



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 8, 2016 – 05:03 PM EDT

PDB ID : 5L59
Title : Plexin A1 full extracellular region, domains 1 to 10, to 6 angstrom, spacegroup P2(1)
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

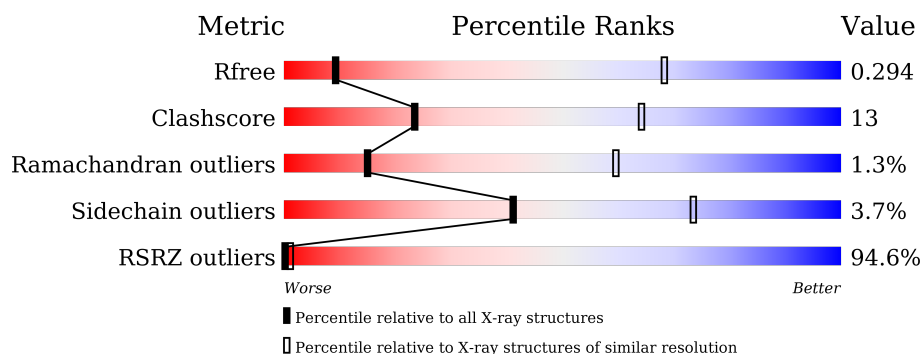
1 Overall quality at a glance

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>91%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div> </div>
1	B	1212	<div> <div>92%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>..</div> </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	1305	-	-	-	X
2	NAG	A	1314	-	-	-	X
2	NAG	A	1329	-	-	-	X
2	NAG	A	1334	X	-	-	-
2	NAG	B	1301	-	-	-	X
2	NAG	B	1305	-	-	-	X
2	NAG	B	1315	-	-	-	X
2	NAG	B	1331	-	-	-	X
2	NAG	B	1337	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19191 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.

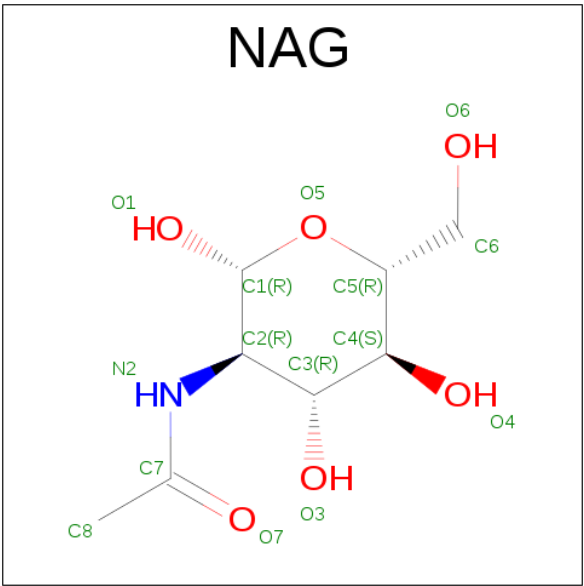
- Molecule 1 is a protein called Plexin-A1.

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

There are 24 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
B	34	GLU	-	expression tag	UNP P70206
B	35	THR	-	expression tag	UNP P70206
B	36	GLY	-	expression tag	UNP P70206
B	1237	ARG	-	expression tag	UNP P70206
B	1238	THR	-	expression tag	UNP P70206
B	1239	LYS	-	expression tag	UNP P70206
B	1240	HIS	-	expression tag	UNP P70206
B	1241	HIS	-	expression tag	UNP P70206
B	1242	HIS	-	expression tag	UNP P70206
B	1243	HIS	-	expression tag	UNP P70206
B	1244	HIS	-	expression tag	UNP P70206
B	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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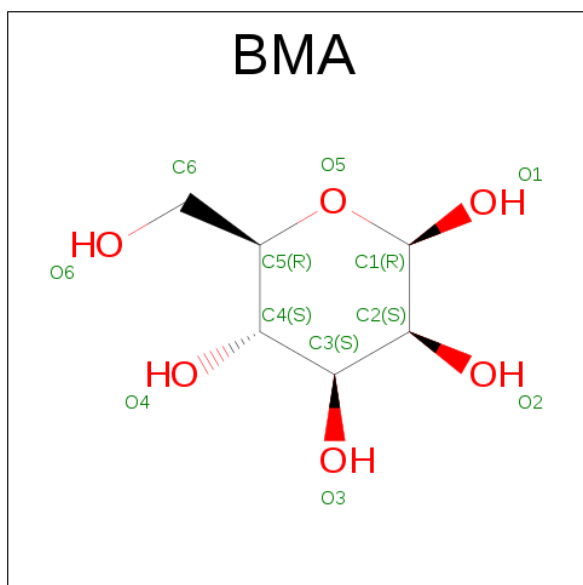
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



