-C1'-C2'	2.04	110.51	108.00
25	C	530	BCR	C38-C26-C27	2.04	117.42	113.47
37	e	105	HEM	CMC-C2C-C3C	2.05	129.09	125.09
35	B	630	HTG	O5-C5-C6	2.05	111.68	106.38
24	a	409	PHO	C3D-C4D-ND	2.05	115.80	109.76
36	h	102	DGD	O1G-C1A-C2A	2.05	118.15	111.85
24	a	408	PHO	C4D-C3D-CAD	2.05	109.40	105.61
25	k	102	BCR	C34-C9-C8	2.05	121.43	118.08
23	d	404	CLA	CMC-C2C-C3C	2.05	131.80	125.91
23	B	612	CLA	C3B-C4B-NB	2.05	111.86	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	d	405	BCR	C34-C9-C8	2.05	121.44	118.08
23	B	611	CLA	CMC-C2C-C3C	2.06	131.82	125.91
25	C	515	BCR	C34-C9-C8	2.06	121.44	118.08
30	B	623	LMT	O5B-C5B-C4B	2.06	113.59	109.67
23	B	603	CLA	CMC-C2C-C1C	2.06	128.05	125.00
25	D	405	BCR	C38-C26-C27	2.06	117.46	113.47
23	B	604	CLA	O2A-CGA-CBA	2.06	118.20	111.85
30	A	416	LMT	O3B-C3B-C4B	2.07	115.02	110.36
23	C	504	CLA	CAC-C3C-C4C	2.07	127.87	124.82
36	c	918	DGD	O6E-C5E-C6E	2.07	111.75	106.38
23	C	508	CLA	CED-O2D-CGD	2.08	120.90	115.97
34	D	412	LMG	C3-C4-C5	2.08	113.93	110.23
30	A	416	LMT	C1B-O5B-C5B	2.08	117.82	113.74
23	c	906	CLA	CMD-C2D-C3D	2.08	129.16	125.09
36	D	407	DGD	C1G-O1G-C1A	2.08	123.20	117.00
23	b	604	CLA	CBA-CAA-C2A	2.08	119.32	113.96
23	C	511	CLA	CBA-CAA-C2A	2.08	119.32	113.96
23	B	603	CLA	C3B-C4B-NB	2.08	111.90	109.21
23	A	408	CLA	CMC-C2C-C3C	2.08	131.90	125.91
34	d	411	LMG	O1-C1-C2	2.08	110.56	108.00
25	T	101	BCR	C34-C9-C8	2.08	121.49	118.08
35	v	204	HTG	O5-C5-C4	2.09	113.65	109.67
25	d	405	BCR	C30-C25-C24	2.09	121.92	115.96
37	e	105	HEM	CMD-C2D-C3D	2.09	129.61	125.24
23	a	410	CLA	C3B-C4B-NB	2.09	111.92	109.21
23	B	604	CLA	CED-O2D-CGD	2.09	120.94	115.97
36	h	102	DGD	C6E-C5E-C4E	2.10	118.24	112.99
23	b	614	CLA	C3B-C4B-NB	2.10	111.92	109.21
23	B	613	CLA	CMD-C2D-C3D	2.10	129.19	125.09
23	B	617	CLA	O2A-CGA-CBA	2.10	118.31	111.85
23	B	614	CLA	C6-C5-C3	2.10	116.54	112.76
23	B	607	CLA	O2A-CGA-CBA	2.10	118.32	111.85
23	C	505	CLA	CMD-C2D-C3D	2.10	129.20	125.09
23	B	608	CLA	C4-C3-C5	2.10	118.58	115.37
23	C	504	CLA	CMD-C2D-C3D	2.10	129.21	125.09
30	e	103	LMT	O5'-C5'-C4'	2.11	114.28	109.78
23	c	907	CLA	O2A-CGA-CBA	2.11	118.35	111.85
23	B	605	CLA	O2A-CGA-CBA	2.12	118.36	111.85
23	B	608	CLA	C3C-C4C-NC	2.12	112.36	110.21
23	d	404	CLA	CAC-C3C-C4C	2.13	127.96	124.82
25	B	620	BCR	C38-C26-C27	2.13	117.59	113.47
23	B	610	CLA	C4-C3-C5	2.13	118.62	115.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	402	LHG	C6-O8-C23	2.14	123.36	117.00
34	J	101	LMG	O7-C10-C11	2.14	116.03	111.53
23	B	613	CLA	CED-O2D-CGD	2.14	121.04	115.97
23	D	404	CLA	CMC-C2C-C1C	2.14	128.16	125.00
25	j	104	BCR	C34-C9-C8	2.14	121.58	118.08
23	c	906	CLA	O2A-CGA-CBA	2.14	118.43	111.85
30	F	101	LMT	O4'-C4B-C5B	2.14	114.86	109.23
23	b	607	CLA	O2A-CGA-CBA	2.14	118.44	111.85
23	B	617	CLA	C4-C3-C5	2.14	118.63	115.37
37	v	203	HEM	CMB-C2B-C3B	2.14	129.28	125.09
23	a	407	CLA	CMC-C2C-C3C	2.14	132.08	125.91
23	b	610	CLA	CED-O2D-CGD	2.15	121.07	115.97
23	d	401	CLA	C4A-NA-C1A	2.15	109.10	106.38
28	D	410	LHG	O4-P-O5	2.15	123.76	112.56
30	B	644	LMT	C1'-O5'-C5'	2.16	117.98	113.74
23	b	615	CLA	C4-C3-C5	2.16	118.66	115.37
23	b	615	CLA	CED-O2D-CGD	2.16	121.10	115.97
36	C	519	DGD	O2G-C1B-C2B	2.16	116.08	111.53
23	D	403	CLA	CMB-C2B-C3B	2.16	129.32	125.09
30	b	621	LMT	C3'-C4'-C5'	2.17	115.80	110.85
23	b	610	CLA	CMD-C2D-C3D	2.17	129.32	125.09
30	F	101	LMT	O1'-C1'-C2'	2.17	110.67	108.00
24	a	409	PHO	C4D-C3D-CAD	2.17	109.63	105.61
23	b	605	CLA	O2A-CGA-CBA	2.17	118.53	111.85
23	b	612	CLA	CMB-C2B-C3B	2.17	129.34	125.09
23	D	404	CLA	C3C-C4C-NC	2.18	112.42	110.21
30	T	103	LMT	O5'-C1'-C2'	2.18	114.80	110.28
23	C	512	CLA	CMB-C2B-C1B	2.18	132.02	128.31
25	Y	101	BCR	C37-C22-C23	2.19	121.65	118.08
35	b	623	HTG	O5-C5-C6	2.19	112.05	106.38
31	U	202	DMS	O-S-C1	2.19	118.80	106.64
23	D	404	CLA	O2A-CGA-CBA	2.19	118.58	111.85
23	B	606	CLA	C3B-C4B-NB	2.19	112.04	109.21
27	A	411	PL9	C20-C19-C21	2.19	118.71	115.37
23	c	904	CLA	CAC-C3C-C4C	2.19	128.06	124.82
23	b	604	CLA	O2A-CGA-CBA	2.19	118.60	111.85
23	C	510	CLA	CMC-C2C-C3C	2.20	132.22	125.91
23	b	608	CLA	O2A-CGA-CBA	2.20	118.61	111.85
23	C	503	CLA	C4-C3-C5	2.20	118.72	115.37
23	b	603	CLA	OBD-CAD-CBD	2.20	129.25	125.94
36	c	917	DGD	C1E-O6E-C5E	2.20	118.06	113.74
25	j	104	BCR	C29-C30-C25	2.20	113.75	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	906	CLA	C4A-NA-C1A	2.20	109.17	106.38
23	B	602	CLA	C3B-C4B-NB	2.20	112.05	109.21
30	B	643	LMT	O1'-C1'-C2'	2.20	110.71	108.00
23	c	913	CLA	CMD-C2D-C3D	2.20	129.40	125.09
23	B	612	CLA	C4A-NA-C1A	2.21	109.18	106.38
34	J	101	LMG	O6-C1-C2	2.21	114.86	110.28
23	a	406	CLA	C3B-C4B-NB	2.21	112.06	109.21
23	c	913	CLA	C3C-C4C-NC	2.21	112.45	110.21
25	b	618	BCR	C35-C13-C12	2.21	121.69	118.08
31	b	639	DMS	C2-S-C1	2.21	110.18	98.50
23	C	514	CLA	CED-O2D-CGD	2.21	121.22	115.97
26	L	102	SQD	O6-C44-C45	2.21	116.25	110.99
23	d	403	CLA	CED-O2D-CGD	2.21	121.22	115.97
25	d	405	BCR	C4-C5-C6	2.21	125.17	122.73
26	a	412	SQD	O48-C23-C24	2.22	118.67	111.85
30	a	422	LMT	O2'-C2'-C1'	2.22	114.92	110.01
23	b	617	CLA	C4A-NA-C1A	2.22	109.19	106.38
23	b	612	CLA	CAC-C3C-C4C	2.22	128.10	124.82
23	A	408	CLA	C3C-C4C-NC	2.22	112.47	110.21
34	d	411	LMG	C9-O8-C28	2.23	123.63	117.00
23	b	615	CLA	O2A-CGA-CBA	2.23	118.70	111.85
34	j	101	LMG	C1-O6-C5	2.23	118.11	113.74
26	a	412	SQD	O8-S-C6	2.23	109.62	104.99
30	Z	101	LMT	O5'-C5'-C4'	2.23	114.53	109.78
26	A	415	SQD	C3-C4-C5	2.23	114.20	110.23
38	H	102	RRX	C32-C1-C6	2.24	113.75	110.33
23	c	909	CLA	C3B-C4B-NB	2.24	112.10	109.21
23	C	506	CLA	C6-C5-C3	2.24	116.78	112.76
30	B	623	LMT	C3B-C4B-C5B	2.24	114.22	110.23
30	T	103	LMT	C4'-C3'-C2'	2.24	114.92	110.79
28	A	412	LHG	C6-O8-C23	2.25	123.69	117.00
28	d	410	LHG	O4-P-O5	2.25	124.25	112.56
23	c	907	CLA	CMC-C2C-C1C	2.25	128.33	125.00
23	C	505	CLA	CAC-C3C-C4C	2.25	128.14	124.82
23	b	603	CLA	O2A-CGA-CBA	2.25	118.77	111.85
23	d	401	CLA	CMD-C2D-C3D	2.25	129.49	125.09
23	b	602	CLA	C3B-C4B-NB	2.25	112.12	109.21
23	C	511	CLA	CMD-C2D-C3D	2.25	129.50	125.09
23	B	610	CLA	CMB-C2B-C3B	2.25	129.50	125.09
34	D	412	LMG	O8-C28-C29	2.25	118.79	111.85
23	c	909	CLA	O2D-CGD-CBD	2.26	114.47	111.22
23	A	408	CLA	C4A-NA-C1A	2.26	109.24	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	h	102	DGD	C6D-C5D-C4D	2.26	117.15	112.00
25	Y	101	BCR	C38-C26-C27	2.26	117.84	113.47
23	a	410	CLA	CMC-C2C-C1C	2.26	128.35	125.00
23	C	504	CLA	O2A-CGA-CBA	2.26	118.82	111.85
23	B	605	CLA	C3B-C4B-NB	2.27	112.15	109.21
30	F	101	LMT	C1'-C2'-C3'	2.27	114.49	109.98
23	B	608	CLA	CMC-C2C-C3C	2.28	132.46	125.91
23	C	512	CLA	C3C-C4C-NC	2.28	112.52	110.21
23	B	613	CLA	C3B-C4B-NB	2.28	112.16	109.21
23	B	605	CLA	C4-C3-C5	2.29	118.85	115.37
28	D	411	LHG	O7-C7-C8	2.29	116.35	111.53
23	A	406	CLA	CMC-C2C-C1C	2.29	128.39	125.00
23	c	904	CLA	CMC-C2C-C1C	2.29	128.40	125.00
35	V	204	HTG	O2-C2-C1	2.29	115.04	110.50
23	b	604	CLA	C3B-C4B-NB	2.30	112.18	109.21
23	B	615	CLA	O2A-CGA-CBA	2.30	118.92	111.85
23	B	602	CLA	C3C-C4C-NC	2.30	112.54	110.21
34	D	412	LMG	C9-O8-C28	2.31	123.87	117.00
23	B	616	CLA	CMB-C2B-C3B	2.31	129.60	125.09
23	d	404	CLA	CMB-C2B-C1B	2.31	132.25	128.31
25	t	101	BCR	C1-C6-C7	2.32	122.58	115.96
23	C	508	CLA	CMB-C2B-C3B	2.32	129.63	125.09
23	c	906	CLA	CAC-C3C-C4C	2.32	128.25	124.82
35	b	623	HTG	C4-C3-C2	2.32	115.06	110.79
23	A	406	CLA	C4-C3-C5	2.32	118.91	115.37
25	D	405	BCR	C2-C3-C4	2.33	117.32	111.42
23	c	913	CLA	O2A-CGA-CBA	2.33	119.03	111.85
36	c	918	DGD	O1G-C1A-C2A	2.34	119.04	111.85
35	c	922	HTG	C1-C2-C3	2.35	115.83	110.58
23	D	404	CLA	CMB-C2B-C3B	2.35	129.69	125.09
23	c	911	CLA	O2A-CGA-CBA	2.35	119.09	111.85
23	B	613	CLA	O2A-CGA-CBA	2.35	119.09	111.85
25	B	619	BCR	C2-C1-C6	2.35	113.98	110.48
30	a	418	LMT	O2'-C2'-C1'	2.36	115.23	110.01
23	B	609	CLA	CMB-C2B-C3B	2.36	129.70	125.09
34	C	531	LMG	O6-C5-C6	2.36	112.50	106.38
23	b	615	CLA	CMD-C2D-C3D	2.37	129.72	125.09
30	B	623	LMT	C1B-O5B-C5B	2.37	118.39	113.74
23	a	410	CLA	CMB-C2B-C3B	2.37	129.72	125.09
23	c	914	CLA	CED-O2D-CGD	2.37	121.60	115.97
34	B	622	LMG	O8-C28-C29	2.37	119.15	111.85
35	B	631	HTG	C1-O5-C5	2.37	117.31	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C3B-C4B-NB	2.37	112.28	109.21
35	b	622	HTG	O2-C2-C1	2.37	115.20	110.50
26	D	408	SQD	O5-C1-O6	2.38	115.69	109.99
36	d	407	DGD	O6D-C5D-C4D	2.38	113.70	109.58
26	A	410	SQD	C3-C4-C5	2.38	114.48	110.23
26	x	101	SQD	C3-C4-C5	2.38	114.48	110.23
23	B	614	CLA	C4A-NA-C1A	2.39	109.41	106.38
30	z	101	LMT	O1'-C1'-C2'	2.39	111.06	108.24
23	C	513	CLA	CMB-C2B-C3B	2.39	129.77	125.09
25	t	101	BCR	C34-C9-C8	2.39	121.99	118.08
24	D	402	PHO	C3D-C4D-ND	2.40	116.83	109.76
23	b	610	CLA	C4-C3-C5	2.40	119.02	115.37
23	d	401	CLA	CMB-C2B-C3B	2.40	129.78	125.09
23	A	405	CLA	O2A-CGA-CBA	2.40	119.23	111.85
25	B	620	BCR	C37-C22-C21	2.40	126.37	122.89
27	d	406	PL9	C35-C34-C36	2.40	119.03	115.37
23	C	506	CLA	O2A-CGA-CBA	2.41	119.25	111.85
27	a	414	PL9	C40-C39-C41	2.41	119.04	115.37
28	d	409	LHG	O8-C23-C24	2.41	119.26	111.85
37	E	105	HEM	CMC-C2C-C3C	2.41	129.80	125.09
23	c	905	CLA	CMC-C2C-C1C	2.41	128.57	125.00
23	c	912	CLA	CMD-C2D-C3D	2.41	129.80	125.09
23	b	611	CLA	C4-C3-C5	2.41	119.05	115.37
23	B	609	CLA	CMD-C2D-C3D	2.42	129.82	125.09
