



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:01 pm GMT

PDB ID : 5L5C
Title : Plexin A1 full extracellular region, domains 1 to 10, to 6 angstrom, spacegroup P4(3)2(1)2
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Deposited on : 2016-05-28
Resolution : 6.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

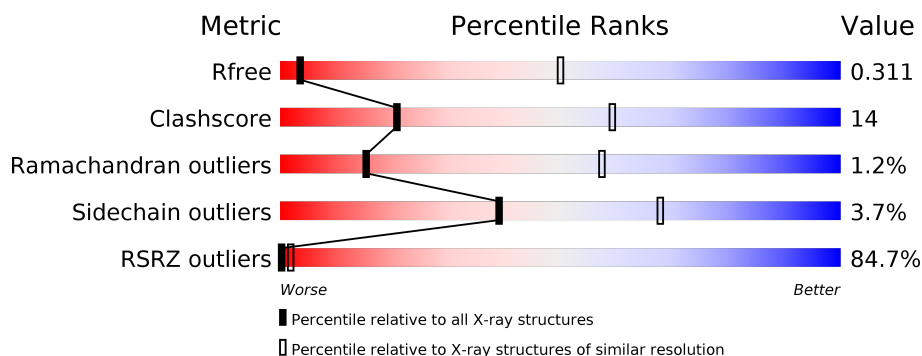
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 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))
R_{free}	100719	1085 (8.30-3.70)
Clashscore	112137	1017 (8.20-3.80)
Ramachandran outliers	110173	1001 (8.20-3.72)
Sidechain outliers	110143	1085 (8.30-3.70)
RSRZ outliers	101464	1094 (8.30-3.70)

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.

Mol	Chain	Length	Quality of chain
1	A	1212	<div> <div>82%</div> <div>70% 25% . .</div> </div>

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
2	NAG	A	1301	-	-	-	X
2	NAG	A	1314	-	-	X	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1331	-	-	-	X
2	NAG	A	1332	X	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9546 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.

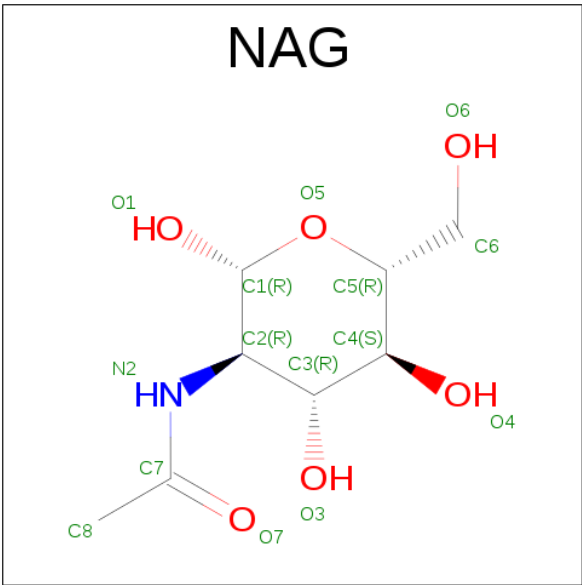
- Molecule 1 is a protein called Plexin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1171	Total	C	N	O	S	0	0	0
			9085	5719	1593	1715	58			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLU	-	expression tag	UNP P70206
A	35	THR	-	expression tag	UNP P70206
A	36	GLY	-	expression tag	UNP P70206
A	1237	ARG	-	expression tag	UNP P70206
A	1238	THR	-	expression tag	UNP P70206
A	1239	LYS	-	expression tag	UNP P70206
A	1240	HIS	-	expression tag	UNP P70206
A	1241	HIS	-	expression tag	UNP P70206
A	1242	HIS	-	expression tag	UNP P70206
A	1243	HIS	-	expression tag	UNP P70206
A	1244	HIS	-	expression tag	UNP P70206
A	1245	HIS	-	expression tag	UNP P70206

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



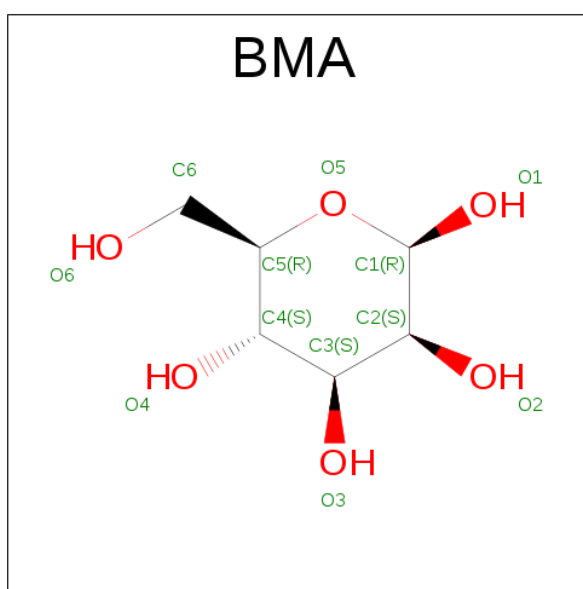
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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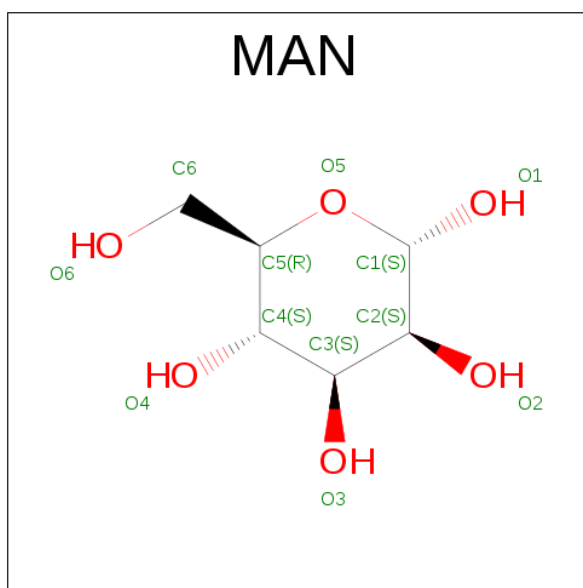
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).

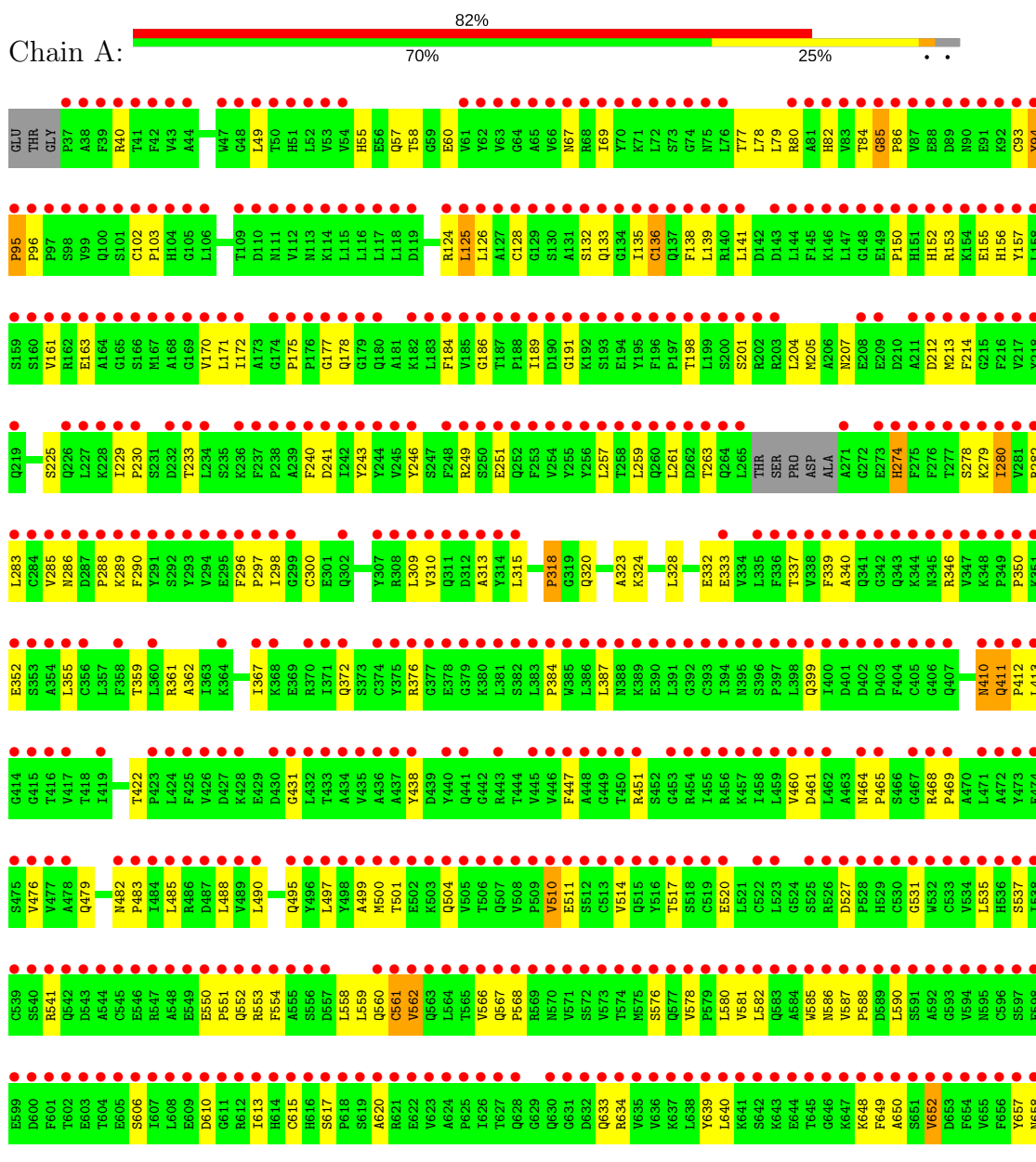


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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

