



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:44 PM GMT

PDB ID : 1GZX
Title : OXY T STATE HAEMOGLOBIN: OXYGEN BOUND AT ALL FOUR HAEMS
Authors : Paoli, M.; Liddington, R.; Tame, J.; Wilkinson, A.; Dodson, G.
Deposited on : 2002-06-07
Resolution : 2.10 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : **FAILED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

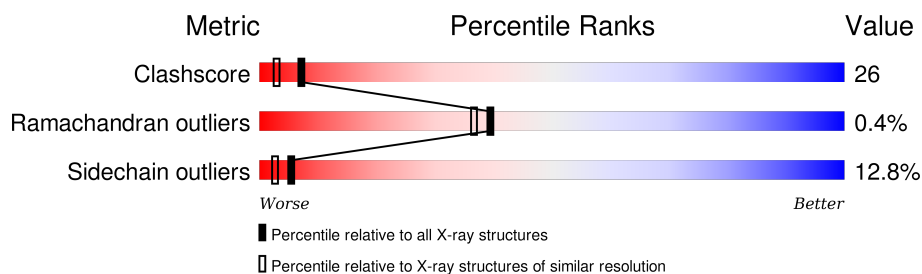
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	141	
1	C	141	
2	B	146	
2	D	146	

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
4	OXY	B	1291	-	-	X	-
4	OXY	D	1691	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4769 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 HEMOGLOBIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			

- Molecule 2 is a protein called HEMOGLOBIN BETA CHAIN.

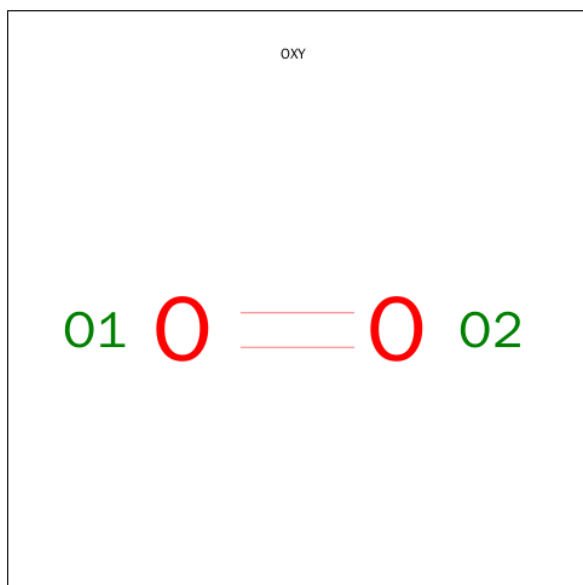
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			
2	D	146	Total	C	N	O	S	0	0	0
			1123	724	195	201	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
3	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	55	Total	O	0	0
			55	55		

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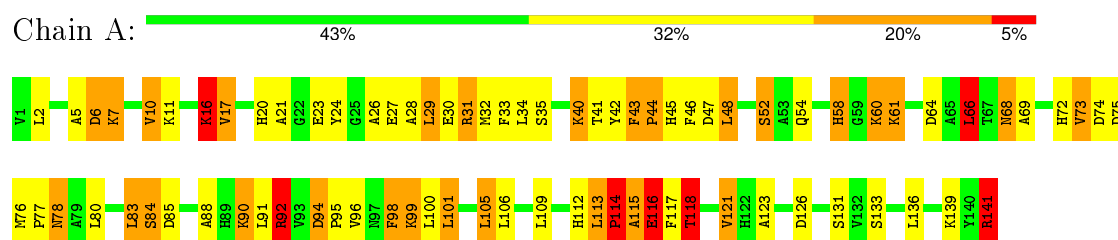
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	45	Total	O	0	0
			45	45		
5	D	43	Total	O	0	0
			43	43		

3 Residue-property plots

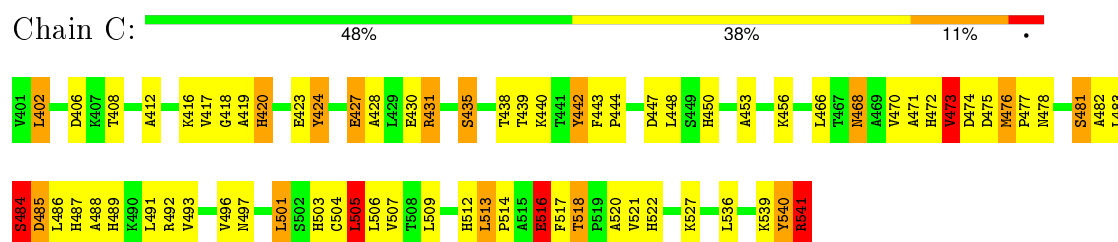
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS failed to run properly.

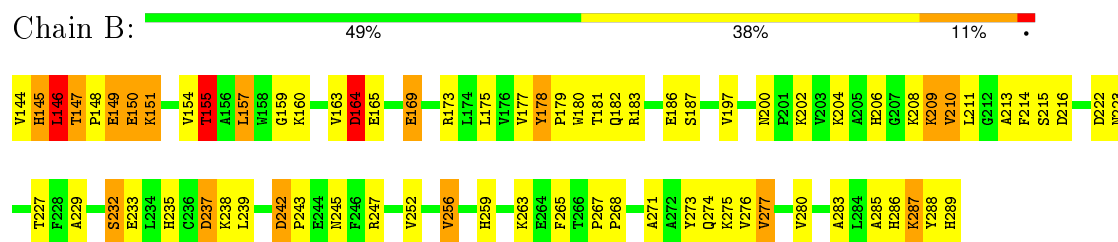
• Molecule 1: HEMOGLOBIN ALPHA CHAIN



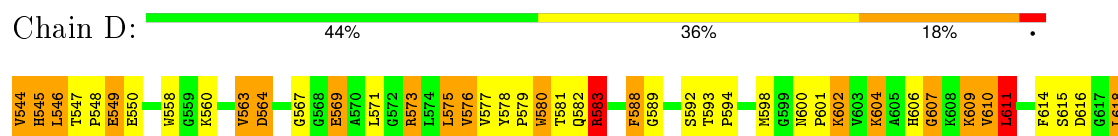
• Molecule 1: HEMOGLOBIN ALPHA CHAIN



• Molecule 2: HEMOGLOBIN BETA CHAIN



• Molecule 2: HEMOGLOBIN BETA CHAIN



L619	L620	L621	L622		L625	L626	L627	L628	L629	L630		L633	L634		L638	L639	L640	L641	L642	L643	L644	L645	L646	L647	L648	L649	L650		L660	L661	L662	L663		L666	L667	L668	L669	L670		L673	L674	L675	L676	L677		L684	L685	L686	L687	L688	L689
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4 Data and refinement statistics

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2 A	Depositor
Cell constants a, b, c, α , β , γ	97.05Å 99.50Å 66.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.10	Depositor
% Data completeness (in resolution range)	95.0 (10.00-2.10)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.199 , 0.221	Depositor
Wilson B-factor (Å ²)	(Not available)	Xtriage
Anisotropy	(Not available)	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtriage
Outliers	(Not available)	Xtriage
Total number of atoms	4769	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HEM, OXY

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	1.13	1/1097 (0.1%)	2.57	80/1491 (5.4%)
1	C	1.11	2/1097 (0.2%)	2.54	68/1491 (4.6%)
2	B	1.13	0/1153	2.76	76/1566 (4.9%)
2	D	1.12	1/1153 (0.1%)	2.44	58/1566 (3.7%)
All	All	1.12	4/4500 (0.1%)	2.58	282/6114 (4.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	487	HIS	CA-CB	6.06	1.67	1.53
2	D	549	GLU	CD-OE2	5.73	1.31	1.25
1	C	541	ARG	CD-NE	-5.41	1.37	1.46
1	A	141	ARG	NE-CZ	5.15	1.39	1.33