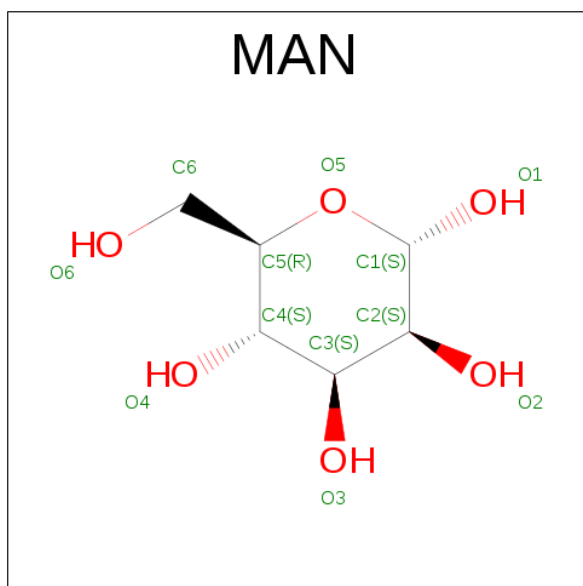
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

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

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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	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

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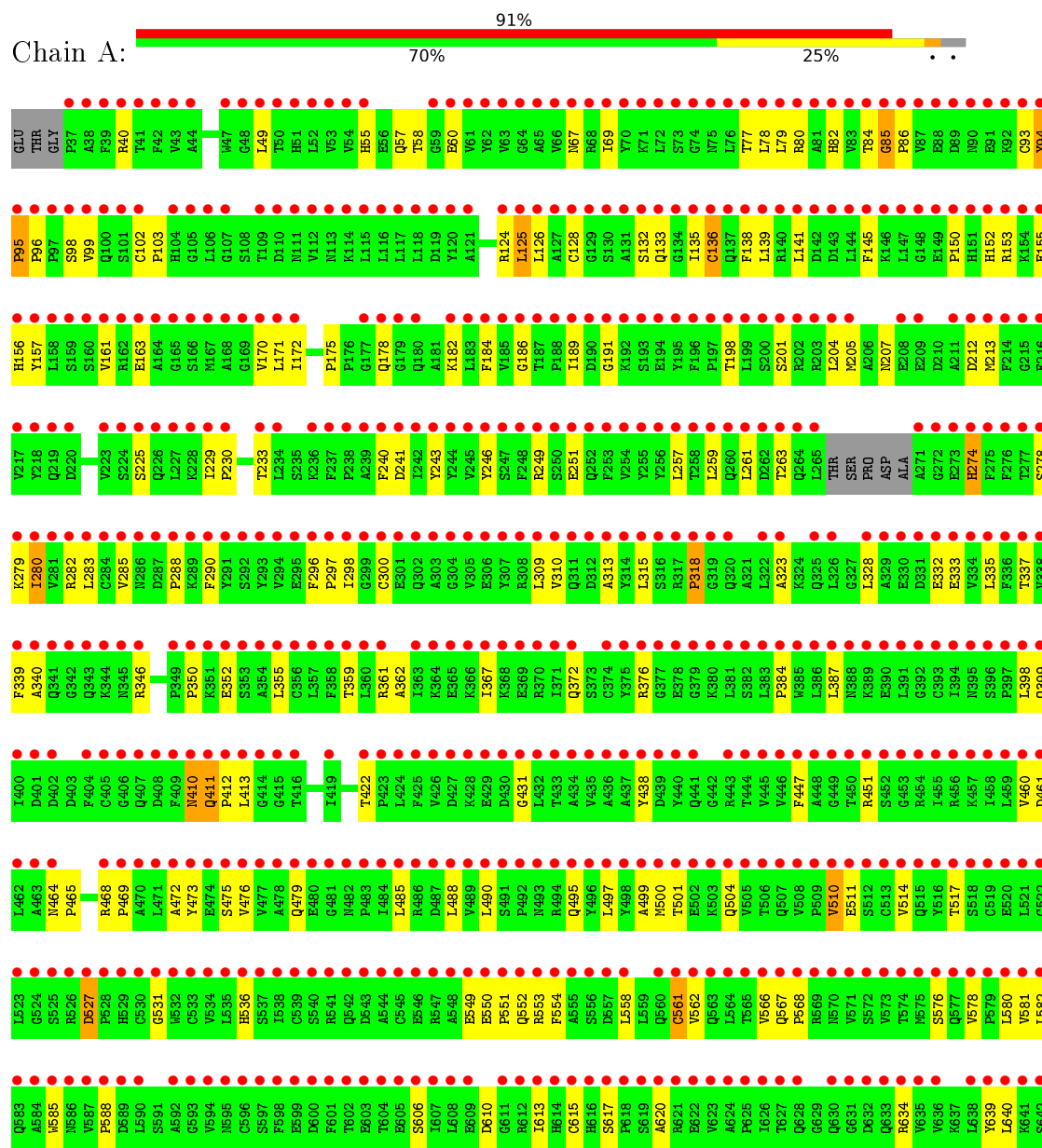
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