• Molecule 1: Plexin-A1



PRO	I1168	I1107	T1047	I1977	P907	P846	V786	K721	C659
GLY	L1169	D1108	I1048	G978	V908	A847	V787	F722	S860
MET	K1170	N1109	L1049	I979	A915	S848	N789	W788	V861
LEU	G1171		R1050	E980	E916	W849	N789	I723	H662
GLN	R1172	R1112	I1051	S982	E917	M850	G790	L725	Q663
VAL	M1173	S1113	D1052	G983	Q917	H851	N791	A726	S664
TYR	L1174	P1053	P1053	H983	T918	A852	F792	A727	C665
SER	L1175	E1054	E1054	L984	V919	H853	R728	L726	L866
ASP	P1176	E1116	W1055	N985	C920	H854	N794	W729	C667
ARG	P1177	L1117	S1056	G987	E921	G855	D795	L730	C668
THR	A1178	G1118	I1057	G987	I922	S856	N796	F731	V669
LYS	P1179	E1119	N1058		G923	S857	F797	Q732	N670
HIS	G1180	R1120	S1059	V990		S858	F798	P733	G671
HIS	N1181	P1121	G1060	A991	T927	C859	N799	Q734	S872
HIS	S1182	D1122	G1061	V992	L928	T860	L800	F674	P673
HIS	R1183	E1123	T1062	S993	R929	D861	Q801	S736	K674
HIS	L1184	I1124	L1063	I994	A930	P862	A802	Q737	C675
HIS	N1185	G1125	L1064		H931	K863	H803	R738	H676
HIS	Y1186	F1126	T1065	C999	D932	I864	L804	W739	W677
	T1187	I1127	V1066	S1000	A933	L867	Y805	Y740	C678
	V1188	M1128	T1067	F1001	L934		K806	E741	K679
	L1189	D1129	G1068		V935	P868	C807	C742	Y680
	I1190	N1130	T1069	R1004	E936	P869	P808	L743	R681
	G1191	V1131	N1070		V937	E870	A809	F744	H682
	S1192	R1132	L1071	R1007	C938	T871	L810	H745	V683
	T1193	T1133	A1072	E1008	V939	G872	R811	L746	C684
	P1194	L1134	T1073	I1009	R940	P873	S813	S749	T685
	C1195	L1135	V1074	R1010	D941	R874	C814	P750	N686
	I1196	V1136	E1075	C1011		Q875	G815	A751	N687
	L1197	L1137	E1076	L1012	L944	G876	L816	F752	A688
	T1198	N1138	P1077	T1013	H945	G877	C817	W753	C691
	V1199	S1139	R1078	P1014	Y946	T878	L818	T754	A692
	S1200	S1140	I1079	P1015	R947	R879	K819	A755	F693
	E1201	S1141	R1080		A948	L880	A820	L756	L694
	T1202	F1142	A1081	T1018		T881	D821	R757	E695
	Q1203	L1143	K1082	P1019	K952	I882	P822	F758	G696
	L1204	Y1144	Y1083	G1020	R953	T883	R823		R697
	L1205	Y1145	G1084	S1021	F954	G884	F824	V698	
	C1206	P1146	G1085	A1022	T955	E885	E825	N699	
	E1207	D1147	T1086	P1023	F956	N886	C826	M700	
	A1208	P1148	E1087	I1024	V957	L887	G827	S701	
	P1209	V1149	R1088	V1025	T958	G888	W828	E702	
	N1210	L1150	E1089	I1026	P959	L889	C829	D703	
LEU		E1151	N1090	N1027	T960	H890	V830	C704	
THR		P1152	S1091	I1028	F961	F891	E831	P705	
GLY		L1153	C1092	N1029	Y962	E892	E832	Q706	
GLN		SER	M1093	R1030	R963	D893	R833	S771	
HIS		PRO	Y1094	Q1031	V964	V894	R834	L708	
	K1216	THR	V1095	Q1032	S965	R895	C835	E772	
	V1217	GLY	N1096	L1033	P966	L896	S836	E773	
	T1218	LEU	D1097		S967	G897	L837	G774	
	V1219	LEU	T1098	V1038	R968	V898	L837		
	R1220	GLU	T1099	K1039	Q969	H899	H838	S778	
	A1221	LEU	M1100	Y1040	P970	V900	H839	D779	
	G1222	LYS	V1101	N1041	L971	G901	H840	L780	
	G1223	PRO	C1102	N1042	S972	K902	C841	P716	
			R1183	T1043	G973	V903	P842	V717	
	F1224	S1164	A1104	E1044	G974	L904	A843	G718	
	E1225	P1165	A1105	D1045	T975	C905	D844	V719	
	F1226	L1167	S1106	P1046	W976	S906	S845	S785	

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	198.15Å 198.15Å 228.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	119.50 – 6.00 119.50 – 6.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (119.50-6.00) 97.7 (119.50-6.00)	Depositor EDS
R_{merge}	0.71	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 6.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.305 , 0.316 0.310 , 0.311	Depositor DCC
R_{free} test set	583 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	326.8	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 511.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9546	wwPDB-VP
Average B, all atoms (Å ²)	283.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.56	5/9294 (0.1%)	0.75	9/12632 (0.1%)

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	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	VAL	C-N	28.43	1.99	1.34
1	A	561	CYS	C-N	21.68	1.83	1.34
1	A	704	CYS	C-N	17.78	1.68	1.34
1	A	1043	THR	C-N	14.17	1.66	1.34
1	A	859	CYS	C-N	-6.73	1.18	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	THR	CA-C-N	-34.31	41.72	117.20
1	A	1043	THR	C-N-CA	-26.50	55.44	121.70
1	A	1043	THR	O-C-N	14.48	145.87	122.70
1	A	859	CYS	O-C-N	-13.80	100.62	122.70
1	A	561	CYS	O-C-N	11.14	140.53	122.70
1	A	859	CYS	C-N-CA	9.32	145.00	121.70
1	A	859	CYS	CA-C-N	9.09	137.19	117.20
1	A	561	CYS	CA-C-N	-9.04	97.30	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	CYS	C-N-CA	-7.86	102.04	121.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1052	ASP	Peptide
1	A	410	ASN	Peptide
1	A	527	ASP	Peptide
1	A	807	CYS	Peptide
1	A	85	GLY	Peptide
1	A	859	CYS	Mainchain
1	A	868	SER	Peptide
1	A	94	TYR	Peptide
1	A	965	SER	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	9085	0	8873	259	28
2	A	252	0	218	23	0
3	A	77	0	61	0	0
4	A	132	0	117	0	0
All	All	9546	0	9269	260	28

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 14.