23	A	408	CLA	CMD-C2D-C3D	2.42	129.82	125.09
23	a	410	CLA	O2A-CGA-CBA	2.42	119.31	111.85
25	D	405	BCR	C2-C1-C6	2.43	114.09	110.48
23	c	903	CLA	C4-C3-C5	2.43	119.07	115.37
23	B	613	CLA	CMB-C2B-C3B	2.43	129.85	125.09
23	B	612	CLA	C4-C3-C5	2.44	119.08	115.37
23	b	611	CLA	CAC-C3C-C4C	2.44	128.42	124.82
23	b	606	CLA	CMB-C2B-C3B	2.44	129.86	125.09
23	c	911	CLA	C3B-C4B-NB	2.44	112.36	109.21
24	A	407	PHO	CED-O2D-CGD	2.44	121.77	115.97
23	C	510	CLA	CMD-C2D-C3D	2.44	129.86	125.09
25	Y	101	BCR	C29-C30-C25	2.44	114.11	110.48
25	d	405	BCR	C36-C18-C19	2.44	122.08	118.08
23	B	613	CLA	C3C-C4C-NC	2.44	112.69	110.21
24	A	407	PHO	C3D-C4D-ND	2.44	116.97	109.76
25	T	101	BCR	C37-C22-C21	2.45	126.44	122.89
23	a	410	CLA	CED-O2D-CGD	2.45	121.79	115.97
23	c	903	CLA	CAC-C3C-C4C	2.45	128.44	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	416	LMT	O5B-C5B-C6B	2.45	112.73	106.38
23	c	908	CLA	CMD-C2D-C3D	2.46	129.90	125.09
34	c	930	LMG	C3-C4-C5	2.46	114.61	110.23
23	c	903	CLA	O2A-CGA-CBA	2.46	119.43	111.85
23	c	913	CLA	CAC-C3C-C4C	2.46	128.46	124.82
23	b	609	CLA	C3B-C4B-NB	2.46	112.40	109.21
23	c	908	CLA	C4A-NA-C1A	2.47	109.51	106.38
23	d	404	CLA	C4-C3-C5	2.47	119.13	115.37
23	b	615	CLA	C4A-NA-C1A	2.48	109.53	106.38
34	c	930	LMG	O8-C28-C29	2.48	119.49	111.85
23	a	407	CLA	CMB-C2B-C3B	2.49	129.95	125.09
23	d	403	CLA	O2D-CGD-CBD	2.49	114.81	111.22
23	B	603	CLA	C4A-NA-C1A	2.49	109.53	106.38
30	I	101	LMT	O1'-C1'-C2'	2.49	111.06	108.00
23	B	607	CLA	C4-C3-C5	2.49	119.17	115.37
26	A	410	SQD	O2-C2-C1	2.49	115.54	110.01
30	z	101	LMT	O1B-C1B-C2B	2.50	114.33	108.12
23	B	602	CLA	C4-C3-C5	2.50	119.18	115.37
23	B	615	CLA	C4-C3-C5	2.50	119.18	115.37
23	b	613	CLA	O2A-CGA-CBA	2.50	119.55	111.85
23	A	405	CLA	CMB-C2B-C3B	2.50	129.99	125.09
34	C	501	LMG	O8-C28-C29	2.50	119.56	111.85
23	c	912	CLA	O2A-CGA-CBA	2.51	119.57	111.85
24	a	408	PHO	O2D-CGD-CBD	2.51	114.84	111.22
25	T	101	BCR	C2-C1-C6	2.51	114.21	110.48
35	b	622	HTG	C1'-S1-C1	2.51	103.82	100.60
23	C	511	CLA	C4A-NA-C1A	2.51	109.56	106.38
27	A	411	PL9	C51-C49-C50	2.51	120.71	114.61
26	x	101	SQD	O8-S-C6	2.51	110.21	104.99
36	c	919	DGD	O3D-C3D-C4D	2.52	116.04	110.36
23	b	604	CLA	CMD-C2D-C3D	2.52	130.01	125.09
23	A	405	CLA	OBD-CAD-CBD	2.52	129.74	125.94
23	b	602	CLA	CED-O2D-CGD	2.52	121.96	115.97
23	b	605	CLA	C3B-C4B-NB	2.52	112.47	109.21
23	B	607	CLA	CMC-C2C-C3C	2.53	133.18	125.91
27	A	411	PL9	C15-C14-C16	2.53	119.23	115.37
23	D	403	CLA	C2A-C3A-C4A	2.54	104.44	101.84
30	A	416	LMT	O5'-C5'-C4'	2.54	115.19	109.78
23	C	508	CLA	C3B-C4B-NB	2.54	112.50	109.21
27	D	406	PL9	C35-C34-C36	2.54	119.25	115.37
23	C	508	CLA	OBD-CAD-CBD	2.55	129.78	125.94
23	C	505	CLA	CMC-C2C-C1C	2.56	128.79	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CMB-C2B-C1B	2.56	132.66	128.31
28	d	410	LHG	O7-C7-C8	2.56	116.92	111.53
36	C	518	DGD	O3G-C1D-C2D	2.56	111.15	108.00
38	H	102	RRX	C34-C9-C8	2.56	122.27	118.08
23	c	912	CLA	C3C-C4C-NC	2.56	112.81	110.21
23	C	514	CLA	CMB-C2B-C3B	2.56	130.10	125.09
23	C	511	CLA	CAC-C3C-C4C	2.56	128.60	124.82
23	b	616	CLA	C3B-C4B-NB	2.57	112.53	109.21
23	b	609	CLA	C4-C3-C5	2.57	119.28	115.37
25	j	104	BCR	C35-C13-C12	2.57	122.28	118.08
23	b	615	CLA	CAC-C3C-C4C	2.57	128.62	124.82
23	A	406	CLA	CMB-C2B-C3B	2.57	130.12	125.09
23	C	511	CLA	C4-C3-C5	2.57	119.29	115.37
27	a	414	PL9	C45-C44-C46	2.58	119.30	115.37
26	a	412	SQD	O5-C1-O6	2.58	116.19	109.99
23	c	902	CLA	CAC-C3C-C4C	2.58	128.63	124.82
23	d	403	CLA	O1D-CGD-CBD	2.59	128.66	124.64
23	C	506	CLA	CMD-C2D-C3D	2.59	130.15	125.09
27	D	406	PL9	C53-C6-C1	2.59	120.17	114.66
36	c	919	DGD	O1G-C1A-C2A	2.59	119.82	111.85
28	D	409	LHG	C6-O8-C23	2.59	124.72	117.00
23	C	507	CLA	CAC-C3C-C4C	2.59	128.64	124.82
23	C	506	CLA	C4A-NA-C1A	2.59	109.67	106.38
30	e	103	LMT	C1-O1'-C1'	2.59	118.53	114.00
23	a	406	CLA	CHC-C1C-NC	2.59	128.72	123.92
23	b	614	CLA	O2A-CGA-CBA	2.60	119.87	111.85
23	b	602	CLA	CMD-C2D-C3D	2.61	130.19	125.09
26	A	415	SQD	C46-O48-C23	2.61	124.77	117.00
23	D	401	CLA	CMB-C2B-C3B	2.61	130.20	125.09
35	c	921	HTG	C3-C4-C5	2.62	114.89	110.23
23	b	606	CLA	C3D-CAD-CBD	2.62	111.30	107.60
23	b	613	CLA	CMD-C2D-C3D	2.62	130.22	125.09
26	x	101	SQD	O47-C7-C8	2.63	120.19	110.82
23	B	615	CLA	CMC-C2C-C1C	2.63	128.90	125.00
35	d	413	HTG	C1-O5-C5	2.63	117.82	112.73
23	b	605	CLA	CMB-C2B-C3B	2.64	130.25	125.09
23	b	611	CLA	CMB-C2B-C3B	2.64	130.25	125.09
23	c	902	CLA	C4-C3-C5	2.65	119.40	115.37
23	C	512	CLA	C4-C3-C5	2.65	119.41	115.37
25	c	916	BCR	C29-C30-C25	2.65	114.42	110.48
35	C	522	HTG	O5-C5-C4	2.65	114.73	109.67
23	D	404	CLA	C4A-NA-C1A	2.65	109.75	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	408	CLA	CED-O2D-CGD	2.66	122.28	115.97
23	B	611	CLA	CMD-C2D-C3D	2.66	130.29	125.09
23	b	615	CLA	C3B-C4B-NB	2.66	112.65	109.21
23	d	401	CLA	C3B-C4B-NB	2.66	112.65	109.21
28	K	101	LHG	O8-C23-C24	2.66	120.05	111.85
25	t	101	BCR	C35-C13-C12	2.67	122.44	118.08
23	C	504	CLA	C3C-C4C-NC	2.67	112.92	110.21
23	d	401	CLA	CED-O2D-CGD	2.67	122.31	115.97
34	C	501	LMG	O7-C10-C11	2.67	117.16	111.53
23	a	406	CLA	CMB-C2B-C3B	2.68	130.32	125.09
23	B	613	CLA	C4A-NA-C1A	2.68	109.78	106.38
35	O	302	HTG	C4-C3-C2	2.68	115.72	110.79
26	x	101	SQD	O5-C5-C4	2.68	114.79	109.67
23	b	608	CLA	CMC-C2C-C1C	2.69	128.98	125.00
23	b	609	CLA	CED-O2D-CGD	2.69	122.35	115.97
23	C	507	CLA	CMB-C2B-C3B	2.69	130.35	125.09
23	C	514	CLA	C4-C3-C5	2.70	119.48	115.37
23	C	503	CLA	CAC-C3C-C4C	2.70	128.80	124.82
25	t	101	BCR	C2-C1-C6	2.70	114.49	110.48
23	C	506	CLA	CMB-C2B-C3B	2.70	130.37	125.09
23	B	617	CLA	C3B-C4B-NB	2.70	112.71	109.21
35	c	922	HTG	C4-C3-C2	2.71	115.78	110.79
23	c	904	CLA	C3C-C4C-NC	2.71	112.96	110.21
36	d	407	DGD	O1G-C1A-C2A	2.71	120.20	111.85
34	d	411	LMG	O6-C1-O1	2.72	116.50	109.99
30	a	418	LMT	O5'-C5'-C4'	2.72	115.57	109.78
24	a	409	PHO	CED-O2D-CGD	2.72	122.43	115.97
34	m	102	LMG	O8-C28-C29	2.72	120.22	111.85
28	E	101	LHG	C6-O8-C23	2.72	125.10	117.00
36	C	517	DGD	C1E-O6E-C5E	2.72	119.08	113.74
23	B	607	CLA	CMB-C2B-C1B	2.72	132.95	128.31
23	B	603	CLA	C4-C3-C5	2.73	119.52	115.37
23	C	511	CLA	C3B-C4B-NB	2.73	112.73	109.21
23	d	403	CLA	CAC-C3C-C4C	2.73	128.85	124.82
23	B	617	CLA	CED-O2D-CGD	2.73	122.45	115.97
23	C	509	CLA	C3C-C4C-NC	2.74	112.98	110.21
23	b	608	CLA	C3B-C4B-NB	2.74	112.75	109.21
27	a	414	PL9	C10-C9-C11	2.74	119.55	115.37
37	e	105	HEM	CAD-CBD-CGD	2.75	118.12	112.78
35	O	302	HTG	C1-O5-C5	2.75	118.03	112.73
23	D	404	CLA	CED-O2D-CGD	2.75	122.50	115.97
23	c	906	CLA	CMB-C2B-C3B	2.75	130.47	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	d	403	CLA	O2A-CGA-CBA	2.76	120.33	111.85
23	c	907	CLA	C3C-C4C-NC	2.76	113.00	110.21
23	C	509	CLA	O2D-CGD-CBD	2.76	115.20	111.22
23	B	615	CLA	C4A-NA-C1A	2.77	109.89	106.38
23	B	609	CLA	CAC-C3C-C4C	2.77	128.91	124.82
25	d	405	BCR	C32-C1-C6	2.77	114.57	110.33
36	C	519	DGD	O1G-C1A-C2A	2.77	120.38	111.85
23	D	404	CLA	C4-C3-C5	2.77	119.60	115.37
28	d	402	LHG	O8-C23-C24	2.78	120.41	111.85
34	j	101	LMG	O7-C10-C11	2.78	117.39	111.53
23	c	908	CLA	O2A-CGA-CBA	2.78	120.42	111.85
23	c	907	CLA	C4-C3-C5	2.78	119.61	115.37
23	B	616	CLA	C3C-C4C-NC	2.79	113.03	110.21
23	C	510	CLA	C3B-C4B-NB	2.79	112.81	109.21
23	D	401	CLA	C3B-C4B-NB	2.79	112.81	109.21
23	c	913	CLA	CMC-C2C-C1C	2.79	129.13	125.00
27	A	411	PL9	C3-C4-C5	2.79	122.67	118.64
23	b	617	CLA	CED-O2D-CGD	2.80	122.62	115.97
23	c	908	CLA	C3C-C4C-NC	2.80	113.05	110.21
23	b	616	CLA	C3C-C4C-NC	2.80	113.05	110.21
23	b	614	CLA	C4A-NA-C1A	2.81	109.94	106.38
23	B	606	CLA	CMD-C2D-C3D	2.81	130.59	125.09
23	B	608	CLA	CAC-C3C-C4C	2.81	128.97	124.82
24	a	408	PHO	C4A-NA-C1A	2.83	110.35	108.22
30	m	103	LMT	C1'-O5'-C5'	2.83	119.30	113.74
23	B	611	CLA	C4A-NA-C1A	2.83	109.97	106.38
28	K	101	LHG	O4-P-O5	2.83	119.87	110.63
23	b	602	CLA	C4-C3-C5	2.83	119.69	115.37
23	B	612	CLA	CMD-C2D-C3D	2.84	130.64	125.09
23	B	607	CLA	C4A-NA-C1A	2.84	109.98	106.38
23	B	603	CLA	OBD-CAD-CBD	2.84	130.22	125.94
23	d	403	CLA	CMD-C2D-C3D	2.84	130.64	125.09
23	D	403	CLA	C3B-C4B-NB	2.84	112.88	109.21
25	d	405	BCR	C2-C1-C6	2.84	114.71	110.48
28	A	412	LHG	O8-C23-C24	2.84	120.59	111.85
23	B	607	CLA	C3B-C4B-NB	2.84	112.88	109.21
23	C	505	CLA	C3B-C4B-NB	2.85	112.89	109.21
23	C	507	CLA	C4-C3-C5	2.85	119.71	115.37
23	B	602	CLA	O2A-CGA-CBA	2.85	120.63	111.85
23	b	607	CLA	CMD-C2D-C3D	2.86	130.68	125.09
35	B	624	HTG	O3-C3-C2	2.86	116.81	110.36
25	c	916	BCR	C36-C18-C19	2.86	122.76	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	CAC-C3C-C4C	2.86	129.04	124.82
23	d	401	CLA	O2D-CGD-CBD	2.87	115.35	111.22
23	B	602	CLA	C4A-NA-C1A	2.87	110.02	106.38
23	c	904	CLA	O2A-CGA-CBA	2.87	120.68	111.85
23	c	902	CLA	C3C-C4C-NC	2.87	113.12	110.21
23	b	617	CLA	CMD-C2D-C3D	2.88	130.72	125.09
28	a	415	LHG	O8-C23-C24	2.88	120.71	111.85
27	d	406	PL9	C3-C4-C5	2.88	122.80	118.64
25	C	516	BCR	C37-C22-C23	2.88	122.80	118.08
34	C	531	LMG	O8-C28-C29	2.89	120.73	111.85
23	b	611	CLA	CMD-C2D-C3D	2.89	130.75	125.09
26	A	410	SQD	O48-C23-C24	2.90	120.76	111.85
27	a	414	PL9	C15-C14-C16	2.90	119.78	115.37
23	c	914	CLA	C4A-NA-C1A	2.90	110.05	106.38
26	D	408	SQD	O48-C23-C24	2.90	120.77	111.85
23	D	403	CLA	CMD-C2D-C3D	2.90	130.76	125.09
24	D	402	PHO	C4A-NA-C1A	2.90	110.41	108.22
