Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2016 – 03:53 PM EDT

PDB ID	:	5L5C
Title	:	Plexin A1 full extracellular region, domains 1 to 10, to 6 angstrom, spacegroup P4(3)2(1)2
Authors	:	Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

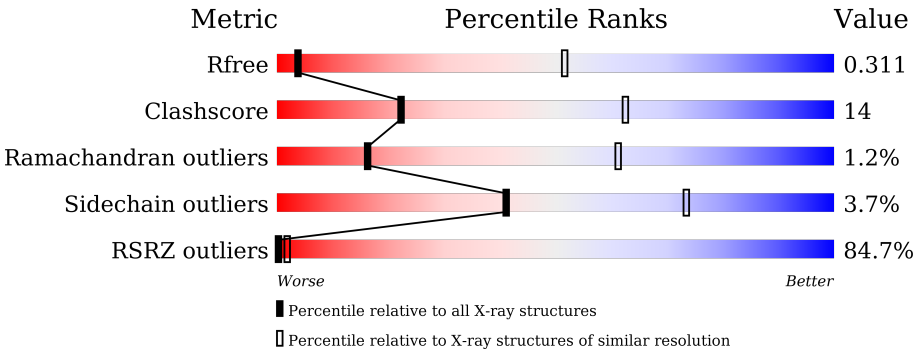
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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}	91344	1002 (8.30-3.66)
Clashscore	102246	1050 (8.30-3.70)
Ramachandran outliers	100387	1023 (8.30-3.66)
Sidechain outliers	100360	1012 (8.30-3.64)
RSRZ outliers	91569	1001 (8.30-3.66)

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 <=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	82% 70% 25%

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.

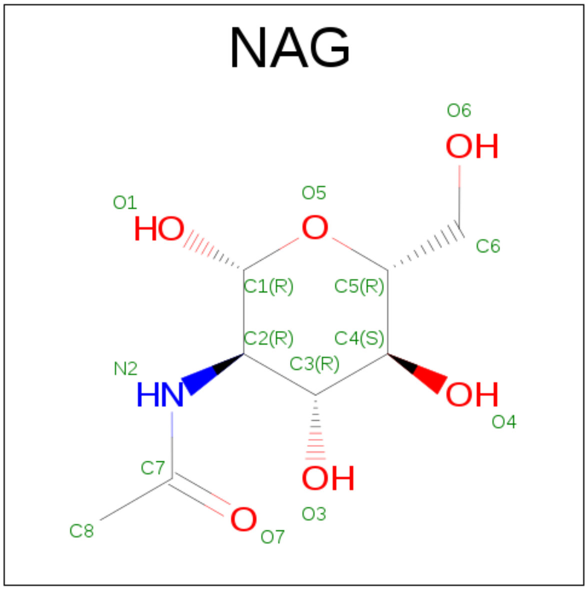
- Molecule 1 is a protein called Plexin-A1.

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

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: $C_8H_{15}NO_6$).