All (260) 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:704:CYS:C	1:A:705:PRO:N	1.68	1.48
1:A:661:VAL:HG13	2:A:1314:NAG:C6	1.47	1.44
1:A:561:CYS:C	1:A:562:VAL:N	1.83	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:VAL:CG1	2:A:1314:NAG:O6	1.88	1.20
1:A:510:VAL:C	1:A:511:GLU:N	1.99	1.15
1:A:553:ARG:HD2	1:A:588:PRO:CB	1.78	1.13
1:A:661:VAL:CG1	2:A:1314:NAG:C6	2.27	1.13
1:A:633:GLN:OE1	1:A:673:PHE:CE1	2.03	1.11
1:A:553:ARG:HD2	1:A:588:PRO:CG	1.81	1.09
1:A:411:GLN:HG2	1:A:412:PRO:HD2	1.35	1.06
1:A:1055:TRP:HH2	1:A:1184:LEU:HD21	1.17	1.06
1:A:860:THR:HA	1:A:946:TYR:CE1	1.93	1.03
1:A:661:VAL:HG13	2:A:1314:NAG:H62	1.06	1.02
1:A:1055:TRP:CH2	1:A:1184:LEU:HD21	1.93	1.02
1:A:661:VAL:HG11	2:A:1314:NAG:O6	1.56	1.00
1:A:661:VAL:HG13	2:A:1314:NAG:O6	1.53	0.99
1:A:661:VAL:CG1	2:A:1314:NAG:H62	1.88	0.98
1:A:661:VAL:CG2	2:A:1314:NAG:O5	2.12	0.97
1:A:553:ARG:HG2	1:A:588:PRO:HB3	1.47	0.95
1:A:633:GLN:OE1	1:A:673:PHE:HE1	1.48	0.94
1:A:553:ARG:HD2	1:A:588:PRO:HG3	1.50	0.93
1:A:553:ARG:CD	1:A:588:PRO:CB	2.46	0.92
1:A:661:VAL:HG21	2:A:1314:NAG:O5	1.67	0.92
1:A:468:ARG:HG2	1:A:469:PRO:HD2	1.51	0.91
1:A:806:LYS:C	1:A:807:CYS:N	2.25	0.90
1:A:860:THR:HA	1:A:946:TYR:HE1	1.28	0.89
1:A:189:ILE:HD12	1:A:198:THR:HG23	1.52	0.88
1:A:94:TYR:CD2	1:A:95:PRO:HD3	2.08	0.88
1:A:661:VAL:HG22	2:A:1314:NAG:C5	2.04	0.87
1:A:808:PRO:HD2	1:A:835:CYS:O	1.76	0.85
1:A:560:GLN:C	1:A:586:ASN:HD22	1.79	0.85
1:A:633:GLN:OE1	1:A:673:PHE:CZ	2.29	0.84
1:A:567:GLN:HB3	1:A:568:PRO:HD3	1.61	0.81
1:A:553:ARG:CG	1:A:588:PRO:HB3	2.09	0.81
1:A:552:GLN:O	1:A:588:PRO:HD3	1.79	0.81
1:A:818:LEU:HB3	1:A:852:ALA:HB2	1.62	0.80
1:A:153:ARG:H	1:A:156:HIS:HD2	1.30	0.78
1:A:789:ASN:HD22	1:A:792:PHE:HE2	1.31	0.78
1:A:560:GLN:O	1:A:586:ASN:HB3	1.82	0.78
1:A:280:ILE:HB	1:A:298:ILE:HD12	1.64	0.78
1:A:553:ARG:CD	1:A:588:PRO:HB2	2.14	0.78
1:A:553:ARG:HD2	1:A:588:PRO:HB2	1.67	0.77
1:A:259:LEU:HD23	1:A:346:ARG:HG3	1.66	0.76
1:A:230:PRO:O	1:A:233:THR:HG22	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:658:ASN:C	1:A:659:CYS:N	2.39	0.76
1:A:535:LEU:HD21	1:A:590:LEU:HD21	1.67	0.75
1:A:923:GLY:HA2	1:A:1030:ARG:HH22	1.52	0.74
1:A:877:GLY:HA3	1:A:1030:ARG:HG3	1.68	0.74
1:A:895:ARG:O	1:A:896:LEU:HB2	1.85	0.74
1:A:411:GLN:CG	1:A:412:PRO:HD2	2.14	0.74
1:A:561:CYS:C	1:A:562:VAL:CA	2.57	0.74
1:A:658:ASN:OD1	1:A:661:VAL:HG23	1.88	0.74
1:A:661:VAL:HG22	2:A:1314:NAG:O5	1.84	0.72
1:A:743:LEU:HD22	1:A:752:ARG:HG2	1.70	0.72
1:A:860:THR:CA	1:A:946:TYR:HE1	2.03	0.72
1:A:561:CYS:CA	1:A:562:VAL:N	2.53	0.71
1:A:852:ALA:HA	1:A:857:SER:OG	1.91	0.71
1:A:1079:ILE:HD11	1:A:1102:CYS:HB3	1.73	0.70
1:A:606:SER:HB3	1:A:615:CYS:HB3	1.74	0.70
1:A:171:LEU:HD22	1:A:204:LEU:HD11	1.72	0.70
1:A:55:HIS:HE2	1:A:141:LEU:HD21	1.57	0.69
1:A:82:HIS:HD2	1:A:84:THR:HG22	1.55	0.69
1:A:310:VAL:HG22	1:A:339:PHE:CE1	2.28	0.69
1:A:560:GLN:HA	1:A:586:ASN:ND2	2.08	0.68
1:A:566:VAL:HG22	1:A:582:LEU:HD23	1.76	0.68
1:A:1055:TRP:CH2	1:A:1176:PRO:HG3	2.28	0.68
1:A:661:VAL:CG2	2:A:1314:NAG:C1	2.72	0.67
1:A:746:ILE:HB	1:A:749:SER:O	1.95	0.67
1:A:175:PRO:HG2	1:A:178:GLN:HG3	1.76	0.67
1:A:1055:TRP:CH2	1:A:1184:LEU:CD2	2.76	0.66
1:A:895:ARG:HA	1:A:907:PRO:HG2	1.76	0.66
1:A:468:ARG:CG	1:A:469:PRO:HD2	2.24	0.65
1:A:315:LEU:HD11	1:A:333:GLU:HB3	1.78	0.64
1:A:560:GLN:O	1:A:586:ASN:CB	2.44	0.64
1:A:553:ARG:CD	1:A:588:PRO:HB3	2.28	0.64
1:A:887:LEU:HB2	1:A:915:ALA:HA	1.80	0.64
1:A:1057:ILE:HD12	1:A:1147:ASP:OD1	1.97	0.64
1:A:550:GLU:HB3	1:A:551:PRO:HD2	1.80	0.63
1:A:1055:TRP:CZ2	1:A:1176:PRO:HG3	2.34	0.63
1:A:58:THR:OG1	1:A:60:GLU:HG2	1.99	0.63
1:A:69:ILE:HD12	1:A:84:THR:HG21	1.79	0.63
1:A:939:VAL:HG22	1:A:946:TYR:HB3	1.82	0.62
1:A:740:TYR:CD1	1:A:788:TRP:HB3	2.36	0.61
1:A:732:GLN:HG2	1:A:757:ARG:HH22	1.66	0.61
1:A:704:CYS:C	1:A:705:PRO:CD	2.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:TYR:CD2	1:A:648:LYS:HD2	2.36	0.60
1:A:259:LEU:HD23	1:A:346:ARG:CG	2.31	0.60
1:A:878:THR:HB	1:A:922:ILE:HD12	1.84	0.59
1:A:153:ARG:N	1:A:156:HIS:HD2	1.99	0.59
1:A:661:VAL:HG21	2:A:1314:NAG:C1	2.33	0.59
1:A:578:VAL:H	1:A:617:SER:HB3	1.66	0.59
1:A:447:PHE:HZ	1:A:510:VAL:HG23	1.69	0.58
1:A:559:LEU:O	1:A:586:ASN:ND2	2.37	0.58
1:A:55:HIS:NE2	1:A:141:LEU:HD21	2.17	0.58
1:A:560:GLN:CA	1:A:586:ASN:ND2	2.67	0.57
1:A:153:ARG:H	1:A:156:HIS:CD2	2.18	0.57
1:A:337:THR:O	1:A:355:LEU:HD12	2.05	0.57
1:A:531:GLY:HA3	1:A:554:PHE:CZ	2.40	0.57
1:A:246:TYR:CD2	1:A:313:ALA:HB3	2.39	0.57
1:A:279:LYS:HG2	1:A:297:PRO:HA	1.87	0.56
1:A:661:VAL:HG22	2:A:1314:NAG:C6	2.34	0.56
1:A:172:ILE:HG22	1:A:249:ARG:HD2	1.87	0.56
1:A:732:GLN:HG2	1:A:757:ARG:NH2	2.20	0.56
1:A:485:LEU:HD12	1:A:500:MET:HG2	1.86	0.56
1:A:789:ASN:HB3	1:A:792:PHE:CD2	2.41	0.56
1:A:808:PRO:HG3	1:A:835:CYS:HB3	1.87	0.56
1:A:537:SER:HB2	1:A:649:PHE:HA	1.88	0.56
1:A:296:PHE:CE1	1:A:367:ILE:HG12	2.41	0.55
1:A:132:SER:HB2	1:A:135:ILE:HG12	1.87	0.55
1:A:488:LEU:HD12	1:A:499:ALA:HA	1.89	0.55
1:A:567:GLN:HB2	1:A:581:VAL:HG22	1.87	0.55
1:A:93:CYS:O	1:A:133:GLN:NE2	2.40	0.55
1:A:737:GLN:HG2	1:A:789:ASN:ND2	2.22	0.55
1:A:318:PRO:HG2	1:A:323:ALA:HB2	1.89	0.55
1:A:658:ASN:CG	1:A:661:VAL:HG23	2.27	0.55
1:A:693:PHE:HZ	1:A:734:GLN:OE1	1.90	0.55
1:A:661:VAL:CG2	2:A:1314:NAG:C5	2.76	0.54
1:A:566:VAL:HG22	1:A:582:LEU:CD2	2.37	0.54
1:A:738:ARG:HB2	1:A:789:ASN:HA	1.89	0.54
1:A:789:ASN:HB3	1:A:792:PHE:HD2	1.73	0.54
1:A:661:VAL:CB	2:A:1314:NAG:H62	2.37	0.54
1:A:278:SER:HB3	1:A:310:VAL:HG23	1.91	0.53
1:A:282:ARG:HG3	1:A:283:LEU:N	2.22	0.53
1:A:205:MET:HG3	1:A:212:ASP:HB3	1.90	0.53
1:A:640:LEU:HD12	1:A:650:ALA:HB3	1.91	0.53
1:A:332:GLU:OE2	1:A:361:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:CB	1:A:60:GLU:HG2	2.39	0.52
1:A:821:ASP:HB2	1:A:824:PHE:CD2	2.44	0.52
1:A:126:LEU:HD11	1:A:136:CYS:SG	2.49	0.52
1:A:677:TRP:HB3	1:A:698:VAL:HB	1.92	0.52
1:A:124:ARG:HD2	1:A:138:PHE:HD2	1.74	0.52
1:A:818:LEU:HB2	1:A:889:LEU:HD11	1.92	0.52
1:A:875:GLN:HB2	1:A:1031:ALA:HB2	1.92	0.51
1:A:438:TYR:CE1	1:A:510:VAL:HG21	2.46	0.51
1:A:461:ASP:HA	1:A:464:ASN:HB3	1.92	0.51
1:A:1061:GLY:O	1:A:1223:GLY:HA3	2.11	0.51
1:A:170:VAL:HG11	1:A:249:ARG:HB2	1.91	0.51
1:A:560:GLN:CA	1:A:586:ASN:HD22	2.24	0.51
1:A:310:VAL:HG22	1:A:339:PHE:HE1	1.72	0.51
1:A:447:PHE:CZ	1:A:510:VAL:HG23	2.45	0.51
2:A:1314:NAG:H61	2:A:1315:NAG:HN2	1.77	0.50
1:A:153:ARG:NH2	1:A:212:ASP:HA	2.26	0.50
1:A:55:HIS:CE1	1:A:57:GLN:HB2	2.46	0.50
1:A:229:ILE:HD12	1:A:240:PHE:HE2	1.76	0.50
1:A:552:GLN:HB2	1:A:587:VAL:C	2.32	0.50
1:A:939:VAL:CG2	1:A:946:TYR:HB3	2.42	0.50
1:A:658:ASN:ND2	1:A:661:VAL:HG21	2.27	0.50
1:A:186:GLY:HA2	1:A:198:THR:O	2.12	0.49
1:A:464:ASN:CG	1:A:465:PRO:HD2	2.32	0.49
1:A:553:ARG:HA	1:A:588:PRO:HG3	1.93	0.49
1:A:323:ALA:HA	1:A:328:LEU:HD12	1.94	0.49
1:A:708:LEU:H	1:A:727:ALA:HA	1.77	0.49
1:A:431:GLY:HA3	1:A:451:ARG:HD2	1.93	0.49
1:A:153:ARG:HB2	1:A:156:HIS:CD2	2.48	0.49
1:A:495:GLN:O	1:A:510:VAL:HG12	2.13	0.49
1:A:560:GLN:C	1:A:586:ASN:ND2	2.57	0.49
1:A:1055:TRP:CZ2	1:A:1184:LEU:CD2	2.96	0.48
1:A:96:PRO:HD2	1:A:157:TYR:CZ	2.48	0.48
1:A:172:ILE:HD11	1:A:184:PHE:HE2	1.77	0.48
1:A:658:ASN:CG	1:A:661:VAL:CG2	2.82	0.48
1:A:468:ARG:HG2	1:A:469:PRO:CD	2.36	0.48
1:A:661:VAL:CG2	2:A:1314:NAG:C6	2.91	0.48
1:A:661:VAL:HG22	2:A:1314:NAG:H62	1.96	0.48
1:A:1055:TRP:CH2	1:A:1184:LEU:HD11	2.49	0.47
1:A:1027:ASN:HB3	1:A:1032:GLN:HG3	1.95	0.47
1:A:460:VAL:HA	1:A:469:PRO:HB3	1.96	0.47
1:A:501:THR:OG1	1:A:504:GLN:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ASP:HB2	1:A:824:PHE:CE2	2.49	0.47
1:A:567:GLN:CB	1:A:581:VAL:HG22	2.44	0.47
1:A:907:PRO:HA	1:A:920:CYS:HA	1.96	0.47
1:A:172:ILE:HD13	1:A:285:VAL:HG13	1.97	0.47
1:A:40:ARG:NH2	2:A:1301:NAG:O3	2.47	0.47
1:A:461:ASP:CA	1:A:464:ASN:HB3	2.45	0.47
1:A:818:LEU:HD22	1:A:852:ALA:H	1.80	0.47
1:A:372:GLN:O	1:A:376:ARG:HD3	2.15	0.47
1:A:447:PHE:CD2	1:A:497:LEU:HD22	2.49	0.47
1:A:566:VAL:CG2	1:A:652:VAL:HG21	2.45	0.46
1:A:806:LYS:CA	1:A:807:CYS:N	2.79	0.46
1:A:860:THR:HG22	1:A:946:TYR:OH	2.16	0.46
1:A:558:LEU:HD12	1:A:561:CYS:SG	2.56	0.46
1:A:934:LEU:HD23	1:A:953:ARG:HB3	1.97	0.46
1:A:887:LEU:HD23	1:A:918:ILE:HD11	1.98	0.46
1:A:661:VAL:HG22	2:A:1314:NAG:H5	1.92	0.45
1:A:201:SER:HB2	1:A:290:PHE:HE1	1.81	0.45
1:A:553:ARG:HD3	1:A:588:PRO:HB2	1.97	0.45
1:A:932:ASP:N	1:A:932:ASP:OD1	2.50	0.45
1:A:125:LEU:HD23	1:A:139:LEU:HB2	1.99	0.45
1:A:79:LEU:O	1:A:80:ARG:HG3	2.16	0.45
1:A:818:LEU:HB3	1:A:852:ALA:CB	2.41	0.45
1:A:132:SER:CB	1:A:135:ILE:HG12	2.47	0.45
1:A:566:VAL:HG23	1:A:652:VAL:HG21	1.98	0.44
1:A:1078:ARG:HG3	1:A:1127:ILE:HB	1.99	0.44
1:A:815:GLY:O	1:A:819:LYS:HB2	2.17	0.44
1:A:894:VAL:HG11	1:A:918:ILE:HD13	1.99	0.44
1:A:576:SER:OG	1:A:620:ALA:N	2.51	0.44
1:A:937:VAL:HG23	1:A:948:ALA:HB3	1.98	0.44
1:A:1088:ARG:HD2	1:A:1106:SER:O	2.18	0.44
1:A:67:ASN:CB	1:A:85:GLY:HA3	2.48	0.44
1:A:261:LEU:HD11	1:A:274:HIS:CB	2.48	0.43
1:A:551:PRO:O	1:A:588:PRO:HA	2.18	0.43
1:A:657:TYR:HB3	1:A:673:PHE:CE2	2.52	0.43
1:A:155:GLU:N	1:A:155:GLU:OE1	2.51	0.43
1:A:1055:TRP:CZ2	1:A:1184:LEU:HD21	2.50	0.43
1:A:150:PRO:HB2	1:A:156:HIS:ND1	2.34	0.43
1:A:49:LEU:HD13	1:A:500:MET:HE2	2.01	0.43
1:A:1104:ALA:HA	1:A:1105:PRO:HD3	1.89	0.43
1:A:952:LYS:HD2	1:A:952:LYS:HA	1.70	0.43
1:A:102:CYS:HA	1:A:103:PRO:HD3	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HB	1:A:60:GLU:HG2	2.01	0.43
1:A:808:PRO:HB2	1:A:811:ARG:H	1.83	0.43
1:A:359:THR:HG23	1:A:362:ALA:CB	2.48	0.43
1:A:476:VAL:HB	1:A:479:GLN:HG2	2.01	0.43
1:A:568:PRO:HG2	1:A:580:LEU:HD23	2.01	0.43
1:A:740:TYR:HE1	1:A:794:ILE:HD11	1.83	0.43
1:A:838:ARG:NH1	1:A:841:CYS:O	2.51	0.43
1:A:959:PRO:HA	1:A:983:HIS:HB2	2.01	0.42
1:A:550:GLU:HB2	1:A:553:ARG:HG3	2.00	0.42
1:A:69:ILE:CD1	1:A:84:THR:HG21	2.48	0.42
1:A:818:LEU:HD22	1:A:852:ALA:N	2.34	0.42
1:A:661:VAL:CG2	2:A:1314:NAG:H62	2.49	0.42
1:A:488:LEU:HG	1:A:497:LEU:HD11	2.02	0.42
1:A:658:ASN:ND2	1:A:661:VAL:CG2	2.82	0.42
1:A:582:LEU:HB2	1:A:613:ILE:HB	2.02	0.42
1:A:161:VAL:HG12	1:A:163:GLU:H	1.83	0.42
1:A:944:LEU:HD12	1:A:944:LEU:H	1.85	0.42
1:A:309:LEU:O	1:A:339:PHE:HA	2.19	0.42
1:A:410:ASN:O	1:A:411:GLN:O	2.37	0.42
1:A:606:SER:CB	1:A:615:CYS:HB3	2.48	0.42
1:A:706:GLN:O	1:A:727:ALA:HB1	2.19	0.42
1:A:661:VAL:HG22	2:A:1314:NAG:C1	2.47	0.41
1:A:263:THR:HB	1:A:384:PRO:HB2	2.02	0.41
1:A:871:THR:HG22	1:A:955:THR:HB	2.02	0.41
1:A:1176:PRO:HA	1:A:1177:PRO:HD3	1.92	0.41
1:A:225:SER:HB3	1:A:288:PRO:O	2.20	0.41
1:A:789:ASN:ND2	1:A:792:PHE:HE2	2.09	0.41
1:A:340:ALA:HB1	1:A:350:PRO:HG2	2.02	0.41
1:A:877:GLY:CA	1:A:1030:ARG:HG3	2.45	0.41
1:A:138:PHE:CZ	1:A:213:MET:CE	3.04	0.41
1:A:1169:LEU:HB2	1:A:1204:LEU:HB2	2.02	0.41
1:A:150:PRO:O	1:A:156:HIS:HB3	2.21	0.41
1:A:261:LEU:HD11	1:A:274:HIS:HB3	2.03	0.41
1:A:541:ARG:HG2	1:A:541:ARG:H	1.74	0.41
1:A:553:ARG:HG2	1:A:588:PRO:CB	2.33	0.41
1:A:138:PHE:CZ	1:A:213:MET:HE2	2.56	0.41
1:A:241:ASP:HB3	1:A:243:TYR:CZ	2.56	0.41
1:A:438:TYR:HB3	1:A:490:LEU:HD11	2.03	0.41
1:A:490:LEU:HD23	1:A:497:LEU:HB2	2.03	0.41
1:A:787:VAL:HG22	1:A:793:VAL:HG22	2.01	0.41
1:A:1001:PHE:HZ	1:A:1004:ARG:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HG22	1:A:191:GLY:H	1.86	0.40
1:A:734:GLN:O	1:A:737:GLN:HB2	2.21	0.40
1:A:836:SER:O	1:A:849:TRP:NE1	2.54	0.40
1:A:136:CYS:HB3	1:A:214:PHE:CZ	2.56	0.40
1:A:461:ASP:CB	1:A:464:ASN:HB3	2.50	0.40
1:A:778:SER:HB3	1:A:810:LEU:HD22	2.02	0.40
1:A:289:LYS:O	1:A:290:PHE:HB2	2.22	0.40
1:A:798:GLN:HG2	1:A:798:GLN:H	1.72	0.40
1:A:482:ASN:HA	1:A:483:PRO:HD3	1.98	0.40
1:A:510:VAL:HG13	1:A:511:GLU:N	2.37	0.40
1:A:520:GLU:HA	1:A:558:LEU:HD11	2.04	0.40