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





I1124	I1064	I1004	I0944	G884	F824	L763	S701	K641	P579	C519	I458	L398	T337	T277
G125	T1065	H1005	H945	E885	E825	Q764	E702	S842	L580	B520	L459	Q399	Y338	S278
F1126	V1066	S1006	T946	M886	C826	Q765	D703	K643	V581	K643	V460	D401	F339	K279
I1127	T1067	R947	R947	M887	G827	Q766	C704	E644	L582	C522	D461	I401	A340	I280
M1128	G1068	E1008	A948	G888	W828	H767	P705	T645	Q583	L523	L462	D402	Q341	R281
M129	T1069	I1009	I949	L889	C829	S768	Q706	G646	A584	G524	A463	D403	G342	V281
N1130	N1070	R1010	S950	R890	R830	S769	T707	K647	K585	S525	N464	F404	Q343	L283
V1131	L1071	C1011	P951	F891	A831	W770	L708	K648	M588	R526	P465	C405	K344	C284
T1132	L1072	K952	K952	E892	E832	S771	P709	F649	V587	D527		G406	R345	V285
T1133	T1073	R1013	R953	F893	R833	W772	S710	A650	P588	P528	R468	Q407	R346	N286
L1134	T1074	P1014	F954	V894	R834	W773	S711	S651	D589	H529	P469	D408		D287
L1135	R1075	P1015	T955	R895	C835	G774	H712	D652	L590	C530	A470	F409	P349	P288
L1136	G1076	G1016	F956	L896	S836	H775	I713	D653	S591	G531	L471	N410	P350	V289
L1137	P1077	H1017	V857	G897	L837	D776	T714	F654	A582	N632	A472	Q411	K351	F290
M1138	R1078	T958	P959	V898	R838	W777	T715	F655	G593	C533	Y473	P412	E352	Y291
S1139	I1079	H1080	P959	H899	H839	S778	P716	F656	V594	V534	E474	L413	S353	S292
S1140	R1080	G1020	T960	V900	H840	D779	G717	N595	M595	L535	S475	G414	A354	Y293
S1141	A1081	S1021	F961	Q901	C941	L780	V718	N658	C596	H536	V476	G415	L355	V294
L1142	K1082	A1022	Y962	K902	P842	S781	W719	C659	S597	S537	V477	T416	C356	E295
L1143	Y1083	P1023	R963	V903	A843	W782	T720	S660	F588	I538	Q478	V417	L357	F296
L1144	G1084	V1024	V964	L904	D844	W783	K721	E599	E599	C539	Q479	T418	F358	P297
Y1145	G1085	V1025	S965	C905	S845	L784	P722	H662	F601	S540	G481	I419	T359	I298
P1146	I1086	I1026	P966	S906	P846	Q663	W723	H663	F601	H541	G481	E420	L360	G299
P1147	E1087	N1027	S967	P907	A847	S664	T724	S664	T602	D542	N482	G421	R361	C301
P1148	R1088	G1028	R968	V908	S848	W787	L725	C665	E603	D543	P483	T422	A362	E501
V1149	E1089	N1029	G969	E909	W849	W788	A726	L666	T604	A544	I484	F423	L363	Q302
L1150	N1090	R1030	P970	S910	H850	A667	A727	A667	E605	C545	R485	F424	K364	A303
E1151	S1091	A1031	L971	E911	H851	Q790	W728	C668	S606	C546	R486	F425	E365	G304
P1152	C1092	Q1032	S972	Y912	A852	W791	N729	V669	I607	H547	D487	V426	K366	V305
L1153	M1093	L1033	G973	I913	H853	F792	L730	N670	L608	A548	L488	D427	I367	E306
SER	V1094	S1034	G974	S914	H854	W793	P731	G671	P609	P549	V489	K428	K368	Y307
PRO	Y1095	N1035	T975	A915	G855	L794	Q732	S672	D610	E560	L490	E429	E369	R308
THR	M1096	P1036	H976	E916	S856	F673	P733	F673	G611	P551	S491	D430	R370	L309
GLY	T1097	E1037	I977	Q917	S857	P674	Q734	P674	I613	Q552	P492	G431	I371	V310
LEU	T1098	Y1038	G978	I918	R858	C675	Q734	C675	I613	H553	J493	L432	Q372	Q311
LEU	T1099	K1039	V919	V919	C859	H676	Q737	H677	C615	A565	R494	T433	S373	D312
GLU	M1100	Y1040	E980	C920	T860	C678	Q738	C678	E616	A566	Q495	A434	C374	A313
LEU	V1101	N1041	G981	E921	D861	Q801	Q738	Q801	S617	S556	Y496	V435	Y375	Y314
LYS	C1102	Y1042	S982	I922	P862	A802	E740	K679	P618	D657	L497	A437	R376	L315
PRO	R1103	T1043	H983	I923	K863	H803	E741	Y680	S619	L558	Y498	Y438	G377	S316
S1164	A1104	E1044	L984	D924	L864	L804	L742	R681	L559	L559	A499	D439	E378	R317
S1165	P1105	D1045	N985	A925	L865	Y805	L743	H682	A620	O560	M500	Y439	O379	P318
P1166	S1106	P1046	A986	S926	K866	K806	F744	V683	R621	C561	T501	Y440	K380	G319
L1167	T1047	T927	G987	T927	L867	C807	H745	C584	E622	V662	E502	Q441	L381	Q320
I1168	D1108	S988	G988	L928	S868	P808	I746	T685	E623	Q563	K503	G442	S382	A321
L1169	M1109	L1049	D989	R929	P869	A809	P747	M686	P624	L564	Q504	R443	P384	L322
K1170	P1110	R1050	V990	A930	E870	L810	G748	M687	A624	T565	V505	V445	V385	K324
G1171	K1111	I1051	A991	H931	T871	R811	S749	A688	P625	V566	Q507	V446	L386	Q325
R1172	R1112	D1052	V992	D932	G872	Q812	P750	A689	T627	D567	L387	F447	L387	L326
M1173	S1113	P1063	S993	A933	P873	S813	A751	D690	Q628	P568	V508	A448	N388	G327
L1174	P1114	E1064	I994	L934	Q874	C814	R752	C691	G629	H569	P509	A449	N389	L328
L1175	E1115	W1055	G995	V935	Q875	G815	W753	A692	Q630	H570	V510	G449	K390	L329
P1176	S1056	P1056	G996	E936	G876	L816	T754	F693	G631	V571	E511	T460	E390	A329
P1177	I1057	R997	R997	V937	G877	C817	A755	D632	S572	S512	S512	R451	L391	E330
A1178	N1058	L1057	P998	C938	T878	L818	L756	E695	Q633	V573	C513	S482	G392	D331
P1179	E1118	K1118	G999	V939	R879	K819	R757	G696	R634	T574	V514	S483	G393	E332
G1180	R1120	G1060	S1000	R940	L880	A850	F758	G697		H575	Q515	R454	I394	E333
S1181	P1121	T1062	F1001	D941	T881	D821	N759	V698	L638	S576	T516	I455	N395	S334
R1182	E1122	G1062	S1002	C942	I882	P822	W760	M699		Q577	T517	R456	S396	L335
R1183	E1123	L1063	W1003	S943	T883	R823		M700	L640	V578	S518	K457	P397	F336

