



wwPDB X-ray Structure Validation Summary 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
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	:	1.7.2 (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

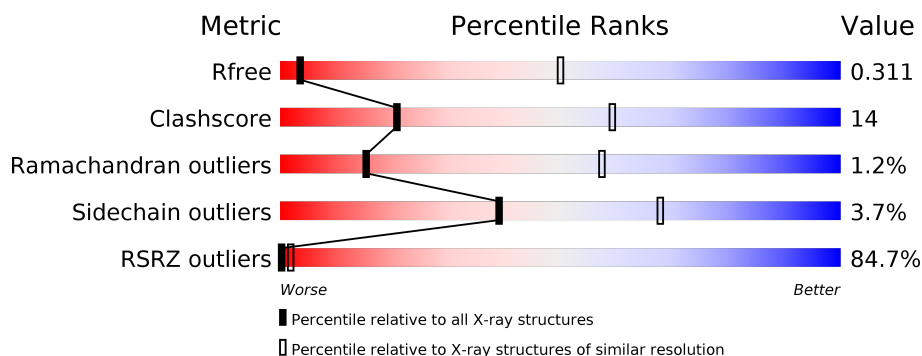
1 Overall quality at a glance

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.

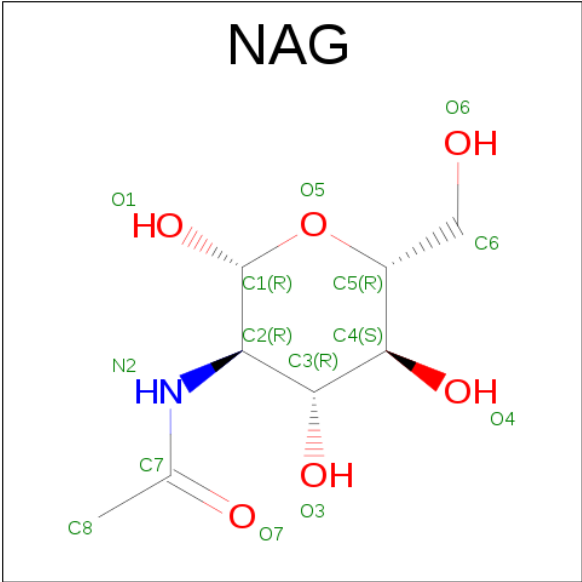
- Molecule 1 is a protein called Plexin-A1.

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).



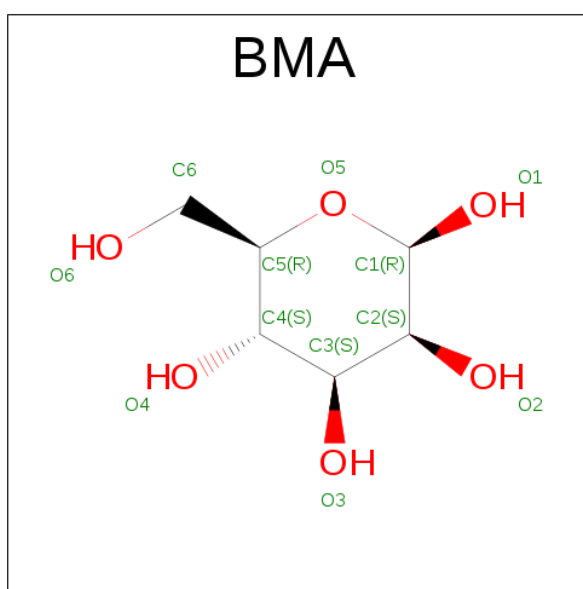
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1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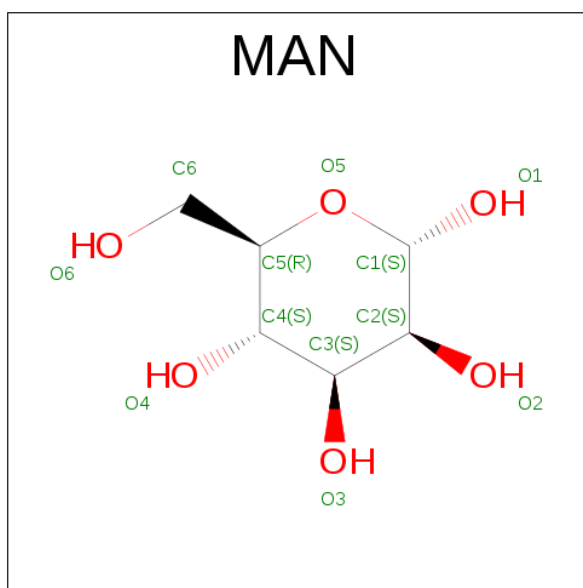
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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).