23	B	616	CLA	CMD-C2D-C3D	2.91	130.77	125.09
23	C	509	CLA	C4A-NA-C1A	2.91	110.07	106.38
23	C	503	CLA	C3C-C4C-NC	2.91	113.16	110.21
34	d	411	LMG	O8-C28-C29	2.91	120.81	111.85
23	b	614	CLA	C3C-C4C-NC	2.91	113.16	110.21
23	b	607	CLA	CAC-C3C-C4C	2.92	129.13	124.82
35	B	625	HTG	O4-C4-C5	2.92	116.92	109.23
23	c	906	CLA	CMC-C2C-C1C	2.92	129.33	125.00
23	c	904	CLA	CMD-C2D-C3D	2.93	130.81	125.09
23	D	403	CLA	C4A-NA-C1A	2.93	110.10	106.38
23	c	903	CLA	C3B-C4B-NB	2.93	113.00	109.21
23	B	616	CLA	C3B-C4B-NB	2.94	113.01	109.21
24	A	407	PHO	C4A-NA-C1A	2.94	110.44	108.22
23	c	903	CLA	C4A-NA-C1A	2.95	110.12	106.38
23	B	610	CLA	CED-O2D-CGD	2.95	122.97	115.97
23	c	910	CLA	O2A-CGA-CBA	2.95	120.92	111.85
35	B	625	HTG	C4-C3-C2	2.95	116.22	110.79
34	d	411	LMG	O6-C5-C6	2.95	114.03	106.38
27	a	414	PL9	C3-C4-C5	2.95	122.91	118.64
23	B	605	CLA	CAC-C3C-C4C	2.96	129.19	124.82
23	C	511	CLA	C3C-C4C-NC	2.96	113.21	110.21
23	c	912	CLA	C4-C3-C5	2.96	119.88	115.37
30	Z	101	LMT	C1'-O5'-C5'	2.96	119.55	113.74
30	a	422	LMT	C1B-O5B-C5B	2.96	119.55	113.74
23	B	604	CLA	CMD-C2D-C3D	2.97	130.89	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	e	103	LMT	O1'-C1'-C2'	2.97	111.65	108.00
23	b	613	CLA	C4-C3-C5	2.97	119.90	115.37
23	B	604	CLA	CBA-CAA-C2A	2.97	121.62	113.96
23	c	907	CLA	C3B-C4B-NB	2.97	113.06	109.21
23	c	903	CLA	C3C-C4C-NC	2.97	113.22	110.21
23	B	611	CLA	O2A-CGA-CBA	2.98	121.03	111.85
23	C	504	CLA	CMB-C2B-C3B	2.99	130.93	125.09
34	C	520	LMG	O6-C5-C6	2.99	114.14	106.38
23	c	903	CLA	CMC-C2C-C1C	2.99	129.44	125.00
23	d	401	CLA	C3C-C4C-NC	3.00	113.25	110.21
23	D	404	CLA	C3B-C4B-NB	3.00	113.09	109.21
23	B	606	CLA	O2D-CGD-CBD	3.00	115.55	111.22
23	b	616	CLA	CAC-C3C-C4C	3.01	129.26	124.82
23	b	609	CLA	CMC-C2C-C1C	3.02	129.47	125.00
23	c	909	CLA	C4A-NA-C1A	3.02	110.21	106.38
24	D	402	PHO	CED-O2D-CGD	3.02	123.15	115.97
28	D	409	LHG	O4-P-O5	3.02	128.28	112.56
35	b	622	HTG	C1-C2-C3	3.02	117.34	110.58
23	c	912	CLA	CMC-C2C-C1C	3.03	129.48	125.00
23	C	512	CLA	C3B-C4B-NB	3.03	113.12	109.21
27	A	411	PL9	C45-C44-C46	3.03	119.98	115.37
23	B	614	CLA	CAC-C3C-C4C	3.03	129.29	124.82
23	B	611	CLA	C3B-C4B-NB	3.03	113.13	109.21
23	b	611	CLA	C3B-C4B-NB	3.03	113.13	109.21
23	c	911	CLA	C4-C3-C5	3.04	120.00	115.37
23	a	406	CLA	O2D-CGD-CBD	3.05	115.61	111.22
23	b	616	CLA	OBD-CAD-CBD	3.05	130.54	125.94
23	D	401	CLA	CMC-C2C-C1C	3.05	129.52	125.00
23	C	502	CLA	C3C-C4C-NC	3.06	113.31	110.21
27	a	414	PL9	C25-C24-C26	3.06	120.04	115.37
23	B	607	CLA	C3C-C4C-NC	3.06	113.32	110.21
34	C	520	LMG	O8-C9-C8	3.07	116.99	108.70
28	d	409	LHG	O7-C7-C8	3.07	118.01	111.53
23	c	908	CLA	C4-C3-C5	3.08	120.06	115.37
23	D	401	CLA	C3C-C4C-NC	3.08	113.33	110.21
27	D	406	PL9	C10-C9-C11	3.08	120.06	115.37
24	a	408	PHO	CMB-C2B-C1B	3.08	129.98	125.06
23	B	604	CLA	CMB-C2B-C3B	3.08	131.11	125.09
23	C	514	CLA	C4A-NA-C1A	3.08	110.29	106.38
34	a	413	LMG	O1-C1-C2	3.08	111.79	108.00
23	b	612	CLA	C3C-C4C-NC	3.09	113.34	110.21
23	B	612	CLA	C3C-C4C-NC	3.09	113.34	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C4A-NA-C1A	3.11	110.32	106.38
23	b	605	CLA	C4A-NA-C1A	3.11	110.33	106.38
24	a	408	PHO	CMC-C2C-C1C	3.12	130.04	125.06
36	c	917	DGD	O2G-C1B-C2B	3.12	118.10	111.53
27	A	411	PL9	C10-C9-C11	3.12	120.13	115.37
23	B	605	CLA	CED-O2D-CGD	3.12	123.39	115.97
36	D	407	DGD	C3G-O3G-C1D	3.13	120.35	113.81
24	D	402	PHO	O2D-CGD-CBD	3.13	115.73	111.22
23	b	607	CLA	C3C-C4C-NC	3.13	113.39	110.21
23	B	609	CLA	CMC-C2C-C1C	3.13	129.65	125.00
26	L	102	SQD	C4-C3-C2	3.14	116.56	110.79
23	C	510	CLA	O2A-CGA-CBA	3.14	121.51	111.85
23	b	617	CLA	CAC-C3C-C4C	3.14	129.45	124.82
23	c	902	CLA	CMC-C2C-C1C	3.15	129.67	125.00
27	a	414	PL9	C20-C19-C21	3.15	120.17	115.37
26	A	410	SQD	O7-S-C6	3.16	109.14	106.92
23	C	514	CLA	O2A-CGA-CBA	3.16	121.58	111.85
23	C	507	CLA	C4A-NA-C1A	3.16	110.39	106.38
24	a	409	PHO	C3C-C4C-NC	3.16	115.30	110.31
23	b	602	CLA	C3C-C4C-NC	3.16	113.42	110.21
23	C	513	CLA	C4A-NA-C1A	3.16	110.39	106.38
23	B	608	CLA	CMD-C2D-C3D	3.17	131.29	125.09
23	B	611	CLA	CAC-C3C-C2C	3.17	132.97	127.51
23	b	605	CLA	CAC-C3C-C4C	3.18	129.51	124.82
35	b	622	HTG	C1-O5-C5	3.18	118.86	112.73
24	D	402	PHO	C2C-C1C-NC	3.18	114.55	109.81
30	A	416	LMT	O2'-C2'-C1'	3.18	117.07	110.01
23	c	914	CLA	CMB-C2B-C3B	3.18	131.32	125.09
23	B	608	CLA	O2D-CGD-CBD	3.19	115.81	111.22
23	D	404	CLA	CAC-C3C-C4C	3.19	129.53	124.82
25	D	405	BCR	C36-C18-C19	3.19	123.30	118.08
23	B	608	CLA	C3B-C4B-NB	3.19	113.34	109.21
23	b	617	CLA	O2A-CGA-CBA	3.20	121.68	111.85
23	c	902	CLA	C3B-C4B-NB	3.20	113.34	109.21
24	a	409	PHO	C2C-C1C-NC	3.20	114.57	109.81
35	c	923	HTG	C1'-S1-C1	3.20	108.98	100.88
23	A	408	CLA	CAC-C3C-C4C	3.20	129.54	124.82
28	L	101	LHG	O4-P-O5	3.20	129.22	112.56
23	b	605	CLA	C3C-C4C-NC	3.20	113.46	110.21
23	b	617	CLA	C3C-C4C-NC	3.20	113.46	110.21
23	b	605	CLA	CMC-C2C-C1C	3.21	129.76	125.00
24	D	402	PHO	C3C-C4C-NC	3.22	115.38	110.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	x	101	SQD	O6-C1-C2	3.22	111.96	108.00
23	B	614	CLA	O2A-CGA-CBA	3.22	121.76	111.85
25	B	620	BCR	C2-C1-C6	3.22	115.27	110.48
25	Y	101	BCR	C4-C5-C6	3.22	126.27	122.73
23	a	406	CLA	O2A-CGA-CBA	3.23	121.78	111.85
23	b	608	CLA	CMD-C2D-C3D	3.23	131.40	125.09
23	C	503	CLA	C3B-C4B-NB	3.23	113.38	109.21
27	A	411	PL9	C25-C24-C26	3.23	120.29	115.37
24	D	402	PHO	CMB-C2B-C1B	3.23	130.23	125.06
23	C	510	CLA	C4A-NA-C1A	3.23	110.48	106.38
30	a	422	LMT	O1'-C1'-C2'	3.25	112.00	108.00
23	c	912	CLA	C4A-NA-C1A	3.25	110.50	106.38
23	D	404	CLA	O2D-CGD-CBD	3.25	115.91	111.22
28	e	101	LHG	O8-C23-C24	3.25	121.85	111.85
23	c	914	CLA	CMC-C2C-C1C	3.25	129.82	125.00
23	B	613	CLA	CMC-C2C-C1C	3.26	129.83	125.00
23	b	603	CLA	C3C-C4C-NC	3.26	113.51	110.21
23	b	611	CLA	CMC-C2C-C1C	3.28	129.85	125.00
23	a	406	CLA	C3C-C4C-NC	3.29	113.54	110.21
23	b	609	CLA	C3C-C4C-NC	3.29	113.54	110.21
23	b	610	CLA	CAC-C3C-C4C	3.29	129.68	124.82
34	c	920	LMG	O7-C10-C11	3.29	118.47	111.53
23	B	606	CLA	CMC-C2C-C1C	3.30	129.89	125.00
23	C	506	CLA	C3C-C4C-NC	3.31	113.56	110.21
23	a	407	CLA	O2A-CGA-CBA	3.31	122.02	111.85
35	V	204	HTG	O5-C1-S1	3.31	118.95	109.89
24	a	408	PHO	C3C-C4C-NC	3.31	115.53	110.31
35	d	413	HTG	O5-C1-C2	3.31	114.75	110.22
23	b	609	CLA	CMB-C2B-C3B	3.32	131.58	125.09
25	d	405	BCR	C29-C30-C25	3.32	115.42	110.48
30	I	101	LMT	O3'-C3'-C4'	3.33	117.77	109.89
25	T	101	BCR	C35-C13-C12	3.34	123.54	118.08
36	H	103	DGD	O1G-C1A-C2A	3.34	122.14	111.85
23	C	513	CLA	C4-C3-C5	3.36	120.48	115.37
23	A	406	CLA	C4A-NA-C1A	3.36	110.64	106.38
23	c	910	CLA	CMD-C2D-C3D	3.36	131.66	125.09
35	v	204	HTG	O3-C3-C2	3.36	117.94	110.36
23	B	615	CLA	C3B-C4B-NB	3.36	113.56	109.21
23	b	614	CLA	CAC-C3C-C4C	3.37	129.79	124.82
23	b	616	CLA	C4-C3-C5	3.37	120.50	115.37
23	C	506	CLA	CAC-C3C-C4C	3.37	129.79	124.82
23	c	906	CLA	C3C-C4C-NC	3.37	113.63	110.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CMB-C2B-C3B	3.37	131.69	125.09
26	a	417	SQD	O9-S-C6	3.38	109.30	106.92
23	C	512	CLA	CMD-C2D-C3D	3.38	131.71	125.09
25	D	405	BCR	C29-C30-C25	3.39	115.53	110.48
23	C	508	CLA	CMC-C2C-C1C	3.40	130.04	125.00
23	a	406	CLA	CMD-C2D-C3D	3.41	131.75	125.09
23	b	602	CLA	C4A-NA-C1A	3.41	110.70	106.38
23	A	408	CLA	C3B-C4B-NB	3.41	113.62	109.21
23	C	509	CLA	CAC-C3C-C4C	3.41	129.86	124.82
24	A	407	PHO	C2B-C1B-NB	3.42	114.90	109.81
23	D	403	CLA	CAC-C3C-C4C	3.42	129.86	124.82
23	C	514	CLA	CMD-C2D-C3D	3.42	131.77	125.09
23	B	616	CLA	C4A-NA-C1A	3.42	110.72	106.38
35	O	302	HTG	C1'-S1-C1	3.42	105.00	100.60
23	B	609	CLA	C3C-C4C-NC	3.43	113.69	110.21
23	b	613	CLA	CMC-C2C-C1C	3.43	130.09	125.00
23	B	603	CLA	CMD-C2D-C3D	3.44	131.81	125.09
28	L	101	LHG	O7-C7-C8	3.44	118.77	111.53
23	C	507	CLA	CMC-C2C-C1C	3.45	130.11	125.00
23	B	604	CLA	CMC-C2C-C1C	3.45	130.11	125.00
23	b	616	CLA	CMC-C2C-C1C	3.45	130.11	125.00
23	B	615	CLA	CAC-C3C-C4C	3.45	129.92	124.82
24	a	408	PHO	C2B-C1B-NB	3.46	114.97	109.81
23	C	513	CLA	CED-O2D-CGD	3.46	124.20	115.97
23	B	614	CLA	C3B-C4B-NB	3.47	113.70	109.21
23	d	403	CLA	C3B-C4B-NB	3.48	113.71	109.21
23	C	507	CLA	CMD-C2D-C3D	3.48	131.90	125.09
26	x	101	SQD	C1-O5-C5	3.49	120.59	113.74
23	C	505	CLA	C4-C3-C5	3.49	120.69	115.37
23	C	510	CLA	C4-C3-C5	3.50	120.70	115.37
23	B	609	CLA	C3B-C4B-NB	3.51	113.74	109.21
36	d	407	DGD	C3D-C4D-C5D	3.52	114.92	109.66
35	B	625	HTG	C1-C2-C3	3.52	118.45	110.58
35	B	625	HTG	C1-O5-C5	3.53	119.54	112.73
28	E	101	LHG	O8-C23-C24	3.54	122.73	111.85
23	B	613	CLA	C4-C3-C5	3.54	120.76	115.37
34	a	413	LMG	O7-C10-C11	3.54	118.98	111.53
36	h	102	DGD	O5D-C1E-C2E	3.54	112.35	108.00
23	a	406	CLA	CAC-C3C-C4C	3.54	130.04	124.82
23	b	617	CLA	C3B-C4B-NB	3.54	113.79	109.21
23	c	914	CLA	O2A-CGA-CBA	3.54	122.75	111.85
23	B	610	CLA	CAC-C3C-C4C	3.55	130.06	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	b	617	CLA	CMB-C2B-C3B	3.55	132.03	125.09
23	b	604	CLA	CAC-C3C-C4C	3.55	130.06	124.82
23	B	617	CLA	CMD-C2D-C3D	3.56	132.05	125.09
23	b	603	CLA	CMC-C2C-C1C	3.57	130.29	125.00
23	b	612	CLA	C6-C5-C3	3.58	119.18	112.76
24	A	407	PHO	C3C-C4C-NC	3.58	115.95	110.31
23	c	911	CLA	CMD-C2D-C3D	3.58	132.09	125.09
23	c	914	CLA	CMD-C2D-C3D	3.59	132.10	125.09
34	a	413	LMG	O8-C28-C29	3.59	122.89	111.85