WORLDWIDE
PDB
PROTEIN DATA BANK

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	139.99Å 196.45Å 144.94Å 90.00° 94.57° 90.00°	Depositor
Resolution (Å)	58.22 – 6.00 58.22 – 6.00	Depositor EDS
% Data completeness (in resolution range)	94.3 (58.22-6.00) 76.2 (58.22-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 6.17Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.274 , 0.299 0.273 , 0.294	Depositor DCC
R_{free} test set	994 reflections (5.13%)	DCC
Wilson B-factor (Å ²)	291.6	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 436.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.077 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	19191	wwPDB-VP
Average B, all atoms (Å ²)	272.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.45	4/9293 (0.0%)	0.60	3/12628 (0.0%)
1	B	0.63	7/9296 (0.1%)	0.77	13/12639 (0.1%)
All	All	0.55	11/18589 (0.1%)	0.69	16/25267 (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	8
1	B	0	10
All	All	0	18

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1147	ASP	C-N	32.49	1.96	1.34
1	B	561	CYS	C-N	28.65	2.00	1.34
1	A	859	CYS	C-N	-19.30	0.89	1.34
1	B	859	CYS	C-N	18.57	1.76	1.34
1	A	510	VAL	C-N	17.80	1.75	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1043	THR	O-C-N	31.38	172.91	122.70
1	B	1043	THR	CA-C-N	-23.75	64.96	117.20
1	B	1043	THR	C-N-CA	-19.45	73.09	121.70
1	B	1147	ASP	O-C-N	-14.82	92.94	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	859	CYS	O-C-N	-13.50	101.10	122.70

There are no chirality outliers.

5 of 18 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	8876	241	22
1	B	9085	0	8877	280	33
2	A	252	0	217	4	0
2	B	252	0	217	2	0
3	A	88	0	72	0	0
3	B	88	0	69	0	0
4	A	154	0	134	1	0
4	B	187	0	164	1	0
All	All	19191	0	18626	504	35

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 13.

The worst 5 of 504 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:855:GLY:HA3	1:A:890:ARG:NH2	1.22	1.48
1:B:1116:GLU:O	1:B:1177:PRO:CD	1.68	1.42
1:A:510:VAL:C	1:A:511:GLU:N	1.75	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:859:CYS:C	1:B:860:THR:N	1.76	1.39
1:B:813:SER:HB2	1:B:886:ASN:OD1	1.22	1.36

The worst 5 of 35 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:399:GLN:N	1:B:1007:ARG:NH2[2_445]	0.67	1.53
1:A:398:LEU:C	1:B:1007:ARG:NH2[2_445]	0.78	1.42
1:A:962:TYR:OH	1:B:361:ARG:NH1[1_656]	1.02	1.18
1:A:398:LEU:O	1:B:1007:ARG:NH1[2_445]	1.61	0.59
1:A:962:TYR:CZ	1:B:361:ARG:NH1[1_656]	1.69	0.51