All (282) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	183	ARG	NE-CZ-NH1	26.47	133.54	120.30
2	B	247	ARG	NE-CZ-NH1	-23.71	108.44	120.30
2	B	247	ARG	CD-NE-CZ	22.18	154.66	123.60
1	A	92	ARG	CD-NE-CZ	20.71	152.59	123.60
1	C	431	ARG	NE-CZ-NH2	-17.30	111.65	120.30
1	A	92	ARG	NE-CZ-NH2	17.23	128.91	120.30
1	C	475	ASP	CB-CG-OD2	-17.00	103.00	118.30
2	B	247	ARG	NE-CZ-NH2	16.57	128.58	120.30
1	C	431	ARG	NE-CZ-NH1	16.42	128.51	120.30
2	B	173	ARG	NE-CZ-NH1	16.40	128.50	120.30
2	B	183	ARG	CD-NE-CZ	15.83	145.76	123.60
1	C	541	ARG	NE-CZ-NH2	15.73	128.16	120.30
2	B	222	ASP	CB-CG-OD1	15.26	132.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	288	TYR	CB-CG-CD1	-15.19	111.89	121.00
1	C	423	GLU	OE1-CD-OE2	13.58	139.60	123.30
1	A	105	LEU	CA-CB-CG	13.32	145.93	115.30
2	D	573	ARG	NE-CZ-NH1	-13.23	113.69	120.30
2	D	573	ARG	NE-CZ-NH2	13.19	126.89	120.30
2	D	622	ASP	CB-CG-OD1	13.13	130.12	118.30
2	B	183	ARG	NH1-CZ-NH2	-12.69	105.44	119.40
2	D	673	TYR	CB-CG-CD2	12.16	128.29	121.00
2	B	273	TYR	CB-CG-CD1	-12.14	113.72	121.00
2	B	169	GLU	OE1-CD-OE2	11.93	137.62	123.30
2	B	216	ASP	CB-CG-OD2	11.87	128.98	118.30
1	A	31	ARG	NE-CZ-NH2	-11.58	114.51	120.30
2	D	622	ASP	CB-CG-OD2	-11.53	107.92	118.30
1	A	31	ARG	NE-CZ-NH1	11.48	126.04	120.30
2	B	149	GLU	CB-CG-CD	11.29	144.69	114.20
2	D	644	GLU	OE1-CD-OE2	11.01	136.52	123.30
1	C	541	ARG	NE-CZ-NH1	-11.00	114.80	120.30
1	A	115	ALA	N-CA-CB	-10.77	95.03	110.10
2	D	588	PHE	C-N-CA	10.73	144.83	122.30
1	A	141	ARG	NE-CZ-NH1	-10.25	115.17	120.30
1	A	60	LYS	CA-CB-CG	9.95	135.29	113.40
2	D	673	TYR	CB-CG-CD1	-9.92	115.05	121.00
2	B	178	TYR	CB-CG-CD1	9.60	126.76	121.00
1	A	141	ARG	CD-NE-CZ	-9.56	110.22	123.60
2	D	633	GLU	OE1-CD-OE2	9.37	134.54	123.30
1	A	83	LEU	CB-CA-C	9.27	127.81	110.20
1	A	74	ASP	CB-CG-OD1	-9.18	110.04	118.30
1	C	541	ARG	CG-CD-NE	9.14	130.99	111.80
2	B	271	ALA	CB-CA-C	9.08	123.72	110.10
1	A	5	ALA	CB-CA-C	8.94	123.51	110.10
2	B	149	GLU	CB-CA-C	8.87	128.14	110.40
1	C	406	ASP	CB-CG-OD2	-8.85	110.33	118.30
2	B	157	LEU	CA-CB-CG	8.78	135.49	115.30
2	B	209	LYS	CA-CB-CG	8.73	132.61	113.40
1	C	408	THR	O-C-N	8.73	136.67	122.70
1	A	31	ARG	CD-NE-CZ	8.73	135.82	123.60
2	B	169	GLU	CG-CD-OE2	-8.68	100.94	118.30
1	C	492	ARG	CD-NE-CZ	-8.47	111.74	123.60
1	A	7	LYS	CG-CD-CE	8.38	137.03	111.90
2	D	545	HIS	O-C-N	8.23	135.87	122.70
2	D	564	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	A	96	VAL	O-C-N	8.10	135.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASP	CB-CG-OD2	-8.03	111.08	118.30
1	C	427	GLU	OE1-CD-OE2	7.93	132.81	123.30
2	D	621	LEU	C-N-CA	7.90	141.45	121.70
1	C	513	LEU	CB-CG-CD1	-7.72	97.88	111.00
2	B	213	ALA	N-CA-CB	7.67	120.83	110.10
1	C	442	TYR	CB-CG-CD1	7.66	125.60	121.00
1	C	489	HIS	O-C-N	7.64	134.93	122.70
1	A	98	PHE	O-C-N	7.64	134.92	122.70
2	B	146	LEU	CA-CB-CG	7.63	132.86	115.30
2	B	222	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	C	540	TYR	CB-CG-CD2	-7.60	116.44	121.00
1	A	115	ALA	CB-CA-C	7.53	121.39	110.10
2	D	576	VAL	CA-CB-CG2	7.51	122.17	110.90
1	C	492	ARG	NE-CZ-NH2	7.46	124.03	120.30
2	D	650	GLY	O-C-N	-7.43	110.81	122.70
1	A	64	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	114	PRO	O-C-N	7.36	134.48	122.70
1	C	520	ALA	CA-C-O	-7.32	104.72	120.10
1	C	430	GLU	OE1-CD-OE2	7.30	132.06	123.30
1	A	118	THR	CA-CB-CG2	7.28	122.59	112.40
2	D	564	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	112	HIS	CA-C-O	-7.25	104.88	120.10
2	D	620	HIS	CA-CB-CG	-7.25	101.28	113.60
2	B	169	GLU	CB-CA-C	-7.20	96.01	110.40
1	A	5	ALA	N-CA-CB	-7.19	100.03	110.10
1	A	75	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	29	LEU	CB-CA-C	7.07	123.64	110.20
2	D	677	VAL	CB-CA-C	7.02	124.73	111.40
2	B	154	VAL	CA-C-O	7.01	134.82	120.10
1	C	423	GLU	CG-CD-OE2	-7.01	104.29	118.30
2	D	583	ARG	CD-NE-CZ	6.93	133.30	123.60
2	B	146	LEU	O-C-N	6.91	133.76	122.70
1	A	73	VAL	CB-CA-C	-6.90	98.30	111.40
1	C	505	LEU	CB-CG-CD2	-6.89	99.29	111.00
1	C	540	TYR	CG-CD2-CE2	-6.88	115.80	121.30
1	A	73	VAL	CA-CB-CG2	6.87	121.21	110.90
1	C	484	SER	O-C-N	6.84	133.65	122.70
2	D	578	TYR	CB-CG-CD1	-6.83	116.90	121.00
2	D	618	LEU	CA-CB-CG	6.83	131.02	115.30
1	C	453	ALA	N-CA-CB	6.83	119.66	110.10
