



wwPDB X-ray Structure Validation Summary Report ⓘ

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 wwPDB X-ray Structure Validation Summary 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 : 1.7.1 (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

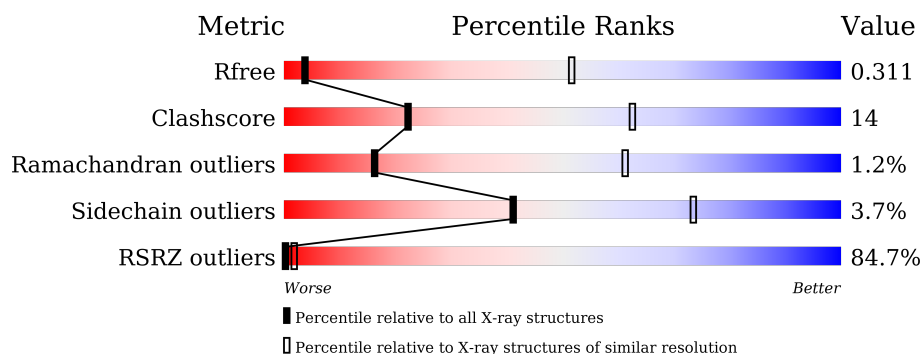
1 Overall quality at a glance

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 $\leq 5\%$. 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).



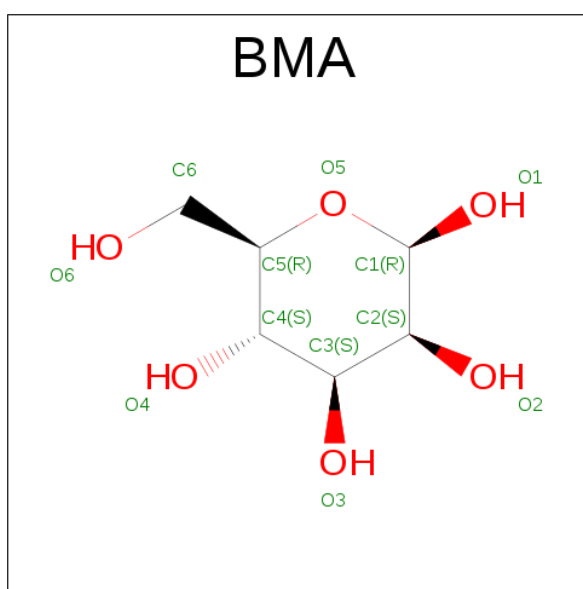
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1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

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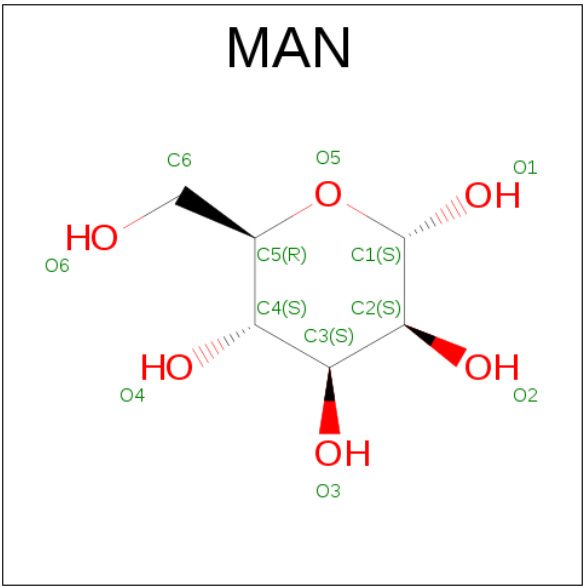
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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).