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	1155/1212 (95%)	1049 (91%)	92 (8%)	14 (1%)	16	61
1	B	1161/1212 (96%)	1048 (90%)	96 (8%)	17 (2%)	13	57
All	All	2316/2424 (96%)	2097 (90%)	188 (8%)	31 (1%)	15	59

5 of 31 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 ⓘ

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
1	B	1015/1051 (97%)	977 (96%)	38 (4%)	41	73
All	All	2030/2102 (97%)	1954 (96%)	76 (4%)	41	73

5 of 76 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1033	LEU
1	B	136	CYS
1	B	1018	THR
1	A	1075	ARG
1	B	77	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

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

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

83 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	0.75	0	15,19,21	1.74	3 (20%)
2	NAG	A	1302	3,2	14,14,15	0.55	0	15,19,21	1.44	1 (6%)
3	BMA	A	1303	2,4	11,11,12	0.65	0	15,15,17	0.83	0
4	MAN	A	1304	3	11,11,12	0.64	0	15,15,17	1.00	1 (6%)
2	NAG	A	1305	1,2	14,14,15	0.64	0	15,19,21	1.22	1 (6%)
2	NAG	A	1306	3,2	14,14,15	0.47	0	15,19,21	1.19	1 (6%)
3	BMA	A	1307	2,4	11,11,12	0.55	0	15,15,17	0.65	0
4	MAN	A	1308	3,4	11,11,12	0.67	0	15,15,17	0.95	1 (6%)
4	MAN	A	1309	4	11,11,12	0.56	0	15,15,17	1.22	2 (13%)
2	NAG	A	1310	1,2	14,14,15	0.62	0	15,19,21	1.14	1 (6%)
2	NAG	A	1311	3,2	14,14,15	0.55	0	15,19,21	1.20	2 (13%)
3	BMA	A	1312	2,4	11,11,12	0.86	1 (9%)	15,15,17	2.24	4 (26%)
4	MAN	A	1313	3	11,11,12	0.58	0	15,15,17	1.05	2 (13%)
2	NAG	A	1314	1,2	14,14,15	0.64	0	15,19,21	1.16	1 (6%)
2	NAG	A	1315	3,2	14,14,15	0.53	0	15,19,21	1.10	1 (6%)
3	BMA	A	1316	2,4	11,11,12	0.60	0	15,15,17	1.65	3 (20%)
4	MAN	A	1317	3	11,11,12	0.59	0	15,15,17	0.88	1 (6%)
4	MAN	A	1318	3,4	11,11,12	0.60	0	15,15,17	0.91	0
4	MAN	A	1319	4	11,11,12	0.51	0	15,15,17	1.22	1 (6%)
4	MAN	A	1320	4	11,11,12	0.57	0	15,15,17	1.32	2 (13%)
2	NAG	A	1321	1	14,14,15	0.60	0	15,19,21	1.21	1 (6%)
2	NAG	A	1322	1,2	14,14,15	0.62	0	15,19,21	0.94	1 (6%)
2	NAG	A	1323	3,2	14,14,15	0.65	0	15,19,21	1.07	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	A	1324	2	11,11,12	0.42	0	15,15,17	1.70	2 (13%)
2	NAG	A	1325	1	14,14,15	0.51	0	15,19,21	0.98	0
2	NAG	A	1326	1,2	14,14,15	0.54	0	15,19,21	1.04	1 (6%)
2	NAG	A	1327	3,2	14,14,15	0.55	0	15,19,21	1.05	1 (6%)
3	BMA	A	1328	2	11,11,12	0.48	0	15,15,17	1.15	2 (13%)
2	NAG	A	1329	1,2	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
2	NAG	A	1330	3,2	14,14,15	0.55	0	15,19,21	1.19	1 (6%)
3	BMA	A	1331	2,4	11,11,12	0.53	0	15,15,17	1.26	2 (13%)
4	MAN	A	1332	3,4	11,11,12	0.74	0	15,15,17	1.34	1 (6%)
4	MAN	A	1333	4	11,11,12	0.59	0	15,15,17	1.05	2 (13%)
2	NAG	A	1334	1,2	14,14,15	0.63	0	15,19,21	1.26	1 (6%)
2	NAG	A	1335	3,2	14,14,15	0.51	0	15,19,21	1.38	2 (13%)
3	BMA	A	1336	2,4	11,11,12	0.36	0	15,15,17	0.76	0
4	MAN	A	1337	3	11,11,12	0.61	0	15,15,17	1.11	2 (13%)
4	MAN	A	1338	3,4	11,11,12	0.62	0	15,15,17	0.93	0
4	MAN	A	1339	4	11,11,12	0.61	0	15,15,17	1.27	1 (6%)
4	MAN	A	1340	4	11,11,12	0.63	0	15,15,17	1.04	1 (6%)
2	NAG	B	1301	1,2	14,14,15	0.76	0	15,19,21	1.74	3 (20%)
2	NAG	B	1302	3,2	14,14,15	0.56	0	15,19,21	1.43	1 (6%)
3	BMA	B	1303	2,4	11,11,12	0.63	0	15,15,17	0.83	0
4	MAN	B	1304	3	11,11,12	0.64	0	15,15,17	1.00	1 (6%)
2	NAG	B	1305	1,2	14,14,15	0.64	0	15,19,21	1.22	1 (6%)
2	NAG	B	1306	3,2	14,14,15	0.48	0	15,19,21	1.19	1 (6%)
3	BMA	B	1307	2,4	11,11,12	0.54	0	15,15,17	0.67	0
4	MAN	B	1308	3	11,11,12	0.58	0	15,15,17	1.06	2 (13%)
4	MAN	B	1309	3,4	11,11,12	0.67	0	15,15,17	0.96	1 (6%)
4	MAN	B	1310	4	11,11,12	0.56	0	15,15,17	1.22	2 (13%)
2	NAG	B	1311	1,2	14,14,15	0.61	0	15,19,21	1.13	1 (6%)
2	NAG	B	1312	3,2	14,14,15	0.53	0	15,19,21	1.21	2 (13%)
3	BMA	B	1313	2,4	11,11,12	0.86	1 (9%)	15,15,17	2.24	4 (26%)
4	MAN	B	1314	3	11,11,12	0.58	0	15,15,17	1.04	2 (13%)
2	NAG	B	1315	1,2	14,14,15	0.63	0	15,19,21	1.16	1 (6%)
2	NAG	B	1316	3,2	14,14,15	0.54	0	15,19,21	1.09	1 (6%)
3	BMA	B	1317	2,4	11,11,12	0.62	0	15,15,17	1.64	3 (20%)
4	MAN	B	1318	3	11,11,12	0.57	0	15,15,17	0.87	1 (6%)
4	MAN	B	1319	3,4	11,11,12	0.62	0	15,15,17	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	B	1320	4	11,11,12	0.53	0	15,15,17	1.22	1 (6%)
4	MAN	B	1321	4	11,11,12	0.58	0	15,15,17	1.31	2 (13%)
2	NAG	B	1322	1	14,14,15	0.59	0	15,19,21	1.22	1 (6%)
2	NAG	B	1323	1,2	14,14,15	0.62	0	15,19,21	0.95	1 (6%)
2	NAG	B	1324	3,2	14,14,15	0.66	0	15,19,21	1.06	1 (6%)
3	BMA	B	1325	2,4	11,11,12	0.43	0	15,15,17	1.70	2 (13%)
4	MAN	B	1326	3	11,11,12	0.54	0	15,15,17	0.88	1 (6%)