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

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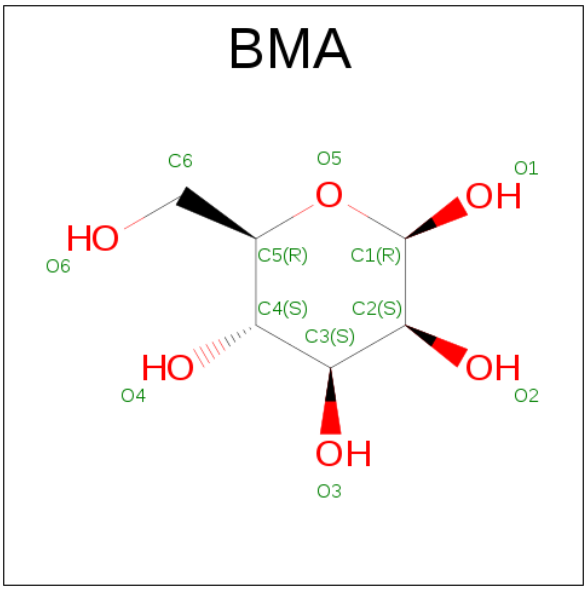
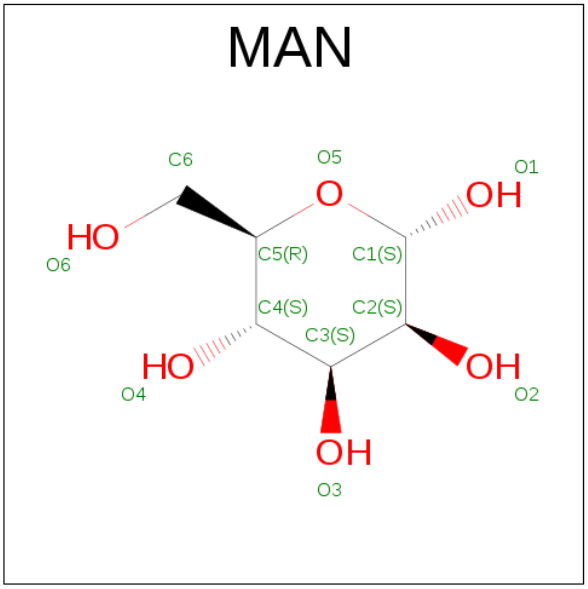
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0

- 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 