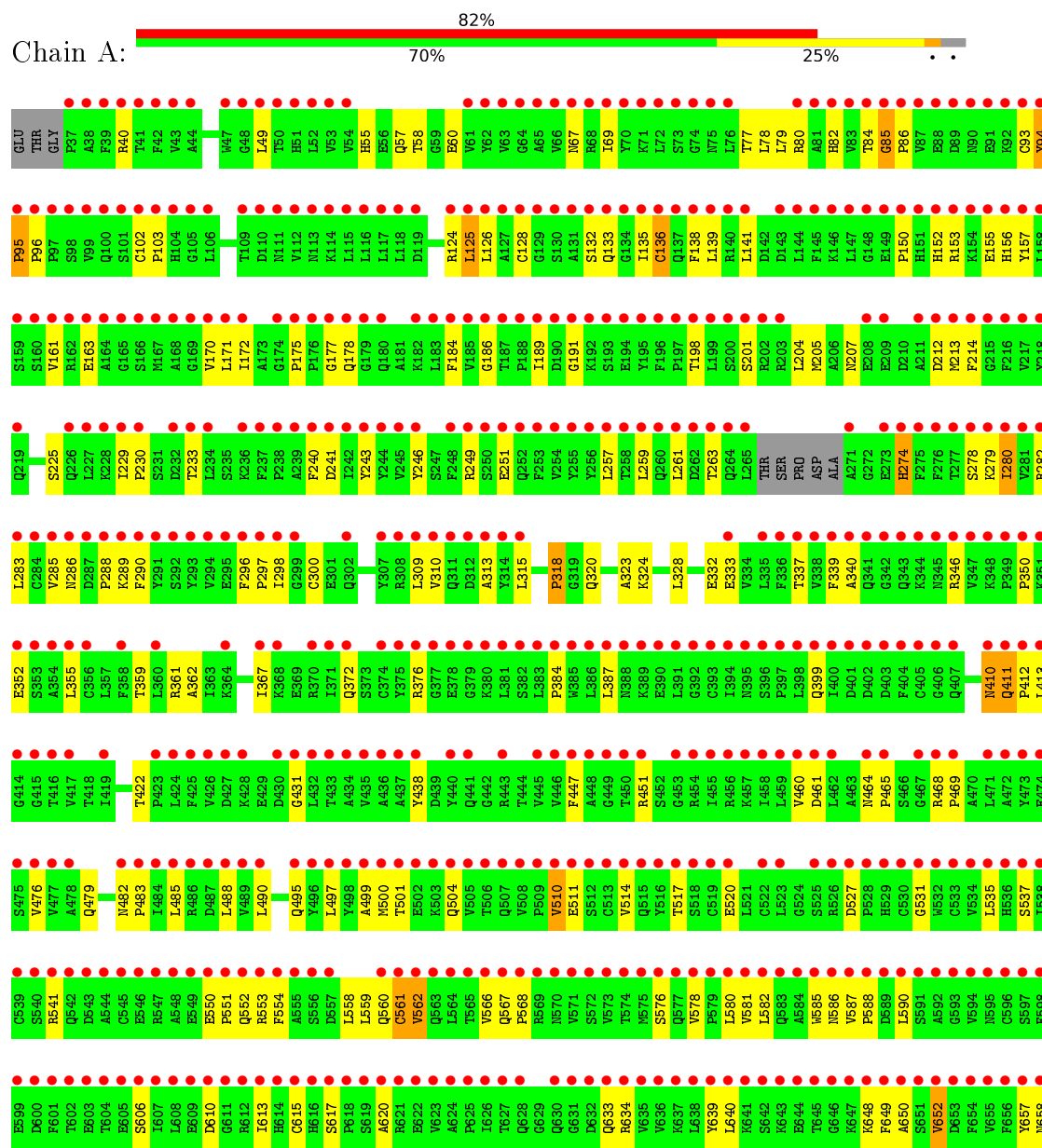


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4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



