



## wwPDB EM Map/Model Validation Report ⓘ

Sep 16, 2016 – 10:30 AM EDT

PDB ID : 5GJV  
EMDB ID: : EMD-9513  
Title : Structure of the mammalian voltage-gated calcium channel Cav1.1 complex at near atomic resolution  
Authors : Wu, J.P.; Yan, Z.; Li, Z.Q.; Zhou, Q.; Yan, N.  
Deposited on : 2016-07-02  
Resolution : 3.60 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.  
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/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
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) : rb-20027939

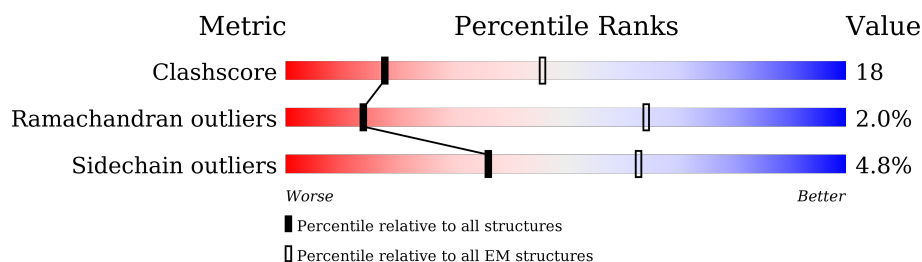
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1873	
2	B	106	
3	C	199	
4	E	222	
5	F	1106	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21904 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Voltage-dependent L-type calcium channel subunit alpha-1S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1276	Total	C	N	O	S	4	0
			10183	6699	1673	1742	69		

- Molecule 2 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	100	Total	C	N	O	S	0	0
			710	455	125	129	1		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	SER	-	expression tag	UNP P19517
B	70	LEU	-	expression tag	UNP P19517
B	71	GLU	-	expression tag	UNP P19517
B	72	VAL	-	expression tag	UNP P19517
B	73	LEU	-	expression tag	UNP P19517
B	74	PHE	-	expression tag	UNP P19517
B	75	GLN	-	expression tag	UNP P19517
B	76	GLY	-	expression tag	UNP P19517
B	77	PRO	-	expression tag	UNP P19517
B	78	HIS	-	expression tag	UNP P19517
B	79	MET	-	expression tag	UNP P19517

- Molecule 3 is a protein called Voltage-dependent L-type calcium channel subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	178	Total	C	N	O	S	0	0
			1367	876	232	254	5		

- Molecule 4 is a protein called Voltage-dependent calcium channel gamma-1 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	166	Total	C	N	O	S	0	0
			1304	860	213	213	18		

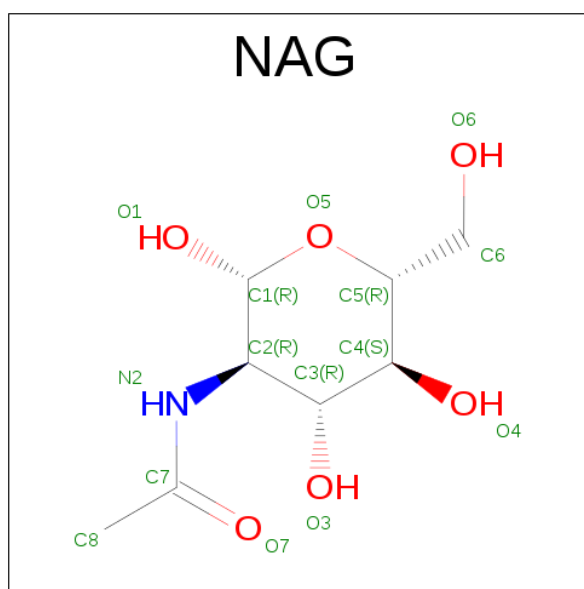
- Molecule 5 is a protein called Voltage-dependent calcium channel subunit alpha-2/delta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	942	Total	C	N	O	S	1	0
			7567	4809	1277	1451	30		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1075	ETA	GLY	conflict	UNP P13806

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



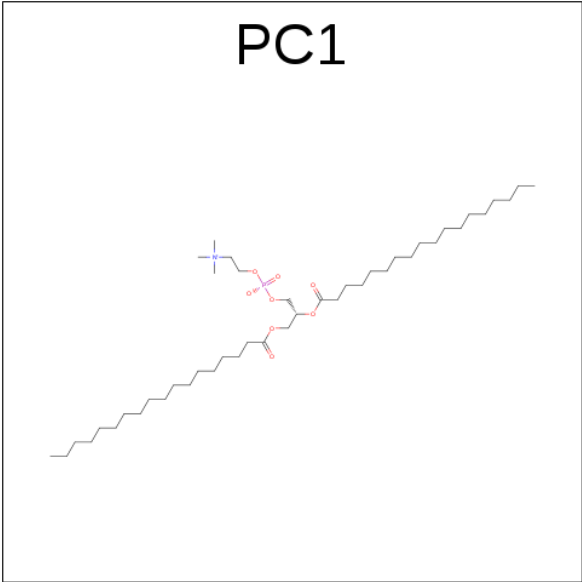
Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	

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Mol	Chain	Residues	Atoms				AltConf
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	
6	F	1	Total	C	N	O	0
			308	176	22	110	

- Molecule 7 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).

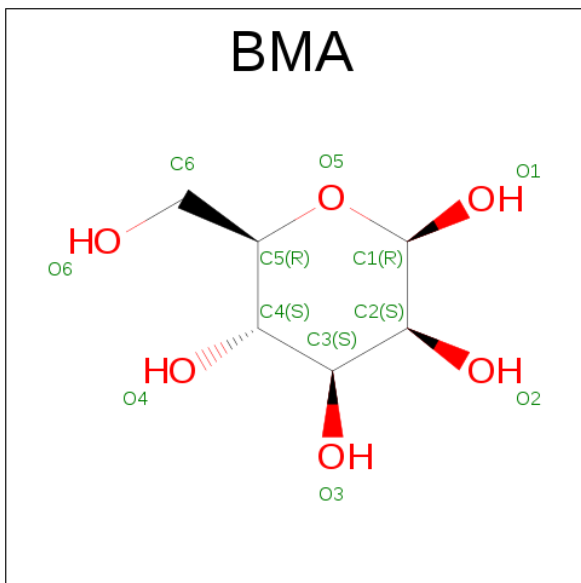


Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	
7	A	1	Total	C	N	O	P	0
			426	356	7	56	7	

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
8	A	2	Total	Ca	0
			2	2	
8	F	1	Total	Ca	0
			1	1	

- Molecule 9 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).

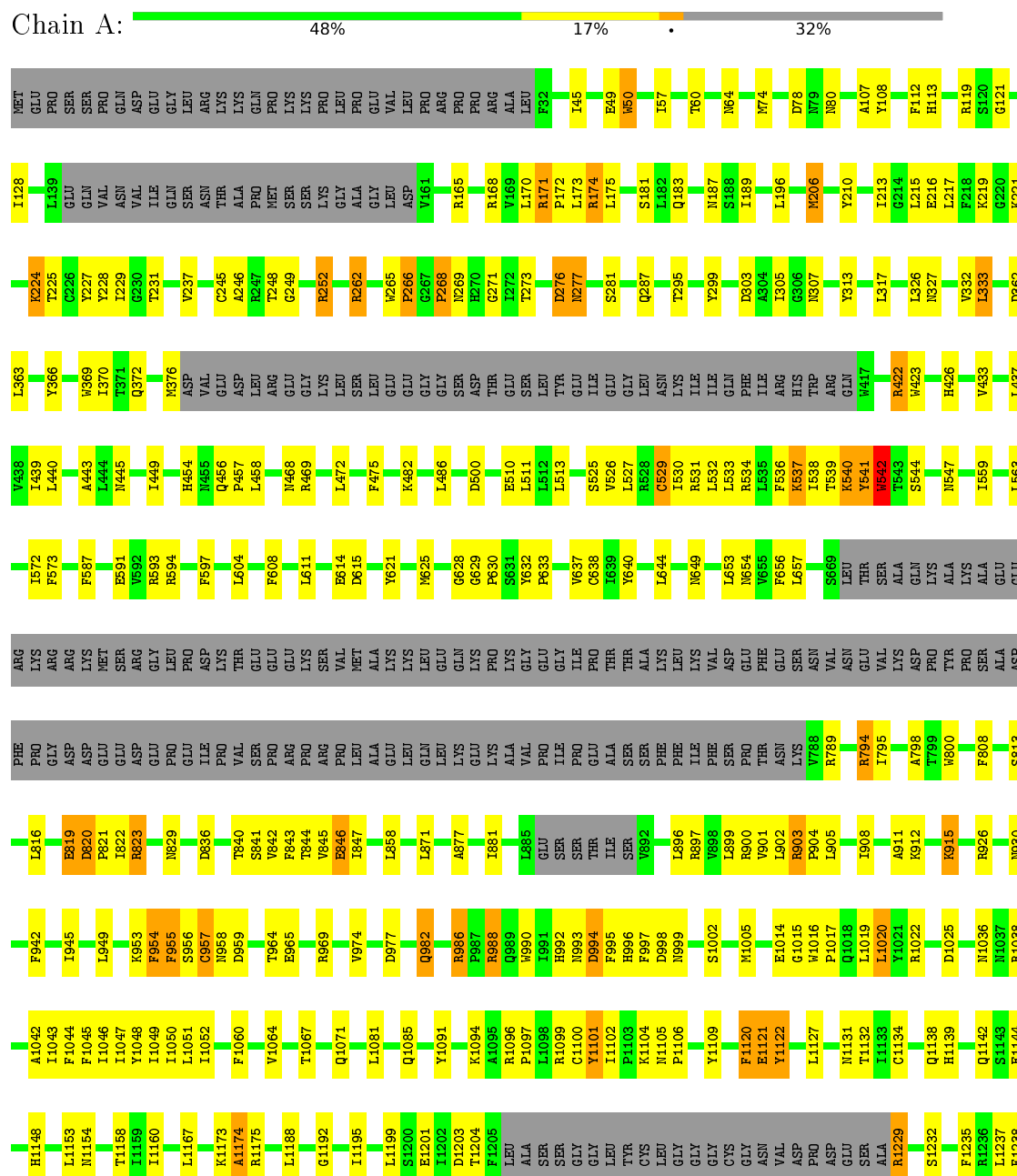


Mol	Chain	Residues	Atoms			AltConf
9	F	1	Total	C	O	0
			22	12	10	
9	F	1	Total	C	O	0
			22	12	10	

### 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. 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. 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: Voltage-dependent L-type calcium channel subunit alpha-1S







Chain F:  55% 24% 6% 15%

MET	ALA	ALA	GLY	ARG	PRO	LEU	ALA	TRP	THR	LEU	THR	LEU	THR	LEU	TRP	GLN	ASP	LEU	ALA	TRP	LEU	ILE	LEU	ILE	LEU	GLY	PRO	SER	SER	SER	GLU	GLU	PRO	F29	P30	W38	V47	T52	G55	L59	E64	Q67	Y70	N75	N76	A77	R78	Q79	L80	V81	R85	S86	K87	A88	L99
V100	R101	E105	A106	S121	ASN	GLU	V126	A131	K132	D133	ASP	LEU	ASP	PRO	GLU	LYS	ASN	ASP	PRO	THR	ASN	ASP	PRO	GLU	GLY	SER	Q145	R146	I147	K148	P149	D153	R159	Q160	Y163	A167	V168	D173	I174	Y175	E176	E184	L185	N186	A190	L191	D192	D193	V194	N198	R199				
E200	E201	L206	W207	Q208	S212	L216	A217	R218	Y219	Y220	P224	W225	V226	ASP	ASN	ARG	THR	ASN	PRO	ASP	K234	L235	D236	R242	R243	P244	W245	Y246	I247	Q248	S252	P253	K254	D255	M256	T270	E283	F290	V291	N297	S298	N299	D302	V303	S304	C305	L309								
W310	Q311	A312	N313	V314	R315	R318	K321	D322	A323	V324	N325	K330	G331	I332	T333	T335	F341	K348	Y349	N350	S351	S352	K353	C356	R357	K358	I359	D365	G366	T381	K382	K383	F389	G392	Q393	R394	N395	Y396	D397	R398	L401	A405	C406	E407	R408	R409									
G410	Y411	Y412	Y413	E414	S417	I418	R422	Y428	L429	L432	L438	Q445	V446	Q447	W448	T449	N450	V451	Y452	L458	V461	L462	T463	G464	T465	L466	F469	E476	N477	K478	T479	N480	L481	K482	L485	V484	S485	L486	D487	D488	L489	K500	R501	L502	T503	P504	R505								
F506	T507	L508	C509	P510	N511	G512	Y513	Y514	F515	D518	P519	N520	G521	Y522	H526	P527	N528	L529	D530	P531	K532	P533	I534	G535	G537	R544	R547	G548	N549	V559	F563	L564	E567	L568	E569	B577	B578	K579	G583	E584	S585	G586	E587	R591	V594	K595	S596	D598							
E599	R600	D603	R607	T608	Y609	T610	W611	P612	P613	W614	N615	A623	L624	T628	Y629	S630	F631	I634	I638	T643	Q644	Y647	S648	E649	N655	F656	G660	Y661	T662	F663	L664	R667	D668	Y669	G670	S671	D672	N679	T680	E681	N685	F686	R692	K693	T694										
PRO	ASN	ASN	PRO	SER	CYS	ASN	T702	R707	L710	D711	W712	A713	G714	T715	L718	Y722	F731	Y732	K733	A734	R735	F736	Y737	V738	T744	W755	P759	Y762	E763	Y767	K768	R769	Y776	F783	N784	Y785	S786	G787	A790	Y791	E792	S793													
G794	I795	M796	I805	Q806	Q807	K808	P812	K818	L819	D820	T831	R834	ASP	PRO	CYS	ASP	ALA	GLY	PRO	VAL	VAL	CYS	ASP	CYS	ALA	LYS	ARG	ASN	SER	ASP	VAL	N851	L856	D857	D858	G859	G860	F878	G879	E880	N886	N891	I892	S893	Y894	Y895	S900	Y901	Q904	A912					
PRO	LYS	GLN	GLY	ALA	GLY	HIS	ARG	SER	ALA	TYR	VAL	PRO	VAL	PRO	SER	ILE	ALA	ASP	ILE	LEU	GLN	ILE	GLY	ILE	GLN	PHE	VAL	VAL	SER	ILE	LEU	GLN	PHE	PHE	PRO	ARG	LEU	SER	LEU	GLY	ALA	ALA	ASP	MET	GLU	ASP	ASP	ASP	PHE	THR	ALA	SER	NET		
S973	T979	E980	Q981	T982	Q983	T984	F985	D989	S990	K991	S992	F993	C1002	F1006	H1007	V1008	E1009	K1010	L1011	H1015	L1016	I1019	M1020	S1023	C1024	G1025	T1026	R1032	L1033	Q1036	A1037	E1038	M1049	V1050	K1051	Q1052	P1053	G1058	P1059	D1060	V1061	C1062	F1063	L1068	E1069	D1070	Y1071								
T1072	D1073	C1074	T1075	GLY	VAL	SER	GLY	ASN	PRO	SER	LEU	TRP	SER	ILE	ILE	GLY	ILE	GLN	PHE	VAL	VAL	SER	GLY	ARG	HIS	CYS	LEU	LEU	R1032	L1033	Q1036	A1037	E1038	M1049	V1050	K1051	Q1052	P1053	G1058	P1059	D1060	V1061	C1062	F1063	L1068	E1069	D1070	Y1071							

## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	527833	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ETA, NAG, BMA, PC1

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  > 2$	RMSZ	# $ Z  > 2$
1	A	0.56	2/10431 (0.0%)	0.73	24/14157 (0.2%)
2	B	0.43	1/723 (0.1%)	0.65	3/979 (0.3%)
3	C	0.34	0/1394	0.50	0/1892
4	E	0.42	1/1336 (0.1%)	0.58	2/1802 (0.1%)
5	F	0.68	13/7721 (0.2%)	0.85	32/10463 (0.3%)
All	All	0.58	17/21605 (0.1%)	0.76	61/29293 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
3	C	0	2
5	F	0	14
All	All	0	27

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ARG	C-O	13.19	1.48	1.23
5	F	647	TYR	C-N	10.24	1.57	1.34
5	F	312	ALA	C-O	7.40	1.37	1.23
2	B	167	SER	CB-OG	6.12	1.50	1.42
5	F	526	HIS	C-N	-6.02	1.22	1.34
5	F	1062	CYS	C-O	-5.84	1.12	1.23
5	F	504	PRO	N-CD	5.50	1.55	1.47
5	F	1053	PRO	N-CD	5.37	1.55	1.47
5	F	225	TRP	CB-CG	-5.31	1.40	1.50
5	F	533	PRO	N-CD	5.29	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	244	PRO	N-CD	5.27	1.55	1.47
5	F	510	PRO	N-CD	5.26	1.55	1.47
5	F	1059	PRO	N-CD	5.20	1.55	1.47
4	E	208	PRO	N-CD	5.19	1.55	1.47
5	F	531	PRO	N-CD	5.05	1.54	1.47
5	F	291	VAL	CB-CG1	-5.03	1.42	1.52
1	A	638	CYS	CB-SG	-5.03	1.73	1.81

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	518	ASP	CB-CA-C	-10.92	88.55	110.40
5	F	469	PHE	CB-CA-C	-9.64	91.12	110.40
5	F	445	GLN	CB-CA-C	9.59	129.57	110.40
1	A	1174	ALA	CB-CA-C	-8.28	97.69	110.10
5	F	175	TYR	N-CA-C	8.25	133.27	111.00
5	F	406	CYS	O-C-N	-8.24	109.52	122.70
5	F	609	TYR	CB-CA-C	7.89	126.17	110.40
5	F	663	PHE	CB-CA-C	-7.64	95.12	110.40
1	A	957	CYS	CB-CA-C	-7.37	95.67	110.40
1	A	181	SER	CB-CA-C	7.31	123.99	110.10
1	A	333	LEU	CA-CB-CG	7.24	131.95	115.30
5	F	607	ARG	N-CA-C	-7.20	91.56	111.00
5	F	216	LEU	CB-CA-C	-7.15	96.61	110.20
1	A	949	LEU	CA-CB-CG	7.10	131.62	115.30
1	A	1417	ILE	CB-CA-C	6.97	125.53	111.60
5	F	407	GLU	CB-CA-C	-6.90	96.59	110.40
5	F	522	TYR	CB-CA-C	-6.80	96.79	110.40
2	B	115	PRO	N-CA-CB	6.75	111.41	103.30
2	B	130	PRO	N-CA-CB	6.56	111.17	103.30
5	F	1002	CYS	CB-CA-C	6.53	123.45	110.40
1	A	281	SER	CB-CA-C	6.35	122.16	110.10
5	F	735	ARG	CB-CA-C	-6.34	97.73	110.40
1	A	954	PHE	CB-CG-CD1	6.32	125.22	120.80
1	A	1461	VAL	CB-CA-C	6.28	123.32	111.40
2	B	113	PRO	N-CA-CB	6.17	110.70	103.30
4	E	210	ASN	C-N-CD	6.10	141.22	128.40
5	F	1006	PHE	CB-CA-C	-6.04	98.31	110.40
1	A	326	LEU	CA-CB-CG	6.04	129.18	115.30
1	A	440	LEU	CB-CA-C	5.99	121.58	110.20
1	A	458	LEU	CA-CB-CG	5.96	129.01	115.30
5	F	664	LEU	CB-CA-C	-5.95	98.90	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	305	CYS	CA-CB-SG	5.92	124.65	114.00
5	F	603	ASP	CB-CA-C	-5.84	98.72	110.40
5	F	405	ALA	O-C-N	-5.83	113.37	122.70
5	F	254	LYS	CB-CA-C	-5.78	98.84	110.40
5	F	624	LEU	CB-CA-C	-5.76	99.25	110.20
1	A	644	LEU	CB-CG-CD2	-5.73	101.25	111.00
1	A	954	PHE	CB-CG-CD2	-5.72	116.80	120.80
5	F	1052	GLN	C-N-CD	5.70	140.37	128.40
4	E	207	MET	C-N-CD	5.68	140.34	128.40
5	F	900	SER	CB-CA-C	-5.64	99.39	110.10
5	F	243	ARG	C-N-CD	5.62	140.20	128.40
1	A	443	ALA	CB-CA-C	5.62	118.53	110.10
5	F	509	CYS	C-N-CD	5.60	140.17	128.40
5	F	1002	CYS	N-CA-C	-5.60	95.87	111.00
5	F	1058	GLY	C-N-CD	5.60	140.17	128.40
5	F	520	ASN	CB-CA-C	-5.57	99.27	110.40
1	A	997	PHE	CB-CG-CD1	5.56	124.69	120.80
1	A	1316	LEU	CB-CG-CD2	-5.53	101.60	111.00
1	A	196	LEU	CA-CB-CG	5.51	127.97	115.30
5	F	783	PHE	C-N-CA	5.47	135.38	121.70
5	F	607	ARG	C-N-CA	5.41	135.22	121.70
5	F	503	THR	C-N-CD	5.33	139.58	128.40
1	A	597	PHE	CB-CG-CD1	5.30	124.51	120.80
1	A	1188	LEU	CA-CB-CG	5.30	127.48	115.30
5	F	609	TYR	CA-CB-CG	5.30	123.46	113.40
1	A	858	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	1337	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	333	LEU	CB-CG-CD2	-5.16	102.22	111.00
5	F	610	THR	CB-CA-C	-5.15	97.68	111.60
1	A	653	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1344	TYR	Peptide
1	A	1440	PRO	Peptide
1	A	1441	HIS	Peptide
1	A	228	TYR	Peptide
1	A	229	ILE	Peptide
1	A	237	VAL	Peptide
1	A	266	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	268	PRO	Peptide
1	A	456	GLN	Peptide
1	A	628	GLY	Peptide
1	A	629	GLY	Peptide
3	C	281	GLY	Mainchain,Peptide
5	F	1023	SER	Peptide
5	F	1024	LYS	Peptide
5	F	1074	CYS	Mainchain,Peptide
5	F	175	TYR	Peptide
5	F	220	TYR	Peptide
5	F	406	CYS	Mainchain
5	F	476	GLU	Peptide
5	F	522	TYR	Peptide
5	F	600	ARG	Peptide
5	F	70	TYR	Peptide
5	F	785	LYS	Peptide
5	F	786	SER	Peptide
5	F	805	ILE	Peptide

## 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	10183	0	10143	394	0
2	B	710	0	633	1	0
3	C	1367	0	1343	9	0
4	E	1304	0	1330	66	0
5	F	7567	0	7404	316	0
6	A	14	0	13	0	0
6	F	308	0	276	6	0
7	A	426	0	675	20	0
8	A	2	0	0	0	0
8	F	1	0	0	0	0
9	F	22	0	20	0	0
All	All	21904	0	21837	768	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 18.