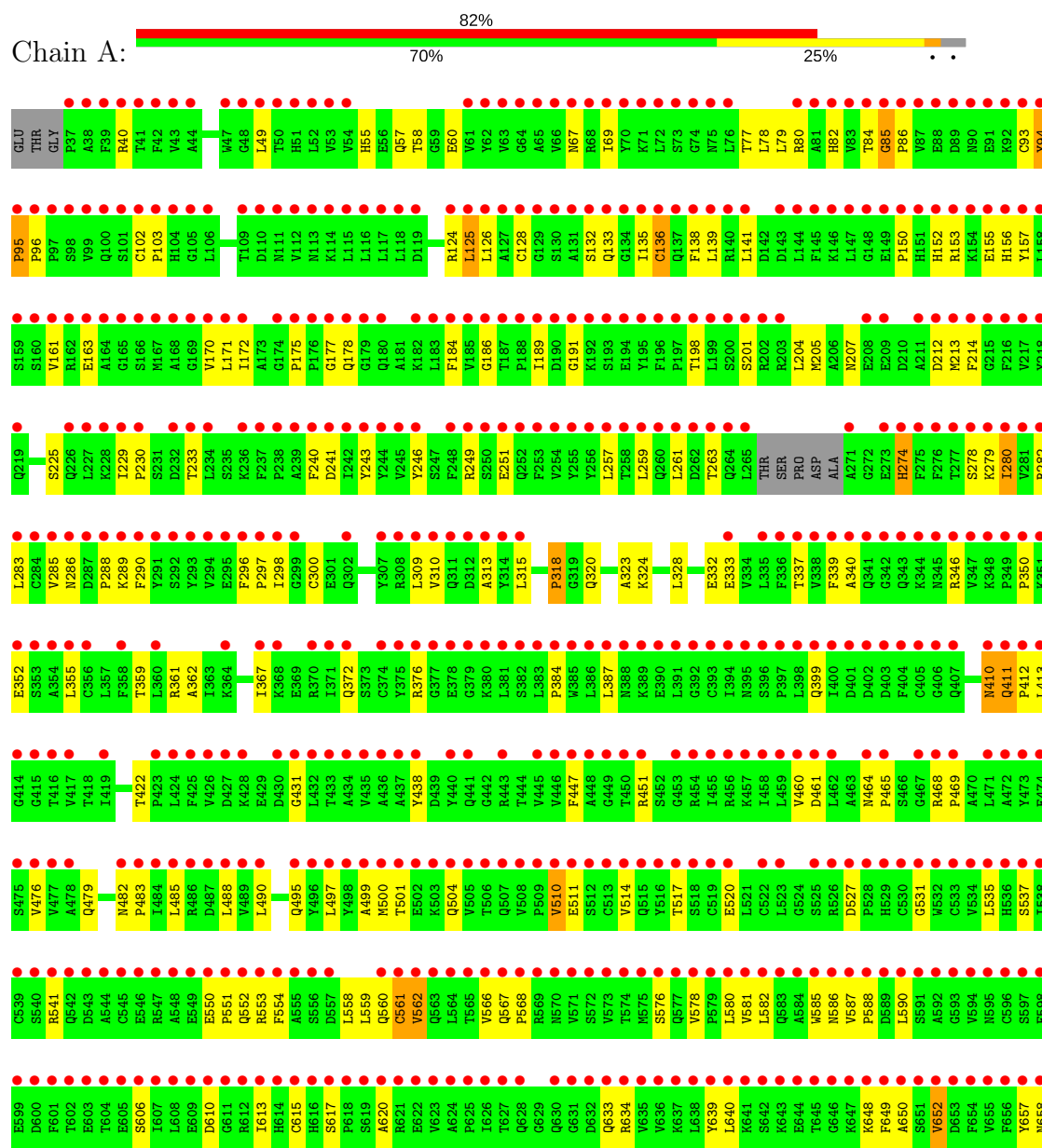


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

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		S948	N789	W788	V861
LEU	G1171		R1050	E980	A915	W849	N789	W724	H662
GLN	R1172		I1051	S982	E916	M850	G790	L725	Q663
VAL	M1173		D1052	G981	Q917	H851	N791	A726	S664
TYR	L1174		P1053	H983	T918	A852	F792	A727	C665
SER	L1175		E1054	L984	V919	H853	R728	L726	L866
ASP	P1176		W1055	M985	C920	H854	V793	W729	C667
ARG	P1177		S1056	G987	E921	G855	L794	L730	C668
THR	A1178		I1057	G987	E922	S856	N796	F731	V669
LYS	P1179		N1058		G923	S857	F797	Q732	N670
HIS	G1180		S1059	V990		S858	F798	P733	G671
HIS	N1181		G1060	A991	T927	C859	N799	Q734	S872
HIS	S1182		T1061	V992	L928	T860	L800	S735	P673
HIS	R1183		G1062	S993	R929	D861	Q801	G736	F874
HIS	L1184		L1063	I994	A930	P862	A802	Q737	C675
HIS	N1185		L1064		H931	K863	H803	R738	H676
	Y1186		T1065	C999	D932	I864	L804	G739	W677
	T1187		V1066	S1000	A933	L867	Y805	Y740	C878
	V1188		T1067	F1001	L934		K806	E741	K879
	L1189		G1068		V935	P869	C807	C742	Y680
	I1190		T1069	R1004	E936	P869	P808	L743	R681
	G1191		N1070		V937	E870	A809	F744	H682
	S1192		L1071	R1007	C938	T871	L810	H745	V683
	T1193		A1072	E1008	V938	G872	R811	L746	C684
	P1194		T1073	I1009	R940	P873	S813		T885
	C1195		V1074	R1010	D941	R874	C814	P750	N686
	I1196		E1075	C1011		Q875	G815	A751	N687
	L1197		E1076	L1012	L944	G876	G815	F752	A688
	T1198		R1077	L1013	H945	G877	L816	R753	
	V1199		P1078	P1014	Y946	T878	C817	W753	C891
	S1200		T1079	P1015	R947	R879	L818	T754	A692
	E1201		R1080		A948	L880	K819	A755	F693
