



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:50 PM GMT

PDB ID : 1FV2
Title : The Hc fragment of tetanus toxin complexed with an analogue of its ganglioside receptor GT1B
Authors : Fotinou, C.; Emsley, P.; Black, I.; Ando, H.; Ishida, H.; Kiso, M.; Sinha, K.A.; Fairweather, N.F.; Isaacs, N.W.
Deposited on : 2000-09-18
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

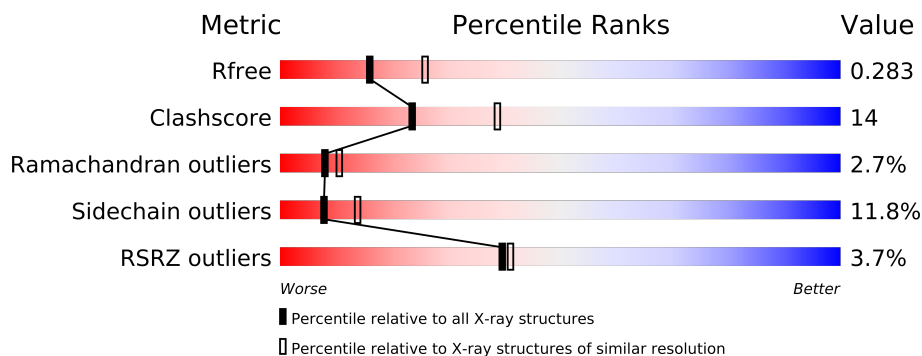
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	472	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	CEQ	A	8[A]	-	X
4	CEQ	A	8[B]	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3893 atoms, of which 0 are hydrogen and 0 are deuterium.

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 TETANUS TOXIN HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	451	3648	2334	611	693	10	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	see remark 999	? P04958
A	845	GLY	-	see remark 999	? P04958
A	846	SER	-	see remark 999	? P04958
A	847	SER	-	see remark 999	? P04958
A	848	HIS	-	see remark 999	? P04958
A	849	HIS	-	see remark 999	? P04958
A	850	HIS	-	see remark 999	? P04958
A	851	HIS	-	see remark 999	? P04958
A	852	HIS	-	see remark 999	? P04958
A	853	HIS	-	see remark 999	? P04958
A	854	SER	-	see remark 999	? P04958
A	855	SER	-	see remark 999	? P04958
A	856	GLY	-	see remark 999	? P04958
A	857	LEU	-	see remark 999	? P04958
A	858	VAL	-	see remark 999	? P04958
A	859	PRO	-	see remark 999	? P04958
A	860	ARG	-	see remark 999	? P04958
A	861	GLY	-	see remark 999	? P04958
A	862	SER	-	see remark 999	? P04958
A	863	HIS	-	see remark 999	? P04958
A	864	MET	-	see remark 999	? P04958

- Molecule 2 is a polymer of unknown type called SUGAR (GLC-GAL-NGA-GAL-NAN-SLB-NAN).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	7	Total	C	N	O	0	0
			108	59	4	45		

There are 21 discrepancies between the modelled and reference sequences:

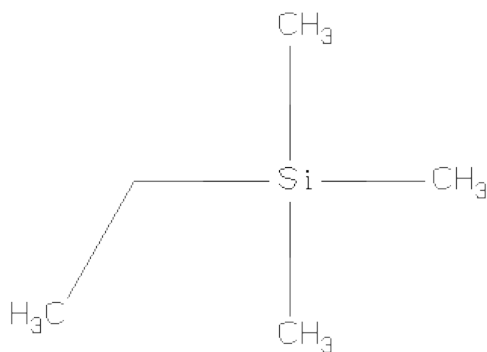
Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	see remark 999	? P04958
A	845	GLY	-	see remark 999	? P04958
A	846	SER	-	see remark 999	? P04958
A	847	SER	-	see remark 999	? P04958
A	848	HIS	-	see remark 999	? P04958
A	849	HIS	-	see remark 999	? P04958
A	850	HIS	-	see remark 999	? P04958
A	851	HIS	-	see remark 999	? P04958
A	852	HIS	-	see remark 999	? P04958
A	853	HIS	-	see remark 999	? P04958
A	854	SER	-	see remark 999	? P04958
A	855	SER	-	see remark 999	? P04958
A	856	GLY	-	see remark 999	? P04958
A	857	LEU	-	see remark 999	? P04958
A	858	VAL	-	see remark 999	? P04958
A	859	PRO	-	see remark 999	? P04958
A	860	ARG	-	see remark 999	? P04958
A	861	GLY	-	see remark 999	? P04958
A	862	SER	-	see remark 999	? P04958
A	863	HIS	-	see remark 999	? P04958
A	864	MET	-	see remark 999	? P04958

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ETHYL-TRIMETHYL-SILANE (three-letter code: CEQ) (formula: C₅H₁₄Si).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	Si	0	1
			12	10	2		

- Molecule 5 is water.