23	c	909	CLA	CMD-C2D-C3D	3.59	132.11	125.09
26	A	415	SQD	O48-C23-C24	3.59	122.89	111.85
23	b	616	CLA	O2D-CGD-CBD	3.59	116.40	111.22
36	H	103	DGD	O2G-C1B-C2B	3.59	119.10	111.53
26	L	102	SQD	O48-C23-C24	3.60	122.93	111.85
24	a	409	PHO	C4-C3-C5	3.60	120.85	115.37
23	B	604	CLA	C6-C5-C3	3.60	119.23	112.76
26	x	101	SQD	O48-C23-C24	3.61	122.97	111.85
23	C	508	CLA	C4A-NA-C1A	3.62	110.97	106.38
23	c	905	CLA	C3B-C4B-NB	3.62	113.89	109.21
23	C	506	CLA	CMC-C2C-C1C	3.63	130.38	125.00
28	D	411	LHG	O4-P-O5	3.64	131.47	112.56
23	b	608	CLA	CAC-C3C-C4C	3.64	130.19	124.82
23	C	504	CLA	C4-C3-C5	3.64	120.91	115.37
23	B	614	CLA	O1D-CGD-CBD	3.64	130.30	124.64
26	D	408	SQD	C3-C4-C5	3.64	116.72	110.23
23	d	403	CLA	C3C-C4C-NC	3.65	113.91	110.21
23	c	912	CLA	O2D-CGD-CBD	3.66	116.49	111.22
30	a	418	LMT	C1-O1'-C1'	3.67	120.41	114.00
36	h	102	DGD	O2G-C1B-C2B	3.68	119.28	111.53
28	d	408	LHG	C6-O8-C23	3.69	128.00	117.00
23	b	604	CLA	CMC-C2C-C1C	3.70	130.48	125.00
26	A	415	SQD	O47-C7-C8	3.70	119.32	111.53
23	C	513	CLA	C3C-C4C-NC	3.70	113.96	110.21
23	b	602	CLA	O2A-CGA-CBA	3.71	123.28	111.85
23	B	608	CLA	CED-O2D-CGD	3.71	124.79	115.97
23	c	910	CLA	CMC-C2C-C1C	3.72	130.51	125.00
23	C	504	CLA	CMC-C2C-C1C	3.73	130.53	125.00
30	m	103	LMT	O1'-C1'-C2'	3.73	112.59	108.00
23	A	406	CLA	C3B-C4B-NB	3.74	114.05	109.21
34	B	622	LMG	O7-C10-C11	3.75	119.43	111.53
23	D	403	CLA	O2D-CGD-CBD	3.75	116.63	111.22
23	c	906	CLA	O2D-CGD-CBD	3.75	116.63	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	402	LHG	O7-C7-C8	3.76	119.45	111.53
23	b	617	CLA	C4-C3-C5	3.76	121.11	115.37
23	c	913	CLA	C4A-NA-C1A	3.77	111.16	106.38
23	A	405	CLA	C3B-C4B-NB	3.77	114.08	109.21
23	C	512	CLA	O2D-CGD-CBD	3.78	116.67	111.22
34	c	920	LMG	O8-C28-C29	3.78	123.48	111.85
23	c	904	CLA	C4A-NA-C1A	3.78	111.18	106.38
24	D	402	PHO	CAC-C3C-C4C	3.78	129.58	125.21
30	F	101	LMT	C2'-C3'-C4'	3.79	118.00	109.63
23	A	406	CLA	C3C-C4C-NC	3.79	114.05	110.21
23	B	604	CLA	C3B-C4B-NB	3.81	114.13	109.21
35	v	204	HTG	O5-C1-S1	3.81	120.33	109.89
26	a	417	SQD	O6-C1-C2	3.82	112.70	108.00
23	D	401	CLA	C4-C3-C5	3.83	121.20	115.37
24	D	402	PHO	C2B-C1B-NB	3.83	115.51	109.81
25	B	619	BCR	C29-C30-C25	3.84	116.19	110.48
23	c	904	CLA	C4-C3-C5	3.84	121.22	115.37
23	C	510	CLA	C3C-C4C-NC	3.84	114.11	110.21
23	a	410	CLA	C4-C3-C5	3.84	121.23	115.37
23	B	611	CLA	C3C-C4C-NC	3.85	114.11	110.21
34	D	412	LMG	O7-C10-C11	3.85	119.64	111.53
30	b	621	LMT	O5'-C5'-C4'	3.86	118.02	109.78
34	C	520	LMG	O8-C28-C29	3.87	123.75	111.85
27	d	406	PL9	C15-C14-C16	3.87	121.27	115.37
23	b	603	CLA	C4-C3-C5	3.87	121.27	115.37
26	B	621	SQD	O47-C7-C8	3.88	119.70	111.53
23	d	404	CLA	O2D-CGD-CBD	3.89	116.83	111.22
23	a	407	CLA	CAC-C3C-C4C	3.91	130.60	124.82
28	e	101	LHG	O7-C7-C8	3.92	119.78	111.53
23	c	905	CLA	O2D-CGD-CBD	3.92	116.88	111.22
36	C	518	DGD	O2G-C1B-C2B	3.94	119.82	111.53
23	c	910	CLA	CAC-C3C-C4C	3.94	130.63	124.82
23	b	612	CLA	C4A-NA-C1A	3.94	111.38	106.38
36	D	407	DGD	C3D-C4D-C5D	3.95	115.56	109.66
23	C	509	CLA	C4-C3-C5	3.98	121.43	115.37
23	a	410	CLA	C3C-C4C-NC	4.01	114.27	110.21
23	C	507	CLA	C3C-C4C-NC	4.03	114.30	110.21
23	c	914	CLA	C3C-C4C-NC	4.04	114.31	110.21
23	b	610	CLA	C3C-C4C-NC	4.06	114.32	110.21
23	b	613	CLA	CAC-C3C-C4C	4.07	130.83	124.82
34	C	520	LMG	O7-C10-C11	4.07	120.11	111.53
23	b	617	CLA	C2C-C1C-NC	4.08	113.03	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	h	102	DGD	O3G-C1D-C2D	4.08	113.02	108.00
23	c	905	CLA	CAC-C3C-C4C	4.08	130.84	124.82
27	a	414	PL9	C53-C6-C1	4.10	123.37	114.66
23	b	606	CLA	CMD-C2D-C3D	4.10	133.10	125.09
23	b	606	CLA	CMC-C2C-C1C	4.10	131.08	125.00
24	D	402	PHO	C2D-C1D-ND	4.11	115.92	109.81
23	c	910	CLA	C3B-C4B-NB	4.11	114.52	109.21
23	C	514	CLA	O2D-CGD-CBD	4.11	117.15	111.22
23	b	615	CLA	C2C-C1C-NC	4.12	113.06	110.22
23	B	612	CLA	O2D-CGD-CBD	4.12	117.16	111.22
23	C	513	CLA	CMD-C2D-C3D	4.12	133.16	125.09
23	C	508	CLA	C4-C3-C5	4.13	121.66	115.37
24	a	409	PHO	C2D-C1D-ND	4.13	115.96	109.81
28	d	408	LHG	O8-C23-C24	4.14	124.58	111.85
23	b	609	CLA	CMD-C2D-C3D	4.14	133.18	125.09
23	B	617	CLA	C3C-C4C-NC	4.14	114.41	110.21
23	B	608	CLA	CMB-C2B-C3B	4.15	133.21	125.09
23	B	606	CLA	C4-C3-C5	4.16	121.71	115.37
23	c	902	CLA	C4A-NA-C1A	4.16	111.66	106.38
23	b	613	CLA	O2D-CGD-CBD	4.16	117.23	111.22
23	b	606	CLA	C3C-C4C-NC	4.16	114.43	110.21
23	B	602	CLA	CMC-C2C-C1C	4.16	131.17	125.00
23	c	909	CLA	C2C-C1C-NC	4.17	113.09	110.22
23	b	604	CLA	C4-C3-C5	4.17	121.72	115.37
34	m	102	LMG	O7-C10-C11	4.17	120.32	111.53
23	c	905	CLA	C4-C3-C5	4.17	121.73	115.37
30	A	416	LMT	O1'-C1'-C2'	4.17	113.14	108.00
23	B	610	CLA	CMD-C2D-C3D	4.18	133.26	125.09
23	B	606	CLA	CAC-C3C-C4C	4.18	130.99	124.82
23	b	611	CLA	O2D-CGD-CBD	4.18	117.25	111.22
23	b	612	CLA	O2D-CGD-CBD	4.19	117.26	111.22
25	b	619	BCR	C29-C30-C25	4.19	116.71	110.48
23	b	608	CLA	C4-C3-C5	4.20	121.76	115.37
26	L	102	SQD	C3-C4-C5	4.20	117.72	110.23
23	c	911	CLA	C3C-C4C-NC	4.20	114.47	110.21
23	b	604	CLA	C3C-C4C-NC	4.20	114.47	110.21
23	C	504	CLA	O2D-CGD-CBD	4.20	117.28	111.22
23	A	405	CLA	CAC-C3C-C4C	4.21	131.04	124.82
26	A	410	SQD	O3-C3-C4	4.23	119.89	110.36
23	C	512	CLA	C4A-NA-C1A	4.23	111.74	106.38
23	B	605	CLA	C3C-C4C-NC	4.23	114.50	110.21
23	b	605	CLA	CMD-C2D-C3D	4.25	133.39	125.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	409	LHG	O8-C23-C24	4.27	124.99	111.85
23	b	610	CLA	O2D-CGD-CBD	4.27	117.38	111.22
26	a	417	SQD	O47-C7-C8	4.27	120.53	111.53
23	b	603	CLA	CMD-C2D-C3D	4.27	133.45	125.09
24	a	409	PHO	C2B-C1B-NB	4.29	116.20	109.81
23	A	405	CLA	C4-C3-C5	4.31	121.93	115.37
23	C	506	CLA	O2D-CGD-CBD	4.32	117.44	111.22
23	b	606	CLA	O2D-CGD-CBD	4.32	117.45	111.22
23	B	613	CLA	O2D-CGD-CBD	4.32	117.46	111.22
24	a	408	PHO	C2D-C1D-ND	4.36	116.30	109.81
30	T	103	LMT	C1'-C2'-C3'	4.36	118.63	109.98
30	F	101	LMT	C1B-O5B-C5B	4.36	122.30	113.74
23	B	612	CLA	CAC-C3C-C4C	4.36	131.26	124.82
23	c	902	CLA	O2D-CGD-CBD	4.37	117.52	111.22
34	C	501	LMG	O1-C1-C2	4.37	113.38	108.00
23	D	401	CLA	CAC-C3C-C4C	4.37	131.27	124.82
28	A	412	LHG	O7-C7-C8	4.37	120.74	111.53
28	K	101	LHG	O7-C7-C8	4.37	120.74	111.53
23	d	404	CLA	C3B-C4B-NB	4.37	114.87	109.21
36	c	918	DGD	O2G-C1B-C2B	4.40	120.80	111.53
26	x	101	SQD	O7-S-C6	4.42	110.03	106.92
27	A	411	PL9	C30-C29-C31	4.42	122.11	115.37
26	D	408	SQD	O47-C7-C8	4.42	120.84	111.53
36	D	407	DGD	C4D-C3D-C2D	4.43	118.94	110.79
23	b	603	CLA	O2D-CGD-CBD	4.45	117.63	111.22
23	B	617	CLA	CAC-C3C-C4C	4.47	131.41	124.82
23	C	513	CLA	C2C-C1C-NC	4.47	113.30	110.22
23	B	604	CLA	C3C-C4C-NC	4.47	114.74	110.21
23	C	511	CLA	O2D-CGD-CBD	4.47	117.67	111.22
23	d	403	CLA	C4-C3-C5	4.48	122.20	115.37
24	a	408	PHO	C2C-C1C-NC	4.49	116.49	109.81
27	d	406	PL9	C40-C39-C41	4.49	122.21	115.37
23	b	605	CLA	O2D-CGD-CBD	4.49	117.70	111.22
23	a	410	CLA	CMD-C2D-C3D	4.49	133.87	125.09
23	A	406	CLA	O2D-CGD-CBD	4.50	117.71	111.22
23	a	406	CLA	C4-C3-C5	4.51	122.24	115.37
23	b	603	CLA	CMB-C2B-C3B	4.55	133.99	125.09
34	C	531	LMG	O7-C10-C11	4.56	121.14	111.53
23	b	606	CLA	CAC-C3C-C4C	4.57	131.56	124.82
23	B	610	CLA	O2D-CGD-CBD	4.60	117.85	111.22
23	c	910	CLA	O2D-CGD-CBD	4.60	117.86	111.22
23	c	910	CLA	C4A-NA-C1A	4.61	112.23	106.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	c	905	CLA	C4A-NA-C1A	4.64	112.26	106.38
23	D	401	CLA	O2D-CGD-CBD	4.66	117.94	111.22
27	A	411	PL9	C53-C6-C1	4.66	124.57	114.66
23	B	607	CLA	O2D-CGD-CBD	4.67	117.95	111.22
23	B	605	CLA	O2D-CGD-CBD	4.67	117.96	111.22
23	c	903	CLA	CMD-C2D-C3D	4.68	134.23	125.09
23	B	603	CLA	O2D-CGD-CBD	4.70	118.00	111.22
36	D	407	DGD	O1G-C1A-C2A	4.73	126.40	111.85
23	b	609	CLA	CAC-C3C-C4C	4.76	131.84	124.82
23	b	609	CLA	O2D-CGD-CBD	4.76	118.08	111.22
26	D	408	SQD	O7-S-C6	4.76	110.28	106.92
23	B	609	CLA	O2D-CGD-CBD	4.76	118.09	111.22
23	B	617	CLA	O2D-CGD-CBD	4.78	118.11	111.22
23	b	617	CLA	O2D-CGD-CBD	4.78	118.12	111.22
23	A	405	CLA	C3C-C4C-NC	4.79	115.06	110.21
34	D	412	LMG	O1-C1-C2	4.80	113.91	108.00
34	c	930	LMG	O7-C10-C11	4.82	121.68	111.53
34	d	411	LMG	O7-C10-C11	4.83	121.69	111.53
23	c	914	CLA	C2C-C1C-NC	4.83	113.54	110.22
23	C	513	CLA	O2D-CGD-CBD	4.85	118.21	111.22
24	A	407	PHO	C2C-C1C-NC	4.85	117.03	109.81
24	a	408	PHO	CMD-C2D-C1D	4.86	132.83	125.06
23	B	606	CLA	C3C-C4C-NC	4.86	115.14	110.21
23	b	608	CLA	O2D-CGD-CBD	4.87	118.24	111.22
34	c	930	LMG	O1-C1-C2	4.88	114.00	108.00
23	c	903	CLA	O2D-CGD-CBD	4.88	118.27	111.22
23	b	616	CLA	CMD-C2D-C3D	4.89	134.66	125.09
24	A	407	PHO	C2D-C1D-ND	4.90	117.10	109.81
28	a	415	LHG	O7-C7-C8	4.90	121.86	111.53
23	B	615	CLA	O2D-CGD-CBD	4.91	118.30	111.22
23	A	406	CLA	CAC-C3C-C4C	4.92	132.08	124.82
26	a	412	SQD	O47-C7-C8	4.94	121.94	111.53
23	a	410	CLA	CAC-C3C-C4C	4.98	132.17	124.82
35	C	522	HTG	C1-O5-C5	4.99	122.37	112.73
24	A	407	PHO	O2D-CGD-CBD	5.01	118.45	111.22
23	a	407	CLA	C3C-C4C-NC	5.04	115.32	110.21
28	E	101	LHG	O7-C7-C8	5.05	122.18	111.53
26	L	102	SQD	O47-C7-C8	5.09	122.26	111.53
23	c	911	CLA	O2D-CGD-CBD	5.09	118.57	111.22
36	d	407	DGD	O2G-C1B-C2B	5.13	122.33	111.53
24	D	402	PHO	CMD-C2D-C1D	5.13	133.26	125.06
23	C	509	CLA	C2C-C1C-NC	5.13	113.75	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	O2D-CGD-CBD	5.16	118.66	111.22