	T1202		A1081	T1018		T881	A820	L756	L694
	Q1203		K1082	P1019	K952	I882	D821	R757	E695
	L1204		Y1083	G1020	R953	T883	P822	F758	G696
	L1205		G1084	S1021	F954	G884	R823		R697
	C1206		G1085	A1022	T955	E885	F824		V698
	E1207		T1086	P1023	F956	N886	E825	S762	N699
	P1208		E1087	I1024	V957	L887	C826	L763	M700
	N1210		R1088	V1025	T958	G888	G827	Q764	S701
	LEU		E1089	I1026	P959	L889	W828	C765	S701
THR	GLY		N1090	N1027	T960	H890	C829	Q766	E702
GLN			S1091	I1028	F961	F891	V830	N767	D703
GLN			C1092	N1029	F962	E892	E831	S768	C704
HIS			M1093	R1030	R963	D893	E832	S769	P705
			V1094	Q1031	V964	R894	R833	Y770	Q706
			Y1095	Q1032	S965	R895	R834	S771	L708
			N1096	L1033	P966	L896	C835	Y772	L708
			D1097		S967	G897	S836	E773	P709
			T1098	V1038	R968	V898	L837	G774	
			T1099	K1039	Q969	H899	L837		H712
			M1100	Y1040	P970	V900	H839		I713
			Y1101	N1041	L971	G901	H840		Y714
			C1102	Y1042	S972	K902	H841		P715
			R1183	T1043	G973	V903	P842		P717
			A1104	E1044	G974	L904	A843		G718
			P1165	D1045	T975	C905	D844		V719
			L1167	P1046	W976	S906	S845		V720

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%)	15 57

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%)	39 68

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	0.78	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%)
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%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

The worst 5 of 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

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.