All (28) 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)
1:A:178:GLN:NE2	1:A:921:GLU:N[5_454]	0.50	1.70
1:A:178:GLN:OE1	1:A:921:GLU:O[5_454]	0.98	1.22
1:A:178:GLN:NE2	1:A:921:GLU:CA[5_454]	0.98	1.22
1:A:177:GLY:O	1:A:907:PRO:O[5_454]	1.54	0.66
1:A:932:ASP:O	1:A:1007:ARG:NH2[8_444]	1.55	0.65
1:A:175:PRO:CB	1:A:921:GLU:OE2[5_454]	1.61	0.59
1:A:178:GLN:CD	1:A:921:GLU:N[5_454]	1.61	0.59
1:A:178:GLN:NE2	1:A:920:CYS:C[5_454]	1.70	0.50
1:A:178:GLN:OE1	1:A:921:GLU:C[5_454]	1.72	0.48
1:A:178:GLN:CD	1:A:921:GLU:CB[5_454]	1.75	0.45
1:A:178:GLN:CB	1:A:906:SER:OG[5_454]	1.80	0.40
1:A:931:HIS:NE2	1:A:982:SER:OG[8_444]	1.84	0.36
1:A:399:GLN:CG	1:A:963:ARG:CZ[4_545]	1.87	0.33
1:A:178:GLN:CD	1:A:921:GLU:C[5_454]	1.91	0.29
1:A:399:GLN:CG	1:A:963:ARG:NH2[4_545]	1.92	0.28
1:A:178:GLN:CD	1:A:921:GLU:O[5_454]	1.94	0.26
1:A:175:PRO:CB	1:A:921:GLU:OE1[5_454]	2.03	0.17
1:A:399:GLN:CD	1:A:963:ARG:NH1[4_545]	2.04	0.16
1:A:178:GLN:NE2	1:A:921:GLU:C[5_454]	2.04	0.16
1:A:175:PRO:CB	1:A:921:GLU:CD[5_454]	2.05	0.15
1:A:177:GLY:O	1:A:907:PRO:C[5_454]	2.08	0.12
1:A:178:GLN:NE2	1:A:921:GLU:CB[5_454]	2.10	0.10
1:A:177:GLY:O	1:A:908:VAL:CA[5_454]	2.10	0.10
1:A:399:GLN:OE1	1:A:963:ARG:NH1[4_545]	2.14	0.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ASN:OD1	1:A:904:LEU:CD1[5_454]	2.16	0.04
1:A:178:GLN:CA	1:A:906:SER:O[5_454]	2.18	0.02
1:A:320:GLN:OE1	1:A:324:LYS:CE[7_555]	2.19	0.01
1:A:178:GLN:CD	1:A:906:SER:O[5_454]	2.19	0.01

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	1157/1212 (96%)	1049 (91%)	94 (8%)	14 (1%)	15 57

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	PRO
1	A	95	PRO
1	A	411	GLN
1	A	869	PRO
1	A	915	ALA
1	A	1192	SER
1	A	251	GLU
1	A	1053	PRO
1	A	1182	SER
1	A	694	LEU
1	A	966	PRO
1	A	318	PRO
1	A	1108	ASP
1	A	774	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1015/1051 (97%)	977 (96%)	38 (4%)	39 68

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	THR
1	A	78	LEU
1	A	125	LEU
1	A	128	CYS
1	A	136	CYS
1	A	152	HIS
1	A	207	ASN
1	A	257	LEU
1	A	274	HIS
1	A	280	ILE
1	A	300	CYS
1	A	352	GLU
1	A	387	LEU
1	A	413	LEU
1	A	422	THR
1	A	514	VAL
1	A	517	THR
1	A	562	VAL
1	A	585	TRP
1	A	610	ASP
1	A	634	ARG
1	A	652	VAL
1	A	693	PHE
1	A	812	GLN
1	A	814	CYS
1	A	821	ASP
1	A	837	LEU
1	A	882	ILE
1	A	929	ARG
1	A	937	VAL

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Mol	Chain	Res	Type
1	A	977	ILE
1	A	982	SER
1	A	1018	THR
1	A	1030	ARG
1	A	1033	LEU
1	A	1075	ARG
1	A	1079	ILE
1	A	1197	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	586	ASN
1	A	706	GLN
1	A	729	ASN
1	A	764	GLN
1	A	899	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 ⓘ

37 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
2	NAG	A	1301	1,2	14,14,15	0.78	0	15,19,21	1.84	3 (20%)
2	NAG	A	1302	3,2	14,14,15	0.57	0	15,19,21	1.60	1 (6%)
3	BMA	A	1303	2,4	11,11,12	0.65	0	13,15,17	0.85	0
4	MAN	A	1304	3	11,11,12	0.67	0	13,15,17	0.94	1 (7%)
2	NAG	A	1305	1,2	14,14,15	0.62	0	15,19,21	1.25	1 (6%)
2	NAG	A	1306	3,2	14,14,15	0.50	0	15,19,21	1.32	1 (6%)
3	BMA	A	1307	2,4	11,11,12	0.55	0	13,15,17	0.63	0
4	MAN	A	1308	3,4	11,11,12	0.69	0	13,15,17	0.88	1 (7%)
4	MAN	A	1309	4	11,11,12	0.59	0	13,15,17	1.30	2 (15%)
2	NAG	A	1310	1,2	14,14,15	0.65	0	15,19,21	1.29	1 (6%)
2	NAG	A	1311	3,2	14,14,15	0.54	0	15,19,21	1.27	2 (13%)
3	BMA	A	1312	2,4	11,11,12	0.88	1 (9%)	13,15,17	2.29	4 (30%)
4	MAN	A	1313	3	11,11,12	0.59	0	13,15,17	1.06	2 (15%)
2	NAG	A	1314	1,2	14,14,15	0.67	0	15,19,21	1.20	1 (6%)
2	NAG	A	1315	3,2	14,14,15	0.53	0	15,19,21	1.26	2 (13%)
3	BMA	A	1316	2,4	11,11,12	0.62	0	13,15,17	1.72	3 (23%)
4	MAN	A	1317	3	11,11,12	0.60	0	13,15,17	0.88	1 (7%)
4	MAN	A	1318	3,4	11,11,12	0.63	0	13,15,17	0.80	0
4	MAN	A	1319	4	11,11,12	0.54	0	13,15,17	1.31	1 (7%)
2	NAG	A	1320	1,2	14,14,15	0.60	0	15,19,21	1.26	1 (6%)
2	NAG	A	1321	2	14,14,15	0.52	0	15,19,21	1.10	1 (6%)
2	NAG	A	1322	1,2	14,14,15	0.62	0	15,19,21	1.06	1 (6%)
2	NAG	A	1323	3,2	14,14,15	0.66	0	15,19,21	1.17	1 (6%)
3	BMA	A	1324	2,4	11,11,12	0.43	0	13,15,17	1.83	2 (15%)
4	MAN	A	1325	3	11,11,12	0.56	0	13,15,17	0.89	1 (7%)
4	MAN	A	1326	3	11,11,12	0.53	0	13,15,17	1.45	2 (15%)
2	NAG	A	1327	1	14,14,15	0.51	0	15,19,21	1.03	1 (6%)
2	NAG	A	1328	1,2	14,14,15	0.58	0	15,19,21	1.15	1 (6%)
2	NAG	A	1329	3,2	14,14,15	0.56	0	15,19,21	1.29	2 (13%)
3	BMA	A	1330	2	11,11,12	0.49	0	13,15,17	1.24	2 (15%)
2	NAG	A	1331	1	14,14,15	0.60	0	15,19,21	1.08	1 (6%)
2	NAG	A	1332	1,2	14,14,15	0.67	0	15,19,21	1.15	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1333	3,2	14,14,15	0.53	0	15,19,21	1.59	3 (20%)
3	BMA	A	1334	2,4	11,11,12	0.40	0	13,15,17	0.77	1 (7%)
4	MAN	A	1335	3	11,11,12	0.61	0	13,15,17	1.12	2 (15%)
4	MAN	A	1336	3,4	11,11,12	0.63	0	13,15,17	0.89	0
4	MAN	A	1337	4	11,11,12	0.63	0	13,15,17	1.21	1 (7%)