26	L	102	SQD	O6-C1-C2	5.16	114.35	108.00
23	A	408	CLA	C4-C3-C5	5.18	123.25	115.37
23	A	405	CLA	CMD-C2D-C3D	5.18	135.22	125.09
35	B	631	HTG	C1'-S1-C1	5.20	107.28	100.60
23	C	504	CLA	C2C-C1C-NC	5.21	113.80	110.22
26	B	621	SQD	O9-S-C6	5.22	110.60	106.92
23	c	914	CLA	O2D-CGD-CBD	5.22	118.75	111.22
23	B	602	CLA	C2C-C1C-NC	5.23	113.82	110.22
27	D	406	PL9	C40-C39-C41	5.24	123.35	115.37
23	D	404	CLA	C2C-C1C-NC	5.26	113.84	110.22
23	c	908	CLA	C2C-C1C-NC	5.28	113.86	110.22
23	c	905	CLA	C2C-C1C-NC	5.30	113.86	110.22
23	b	606	CLA	C4-C3-C5	5.31	123.45	115.37
36	D	407	DGD	O2G-C1B-C2B	5.31	122.71	111.53
26	A	410	SQD	O47-C7-C8	5.32	122.75	111.53
23	b	607	CLA	O2D-CGD-CBD	5.32	118.90	111.22
23	B	613	CLA	CAC-C3C-C4C	5.34	132.71	124.82
23	B	611	CLA	O2D-CGD-CBD	5.37	118.97	111.22
23	D	403	CLA	CMC-C2C-C1C	5.38	132.97	125.00
23	B	610	CLA	C3C-C4C-NC	5.38	115.66	110.21
23	A	408	CLA	O2D-CGD-CBD	5.41	119.02	111.22
23	C	510	CLA	O2D-CGD-CBD	5.47	119.12	111.22
23	C	505	CLA	O2D-CGD-CBD	5.50	119.15	111.22
23	c	903	CLA	C2C-C1C-NC	5.52	114.02	110.22
23	C	503	CLA	O2D-CGD-CBD	5.55	119.22	111.22
35	B	625	HTG	C1'-S1-C1	5.61	107.81	100.60
23	b	604	CLA	O2D-CGD-CBD	5.61	119.32	111.22
23	C	514	CLA	C2C-C1C-NC	5.68	114.13	110.22
23	b	612	CLA	C2C-C1C-NC	5.76	114.19	110.22
30	I	101	LMT	O1B-C4'-C3'	5.78	122.27	107.18
23	c	908	CLA	O2D-CGD-CBD	5.79	119.57	111.22
23	c	907	CLA	O2D-CGD-CBD	5.80	119.59	111.22
23	b	615	CLA	O2D-CGD-CBD	5.82	119.61	111.22
26	D	408	SQD	O9-S-C6	5.82	111.02	106.92
23	c	904	CLA	C2C-C1C-NC	5.85	114.25	110.22
23	b	611	CLA	C2C-C1C-NC	5.88	114.27	110.22
23	b	613	CLA	C3C-C4C-NC	5.92	116.20	110.21
23	c	911	CLA	C2C-C1C-NC	5.95	114.31	110.22
23	b	607	CLA	C2C-C1C-NC	5.97	114.33	110.22
35	B	624	HTG	C1'-S1-C1	5.99	108.29	100.60
23	c	913	CLA	O2D-CGD-CBD	6.02	119.91	111.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	401	CLA	CMD-C2D-C3D	6.04	136.90	125.09
23	c	912	CLA	C2C-C1C-NC	6.06	114.39	110.22
24	a	409	PHO	CMD-C2D-C1D	6.06	134.75	125.06
23	a	406	CLA	C2C-C1C-NC	6.06	114.39	110.22
23	c	907	CLA	C2C-C1C-NC	6.07	114.39	110.22
23	b	602	CLA	C2C-C1C-NC	6.07	114.40	110.22
23	a	410	CLA	O2D-CGD-CBD	6.19	120.15	111.22
23	c	910	CLA	C2C-C1C-NC	6.20	114.48	110.22
23	C	507	CLA	C2C-C1C-NC	6.20	114.48	110.22
26	B	621	SQD	O6-C1-C2	6.23	115.66	108.00
23	c	913	CLA	C2C-C1C-NC	6.29	114.55	110.22
26	L	102	SQD	O9-S-C6	6.30	111.36	106.92
35	c	921	HTG	C1'-S1-C1	6.37	108.79	100.60
23	B	614	CLA	C2C-C1C-NC	6.38	114.61	110.22
35	B	630	HTG	C1'-S1-C1	6.38	108.80	100.60
26	A	410	SQD	O6-C1-C2	6.40	115.88	108.00
24	a	409	PHO	O2D-CGD-CBD	6.42	120.48	111.22
23	B	606	CLA	C2C-C1C-NC	6.42	114.64	110.22
23	C	502	CLA	C2C-C1C-NC	6.44	114.65	110.22
23	D	403	CLA	C3C-C4C-NC	6.46	116.76	110.21
23	C	507	CLA	O2D-CGD-CBD	6.47	120.55	111.22
23	b	608	CLA	C2C-C1C-NC	6.47	114.67	110.22
35	b	627	HTG	C1'-S1-C1	6.50	108.96	100.60
23	A	408	CLA	C2C-C1C-NC	6.53	114.72	110.22
23	b	616	CLA	C2C-C1C-NC	6.55	114.72	110.22
23	C	508	CLA	O2D-CGD-CBD	6.55	120.67	111.22
23	B	603	CLA	C2C-C1C-NC	6.60	114.76	110.22
23	b	610	CLA	C2C-C1C-NC	6.61	114.77	110.22
23	B	615	CLA	C2C-C1C-NC	6.76	114.87	110.22
23	a	410	CLA	C2C-C1C-NC	6.91	114.97	110.22
23	B	611	CLA	C2C-C1C-NC	6.93	114.99	110.22
23	b	606	CLA	C2C-C1C-NC	6.93	114.99	110.22
23	C	508	CLA	C2C-C1C-NC	6.93	114.99	110.22
23	B	607	CLA	C2C-C1C-NC	6.96	115.01	110.22
23	A	405	CLA	C2C-C1C-NC	7.00	115.04	110.22
24	A	407	PHO	CMD-C2D-C1D	7.01	136.27	125.06
36	D	407	DGD	O3G-C1D-C2D	7.04	116.67	108.00
23	c	906	CLA	C2C-C1C-NC	7.16	115.15	110.22
23	D	401	CLA	C2C-C1C-NC	7.18	115.16	110.22
23	B	604	CLA	O2D-CGD-CBD	7.30	121.75	111.22
23	b	609	CLA	C2C-C1C-NC	7.30	115.24	110.22
23	b	603	CLA	C2C-C1C-NC	7.30	115.25	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	C2C-C1C-NC	7.32	115.25	110.22
23	C	503	CLA	C2C-C1C-NC	7.33	115.26	110.22
23	b	605	CLA	C2C-C1C-NC	7.36	115.28	110.22
23	B	609	CLA	C2C-C1C-NC	7.40	115.31	110.22
23	B	617	CLA	C2C-C1C-NC	7.45	115.34	110.22
23	B	612	CLA	C2C-C1C-NC	7.48	115.36	110.22
23	B	613	CLA	C2C-C1C-NC	7.50	115.38	110.22
23	C	512	CLA	C2C-C1C-NC	7.55	115.41	110.22
35	D	414	HTG	C1'-S1-C1	7.56	110.31	100.60
23	c	902	CLA	C2C-C1C-NC	7.73	115.54	110.22
23	B	616	CLA	C2C-C1C-NC	7.73	115.54	110.22
23	B	605	CLA	C2C-C1C-NC	7.84	115.62	110.22
23	b	602	CLA	O2D-CGD-CBD	7.86	122.56	111.22
23	b	614	CLA	C2C-C1C-NC	7.90	115.65	110.22
23	B	608	CLA	C2C-C1C-NC	7.94	115.68	110.22
23	C	510	CLA	C2C-C1C-NC	7.96	115.69	110.22
23	C	511	CLA	C2C-C1C-NC	7.99	115.71	110.22
23	C	502	CLA	O2D-CGD-CBD	8.04	122.83	111.22
26	L	102	SQD	O7-S-C6	8.07	112.61	106.92
23	d	403	CLA	C2C-C1C-NC	8.10	115.79	110.22
23	b	613	CLA	C2C-C1C-NC	8.23	115.88	110.22
26	A	415	SQD	O6-C1-C2	8.32	118.23	108.00
23	d	401	CLA	C2C-C1C-NC	8.42	116.01	110.22
23	C	505	CLA	C2C-C1C-NC	8.46	116.04	110.22
35	C	522	HTG	C1'-S1-C1	8.54	111.58	100.60
35	b	628	HTG	C1'-S1-C1	8.67	111.75	100.60
35	c	922	HTG	C1'-S1-C1	8.73	111.82	100.60
23	b	604	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	C	506	CLA	C2C-C1C-NC	8.90	116.34	110.22
23	d	404	CLA	C2C-C1C-NC	8.91	116.35	110.22
35	B	626	HTG	C1'-S1-C1	8.92	112.07	100.60
23	B	602	CLA	O2D-CGD-CBD	8.96	124.15	111.22
26	A	410	SQD	O9-S-C6	9.12	113.34	106.92
23	A	406	CLA	C2C-C1C-NC	9.15	116.52	110.22
26	A	415	SQD	O9-S-C6	9.66	113.73	106.92
35	b	623	HTG	C1'-S1-C1	9.73	113.11	100.60
26	B	621	SQD	O7-S-C6	10.00	113.97	106.92
35	C	521	HTG	C1'-S1-C1	10.01	113.47	100.60
23	D	403	CLA	C2C-C1C-NC	10.18	117.22	110.22
26	a	412	SQD	O6-C1-C2	10.44	120.85	108.00
35	C	523	HTG	C1'-S1-C1	10.45	114.04	100.60
35	d	413	HTG	C1'-S1-C1	10.65	114.30	100.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	a	407	CLA	C2C-C1C-NC	11.06	117.83	110.22
23	B	604	CLA	C2C-C1C-NC	11.29	117.98	110.22
26	D	408	SQD	O6-C1-C2	11.73	122.43	108.00
26	a	412	SQD	O9-S-C6	12.34	115.62	106.92
35	v	204	HTG	C1'-S1-C1	13.11	117.46	100.60

All (169) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	b	605	CLA	NC
23	b	605	CLA	ND
23	b	605	CLA	NA
23	C	504	CLA	NC
23	C	504	CLA	NA
23	a	407	CLA	NC
23	a	407	CLA	NA
23	A	405	CLA	NC
23	A	405	CLA	NA
23	c	912	CLA	NC
23	c	912	CLA	NA
23	d	403	CLA	ND
23	d	403	CLA	NA
23	B	605	CLA	NC
23	B	605	CLA	ND
23	B	605	CLA	NA
23	c	910	CLA	NC
23	c	910	CLA	ND
23	c	910	CLA	NA
23	a	406	CLA	NC
23	a	406	CLA	ND
23	a	406	CLA	NA
23	b	613	CLA	NA
23	b	613	CLA	NC
23	b	613	CLA	ND
23	A	406	CLA	NC
23	A	406	CLA	NA
23	C	513	CLA	NC
23	C	513	CLA	ND
23	C	513	CLA	NA
23	B	602	CLA	NC
23	B	602	CLA	ND
23	C	514	CLA	NC

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Mol	Chain	Res	Type	Atom
23	D	403	CLA	ND
23	B	614	CLA	NC
23	B	614	CLA	ND
23	B	614	CLA	NA
23	b	615	CLA	NC
23	b	615	CLA	ND
23	b	615	CLA	NA
23	a	410	CLA	NC
23	B	604	CLA	NC
23	B	604	CLA	ND
23	B	604	CLA	NA
23	B	613	CLA	NA
23	B	613	CLA	NC
23	B	613	CLA	ND
23	B	603	CLA	NC
23	B	603	CLA	ND
23	B	603	CLA	NA
23	b	607	CLA	NC
23	b	607	CLA	ND
23	b	607	CLA	NA
23	c	903	CLA	NC
23	c	903	CLA	NA
23	D	401	CLA	NA
23	c	902	CLA	NC
23	c	902	CLA	ND
23	c	902	CLA	NA
23	C	505	CLA	NC
23	C	505	CLA	ND
23	C	505	CLA	NA
23	b	614	CLA	NC
23	b	614	CLA	ND
23	b	614	CLA	NA
23	c	907	CLA	ND
23	c	907	CLA	NA
23	c	908	CLA	NC
23	c	908	CLA	ND
23	c	908	CLA	NA
23	C	510	CLA	NC
23	C	510	CLA	NA
23	C	510	CLA	ND
23	B	616	CLA	NC
23	B	616	CLA	ND

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Mol	Chain	Res	Type	Atom
23	B	616	CLA	NA
23	c	911	CLA	NC
23	c	911	CLA	ND
23	c	911	CLA	NA
23	A	408	CLA	NC
23	A	408	CLA	NA
23	B	609	CLA	NC
23	B	615	CLA	NC
23	B	615	CLA	ND
23	B	615	CLA	NA
23	c	909	CLA	NC
23	c	909	CLA	NA
23	C	502	CLA	NC
23	C	502	CLA	ND
23	C	502	CLA	NA
23	B	606	CLA	NC
23	B	606	CLA	ND
23	B	606	CLA	NA
23	b	602	CLA	NC
23	b	602	CLA	ND
23	b	602	CLA	NA
23	C	508	CLA	NC
23	C	508	CLA	ND
23	C	508	CLA	NA
23	b	609	CLA	NC
23	b	606	CLA	NC
23	b	606	CLA	ND
23	b	606	CLA	NA
23	C	509	CLA	NC
23	C	509	CLA	ND
23	C	509	CLA	NA
23	b	611	CLA	NC
23	b	611	CLA	ND
23	b	611	CLA	NA
23	C	507	CLA	NC
23	C	507	CLA	ND
23	C	507	CLA	NA
23	d	401	CLA	NA
23	d	404	CLA	NC
23	b	604	CLA	NC
23	b	604	CLA	ND
23	b	604	CLA	NA

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Mol	Chain	Res	Type	Atom
23	B	612	CLA	NC
23	B	612	CLA	ND
23	B	612	CLA	NA
23	C	511	CLA	NA
23	C	511	CLA	NC
23	C	511	CLA	ND
23	c	904	CLA	NC
23	c	913	CLA	NC
23	c	913	CLA	ND
23	c	913	CLA	NA
23	b	617	CLA	NC
23	b	617	CLA	ND
23	b	617	CLA	NA
23	c	914	CLA	NC
23	D	404	CLA	NC
23	D	404	CLA	ND
23	D	404	CLA	NA
23	C	506	CLA	ND
23	C	506	CLA	NA
23	B	608	CLA	NC
23	B	608	CLA	ND
23	B	608	CLA	NA
23	b	610	CLA	NC
23	b	610	CLA	NA
23	B	607	CLA	NC
23	B	607	CLA	ND
23	B	607	CLA	NA
23	B	610	CLA	NC
23	B	610	CLA	NA
23	C	512	CLA	NC
23	C	512	CLA	NA
23	B	617	CLA	NC
23	B	617	CLA	ND
23	B	617	CLA	NA
23	C	503	CLA	NA
23	B	611	CLA	NC
23	B	611	CLA	ND
23	B	611	CLA	NA
23	b	616	CLA	NC
23	b	616	CLA	ND
23	b	616	CLA	NA
23	b	603	CLA	NC

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Mol	Chain	Res	Type	Atom
23	b	603	CLA	ND
23	b	603	CLA	NA
23	b	608	CLA	NC
23	b	608	CLA	ND
23	b	608	CLA	NA
23	c	906	CLA	ND
23	c	906	CLA	NA
23	c	905	CLA	NC
23	c	905	CLA	NA
23	b	612	CLA	NC

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	d	413	HTG	O5-C1-S1-C1'
26	L	102	SQD	C45-O47-C7-C8

There are no ring outliers.