2	NAG	B	1327	1	14,14,15	0.51	0	15,19,21	0.97	0
2	NAG	B	1328	1,2	14,14,15	0.56	0	15,19,21	1.05	1 (6%)
2	NAG	B	1329	3,2	14,14,15	0.54	0	15,19,21	1.06	1 (6%)
3	BMA	B	1330	2	11,11,12	0.48	0	15,15,17	1.16	2 (13%)
2	NAG	B	1331	1,2	14,14,15	0.58	0	15,19,21	1.05	1 (6%)
2	NAG	B	1332	3,2	14,14,15	0.56	0	15,19,21	1.20	1 (6%)
3	BMA	B	1333	2,4	11,11,12	0.55	0	15,15,17	1.25	2 (13%)
4	MAN	B	1334	3	11,11,12	0.65	0	15,15,17	0.87	1 (6%)
4	MAN	B	1335	3,4	11,11,12	0.75	0	15,15,17	1.34	1 (6%)
4	MAN	B	1336	4	11,11,12	0.59	0	15,15,17	1.06	2 (13%)
2	NAG	B	1337	1,2	14,14,15	0.63	0	15,19,21	1.27	2 (13%)
2	NAG	B	1338	3,2	14,14,15	0.51	0	15,19,21	1.38	2 (13%)
3	BMA	B	1339	2,4	11,11,12	0.38	0	15,15,17	0.76	0
4	MAN	B	1340	3	11,11,12	0.62	0	15,15,17	1.11	2 (13%)
4	MAN	B	1341	3,4	11,11,12	0.63	0	15,15,17	0.92	0
4	MAN	B	1342	4	11,11,12	0.61	0	15,15,17	1.28	1 (6%)
4	MAN	B	1343	4	11,11,12	0.62	0	15,15,17	1.04	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
4	MAN	A	1320	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1321	1	-	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	-	0/2/19/22	0/1/1/1
2	NAG	A	1325	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1326	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1327	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1328	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1329	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1330	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1331	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1332	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1333	4	-	0/2/19/22	0/1/1/1
2	NAG	A	1334	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1335	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1336	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1337	3	-	0/2/19/22	0/1/1/1
4	MAN	A	1338	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	1339	4	-	0/2/19/22	0/1/1/1
4	MAN	A	1340	4	-	0/2/19/22	0/1/1/1
2	NAG	B	1301	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1302	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1303	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1304	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1305	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1306	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1307	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1308	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1309	3,4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	B	1310	4	-	0/2/19/22	0/1/1/1
2	NAG	B	1311	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1312	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1313	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1314	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1315	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1316	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1317	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1318	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1319	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1320	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1321	4	-	0/2/19/22	0/1/1/1
2	NAG	B	1322	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1323	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1324	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1325	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1326	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1327	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1328	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1329	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1330	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1331	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1332	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1333	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1334	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1335	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1336	4	-	0/2/19/22	0/1/1/1
2	NAG	B	1337	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1338	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1339	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1340	3	-	0/2/19/22	0/1/1/1
4	MAN	B	1341	3,4	-	0/2/19/22	0/1/1/1
4	MAN	B	1342	4	-	0/2/19/22	0/1/1/1
4	MAN	B	1343	4	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1312	BMA	C2-C3	2.30	1.55	1.52
3	B	1313	BMA	C2-C3	2.31	1.55	1.52