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
2	NAG	A	1301	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1302	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1303	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1304	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1305	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1306	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1307	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1308	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1309	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1310	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1311	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1312	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1313	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1314	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1315	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1316	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1317	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1318	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1319	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1320	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1321	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1322	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1323	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1324	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1325	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1326	3	-	0/2/19/22	1/1/1/1
2	NAG	A	1327	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1328	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1329	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1330	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1331	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1332	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1333	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1334	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1335	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1336	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1337	4	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1312	BMA	C2-C3	2.37	1.55	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1333	NAG	O5-C1-C2	-2.93	107.39	111.47
2	A	1329	NAG	O5-C1-C2	-2.70	107.71	111.47
2	A	1315	NAG	O5-C1-C2	-2.46	108.05	111.47
3	A	1334	BMA	C1-O5-C5	2.06	115.00	112.17
4	A	1313	MAN	C1-C2-C3	2.10	112.31	109.65
2	A	1301	NAG	C2-N2-C7	2.12	126.03	122.94
3	A	1312	BMA	C1-O5-C5	2.12	115.08	112.17
4	A	1317	MAN	C1-O5-C5	2.18	115.18	112.17
4	A	1335	MAN	C1-O5-C5	2.23	115.24	112.17
4	A	1313	MAN	C1-O5-C5	2.24	115.25	112.17
2	A	1327	NAG	C4-C3-C2	2.24	114.31	111.02
3	A	1312	BMA	O5-C1-C2	2.26	114.34	110.79
2	A	1315	NAG	C3-C4-C5	2.27	114.22	110.22
3	A	1312	BMA	C2-C3-C4	2.32	114.92	110.88
2	A	1332	NAG	C4-C3-C2	2.33	114.43	111.02
4	A	1326	MAN	C1-C2-C3	2.41	112.70	109.65
4	A	1308	MAN	C1-C2-C3	2.49	112.81	109.65
4	A	1304	MAN	C1-C2-C3	2.51	112.83	109.65
3	A	1330	BMA	C1-C2-C3	2.53	112.86	109.65
4	A	1325	MAN	C1-O5-C5	2.54	115.67	112.17
2	A	1311	NAG	C4-C3-C2	2.67	114.93	111.02
4	A	1335	MAN	C1-C2-C3	2.80	113.21	109.65
4	A	1309	MAN	C1-C2-C3	2.82	113.23	109.65
2	A	1305	NAG	C4-C3-C2	2.85	115.19	111.02
2	A	1311	NAG	C1-O5-C5	2.91	116.18	112.17
3	A	1316	BMA	C2-C3-C4	2.98	116.08	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1333	NAG	C3-C4-C5	2.98	115.48	110.22
2	A	1322	NAG	C4-C3-C2	2.99	115.40	111.02
2	A	1329	NAG	C4-C3-C2	2.99	115.41	111.02
2	A	1333	NAG	C4-C3-C2	3.05	115.48	111.02
2	A	1323	NAG	C4-C3-C2	3.07	115.52	111.02
3	A	1316	BMA	C1-C2-C3	3.07	113.55	109.65
2	A	1301	NAG	C3-C4-C5	3.10	115.68	110.22
3	A	1330	BMA	C1-O5-C5	3.16	116.52	112.17
2	A	1331	NAG	C1-O5-C5	3.27	116.67	112.17
2	A	1320	NAG	C4-C3-C2	3.27	115.82	111.02
2	A	1328	NAG	C4-C3-C2	3.29	115.84	111.02
4	A	1337	MAN	C1-C2-C3	3.35	113.90	109.65
4	A	1309	MAN	C1-O5-C5	3.41	116.86	112.17
2	A	1321	NAG	C1-O5-C5	3.62	117.16	112.17
3	A	1324	BMA	C1-C2-C3	3.69	114.33	109.65
3	A	1316	BMA	C3-C4-C5	3.78	116.88	110.22
2	A	1306	NAG	C1-O5-C5	3.97	117.64	112.17
2	A	1314	NAG	C4-C3-C2	4.00	116.88	111.02
2	A	1310	NAG	C4-C3-C2	4.08	117.00	111.02
4	A	1319	MAN	C1-O5-C5	4.12	117.84	112.17
4	A	1326	MAN	C1-O5-C5	4.42	118.25	112.17
3	A	1324	BMA	C1-O5-C5	4.50	118.36	112.17
2	A	1302	NAG	C4-C3-C2	4.90	118.20	111.02
2	A	1301	NAG	C4-C3-C2	5.16	118.58	111.02
3	A	1312	BMA	C1-C2-C3	7.06	118.60	109.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1332	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1326	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1314	NAG	22	0
2	A	1315	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	8

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1147:ASP	C	1148:PRO	N	4.89
1	A	658:ASN	C	659:CYS	N	2.39
1	A	806:LYS	C	807:CYS	N	2.25
1	A	510:VAL	C	511:GLU	N	1.99
1	A	561:CYS	C	562:VAL	N	1.83
1	A	704:CYS	C	705:PRO	N	1.68
1	A	1043:THR	C	1044:GLU	N	1.66
1	A	859:CYS	C	860:THR	N	1.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1171/1212 (96%)	7.82	992 (84%) 0 2	235, 263, 432, 432	0

All (992) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1218	THR	54.7
1	A	1062	THR	52.4
1	A	1104	ALA	45.8
1	A	1221	ALA	38.1
1	A	1105	PRO	37.1
1	A	1173	ASN	36.2
1	A	1102	CYS	35.4
1	A	1060	GLY	33.5
1	A	1061	GLY	32.5
1	A	1188	VAL	31.6
1	A	1052	ASP	31.5
1	A	1077	PRO	31.4
1	A	1090	ASN	30.9
1	A	1186	TYR	30.8
1	A	1220	ARG	30.4
1	A	1219	VAL	29.5
1	A	1064	LEU	29.0
1	A	1187	THR	28.7
1	A	1053	PRO	27.8
1	A	1175	LEU	27.6
1	A	1148	PRO	27.2
1	A	1222	GLY	27.2
1	A	1225	GLU	27.0
1	A	1151	GLU	26.9
1	A	1092	CYS	26.7
1	A	1184	LEU	26.7
1	A	1046	PRO	26.6

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Mol	Chain	Res	Type	RSRZ
1	A	1150	LEU	26.2
1	A	1174	LEU	25.6
1	A	1070	ASN	25.6
1	A	1199	VAL	25.6
1	A	1183	ARG	25.5
1	A	1134	LEU	25.3
1	A	1106	SER	25.3
1	A	1182	SER	25.0
1	A	1050	ARG	24.8
1	A	1065	THR	24.2
1	A	1224	PHE	24.1
1	A	1185	ASN	24.1
1	A	1067	THR	24.1
1	A	1055	TRP	23.9
1	A	1136	VAL	23.6
1	A	1178	ALA	23.5
1	A	1179	PRO	23.3
1	A	1059	SER	23.2
1	A	1176	PRO	23.0
1	A	1056	SER	22.8
1	A	1189	LEU	22.5
1	A	1125	GLY	22.3
1	A	1066	VAL	22.2
1	A	1195	CYS	22.0
1	A	1200	SER	21.8
1	A	1172	ARG	21.7
1	A	1168	ILE	21.7
1	A	1201	GLU	21.5
1	A	1063	LEU	21.4
1	A	1124	ILE	21.4
1	A	1210	ASN	21.3
1	A	1103	ARG	21.3
1	A	1128	MET	21.2
1	A	148	GLY	21.0
1	A	1054	GLU	21.0
1	A	1149	VAL	20.9
1	A	1073	THR	20.8
1	A	150	PRO	20.6
1	A	1116	GLU	20.4
1	A	1147	ASP	20.4
1	A	1227	SER	20.4
1	A	1208	ALA	20.3

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Mol	Chain	Res	Type	RSRZ
1	A	1171	GLY	20.3
1	A	1209	PRO	20.2
1	A	1152	PRO	20.1
1	A	1129	ASP	20.0
1	A	1197	LEU	19.7
1	A	1194	PRO	19.7
1	A	1091	SER	19.7
1	A	240	PHE	19.5
1	A	1047	THR	19.2
1	A	1226	PHE	18.7
1	A	241	ASP	18.7
1	A	1223	GLY	18.6
1	A	1078	ARG	18.5
1	A	1071	LEU	18.5
1	A	555	ALA	18.4
1	A	1135	LEU	18.4
1	A	1048	ILE	18.3
1	A	1074	VAL	18.3
1	A	1177	PRO	18.1
1	A	1051	ILE	18.0
1	A	1207	GLU	18.0
1	A	1217	VAL	17.9
1	A	1126	PHE	17.8
1	A	160	SER	17.8
1	A	1192	SER	17.8
1	A	859	CYS	17.7
1	A	1140	SER	17.6
1	A	1198	THR	17.6
1	A	1193	THR	17.4
1	A	1170	LYS	17.4
1	A	1131	VAL	17.2
1	A	1133	THR	17.2
1	A	1190	ILE	17.2
1	A	1138	ASN	17.2
1	A	1204	LEU	17.0
1	A	1123	GLU	16.9
1	A	1164	SER	16.9
1	A	1057	ILE	16.9
1	A	597	SER	16.9
1	A	1081	ALA	16.9
1	A	414	GLY	16.8
1	A	1127	ILE	16.8