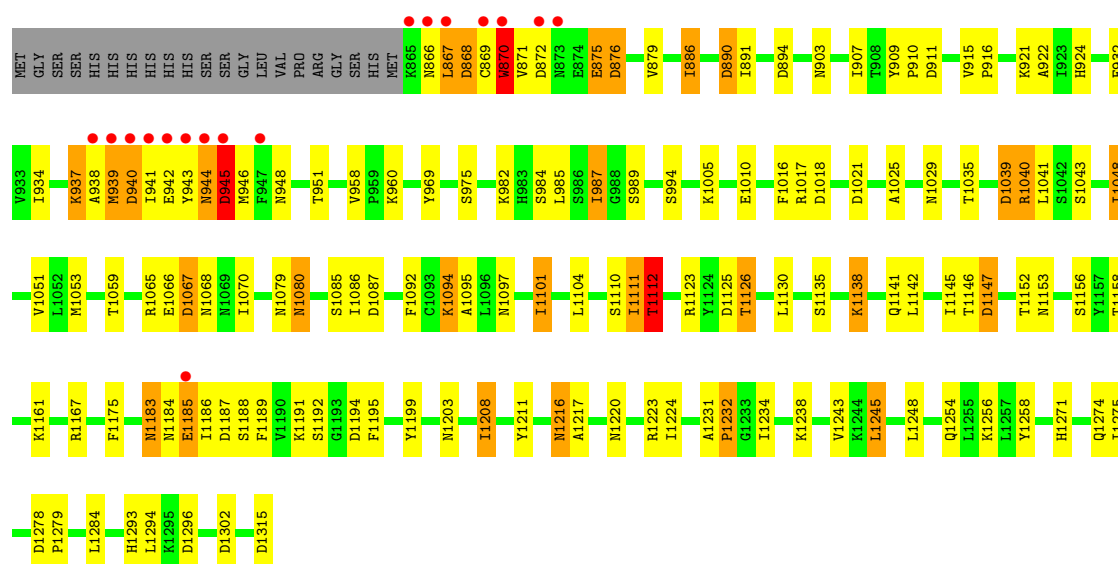
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	120	Total 120	O 120	0	0

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: TETANUS TOXIN HEAVY CHAIN

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	45.85Å 52.17Å 117.35Å 90.00° 99.55° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 39.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.50) 99.3 (39.93-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.224 , 0.276 0.232 , 0.283	Depositor DCC
R_{free} test set	583 reflections (3.15%)	DCC
Wilson B-factor (Å ²)	41.5	Xtriage
Anisotropy	0.554	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.2	EDS
Estimated twinning fraction	0.038 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 19086 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3893	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NGA, PO4, SIA, GAL, CEQ, SLB

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	0.86	0/3731	1.07	14/5064 (0.3%)

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
2	A	1	0

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	894	ASP	CB-CG-OD2	8.02	125.51	118.30
1	A	1039	ASP	CB-CG-OD2	7.84	125.35	118.30
1	A	1067	ASP	CB-CG-OD2	7.59	125.14	118.30
1	A	911	ASP	CB-CG-OD2	7.41	124.96	118.30
1	A	890	ASP	CB-CG-OD2	6.57	124.21	118.30
1	A	1147	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	1101	ILE	CG1-CB-CG2	-5.91	98.39	111.40
1	A	945	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	1183	ASN	N-CA-C	5.69	126.37	111.00
1	A	868	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	1125	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	1021	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	940	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	1315	ASP	CB-CG-OD2	5.36	123.13	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	6	SLB	C8