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0
3	A	1	Total C O 11 6 5	0	0

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



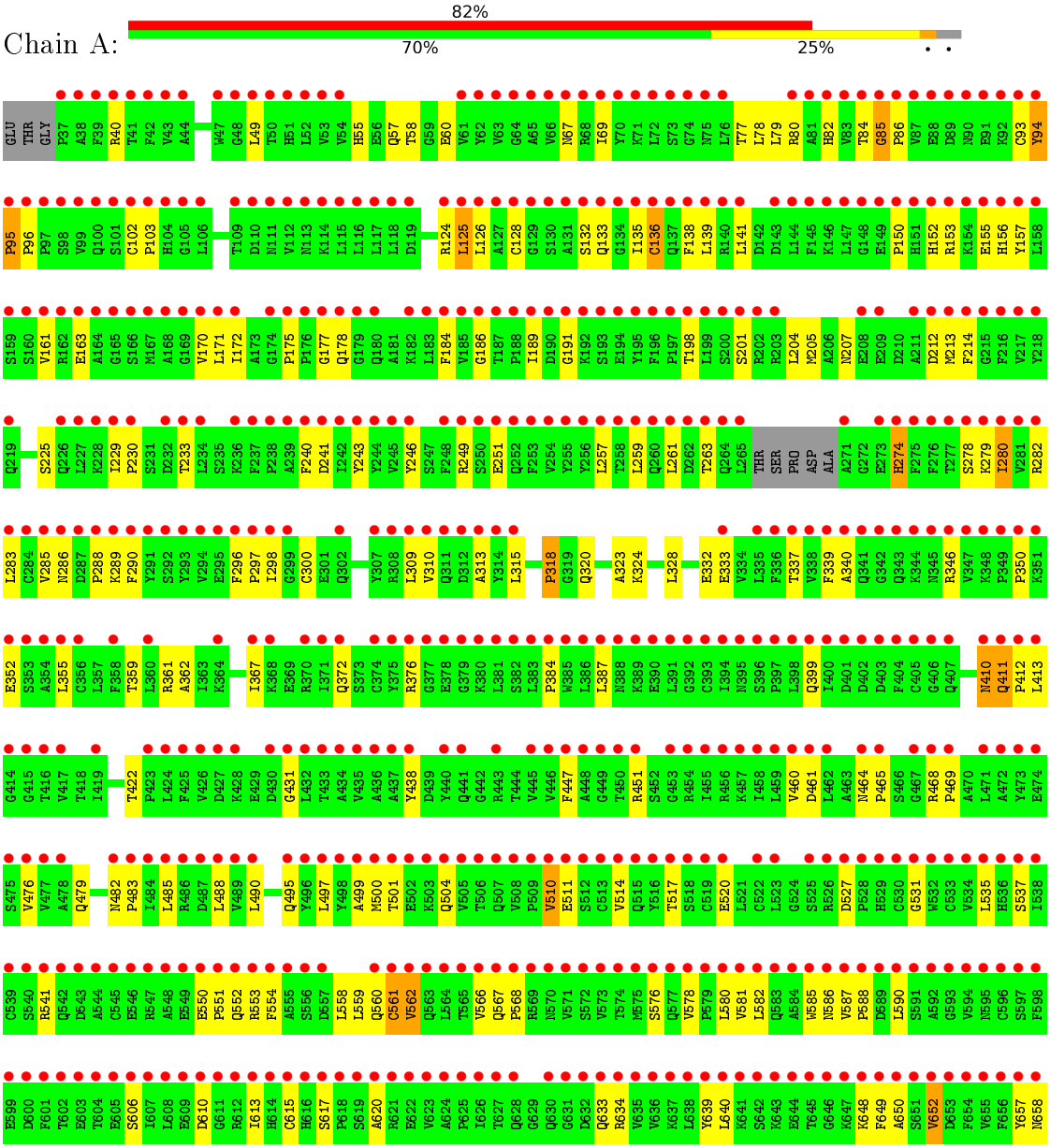
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11 6 5	0	0
4	A	1	Total C O 11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