All (768) 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)
1:A:1389:ARG:HD2	1:A:1391:TRP:CE3	1.43	1.51
5:F:669:TYR:HD1	5:F:670:CYS:N	1.28	1.29
4:E:208:PRO:CG	4:E:214:SER:HA	1.64	1.26
1:A:1203:ASP:OD2	1:A:1229:ARG:HD2	1.15	1.24
1:A:1389:ARG:HB2	1:A:1391:TRP:CZ3	1.71	1.24
5:F:411:TYR:CD1	5:F:1074:CYS:HA	1.71	1.22
4:E:15:CYS:SG	4:E:191:LEU:CD2	2.28	1.21
1:A:956:SER:HB3	1:A:1022:ARG:NH1	1.53	1.21
1:A:475:PHE:CE2	1:A:537:LYS:HE3	1.77	1.20
1:A:224:LYS:O	1:A:266:PRO:HG3	1.44	1.16
1:A:1389:ARG:HD2	1:A:1391:TRP:CD2	1.82	1.15
5:F:529:LEU:O	5:F:530:GLN:HG2	1.48	1.14
4:E:15:CYS:SG	4:E:191:LEU:HD21	1.87	1.13
5:F:315[B]:ARG:HH21	5:F:1049:MET:HE2	1.07	1.12
1:A:1060:PHE:HZ	1:A:1376:PHE:CE1	1.68	1.10
1:A:1015:GLY:HA3	1:A:1326:GLN:HE22	1.03	1.09
1:A:1389:ARG:CD	1:A:1391:TRP:CE3	2.34	1.09
1:A:956:SER:HB3	1:A:1022:ARG:HH11	0.92	1.08
4:E:208:PRO:HG3	4:E:214:SER:HA	1.28	1.08
1:A:1262:LYS:HE3	4:E:209:GLN:O	1.52	1.08
5:F:564:LEU:HD11	5:F:569:GLU:HG3	1.31	1.07
1:A:1046:ILE:HD12	7:A:1914:PC1:H392	1.36	1.06
5:F:174:ILE:HG22	5:F:175:TYR:H	1.21	1.06
5:F:669:TYR:CD1	5:F:670:CYS:N	2.09	1.05
1:A:128:ILE:HG13	1:A:171:ARG:HH11	1.16	1.05
1:A:1391:TRP:HE1	1:A:1397:HIS:CD2	1.73	1.04
5:F:564:LEU:CD1	5:F:569:GLU:HG3	1.87	1.04
4:E:19:GLY:HA3	4:E:191:LEU:CD1	1.88	1.04
1:A:587:PHE:HE2	1:A:625:MET:HE2	1.23	1.03
5:F:894:VAL:HG21	5:F:993:PHE:CE2	1.93	1.03
5:F:297:ASN:ND2	5:F:330:LYS:O	1.91	1.03
4:E:208:PRO:HG2	4:E:214:SER:HA	1.39	1.02
5:F:661:TYR:CE2	5:F:663:PHE:CZ	2.48	1.02
4:E:19:GLY:CA	4:E:191:LEU:CD1	2.38	1.02
1:A:362:ASP:OD1	3:C:437:ASN:ND2	1.93	1.01
5:F:643:THR:HG22	5:F:647:TYR:CE2	1.95	1.01
5:F:647:TYR:CE1	5:F:713:GLY:HA3	1.96	1.00
5:F:644:GLN:HA	5:F:647:TYR:HD2	1.25	1.00
5:F:534:ILE:HG22	5:F:904:GLN:HG2	1.40	0.99
1:A:1015:GLY:CA	1:A:1326:GLN:HE22	1.75	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:PHE:HD2	1:A:1048:TYR:CD1	1.81	0.99
1:A:1337:LEU:CD1	1:A:1350:TYR:HE1	1.76	0.98
5:F:248:GLN:OE1	5:F:447:GLN:HB3	1.63	0.98
1:A:1203:ASP:OD2	1:A:1229:ARG:CD	2.11	0.98
1:A:529:CYS:SG	1:A:945:ILE:HG13	2.03	0.97
1:A:1015:GLY:HA3	1:A:1326:GLN:NE2	1.80	0.97
4:E:19:GLY:CA	4:E:191:LEU:HD12	1.94	0.97
5:F:732:VAL:O	5:F:820:ASP:HB2	1.63	0.96
1:A:942:PHE:HD2	1:A:1048:TYR:HD1	1.00	0.96
5:F:174:ILE:HG22	5:F:175:TYR:N	1.75	0.96
5:F:315[B]:ARG:HH21	5:F:1049:MET:CE	1.78	0.96
1:A:955:PHE:CE1	1:A:992:HIS:ND1	2.34	0.95
4:E:19:GLY:HA3	4:E:191:LEU:HD13	1.48	0.95
1:A:1262:LYS:CE	4:E:209:GLN:O	2.15	0.95
5:F:528:ASN:O	5:F:528:ASN:ND2	1.98	0.95
1:A:955:PHE:CE1	1:A:992:HIS:CE1	2.54	0.95
1:A:614:GLU:OE2	1:A:615:ASP:HB2	1.68	0.94
6:F:1204:NAG:C6	6:F:1205:NAG:H82	1.98	0.94
4:E:19:GLY:N	4:E:191:LEU:CD1	2.32	0.93
1:A:1390:ASP:O	1:A:1392:SER:N	2.02	0.93
5:F:382:LYS:NZ	5:F:407:GLU:O	2.02	0.93
1:A:1042:ALA:O	1:A:1046:ILE:HG13	1.69	0.92
1:A:1389:ARG:HB2	1:A:1391:TRP:HZ3	1.25	0.92
5:F:1036:GLN:HE21	5:F:1037:ALA:H	1.17	0.92
5:F:174:ILE:CG2	5:F:175:TYR:H	1.81	0.92
5:F:661:TYR:CD2	5:F:663:PHE:CZ	2.58	0.92
1:A:1299:GLN:NE2	1:A:1327:GLU:OE1	2.03	0.92
1:A:836:ASP:OD2	1:A:900:ARG:NH1	2.02	0.92
5:F:290:PHE:HD2	5:F:310:VAL:O	1.52	0.91
5:F:647:TYR:CD1	5:F:713:GLY:HA3	2.05	0.91
1:A:942:PHE:CD2	1:A:1048:TYR:HD1	1.88	0.91
1:A:1043:ILE:HG12	1:A:1047:ILE:HD11	1.52	0.90
1:A:1337:LEU:HG	1:A:1350:TYR:CE1	2.05	0.90
1:A:956:SER:CB	1:A:1022:ARG:HH11	1.84	0.90
1:A:1389:ARG:HB2	1:A:1391:TRP:CE3	2.06	0.89
1:A:1060:PHE:CZ	1:A:1376:PHE:CE1	2.60	0.89
5:F:30:PRO:CG	5:F:1020:MET:HE1	2.03	0.89
5:F:315[B]:ARG:NH2	5:F:1049:MET:HE2	1.88	0.88
1:A:587:PHE:HE2	1:A:625:MET:CE	1.85	0.88
1:A:820:ASP:HB2	1:A:821:PRO:HA	1.56	0.86
1:A:1096:ARG:NH2	4:E:213:GLU:OE2	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:1062:CYS:O	5:F:1063:PHE:CD1	2.28	0.86
5:F:536:VAL:HG12	5:F:537:GLY:H	1.37	0.86
5:F:510:PRO:HG2	5:F:767:TYR:CE2	2.11	0.86
5:F:478:LYS:O	5:F:480:ASN:N	2.09	0.85
5:F:477:ASN:O	5:F:478:LYS:HB2	1.75	0.85
1:A:510:GLU:OE2	1:A:531:ARG:HD3	1.76	0.85
5:F:297:ASN:HD21	5:F:331:GLY:HA3	1.40	0.85
1:A:1391:TRP:NE1	1:A:1397:HIS:CD2	2.45	0.85
4:E:15:CYS:SG	4:E:191:LEU:HD23	2.14	0.84
5:F:661:TYR:HD2	5:F:663:PHE:CE2	1.96	0.84
5:F:30:PRO:HG2	5:F:1020:MET:HE1	1.60	0.84
1:A:841:SER:O	1:A:845:VAL:HG23	1.76	0.84
5:F:1036:GLN:NE2	5:F:1037:ALA:H	1.75	0.84
5:F:643:THR:HG22	5:F:647:TYR:HE2	1.42	0.83
5:F:894:VAL:HG11	5:F:993:PHE:CE2	2.13	0.83
1:A:965:GLU:OE1	1:A:990:TRP:NE1	2.11	0.83
1:A:1134:CYS:SG	1:A:1153:LEU:CD1	2.67	0.83
1:A:1391:TRP:NE1	1:A:1397:HIS:HD2	1.76	0.83
5:F:894:VAL:HG21	5:F:993:PHE:HE2	1.41	0.82
5:F:534:ILE:HG22	5:F:904:GLN:CG	2.09	0.82
1:A:1262:LYS:HE3	4:E:209:GLN:C	1.98	0.82
1:A:538:ILE:O	1:A:541:TYR:HD1	1.62	0.82
5:F:290:PHE:CD2	5:F:310:VAL:O	2.32	0.82
5:F:661:TYR:HE2	5:F:663:PHE:CZ	1.94	0.81
5:F:894:VAL:HG21	5:F:993:PHE:CZ	2.14	0.81
4:E:208:PRO:HG2	4:E:214:SER:CA	2.10	0.81
5:F:515:PHE:HE2	5:F:563:PHE:CE1	1.97	0.81
5:F:247:ILE:HG23	5:F:429:LEU:HD11	1.61	0.81
1:A:262:ARG:HH11	1:A:262:ARG:HG2	1.46	0.81
1:A:1046:ILE:CD1	7:A:1914:PC1:H392	2.11	0.80
1:A:128:ILE:HG13	1:A:171:ARG:NH1	1.94	0.80
5:F:174:ILE:CG2	5:F:175:TYR:N	2.43	0.80
1:A:1134:CYS:SG	1:A:1153:LEU:HD12	2.22	0.80
5:F:671:SER:O	5:F:672:ASP:OD1	1.99	0.80
1:A:840:THR:O	1:A:844:THR:HG23	1.82	0.79
5:F:733:LYS:NZ	5:F:792:GLU:O	2.14	0.79
1:A:1337:LEU:CD1	1:A:1350:TYR:CE1	2.66	0.79
1:A:955:PHE:HE1	1:A:992:HIS:CE1	2.00	0.79
1:A:1046:ILE:O	1:A:1049:ILE:HG22	1.84	0.78
1:A:591:GLU:OE2	1:A:593:ARG:NH1	2.15	0.78
5:F:353:ARG:HH11	5:F:353:ARG:HB2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:PHE:CD1	1:A:992:HIS:ND1	2.51	0.78
1:A:587:PHE:CE2	1:A:625:MET:CE	2.68	0.77
1:A:1384:PHE:O	1:A:1388:THR:HG23	1.85	0.77
1:A:215:LEU:O	1:A:219:LYS:HG3	1.83	0.77
1:A:587:PHE:CE2	1:A:625:MET:HE2	2.15	0.77
5:F:644:GLN:HA	5:F:647:TYR:CD2	2.16	0.77
5:F:1061:VAL:HG23	5:F:1062:CYS:H	1.48	0.77
5:F:564:LEU:CD1	5:F:569:GLU:CG	2.63	0.77
1:A:821:PRO:HG3	1:A:1286:MET:HG2	1.67	0.77
5:F:411:TYR:CE1	5:F:1074:CYS:HA	2.19	0.77
5:F:894:VAL:HG11	5:F:993:PHE:HE2	1.49	0.77
1:A:1020:LEU:O	1:A:1020:LEU:HD12	1.85	0.76
1:A:903:ARG:HB2	1:A:904:PRO:HD3	1.66	0.76
1:A:1337:LEU:HD12	1:A:1350:TYR:HE1	1.50	0.76
1:A:820:ASP:H	1:A:821:PRO:HA	1.50	0.76
1:A:955:PHE:CD1	1:A:992:HIS:CE1	2.73	0.76
1:A:1390:ASP:HB3	1:A:1393:ILE:CD1	2.16	0.75
5:F:661:TYR:CD2	5:F:663:PHE:CE2	2.74	0.75
5:F:411:TYR:CD1	5:F:1074:CYS:CA	2.63	0.75
5:F:76:ASN:O	5:F:78:ARG:N	2.20	0.75
5:F:894:VAL:CG2	5:F:993:PHE:CE2	2.69	0.75
1:A:1060:PHE:HZ	1:A:1376:PHE:CD1	2.04	0.75
1:A:468:ASN:ND2	1:A:531:ARG:NH2	2.35	0.75
1:A:475:PHE:CZ	1:A:537:LYS:HE3	2.21	0.75
1:A:902:LEU:HD11	1:A:905:LEU:HD12	1.69	0.75
1:A:1325:TRP:HA	1:A:1328:ILE:HD12	1.68	0.74
4:E:19:GLY:CA	4:E:191:LEU:HD13	2.11	0.74
5:F:503:THR:HB	5:F:514:TYR:HD2	1.53	0.74
5:F:510:PRO:HG2	5:F:767:TYR:HE2	1.52	0.74
1:A:1389:ARG:CB	1:A:1391:TRP:CZ3	2.63	0.74
4:E:19:GLY:HA3	4:E:191:LEU:HD12	1.60	0.74
5:F:450:ASN:O	5:F:451:VAL:HG22	1.88	0.74
5:F:452:TYR:OH	5:F:463:THR:CG2	2.36	0.73
1:A:820:ASP:HB2	1:A:821:PRO:CA	2.18	0.73
5:F:661:TYR:CE2	5:F:663:PHE:HZ	2.02	0.73
1:A:171:ARG:O	1:A:174:ARG:HB2	1.88	0.73
1:A:819:GLU:CD	1:A:897:ARG:HH21	1.91	0.73
1:A:224:LYS:O	1:A:266:PRO:CG	2.32	0.73
5:F:315[B]:ARG:NH2	5:F:1049:MET:CE	2.46	0.73
5:F:598:ASP:C	5:F:599:GLU:HG3	2.08	0.73
5:F:732:VAL:HG23	5:F:733:LYS:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:PHE:HE2	4:E:153:VAL:CG2	2.02	0.73
1:A:1389:ARG:HE	1:A:1391:TRP:HB2	1.54	0.72
1:A:902:LEU:CD1	1:A:905:LEU:HD12	2.19	0.72
5:F:478:LYS:O	5:F:479:THR:C	2.27	0.72
5:F:586:GLY:HA3	5:F:611:TRP:CZ2	2.24	0.72
1:A:262:ARG:NH1	1:A:262:ARG:HG2	1.99	0.72
1:A:820:ASP:CB	1:A:821:PRO:CA	2.68	0.72
4:E:19:GLY:H	4:E:191:LEU:CD1	2.01	0.72
5:F:530:GLN:OE1	5:F:532:LYS:NZ	2.22	0.72
1:A:1195:ILE:HD11	4:E:113:PHE:CD2	2.25	0.72
1:A:1299:GLN:HG2	1:A:1327:GLU:HB3	1.71	0.72
5:F:1074:CYS:SG	5:F:1075:ETA:N	2.63	0.72
5:F:30:PRO:HG3	5:F:1020:MET:CE	2.19	0.72
5:F:30:PRO:HG3	5:F:1020:MET:HE1	1.69	0.72
1:A:544:SER:OG	1:A:547:ASN:HB3	1.90	0.71
1:A:843:PHE:CE2	1:A:871:LEU:HA	2.25	0.71
1:A:1134:CYS:SG	1:A:1153:LEU:HD13	2.30	0.71
5:F:669:TYR:CE1	5:F:670:CYS:HB2	2.25	0.71
5:F:353:ARG:NH1	5:F:353:ARG:HB2	2.05	0.71
1:A:439:ILE:HG12	1:A:541:TYR:OH	1.91	0.71
5:F:366:GLY:HA2	5:F:401:ILE:HD11	1.72	0.71
1:A:1014:GLU:OE2	1:A:1326:GLN:NE2	2.23	0.71
1:A:1329:LEU:HD11	1:A:1358:TYR:CD1	2.26	0.70
1:A:908:ILE:HD11	1:A:1276:MET:HG2	1.74	0.70
5:F:409:LYS:HE2	5:F:1071:TYR:CE1	2.26	0.70
1:A:1391:TRP:CD1	1:A:1397:HIS:HD2	2.09	0.70
5:F:892:ILE:HD12	5:F:892:ILE:O	1.91	0.70
1:A:632:TYR:HB3	1:A:633:PRO:HD3	1.71	0.70
1:A:911:ALA:O	1:A:915:LYS:HE3	1.92	0.70
5:F:529:LEU:O	5:F:530:GLN:CG	2.35	0.70
1:A:1249[A]:ARG:HD3	1:A:1249[A]:ARG:O	1.92	0.69
1:A:538:ILE:O	1:A:541:TYR:CD1	2.46	0.69
5:F:595:LYS:HE3	5:F:983:GLN:HE22	1.56	0.69
1:A:245:CYS:SG	1:A:246:ALA:N	2.66	0.69
1:A:268:PRO:HB2	1:A:273:THR:HB	1.73	0.69
5:F:511:ASN:HB3	5:F:607:ARG:HH12	1.56	0.69
1:A:1235:PHE:HE2	4:E:153:VAL:HG21	1.58	0.69
1:A:994:ASP:HB3	1:A:1330:LEU:HD21	1.75	0.68
4:E:208:PRO:O	4:E:210:ASN:N	2.27	0.68
6:F:1204:NAG:H62	6:F:1205:NAG:H82	1.76	0.68
5:F:318:LYS:HG2	5:F:536:VAL:HG13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1235:PHE:CE2	4:E:153:VAL:HG21	2.28	0.68
1:A:1337:LEU:CG	1:A:1350:TYR:CE1	2.76	0.68
5:F:564:LEU:HD12	5:F:569:GLU:CG	2.24	0.68
1:A:820:ASP:CB	1:A:821:PRO:HA	2.19	0.68
1:A:1071:GLN:NE2	1:A:1381:MET:SD	2.67	0.68
5:F:351:VAL:HG12	5:F:352:SER:N	2.09	0.67
1:A:1417:ILE:O	1:A:1460:THR:HA	1.95	0.67
1:A:843:PHE:HE2	1:A:871:LEU:CA	2.07	0.67
1:A:1305:ASN:HD22	1:A:1311:GLN:HG3	1.59	0.66
1:A:1047:ILE:O	1:A:1051:LEU:HG	1.94	0.66
1:A:1391:TRP:CZ2	1:A:1396:PRO:HD2	2.30	0.66
5:F:77:ALA:O	5:F:81:VAL:HG23	1.95	0.66
6:F:1204:NAG:H61	6:F:1205:NAG:H82	1.75	0.66
5:F:503:THR:HB	5:F:514:TYR:CD2	2.29	0.66
1:A:843:PHE:O	1:A:846:GLU:HG3	1.95	0.66
5:F:649:GLU:OE1	5:F:655:ASN:ND2	2.29	0.66
5:F:302:ASP:O	5:F:304:SER:N	2.29	0.66
1:A:996:HIS:ND1	1:A:998:ASP:HB2	2.11	0.65
5:F:586:GLY:O	5:F:611:TRP:CD2	2.49	0.65
5:F:991:LYS:HB3	5:F:1010:LYS:HB2	1.78	0.65
5:F:506:PHE:HA	5:F:762:TYR:HE2	1.60	0.65
5:F:667:ARG:NH1	5:F:668:ASP:O	2.30	0.65
1:A:915:LYS:N	1:A:915:LYS:HD3	2.11	0.65
1:A:1264:PHE:CE1	1:A:1267:LEU:HD23	2.32	0.65
1:A:231:THR:O	1:A:262:ARG:NH2	2.29	0.65
1:A:1192:GLY:HA3	1:A:1238:PHE:CD2	2.31	0.65
1:A:1060:PHE:CZ	1:A:1376:PHE:CD1	2.82	0.65
1:A:439:ILE:CG1	1:A:541:TYR:OH	2.45	0.65
1:A:45:ILE:HG12	1:A:107:ALA:HA	1.78	0.65
1:A:843:PHE:CE2	1:A:871:LEU:CA	2.80	0.65
5:F:297:ASN:ND2	5:F:331:GLY:HA3	2.10	0.65
1:A:1430:GLN:HG3	1:A:1432:PRO:HD2	1.79	0.64
5:F:536:VAL:HG12	5:F:537:GLY:N	2.10	0.64
1:A:1060:PHE:HZ	1:A:1376:PHE:CZ	2.14	0.64
1:A:1248:SER:HB3	1:A:1249[B]:ARG:HD3	1.78	0.64
5:F:647:TYR:CD1	5:F:713:GLY:CA	2.78	0.64
1:A:1334:TYR:CE1	1:A:1351:THR:HG23	2.33	0.64
5:F:449:THR:O	5:F:462:ILE:HG13	1.97	0.64
5:F:661:TYR:HE2	5:F:663:PHE:HZ	1.38	0.64
5:F:671:SER:C	5:F:672:ASP:OD1	2.35	0.64
5:F:736:PHE:CZ	5:F:796:MET:SD	2.90	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1139:HIS:CD2	1:A:1142:GLN:HB3	2.33	0.64
5:F:76:ASN:ND2	5:F:79:GLN:HB2	2.13	0.64
5:F:283:GLU:OE2	5:F:321:LYS:NZ	2.31	0.64
5:F:597:GLN:NE2	5:F:763:GLU:O	2.31	0.63
5:F:153:ASP:OD1	5:F:160:GLN:HG2	1.98	0.63
1:A:303:ASP:OD2	1:A:1302:ARG:NH1	2.31	0.63
1:A:372:GLN:NE2	1:A:486:LEU:O	2.31	0.63
5:F:667:ARG:HH21	5:F:686:PHE:HE1	1.45	0.63
5:F:894:VAL:CB	5:F:993:PHE:CE2	2.82	0.63
1:A:1195:ILE:HD11	4:E:113:PHE:HD2	1.62	0.63