1	A	94	ASP	CB-CG-OD2	6.79	124.41	118.30
2	D	611	LEU	CB-CA-C	6.79	123.09	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	688	TYR	CB-CG-CD1	6.78	125.06	121.00
2	B	242	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	C	473	VAL	CA-C-N	-6.74	102.37	117.20
2	D	622	ASP	CA-CB-CG	6.73	128.21	113.40
2	B	173	ARG	NH1-CZ-NH2	-6.73	112.00	119.40
2	D	647	ARG	NE-CZ-NH1	6.73	123.66	120.30
2	D	546	LEU	C-N-CA	6.72	138.50	121.70
2	D	638	LYS	CB-CA-C	-6.65	97.10	110.40
1	A	116	GLU	CG-CD-OE1	6.61	131.51	118.30
2	D	626	GLY	O-C-N	6.55	133.18	122.70
1	A	131	SER	CB-CA-C	6.53	122.50	110.10
1	A	6	ASP	CB-CG-OD2	6.52	124.16	118.30
1	A	78	ASN	CB-CG-OD1	6.51	134.62	121.60
1	C	406	ASP	OD1-CG-OD2	6.49	135.62	123.30
2	B	286	HIS	O-C-N	-6.46	112.36	122.70
2	D	626	GLY	CA-C-O	-6.45	108.98	120.60
1	C	507	VAL	O-C-N	-6.45	112.38	122.70
2	D	549	GLU	CG-CD-OE1	6.43	131.16	118.30
1	C	518	THR	CA-CB-CG2	6.42	121.38	112.40
1	A	61	LYS	CB-CG-CD	-6.38	95.00	111.60
2	B	146	LEU	N-CA-C	-6.37	93.79	111.00
2	B	277	VAL	N-CA-CB	-6.33	97.57	111.50
1	A	60	LYS	CB-CG-CD	6.32	128.03	111.60
2	D	577	VAL	C-N-CA	6.30	137.45	121.70
2	B	214	PHE	CZ-CE2-CD2	-6.29	112.55	120.10
2	B	277	VAL	CB-CA-C	6.29	123.35	111.40
1	A	72	HIS	CA-CB-CG	-6.28	102.92	113.60
2	D	604	LYS	CB-CA-C	-6.26	97.88	110.40
2	D	569	GLU	CG-CD-OE2	-6.25	105.80	118.30
1	A	112	HIS	CA-CB-CG	6.24	124.21	113.60
2	B	277	VAL	CA-CB-CG1	6.23	120.24	110.90
1	C	504	CYS	CA-CB-SG	-6.22	102.80	114.00
1	C	483	LEU	CA-C-O	-6.21	107.05	120.10
1	A	40	LYS	CD-CE-NZ	-6.17	97.51	111.70
1	A	46	PHE	CB-CG-CD1	-6.17	116.48	120.80
2	B	285	ALA	O-C-N	-6.16	112.84	122.70
2	D	677	VAL	N-CA-CB	-6.15	97.97	111.50
2	B	237	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	475	ASP	O-C-N	6.12	132.50	122.70
2	B	256	VAL	CA-CB-CG1	6.12	120.08	110.90
2	B	181	THR	CA-CB-CG2	-6.05	103.92	112.40
1	C	447	ASP	CB-CG-OD2	-6.05	112.85	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	VAL	CA-C-O	6.01	132.73	120.10
2	D	589	GLY	N-CA-C	6.01	128.13	113.10
2	D	607	GLY	O-C-N	-5.99	113.12	122.70
2	B	288	TYR	CD1-CG-CD2	5.98	124.48	117.90
1	C	517	PHE	CB-CG-CD1	-5.98	116.61	120.80
1	A	72	HIS	O-C-N	5.95	132.22	122.70
1	A	68	ASN	CB-CG-OD1	-5.94	109.71	121.60
1	A	28	ALA	N-CA-CB	5.93	118.41	110.10
2	D	578	TYR	CB-CG-CD2	5.93	124.56	121.00
1	A	133	SER	O-C-N	-5.92	113.22	122.70
1	A	92	ARG	C-N-CA	5.92	136.49	121.70
1	A	42	TYR	CB-CG-CD1	5.91	124.55	121.00
1	C	420	HIS	O-C-N	5.90	132.14	122.70
2	B	145	HIS	CA-C-N	-5.89	104.24	117.20
1	A	54	GLN	N-CA-CB	5.87	121.17	110.60
2	B	177	VAL	C-N-CA	5.87	136.38	121.70
1	C	471	ALA	CA-C-O	-5.86	107.79	120.10
1	A	92	ARG	NE-CZ-NH1	-5.84	117.38	120.30
2	B	150	GLU	OE1-CD-OE2	5.84	130.31	123.30
2	B	151	LYS	N-CA-CB	5.81	121.06	110.60
2	D	602	LYS	CA-CB-CG	5.79	126.14	113.40
1	C	483	LEU	CA-CB-CG	5.79	128.61	115.30
2	D	628	PHE	CA-C-O	-5.77	107.99	120.10
2	B	252	VAL	CG1-CB-CG2	5.75	120.11	110.90
1	C	522	HIS	CA-CB-CG	5.75	123.38	113.60
1	A	101	LEU	CB-CG-CD1	-5.74	101.24	111.00
2	B	256	VAL	CB-CA-C	5.74	122.31	111.40
2	B	165	GLU	CG-CD-OE1	5.74	129.77	118.30
1	C	496	VAL	CA-C-O	-5.72	108.08	120.10
1	A	41	THR	CA-CB-CG2	5.72	120.40	112.40
1	A	116	GLU	CA-CB-CG	5.71	125.97	113.40
2	D	640	HIS	CA-CB-CG	-5.71	103.89	113.60
2	B	288	TYR	CG-CD1-CE1	-5.71	116.73	121.30
1	C	475	ASP	OD1-CG-OD2	5.67	134.08	123.30
1	A	136	LEU	CB-CG-CD2	-5.65	101.40	111.00
1	A	68	ASN	CA-C-N	5.63	129.60	117.20
1	A	72	HIS	CA-C-O	-5.63	108.27	120.10
1	C	505	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	141	ARG	CB-CG-CD	5.62	126.22	111.60
2	B	151	LYS	CB-CA-C	-5.60	99.20	110.40
1	C	540	TYR	O-C-N	5.60	131.66	122.70
2	B	187	SER	N-CA-CB	-5.60	102.10	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	540	TYR	CA-C-N	-5.59	104.90	117.20
1	A	21	ALA	N-CA-CB	-5.57	102.30	110.10
1	A	20	HIS	CA-CB-CG	-5.57	104.14	113.60
1	A	117	PHE	C-N-CA	5.56	135.61	121.70
1	A	21	ALA	CB-CA-C	5.55	118.43	110.10
1	C	485	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	66	LEU	CB-CG-CD1	5.55	120.44	111.00
2	B	273	TYR	CB-CG-CD2	5.55	124.33	121.00
2	D	560	LYS	C-N-CA	5.54	135.55	121.70
1	A	16	LYS	CD-CE-NZ	5.51	124.37	111.70
2	B	273	TYR	CD1-CE1-CZ	-5.50	114.85	119.80
2	B	150	GLU	N-CA-CB	5.50	120.50	110.60