107 monomers are involved in 318 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	A	405	CLA	4	0
23	A	406	CLA	6	0
24	A	407	PHO	2	0
23	A	408	CLA	2	0
25	A	409	BCR	3	0
26	A	410	SQD	9	0
27	A	411	PL9	12	0
28	A	412	LHG	1	0
26	A	415	SQD	2	0
30	A	416	LMT	2	0
31	A	421	DMS	1	0
31	A	422	DMS	1	0
31	A	424	DMS	2	0
23	B	602	CLA	4	0
23	B	603	CLA	4	0
23	B	604	CLA	3	0
23	B	605	CLA	2	0
23	B	606	CLA	7	0
23	B	607	CLA	1	0
23	B	609	CLA	1	0
23	B	610	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	611	CLA	7	0
23	B	612	CLA	2	0
23	B	613	CLA	4	0
23	B	614	CLA	6	0
23	B	615	CLA	5	0
23	B	616	CLA	5	0
23	B	617	CLA	13	0
25	B	618	BCR	1	0
25	B	619	BCR	5	0
25	B	620	BCR	9	0
26	B	621	SQD	4	0
34	B	622	LMG	2	0
30	B	623	LMT	2	0
35	B	625	HTG	1	0
31	B	636	DMS	5	0
31	B	639	DMS	10	0
31	B	641	DMS	3	0
30	B	644	LMT	1	0
31	B	645	DMS	4	0
31	B	646	DMS	3	0
31	B	648	DMS	1	0
34	C	501	LMG	1	0
23	C	502	CLA	2	0
23	C	503	CLA	3	0
23	C	504	CLA	5	0
23	C	505	CLA	1	0
23	C	506	CLA	1	0
23	C	507	CLA	5	0
23	C	508	CLA	2	0
23	C	509	CLA	3	0
23	C	510	CLA	3	0
23	C	511	CLA	5	0
23	C	512	CLA	3	0
23	C	513	CLA	6	0
23	C	514	CLA	5	0
25	C	515	BCR	4	0
25	C	516	BCR	2	0
36	C	517	DGD	1	0
36	C	518	DGD	1	0
35	C	521	HTG	1	0
31	C	525	DMS	1	0
31	C	526	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	C	529	DMS	1	0
25	C	530	BCR	2	0
34	C	531	LMG	3	0
23	D	401	CLA	6	0
24	D	402	PHO	3	0
23	D	403	CLA	3	0
23	D	404	CLA	3	0
25	D	405	BCR	6	0
36	D	407	DGD	10	0
26	D	408	SQD	2	0
28	D	409	LHG	2	0
28	D	410	LHG	1	0
28	D	411	LHG	5	0
34	D	412	LMG	5	0
35	D	414	HTG	3	0
31	D	415	DMS	1	0
31	D	416	DMS	6	0
28	E	101	LHG	7	0
37	E	105	HEM	1	0
31	F	102	DMS	6	0
31	H	101	DMS	3	0
31	H	105	DMS	3	0
30	I	101	LMT	2	0
34	J	101	LMG	3	0
28	L	101	LHG	1	0
26	L	102	SQD	3	0
30	M	101	LMT	1	0
35	O	302	HTG	2	0
31	O	303	DMS	3	0
31	O	304	DMS	3	0
31	O	305	DMS	6	0
31	O	308	DMS	5	0
31	O	311	DMS	3	0
25	T	101	BCR	9	0
31	U	202	DMS	1	0
31	U	204	DMS	3	0
31	V	202	DMS	1	0
35	V	204	HTG	2	0
31	V	206	DMS	3	0
31	V	207	DMS	4	0
31	V	209	DMS	5	0
31	V	210	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Y	101	BCR	1	0
30	Z	101	LMT	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	334/344 (97%)	-0.26	4 (1%) 81 83	14, 21, 43, 67	0
1	a	334/344 (97%)	-0.09	9 (2%) 58 60	14, 21, 44, 91	0
2	B	505/505 (100%)	0.00	28 (5%) 29 30	17, 26, 50, 81	0
2	b	501/505 (99%)	0.01	32 (6%) 23 24	16, 25, 53, 109	0
3	C	451/455 (99%)	-0.03	14 (3%) 52 54	18, 30, 46, 73	0
3	c	455/455 (100%)	-0.00	15 (3%) 50 52	20, 31, 43, 68	0
4	D	342/342 (100%)	-0.24	3 (0%) 85 87	15, 22, 41, 88	0
4	d	342/342 (100%)	-0.30	3 (0%) 85 87	15, 22, 40, 73	0
5	E	81/83 (97%)	1.43	24 (29%) 1 0	25, 45, 75, 97	0
5	e	79/83 (95%)	0.86	13 (16%) 2 2	28, 42, 67, 87	0
6	F	35/44 (79%)	0.43	6 (17%) 2 2	24, 35, 59, 96	0
6	f	32/44 (72%)	0.03	2 (6%) 23 25	26, 31, 70, 82	0
7	H	63/65 (96%)	-0.00	2 (3%) 51 53	24, 34, 44, 77	0
7	h	63/65 (96%)	0.35	5 (7%) 15 16	23, 34, 46, 72	0
8	I	34/38 (89%)	-0.19	0 100 100	27, 35, 58, 77	0
8	i	37/38 (97%)	0.23	3 (8%) 15 16	26, 32, 84, 89	0
9	J	36/40 (90%)	0.21	3 (8%) 14 15	24, 38, 65, 81	0
9	j	40/40 (100%)	0.22	5 (12%) 5 5	24, 36, 69, 76	0
10	K	37/37 (100%)	0.05	2 (5%) 29 31	31, 37, 47, 56	0
10	k	37/37 (100%)	0.24	2 (5%) 29 31	29, 37, 55, 66	0
11	L	37/37 (100%)	-0.10	3 (8%) 15 16	15, 20, 62, 80	0
11	l	36/37 (97%)	-0.04	2 (5%) 28 30	17, 20, 68, 76	0
12	M	34/36 (94%)	-0.16	2 (5%) 26 27	19, 23, 52, 75	0
12	m	34/36 (94%)	0.11	2 (5%) 26 27	19, 24, 53, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	O	243/244 (99%)	0.08	17 (6%) 19 20	16, 30, 55, 86	0
13	o	243/244 (99%)	0.17	29 (11%) 6 6	16, 32, 65, 86	0
14	T	29/32 (90%)	0.26	1 (3%) 49 50	17, 21, 45, 81	0
14	t	30/32 (93%)	0.29	2 (6%) 21 22	18, 22, 55, 85	0
15	U	97/104 (93%)	-0.22	0 100 100	20, 28, 46, 59	0
15	u	97/104 (93%)	-0.37	1 (1%) 84 85	22, 27, 40, 63	0
16	V	137/137 (100%)	-0.35	0 100 100	20, 26, 41, 59	0
16	v	137/137 (100%)	0.23	9 (6%) 22 23	23, 33, 51, 71	0
17	Y	29/30 (96%)	1.27	9 (31%) 1 0	38, 46, 69, 72	0
17	y	29/30 (96%)	0.85	6 (20%) 1 1	38, 47, 59, 69	0
18	X	38/40 (95%)	0.58	6 (15%) 3 3	29, 39, 58, 62	0
18	x	38/40 (95%)	0.82	6 (15%) 3 3	31, 38, 83, 98	0
19	Z	62/62 (100%)	1.61	21 (33%) 0 0	36, 45, 83, 96	0
19	z	61/62 (98%)	1.64	23 (37%) 0 0	42, 52, 83, 103	0
All	All	5249/5350 (98%)	0.05	314 (5%) 25 27	14, 28, 55, 109	0

All (314) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	b	487	SER	9.5
6	F	11	VAL	8.0
2	b	496	TYR	7.7
19	z	3	ILE	7.4
18	x	37	VAL	7.3
14	T	30	THR	7.2
2	b	503	THR	7.1
2	B	494	GLY	6.9
2	b	495	PHE	6.9
2	B	486	LEU	6.6
5	E	84	LYS	6.5
2	b	493	TRP	6.4
2	B	495	PHE	6.4
19	Z	33	TRP	6.3
2	b	502	VAL	6.3
5	E	79	PHE	6.2
5	E	83	LEU	6.2
6	F	12	SER	6.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
18	x	38	GLN	6.1
13	o	36	GLN	6.1
11	L	1	MET	5.9
14	t	31	LYS	5.9
7	H	64	ALA	5.8
1	a	13	LEU	5.7
13	o	246	ALA	5.7
7	h	64	ALA	5.7
19	z	4	LEU	5.5
1	A	11	ALA	5.4
19	z	2	THR	5.4
2	B	496	TYR	5.3
2	b	484	PRO	5.3
19	Z	35	ARG	5.3
2	b	491	VAL	5.2
17	y	18	VAL	5.2
18	X	37	VAL	5.2
3	C	23	ALA	5.0
19	Z	32	ASP	5.0
18	x	39	ARG	5.0
2	B	293	ALA	5.0
1	a	11	ALA	4.9
9	j	1	MET	4.9
18	x	2	THR	4.8
11	L	2	GLU	4.8
5	E	82	GLN	4.8
19	Z	30	PRO	4.8
19	z	5	PHE	4.7
2	b	504	THR	4.7
9	J	5	GLY	4.7
17	Y	18	VAL	4.7
13	o	35	SER	4.6
19	Z	60	PHE	4.6
6	F	15	ILE	4.6
19	Z	31	GLN	4.5
2	B	505	ARG	4.5
5	E	74	GLN	4.5
5	E	17	VAL	4.4
6	F	16	PHE	4.4
2	b	494	GLY	4.4
13	o	32	ILE	4.4
2	B	487	SER	4.4

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Mol	Chain	Res	Type	RSRZ
19	z	7	LEU	4.3
5	E	20	TRP	4.2
19	Z	41	PHE	4.2
12	M	34	LYS	4.2
3	C	143	TYR	4.2
4	d	11	GLU	4.2
2	b	488	PRO	4.2
3	C	155[A]	ASN	4.1
2	B	506	LYS	4.1
19	Z	3	ILE	4.0
5	e	59	GLU	4.0
10	k	18	PHE	4.0
5	E	80	LEU	4.0
19	Z	4	LEU	4.0
5	E	22	ILE	3.9
11	L	3	PRO	3.9
5	E	25	ILE	3.9
17	Y	19	ILE	3.9
17	y	19	ILE	3.9
16	v	16	GLY	3.9
19	z	60	PHE	3.9
9	j	2	MET	3.9
13	o	27	ARG	3.9
13	o	38	TYR	3.9
13	o	4	THR	3.8
2	B	485	GLU	3.8
5	E	81	GLU	3.8
3	C	257	PHE	3.8
5	e	72	ALA	3.8
19	Z	1	MET	3.8
12	M	33	GLN	3.8
8	i	37	LEU	3.7
18	X	34	ILE	3.7
19	Z	38	GLN	3.7
9	J	6	GLY	3.7
5	e	84	LYS	3.7
2	b	295	GLY	3.7
15	u	8	GLU	3.7
16	v	21	LEU	3.7
2	b	490	GLN	3.7
13	o	34	SER	3.7
19	z	61	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	504	THR	3.6
13	O	60	ARG	3.6
13	o	133	VAL	3.6
6	F	13	TYR	3.6
10	k	17	ILE	3.6
5	E	77	GLU	3.6
19	Z	36	SER	3.6
2	b	500	GLY	3.6
18	X	2	THR	3.6
17	y	20	ALA	3.5
2	b	499	VAL	3.5
19	z	6	GLN	3.5
13	o	135	SER	3.5
5	E	78	THR	3.5
5	E	6	GLY	3.5
13	o	26	ALA	3.4
5	e	25	ILE	3.4
5	E	72	ALA	3.4
2	B	500	GLY	3.4
3	c	21	ILE	3.4
16	v	14	SER	3.4
5	E	21	VAL	3.4
2	B	488	PRO	3.3
9	J	8	ILE	3.3
11	l	3	PRO	3.3
13	O	25	THR	3.3
19	z	1	MET	3.3
6	f	14	PRO	3.3
19	Z	34	ASP	3.3
13	o	134	THR	3.3
19	z	38	GLN	3.3
1	A	12	ASN	3.3
16	v	19	ILE	3.3
17	y	22	LEU	3.2
4	D	11	GLU	3.2
2	b	129	GLY	3.2
2	b	489	GLU	3.2
19	z	9	LEU	3.1
4	D	12	ARG	3.1
1	a	15[A]	GLU	3.1
19	z	59	PHE	3.1
3	c	279	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
5	E	61	ARG	3.1
18	X	39	ARG	3.1
8	i	38	GLU	3.1
13	o	60	ARG	3.1
17	Y	22	LEU	3.1
19	Z	39	LEU	3.1
5	E	73	LYS	3.1
2	B	503	THR	3.1
16	v	18	THR	3.1
5	E	76	VAL	3.0
19	Z	61	VAL	3.0
19	z	32	ASP	3.0
19	Z	42	LEU	3.0
13	O	136	ILE	3.0
19	Z	2	THR	3.0
1	A	16	ARG	3.0
5	e	61	ARG	3.0
2	B	501	ASP	3.0
2	b	492	GLU	2.9
19	z	39	LEU	2.9
3	C	259	TRP	2.9
19	z	35	ARG	2.9
3	c	432	VAL	2.9
19	z	41	PHE	2.9
13	o	132	ASN	2.9
5	e	21	VAL	2.9
13	o	37	THR	2.9
2	b	292	LEU	2.9
2	B	484	PRO	2.9
17	Y	20	ALA	2.9
13	O	87	VAL	2.9
13	O	26	ALA	2.9
3	c	143	TYR	2.9
13	O	130	GLN	2.9
13	o	136	ILE	2.9
1	a	262	TYR	2.8
13	o	23	ASP	2.8
13	o	25	THR	2.8
3	c	433	LEU	2.8
5	E	4	THR	2.8
1	a	235	TYR	2.8
13	O	27	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
12	m	5	GLN	2.8
13	o	30	TYR	2.8
13	o	87	VAL	2.8
3	c	434	ALA	2.7
19	Z	7	LEU	2.7
19	z	30	PRO	2.7
3	C	25	ASN	2.7
17	y	40	ALA	2.7
19	Z	29	SER	2.7
2	b	126	PRO	2.7
13	o	33	ASP	2.7
17	Y	21	GLN	2.7
13	o	204	VAL	2.7
13	o	245	PRO	2.7
13	O	133	VAL	2.7
4	D	240	ALA	2.6
4	d	240	ALA	2.6
13	O	207	ARG	2.6
13	o	24	ASP	2.6
19	z	33	TRP	2.6
5	e	6	GLY	2.6
17	Y	40	ALA	2.6
2	B	483	ASP	2.6
1	a	16	ARG	2.6
13	O	30	TYR	2.6
13	o	131	PRO	2.6
2	b	297	THR	2.6
2	B	499	VAL	2.6
4	d	12	ARG	2.5
6	F	14	PRO	2.5
7	h	23	PRO	2.5
18	x	34	ILE	2.5
19	Z	62	VAL	2.5
1	a	12	ASN	2.5
2	B	247	PHE	2.5
3	c	20	SER	2.5
16	v	5	PRO	2.5
3	c	207	ARG	2.5
2	b	218	LEU	2.5
2	b	501	ASP	2.5
16	v	15	GLU	2.5
2	B	298	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
9	j	4	GLU	2.5
13	O	206	GLY	2.4
5	e	32	ILE	2.4
13	O	135	SER	2.4
13	o	130	GLN	2.4
2	b	483	ASP	2.4
2	b	293	ALA	2.4
3	C	434	ALA	2.4
18	x	36	LYS	2.4
3	c	435	PHE	2.4
2	B	253	ALA	2.4
16	v	12	LEU	2.4
14	t	30	THR	2.4
2	b	161	LEU	2.3
2	B	296	ALA	2.3
7	h	57	GLY	2.3
8	i	36	ASP	2.3
2	B	490	GLN	2.3
19	Z	57	LEU	2.3
3	C	252	ILE	2.3
13	o	58	ASN	2.3
2	B	295	GLY	2.3
9	j	6	GLY	2.3
5	e	26	THR	2.3
3	C	431	PHE	2.3
5	E	71	GLU	2.3
10	K	14	ALA	2.3
3	C	255	THR	2.3
1	a	230	THR	2.3
1	A	243	GLU	2.3
2	B	489	GLU	2.3
9	j	5	GLY	2.2
7	h	56	ASP	2.2
2	B	497	GLN	2.2
2	B	479	PHE	2.2
6	f	16	PHE	2.2
5	E	18	ARG	2.2
13	o	89	SER	2.2
2	B	297	THR	2.2
5	e	79	PHE	2.2
5	e	23	HIS	2.2
16	v	8	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	b	479	PHE	2.2
3	c	436	PHE	2.2
19	z	10	ALA	2.2
18	X	33	GLN	2.2
5	E	19	TYR	2.2
19	z	58	ASN	2.2
3	c	146	PHE	2.2
13	O	204	VAL	2.2
5	E	32	ILE	2.1
19	z	57	LEU	2.1
12	m	33	GLN	2.1
3	C	256	PRO	2.1
2	b	461	LEU	2.1
19	z	42	LEU	2.1
2	B	248	ALA	2.1
1	a	243	GLU	2.1
3	c	257	PHE	2.1
3	c	201	ASN	2.1
3	C	285	ILE	2.1
11	l	2	GLU	2.1