1:A:1389:ARG:HD2	1:A:1391:TRP:CZ3	2.25	0.63
5:F:407:GLU:O	5:F:407:GLU:HG2	1.98	0.63
5:F:452:TYR:OH	5:F:463:THR:HG21	1.99	0.62
1:A:468:ASN:HD21	1:A:531:ARG:HD3	1.65	0.62
4:E:206:ARG:O	4:E:207:MET:C	2.36	0.62
1:A:1019:LEU:HD21	1:A:1045:PHE:CZ	2.35	0.62
1:A:822:ILE:O	1:A:822:ILE:HD12	2.00	0.61
1:A:608:PHE:CZ	1:A:1050:ILE:HD11	2.35	0.61
1:A:820:ASP:N	1:A:821:PRO:HA	2.11	0.61
1:A:843:PHE:O	1:A:846:GLU:CG	2.48	0.61
1:A:1258:TRP:HE1	4:E:208:PRO:HD2	1.64	0.61
5:F:351:VAL:O	5:F:352:SER:HB3	1.98	0.61
5:F:482:LYS:O	5:F:482:LYS:HG2	1.99	0.61
5:F:647:TYR:HE1	5:F:713:GLY:HA3	1.60	0.61
1:A:1260:PHE:HA	1:A:1263:SER:OG	1.99	0.61
1:A:823:ARG:HH21	1:A:823:ARG:HG2	1.65	0.61
5:F:858:ASP:HB2	5:F:1015:ASN:OD1	1.99	0.61
5:F:669:TYR:HE1	5:F:670:CYS:HB2	1.64	0.61
5:F:163:TYR:OH	5:F:199:ARG:NH2	2.34	0.61
5:F:894:VAL:CG1	5:F:993:PHE:CE2	2.84	0.61
4:E:30:ASP:OD2	4:E:55:ARG:NH2	2.34	0.61
5:F:531:PRO:O	5:F:532:LYS:HG3	2.01	0.60
5:F:731:GLY:O	5:F:732:VAL:HG22	2.01	0.60
5:F:310:VAL:HG12	5:F:1050:VAL:HG21	1.83	0.60
5:F:101:ARG:HH12	5:F:201:GLU:HG2	1.64	0.60
1:A:265:TRP:HZ2	1:A:271:GLY:HA2	1.66	0.60
1:A:823:ARG:HH21	1:A:823:ARG:CG	2.14	0.60
1:A:942:PHE:HA	1:A:945:ILE:HG22	1.83	0.60
1:A:1389:ARG:CB	1:A:1391:TRP:CE3	2.81	0.60
5:F:579:LYS:O	5:F:583:GLY:HA3	2.01	0.60
1:A:1016:TRP:CD1	1:A:1017:PRO:HD3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:243:ARG:CG	5:F:243:ARG:HH11	2.15	0.60
5:F:411:TYR:HD1	5:F:1074:CYS:HA	1.56	0.59
1:A:637:VAL:HG22	7:A:1903:PC1:H291	1.84	0.59
1:A:541:TYR:O	1:A:542:TRP:HB2	2.02	0.59
5:F:309:LEU:HD12	5:F:353:ARG:HD2	1.84	0.59
5:F:981:GLN:NE2	5:F:1038:GLU:OE2	2.35	0.59
1:A:587:PHE:CE2	1:A:625:MET:HE3	2.38	0.59
5:F:529:LEU:C	5:F:530:GLN:HG2	2.20	0.59
5:F:586:GLY:O	5:F:611:TRP:CE2	2.56	0.59
1:A:1195:ILE:CD1	4:E:113:PHE:CD2	2.86	0.59
5:F:256:MET:HB3	5:F:291:VAL:HG12	1.83	0.59
5:F:303:VAL:HG22	5:F:303:VAL:O	2.02	0.59
5:F:309:LEU:HD12	5:F:353:ARG:CD	2.33	0.59
1:A:206:MET:HE2	1:A:317:LEU:HD12	1.85	0.58
5:F:302:ASP:OD1	5:F:341:PHE:HE2	1.86	0.58
5:F:894:VAL:CG1	5:F:993:PHE:HE2	2.15	0.58
5:F:643:THR:O	5:F:647:TYR:CD2	2.57	0.58
1:A:822:ILE:HG21	1:A:1291:LYS:H	1.68	0.58
5:F:225:TRP:NE1	5:F:236:ASP:OD2	2.36	0.58
1:A:982:GLN:HG2	5:F:547:ARG:HE	1.67	0.58
1:A:1016:TRP:O	1:A:1020:LEU:N	2.28	0.58
1:A:469:ARG:HG2	1:A:511:LEU:HD11	1.85	0.58
4:E:208:PRO:CG	4:E:214:SER:CA	2.58	0.58
5:F:206:LEU:HD13	5:F:458:LEU:HD21	1.85	0.58
1:A:262:ARG:HH11	1:A:262:ARG:CG	2.15	0.58
5:F:894:VAL:CG2	5:F:993:PHE:HE2	2.10	0.58
1:A:108:TYR:HB2	1:A:112:PHE:HB2	1.86	0.57
1:A:482:LYS:HE2	1:A:486:LEU:HD22	1.86	0.57
1:A:183:GLN:O	1:A:187:ASN:ND2	2.38	0.57
1:A:591:GLU:OE2	1:A:593:ARG:NH2	2.36	0.57
5:F:365:ASP:O	5:F:394:HIS:NE2	2.37	0.57
5:F:679:ASN:HD21	5:F:759:PRO:HG3	1.68	0.57
1:A:1094:LYS:HD3	4:E:212:TRP:CZ2	2.40	0.57
1:A:225:THR:HG23	1:A:266:PRO:HB3	1.86	0.57
1:A:1416:ARG:HA	1:A:1461:VAL:O	2.04	0.57
1:A:900:ARG:HD2	1:A:903:ARG:HH11	1.70	0.57
1:A:1262:LYS:HE2	4:E:209:GLN:OE1	2.04	0.57
1:A:1249[A]:ARG:CG	1:A:1249[A]:ARG:HH21	2.17	0.57
1:A:369:TRP:O	1:A:369:TRP:HD1	1.87	0.57
1:A:468:ASN:HD22	1:A:531:ARG:NH2	2.02	0.57
5:F:505:ARG:O	5:F:505:ARG:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:586:GLY:CA	5:F:611:TRP:CZ2	2.88	0.57
1:A:965:GLU:CD	1:A:990:TRP:HE1	2.08	0.57
1:A:1244:ILE:CG2	1:A:1247:LEU:HD21	2.35	0.56
1:A:529:CYS:SG	1:A:945:ILE:CG1	2.89	0.56
1:A:206:MET:CE	1:A:317:LEU:HD12	2.34	0.56
1:A:475:PHE:CE2	1:A:537:LYS:CE	2.70	0.56
4:E:206:ARG:HB3	4:E:206:ARG:CZ	2.33	0.56
5:F:638:ILE:HG21	5:F:644:GLN:HB3	1.87	0.56
4:E:19:GLY:N	4:E:191:LEU:HD13	2.14	0.56
1:A:542:TRP:HE3	1:A:542:TRP:N	2.04	0.56
1:A:1144:GLU:O	1:A:1148:HIS:ND1	2.30	0.56
1:A:1390:ASP:HB3	1:A:1393:ILE:HD12	1.86	0.56
1:A:1339:ASP:O	1:A:1341:GLU:N	2.34	0.56
5:F:981:GLN:HG2	5:F:1038:GLU:HG2	1.87	0.56
5:F:515:PHE:HD1	5:F:623:ALA:O	1.89	0.56
1:A:252:ARG:HD2	1:A:1302:ARG:HH11	1.70	0.56
5:F:270:THR:HG22	5:F:392:GLY:HA3	1.87	0.56
5:F:356:CYS:SG	5:F:357:ASN:N	2.76	0.56
1:A:843:PHE:CD2	1:A:871:LEU:HA	2.41	0.56
1:A:1099:ARG:O	1:A:1100:CYS:SG	2.63	0.56
1:A:1389:ARG:CD	1:A:1391:TRP:CD2	2.73	0.56
1:A:959:ASP:OD2	1:A:988:ARG:NH1	2.38	0.56
1:A:454:HIS:HB2	1:A:998:ASP:OD1	2.05	0.56
5:F:64:GLU:O	5:F:67:GLN:NE2	2.38	0.55
1:A:1264:PHE:CE1	1:A:1267:LEU:CD2	2.90	0.55
5:F:452:TYR:CD1	5:F:452:TYR:N	2.73	0.55
7:A:1911:PC1:H262	7:A:1911:PC1:H322	1.89	0.55
1:A:445:ASN:HD21	1:A:534:ARG:HD3	1.71	0.55
5:F:1036:GLN:HE21	5:F:1037:ALA:N	1.97	0.55
5:F:389:PHE:CD1	5:F:389:PHE:N	2.73	0.55
5:F:497:GLU:O	5:F:501:ARG:HD3	2.05	0.55
1:A:1389:ARG:CG	1:A:1391:TRP:CE3	2.88	0.55
5:F:732:VAL:O	5:F:820:ASP:CB	2.48	0.55
1:A:1139:HIS:HD2	1:A:1142:GLN:HB3	1.69	0.55
1:A:1020:LEU:C	1:A:1020:LEU:HD12	2.27	0.55
5:F:530:GLN:HG2	5:F:904:GLN:HE22	1.70	0.55
1:A:74:MET:HB3	1:A:78:ASP:HB3	1.88	0.55
1:A:1043:ILE:O	1:A:1047:ILE:HG13	2.07	0.55
5:F:518:ASP:O	5:F:520:ASN:N	2.40	0.55
1:A:1391:TRP:CE2	1:A:1396:PRO:HD2	2.42	0.55
1:A:1019:LEU:CD2	1:A:1045:PHE:CZ	2.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1046:ILE:O	1:A:1050:ILE:HG12	2.07	0.54
4:E:15:CYS:O	4:E:191:LEU:HD11	2.07	0.54
5:F:510:PRO:HG3	5:F:762:TYR:CD1	2.42	0.54
5:F:647:TYR:HD1	5:F:713:GLY:CA	2.20	0.54
4:E:37:PRO:HA	4:E:174:ILE:HA	1.90	0.54
5:F:880:GLU:HA	5:F:1033:LEU:HD22	1.89	0.54
1:A:1046:ILE:HD13	7:A:1914:PC1:H381	1.90	0.54
5:F:247:ILE:O	5:F:247:ILE:HG22	2.08	0.54
1:A:513:LEU:HD23	1:A:527:LEU:HD11	1.90	0.54
1:A:1262:LYS:CD	4:E:209:GLN:O	2.56	0.54
1:A:216:GLU:OE2	1:A:1239:ARG:NH2	2.37	0.54
4:E:19:GLY:N	4:E:191:LEU:HD11	2.18	0.54
4:E:206:ARG:HB3	4:E:206:ARG:NH1	2.23	0.54
1:A:820:ASP:OD2	1:A:829:ASN:ND2	2.40	0.54
1:A:1173:LYS:O	1:A:1175:ARG:N	2.40	0.54
1:A:1043:ILE:CG2	7:A:1904:PC1:H291	2.37	0.54
1:A:957:CYS:SG	1:A:958:ASN:N	2.81	0.54
1:A:1016:TRP:CG	1:A:1017:PRO:HD3	2.43	0.54
1:A:369:TRP:NE1	3:C:293:MET:HA	2.23	0.53
5:F:510:PRO:HG2	5:F:767:TYR:CD2	2.42	0.53
5:F:634:ILE:HB	5:F:707:ARG:HH12	1.73	0.53
1:A:1244:ILE:O	1:A:1247:LEU:HD23	2.09	0.53
1:A:942:PHE:CD2	1:A:1048:TYR:CD1	2.73	0.53
1:A:573:PHE:O	1:A:640:TYR:OH	2.25	0.53
1:A:969:ARG:HB3	5:F:176:GLU:HG3	1.90	0.53
1:A:541:TYR:N	1:A:541:TYR:CD1	2.76	0.53
5:F:252:SER:OG	5:F:357:ASN:OD1	2.26	0.53
1:A:1264:PHE:CZ	1:A:1267:LEU:HD23	2.44	0.53
1:A:1334:TYR:CE1	1:A:1351:THR:CG2	2.92	0.53
5:F:452:TYR:N	5:F:452:TYR:HD1	2.05	0.53
5:F:669:TYR:CD1	5:F:670:CYS:CB	2.92	0.53
5:F:1061:VAL:HG23	5:F:1062:CYS:N	2.20	0.53
1:A:333:LEU:HD11	1:A:1064:VAL:HG11	1.91	0.53
1:A:1101:TYR:HD1	1:A:1101:TYR:H	1.56	0.53
1:A:1337:LEU:HD12	1:A:1350:TYR:CE1	2.39	0.53
1:A:820:ASP:HB2	1:A:821:PRO:C	2.30	0.53
1:A:1101:TYR:CD1	1:A:1101:TYR:N	2.74	0.53
5:F:55:GLY:HA3	5:F:718:LEU:HD11	1.91	0.52
1:A:542:TRP:N	1:A:542:TRP:CE3	2.76	0.52
1:A:816:LEU:HD21	1:A:901:VAL:HG12	1.91	0.52
5:F:411:TYR:CE1	5:F:1074:CYS:CA	2.88	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:GLU:OE2	1:A:1015:GLY:N	2.43	0.52
1:A:1015:GLY:CA	1:A:1326:GLN:NE2	2.55	0.52
5:F:669:TYR:HD1	5:F:670:CYS:CA	2.15	0.52
5:F:515:PHE:CD1	5:F:623:ALA:O	2.63	0.52
5:F:515:PHE:CE2	5:F:563:PHE:CE1	2.88	0.52
5:F:77:ALA:HA	5:F:624:LEU:CD2	2.38	0.52
1:A:953:LYS:HE2	1:A:1038:ARG:HH12	1.75	0.52
5:F:359:ILE:HD11	5:F:432:LEU:HD21	1.91	0.52
1:A:217:LEU:HD11	1:A:1237:LEU:HD11	1.91	0.52
1:A:276:ASP:O	1:A:277:ASN:CB	2.57	0.52
1:A:366:TYR:O	1:A:369:TRP:HB3	2.10	0.52
1:A:632:TYR:HB3	1:A:633:PRO:CD	2.39	0.52
5:F:243:ARG:HG3	5:F:243:ARG:NH1	2.24	0.52
5:F:303:VAL:O	5:F:323:ALA:HB1	2.10	0.52
5:F:321:LYS:O	5:F:325:ASN:ND2	2.43	0.52
5:F:733:LYS:NZ	5:F:793:SER:HA	2.25	0.52
5:F:805:ILE:O	5:F:807:GLY:N	2.38	0.52
1:A:1306:PHE:CD2	1:A:1315:LEU:HD13	2.45	0.52
4:E:7:PRO:HA	4:E:10:ARG:HB2	1.92	0.52
5:F:1011:LEU:HD22	5:F:1016:LEU:HD12	1.92	0.51
1:A:1016:TRP:N	1:A:1017:PRO:CD	2.73	0.51
5:F:1007:HIS:NE2	5:F:1009:GLU:OE2	2.43	0.51
1:A:843:PHE:HE2	1:A:871:LEU:HA	1.68	0.51
5:F:309:LEU:HD12	5:F:353:ARG:CG	2.40	0.51
1:A:1416:ARG:HB3	1:A:1460:THR:HB	1.91	0.51
1:A:843:PHE:HE2	1:A:871:LEU:N	2.09	0.51
1:A:819:GLU:CG	1:A:897:ARG:HH21	2.24	0.51
5:F:1008:VAL:HG22	5:F:1019:ILE:HG12	1.92	0.51
1:A:225:THR:HA	1:A:266:PRO:HB3	1.92	0.51
4:E:131:LYS:HB3	4:E:133:ARG:HE	1.76	0.51
5:F:398:ARG:NH1	5:F:414:GLU:OE2	2.43	0.51
5:F:510:PRO:HG3	5:F:762:TYR:CE1	2.46	0.51
1:A:468:ASN:HD21	1:A:531:ARG:HH21	1.59	0.51
5:F:669:TYR:CD1	5:F:670:CYS:HB2	2.46	0.51
1:A:1249[A]:ARG:HG2	1:A:1249[A]:ARG:NH2	2.24	0.51
4:E:19:GLY:H	4:E:191:LEU:HD13	1.70	0.51
5:F:198:ASN:HB2	5:F:208:GLN:HE22	1.76	0.51
5:F:894:VAL:HG11	5:F:993:PHE:CD2	2.44	0.51
1:A:287:GLN:NE2	1:A:621:TYR:OH	2.35	0.51
3:C:265:VAL:O	3:C:265:VAL:HG12	2.10	0.51
5:F:131:ALA:HB2	5:F:167:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:ND2	1:A:531:ARG:HH21	2.08	0.50
5:F:243:ARG:NH1	5:F:243:ARG:CG	2.73	0.50
1:A:974:VAL:HG21	1:A:986:ARG:HD2	1.93	0.50
1:A:1235:PHE:CE2	4:E:153:VAL:CG2	2.87	0.50
1:A:1244:ILE:HG23	1:A:1247:LEU:HD21	1.93	0.50
5:F:1052:GLN:O	5:F:1052:GLN:HG2	2.12	0.50
6:F:1204:NAG:H61	6:F:1205:NAG:C8	2.41	0.50
1:A:1337:LEU:HD11	1:A:1350:TYR:HE1	1.70	0.50
1:A:526:VAL:O	1:A:530:ILE:HG13	2.10	0.50
5:F:886:MET:CE	5:F:895:TYR:HH	2.25	0.50
5:F:77:ALA:HA	5:F:624:LEU:HD21	1.93	0.50
5:F:993:PHE:HB2	5:F:1008:VAL:HB	1.94	0.50
1:A:1005:MET:HB2	7:A:1911:PC1:H352	1.92	0.50
5:F:245:TRP:O	5:F:465:THR:HG21	2.12	0.50
1:A:1418:LYS:HG3	1:A:1420:LEU:H	1.77	0.50
5:F:173:ASP:CB	5:F:422:ARG:HH22	2.25	0.50
5:F:75:ASN:O	5:F:76:ASN:HB3	2.11	0.50
1:A:529:CYS:HA	1:A:532:LEU:HD12	1.94	0.50
1:A:57:ILE:HA	1:A:60:THR:HG22	1.93	0.50
1:A:591:GLU:OE2	1:A:593:ARG:CZ	2.59	0.50
4:E:107:ALA:HA	4:E:110:ILE:HD12	1.93	0.50
5:F:428:TYR:C	5:F:428:TYR:CD1	2.85	0.49
5:F:638:ILE:HD11	5:F:710:LEU:HB2	1.94	0.49
1:A:1106:PRO:HA	1:A:1109:TYR:HB3	1.95	0.49
1:A:915:LYS:HD3	1:A:915:LYS:H	1.75	0.49
1:A:170:LEU:HD12	1:A:173:LEU:HD13	1.95	0.49
7:A:1902:PC1:H321	7:A:1902:PC1:H221	1.94	0.49
5:F:438:LEU:HD12	5:F:1068:LEU:HD12	1.95	0.49
1:A:1046:ILE:CD1	7:A:1914:PC1:C39	2.89	0.49
1:A:844:THR:O	1:A:847:ILE:HG13	2.12	0.49
1:A:993:ASN:O	1:A:995:PHE:N	2.39	0.49
5:F:394:HIS:HD2	5:F:396:TYR:HB2	1.78	0.49
5:F:985:PHE:HZ	6:F:1215:NAG:H61	1.77	0.49
5:F:389:PHE:HD1	5:F:389:PHE:N	2.10	0.49
5:F:482:LYS:HE3	5:F:485:LEU:HD12	1.93	0.49
5:F:584:GLU:O	5:F:613:PRO:HD3	2.12	0.49
5:F:153:ASP:OD1	5:F:160:GLN:CG	2.59	0.49
5:F:564:LEU:HD12	5:F:569:GLU:CB	2.43	0.49
5:F:744:THR:HG1	5:F:755:TRP:HZ3	1.60	0.49
1:A:1060:PHE:CZ	1:A:1376:PHE:CZ	2.96	0.49
1:A:49:GLU:O	1:A:50:TRP:O	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:TYR:CZ	1:A:1351:THR:HG23	2.47	0.49
1:A:363:LEU:HD22	3:C:399:ARG:HD3	1.95	0.49
5:F:417:SER:OG	5:F:418:ILE:N	2.46	0.49
5:F:513:TYR:OH	5:F:567:GLU:OE2	2.28	0.49
5:F:95:ARG:HD3	5:F:494:VAL:HG22	1.95	0.49
1:A:808:PHE:HE2	1:A:903:ARG:HH22	1.61	0.48
5:F:333:THR:HG21	5:F:335:TYR:CE2	2.47	0.48
5:F:564:LEU:CD1	5:F:569:GLU:CB	2.90	0.48
5:F:733:LYS:HD2	5:F:793:SER:O	2.13	0.48
5:F:733:LYS:HZ3	5:F:793:SER:HA	1.78	0.48
1:A:842:VAL:O	1:A:845:VAL:HB	2.14	0.48
5:F:333:THR:HG21	5:F:335:TYR:HE2	1.78	0.48
5:F:733:LYS:CD	5:F:793:SER:O	2.61	0.48
1:A:1318:ARG:HH21	1:A:1328:ILE:HD11	1.79	0.48
1:A:1293:ALA:HB2	1:A:1339:ASP:H	1.77	0.48
1:A:974:VAL:HG23	1:A:986:ARG:HG3	1.95	0.48
4:E:208:PRO:HG2	4:E:214:SER:CB	2.43	0.48
5:F:184:GLU:OE2	5:F:212:SER:OG	2.27	0.48
5:F:744:THR:HB	5:F:755:TRP:CH2	2.48	0.48
1:A:269:ASN:ND2	1:A:273:THR:OG1	2.42	0.48
5:F:1062:CYS:O	5:F:1063:PHE:HD1	1.88	0.48
1:A:1081:LEU:HD22	1:A:1085:GLN:HE21	1.79	0.48