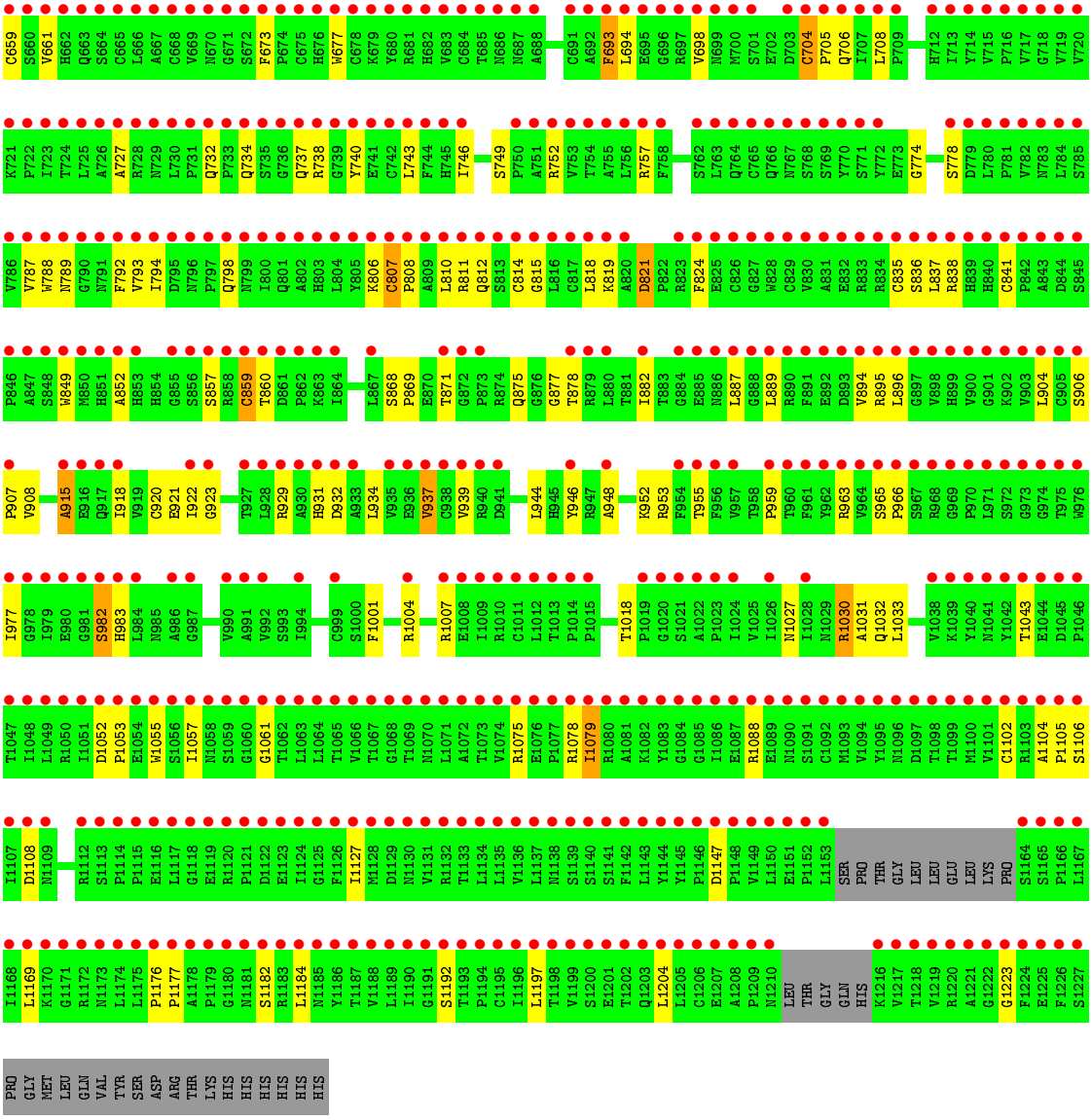
3 Residue-property plots (i)