1	A	121	VAL	CA-CB-CG1	5.50	119.15	110.90
2	D	558	TRP	CB-CG-CD1	5.49	134.13	127.00
1	C	424	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	A	116	GLU	CG-CD-OE2	-5.48	107.34	118.30
1	C	412	ALA	CA-C-O	-5.47	108.62	120.10
2	B	216	ASP	CA-C-O	5.44	131.53	120.10
2	B	155	THR	OG1-CB-CG2	5.44	122.51	110.00
1	A	30	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	A	54	GLN	O-C-N	5.42	131.37	122.70
2	B	223	ASN	CB-CA-C	5.41	121.22	110.40
2	B	222	ASP	O-C-N	5.41	131.35	122.70
1	A	44	PRO	O-C-N	-5.40	114.05	122.70
2	B	177	VAL	CA-C-N	5.40	129.09	117.20
1	C	491	LEU	CA-C-O	-5.40	108.77	120.10
1	A	26	ALA	C-N-CA	5.39	135.17	121.70
1	C	431	ARG	CD-NE-CZ	-5.37	116.08	123.60
2	B	164	ASP	CB-CG-OD1	5.37	123.13	118.30
2	B	210	VAL	CG1-CB-CG2	5.37	119.48	110.90
2	B	265	PHE	CB-CA-C	5.36	121.12	110.40
2	D	662	GLY	C-N-CA	5.35	135.07	121.70
2	D	670	GLN	CA-CB-CG	-5.35	101.63	113.40
2	B	227	THR	CA-CB-CG2	5.35	119.89	112.40
2	D	689	HIS	CA-C-O	-5.34	108.88	120.10
1	C	483	LEU	CA-C-N	5.34	128.95	117.20
1	A	58	HIS	CB-CA-C	5.33	121.06	110.40
2	B	165	GLU	CA-CB-CG	5.33	125.13	113.40
1	C	516	GLU	CB-CA-C	-5.33	99.74	110.40
2	B	232	SER	O-C-N	-5.32	114.19	122.70
1	C	476	MET	CB-CA-C	5.31	121.02	110.40
1	C	423	GLU	CB-CA-C	-5.31	99.79	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	569	GLU	CB-CA-C	-5.30	99.80	110.40
1	A	100	LEU	O-C-N	5.30	131.18	122.70
1	A	43	PHE	CZ-CE2-CD2	-5.30	113.75	120.10
1	C	487	HIS	N-CA-CB	5.30	120.14	110.60
2	D	673	TYR	CG-CD2-CE2	5.29	125.53	121.30
2	B	285	ALA	N-CA-CB	-5.28	102.71	110.10
1	A	91	LEU	O-C-N	5.26	131.12	122.70
2	B	157	LEU	CB-CG-CD1	5.25	119.93	111.00
1	A	92	ARG	NH1-CZ-NH2	-5.25	113.63	119.40
2	D	663	LYS	CA-CB-CG	5.25	124.95	113.40
1	C	468	ASN	CB-CA-C	5.24	120.88	110.40
2	B	271	ALA	O-C-N	-5.24	114.32	122.70
2	D	687	LYS	CD-CE-NZ	5.23	123.74	111.70
1	A	48	LEU	O-C-N	5.23	131.07	122.70
2	B	145	HIS	CA-CB-CG	-5.23	104.71	113.60
2	B	237	ASP	C-N-CA	-5.22	108.64	121.70
2	B	256	VAL	CA-C-N	5.20	128.63	117.20
1	C	471	ALA	CA-C-N	5.19	128.62	117.20
1	C	503	HIS	C-N-CA	5.18	134.64	121.70
1	A	73	VAL	CA-CB-CG1	-5.17	103.14	110.90
2	D	686	HIS	CA-CB-CG	-5.17	104.81	113.60
1	C	430	GLU	O-C-N	-5.17	114.43	122.70
2	D	545	HIS	N-CA-CB	5.16	119.89	110.60
2	B	165	GLU	CG-CD-OE2	-5.16	107.98	118.30
2	B	287	LYS	CG-CD-CE	-5.16	96.42	111.90
1	C	420	HIS	CB-CA-C	-5.16	100.08	110.40
1	C	481	SER	CA-C-O	-5.16	109.28	120.10
1	C	450	HIS	CB-CA-C	-5.15	100.10	110.40
2	B	178	TYR	CD1-CG-CD2	-5.14	112.25	117.90
1	A	113	LEU	CA-CB-CG	5.13	127.11	115.30
1	C	478	ASN	OD1-CG-ND2	5.13	133.70	121.90
1	C	474	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	C	536	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	A	17	VAL	N-CA-CB	5.10	122.73	111.50
2	D	688	TYR	N-CA-CB	5.09	119.77	110.60
1	C	420	HIS	CA-CB-CG	-5.09	104.94	113.60
2	D	610	VAL	O-C-N	-5.09	114.56	122.70
1	C	475	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	131	SER	CA-C-N	5.08	128.38	117.20
1	A	10	VAL	CG1-CB-CG2	5.08	119.03	110.90
1	C	424	TYR	O-C-N	5.07	131.82	123.20
2	D	660	HIS	CB-CA-C	-5.07	100.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	424	TYR	CA-C-O	-5.07	109.45	120.10
1	A	29	LEU	CA-CB-CG	5.07	126.95	115.30
1	A	21	ALA	O-C-N	-5.07	114.59	123.20
2	B	146	LEU	C-N-CA	5.07	134.36	121.70
2	B	283	ALA	CB-CA-C	5.06	117.69	110.10
1	A	114	PRO	CA-CB-CG	-5.06	94.39	104.00
2	D	580	TRP	CE3-CZ3-CH2	-5.05	115.64	121.20
1	C	520	ALA	CA-C-N	5.04	128.30	117.20
1	C	435	SER	O-C-N	5.04	130.77	122.70
2	D	634	LEU	CA-CB-CG	-5.04	103.71	115.30
2	D	615	SER	CA-C-O	5.03	130.66	120.10
2	B	222	ASP	C-N-CA	-5.02	109.14	121.70
2	D	611	LEU	CB-CG-CD2	-5.01	102.47	111.00
1	C	486	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	A	24	TYR	CA-CB-CG	5.01	122.92	113.40
2	B	237	ASP	CB-CG-OD1	5.01	122.81	118.30
2	D	619	ALA	CB-CA-C	5.00	117.60	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1069	0	1073	46	0
1	C	1069	0	1070	50	0
2	B	1123	0	1115	53	0
2	D	1123	0	1112	105	0
3	A	43	0	30	3	0
3	B	43	0	30	1	0
3	C	43	0	30	0	0
3	D	43	0	30	9	0
4	A	2	0	0	0	0
4	B	2	0	0	2	0
4	C	2	0	0	0	0
4	D	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	62	0	0	4	0
5	B	55	0	0	7	0
5	C	45	0	0	2	1
5	D	43	0	0	8	0
All	All	4769	0	4490	237	1