1:A:510:GLU:OE2	1:A:531:ARG:CD	2.55	0.48
1:A:542:TRP:H	1:A:542:TRP:HE3	1.61	0.48
1:A:820:ASP:CG	1:A:829:ASN:HD21	2.17	0.48
4:E:161:SER:HA	4:E:164:ARG:HD3	1.95	0.48
5:F:105:GLU:HG3	5:F:194:VAL:HG21	1.95	0.48
1:A:172:PRO:HB2	1:A:572:ILE:HD11	1.95	0.48
1:A:974:VAL:CG2	1:A:986:ARG:HG3	2.44	0.48
5:F:173:ASP:OD2	5:F:422:ARG:NH2	2.47	0.48
5:F:531:PRO:C	5:F:532:LYS:HG3	2.34	0.48
5:F:726:GLN:HB3	5:F:729:ILE:HD11	1.96	0.48
5:F:586:GLY:C	5:F:611:TRP:CZ2	2.87	0.48
1:A:500:ASP:OD1	1:A:537:LYS:NZ	2.47	0.47
1:A:1258:TRP:NE1	4:E:208:PRO:HD2	2.29	0.47
5:F:478:LYS:O	5:F:480:ASN:CG	2.52	0.47
5:F:478:LYS:C	5:F:480:ASN:N	2.66	0.47
4:E:207:MET:O	4:E:209:GLN:N	2.47	0.47
5:F:615:ASN:OD1	6:F:1204:NAG:O5	2.32	0.47
1:A:587:PHE:CD2	1:A:625:MET:HE3	2.50	0.47
4:E:19:GLY:HA2	4:E:191:LEU:HD12	1.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:LYS:CG	4:E:209:GLN:O	2.62	0.47
5:F:732:VAL:HG23	5:F:733:LYS:H	1.74	0.47
5:F:644:GLN:CA	5:F:647:TYR:HD2	2.12	0.47
1:A:594:ARG:NH2	1:A:1025:ASP:OD1	2.31	0.47
1:A:1390:ASP:HB3	1:A:1393:ILE:HD13	1.94	0.47
1:A:534:ARG:O	1:A:537:LYS:HB2	2.14	0.47
1:A:965:GLU:HA	1:A:990:TRP:CZ2	2.49	0.47
5:F:348:ASN:O	5:F:350:ASN:N	2.47	0.47
1:A:1199:LEU:HD12	1:A:1232:SER:HB3	1.96	0.47
4:E:15:CYS:O	4:E:191:LEU:HD21	2.15	0.47
5:F:38:TRP:HE1	5:F:831:THR:HB	1.79	0.47
1:A:1296:ASP:OD2	1:A:1302:ARG:NH2	2.47	0.47
1:A:433:VAL:O	1:A:437:LEU:N	2.44	0.47
1:A:813:SER:HA	1:A:816:LEU:HB3	1.96	0.47
1:A:820:ASP:CB	1:A:821:PRO:C	2.83	0.47
1:A:843:PHE:CE2	1:A:871:LEU:CB	2.98	0.47
1:A:1067:THR:HG21	1:A:1377:VAL:HG13	1.97	0.47
1:A:1429:ILE:HG21	1:A:1433:LEU:HD12	1.96	0.46
5:F:1068:LEU:HD23	5:F:1068:LEU:N	2.30	0.46
5:F:302:ASP:OD1	5:F:341:PHE:CE2	2.67	0.46
5:F:598:ASP:O	5:F:599:GLU:HG3	2.14	0.46
5:F:669:TYR:HD1	5:F:670:CYS:CB	2.26	0.46
4:E:211:PRO:O	4:E:212:TRP:CD1	2.68	0.46
5:F:536:VAL:CG1	5:F:537:GLY:H	2.18	0.46
5:F:563:PHE:HB3	5:F:577:ARG:HD3	1.97	0.46
1:A:1154:ASN:O	1:A:1158:THR:HG23	2.15	0.46
1:A:165:ARG:HG3	1:A:165:ARG:HH11	1.80	0.46
1:A:533:LEU:HG	1:A:533:LEU:O	2.14	0.46
5:F:297:ASN:HD21	5:F:331:GLY:CA	2.21	0.46
5:F:656:PHE:O	5:F:660:GLY:HA2	2.14	0.46
1:A:213:ILE:HG13	1:A:1240:VAL:HG11	1.97	0.46
5:F:159:ARG:NH2	5:F:224:PRO:O	2.49	0.46
5:F:219:TYR:O	5:F:219:TYR:CD2	2.68	0.46
5:F:597:GLN:HB2	5:F:768:LYS:HZ1	1.80	0.46
1:A:332:VAL:HB	1:A:657:LEU:HD11	1.97	0.46
5:F:106:ALA:HB2	5:F:191:LEU:HD21	1.97	0.46
5:F:563:PHE:HD2	5:F:577:ARG:HD3	1.80	0.46
1:A:121:GLY:HA3	1:A:174:ARG:NH2	2.31	0.46
1:A:912[B]:LYS:HA	1:A:915:LYS:HE3	1.97	0.46
5:F:518:ASP:O	5:F:521:GLY:N	2.39	0.46
5:F:795:ILE:O	5:F:819:ILE:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1016:TRP:CZ3	1:A:1020:LEU:HD23	2.51	0.46
1:A:911:ALA:O	1:A:915:LYS:CE	2.63	0.46
1:A:823:ARG:NH2	1:A:823:ARG:CG	2.73	0.46
5:F:30:PRO:CG	5:F:1020:MET:CE	2.79	0.46
5:F:979:THR:HB	5:F:1038:GLU:HB3	1.98	0.46
7:A:1915:PC1:H31	7:A:1915:PC1:H321	1.71	0.45
5:F:458:LEU:HD23	5:F:461:VAL:HG11	1.97	0.45
5:F:445:GLN:O	5:F:466:LEU:CD1	2.64	0.45
1:A:1305:ASN:HD22	1:A:1311:GLN:CG	2.28	0.45
5:F:1073:ASP:O	5:F:1074:CYS:C	2.54	0.45
5:F:242:ARG:HA	5:F:247:ILE:HD11	1.99	0.45
1:A:1016:TRP:CZ3	1:A:1020:LEU:CD2	3.00	0.45
1:A:614:GLU:HG3	1:A:1017:PRO:HG2	1.99	0.45
1:A:877:ALA:O	1:A:881:ILE:N	2.46	0.45
1:A:903:ARG:CB	1:A:904:PRO:HD3	2.42	0.45
5:F:586:GLY:O	5:F:611:TRP:CE3	2.69	0.45
5:F:207:TRP:HE1	5:F:458:LEU:HD22	1.82	0.45
1:A:1261:ILE:HG22	4:E:207:MET:SD	2.57	0.45
1:A:1281:TYR:O	1:A:1360:TYR:OH	2.33	0.45
1:A:276:ASP:O	1:A:277:ASN:HB3	2.16	0.45
5:F:1068:LEU:HB2	5:F:1069:GLU:H	1.66	0.45
5:F:47:VAL:HG13	5:F:776:TYR:HE2	1.81	0.45
5:F:531:PRO:C	5:F:532:LYS:CG	2.85	0.45
5:F:587:GLU:HB3	5:F:610:THR:HG22	1.99	0.45
5:F:733:LYS:HB3	5:F:818:LYS:O	2.17	0.45
1:A:1334:TYR:O	1:A:1334:TYR:CG	2.70	0.44
1:A:295:THR:HG22	1:A:1323:GLU:OE2	2.17	0.44
1:A:376:MET:SD	1:A:422:ARG:NH1	2.90	0.44
5:F:1020:MET:HB3	5:F:1020:MET:HE2	1.77	0.44
1:A:1254:ARG:HG3	1:A:1255:THR:N	2.32	0.44
5:F:900:SER:OG	5:F:901:TYR:N	2.50	0.44
1:A:210:TYR:O	1:A:313:TYR:OH	2.35	0.44
1:A:820:ASP:N	1:A:821:PRO:CA	2.79	0.44
1:A:964:THR:OG1	1:A:965:GLU:N	2.50	0.44
1:A:305:ILE:HG23	7:A:1902:PC1:H121	1.99	0.44
1:A:896:LEU:HD23	1:A:899:LEU:HD12	2.00	0.44
4:E:19:GLY:H	4:E:191:LEU:HD11	1.77	0.44
5:F:96:SER:O	5:F:99:LEU:HB2	2.18	0.44
1:A:1244:ILE:O	1:A:1247:LEU:CD2	2.65	0.44
1:A:587:PHE:HB3	1:A:593:ARG:HH21	1.82	0.44
1:A:1094:LYS:HD3	4:E:212:TRP:CH2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:894:VAL:HA	5:F:895:TYR:HA	1.68	0.44
1:A:536:PHE:O	1:A:539:THR:OG1	2.30	0.44
1:A:1262:LYS:CE	4:E:209:GLN:OE1	2.65	0.44
5:F:147:ILE:HG22	5:F:149:PRO:HD3	1.99	0.44
1:A:1120:PHE:HZ	1:A:1167:LEU:HD12	1.83	0.44
1:A:1121:GLU:CG	1:A:1249[A]:ARG:HH22	2.30	0.44
1:A:468:ASN:ND2	1:A:531:ARG:CZ	2.81	0.44
1:A:475:PHE:CZ	1:A:537:LYS:CE	2.99	0.44
4:E:209:GLN:HG3	4:E:210:ASN:N	2.33	0.44
5:F:564:LEU:HD12	5:F:569:GLU:HB2	1.99	0.44
5:F:738:VAL:HG13	5:F:744:THR:HG22	2.00	0.44
5:F:892:ILE:O	5:F:893:SER:HB3	2.18	0.44
1:A:1046:ILE:HA	1:A:1049:ILE:HG22	2.00	0.43
1:A:1334:TYR:O	1:A:1334:TYR:CD1	2.70	0.43
1:A:539:THR:C	1:A:541:TYR:N	2.68	0.43
1:A:902:LEU:HD12	1:A:905:LEU:HD12	1.95	0.43
3:C:398:GLN:HG2	3:C:402:LYS:HD2	2.00	0.43
5:F:428:TYR:O	5:F:428:TYR:CD1	2.70	0.43
5:F:508:LEU:N	5:F:508:LEU:HD23	2.33	0.43
1:A:423:TRP:HA	1:A:426:HIS:HD2	1.83	0.43
5:F:1068:LEU:O	5:F:1070:ASP:N	2.52	0.43
5:F:168:VAL:HG22	5:F:218:ARG:HG2	2.00	0.43
5:F:594:VAL:HG21	5:F:607:ARG:HH21	1.84	0.43
1:A:468:ASN:HD21	1:A:531:ARG:CD	2.30	0.43
5:F:190:ALA:C	5:F:192:ASP:H	2.21	0.43
5:F:509:CYS:O	5:F:511:ASN:N	2.52	0.43
5:F:860:GLY:O	5:F:878:PHE:N	2.44	0.43
1:A:1016:TRP:HZ3	1:A:1020:LEU:CD2	2.31	0.43
1:A:225:THR:HG21	1:A:227:TYR:CZ	2.53	0.43
1:A:307:ASN:N	1:A:307:ASN:OD1	2.46	0.43
1:A:540:LYS:HE3	1:A:540:LYS:HB2	1.74	0.43
1:A:846:GLU:HG3	1:A:847:ILE:N	2.33	0.43
5:F:656:PHE:CD1	5:F:660:GLY:O	2.71	0.43
1:A:1044:PHE:HB2	7:A:1904:PC1:H2A1	2.00	0.43
1:A:794[B]:ARG:HE	1:A:794[B]:ARG:HB3	1.54	0.43
5:F:298:SER:OG	5:F:299:ASN:N	2.51	0.43
5:F:598:ASP:OD1	5:F:598:ASP:N	2.50	0.43
1:A:1263:SER:O	1:A:1265:GLN:N	2.41	0.43
1:A:1403:LYS:HA	1:A:1406:TRP:HD1	1.83	0.43
2:B:169:ARG:NH1	2:B:173:GLU:OE1	2.51	0.43
4:E:17:LEU:HD23	4:E:20:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1384:PHE:CE1	1:A:1388:THR:HG21	2.53	0.43
5:F:411:TYR:HA	5:F:1074:CYS:HB2	1.99	0.43
1:A:1046:ILE:C	1:A:1049:ILE:HG22	2.37	0.43
1:A:1331:ALA:O	1:A:1336:LYS:HG3	2.19	0.43
1:A:1321:THR:HG22	7:A:1909:PC1:H3D2	2.00	0.43
1:A:1370:PHE:CD1	1:A:1370:PHE:C	2.91	0.43
5:F:712:ALA:HA	5:F:715:THR:HG22	2.01	0.43
1:A:1244:ILE:HG22	1:A:1247:LEU:HD21	2.00	0.42
1:A:165:ARG:O	1:A:168:ARG:HG2	2.19	0.42
1:A:172:PRO:O	1:A:175:LEU:HB3	2.19	0.42
1:A:252:ARG:HD2	1:A:1302:ARG:NH1	2.33	0.42
1:A:449:ILE:HA	1:A:449:ILE:HD12	1.90	0.42
5:F:661:TYR:HD2	5:F:663:PHE:CZ	2.13	0.42
5:F:790:ALA:N	5:F:793:SER:OG	2.52	0.42
1:A:1091:TYR:CZ	1:A:1399:LEU:HB3	2.54	0.42
1:A:1104:LYS:HG3	1:A:1105:ASN:H	1.84	0.42
1:A:1389:ARG:HE	1:A:1391:TRP:CB	2.29	0.42
7:A:1912:PC1:H142	7:A:1912:PC1:H112	1.86	0.42
5:F:989:ASP:HB3	5:F:990:SER:H	1.69	0.42
1:A:370:ILE:HG21	3:C:404:ARG:NH1	2.34	0.42
5:F:309:LEU:HD12	5:F:353:ARG:HG2	2.00	0.42
5:F:509:CYS:C	5:F:511:ASN:N	2.73	0.42
1:A:1127:LEU:HD13	1:A:1160:ILE:HG21	2.00	0.42
5:F:381:ASP:HB3	5:F:383:LYS:HE3	2.00	0.42
1:A:1195:ILE:CD1	4:E:113:PHE:CE2	3.03	0.42
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.33	0.42
1:A:559:ILE:HG22	1:A:563:LEU:HB2	2.01	0.42
1:A:614:GLU:HG3	1:A:1017:PRO:CG	2.49	0.42
5:F:52:THR:O	5:F:722:TYR:OH	2.30	0.42
5:F:784:ASN:O	5:F:787:GLY:N	2.50	0.42
1:A:1293:ALA:O	1:A:1295:VAL:N	2.52	0.42
4:E:55:ARG:HD2	4:E:80:CYS:HB3	2.01	0.42
1:A:1249[A]:ARG:NH2	1:A:1249[A]:ARG:CG	2.75	0.42
5:F:248:GLN:HE21	5:F:248:GLN:HB3	1.66	0.42
5:F:515:PHE:HE2	5:F:563:PHE:HE1	1.59	0.42
1:A:1132:THR:HG21	7:A:1912:PC1:H3A1	2.01	0.42
1:A:902:LEU:O	1:A:905:LEU:HB2	2.20	0.42
5:F:805:ILE:HB	5:F:808:LYS:HE2	2.02	0.42
5:F:886:MET:SD	5:F:895:TYR:CE1	3.13	0.42
5:F:496:LEU:HD23	5:F:499:ILE:HD12	2.02	0.42
1:A:1020:LEU:HD13	1:A:1045:PHE:HD2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1262:LYS:HG2	4:E:209:GLN:HA	2.01	0.41
1:A:1304:ASN:HA	1:A:1304:ASN:HD22	1.60	0.41
1:A:945:ILE:HD11	7:A:1904:PC1:H361	2.02	0.41
1:A:632:TYR:CB	1:A:633:PRO:CD	2.98	0.41
5:F:1061:VAL:CG2	5:F:1062:CYS:H	2.19	0.41
5:F:594:VAL:HG21	5:F:607:ARG:HE	1.85	0.41
5:F:586:GLY:CA	5:F:611:TRP:CE2	3.02	0.41
5:F:856:LEU:HD12	5:F:856:LEU:HA	1.91	0.41
1:A:1265:GLN:HB3	1:A:1265:GLN:HE21	1.65	0.41
1:A:1389:ARG:HH21	1:A:1389:ARG:HG2	1.84	0.41
5:F:1073:ASP:O	5:F:1074:CYS:O	2.38	0.41
5:F:348:ASN:C	5:F:350:ASN:N	2.71	0.41
5:F:598:ASP:C	5:F:599:GLU:CG	2.85	0.41
1:A:1049:ILE:HG23	1:A:1050:ILE:N	2.34	0.41
1:A:632:TYR:C	1:A:632:TYR:CD1	2.92	0.41
1:A:1096:ARG:HB3	1:A:1097:PRO:HD2	2.02	0.41
1:A:1102:ILE:HG13	1:A:1411:PRO:HB2	2.02	0.41
1:A:265:TRP:CZ2	1:A:271:GLY:HA2	2.52	0.41
3:C:282:PRO:HA	3:C:389:ILE:O	2.21	0.41
5:F:413:TYR:OH	5:F:428:TYR:HA	2.20	0.41
5:F:76:ASN:HD22	5:F:79:GLN:HB2	1.84	0.41
5:F:767:TYR:OH	5:F:812:PRO:O	2.35	0.41
5:F:769:ARG:HH22	5:F:858:ASP:HB3	1.86	0.41
5:F:878:PHE:HB3	5:F:886:MET:HE3	2.02	0.41
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.92	0.41
1:A:526:VAL:HG22	7:A:1904:PC1:H331	2.02	0.41
5:F:509:CYS:HB2	5:F:630:SER:HB3	2.03	0.41
1:A:999:ASN:HB2	1:A:1002:SER:H	1.86	0.41
1:A:1052:ILE:HA	1:A:1052:ILE:HD13	1.90	0.41
7:A:1903:PC1:H3C2	7:A:1903:PC1:H2E2	2.03	0.41
5:F:55:GLY:O	5:F:59:LEU:N	2.46	0.41
5:F:382:LYS:NZ	5:F:407:GLU:HG2	2.35	0.41
5:F:681:GLU:O	5:F:685:ASN:ND2	2.54	0.41
5:F:894:VAL:CB	5:F:993:PHE:HE2	2.29	0.41
1:A:113:HIS:O	1:A:119:ARG:NE	2.36	0.41
1:A:1389:ARG:NE	1:A:1391:TRP:HB2	2.29	0.41
7:A:1909:PC1:H3C2	7:A:1909:PC1:H391	1.74	0.41
5:F:243:ARG:HG3	5:F:243:ARG:HH11	1.84	0.41
5:F:303:VAL:HG13	5:F:303:VAL:O	2.21	0.41
1:A:1043:ILE:CG1	1:A:1047:ILE:HD11	2.37	0.41
1:A:369:TRP:O	1:A:369:TRP:CD1	2.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1912:PC1:H261	7:A:1912:PC1:H231	1.53	0.41
1:A:248:THR:HG22	1:A:249:GLY:H	1.86	0.41
1:A:604:LEU:HA	1:A:604:LEU:HD12	1.89	0.41
1:A:189:ILE:HG13	1:A:654:ASN:HD22	1.85	0.41
1:A:794[B]:ARG:NH2	1:A:795:ILE:HD11	2.36	0.41
1:A:821:PRO:HG3	1:A:1286:MET:CG	2.42	0.41
1:A:965:GLU:HA	1:A:990:TRP:HZ2	1.85	0.41
5:F:736:PHE:CE1	5:F:796:MET:SD	3.14	0.41
4:E:113:PHE:HD1	4:E:113:PHE:HA	1.69	0.41
4:E:211:PRO:C	4:E:212:TRP:CD1	2.95	0.41
4:E:207:MET:C	4:E:209:GLN:N	2.75	0.40
1:A:1201:GLU:O	1:A:1204:THR:OG1	2.37	0.40
1:A:1391:TRP:CD1	1:A:1397:HIS:CD2	2.98	0.40
1:A:794[A]:ARG:NH1	1:A:798:ALA:CB	2.84	0.40
4:E:207:MET:C	4:E:209:GLN:H	2.24	0.40
5:F:628:THR:HA	5:F:631:PHE:HE2	1.86	0.40
1:A:1122:TYR:HA	1:A:1122:TYR:HD1	1.77	0.40
1:A:1391:TRP:CZ2	1:A:1396:PRO:CD	3.02	0.40
1:A:656:PHE:CE1	1:A:1060:PHE:HD2	2.39	0.40
3:C:388:TYR:HB2	3:C:430:PHE:CD1	2.56	0.40
5:F:895:TYR:N	5:F:895:TYR:CD1	2.90	0.40
5:F:530:GLN:CG	5:F:904:GLN:HE22	2.34	0.40
1:A:299:TYR:O	1:A:303:ASP:HB2	2.22	0.40
1:A:611:LEU:HA	1:A:611:LEU:HD12	1.86	0.40
1:A:369:TRP:CD1	3:C:293:MET:HA	2.56	0.40
4:E:15:CYS:O	4:E:191:LEU:CD1	2.70	0.40
5:F:451:VAL:HG23	5:F:559:VAL:O	2.20	0.40
5:F:584:GLU:O	5:F:613:PRO:CD	2.69	0.40
1:A:1249[B]:ARG:HD2	1:A:1249[B]:ARG:HA	1.97	0.40
1:A:1441:HIS:HB3	1:A:1443:VAL:N	2.36	0.40
5:F:1002:CYS:SG	5:F:1026:THR:OG1	2.76	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 PDB entries followed by that with respect to all EM entries.