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

- Molecule 1: Plexin-A1

Chain A:




C659 S660 V661 H662 Q663 S664 C665 L666 A667 C668 V669 H670 G671 S672 F673 P674 C675 H676 W677 C678 K679 Y680 R681 H682 V683 C684 T685 N686 N687 A688 C691 A692 F693 L694 E695 G696 R697 V698 H699 M700 S701 E702 D703 C704 P705 Q706 I707 L708 P709 H712 I713 Y714 V715 P716 V717 G718 V719 V720
K721 P722 I723 T724 L725 A726 A727 R728 N729 L730 P731 Q732 P733 Q734 S735 G736 Q737 R738 G739 Y740 E741 C742 L743 F744 H745 I746 S749 P750 A751 R752 V753 T754 A755 L756 R757 F758 S762 L763 Q764 C765 Q766 N767 S768 S769 Y770 S771 Y772 E773 G774 S778 D779 L780 P781 V782 N783 L784 S785
V786 V787 W788 N789 G790 N791 F792 V793 I794 D795 N796 P797 Q798 N799 I800 Q801 A802 H803 L804 Y805 K806 C807 P808 A809 L810 R811 Q812 S813 C814 G815 L816 C817 L818 K819 A820 D821 P822 R823 F824 E825 C826 G827 W828 C829 V830 A831 E832 R833 R834 C835 S836 L837 R838 H839 H840 C841 P842 A843 D844 S845
P846 A847 S848 W849 M850 H851 A852 H853 H854 G855 S856 S857 R858 C859 T860 D861 P862 K863 I864 L867 S868 P869 E870 T871 G872 P873 R874 Q875 G876 G877 T878 R879 L880 T881 I882 T883 G884 E885 H886 L887 G888 L889 R890 F891 E892 D893 V894 R895 L896 G897 V898 H899 V900 G901 K902 V903 L904 C905 S906
P907 V908 A915 E916 Q917 I918 V919 C920 E921 I922 G923 T927 L928 R929 A930 H931 D932 A933 L934 V935 E936 V937 C938 V939 H940 D941 L944 H945 Y946 R947 A948 K952 R953 P954 T955 F956 V957 T958 P959 T960 F961 Y962 R963 V964 S965 P966 S967 R968 G969 P970 L971 S972 G973 G974 T975 W976
I977 G978 I979 E980 G981 S982 H983 L984 N985 A986 G987 V990 A991 V992 S993 I994 C999 S1000 F1001 R1004 R1007 E1008 I1009 R1010 C1011 L1012 T1013 P1014 P1015 T1018 P1019 G1020 S1021 A1022 P1023 I1024 V1025 I1026 N1027 I1028 N1029 R1030 A1031 Q1032 L1033 V1038 K1039 Y1040 N1041 Y1042 T1043 E1044 D1045 P1046
T1047 I1048 L1049 R1050 I1051 D1052 P1053 E1054 W1055 S1056 I1057 N1058 S1059 G1060 G1061 T1062 L1063 L1064 T1065 V1066 T1067 G1068 T1069 N1070 L1071 A1072 T1073 V1074 R1075 E1076 P1077 R1078 T1079 R1080 A1081 K1082 Y1083 G1084 G1085 I1086 E1087 R1088 E1089 N1090 S1091 C1092 M1093 V1094 Y1095 N1096 D1097 T1098 T1099 M1100 V1101 C1102 R1103 A1104 P1105 S1106
I1107 D1108 M1109 R1112 S1113 P1114 P1115 E1116 L1117 G1118 E1119 R1120 P1121 D1122 E1123 I1124 G1125 F1126 I1127 M1128 D1129 N1130 V1131 R1132 T1133 I1134 L1135 V1136 I1137 N1138 S1139 S1140 S1141 F1142 L1143 Y1144 Y1145 P1146 D1147 P1148 V1149 L1150 E1151 P1152 L1153 SER PRO THR GLY LEU LEU GLU LEU LYS PRO S1164 S1165 P1166 L1167
I1168 L1169 K1170 G1171 R1172 N1173 L1174 L1175 P1176 P1177 A1178 P1179 G1180 N1181 S1182 R1183 L1184 N1185 Y1186 T1187 V1188 L1189 I1190 G1191 S1192 T1193 P1194 C1195 I1196 L1197 T1198 V1199 S1200 E1201 T1202 Q1203 L1204 L1205 C1206 E1207 A1208 P1209 N1210 LEU THR GLY GLN HIS K1216 V1217 T1218 V1219 R1220 A1221 G1222 G1223 F1224 E1225 F1226 S1227
PRO GLY MET LEU GLN VAL TYR SER ASP ARG THR LYS HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:172:ILE:HG22	1:A:249:ARG:HD2	1.87	0.56
1:A:661:VAL:HG22	2:A:1314:NAG:C6	2.34	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:737:GLN:HG2	1:A:789:ASN:ND2	2.22	0.55
1:A:93:CYS:O	1:A:133:GLN:NE2	2.40	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:566:VAL:HG22	1:A:582:LEU:CD2	2.37	0.54
1:A:661:VAL:CG2	2:A:1314:NAG:C5	2.76	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:461:ASP:HA	1:A:464:ASN:HB3	1.92	0.51
1:A:438:TYR:CE1	1:A:510:VAL:HG21	2.46	0.51
1:A:875:GLN:HB2	1:A:1031:ALA:HB2	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:488:LEU:HG	1:A:497:LEU:HD11	2.02	0.42
1:A:661:VAL:CG2	2:A:1314:NAG:H62	2.49	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1157/1212 (96%)	1049 (91%)	94 (8%)	14 (1%)	16 61

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1015/1051 (97%)	977 (96%)	38 (4%)	41 73