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 26.

All (237) 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:D:638:LYS:NZ	2:D:638:LYS:HB2	1.27	1.28
1:C:470:VAL:O	1:C:473:VAL:HG22	1.39	1.18
2:D:547:THR:HG22	2:D:549:GLU:N	1.64	1.13
2:D:649:LEU:HD23	3:D:1690:HEM:HBB2	1.32	1.09
2:D:638:LYS:NZ	2:D:638:LYS:CB	2.17	1.08
2:D:544:VAL:HG13	2:D:546:LEU:HD13	1.36	1.07
2:D:547:THR:HG22	2:D:549:GLU:H	0.82	0.97
2:B:144:VAL:HG22	2:B:145:HIS:H	1.31	0.95
2:D:620:HIS:HB2	5:D:2022:HOH:O	1.65	0.95
1:C:470:VAL:O	1:C:473:VAL:CG2	2.15	0.94
2:D:547:THR:CG2	2:D:549:GLU:H	1.78	0.94
2:D:563:VAL:HG22	2:D:611:LEU:HD12	1.51	0.93
1:A:16:LYS:HB3	1:A:16:LYS:NZ	1.84	0.91
2:D:620:HIS:CD2	2:D:620:HIS:N	2.36	0.90
2:D:638:LYS:CB	2:D:638:LYS:HZ2	1.79	0.89
2:D:638:LYS:HB2	2:D:638:LYS:HZ3	1.38	0.89
2:D:627:THR:CB	5:D:2022:HOH:O	2.20	0.89
2:D:610:VAL:HG21	4:D:1691:OXY:O1	1.73	0.89
1:C:513:LEU:HB3	1:C:516:GLU:HG2	1.53	0.88
2:D:544:VAL:CG1	2:D:546:LEU:HD13	2.05	0.87
2:D:638:LYS:HB2	2:D:638:LYS:HZ2	0.90	0.85
2:D:547:THR:HG21	2:D:549:GLU:HB2	1.57	0.84
2:D:627:THR:OG1	5:D:2022:HOH:O	1.94	0.82
1:A:84:SER:HB2	1:A:139:LYS:HD2	1.60	0.81
2:D:620:HIS:HD2	2:D:620:HIS:N	1.76	0.81
2:D:544:VAL:HG13	2:D:546:LEU:CD1	2.10	0.80
2:B:144:VAL:HG22	2:B:145:HIS:N	1.95	0.80
2:D:667:PRO:N	2:D:668:PRO:CD	2.45	0.80
1:C:439:THR:HG22	1:C:497:ASN:HD22	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:PRO:HD2	2:B:268:PRO:HD3	1.62	0.79
1:C:512:HIS:C	1:C:514:PRO:HD3	2.03	0.79
1:C:518:THR:HG23	1:C:521:VAL:H	1.48	0.79
2:D:638:LYS:HA	2:D:638:LYS:HE3	1.62	0.78
1:A:35:SER:HB3	2:B:274:GLN:HG3	1.64	0.78
2:B:180:TRP:HZ3	1:C:541:ARG:HG2	1.50	0.77
2:D:634:LEU:HD12	2:D:638:LYS:HZ3	1.52	0.75
1:C:443:PHE:N	1:C:444:PRO:CD	2.50	0.74
2:B:267:PRO:CD	2:B:268:PRO:HD3	2.18	0.74
1:A:114:PRO:O	2:B:259:HIS:NE2	2.20	0.74
2:D:649:LEU:CD2	3:D:1690:HEM:HBB2	2.13	0.74
2:D:638:LYS:CA	2:D:638:LYS:HE3	2.17	0.74
2:B:144:VAL:CG2	2:B:145:HIS:H	2.01	0.74
1:A:99:LYS:N	1:A:99:LYS:HD2	2.03	0.73
2:D:563:VAL:HG22	2:D:611:LEU:CD1	2.17	0.73
1:A:92:ARG:HB3	2:D:580:TRP:HB2	1.71	0.73
2:D:547:THR:CG2	2:D:549:GLU:HB2	2.17	0.72
1:C:485:ASP:OD1	1:C:539:LYS:HE2	1.88	0.72
2:D:634:LEU:O	2:D:638:LYS:HB3	1.90	0.71
2:D:667:PRO:N	2:D:668:PRO:HD2	2.05	0.71
2:B:186:GLU:HG2	5:B:2012:HOH:O	1.91	0.71
1:C:476:MET:N	1:C:477:PRO:CD	2.54	0.70
1:A:99:LYS:H	1:A:99:LYS:HD2	1.56	0.70
1:C:428:ALA:CB	1:C:505:LEU:HD13	2.22	0.69
2:D:600:ASN:OD1	2:D:602:LYS:N	2.22	0.69
2:D:619:ALA:C	2:D:620:HIS:HD2	1.96	0.69
2:D:687:LYS:HD2	5:D:2040:HOH:O	1.94	0.68
2:D:619:ALA:C	2:D:620:HIS:CD2	2.66	0.68
2:B:164:ASP:OD2	2:B:208:LYS:HD2	1.95	0.67
2:B:267:PRO:N	2:B:268:PRO:CD	2.58	0.66
1:A:114:PRO:HG2	1:A:115:ALA:N	2.09	0.66
1:A:90:LYS:HB2	1:A:90:LYS:NZ	2.10	0.66
2:D:667:PRO:CD	2:D:668:PRO:CD	2.73	0.66
1:A:90:LYS:HB2	1:A:90:LYS:HZ2	1.60	0.66
2:D:610:VAL:CG2	4:D:1691:OXY:O1	2.44	0.65
2:B:209:LYS:HE2	5:B:2054:HOH:O	1.97	0.64
2:B:237:ASP:OD2	2:B:289:HIS:NE2	2.30	0.64
2:B:164:ASP:CG	2:B:208:LYS:HD2	2.17	0.64
1:C:513:LEU:N	1:C:514:PRO:HD3	2.13	0.64
1:C:518:THR:CG2	1:C:521:VAL:HG23	2.27	0.64
2:D:614:PHE:CE1	5:D:2005:HOH:O	2.50	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:ALA:HB2	1:C:505:LEU:HD13	1.79	0.64
2:D:609:LYS:HD3	3:D:1690:HEM:HAA2	1.79	0.63
1:C:468:ASN:O	1:C:472:HIS:HD2	1.80	0.63
2:D:569:GLU:O	2:D:573:ARG:HG3	1.98	0.63
2:D:634:LEU:HD12	2:D:638:LYS:NZ	2.13	0.63
2:D:667:PRO:HD2	2:D:668:PRO:CD	2.28	0.62
1:C:518:THR:HG22	1:C:521:VAL:CG2	2.29	0.62
2:B:144:VAL:HG13	2:B:146:LEU:HD23	1.82	0.62
2:D:667:PRO:CD	2:D:668:PRO:HD3	2.29	0.62
2:B:229:ALA:O	2:B:233:GLU:HG3	2.00	0.61
1:A:92:ARG:HB2	2:D:583:ARG:HD3	1.82	0.61
2:D:594:PRO:O	2:D:598:MET:HG2	2.00	0.61
2:B:150:GLU:OE2	2:B:275:LYS:NZ	2.33	0.61
2:D:625:LYS:HD3	2:D:686:HIS:CG	2.36	0.60
2:D:638:LYS:CA	2:D:638:LYS:CE	2.76	0.60
2:B:151:LYS:O	2:B:155:THR:HB	2.01	0.60
1:C:443:PHE:N	1:C:444:PRO:HD3	2.17	0.59
1:A:85:ASP:OD1	1:A:139:LYS:HD3	2.03	0.59
1:C:484:SER:HB2	5:C:2029:HOH:O	2.03	0.59
2:B:146:LEU:HD13	2:B:150:GLU:HB3	1.85	0.59
1:C:501:LEU:HD22	1:C:505:LEU:HD22	1.85	0.59
2:B:276:VAL:O	2:B:280:VAL:HG23	2.03	0.59
2:D:667:PRO:HD2	2:D:668:PRO:HD3	1.84	0.58
1:A:6:ASP:O	1:A:10:VAL:HG23	2.03	0.58
2:B:287:LYS:HE2	5:B:2052:HOH:O	2.02	0.58
2:D:627:THR:HB	5:D:2022:HOH:O	1.94	0.58
1:C:439:THR:HG22	1:C:497:ASN:ND2	2.17	0.58
2:B:144:VAL:HG21	5:B:2047:HOH:O	2.04	0.58
1:A:114:PRO:HA	2:B:259:HIS:CD2	2.38	0.58
2:D:547:THR:CG2	2:D:548:PRO:CD	2.82	0.57
1:C:518:THR:HG22	1:C:521:VAL:HB	1.85	0.57
2:D:547:THR:HG23	2:D:548:PRO:CD	2.33	0.57
2:D:588:PHE:N	2:D:588:PHE:HD2	2.02	0.57
2:D:625:LYS:HE3	2:D:686:HIS:CD2	2.40	0.56
1:A:16:LYS:HZ3	1:A:16:LYS:HB3	1.64	0.56
1:A:33:PHE:CE2	1:A:48:LEU:HD22	2.40	0.56
2:D:576:VAL:HG22	2:D:594:PRO:HA	1.87	0.56
2:D:588:PHE:CD2	2:D:588:PHE:N	2.72	0.56
1:A:114:PRO:HG2	1:A:115:ALA:H	1.71	0.56
2:D:667:PRO:CD	2:D:668:PRO:HD2	2.35	0.55
2:D:571:LEU:HD21	2:D:606:HIS:HD2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:HB1	5:A:2054:HOH:O	2.06	0.54
2:D:544:VAL:HG23	5:D:2035:HOH:O	2.06	0.54
1:C:440:LYS:HG2	1:C:448:LEU:HD13	1.90	0.54
1:C:518:THR:HG22	1:C:521:VAL:HG23	1.88	0.54
1:A:114:PRO:HA	2:B:259:HIS:NE2	2.23	0.54
5:A:2050:HOH:O	2:B:263:LYS:HD2	2.07	0.54
2:B:147:THR:O	2:B:150:GLU:HB2	2.08	0.54