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	1268/1873 (68%)	1103 (87%)	143 (11%)	22 (2%)	11	55
2	B	98/106 (92%)	90 (92%)	8 (8%)	0	100	100
3	C	174/199 (87%)	171 (98%)	3 (2%)	0	100	100
4	E	156/222 (70%)	142 (91%)	12 (8%)	2 (1%)	15	60
5	F	929/1106 (84%)	764 (82%)	137 (15%)	28 (3%)	5	44
All	All	2625/3506 (75%)	2270 (86%)	303 (12%)	52 (2%)	14	53

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	977	ASP
1	A	1174	ALA
1	A	1391	TRP
1	A	1441	HIS
5	F	77	ALA
5	F	303	VAL
5	F	351	VAL
5	F	352	SER
5	F	451	VAL
5	F	478	LYS
5	F	479	THR
5	F	536	VAL
5	F	598	ASP
5	F	785	LYS
5	F	806	GLN
5	F	1061	VAL
1	A	80	ASN
1	A	1440	PRO
4	E	209	GLN
5	F	732	VAL
5	F	733	LYS
5	F	1068	LEU
1	A	819	GLU
1	A	1344	TYR
1	A	1354	THR
5	F	297	ASN
5	F	349	TYR

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Mol	Chain	Res	Type
5	F	353	ARG
5	F	531	PRO
5	F	786	SER
1	A	994	ASP
1	A	1138	GLN
1	A	1333	SER
1	A	1355	ASN
5	F	175	TYR
5	F	313	ASN
5	F	734	ALA
5	F	1069	GLU
1	A	820	ASP
1	A	903	ARG
1	A	1323	GLU
4	E	212	TRP
1	A	542	TRP
1	A	1294	LEU
5	F	532	LYS
5	F	894	VAL
5	F	1062	CYS
5	F	519	PRO
1	A	457	PRO
1	A	252	ARG
1	A	630	PRO