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	0.76	0	15,19,21	1.74	3 (20%)
2	NAG	A	1302	3,2	14,14,15	0.56	0	15,19,21	1.44	1 (6%)
3	BMA	A	1303	2,4	11,11,12	0.64	0	15,15,17	0.82	0
4	MAN	A	1304	3	11,11,12	0.66	0	15,15,17	1.01	1 (6%)
2	NAG	A	1305	1,2	14,14,15	0.61	0	15,19,21	1.23	1 (6%)
2	NAG	A	1306	3,2	14,14,15	0.49	0	15,19,21	1.19	1 (6%)
3	BMA	A	1307	2,4	11,11,12	0.54	0	15,15,17	0.67	0
4	MAN	A	1308	3,4	11,11,12	0.68	0	15,15,17	0.95	1 (6%)
4	MAN	A	1309	4	11,11,12	0.58	0	15,15,17	1.24	2 (13%)
2	NAG	A	1310	1,2	14,14,15	0.63	0	15,19,21	1.13	1 (6%)
2	NAG	A	1311	3,2	14,14,15	0.53	0	15,19,21	1.20	2 (13%)
3	BMA	A	1312	2,4	11,11,12	0.87	1 (9%)	15,15,17	2.24	4 (26%)
4	MAN	A	1313	3	11,11,12	0.58	0	15,15,17	1.03	2 (13%)
2	NAG	A	1314	1,2	14,14,15	0.65	0	15,19,21	1.17	1 (6%)
2	NAG	A	1315	3,2	14,14,15	0.53	0	15,19,21	1.09	1 (6%)
3	BMA	A	1316	2,4	11,11,12	0.61	0	15,15,17	1.65	3 (20%)
4	MAN	A	1317	3	11,11,12	0.59	0	15,15,17	0.87	1 (6%)
4	MAN	A	1318	3,4	11,11,12	0.62	0	15,15,17	0.91	0
4	MAN	A	1319	4	11,11,12	0.53	0	15,15,17	1.21	1 (6%)
2	NAG	A	1320	1,2	14,14,15	0.59	0	15,19,21	1.21	1 (6%)
2	NAG	A	1321	2	14,14,15	0.50	0	15,19,21	1.05	1 (6%)
2	NAG	A	1322	1,2	14,14,15	0.61	0	15,19,21	0.94	1 (6%)
2	NAG	A	1323	3,2	14,14,15	0.64	0	15,19,21	1.07	1 (6%)
3	BMA	A	1324	2,4	11,11,12	0.41	0	15,15,17	1.70	2 (13%)
4	MAN	A	1325	3	11,11,12	0.55	0	15,15,17	0.88	1 (6%)
4	MAN	A	1326	3	11,11,12	0.52	0	15,15,17	1.46	2 (13%)
2	NAG	A	1327	1	14,14,15	0.50	0	15,19,21	0.97	0
2	NAG	A	1328	1,2	14,14,15	0.56	0	15,19,21	1.04	1 (6%)
2	NAG	A	1329	3,2	14,14,15	0.55	0	15,19,21	1.06	1 (6%)
3	BMA	A	1330	2	11,11,12	0.48	0	15,15,17	1.15	2 (13%)
2	NAG	A	1331	1	14,14,15	0.58	0	15,19,21	1.06	1 (6%)
2	NAG	A	1332	1,2	14,14,15	0.66	0	15,19,21	1.27	2 (13%)
2	NAG	A	1333	3,2	14,14,15	0.52	0	15,19,21	1.39	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BMA	A	1334	2,4	11,11,12	0.39	0	15,15,17	0.76	0
4	MAN	A	1335	3	11,11,12	0.60	0	15,15,17	1.11	2 (13%)
4	MAN	A	1336	3,4	11,11,12	0.62	0	15,15,17	0.93	0
4	MAN	A	1337	4	11,11,12	0.62	0	15,15,17	1.27	1 (6%)