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Mol	Chain	Res	Type	RSRZ
1	A	383	LEU	16.7
1	A	260	GLN	16.7
1	A	48	GLY	16.6
1	A	650	ALA	16.6
1	A	1202	THR	16.5
1	A	1089	GLU	16.5
1	A	1146	PRO	16.4
1	A	1072	ALA	16.4
1	A	1191	GLY	16.4
1	A	311	GLN	16.3
1	A	1203	GLN	16.3
1	A	1079	ILE	16.3
1	A	596	CYS	16.2
1	A	535	LEU	16.2
1	A	1141	SER	16.1
1	A	1080	ARG	16.1
1	A	699	ASN	16.0
1	A	675	CYS	15.8
1	A	131	ALA	15.8
1	A	658	ASN	15.7
1	A	1076	GLU	15.7
1	A	1169	LEU	15.6
1	A	1096	ASN	15.6
1	A	1097	ASP	15.5
1	A	1100	MET	15.4
1	A	382	SER	15.4
1	A	1180	GLY	15.2
1	A	732	GLN	15.2
1	A	673	PHE	15.2
1	A	399	GLN	15.2
1	A	1181	ASN	15.1
1	A	657	TYR	15.1
1	A	1121	PRO	15.0
1	A	1137	LEU	15.0
1	A	655	VAL	15.0
1	A	190	ASP	15.0
1	A	698	VAL	15.0
1	A	966	PRO	15.0
1	A	91	GLU	14.9
1	A	795	ASP	14.9
1	A	1132	ARG	14.6
1	A	1139	SER	14.5

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Mol	Chain	Res	Type	RSRZ
1	A	680	TYR	14.4
1	A	1069	THR	14.4
1	A	385	TRP	14.4
1	A	1166	PRO	14.3
1	A	1206	CYS	14.3
1	A	162	ARG	14.3
1	A	969	GLY	14.2
1	A	968	ARG	14.2
1	A	1068	GLY	14.2
1	A	641	LYS	14.1
1	A	604	THR	14.1
1	A	1167	LEU	14.1
1	A	814	CYS	14.1
1	A	531	GLY	14.0
1	A	136	CYS	14.0
1	A	662	HIS	14.0
1	A	1049	LEU	14.0
1	A	157	TYR	13.9
1	A	1142	PHE	13.9
1	A	1122	ASP	13.8
1	A	1144	TYR	13.8
1	A	648	LYS	13.8
1	A	263	THR	13.8
1	A	570	ASN	13.8
1	A	1094	VAL	13.8
1	A	645	THR	13.7
1	A	1045	ASP	13.7
1	A	595	ASN	13.6
1	A	96	PRO	13.6
1	A	634	ARG	13.5
1	A	659	CYS	13.5
1	A	602	THR	13.5
1	A	295	GLU	13.5
1	A	1165	SER	13.4
1	A	731	PRO	13.4
1	A	1196	ILE	13.4
1	A	159	SER	13.4
1	A	1101	VAL	13.3
1	A	98	SER	13.3
1	A	536	HIS	13.2
1	A	1205	LEU	13.2
1	A	487	ASP	13.2

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Mol	Chain	Res	Type	RSRZ
1	A	401	ASP	13.2
1	A	886	ASN	13.1
1	A	137	GLN	13.1
1	A	665	CYS	13.1
1	A	1058	ASN	13.0
1	A	1130	ASN	13.0
1	A	161	VAL	13.0
1	A	149	GLU	12.9
1	A	649	PHE	12.9
1	A	639	TYR	12.8
1	A	276	PHE	12.7
1	A	1145	TYR	12.6
1	A	99	VAL	12.5
1	A	1040	TYR	12.5
1	A	500	MET	12.4
1	A	188	PRO	12.3
1	A	532	TRP	12.3
1	A	534	VAL	12.3
1	A	415	GLY	12.2
1	A	603	GLU	12.1
1	A	499	ALA	12.0
1	A	97	PRO	12.0
1	A	197	PRO	11.9
1	A	402	ASP	11.9
1	A	965	SER	11.9
1	A	189	ILE	11.9
1	A	554	PHE	11.8
1	A	677	TRP	11.8
1	A	1107	ILE	11.8
1	A	1098	THR	11.8
1	A	733	PRO	11.8
1	A	967	SER	11.7
1	A	277	THR	11.7
1	A	571	VAL	11.7
1	A	1216	LYS	11.7
1	A	572	SER	11.7
1	A	152	HIS	11.7
1	A	94	TYR	11.6
1	A	533	CYS	11.6
1	A	146	LYS	11.6
1	A	384	PRO	11.6
1	A	656	PHE	11.6

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Mol	Chain	Res	Type	RSRZ
1	A	826	CYS	11.6
1	A	1044	GLU	11.6
1	A	196	PHE	11.6
1	A	599	GLU	11.5
1	A	133	GLN	11.5
1	A	573	VAL	11.5
1	A	400	ILE	11.5
1	A	1120	ARG	11.5
1	A	346	ARG	11.4
1	A	970	PRO	11.4
1	A	82	HIS	11.4
1	A	964	VAL	11.4
1	A	50	THR	11.3
1	A	813	SER	11.3
1	A	963	ARG	11.2
1	A	433	THR	11.2
1	A	537	SER	11.2
1	A	766	GLN	11.2
1	A	449	GLY	11.2
1	A	477	VAL	11.2
1	A	835	CYS	11.1
1	A	448	ALA	11.1
1	A	654	PHE	11.1
1	A	568	PRO	11.1
1	A	245	VAL	11.1
1	A	529	HIS	11.0
1	A	151	HIS	11.0
1	A	642	SER	11.0
1	A	1143	LEU	11.0
1	A	556	SER	11.0
1	A	506	THR	11.0
1	A	395	ASN	10.9
1	A	413	LEU	10.9
1	A	434	ALA	10.9
1	A	1082	LYS	10.9
1	A	49	LEU	10.8
1	A	390	GLU	10.8
1	A	138	PHE	10.8
1	A	828	TRP	10.8
1	A	191	GLY	10.8
1	A	498	TYR	10.8
1	A	381	LEU	10.8

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Mol	Chain	Res	Type	RSRZ
1	A	669	VAL	10.7
1	A	1117	LEU	10.7
1	A	651	SER	10.7
1	A	940	ARG	10.6
1	A	679	LYS	10.6
1	A	674	PRO	10.5
1	A	682	HIS	10.5
1	A	705	PRO	10.5
1	A	545	CYS	10.5
1	A	807	CYS	10.4
1	A	588	PRO	10.4
1	A	644	GLU	10.4
1	A	851	HIS	10.4
1	A	975	THR	10.3
1	A	756	LEU	10.3
1	A	229	ILE	10.3
1	A	261	LEU	10.2
1	A	640	LEU	10.2
1	A	163	GLU	10.2
1	A	606	SER	10.2
1	A	594	VAL	10.2
1	A	726	ALA	10.2
1	A	811	ARG	10.2
1	A	1119	GLU	10.2
1	A	128	CYS	10.1
1	A	114	LYS	10.1
1	A	858	ARG	10.1
1	A	598	PHE	10.1
1	A	501	THR	10.1
1	A	1084	GLY	10.1
1	A	432	LEU	10.0
1	A	486	ARG	10.0
1	A	510	VAL	10.0
1	A	676	HIS	10.0
1	A	1095	TYR	10.0
1	A	343	GLN	10.0
1	A	228	LYS	10.0
1	A	818	LEU	10.0
1	A	405	CYS	10.0
1	A	1153	LEU	9.9
1	A	1043	THR	9.9
1	A	488	LEU	9.9

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Mol	Chain	Res	Type	RSRZ
1	A	129	GLY	9.9
1	A	638	LEU	9.9
1	A	1118	GLY	9.9
1	A	815	GLY	9.8
1	A	310	VAL	9.8
1	A	740	TYR	9.8
1	A	668	CYS	9.8
1	A	51	HIS	9.8
1	A	716	PRO	9.7
1	A	1083	TYR	9.7
1	A	1115	PRO	9.7
1	A	52	LEU	9.7
1	A	403	ASP	9.7
1	A	242	ILE	9.7
1	A	164	ALA	9.7
1	A	605	GLU	9.6
1	A	633	GLN	9.6
1	A	653	ASP	9.6
1	A	755	ALA	9.5
1	A	977	ILE	9.5
1	A	1088	ARG	9.5
1	A	132	SER	9.5
1	A	192	LYS	9.4
1	A	672	SER	9.4
1	A	259	LEU	9.4
1	A	717	VAL	9.4
1	A	89	ASP	9.4
1	A	312	ASP	9.3
1	A	593	GLY	9.3
1	A	527	ASP	9.3
1	A	435	VAL	9.3
1	A	707	ILE	9.3
1	A	652	VAL	9.3
1	A	850	MET	9.3
1	A	647	LYS	9.3
1	A	90	ASN	9.2
1	A	135	ILE	9.2
1	A	857	SER	9.2
1	A	116	LEU	9.2
1	A	130	SER	9.1
1	A	158	LEU	9.1
1	A	939	VAL	9.1

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Mol	Chain	Res	Type	RSRZ
1	A	962	TYR	9.1
1	A	788	TRP	9.1
1	A	860	THR	9.1
1	A	540	SER	9.1
1	A	127	ALA	9.0
1	A	734	GLN	9.0
1	A	805	TYR	9.0
1	A	767	ASN	9.0
1	A	39	PHE	9.0
1	A	404	PHE	9.0
1	A	476	VAL	8.9
1	A	706	GLN	8.9
1	A	757	ARG	8.9
1	A	511	GLU	8.9
1	A	436	ALA	8.9
1	A	95	PRO	8.9
1	A	546	GLU	8.9
1	A	165	GLY	8.9
1	A	862	PRO	8.9
1	A	113	ASN	8.8
1	A	243	TYR	8.8
1	A	456	ARG	8.8
1	A	737	GLN	8.8
1	A	794	ILE	8.8
1	A	410	ASN	8.8
1	A	817	CYS	8.8
1	A	515	GLN	8.8
1	A	636	VAL	8.8
1	A	100	GLN	8.7
1	A	684	CYS	8.7
1	A	663	GLN	8.7
1	A	764	GLN	8.7
1	A	553	ARG	8.7
1	A	1093	MET	8.7
1	A	632	ASP	8.7
1	A	1041	ASN	8.7
1	A	70	TYR	8.7
1	A	475	SER	8.6
1	A	338	VAL	8.6
1	A	1099	THR	8.6
1	A	528	PRO	8.6
1	A	574	THR	8.6

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Mol	Chain	Res	Type	RSRZ
1	A	1114	PRO	8.6
1	A	214	PHE	8.6
1	A	660	SER	8.6
1	A	512	SER	8.5
1	A	770	TYR	8.5
1	A	796	ASN	8.5
1	A	147	LEU	8.5
1	A	115	LEU	8.4
1	A	397	PRO	8.4
1	A	1087	GLU	8.4
1	A	600	ASP	8.4
1	A	888	GLY	8.4
1	A	678	CYS	8.4
1	A	806	LYS	8.3
1	A	509	PRO	8.3
1	A	262	ASP	8.3
1	A	239	ALA	8.3
1	A	765	CYS	8.3
1	A	566	VAL	8.3
1	A	258	THR	8.3
1	A	69	ILE	8.3
1	A	398	LEU	8.3
1	A	785	SER	8.3
1	A	489	VAL	8.2
1	A	117	LEU	8.2
1	A	832	GLU	8.2
1	A	646	GLY	8.2
1	A	643	LYS	8.2
1	A	808	PRO	8.1
1	A	889	LEU	8.1
1	A	396	SER	8.1
1	A	587	VAL	8.1
1	A	541	ARG	8.1
1	A	686	ASN	8.1
1	A	929	ARG	8.1
1	A	615	CYS	8.1
1	A	64	GLY	8.1
1	A	156	HIS	8.1
1	A	386	LEU	8.1
1	A	392	GLY	8.1
1	A	166	SER	8.0
1	A	101	SER	8.0