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1332	NAG	O5-C5-C4	-2.42	106.13	110.13
2	A	1330	NAG	O5-C5-C4	-2.39	106.17	110.13
2	B	1337	NAG	O5-C5-C4	-2.27	106.38	110.13
2	A	1334	NAG	O5-C5-C4	-2.25	106.40	110.13
2	B	1337	NAG	C4-C3-C2	2.03	114.49	111.34

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1337	NAG	C1
2	A	1334	NAG	C1

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	NAG	1	0
2	A	1314	NAG	3	0
2	A	1315	NAG	1	0
4	A	1320	MAN	1	0
2	B	1301	NAG	1	0
2	B	1315	NAG	1	0
2	B	1316	NAG	1	0
4	B	1321	MAN	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	B	7
1	A	6

The worst 5 of 13 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	3.75
1	A	1043:THR	C	1044:GLU	N	2.21
1	B	658:ASN	C	659:CYS	N	2.12
1	A	704:CYS	C	705:PRO	N	2.07
1	A	658:ASN	C	659:CYS	N	2.04

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%)	8.80	1099 (93%) 0 1	241, 248, 360, 360	0
1	B	1171/1212 (96%)	9.89	1117 (95%) 0 1	243, 247, 397, 397	0
All	All	2342/2424 (96%)	9.35	2216 (94%) 0 1	241, 248, 365, 397	0

The worst 5 of 2216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1073	THR	44.3
1	B	1068	GLY	40.0
1	B	835	CYS	37.1
1	A	1070	ASN	36.1
1	B	1203	GLN	35.6