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
2	NAG	A	1331	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1332	NAG	O5-C5-C4	-2.27	106.38	110.13
3	A	1312	BMA	C1-O5-C5	2.00	115.08	112.14
2	A	1332	NAG	O5-C5-C6	2.01	111.65	107.34
4	A	1317	MAN	C1-O5-C5	2.06	115.18	112.14
4	A	1335	MAN	C1-O5-C5	2.11	115.24	112.14
4	A	1313	MAN	C1-O5-C5	2.12	115.25	112.14
3	A	1312	BMA	O5-C1-C2	2.15	114.34	110.89
3	A	1312	BMA	C2-C3-C4	2.22	114.92	111.05
2	A	1315	NAG	C3-C4-C5	2.24	114.22	110.23
2	A	1301	NAG	C2-N2-C7	2.25	126.03	123.11
4	A	1313	MAN	C1-C2-C3	2.28	112.31	109.55
2	A	1311	NAG	C4-C3-C2	2.31	114.93	111.34
4	A	1325	MAN	C1-O5-C5	2.40	115.67	112.14
2	A	1305	NAG	C4-C3-C2	2.48	115.19	111.34
4	A	1326	MAN	C1-C2-C3	2.60	112.70	109.55
2	A	1322	NAG	C4-C3-C2	2.62	115.40	111.34
2	A	1329	NAG	C4-C3-C2	2.62	115.41	111.34
2	A	1333	NAG	C4-C3-C2	2.67	115.48	111.34
4	A	1308	MAN	C1-C2-C3	2.69	112.81	109.55
2	A	1323	NAG	C4-C3-C2	2.69	115.52	111.34
4	A	1304	MAN	C1-C2-C3	2.71	112.83	109.55
3	A	1330	BMA	C1-C2-C3	2.73	112.86	109.55
2	A	1311	NAG	C1-O5-C5	2.75	116.18	112.14
3	A	1316	BMA	C2-C3-C4	2.88	116.08	111.05
2	A	1320	NAG	C4-C3-C2	2.88	115.82	111.34
2	A	1328	NAG	C4-C3-C2	2.90	115.84	111.34
2	A	1333	NAG	C3-C4-C5	2.94	115.48	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1330	BMA	C1-O5-C5	2.98	116.52	112.14
4	A	1335	MAN	C1-C2-C3	3.02	113.21	109.55
4	A	1309	MAN	C1-C2-C3	3.03	113.23	109.55
2	A	1301	NAG	C3-C4-C5	3.06	115.68	110.23
2	A	1331	NAG	C1-O5-C5	3.08	116.67	112.14
4	A	1309	MAN	C1-O5-C5	3.21	116.86	112.14
3	A	1316	BMA	C1-C2-C3	3.30	113.55	109.55
2	A	1321	NAG	C1-O5-C5	3.41	117.16	112.14
2	A	1314	NAG	C4-C3-C2	3.57	116.88	111.34
4	A	1337	MAN	C1-C2-C3	3.59	113.90	109.55
2	A	1310	NAG	C4-C3-C2	3.65	117.00	111.34
3	A	1316	BMA	C3-C4-C5	3.73	116.88	110.23
2	A	1306	NAG	C1-O5-C5	3.74	117.64	112.14
4	A	1319	MAN	C1-O5-C5	3.88	117.84	112.14
3	A	1324	BMA	C1-C2-C3	3.94	114.33	109.55
4	A	1326	MAN	C1-O5-C5	4.16	118.25	112.14
3	A	1324	BMA	C1-O5-C5	4.23	118.36	112.14
2	A	1302	NAG	C4-C3-C2	4.42	118.20	111.34
2	A	1301	NAG	C4-C3-C2	4.67	118.58	111.34
3	A	1312	BMA	C1-C2-C3	7.47	118.60	109.55

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
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, 95^{th} 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	1168	ILE	21.7
1	A	1172	ARG	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	1206	CYS	14.3
1	A	1166	PRO	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	11.4
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	652	VAL	9.3
1	A	707	ILE	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	789	ASN	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	718	GLY	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	5.1
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	801	GLN	4.3
1	A	843	ALA	4.3
1	A	769	SER	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	460	VAL	3.5
1	A	878	THR	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, 95^{th} 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(Å^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.