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Mol	Chain	Res	Type	RSRZ
1	A	812	GLN	8.0
1	A	938	CYS	8.0
1	A	179	GLY	7.9
1	A	601	PHE	7.9
1	A	834	ARG	7.9
1	A	836	SER	7.9
1	A	530	CYS	7.9
1	A	111	ASN	7.9
1	A	484	ILE	7.9
1	A	617	SER	7.8
1	A	92	LYS	7.8
1	A	110	ASP	7.8
1	A	721	LYS	7.8
1	A	670	ASN	7.8
1	A	412	PRO	7.8
1	A	1075	ARG	7.7
1	A	502	GLU	7.7
1	A	63	VAL	7.7
1	A	661	VAL	7.7
1	A	1085	GLY	7.7
1	A	825	GLU	7.7
1	A	849	TRP	7.7
1	A	786	VAL	7.7
1	A	193	SER	7.7
1	A	793	VAL	7.6
1	A	580	LEU	7.6
1	A	664	SER	7.6
1	A	508	VAL	7.6
1	A	738	ARG	7.6
1	A	286	ASN	7.6
1	A	353	SER	7.6
1	A	264	GLN	7.6
1	A	68	ARG	7.6
1	A	38	ALA	7.6
1	A	485	LEU	7.6
1	A	81	ALA	7.5
1	A	708	LEU	7.5
1	A	562	VAL	7.5
1	A	739	GLY	7.5
1	A	278	SER	7.5
1	A	447	PHE	7.5
1	A	715	VAL	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	768	SER	7.4
1	A	126	LEU	7.4
1	A	507	GLN	7.4
1	A	497	LEU	7.3
1	A	727	ALA	7.3
1	A	337	THR	7.3
1	A	722	PRO	7.3
1	A	887	LEU	7.3
1	A	104	HIS	7.3
1	A	569	ARG	7.3
1	A	84	THR	7.3
1	A	931	HIS	7.3
1	A	978	GLY	7.3
1	A	391	LEU	7.3
1	A	895	ARG	7.2
1	A	724	THR	7.2
1	A	763	LEU	7.2
1	A	519	CYS	7.2
1	A	582	LEU	7.2
1	A	134	GLY	7.2
1	A	575	MET	7.2
1	A	387	LEU	7.1
1	A	618	PRO	7.1
1	A	47	TRP	7.1
1	A	282	ARG	7.1
1	A	627	THR	7.1
1	A	827	GLY	7.1
1	A	829	CYS	7.0
1	A	974	GLY	7.0
1	A	388	ASN	7.0
1	A	1113	SER	7.0
1	A	930	ALA	6.9
1	A	616	HIS	6.9
1	A	296	PHE	6.9
1	A	538	ILE	6.9
1	A	552	GLN	6.9
1	A	195	TYR	6.9
1	A	704	CYS	6.9
1	A	714	TYR	6.9
1	A	564	LEU	6.9
1	A	238	PRO	6.8
1	A	380	LYS	6.8