### 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 PDB entries followed by that with respect to all EM entries.

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	1073/1628 (66%)	1020 (95%)	53 (5%)	31	71
2	B	59/91 (65%)	56 (95%)	3 (5%)	29	70
3	C	143/179 (80%)	141 (99%)	2 (1%)	74	91
4	E	141/192 (73%)	134 (95%)	7 (5%)	30	70
5	F	837/974 (86%)	793 (95%)	44 (5%)	28	69
All	All	2253/3064 (74%)	2144 (95%)	109 (5%)	36	72

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	174	ARG
1	A	206	MET
1	A	221	LYS
1	A	224	LYS
1	A	262	ARG
1	A	276	ASP
1	A	277	ASN
1	A	327	ASN
1	A	422	ARG
1	A	525	SER
1	A	529	CYS
1	A	537	LYS
1	A	540	LYS
1	A	541	TYR
1	A	542	TRP
1	A	649	ASN
1	A	789	ARG
1	A	794[A]	ARG
1	A	794[B]	ARG
1	A	800	TRP
1	A	823	ARG
1	A	846	GLU
1	A	915	LYS
1	A	926	ARG
1	A	930	ASN
1	A	954	PHE
1	A	955	PHE
1	A	982	GLN
1	A	986	ARG
1	A	988	ARG
1	A	1020	LEU
1	A	1036	ASN
1	A	1101	TYR
1	A	1120	PHE
1	A	1121	GLU
1	A	1122	TYR
1	A	1131	ASN
1	A	1229	ARG
1	A	1239	ARG
1	A	1247	LEU
1	A	1249[A]	ARG