18	X	3	ILE	2.1
2	b	294	SER	2.1
13	O	132	ASN	2.1
3	C	146	PHE	2.1
3	c	200	THR	2.1
17	Y	34	MET	2.1
2	b	298	LEU	2.1
3	C	253	LEU	2.1
13	o	139	SER	2.1
2	b	246	PHE	2.1
13	O	89	SER	2.1
10	K	17	ILE	2.1
13	O	24	ASP	2.0
7	h	22	ALA	2.0
3	c	426	LEU	2.0
5	e	14	ILE	2.0
13	O	23	ASP	2.0
17	y	21	GLN	2.0
2	b	459	ALA	2.0
7	H	56[A]	ASP	2.0
17	Y	30	ILE	2.0
5	e	24	SER	2.0

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Mol	Chain	Res	Type	RSRZ
19	z	29	SER	2.0
17	Y	42	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
14	FME	T	1	10/11	0.97	0.07	-	19,26,45,49	0
8	FME	I	1	10/11	0.97	0.09	-	27,32,36,36	0
8	FME	i	1	10/11	0.98	0.08	-	28,29,33,33	0
14	FME	t	1	10/11	0.97	0.08	-	18,24,45,50	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
31	DMS	b	637	4/4	0.89	0.32	23.67	61,63,68,74	0
29	UNL	T	102	13/-	0.80	0.50	22.60	62,68,75,75	0
29	UNL	A	417	4/-	0.92	0.52	17.13	58,61,63,67	0
31	DMS	b	640	4/4	0.86	0.19	15.87	67,70,78,83	0
31	DMS	b	645	4/4	0.82	0.46	15.86	70,77,83,84	0
29	UNL	J	104	16/-	0.54	0.37	14.81	62,82,99,99	0
31	DMS	O	311	4/4	0.84	0.27	14.36	59,59,71,73	0
29	UNL	t	102	16/-	0.76	0.37	13.77	53,62,74,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
29	UNL	a	419	6/-	0.81	0.36	11.31	47,53,53,53	0
31	DMS	b	644	4/4	0.46	0.39	10.59	73,76,78,96	0
31	DMS	U	202	4/4	0.88	0.22	10.53	33,45,50,55	0
31	DMS	C	525	4/4	0.93	0.19	10.40	39,39,43,46	0
30	LMT	F	101	35/35	0.66	0.39	10.39	64,88,93,96	0
36	DGD	D	407	50/66	0.61	0.31	9.92	54,71,97,97	0
31	DMS	O	304	4/4	0.66	0.26	9.78	69,71,78,87	0
31	DMS	u	206	4/4	0.75	0.30	9.70	70,71,76,93	0
31	DMS	V	211	4/4	0.52	0.36	9.49	61,61,68,79	0
31	DMS	A	421	4/4	0.83	0.25	9.36	57,63,74,78	0
31	DMS	b	646	4/4	0.81	0.36	9.27	84,87,89,96	0
31	DMS	c	929	4/4	0.81	0.43	8.93	46,62,67,70	0
35	HTG	d	413	19/19	0.65	0.27	8.47	62,86,104,106	0
31	DMS	o	303	4/4	0.94	0.23	8.34	51,55,67,70	0
35	HTG	D	414	19/19	0.59	0.37	8.09	76,92,111,112	0
29	UNL	B	629	14/-	0.54	0.28	7.79	62,72,81,82	0
31	DMS	u	203	4/4	0.94	0.21	7.32	38,50,51,52	0
31	DMS	C	529	4/4	0.89	0.29	7.29	54,66,72,74	0
31	DMS	c	932	4/4	0.95	0.32	7.28	54,57,63,64	0
29	UNL	e	102	16/-	0.72	0.38	7.09	54,61,69,72	0
31	DMS	o	304	4/4	0.73	0.28	7.04	63,68,70,84	0
29	UNL	x	103	15/-	0.87	0.17	6.73	31,40,57,58	0
29	UNL	E	102	16/-	0.68	0.39	6.59	58,61,76,77	0
31	DMS	c	925	4/4	0.96	0.16	6.29	35,37,42,49	0
29	UNL	i	103	16/-	0.73	0.33	6.20	58,61,67,70	0
35	HTG	b	622	19/19	0.88	0.23	5.97	28,41,57,64	0
36	DGD	d	407	50/66	0.63	0.27	5.92	58,74,97,98	0
29	UNL	D	413	16/-	0.92	0.21	5.91	36,42,57,58	0
29	UNL	b	626	16/-	0.63	0.28	5.64	59,68,73,73	0
35	HTG	c	922	19/19	0.68	0.41	5.49	53,84,96,100	0
29	UNL	E	103	13/-	0.71	0.34	5.38	63,68,85,87	0
27	PL9	A	411	55/55	0.73	0.25	5.36	45,59,80,84	0
29	UNL	u	202	16/-	0.79	0.28	5.35	41,54,60,62	0
30	LMT	e	103	25/35	0.75	0.32	5.15	60,77,93,95	0
31	DMS	C	527	4/4	0.92	0.19	5.14	58,68,73,83	0
29	UNL	d	412	16/-	0.89	0.25	4.82	31,40,54,57	0
35	HTG	C	522	19/19	0.72	0.35	4.66	41,78,86,87	0
30	LMT	A	416	35/35	0.82	0.20	4.65	42,63,86,98	0
28	LHG	K	101	44/49	0.67	0.32	4.57	63,93,124,137	0
27	PL9	a	414	55/55	0.71	0.24	4.55	46,61,86,88	0
31	DMS	O	305	4/4	0.95	0.41	4.54	65,70,70,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
30	LMT	T	103	24/35	0.84	0.20	4.45	34,56,76,83	0
31	DMS	B	636	4/4	0.97	0.12	4.33	18,20,22,28	0
31	DMS	B	638	4/4	0.95	0.17	4.32	55,60,62,71	0
31	DMS	B	645	4/4	0.85	0.24	4.30	50,61,64,69	0
31	DMS	v	209	4/4	0.92	0.15	4.27	49,50,58,64	0
30	LMT	B	644	24/35	0.82	0.21	4.08	34,52,81,87	0
29	UNL	I	103	16/-	0.72	0.28	3.95	51,57,70,74	0
30	LMT	B	643	24/35	0.71	0.23	3.94	50,77,114,118	0
31	DMS	O	308	4/4	0.85	0.27	3.86	54,64,77,81	0
31	DMS	F	102	4/4	0.97	0.14	3.77	48,48,50,64	0
30	LMT	a	418	35/35	0.73	0.23	3.73	44,63,79,80	0
35	HTG	B	625	19/19	0.85	0.17	3.72	28,42,49,51	0
29	UNL	k	101	8/-	0.77	0.18	3.57	59,71,78,80	0
31	DMS	A	419	4/4	0.67	0.37	3.52	75,76,91,97	0
39	MG	j	102	1/1	0.99	0.14	3.49	28,28,28,28	0
28	LHG	d	402	44/49	0.62	0.23	3.47	59,78,125,135	0
31	DMS	d	415	4/4	0.93	0.20	3.45	45,53,57,73	0
23	CLA	B	602	65/65	0.93	0.19	3.41	28,39,75,85	0
29	UNL	B	632	16/-	0.76	0.25	3.21	44,61,68,70	0
35	HTG	C	523	19/19	0.82	0.29	3.16	60,78,95,97	0
26	SQD	B	621	54/54	0.68	0.24	3.13	43,63,88,93	0
31	DMS	k	103	4/4	0.72	0.33	3.11	90,92,93,104	0
35	HTG	c	923	13/19	0.68	0.34	3.09	59,72,86,87	0
25	BCR	D	405	40/40	0.95	0.16	3.06	22,28,54,57	0
29	UNL	U	201	14/-	0.79	0.26	3.06	38,50,58,61	0
25	BCR	B	619	40/40	0.96	0.19	3.02	20,25,41,45	0
28	LHG	E	101	49/49	0.70	0.28	2.99	39,83,104,109	0
34	LMG	C	531	51/55	0.76	0.22	2.98	38,78,93,98	0
28	LHG	A	412	49/49	0.63	0.35	2.94	59,83,104,111	0
31	DMS	C	526	4/4	0.92	0.16	2.87	49,56,57,62	0
34	LMG	J	101	51/55	0.93	0.17	2.86	25,31,85,93	0
34	LMG	d	411	51/55	0.77	0.23	2.85	39,70,101,108	0
29	UNL	Z	102	14/-	0.76	0.32	2.82	63,67,74,76	0
26	SQD	a	417	54/54	0.81	0.17	2.79	38,53,72,73	0
36	DGD	C	519	62/66	0.95	0.12	2.60	21,28,68,83	0
31	DMS	v	202	4/4	0.93	0.17	2.60	68,74,76,81	0
28	LHG	e	101	40/49	0.61	0.25	2.58	55,93,121,126	0
31	DMS	O	303	4/4	0.94	0.21	2.56	59,66,69,73	0
29	UNL	A	414	13/-	0.62	0.34	2.55	58,71,83,83	0
29	UNL	j	103	16/-	0.81	0.17	2.52	45,56,61,62	0
31	DMS	B	641	4/4	0.83	0.21	2.52	62,63,65,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
25	BCR	d	405	40/40	0.95	0.09	2.51	21,27,50,54	0
26	SQD	L	102	54/54	0.75	0.20	2.50	42,58,87,90	0
35	HTG	O	302	19/19	0.93	0.12	2.49	36,39,48,49	0
29	UNL	J	103	16/-	0.82	0.17	2.47	46,54,60,63	0
34	LMG	c	930	51/55	0.77	0.22	2.47	33,69,81,84	0
31	DMS	c	933	4/4	0.80	0.17	2.46	61,64,65,77	0
28	LHG	d	408	49/49	0.94	0.20	2.45	25,33,43,44	0
31	DMS	V	210	4/4	0.90	0.15	2.39	64,65,67,73	0
31	DMS	D	417	4/4	0.86	0.23	2.35	53,54,58,59	0
31	DMS	D	416	4/4	0.97	0.20	2.35	56,57,58,62	0
23	CLA	b	602	65/65	0.92	0.17	2.26	29,42,66,71	0
31	DMS	b	635	4/4	0.89	0.17	2.19	53,63,69,71	0
35	HTG	V	204	14/19	0.90	0.18	2.19	42,45,71,82	0
29	UNL	J	105	11/-	0.54	0.27	2.19	61,67,75,78	0
29	UNL	z	102	13/-	0.72	0.23	2.17	53,62,72,75	0
31	DMS	b	638	4/4	0.75	0.20	2.17	54,60,67,74	0
35	HTG	v	204	19/19	0.69	0.33	2.13	62,70,81,91	0
31	DMS	V	202	4/4	0.91	0.16	2.13	31,32,38,48	0
29	UNL	X	101	16/-	0.84	0.17	2.11	33,37,60,61	0
31	DMS	v	201	4/4	0.98	0.12	2.10	46,48,51,51	0
29	UNL	u	201	11/-	0.81	0.28	2.09	39,50,60,61	0
30	LMT	z	101	32/35	0.78	0.23	2.07	43,88,96,99	0
26	SQD	A	415	54/54	0.84	0.18	2.02	39,54,72,76	0
25	BCR	T	101	40/40	0.96	0.16	2.02	22,29,40,41	0
31	DMS	b	647	4/4	0.87	0.28	2.01	67,78,85,86	0
30	LMT	I	101	35/35	0.77	0.30	2.00	63,75,85,91	0
35	HTG	b	627	19/19	0.89	0.14	1.97	39,59,72,82	0
26	SQD	D	408	45/54	0.85	0.29	1.96	45,67,86,93	0
31	DMS	i	105	4/4	0.94	0.24	1.90	61,64,71,73	0
34	LMG	a	413	51/55	0.81	0.19	1.90	41,53,68,74	0
28	LHG	a	415	49/49	0.53	0.34	1.89	56,72,99,108	0
34	LMG	C	501	51/55	0.83	0.20	1.86	37,51,63,70	0
29	UNL	E	104	16/-	0.71	0.23	1.77	67,71,74,76	0
26	SQD	A	410	54/54	0.90	0.17	1.77	31,55,74,80	0
34	LMG	D	412	51/55	0.66	0.25	1.76	37,65,106,119	0
31	DMS	B	639	4/4	0.95	0.15	1.75	44,48,51,54	0
31	DMS	c	926	4/4	0.97	0.15	1.72	66,68,69,77	0
31	DMS	b	633	4/4	0.98	0.10	1.72	21,23,24,25	0
34	LMG	B	622	51/55	0.85	0.17	1.71	31,41,52,67	0
34	LMG	m	102	51/55	0.83	0.19	1.70	33,41,54,61	0
26	SQD	x	101	41/54	0.84	0.24	1.70	54,76,95,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	a	407	65/65	0.97	0.13	1.59	17,20,95,102	0
23	CLA	A	406	65/65	0.97	0.14	1.59	18,20,90,96	0
31	DMS	b	636	4/4	0.95	0.17	1.58	44,48,50,52	0
26	SQD	a	412	54/54	0.91	0.15	1.57	31,53,72,76	0
23	CLA	B	611	65/65	0.96	0.13	1.57	20,24,33,39	0
25	BCR	b	619	40/40	0.96	0.18	1.57	20,27,41,43	0
28	LHG	D	411	46/49	0.96	0.12	1.53	25,30,82,85	0
30	LMT	a	422	35/35	0.83	0.35	1.51	61,74,82,85	0
28	LHG	d	409	49/49	0.95	0.13	1.49	18,24,44,47	0
36	DGD	C	518	62/66	0.93	0.13	1.47	24,33,70,80	0
28	LHG	D	409	49/49	0.93	0.15	1.47	27,34,41,47	0
31	DMS	H	101	4/4	0.83	0.28	1.46	54,58,62,65	0
25	BCR	B	618	40/40	0.96	0.12	1.44	19,24,30,33	0
36	DGD	h	102	62/66	0.88	0.18	1.42	24,31,41,47	0
28	LHG	L	101	49/49	0.94	0.12	1.41	22,31,42,48	0
23	CLA	B	606	65/65	0.97	0.16	1.41	18,22,32,34	0
36	DGD	H	103	62/66	0.92	0.18	1.38	23,32,38,39	0
31	DMS	c	927	4/4	0.93	0.15	1.38	30,37,37,44	0
36	DGD	C	517	62/66	0.95	0.17	1.37	21,29,69,71	0
24	PHO	a	409	64/64	0.97	0.13	1.35	17,22,27,30	0
31	DMS	a	421	4/4	0.88	0.28	1.34	81,84,85,92	0
23	CLA	b	608	65/65	0.97	0.14	1.30	16,20,28,36	0
35	HTG	B	630	19/19	0.87	0.13	1.29	41,55,62,66	0
28	LHG	d	410	46/49	0.96	0.14	1.29	24,27,73,84	0
31	DMS	d	416	4/4	0.96	0.15	1.25	47,52,59,64	0
23	CLA	B	608	65/65	0.97	0.13	1.24	16,19,32,35	0
25	BCR	C	516	40/40	0.94	0.12	1.23	28,34,40,43	0
34	LMG	j	101	51/55	0.94	0.10	1.20	22,33,80,85	0
30	LMT	m	103	35/35	0.71	0.19	1.20	48,92,102,103	0
30	LMT	Z	101	35/35	0.70	0.25	1.18	41,88,100,102	0
34	LMG	C	520	51/55	0.84	0.20	1.17	31,61,74,79	0
35	HTG	B	624	19/19	0.93	0.12	1.16	35,39,46,47	0
25	BCR	A	409	40/40	0.97	0.12	1.13	19,23,29,32	0
23	CLA	c	909	65/65	0.95	0.16	1.12	22,26,79,92	0
27	PL9	d	406	55/55	0.96	0.12	1.10	16,21,27,34	0
23	CLA	c	910	65/65	0.96	0.17	1.08	23,27,49,60	0
23	CLA	d	401	65/65	0.98	0.12	1.06	15,17,26,31	0
34	LMG	c	920	51/55	0.84	0.19	1.04	27,55,81,84	0
28	LHG	l	101	49/49	0.94	0.15	1.02	20,28,48,52	0
25	BCR	t	101	40/40	0.95	0.14	1.00	19,26,38,40	0
23	CLA	c	911	65/65	0.97	0.21	0.98	20,26,36,40	0