2:B:169:GLU:HG2	2:B:256:VAL:HG13	1.89	0.54
2:D:609:LYS:HD3	3:D:1690:HEM:CAA	2.37	0.54
2:B:267:PRO:CD	2:B:268:PRO:CD	2.86	0.54
1:C:424:TYR:CD2	1:C:424:TYR:N	2.75	0.54
2:D:592:SER:C	2:D:593:THR:HG23	2.28	0.53
2:D:639:LEU:HD13	3:D:1690:HEM:C3D	2.42	0.53
2:B:267:PRO:HD2	2:B:268:PRO:CD	2.34	0.53
2:D:547:THR:HG23	2:D:548:PRO:HD2	1.90	0.53
1:A:16:LYS:HZ2	1:A:16:LYS:HB3	1.72	0.53
2:B:202:LYS:HG3	5:B:2020:HOH:O	2.09	0.53
1:A:118:THR:HG23	5:A:2051:HOH:O	2.09	0.52
1:C:488:ALA:HA	1:C:540:TYR:CE2	2.45	0.52
2:D:547:THR:HB	2:D:550:GLU:HG3	1.91	0.51
2:D:571:LEU:CD2	2:D:606:HIS:HD2	2.23	0.51
2:B:186:GLU:HG3	5:B:2014:HOH:O	2.08	0.51
1:A:141:ARG:HD3	1:C:527:LYS:HG2	1.93	0.51
2:D:576:VAL:CG2	2:D:594:PRO:HA	2.40	0.51
2:D:667:PRO:HD2	2:D:668:PRO:HD2	1.92	0.51
1:C:518:THR:HG22	1:C:521:VAL:CB	2.40	0.51
2:B:235:HIS:HA	2:B:239:LEU:HB2	1.94	0.50
2:B:144:VAL:CG2	2:B:145:HIS:N	2.62	0.50
2:B:147:THR:HG23	2:B:148:PRO:HD2	1.93	0.50
1:C:513:LEU:N	1:C:514:PRO:CD	2.74	0.50
2:B:267:PRO:CB	2:B:268:PRO:HD3	2.41	0.50
2:D:643:PRO:HA	2:D:646:PHE:CD2	2.46	0.50
2:B:242:ASP:OD1	1:C:442:TYR:OH	2.24	0.50
2:D:592:SER:O	2:D:593:THR:CG2	2.60	0.50
2:B:210:VAL:HG21	4:B:1291:OXY:O1	2.12	0.50
1:A:43:PHE:N	1:A:44:PRO:CD	2.75	0.49
1:A:47:ASP:OD2	1:A:52:SER:HB2	2.12	0.49
2:D:666:THR:OG1	2:D:669:VAL:HG23	2.13	0.49
1:C:476:MET:N	1:C:477:PRO:HD2	2.28	0.49
2:D:634:LEU:CD1	2:D:638:LYS:HZ3	2.23	0.48
2:D:563:VAL:CG2	2:D:611:LEU:HD12	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:PRO:HB2	2:B:268:PRO:HD3	1.95	0.48
2:B:287:LYS:CE	5:B:2052:HOH:O	2.61	0.48
2:D:600:ASN:OD1	2:D:600:ASN:C	2.52	0.48
1:C:440:LYS:HG2	1:C:448:LEU:CD1	2.43	0.48
1:A:113:LEU:HB3	1:A:116:GLU:HG2	1.96	0.48
2:B:146:LEU:CD1	2:B:150:GLU:HB3	2.44	0.48
2:D:684:LEU:CD1	3:D:1690:HEM:HAB	2.44	0.48
1:C:431:ARG:HD3	2:D:670:GLN:OE1	2.14	0.48
1:A:92:ARG:HB2	2:D:583:ARG:CD	2.44	0.47
2:D:567:GLY:O	2:D:607:GLY:HA3	2.14	0.47
1:A:7:LYS:O	1:A:11:LYS:HG2	2.13	0.47
3:D:1690:HEM:HHA	3:D:1690:HEM:HBA2	1.96	0.47
1:C:442:TYR:CE1	1:C:493:VAL:HA	2.50	0.47
2:D:592:SER:O	2:D:593:THR:HG23	2.15	0.47
1:C:484:SER:O	1:C:488:ALA:CB	2.63	0.47
1:A:114:PRO:HA	2:B:259:HIS:HE2	1.80	0.47
2:D:661:PHE:O	2:D:662:GLY:C	2.53	0.47
1:A:88:ALA:HB2	5:A:2061:HOH:O	2.15	0.46
1:C:442:TYR:C	1:C:444:PRO:CD	2.82	0.46
2:D:547:THR:HG22	2:D:548:PRO:N	2.31	0.46
1:A:83:LEU:HD11	3:A:1142:HEM:C3A	2.51	0.46
2:D:575:LEU:HG	2:D:582:GLN:HG2	1.96	0.46
2:D:666:THR:C	2:D:668:PRO:HD2	2.36	0.46
2:B:200:ASN:OD1	2:B:202:LYS:HB2	2.16	0.46
2:B:243:PRO:HG2	1:C:438:THR:CG2	2.45	0.46
1:A:29:LEU:HD11	1:A:58:HIS:HD2	1.80	0.45
2:D:544:VAL:CG1	2:D:546:LEU:CD1	2.83	0.45
2:D:547:THR:HG22	2:D:549:GLU:CA	2.43	0.45
1:C:482:ALA:O	1:C:485:ASP:HB2	2.17	0.45
1:C:516:GLU:H	1:C:516:GLU:CD	2.19	0.45
2:D:634:LEU:O	2:D:638:LYS:CB	2.63	0.44
1:C:442:TYR:C	1:C:444:PRO:HD2	2.38	0.44
1:C:506:LEU:HA	1:C:506:LEU:HD12	1.73	0.44
2:B:243:PRO:HG2	1:C:438:THR:HG22	1.98	0.44
1:A:84:SER:CB	1:A:139:LYS:HD2	2.42	0.44
1:A:27:GLU:O	1:A:31:ARG:HG3	2.17	0.44
1:C:418:GLY:O	1:C:420:HIS:N	2.51	0.44
2:D:649:LEU:HD22	3:D:1690:HEM:HMC3	1.99	0.44
2:D:547:THR:CG2	2:D:548:PRO:HD2	2.48	0.44
1:A:66:LEU:HD21	1:A:105:LEU:HD21	1.99	0.44
1:C:427:GLU:O	1:C:431:ARG:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:157:LEU:C	2:B:159:GLY:N	2.71	0.43
1:A:78:ASN:HA	1:A:78:ASN:HD22	1.58	0.43
2:D:547:THR:CG2	2:D:549:GLU:CB	2.94	0.43
2:D:579:PRO:O	2:D:582:GLN:HG3	2.19	0.43
1:C:466:LEU:O	1:C:470:VAL:HG23	2.19	0.43
1:C:402:LEU:HD12	1:C:402:LEU:HA	1.83	0.43
2:D:667:PRO:CB	2:D:668:PRO:HD3	2.48	0.43
2:D:625:LYS:NZ	5:D:2020:HOH:O	2.52	0.43
1:A:43:PHE:CD1	1:A:43:PHE:N	2.87	0.43
1:A:76:MET:N	1:A:77:PRO:CD	2.81	0.43
2:B:178:TYR:N	2:B:179:PRO:CD	2.80	0.43
2:D:575:LEU:HD12	2:D:581:THR:OG1	2.19	0.43
1:A:61:LYS:HD3	3:A:1142:HEM:HAA2	2.01	0.42
2:D:545:HIS:O	2:D:675:LYS:HE2	2.19	0.42
2:D:666:THR:HB	2:D:668:PRO:HD2	2.02	0.42
2:D:547:THR:CG2	2:D:548:PRO:N	2.82	0.42
2:D:625:LYS:HD3	2:D:686:HIS:CD2	2.54	0.42
1:C:444:PRO:HG2	5:C:2017:HOH:O	2.18	0.42
1:A:94:ASP:HA	1:A:95:PRO:HD3	1.85	0.42
2:D:571:LEU:HD12	2:D:571:LEU:HA	1.71	0.42
1:A:98:PHE:HD1	3:A:1142:HEM:HBB2	1.85	0.42
1:A:114:PRO:C	2:B:259:HIS:HE2	2.17	0.42
2:D:634:LEU:HD12	2:D:638:LYS:HB2	2.02	0.42
1:C:435:SER:HB3	2:D:674:GLN:HG3	2.01	0.42
1:A:69:ALA:HB2	1:A:80:LEU:HD21	2.02	0.41
2:D:611:LEU:HD22	2:D:611:LEU:HA	1.68	0.41
1:A:33:PHE:CD1	1:A:40:LYS:HG2	2.55	0.41
2:D:616:ASP:O	2:D:620:HIS:CD2	2.72	0.41
2:D:642:ASP:HA	2:D:643:PRO:HD3	1.82	0.41
2:B:175:LEU:HG	2:B:182:GLN:HG2	2.01	0.41
1:C:484:SER:O	1:C:488:ALA:HB3	2.20	0.41
1:C:424:TYR:N	1:C:424:TYR:HD2	2.15	0.41
2:D:592:SER:C	2:D:593:THR:CG2	2.89	0.41
2:B:232:SER:HB3	2:B:287:LYS:HG2	2.02	0.41
1:A:118:THR:HG22	1:A:121:VAL:H	1.86	0.41
2:D:609:LYS:HE2	3:D:1690:HEM:O1A	2.20	0.41
1:A:34:LEU:HD12	2:B:267:PRO:HB2	2.03	0.41
1:A:43:PHE:HA	1:A:45:HIS:CE1	2.55	0.40
2:B:148:PRO:HA	2:B:151:LYS:HG3	2.02	0.40
2:D:643:PRO:HA	2:D:646:PHE:CE2	2.56	0.40
2:B:206:HIS:NE2	4:B:1291:OXY:O1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ARG:HA	2:D:667:PRO:HB3	2.03	0.40
2:B:245:ASN:HB3	3:B:1290:HEM:HMC1	2.02	0.40
2:D:625:LYS:CD	2:D:686:HIS:CD2	3.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:2027:HOH:O	5:C:2027:HOH:O[2_545]	1.90	0.30