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Mol	Chain	Res	Type
1	A	1249[B]	ARG
1	A	1262	LYS
1	A	1264	PHE
1	A	1265	GLN
1	A	1276	MET
1	A	1302	ARG
1	A	1304	ASN
1	A	1306	PHE
1	A	1370	PHE
1	A	1376	PHE
1	A	1388	THR
2	B	115	PRO
2	B	167	SER
2	B	170	LEU
3	C	299	ASP
3	C	310	SER
4	E	10	ARG
4	E	15	CYS
4	E	113	PHE
4	E	191	LEU
4	E	206	ARG
4	E	207	MET
4	E	212	TRP
5	F	95	ARG
5	F	97	LYS
5	F	148	LYS
5	F	186	ASN
5	F	243	ARG
5	F	248	GLN
5	F	299	ASN
5	F	311	GLN
5	F	333	THR
5	F	348	ASN
5	F	353	ARG
5	F	389	PHE
5	F	428	TYR
5	F	447	GLN
5	F	452	TYR
5	F	478	LYS
5	F	501	ARG
5	F	508	LEU
5	F	509	CYS

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Mol	Chain	Res	Type
5	F	515	PHE
5	F	528	ASN
5	F	529	LEU
5	F	544	ARG
5	F	564	LEU
5	F	591	ARG
5	F	597	GLN
5	F	599	GLU
5	F	615	ASN
5	F	692	ARG
5	F	733	LYS
5	F	755	TRP
5	F	891	ASN
5	F	895	TYR
5	F	989	ASP
5	F	991	LYS
5	F	1020	MET
5	F	1032	ARG
5	F	1036	GLN
5	F	1049	MET
5	F	1052	GLN
5	F	1062	CYS
5	F	1068	LEU
5	F	1070	ASP
5	F	1071	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	ASN
1	A	372	GLN
1	A	426	HIS
1	A	445	ASN
1	A	468	ASN
1	A	916	HIS
1	A	1036	ASN
1	A	1071	GLN
1	A	1085	GLN
1	A	1139	HIS
1	A	1154	ASN
1	A	1265	GLN
1	A	1304	ASN

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Mol	Chain	Res	Type
1	A	1305	ASN
1	A	1311	GLN
1	A	1326	GLN
1	A	1397	HIS
5	F	76	ASN
5	F	311	GLN
5	F	313	ASN
5	F	316	ASN
5	F	348	ASN
5	F	480	ASN
5	F	511	ASN
5	F	556	GLN
5	F	655	ASN
5	F	679	ASN
5	F	685	ASN
5	F	1036	GLN
5	F	1052	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
5	ETA	F	1075	5	3,3,3	0.46	0	2,2,2	0.54	0

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
5	ETA	F	1075	5	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1075	ETA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 3 are monoatomic - leaving 39 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	$\# Z  > 2$
6	NAG	A	1901	1	14,14,15	0.38	0	15,19,21	0.47	0
7	PC1	A	1902	-	43,43,53	1.17	4 (9%)	47,51,61	1.22	3 (6%)
7	PC1	A	1903	-	53,53,53	1.07	3 (5%)	57,61,61	1.05	3 (5%)
7	PC1	A	1904	-	41,41,53	1.20	4 (9%)	45,49,61	1.21	3 (6%)
7	PC1	A	1905	-	37,37,53	1.22	2 (5%)	41,45,61	1.18	4 (9%)
7	PC1	A	1906	-	17,17,53	0.68	0	16,16,61	0.49	0
7	PC1	A	1907	-	11,11,53	0.70	0	10,10,61	0.38	0
7	PC1	A	1908	-	11,11,53	0.61	0	10,10,61	0.33	0
7	PC1	A	1909	-	14,14,53	0.62	0	13,13,61	0.44	0
7	PC1	A	1910	-	17,17,53	0.76	0	16,16,61	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	PC1	A	1911	-	47,47,53	1.06	3 (6%)	51,55,61	1.12	4 (7%)
7	PC1	A	1912	-	44,44,53	1.16	3 (6%)	48,52,61	1.12	3 (6%)
7	PC1	A	1913	-	17,17,53	0.72	0	16,16,61	0.40	0
7	PC1	A	1914	-	13,13,53	0.57	0	12,12,61	0.49	0
7	PC1	A	1915	-	47,47,53	1.15	3 (6%)	51,55,61	1.24	4 (7%)
6	NAG	F	1201	5,6	14,14,15	0.62	1 (7%)	15,19,21	0.86	1 (6%)
6	NAG	F	1202	6	14,14,15	0.46	0	15,19,21	0.33	0
6	NAG	F	1203	5	14,14,15	0.29	0	15,19,21	0.36	0
6	NAG	F	1204	5,6	14,14,15	0.28	0	15,19,21	0.54	0
6	NAG	F	1205	6	14,14,15	0.28	0	15,19,21	0.53	0
6	NAG	F	1206	5	14,14,15	0.49	0	15,19,21	0.26	0
9	BMA	F	1207	6	11,11,12	0.88	1 (9%)	15,15,17	0.80	0
6	NAG	F	1208	9,6	14,14,15	0.26	0	15,19,21	0.76	1 (6%)
6	NAG	F	1209	5,6	14,14,15	0.66	0	15,19,21	0.52	0
6	NAG	F	1210	5,6	14,14,15	0.31	0	15,19,21	0.70	0
6	NAG	F	1211	9,6	14,14,15	0.33	0	15,19,21	0.52	0
9	BMA	F	1212	6	11,11,12	0.59	0	15,15,17	0.91	2 (13%)
6	NAG	F	1213	5	14,14,15	0.43	0	15,19,21	0.63	1 (6%)
6	NAG	F	1214	5	14,14,15	0.64	0	15,19,21	0.56	0
6	NAG	F	1215	5,6	14,14,15	0.25	0	15,19,21	0.43	0
6	NAG	F	1216	6	14,14,15	0.26	0	15,19,21	0.43	0
6	NAG	F	1217	5,6	14,14,15	0.57	0	15,19,21	0.92	1 (6%)
6	NAG	F	1218	6	14,14,15	0.58	0	15,19,21	0.98	1 (6%)
6	NAG	F	1219	5	14,14,15	0.37	0	15,19,21	0.36	0
6	NAG	F	1220	5	14,14,15	0.81	1 (7%)	15,19,21	1.04	1 (6%)
6	NAG	F	1221	5	14,14,15	0.57	0	15,19,21	0.58	0
6	NAG	F	1222	6	14,14,15	0.43	0	15,19,21	0.64	1 (6%)
6	NAG	F	1223	6	14,14,15	0.31	0	15,19,21	0.84	1 (6%)
6	NAG	F	1224	5,6	14,14,15	0.33	0	15,19,21	0.64	0

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
6	NAG	A	1901	1	-	0/6/23/26	0/1/1/1
7	PC1	A	1902	-	-	0/47/47/57	0/0/0/0
7	PC1	A	1903	-	-	0/57/57/57	0/0/0/0
7	PC1	A	1904	-	-	1/45/45/57	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PC1	A	1905	-	-	0/41/41/57	0/0/0/0
7	PC1	A	1906	-	-	0/15/15/57	0/0/0/0
7	PC1	A	1907	-	-	0/9/9/57	0/0/0/0
7	PC1	A	1908	-	-	0/9/9/57	0/0/0/0
7	PC1	A	1909	-	-	0/12/12/57	0/0/0/0
7	PC1	A	1910	-	-	0/15/15/57	0/0/0/0
7	PC1	A	1911	-	-	1/51/51/57	0/0/0/0
7	PC1	A	1912	-	-	0/48/48/57	0/0/0/0
7	PC1	A	1913	-	-	0/15/15/57	0/0/0/0
7	PC1	A	1914	-	-	0/11/11/57	0/0/0/0
7	PC1	A	1915	-	-	2/51/51/57	0/0/0/0
6	NAG	F	1201	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1202	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1203	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1204	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1205	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1206	5	-	0/6/23/26	0/1/1/1
9	BMA	F	1207	6	-	0/2/19/22	0/1/1/1
6	NAG	F	1208	9,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1209	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1210	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1211	9,6	-	0/6/23/26	0/1/1/1
9	BMA	F	1212	6	-	0/2/19/22	0/1/1/1
6	NAG	F	1213	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1214	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1215	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1216	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1217	5,6	-	0/6/23/26	0/1/1/1
6	NAG	F	1218	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1219	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1220	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1221	5	-	0/6/23/26	0/1/1/1
6	NAG	F	1222	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1223	6	-	0/6/23/26	0/1/1/1
6	NAG	F	1224	5,6	-	0/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1911	PC1	O21-C2	-2.58	1.39	1.46
7	A	1912	PC1	O21-C2	-2.50	1.39	1.46
7	A	1915	PC1	O21-C2	-2.48	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1903	PC1	O21-C2	-2.29	1.40	1.46
7	A	1904	PC1	O21-C2	-2.27	1.40	1.46
7	A	1902	PC1	O21-C2	-2.03	1.41	1.46
7	A	1904	PC1	C22-C21	2.03	1.56	1.50
9	F	1207	BMA	C2-C3	2.07	1.55	1.52
7	A	1902	PC1	C22-C21	2.15	1.56	1.50
6	F	1201	NAG	C1-C2	2.16	1.55	1.52
6	F	1220	NAG	C1-C2	2.35	1.55	1.52
7	A	1911	PC1	O21-C21	2.47	1.41	1.34
7	A	1911	PC1	O31-C31	2.63	1.41	1.33
7	A	1912	PC1	O21-C21	2.64	1.42	1.34
7	A	1904	PC1	O21-C21	2.77	1.42	1.34
7	A	1903	PC1	O21-C21	2.84	1.42	1.34
7	A	1902	PC1	O31-C31	2.93	1.42	1.33
7	A	1905	PC1	O31-C31	2.97	1.42	1.33
7	A	1915	PC1	O21-C21	2.97	1.43	1.34
7	A	1905	PC1	O21-C21	2.99	1.43	1.34
7	A	1902	PC1	O21-C21	3.11	1.43	1.34
7	A	1915	PC1	O31-C31	3.14	1.42	1.33
7	A	1903	PC1	O31-C31	3.17	1.42	1.33
7	A	1912	PC1	O31-C31	3.17	1.42	1.33
7	A	1904	PC1	O31-C31	3.24	1.43	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1915	PC1	O21-C21-O22	-2.07	118.03	123.67
7	A	1911	PC1	C2-O21-C21	-2.07	112.79	117.91
9	F	1212	BMA	O2-C2-C3	-2.03	106.10	110.19
7	A	1905	PC1	O21-C2-C1	2.05	115.58	108.36
9	F	1212	BMA	C1-O5-C5	2.09	115.21	112.14
6	F	1213	NAG	C1-O5-C5	2.11	115.24	112.14
6	F	1222	NAG	C1-O5-C5	2.19	115.36	112.14
7	A	1905	PC1	O31-C31-C32	2.26	118.79	111.85
7	A	1911	PC1	O31-C31-C32	2.47	119.44	111.85
6	F	1208	NAG	C1-O5-C5	2.49	115.80	112.14
7	A	1912	PC1	O31-C31-C32	2.54	119.66	111.85
7	A	1902	PC1	O31-C31-C32	2.69	120.13	111.85
6	F	1223	NAG	C1-O5-C5	2.70	116.11	112.14
6	F	1201	NAG	C2-N2-C7	2.88	126.85	123.11
7	A	1903	PC1	O31-C31-C32	2.90	120.76	111.85
7	A	1915	PC1	O31-C31-C32	3.03	121.19	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	1218	NAG	C2-N2-C7	3.16	127.21	123.11
6	F	1217	NAG	C1-O5-C5	3.16	116.79	112.14
7	A	1915	PC1	C15-N-C13	3.34	117.60	108.96
7	A	1904	PC1	O31-C31-C32	3.38	122.25	111.85
6	F	1220	NAG	C1-O5-C5	3.47	117.24	112.14
7	A	1911	PC1	O21-C21-C22	3.50	118.89	111.53
7	A	1912	PC1	C15-N-C13	3.50	118.02	108.96
7	A	1905	PC1	O21-C21-C22	3.59	119.10	111.53
7	A	1903	PC1	C15-N-C13	3.62	118.32	108.96
7	A	1903	PC1	O21-C21-C22	3.62	119.16	111.53
7	A	1902	PC1	C15-N-C13	3.68	118.49	108.96
7	A	1911	PC1	C15-N-C13	3.68	118.49	108.96
7	A	1905	PC1	C15-N-C13	3.80	118.80	108.96
7	A	1904	PC1	C15-N-C13	4.00	119.32	108.96
7	A	1904	PC1	O21-C21-C22	4.16	120.28	111.53
7	A	1912	PC1	O21-C21-C22	4.45	120.91	111.53
7	A	1902	PC1	O21-C21-C22	5.15	122.38	111.53
7	A	1915	PC1	O21-C21-C22	5.52	123.15	111.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1911	PC1	C2-O21-C21-C22
7	A	1904	PC1	C2-O21-C21-C22
7	A	1915	PC1	C2-O21-C21-O22
7	A	1915	PC1	C2-O21-C21-C22

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1902	PC1	2	0
7	A	1903	PC1	2	0
7	A	1904	PC1	4	0
7	A	1909	PC1	2	0
7	A	1911	PC1	2	0
7	A	1912	PC1	3	0
7	A	1914	PC1	4	0
7	A	1915	PC1	1	0
6	F	1204	NAG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	1205	NAG	4	0
6	F	1215	NAG	1	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.