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Mol	Chain	Res	Type	RSRZ
1	A	457	LYS	6.8
1	A	667	ALA	6.8
1	A	187	THR	6.8
1	A	93	CYS	6.8
1	A	102	CYS	6.8
1	A	125	LEU	6.8
1	A	581	VAL	6.8
1	A	696	GLY	6.8
1	A	490	LEU	6.8
1	A	614	HIS	6.7
1	A	803	HIS	6.7
1	A	852	ALA	6.7
1	A	406	GLY	6.7
1	A	139	LEU	6.7
1	A	53	VAL	6.7
1	A	725	LEU	6.7
1	A	723	ILE	6.7
1	A	539	CYS	6.7
1	A	112	VAL	6.7
1	A	893	ASP	6.7
1	A	885	GLU	6.6
1	A	681	ARG	6.6
1	A	293	TYR	6.6
1	A	309	LEU	6.6
1	A	586	ASN	6.6
1	A	861	ASP	6.6
1	A	838	ARG	6.6
1	A	208	GLU	6.6
1	A	455	ILE	6.5
1	A	523	LEU	6.5
1	A	719	VAL	6.5
1	A	416	THR	6.5
1	A	378	GLU	6.5
1	A	167	MET	6.5
1	A	198	THR	6.5
1	A	976	TRP	6.5
1	A	516	TYR	6.5
1	A	840	HIS	6.5
1	A	1108	ASP	6.5
1	A	1022	ALA	6.4
1	A	683	VAL	6.4
1	A	454	ARG	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	613	ILE	6.4
1	A	623	VAL	6.4
1	A	313	ALA	6.3
1	A	787	VAL	6.3
1	A	567	GLN	6.3
1	A	118	LEU	6.3
1	A	376	ARG	6.3
1	A	184	PHE	6.3
1	A	336	PHE	6.3
1	A	237	PHE	6.2
1	A	980	GLU	6.2
1	A	294	VAL	6.2
1	A	155	GLU	6.2
1	A	83	VAL	6.2
1	A	626	ILE	6.2
1	A	379	GLY	6.2
1	A	839	HIS	6.2
1	A	800	ILE	6.2
1	A	389	LYS	6.2
1	A	584	ALA	6.2
1	A	590	LEU	6.2
1	A	504	GLN	6.2
1	A	548	ALA	6.1
1	A	611	GLY	6.1
1	A	622	GLU	6.1
1	A	631	GLY	6.1
1	A	285	VAL	6.1
1	A	972	SER	6.1
1	A	579	PRO	6.1
1	A	752	ARG	6.1
1	A	791	ASN	6.0
1	A	671	GLY	6.0
1	A	729	ASN	6.0
1	A	244	TYR	6.0
1	A	153	ARG	6.0
1	A	354	ALA	6.0
1	A	804	LEU	6.0
1	A	697	ARG	6.0
1	A	236	LYS	6.0
1	A	685	THR	6.0
1	A	896	LEU	5.9
1	A	718	GLY	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	789	ASN	5.9
1	A	837	LEU	5.9
1	A	589	ASP	5.9
1	A	503	LYS	5.9
1	A	505	VAL	5.8
1	A	897	GLY	5.8
1	A	542	GLN	5.8
1	A	637	LYS	5.8
1	A	154	LYS	5.8
1	A	713	ILE	5.8
1	A	375	TYR	5.8
1	A	281	VAL	5.8
1	A	425	PHE	5.8
1	A	576	SER	5.8
1	A	265	LEU	5.7
1	A	560	GLN	5.7
1	A	1013	THR	5.7
1	A	932	ASP	5.7
1	A	730	LEU	5.7
1	A	274	HIS	5.7
1	A	819	LYS	5.7
1	A	144	LEU	5.7
1	A	230	PRO	5.7
1	A	426	VAL	5.7
1	A	275	PHE	5.7
1	A	802	ALA	5.7
1	A	66	VAL	5.6
1	A	257	LEU	5.6
1	A	987	GLY	5.6
1	A	771	SER	5.6
1	A	513	CYS	5.6
1	A	65	ALA	5.6
1	A	227	LEU	5.6
1	A	226	GLN	5.6
1	A	792	PHE	5.5
1	A	973	GLY	5.5
1	A	956	PHE	5.5
1	A	635	VAL	5.5
1	A	279	LYS	5.5
1	A	1021	SER	5.5
1	A	394	ILE	5.5
1	A	742	CYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	820	ALA	5.5
1	A	446	VAL	5.5
1	A	809	ALA	5.4
1	A	844	ASP	5.4
1	A	692	ALA	5.4
1	A	782	VAL	5.4
1	A	202	ARG	5.4
1	A	271	ALA	5.4
1	A	693	PHE	5.4
1	A	744	PHE	5.3
1	A	62	TYR	5.3
1	A	1039	LYS	5.3
1	A	583	GLN	5.3
1	A	280	ILE	5.3
1	A	784	LEU	5.3
1	A	1042	TYR	5.3
1	A	701	SER	5.3
1	A	344	LYS	5.2
1	A	251	GLU	5.2
1	A	741	GLU	5.2
1	A	514	VAL	5.2
1	A	180	GLN	5.2
1	A	898	VAL	5.2
1	A	42	PHE	5.2
1	A	979	ILE	5.1
1	A	743	LEU	5.1
1	A	54	VAL	5.1
1	A	816	LEU	5.1
1	A	561	CYS	5.1
1	A	67	ASN	5.1
1	A	753	VAL	5.1
1	A	863	LYS	5.1
1	A	74	GLY	5.0
1	A	256	TYR	5.0
1	A	621	ARG	5.0
1	A	393	CYS	5.0
1	A	246	TYR	5.0
1	A	124	ARG	5.0
1	A	608	LEU	4.9
1	A	185	VAL	4.9
1	A	894	VAL	4.9
1	A	666	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	833	ARG	4.9
1	A	252	GLN	4.9
1	A	284	CYS	4.9
1	A	709	PRO	4.9
1	A	754	THR	4.9
1	A	411	GLN	4.9
1	A	612	ARG	4.9
1	A	1086	ILE	4.9
1	A	349	PRO	4.9
1	A	578	VAL	4.8
1	A	522	CYS	4.8
1	A	483	PRO	4.8
1	A	355	LEU	4.8
1	A	630	GLN	4.8
1	A	824	PHE	4.8
1	A	86	PRO	4.8
1	A	550	GLU	4.8
1	A	200	SER	4.7
1	A	37	PRO	4.7
1	A	735	SER	4.7
1	A	577	GLN	4.7
1	A	900	VAL	4.7
1	A	758	PHE	4.7
1	A	695	GLU	4.7
1	A	986	ALA	4.7
1	A	563	GLN	4.6
1	A	772	TYR	4.6
1	A	797	PRO	4.6
1	A	478	ALA	4.6
1	A	80	ARG	4.6
1	A	1038	VAL	4.6
1	A	109	THR	4.6
1	A	841	CYS	4.6
1	A	720	VAL	4.6
1	A	145	PHE	4.5
1	A	254	VAL	4.5
1	A	547	ARG	4.5
1	A	199	LEU	4.5
1	A	830	VAL	4.5
1	A	427	ASP	4.5
1	A	40	ARG	4.5
1	A	372	GLN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	525	SER	4.5
1	A	517	THR	4.4
1	A	1112	ARG	4.4
1	A	339	PHE	4.4
1	A	607	ILE	4.4
1	A	44	ALA	4.4
1	A	981	GLY	4.4
1	A	610	ASP	4.4
1	A	890	ARG	4.4
1	A	769	SER	4.3
1	A	801	GLN	4.3
1	A	843	ALA	4.3
1	A	728	ARG	4.3
1	A	364	LYS	4.3
1	A	371	ILE	4.3
1	A	350	PRO	4.3
1	A	419	ILE	4.3
1	A	298	ILE	4.3
1	A	848	SER	4.3
1	A	450	THR	4.3
1	A	352	GLU	4.3
1	A	194	GLU	4.3
1	A	831	ALA	4.2
1	A	233	THR	4.2
1	A	941	ASP	4.2
1	A	907	PRO	4.2
1	A	41	THR	4.2
1	A	937	VAL	4.2
1	A	496	TYR	4.2
1	A	609	GLU	4.2
1	A	168	ALA	4.2
1	A	549	GLU	4.2
1	A	103	PRO	4.2
1	A	106	LEU	4.2
1	A	283	LEU	4.2
1	A	473	TYR	4.2
1	A	565	THR	4.1
1	A	783	ASN	4.1
1	A	1011	CYS	4.1
1	A	347	VAL	4.1
1	A	87	VAL	4.1
1	A	217	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	751	ALA	4.1
1	A	625	PRO	4.1
1	A	948	ALA	4.1
1	A	551	PRO	4.1
1	A	745	HIS	4.1
1	A	779	ASP	4.1
1	A	990	VAL	4.1
1	A	288	PRO	4.1
1	A	292	SER	4.0
1	A	781	PRO	4.0
1	A	43	VAL	4.0
1	A	453	GLY	4.0
1	A	780	LEU	4.0
1	A	424	LEU	4.0
1	A	203	ARG	4.0
1	A	592	ALA	4.0
1	A	377	GLY	4.0
1	A	903	VAL	4.0
1	A	431	GLY	3.9
1	A	458	ILE	3.9
1	A	842	PRO	3.9
1	A	459	LEU	3.9
1	A	216	PHE	3.9
1	A	482	ASN	3.9
1	A	171	LEU	3.9
1	A	341	GLN	3.9
1	A	345	ASN	3.8
1	A	474	GLU	3.8
1	A	982	SER	3.8
1	A	946	TYR	3.8
1	A	1009	ILE	3.8
1	A	297	PRO	3.8
1	A	342	GLY	3.8
1	A	1024	ILE	3.8
1	A	872	GLY	3.8
1	A	619	SER	3.7
1	A	209	GLU	3.7
1	A	367	ILE	3.7
1	A	762	SER	3.7
1	A	170	VAL	3.7
1	A	445	VAL	3.7
1	A	219	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	105	GLY	3.7
1	A	61	VAL	3.7
1	A	370	ARG	3.7
1	A	423	PRO	3.7
1	A	544	ALA	3.7
1	A	85	GLY	3.6
1	A	169	GLY	3.6
1	A	620	ALA	3.6
1	A	1020	GLY	3.6
1	A	790	GLY	3.6
1	A	856	SER	3.6
1	A	451	ARG	3.6
1	A	250	SER	3.6
1	A	961	PHE	3.6
1	A	211	ALA	3.5
1	A	585	TRP	3.5
1	A	992	VAL	3.5
1	A	891	PHE	3.5
1	A	437	ALA	3.5
1	A	201	SER	3.5
1	A	736	GLY	3.5
1	A	624	ALA	3.5
1	A	314	TYR	3.5
1	A	954	PHE	3.5
1	A	374	CYS	3.5
1	A	878	THR	3.5
1	A	460	VAL	3.5
1	A	798	GLN	3.4
1	A	186	GLY	3.4
1	A	255	TYR	3.4
1	A	879	ARG	3.4
1	A	290	PHE	3.4
1	A	904	LEU	3.4
1	A	557	ASP	3.4
1	A	308	ARG	3.4
1	A	440	TYR	3.4
1	A	175	PRO	3.4
1	A	469	PRO	3.4
1	A	778	SER	3.4
1	A	76	LEU	3.4
1	A	971	LEU	3.4
1	A	591	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	933	ALA	3.3
1	A	71	LYS	3.3
1	A	855	GLY	3.3
1	A	918	ILE	3.3
1	A	1008	GLU	3.3
1	A	892	GLU	3.3
1	A	183	LEU	3.3
1	A	936	GLU	3.3
1	A	1109	ASN	3.3
1	A	335	LEU	3.2
1	A	273	GLU	3.2
1	A	518	SER	3.2
1	A	935	VAL	3.2
1	A	438	TYR	3.2
1	A	249	ARG	3.2
1	A	368	LYS	3.2
1	A	340	ALA	3.2
1	A	348	LYS	3.2
1	A	88	GLU	3.2
1	A	922	ILE	3.1
1	A	141	LEU	3.1
1	A	234	LEU	3.1
1	A	1007	ARG	3.1
1	A	178	GLN	3.1
1	A	628	GLN	3.1
1	A	176	PRO	3.1
1	A	526	ARG	3.1
1	A	845	SER	3.1
1	A	417	VAL	3.0
1	A	905	CYS	3.0
1	A	873	PRO	3.0
1	A	289	LYS	3.0
1	A	902	LYS	3.0
1	A	687	ASN	3.0
1	A	700	MET	3.0
1	A	333	GLU	2.9
1	A	928	LEU	2.9
1	A	177	GLY	2.9
1	A	864	ILE	2.9
1	A	1023	PRO	2.9
1	A	213	MET	2.8
1	A	871	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1004	ARG	2.8
1	A	712	HIS	2.8
1	A	799	ASN	2.8
1	A	906	SER	2.8
1	A	315	LEU	2.8
1	A	1019	PRO	2.8
1	A	495	GLN	2.8
1	A	441	GLN	2.7
1	A	461	ASP	2.7
1	A	960	THR	2.7
1	A	846	PRO	2.7
1	A	212	ASP	2.7
1	A	215	GLY	2.7
1	A	688	ALA	2.7
1	A	248	PHE	2.7
1	A	232	ASP	2.7
1	A	810	LEU	2.7
1	A	847	ALA	2.7
1	A	75	ASN	2.7
1	A	691	CYS	2.7
1	A	899	HIS	2.7
1	A	923	GLY	2.6
1	A	72	LEU	2.6
1	A	140	ARG	2.6
1	A	182	LYS	2.6
1	A	959	PRO	2.6
1	A	543	ASP	2.6
1	A	119	ASP	2.6
1	A	1012	LEU	2.6
1	A	882	ILE	2.6
1	A	880	LEU	2.6
1	A	999	CYS	2.6
1	A	351	LYS	2.5
1	A	1014	PRO	2.5
1	A	468	ARG	2.5
1	A	1010	ARG	2.5
1	A	994	ILE	2.5
1	A	430	ASP	2.5
1	A	428	LYS	2.5
1	A	464	ASN	2.4
1	A	1028	ILE	2.4
1	A	218	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	853	HIS	2.4
1	A	703	ASP	2.4
1	A	1015	PRO	2.4
1	A	467	GLY	2.4
1	A	750	PRO	2.4
1	A	302	GLN	2.4
1	A	983	HIS	2.4
1	A	471	LEU	2.4
1	A	143	ASP	2.4
1	A	867	LEU	2.4
1	A	955	THR	2.4
1	A	927	THR	2.4
1	A	1026	ILE	2.4
1	A	465	PRO	2.3
1	A	746	ILE	2.3
1	A	172	ILE	2.3
1	A	957	VAL	2.3
1	A	984	LEU	2.3
1	A	991	ALA	2.3
1	A	360	LEU	2.3
1	A	823	ARG	2.3
1	A	916	GLU	2.3
1	A	901	GLY	2.3
1	A	884	GLY	2.3
1	A	287	ASP	2.3
1	A	917	GLN	2.2
1	A	299	GLY	2.2
1	A	443	ARG	2.2
1	A	174	GLY	2.2
1	A	407	GLN	2.2
1	A	472	ALA	2.2
1	A	358	PHE	2.1
1	A	291	TYR	2.1
1	A	253	PHE	2.1
1	A	694	LEU	2.1
1	A	73	SER	2.1
1	A	307	TYR	2.1
1	A	915	ALA	2.1
1	A	520	GLU	2.1
1	A	462	LEU	2.0
1	A	356	CYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	A	1332	14/15	0.33	3.93	2.87	431,431,431,431	0
2	NAG	A	1314	14/15	0.77	1.64	-0.30	269,269,269,269	0
2	NAG	A	1331	14/15	0.29	1.85	-0.33	268,268,268,268	0
2	NAG	A	1301	14/15	0.53	0.48	-0.88	262,262,262,262	0
2	NAG	A	1311	14/15	0.53	1.38	-	269,269,269,269	0
4	MAN	A	1319	11/12	0.72	1.02	-	269,269,269,269	0
3	BMA	A	1307	11/12	0.11	0.57	-	269,269,269,269	0
4	MAN	A	1317	11/12	0.69	0.32	-	269,269,269,269	0
2	NAG	A	1320	14/15	0.74	1.10	-	252,252,252,252	0
2	NAG	A	1322	14/15	0.36	0.64	-	252,252,252,252	0
3	BMA	A	1316	11/12	0.17	0.36	-	269,269,269,269	0
2	NAG	A	1306	14/15	0.49	0.80	-	269,269,269,269	0
4	MAN	A	1325	11/12	0.84	0.41	-	252,252,252,252	0
3	BMA	A	1330	11/12	0.33	0.68	-	252,252,252,252	0
3	BMA	A	1334	11/12	-0.09	0.79	-	431,431,431,431	0
4	MAN	A	1313	11/12	0.89	0.34	-	269,269,269,269	0
4	MAN	A	1318	11/12	0.43	0.65	-	269,269,269,269	0
4	MAN	A	1337	11/12	-0.04	3.96	-	431,431,431,431	0
2	NAG	A	1310	14/15	0.66	2.19	-	269,269,269,269	0
4	MAN	A	1308	11/12	0.21	0.56	-	269,269,269,269	0
2	NAG	A	1329	14/15	0.42	0.63	-	252,252,252,252	0
2	NAG	A	1333	14/15	0.32	2.67	-	431,431,431,431	0
2	NAG	A	1305	14/15	0.60	1.53	-	269,269,269,269	0
2	NAG	A	1315	14/15	0.79	1.41	-	269,269,269,269	0
2	NAG	A	1302	14/15	0.73	0.31	-	262,262,262,262	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	A	1323	14/15	0.34	0.73	-	252,252,252,252	0
4	MAN	A	1304	11/12	0.66	0.67	-	262,262,262,262	0
2	NAG	A	1321	14/15	0.39	0.76	-	252,252,252,252	0
3	BMA	A	1312	11/12	0.86	0.46	-	269,269,269,269	0
2	NAG	A	1328	14/15	0.72	0.95	-	252,252,252,252	0
2	NAG	A	1327	14/15	0.56	1.49	-	252,252,252,252	0
4	MAN	A	1309	11/12	0.56	0.51	-	269,269,269,269	0
4	MAN	A	1336	11/12	0.26	2.31	-	431,431,431,431	0
4	MAN	A	1326	11/12	0.33	0.90	-	252,252,252,252	0
4	MAN	A	1335	11/12	0.46	0.55	-	431,431,431,431	0
3	BMA	A	1324	11/12	0.55	0.38	-	252,252,252,252	0
3	BMA	A	1303	11/12	0.59	0.36	-	262,262,262,262	0

6.5 Other polymers [i](#)

There are no such residues in this entry.