23	CLA	C	506	65/65	0.96	0.13	0.94	25,31,40,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	d	414	4/4	0.94	0.11	0.93	62,66,71,78	0
35	HTG	b	623	19/19	0.80	0.25	0.92	47,76,83,84	0
23	CLA	b	612	65/65	0.96	0.16	0.91	18,21,36,42	0
30	LMT	b	621	25/35	0.71	0.19	0.90	45,70,90,91	0
36	DGD	c	917	62/66	0.95	0.15	0.90	20,30,74,77	0
23	CLA	b	606	65/65	0.97	0.12	0.88	18,22,29,33	0
23	CLA	C	509	65/65	0.95	0.13	0.88	24,29,76,85	0
36	DGD	c	919	62/66	0.94	0.11	0.87	22,29,50,56	0
23	CLA	B	610	65/65	0.88	0.13	0.87	21,28,32,34	0
23	CLA	b	614	65/65	0.97	0.18	0.86	17,21,47,54	0
23	CLA	B	605	65/65	0.97	0.17	0.83	18,21,52,53	0
31	DMS	B	648	4/4	0.93	0.31	0.82	43,45,47,48	0
23	CLA	B	617	65/65	0.96	0.11	0.81	20,27,93,106	0
23	CLA	D	404	65/65	0.94	0.13	0.79	23,27,67,73	0
24	PHO	D	402	64/64	0.97	0.13	0.79	16,21,25,29	0
23	CLA	a	410	65/65	0.97	0.10	0.79	17,22,91,94	0
23	CLA	B	613	65/65	0.96	0.13	0.78	18,23,28,31	0
30	LMT	m	104	35/35	0.74	0.20	0.77	34,51,56,58	0
31	DMS	u	205	4/4	0.91	0.21	0.77	41,50,54,58	0
23	CLA	A	408	65/65	0.97	0.11	0.76	18,22,89,96	0
23	CLA	C	502	65/65	0.95	0.14	0.75	25,31,41,51	0
23	CLA	b	609	65/65	0.97	0.15	0.75	19,23,31,32	0
30	LMT	M	101	35/35	0.71	0.22	0.75	31,50,59,60	0
28	LHG	D	410	49/49	0.96	0.11	0.73	20,27,42,46	0
23	CLA	b	615	65/65	0.96	0.14	0.73	19,24,71,76	0
23	CLA	B	614	65/65	0.98	0.15	0.72	18,20,44,51	0
31	DMS	b	634	4/4	0.97	0.11	0.70	42,45,48,48	0
24	PHO	A	407	64/64	0.97	0.11	0.69	17,19,22,22	0
31	DMS	V	208	4/4	0.93	0.13	0.67	69,70,71,72	0
23	CLA	c	904	65/65	0.93	0.15	0.67	25,32,37,40	0
23	CLA	b	604	65/65	0.96	0.13	0.65	19,23,29,32	0
23	CLA	c	903	65/65	0.95	0.18	0.61	20,24,37,43	0
23	CLA	B	612	65/65	0.97	0.12	0.61	17,20,36,52	0
25	BCR	b	618	40/40	0.96	0.13	0.59	20,25,32,33	0
25	BCR	b	620	40/40	0.96	0.11	0.59	25,29,40,44	0
23	CLA	d	403	65/65	0.97	0.11	0.56	13,18,36,42	0
23	CLA	C	510	65/65	0.95	0.12	0.55	25,31,52,55	0
23	CLA	c	902	65/65	0.96	0.12	0.54	24,27,38,46	0
27	PL9	D	406	55/55	0.96	0.09	0.53	17,22,28,30	0
23	CLA	B	616	65/65	0.95	0.10	0.52	23,27,43,49	0
23	CLA	C	505	65/65	0.96	0.13	0.52	25,28,58,60	0
23	CLA	B	604	65/65	0.96	0.14	0.52	18,21,30,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
23	CLA	C	504	65/65	0.95	0.10	0.52	24,31,36,41	0
23	CLA	B	609	65/65	0.97	0.14	0.50	19,23,28,29	0
23	CLA	b	607	65/65	0.93	0.11	0.47	22,27,54,63	0
31	DMS	V	201	4/4	0.98	0.10	0.47	41,46,47,47	0
30	LMT	B	623	35/35	0.74	0.21	0.46	48,72,89,93	0
31	DMS	B	637	4/4	0.97	0.11	0.41	35,38,40,42	0
23	CLA	D	403	65/65	0.96	0.10	0.40	13,17,33,41	0
23	CLA	c	905	65/65	0.95	0.16	0.40	21,27,51,54	0
23	CLA	B	603	65/65	0.92	0.13	0.39	20,26,33,36	0
23	CLA	B	615	65/65	0.96	0.11	0.38	18,23,66,71	0
23	CLA	c	913	65/65	0.92	0.12	0.37	30,39,65,68	0
31	DMS	V	209	4/4	0.94	0.12	0.36	58,59,62,65	0
23	CLA	b	610	65/65	0.91	0.11	0.35	22,27,31,39	0
31	DMS	h	101	4/4	0.94	0.17	0.34	47,51,52,53	0
38	RRX	H	102	41/41	0.89	0.13	0.32	25,29,38,44	0
24	PHO	a	408	64/64	0.97	0.11	0.32	15,18,20,22	0
21	FE2	a	403	1/1	0.99	0.07	0.31	25,25,25,25	0
22	CL	A	403	1/1	1.00	0.07	0.30	19,19,19,19	0
23	CLA	c	914	65/65	0.92	0.12	0.30	36,44,76,80	0
23	CLA	C	514	65/65	0.89	0.15	0.29	37,47,67,72	0
23	CLA	b	605	65/65	0.96	0.14	0.28	17,22,53,55	0
23	CLA	D	401	65/65	0.98	0.09	0.27	13,17,27,35	0
23	CLA	C	511	65/65	0.96	0.12	0.17	24,30,35,40	0
23	CLA	A	405	65/65	0.97	0.09	0.17	14,17,26,34	0
23	CLA	b	613	65/65	0.97	0.13	0.16	18,24,29,34	0
23	CLA	d	404	65/65	0.96	0.10	0.12	22,27,66,72	0
23	CLA	b	603	65/65	0.93	0.12	0.11	21,24,33,41	0
23	CLA	c	906	65/65	0.95	0.10	0.08	25,29,44,47	0
23	CLA	a	406	65/65	0.97	0.11	0.07	14,17,25,37	0
36	DGD	c	918	62/66	0.95	0.13	0.07	24,30,75,84	0
23	CLA	b	611	65/65	0.96	0.10	0.05	19,24,32,37	0
25	BCR	Y	101	40/40	0.95	0.09	0.05	29,33,40,41	0
23	CLA	B	607	65/65	0.94	0.10	0.05	20,26,53,60	0
38	RRX	x	102	41/41	0.88	0.13	0.04	23,29,46,52	0
23	CLA	C	507	65/65	0.90	0.13	0.02	25,42,79,81	0
23	CLA	c	908	65/65	0.95	0.11	-0.02	23,28,46,54	0
23	CLA	C	503	65/65	0.96	0.12	-0.05	23,27,37,42	0
25	BCR	a	411	40/40	0.95	0.08	-0.07	20,23,27,28	0
25	BCR	k	102	40/40	0.93	0.11	-0.08	27,32,38,40	0
23	CLA	C	513	65/65	0.93	0.11	-0.09	34,42,73,76	0
25	BCR	c	916	40/40	0.94	0.10	-0.13	25,32,38,38	0
37	HEM	e	105	43/43	0.98	0.15	-0.13	35,39,51,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	v	207	4/4	0.96	0.14	-0.16	53,54,54,60	0
23	CLA	b	617	65/65	0.94	0.12	-0.18	20,30,81,89	0
25	BCR	B	620	40/40	0.95	0.09	-0.22	21,29,41,42	0
23	CLA	c	907	65/65	0.93	0.10	-0.36	23,36,73,76	0
23	CLA	C	508	65/65	0.94	0.10	-0.36	28,35,49,55	0
37	HEM	V	203	43/43	0.98	0.07	-0.38	19,22,26,29	0
31	DMS	e	104	4/4	0.95	0.11	-0.38	72,73,78,83	0
25	BCR	c	915	40/40	0.94	0.10	-0.40	36,44,48,50	0
37	HEM	E	105	43/43	0.95	0.12	-0.40	36,42,46,47	0
25	BCR	C	515	40/40	0.93	0.09	-0.42	35,43,46,48	0
39	MG	J	102	1/1	0.99	0.09	-0.44	30,30,30,30	0
25	BCR	C	530	40/40	0.95	0.08	-0.47	27,32,36,37	0
37	HEM	v	203	43/43	0.98	0.08	-0.48	22,27,29,32	0
23	CLA	c	912	65/65	0.96	0.09	-0.54	26,31,37,41	0
25	BCR	j	104	40/40	0.95	0.08	-0.59	27,32,39,43	0
20	OEX	a	402	10/10	1.00	0.09	-0.71	21,23,24,24	0
20	OEX	A	401	10/10	1.00	0.08	-0.73	19,21,23,24	0
23	CLA	b	616	65/65	0.95	0.09	-0.76	21,26,42,44	0
23	CLA	C	512	65/65	0.94	0.08	-0.77	26,34,39,40	0
32	BCT	A	420	4/4	0.95	0.07	-0.78	31,32,35,40	0
32	BCT	a	424	4/4	0.97	0.06	-0.83	32,35,37,41	0
31	DMS	D	415	4/4	0.98	0.09	-1.16	50,53,56,59	0
22	CL	a	405	1/1	0.99	0.09	-1.53	21,21,21,21	0
21	FE2	A	402	1/1	0.99	0.04	-1.86	28,28,28,28	0
22	CL	a	404	1/1	0.99	0.06	-2.21	19,19,19,19	0
22	CL	A	404	1/1	1.00	0.08	-2.37	20,20,20,20	0
33	CA	o	302	1/1	0.94	0.06	-3.20	43,43,43,43	0
33	CA	c	901	1/1	0.98	0.04	-3.49	39,39,39,39	0
33	CA	O	301	1/1	0.95	0.08	-4.40	42,42,42,42	0
31	DMS	v	210	4/4	0.94	0.21	-	62,65,68,72	0
29	UNL	d	417	11/-	0.83	0.17	-	48,63,69,71	0
31	DMS	A	422	4/4	0.93	0.20	-	65,68,68,71	0
29	UNL	A	413	16/-	0.93	0.14	-	38,43,70,76	0
29	UNL	B	633	16/-	0.59	0.30	-	61,80,87,88	0
31	DMS	d	419	4/4	0.87	0.23	-	63,70,76,82	0
31	DMS	B	649	4/4	0.86	0.28	-	70,71,73,84	0
31	DMS	u	204	4/4	0.92	0.14	-	62,68,68,73	0
31	DMS	C	524	4/4	0.99	0.10	-	32,33,36,36	0
31	DMS	a	420	4/4	0.93	0.32	-	48,61,64,66	0
29	UNL	b	632	16/-	0.59	0.34	-	58,83,101,101	0
29	UNL	B	634	16/-	0.50	0.27	-	73,80,95,97	0
31	DMS	a	423	4/4	0.94	0.17	-	53,56,63,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	B	646	4/4	0.85	0.19	-	76,77,77,84	0
33	CA	B	601	1/1	0.96	0.10	-	41,41,41,41	0
31	DMS	c	936	4/4	0.65	0.29	-	80,80,81,90	0
31	DMS	B	647	4/4	0.80	0.37	-	81,85,85,89	0
31	DMS	v	205	4/4	0.95	0.11	-	63,66,68,69	0
31	DMS	h	105	4/4	0.80	0.19	-	76,83,89,90	0
31	DMS	b	641	4/4	0.92	0.21	-	52,59,66,66	0
31	DMS	b	643	4/4	0.83	0.33	-	81,82,85,85	0
29	UNL	b	631	16/-	0.41	0.23	-	61,73,81,82	0
29	UNL	I	104	16/-	0.50	0.29	-	69,76,89,92	0
31	DMS	i	106	4/4	0.17	0.34	-	120,121,124,138	0
31	DMS	U	204	4/4	0.61	0.21	-	53,62,62,80	0
31	DMS	l	102	4/4	0.88	0.14	-	64,65,70,84	0
29	UNL	Z	103	9/-	0.74	0.22	-	50,61,69,70	0
35	HTG	B	631	19/19	0.64	0.21	-	41,88,97,100	0
29	UNL	B	628	10/-	0.73	0.42	-	62,67,70,71	0
29	UNL	M	102	11/-	0.90	0.21	-	45,50,63,69	0
31	DMS	O	309	4/4	0.85	0.22	-	53,63,64,70	0
31	DMS	V	207	4/4	0.82	0.15	-	51,52,60,62	0
31	DMS	A	424	4/4	0.90	0.21	-	53,54,58,69	0
35	HTG	C	521	19/19	0.90	0.19	-	61,66,74,77	0
35	HTG	b	628	19/19	0.61	0.22	-	52,96,109,112	0
29	UNL	i	104	16/-	0.63	0.35	-	69,76,78,79	0
31	DMS	C	533	4/4	0.94	0.17	-	67,67,68,71	0
31	DMS	B	642	4/4	0.91	0.30	-	46,54,59,67	0
31	DMS	V	205	4/4	0.90	0.23	-	49,60,60,63	0
29	UNL	b	625	10/-	0.86	0.28	-	44,59,68,68	0
29	UNL	a	416	10/-	0.77	0.33	-	54,68,75,76	0
31	DMS	V	206	4/4	0.95	0.25	-	55,55,55,61	0
31	DMS	B	640	4/4	0.89	0.25	-	50,56,60,61	0
29	UNL	c	931	10/-	0.83	0.21	-	55,60,62,64	0
31	DMS	A	418	4/4	0.88	0.29	-	70,79,79,85	0
31	DMS	c	937	4/4	0.95	0.30	-	76,80,84,84	0
31	DMS	A	423	4/4	0.99	0.09	-	23,27,27,28	0
29	UNL	b	624	16/-	0.88	0.13	-	42,51,58,60	0
31	DMS	b	639	4/4	0.84	0.26	-	41,55,63,67	0
31	DMS	c	928	4/4	0.96	0.14	-	57,59,61,61	0
31	DMS	H	105	4/4	0.89	0.26	-	60,74,74,84	0
29	UNL	B	627	16/-	0.82	0.15	-	38,45,55,60	0
31	DMS	h	103	4/4	0.92	0.16	-	82,84,97,101	0
31	DMS	a	401	4/4	0.78	0.27	-	75,81,85,96	0
29	UNL	i	102	16/-	0.73	0.21	-	52,62,75,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	DMS	v	206	4/4	0.90	0.26	-	66,68,76,78	0
29	UNL	B	635	9/-	0.77	0.20	-	60,67,76,77	0
31	DMS	d	418	4/4	0.90	0.28	-	68,69,71,71	0
35	HTG	B	626	19/19	0.66	0.46	-	52,88,96,96	0
31	DMS	O	307	4/4	0.79	0.21	-	64,69,69,84	0
29	UNL	m	101	11/-	0.92	0.18	-	47,51,56,58	0
29	UNL	H	104	14/-	0.64	0.42	-	64,69,74,76	0
31	DMS	O	306	4/4	0.95	0.28	-	68,68,73,76	0
31	DMS	U	203	4/4	0.60	0.32	-	70,74,80,89	0
31	DMS	o	301	4/4	0.99	0.08	-	22,27,28,31	0
33	CA	b	601	1/1	0.98	0.08	-	41,41,41,41	0
31	DMS	c	935	4/4	0.86	0.28	-	71,72,75,83	0
29	UNL	I	102	13/-	0.83	0.16	-	47,53,65,69	0
29	UNL	b	629	12/-	0.84	0.34	-	49,59,70,71	0
31	DMS	O	310	4/4	0.86	0.25	-	61,67,74,76	0
31	DMS	c	924	4/4	0.99	0.09	-	31,33,36,36	0
31	DMS	C	528	4/4	0.91	0.15	-	60,63,65,66	0
29	UNL	i	101	16/-	0.91	0.13	-	37,43,60,60	0
35	HTG	c	921	19/19	0.84	0.21	-	68,82,88,91	0
31	DMS	b	642	4/4	0.70	0.34	-	90,90,97,101	0
31	DMS	c	934	4/4	0.86	0.27	-	87,87,89,99	0
29	UNL	C	532	11/-	0.88	0.23	-	54,59,66,66	0
31	DMS	h	104	4/4	0.87	0.27	-	97,99,103,103	0
31	DMS	v	208	4/4	0.89	0.22	-	54,67,71,87	0
29	UNL	b	630	16/-	0.38	0.34	-	74,86,106,110	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.