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
1	C	139/141 (99%)	128 (92%)	10 (7%)	1 (1%)	26	21
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	D	144/146 (99%)	138 (96%)	5 (4%)	1 (1%)	26	21
All	All	566/574 (99%)	543 (96%)	21 (4%)	2 (0%)	39	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	419	ALA
2	D	663	LYS

5.3.2 Protein sidechains [i](#)

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	113/113 (100%)	92 (81%)	21 (19%)	2	1
1	C	113/113 (100%)	101 (89%)	12 (11%)	8	5
2	B	118/118 (100%)	106 (90%)	12 (10%)	9	5
2	D	118/118 (100%)	104 (88%)	14 (12%)	6	3
All	All	462/462 (100%)	403 (87%)	59 (13%)	5	3

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	16	LYS
1	A	17	VAL
1	A	23	GLU
1	A	32	MET
1	A	52	SER
1	A	60	LYS
1	A	66	LEU
1	A	68	ASN
1	A	73	VAL
1	A	84	SER
1	A	90	LYS
1	A	92	ARG
1	A	99	LYS
1	A	101	LEU
1	A	106	LEU
1	A	109	LEU
1	A	114	PRO
1	A	116	GLU
1	A	118	THR
1	A	141	ARG
2	B	146	LEU
2	B	147	THR
2	B	149	GLU
2	B	155	THR
2	B	160	LYS
2	B	163	VAL
2	B	164	ASP

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Mol	Chain	Res	Type
2	B	204	LYS
2	B	211	LEU
2	B	215	SER
2	B	238	LYS
2	B	277	VAL
1	C	402	LEU
1	C	416	LYS
1	C	417	VAL
1	C	456	LYS
1	C	473	VAL
1	C	481	SER
1	C	484	SER
1	C	501	LEU
1	C	505	LEU
1	C	509	LEU
1	C	516	GLU
1	C	541	ARG
2	D	544	VAL
2	D	563	VAL
2	D	564	ASP
2	D	575	LEU
2	D	583	ARG
2	D	601	PRO
2	D	604	LYS
2	D	609	LYS
2	D	611	LEU
2	D	618	LEU
2	D	630	THR
2	D	638	LYS
2	D	647	ARG
2	D	687	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	97	ASN
2	B	245	ASN
2	B	260	HIS
1	C	472	HIS
1	C	497	ASN
2	D	620	HIS

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Mol	Chain	Res	Type
2	D	623	ASN
2	D	686	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands 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$
3	HEM	A	1142	1,4	30,50,50	2.77	11 (36%)	24,82,82	3.56	16 (66%)
4	OXY	A	1143	3	1,1,1	0.10	0	0,0,0	0.00	-
3	HEM	B	1290	2,4	30,50,50	2.53	8 (26%)	24,82,82	3.65	15 (62%)
4	OXY	B	1291	3	1,1,1	0.40	0	0,0,0	0.00	-
3	HEM	C	1542	1,4	30,50,50	2.69	8 (26%)	24,82,82	2.84	13 (54%)
4	OXY	C	1543	3	1,1,1	0.32	0	0,0,0	0.00	-
3	HEM	D	1690	2,4	30,50,50	2.87	12 (40%)	24,82,82	3.36	12 (50%)
4	OXY	D	1691	3	1,1,1	0.04	0	0,0,0	0.00	-

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
3	HEM	A	1142	1,4	-	0/10/54/54	0/0/8/8
4	OXY	A	1143	3	-	0/0/0/0	0/0/0/0
3	HEM	B	1290	2,4	-	0/10/54/54	0/0/8/8
4	OXY	B	1291	3	-	0/0/0/0	0/0/0/0
3	HEM	C	1542	1,4	-	0/10/54/54	0/0/8/8
4	OXY	C	1543	3	-	0/0/0/0	0/0/0/0
3	HEM	D	1690	2,4	-	0/10/54/54	0/0/8/8
4	OXY	D	1691	3	-	0/0/0/0	0/0/0/0