PRO	I1168	I1107	T1047	1977	P907	P846	V786	K721	C659
GLY	L1169	D1108	I1048	G978	V908	A847	V787	F722	S660
MET	K1170	M1109	I1049	E980	A915	S948	W788	W723	H661
LEU	G1171		R1050	E980	A915	W849	W789	T724	H662
GLN	R1172	R1112	I1051	S982	E916	H850	G790	L725	Q663
VAL	M1173	S1113	D1052	G981	D917	H851	G791	A726	S664
TYR	L1174	P1053	P1053	H983	T918	A852	G792	A727	C665
SER	L1175	E1054	E1054	L984	V919	H853	G793	R728	L666
ASP	P1176	E1116	W1055	L984	C920	H854	W729	W729	A667
ARG	P1177	L1117	S1056	A986	E921	G855	L730	C668	C668
THR	A1178	G1118	I1057	G987	E922	S856	W796	F731	G669
LYS	P1179	N1058	N1058		G923	S857	G797	Q732	N670
HIS	G1180	S1059	S1059	V690		R858	Q798	P733	G571
HIS	N1181	R1120	G1060	A991	T927	C859	N799	P733	G571
HIS	S1182	P1121	G1061	V992	L928	T860	W735	Q734	S672
HIS	R1183	E1123	T1062	S993	R929	D861	L800	G736	F673
HIS	L1184	I1124	L1063	1994	A930	P862	Q801	P674	
HIS	N1185	G1125	L1064		H931	K863	A802	Q737	C675
	Y1186	F1126	T1065	C999	D932	I864	H803	R738	H676
	T1187	I1127	V1066	S1000	A933		L804	G739	H677
	V1188	M1128	T1067	F1001	L867		K805	Y740	C678
	L1189	D1129	G1068	R1004	S868		C807	E741	C679
	I1190	M1130	T1069		P869		W680	G742	Y680
	G1191	V1131	N1070	R1004	E936		P808	L743	H681
	S1192	R1132	L1071	R1007	V937		A809	F744	H682
	T1193	T1133	A1072	E1008	C938		L811	H745	H683
	P1194	L1134	T1073	I1009	V938		K812	C684	C684
	C1195	L1135	W1074	R1010	D941		S813	W749	H686
	I1196	V1136	E1075	C1011			G814	P750	N687
	L1197	L1137	E1076	L1012	L944		G815	A751	A688
	T1198	M1138	P1077	T1013	H945		L816	R752	
	V1199	S1139	I1078	P1014	V946		C817	W753	C691
	S1200	S1140	I1079	P1015	A947		L818	T754	A692
	E1201	F1141	R1080	T1018	A948		K819	A755	F693
	T1202	L1142	A1081				A820	L756	L694
	Q1203	L1143	K1082	P1019	K952		D821	R757	E695
	L1204	Y1144	Y1083	G1020	R953		P822	F758	G696
	L1205	Y1145	G1084	S1021	T954		R823		R697
	C1206	P1146	G1085	A1022	T955		F824		V698
	E1207	D1147	I1086	P1023	F956		E825		H699
	A1208	P1148	E1087	I1024	V957		C826		W700
	P1209	V1149	N1088	V1025	T958		G827		S701
	N1210	L1150	E1089	I1026	P959		W828		E702
LEU		E1151	N1090	N1027	T960		C829		D703
THR		P1152	S1091	I1028	F961		V830		C704
GLY		L1153	C1092	N1029	V962		E831		P705
GLN		SER	M1093	R1030	R963		E832		Q706
HIS		PRO	V1094	A1031	V964		R833		I707
	K1216	THR	Y1095	Q1032	S965		R834		L708
V1217		GLY	N1096	L1033	P966		C835		P709
T1218		LEU	D1097		S967		S836		
V1219		LEU	T1098	V1038	R968		L837		H712
R1220		GLU	T1099	K1039	G969		H838		I713
A1221		LEU	M1100	Y1040	P970		H839		Y714
G1222		LYS	V1101	N1041	L971		H840		W715
		PRO	C1102	Y1042	S972		C841		P716
			R1103	T1043	G973		P842		V717
F1224		S1164	A1104	E1044	G974		A843		G718
E1225		P1165	P1105	D1045	T975		L784		V719
F1226		P1166					S785		V720
S1227		L1167		P1046	N976				

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 [i](#)

5.1 Standard geometry [i](#)

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

The worst 5 of 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

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	ASN	Peptide
1	A	527	ASP	Peptide
1	A	807	CYS	Peptide
1	A	85	GLY	Peptide
1	A	94	TYR	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.

The worst 5 of 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
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

The worst 5 of 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ASP:O	1:A:1007:ARG:NH2[8_444]	1.55	0.65

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%)	16 61

5 of 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

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

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	562	VAL

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Mol	Chain	Res	Type
1	A	652	VAL
1	A	1075	ARG
1	A	610	ASP
1	A	693	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	8

The worst 5 of 8 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

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

The worst 5 of 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

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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 ⓘ

There are no such residues in this entry.