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(\AA^2)	Q<0.9
2	NAG	A	1314	14/15	0.46	2.21	0.03	271,271,271,271	0
2	NAG	A	1301	14/15	0.44	1.71	0.01	242,242,242,242	0
2	NAG	B	1305	14/15	0.79	1.81	-0.01	282,282,282,282	0
2	NAG	B	1315	14/15	0.48	2.13	-0.19	282,282,282,282	0
2	NAG	B	1301	14/15	0.33	1.67	-0.43	243,243,243,243	0
2	NAG	B	1331	14/15	-0.52	3.55	-0.58	308,308,308,308	0
2	NAG	A	1329	14/15	-0.35	2.59	-0.76	314,314,314,314	0
2	NAG	A	1305	14/15	0.59	1.75	-1.15	271,271,271,271	0
2	NAG	B	1327	14/15	0.14	2.40	-	270,270,270,270	0
2	NAG	A	1311	14/15	0.65	1.67	-	271,271,271,271	0
3	BMA	B	1313	11/12	0.09	1.03	-	282,282,282,282	0
2	NAG	A	1335	14/15	0.09	3.39	-	359,359,359,359	0
2	NAG	A	1310	14/15	0.71	1.99	-	271,271,271,271	0
4	MAN	B	1336	11/12	-0.34	1.17	-	308,308,308,308	0
3	BMA	B	1317	11/12	0.73	0.94	-	282,282,282,282	0
3	BMA	A	1328	11/12	-0.16	0.89	-	248,248,248,248	0
4	MAN	B	1340	11/12	0.09	1.51	-	365,365,365,365	0
2	NAG	B	1322	14/15	-0.01	1.98	-	251,251,251,251	0
4	MAN	A	1340	11/12	-0.30	1.60	-	359,359,359,359	0
3	BMA	B	1330	11/12	-0.10	1.55	-	270,270,270,270	0
3	BMA	B	1333	11/12	0.04	1.39	-	308,308,308,308	0
3	BMA	B	1325	11/12	0.71	0.54	-	270,270,270,270	0
2	NAG	A	1323	14/15	0.59	0.62	-	248,248,248,248	0
2	NAG	B	1329	14/15	0.63	1.51	-	270,270,270,270	0
4	MAN	A	1318	11/12	0.41	0.72	-	271,271,271,271	0
4	MAN	B	1321	11/12	-0.21	3.33	-	282,282,282,282	0
2	NAG	B	1306	14/15	0.77	2.40	-	282,282,282,282	0
2	NAG	B	1332	14/15	-0.15	3.29	-	308,308,308,308	0
4	MAN	A	1339	11/12	-0.01	2.96	-	359,359,359,359	0
2	NAG	B	1311	14/15	0.59	2.07	-	282,282,282,282	0
4	MAN	B	1341	11/12	0.10	2.90	-	365,365,365,365	0
3	BMA	A	1312	11/12	0.54	0.80	-	271,271,271,271	0
3	BMA	B	1303	11/12	0.83	0.51	-	243,243,243,243	0
2	NAG	B	1337	14/15	-0.24	2.82	-	365,365,365,365	0
4	MAN	A	1333	11/12	-0.52	2.47	-	314,314,314,314	0
3	BMA	B	1307	11/12	0.28	2.38	-	282,282,282,282	0
4	MAN	A	1304	11/12	0.46	0.98	-	242,242,242,242	0
2	NAG	A	1322	14/15	0.54	0.70	-	248,248,248,248	0
4	MAN	B	1343	11/12	-0.16	1.76	-	365,365,365,365	0
4	MAN	A	1313	11/12	0.60	0.43	-	271,271,271,271	0
2	NAG	A	1326	14/15	0.49	2.04	-	248,248,248,248	0
2	NAG	A	1321	14/15	0.19	1.53	-	240,240,240,240	0
4	MAN	A	1319	11/12	0.09	0.53	-	271,271,271,271	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	1324	14/15	0.10	1.18	-	270,270,270,270	0
3	BMA	A	1331	11/12	-0.17	1.93	-	314,314,314,314	0
4	MAN	B	1326	11/12	0.51	0.39	-	270,270,270,270	0
4	MAN	A	1309	11/12	0.44	1.20	-	271,271,271,271	0
4	MAN	B	1318	11/12	0.76	1.10	-	282,282,282,282	0
3	BMA	A	1303	11/12	0.51	1.03	-	242,242,242,242	0
4	MAN	A	1337	11/12	-0.30	1.50	-	359,359,359,359	0
3	BMA	A	1336	11/12	0.10	2.79	-	359,359,359,359	0
2	NAG	A	1306	14/15	0.82	1.29	-	271,271,271,271	0
4	MAN	B	1319	11/12	0.38	0.93	-	282,282,282,282	0
2	NAG	A	1302	14/15	0.76	1.03	-	242,242,242,242	0
4	MAN	A	1332	11/12	0.18	2.39	-	314,314,314,314	0
2	NAG	A	1325	14/15	0.10	0.83	-	248,248,248,248	0
2	NAG	B	1316	14/15	0.83	1.39	-	282,282,282,282	0
4	MAN	B	1309	11/12	0.29	1.67	-	282,282,282,282	0
2	NAG	B	1312	14/15	0.38	1.19	-	282,282,282,282	0
3	BMA	A	1324	11/12	0.80	0.36	-	248,248,248,248	0
4	MAN	B	1308	11/12	0.19	1.73	-	282,282,282,282	0
4	MAN	B	1320	11/12	0.42	0.64	-	282,282,282,282	0
4	MAN	A	1308	11/12	0.54	0.79	-	271,271,271,271	0
4	MAN	A	1320	11/12	-0.02	1.13	-	271,271,271,271	0
2	NAG	A	1327	14/15	0.59	1.92	-	248,248,248,248	0
2	NAG	B	1323	14/15	0.01	0.96	-	270,270,270,270	0
4	MAN	A	1338	11/12	-0.04	2.37	-	359,359,359,359	0
4	MAN	B	1342	11/12	-0.54	3.79	-	365,365,365,365	0
4	MAN	B	1314	11/12	-0.03	1.35	-	282,282,282,282	0
2	NAG	A	1315	14/15	0.58	1.67	-	271,271,271,271	0
4	MAN	B	1310	11/12	0.19	0.92	-	282,282,282,282	0
2	NAG	B	1302	14/15	0.85	0.89	-	243,243,243,243	0
4	MAN	B	1334	11/12	0.34	0.40	-	308,308,308,308	0
4	MAN	A	1317	11/12	-0.03	0.98	-	271,271,271,271	0
2	NAG	B	1338	14/15	0.19	2.87	-	365,365,365,365	0
2	NAG	B	1328	14/15	0.72	1.08	-	270,270,270,270	0
3	BMA	A	1316	11/12	0.70	1.08	-	271,271,271,271	0
4	MAN	B	1335	11/12	0.43	1.53	-	308,308,308,308	0
3	BMA	B	1339	11/12	0.24	2.98	-	365,365,365,365	0
2	NAG	A	1334	14/15	0.10	2.66	-	359,359,359,359	0
3	BMA	A	1307	11/12	0.68	0.78	-	271,271,271,271	0
2	NAG	A	1330	14/15	0.24	2.91	-	314,314,314,314	0
4	MAN	B	1304	11/12	0.75	0.54	-	243,243,243,243	0

6.5 Other polymers [i](#)

There are no such residues in this entry.