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1690	HEM	C3B-C4B	-8.48	1.44	1.51
3	A	1142	HEM	C3B-C4B	-7.97	1.44	1.51
3	C	1542	HEM	C2D-C3D	-7.35	1.32	1.54
3	D	1690	HEM	C2D-C3D	-7.20	1.32	1.54
3	B	1290	HEM	C3B-C4B	-6.82	1.45	1.51
3	B	1290	HEM	C2D-C3D	-6.72	1.34	1.54
3	A	1142	HEM	C2D-C3D	-6.22	1.35	1.54
3	B	1290	HEM	C3D-C4D	-6.19	1.43	1.51
3	C	1542	HEM	C3D-C4D	-5.99	1.43	1.51
3	D	1690	HEM	C3D-C4D	-5.83	1.44	1.51
3	C	1542	HEM	C3B-C4B	-5.48	1.47	1.51
3	A	1142	HEM	C3D-C4D	-5.39	1.44	1.51
3	A	1142	HEM	C2C-C1C	-4.38	1.44	1.52
3	C	1542	HEM	C2C-C1C	-3.96	1.45	1.52
3	D	1690	HEM	C2C-C1C	-3.82	1.45	1.52
3	D	1690	HEM	C2B-C1B	-2.63	1.43	1.51
3	B	1290	HEM	C2C-C1C	-2.60	1.47	1.52
3	D	1690	HEM	C2D-C1D	-2.57	1.43	1.51
3	B	1290	HEM	C2D-C1D	-2.40	1.44	1.51
3	D	1690	HEM	C2A-C3A	-2.36	1.30	1.37
3	A	1142	HEM	C2B-C1B	-2.34	1.44	1.51
3	A	1142	HEM	C2D-C1D	-2.12	1.44	1.51
3	A	1142	HEM	C2A-C3A	-2.11	1.31	1.37
3	C	1542	HEM	C2D-C1D	-2.08	1.45	1.51
3	A	1142	HEM	FE-NC	2.19	2.04	1.95
3	D	1690	HEM	CHD-C4C	2.35	1.41	1.36
3	C	1542	HEM	FE-NC	2.42	2.05	1.95
3	B	1290	HEM	C3C-CAC	2.51	1.56	1.51
3	D	1690	HEM	C3C-CAC	2.73	1.56	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1290	HEM	C1C-NC	2.78	1.39	1.36
3	D	1690	HEM	FE-NC	2.92	2.07	1.95
3	D	1690	HEM	C4C-NC	3.00	1.39	1.36
3	A	1142	HEM	CHC-C1C	3.10	1.43	1.36
3	A	1142	HEM	C3C-CAC	3.11	1.57	1.51
3	C	1542	HEM	C1C-NC	3.53	1.40	1.36
3	D	1690	HEM	C1C-NC	3.55	1.40	1.36
3	B	1290	HEM	FE-NC	3.63	2.10	1.95
3	A	1142	HEM	C1C-NC	4.36	1.41	1.36
3	C	1542	HEM	C4C-NC	5.39	1.42	1.36

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1142	HEM	CAA-C2A-C1A	-9.10	117.13	127.01
3	B	1290	HEM	CAA-C2A-C1A	-8.51	117.77	127.01
3	D	1690	HEM	CMA-C3A-C4A	-6.00	118.44	128.36
3	B	1290	HEM	CMA-C3A-C4A	-5.76	118.83	128.36
3	D	1690	HEM	CAA-C2A-C1A	-5.59	120.94	127.01
3	D	1690	HEM	CBA-CAA-C2A	-5.01	103.55	112.53
3	B	1290	HEM	C3C-CAC-CBC	-4.01	118.30	124.46
3	B	1290	HEM	C3B-CAB-CBB	-4.00	118.33	124.46
3	C	1542	HEM	CMA-C3A-C4A	-3.79	122.09	128.36
3	D	1690	HEM	C4B-CHC-C1C	-3.70	119.64	125.82
3	A	1142	HEM	CBA-CAA-C2A	-3.51	106.23	112.53
3	A	1142	HEM	CAA-CBA-CGA	-3.49	106.35	112.75
3	C	1542	HEM	CBD-CAD-C3D	-3.02	104.77	113.55
3	A	1142	HEM	CBD-CAD-C3D	-2.99	104.85	113.55
3	C	1542	HEM	CAA-C2A-C1A	-2.75	124.02	127.01
3	A	1142	HEM	CMA-C3A-C4A	-2.40	124.39	128.36
3	B	1290	HEM	C1D-CHD-C4C	-2.18	122.17	125.82
3	B	1290	HEM	CBA-CAA-C2A	-2.12	108.73	112.53
3	C	1542	HEM	C3B-CAB-CBB	-2.12	121.21	124.46
3	B	1290	HEM	C4B-CHC-C1C	2.20	129.51	125.82
3	B	1290	HEM	CAA-C2A-C3A	2.23	135.36	129.00
3	B	1290	HEM	C2C-C1C-CHC	2.28	127.14	123.68
3	A	1142	HEM	CMA-C3A-C2A	2.36	130.18	125.24
3	D	1690	HEM	CAD-CBD-CGD	2.65	123.84	113.02
3	A	1142	HEM	CMD-C2D-C3D	2.68	126.19	114.35
3	A	1142	HEM	CAD-C3D-C4D	2.78	122.27	112.47
3	C	1542	HEM	CMA-C3A-C2A	2.78	131.06	125.24
3	A	1142	HEM	C2C-C1C-CHC	2.98	128.22	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1290	HEM	CMA-C3A-C2A	3.06	131.63	125.24
3	C	1542	HEM	CAA-CBA-CGA	3.07	118.37	112.75
3	C	1542	HEM	CMD-C2D-C3D	3.12	128.17	114.35
3	A	1142	HEM	C1D-CHD-C4C	3.14	131.06	125.82
3	D	1690	HEM	CAD-C3D-C4D	3.14	123.54	112.47
3	A	1142	HEM	C3B-C4B-CHC	3.22	127.70	123.16
3	C	1542	HEM	CAD-C3D-C4D	3.32	124.17	112.47
3	B	1290	HEM	CMD-C2D-C3D	3.45	129.59	114.35
3	B	1290	HEM	CMB-C2B-C3B	3.71	125.80	116.53
3	A	1142	HEM	C3B-CAB-CBB	3.80	130.28	124.46
3	D	1690	HEM	CMD-C2D-C3D	4.03	132.16	114.35
3	D	1690	HEM	CMA-C3A-C2A	4.45	134.55	125.24
3	D	1690	HEM	C2D-C3D-C4D	4.46	109.07	101.50
3	C	1542	HEM	CBA-CAA-C2A	4.53	120.65	112.53
3	A	1142	HEM	C2D-C3D-C4D	4.56	109.22	101.50
3	C	1542	HEM	CAD-C3D-C2D	4.58	126.39	113.22
3	B	1290	HEM	C2D-C3D-C4D	4.67	109.41	101.50
3	C	1542	HEM	C2D-C3D-C4D	4.68	109.44	101.50
3	C	1542	HEM	CMB-C2B-C3B	4.71	128.28	116.53
3	D	1690	HEM	CAD-C3D-C2D	4.89	127.27	113.22
3	D	1690	HEM	CMB-C2B-C3B	5.05	129.15	116.53
3	A	1142	HEM	CAD-C3D-C2D	5.29	128.44	113.22
3	C	1542	HEM	CMC-C2C-C3C	5.46	130.15	116.53
3	A	1142	HEM	CMC-C2C-C3C	5.56	130.41	116.53
3	A	1142	HEM	CMB-C2B-C3B	5.62	130.55	116.53
3	D	1690	HEM	CMC-C2C-C3C	5.67	130.68	116.53
3	B	1290	HEM	CAD-C3D-C2D	6.62	132.26	113.22
3	B	1290	HEM	CMC-C2C-C3C	6.84	133.61	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1142	HEM	3	0
3	B	1290	HEM	1	0
4	B	1291	OXY	2	0
3	D	1690	HEM	9	0
4	D	1691	OXY	2	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 ⓘ

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands ⓘ

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS failed to run properly - this section will therefore be empty.