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3648	0	3588	93	0
2	A	108	0	86	21	0
3	A	5	0	0	0	0
4	A	12	0	0	0	0
5	A	120	0	0	5	0
All	All	3893	0	3674	107	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (107) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:5:SIA:O2	2:A:5:SIA:C2	1.65	1.44
1:A:987:ILE:HD12	1:A:987:ILE:H	1.18	1.03
2:A:7:SIA:H7	2:A:7:SIA:H112	1.39	1.00
2:A:7:SIA:H7	2:A:7:SIA:C11	1.96	0.95
1:A:1271:HIS:HB2	2:A:4:GAL:O6	1.64	0.95
2:A:7:SIA:C7	2:A:7:SIA:H112	2.01	0.91
1:A:946:MET:SD	1:A:1065:ARG:HG2	2.13	0.89
1:A:987:ILE:H	1:A:987:ILE:CD1	1.93	0.80
1:A:1293:HIS:HB3	1:A:1296:ASP:OD2	1.83	0.79
1:A:869:CYS:HB2	1:A:870:TRP:CD1	2.18	0.78
1:A:939:MET:HA	1:A:942:GLU:CD	2.10	0.72
2:A:5:SIA:O2	2:A:5:SIA:C3	2.39	0.71
1:A:944:ASN:O	1:A:948:ASN:HB2	1.91	0.71
1:A:1040:ARG:HD3	5:A:1428:HOH:O	1.92	0.69
1:A:1271:HIS:CB	2:A:4:GAL:O6	2.41	0.69
1:A:1048:ILE:HG13	1:A:1053:MET:HG3	1.73	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1123:ARG:HE	1:A:1189:PHE:HE1	1.41	0.68
1:A:1186:ILE:HG22	1:A:1187:ASP:H	1.57	0.68
1:A:903:ASN:O	1:A:938:ALA:HB2	1.94	0.68
1:A:868:ASP:HB3	1:A:1094:LYS:HB2	1.76	0.67
1:A:1195:PHE:HE1	1:A:1258:TYR:CE1	2.13	0.65
1:A:1231:ALA:HB1	1:A:1232:PRO:HD2	1.79	0.65
1:A:869:CYS:HB2	1:A:870:TRP:HD1	1.60	0.65
2:A:5:SIA:O6	2:A:5:SIA:O2	2.13	0.64
1:A:938:ALA:O	1:A:942:GLU:HG3	1.97	0.64
1:A:1138:LYS:HE3	1:A:1153:ASN:OD1	1.98	0.64
2:A:5:SIA:O2	2:A:5:SIA:C1	2.41	0.64
1:A:945:ASP:CB	1:A:1066:GLU:OE1	2.46	0.63
1:A:1216:ASN:HD22	1:A:1217:ALA:H	1.45	0.63
1:A:1080:ASN:HB2	5:A:1355:HOH:O	1.99	0.63
1:A:876:ASP:HB2	1:A:879:VAL:HG23	1.79	0.62
1:A:945:ASP:HB2	1:A:1066:GLU:OE1	2.00	0.62
1:A:1271:HIS:HB2	2:A:4:GAL:C6	2.29	0.61
1:A:909:TYR:HB3	1:A:910:PRO:HD2	1.83	0.61
2:A:7:SIA:H112	2:A:7:SIA:O7	2.03	0.58
1:A:1141:GLN:HG3	1:A:1142:LEU:N	2.19	0.57
1:A:1254:GLN:NE2	1:A:1302:ASP:OD1	2.36	0.57
2:A:5:SIA:C10	2:A:5:SIA:H7	2.35	0.57
1:A:1216:ASN:HD22	1:A:1217:ALA:N	2.03	0.56
1:A:1211:TYR:CE1	1:A:1223:ARG:HB3	2.41	0.56
1:A:1141:GLN:HG3	1:A:1142:LEU:H	1.71	0.56
1:A:987:ILE:HD12	1:A:987:ILE:N	2.02	0.56
1:A:1199:TYR:CE2	1:A:1208:ILE:HG12	2.42	0.54
1:A:870:TRP:CD1	1:A:870:TRP:N	2.75	0.54
1:A:943:TYR:CE1	1:A:946:MET:HB3	2.43	0.53
1:A:1186:ILE:HG22	1:A:1187:ASP:N	2.23	0.53
1:A:909:TYR:HB3	1:A:910:PRO:CD	2.39	0.53
1:A:1183:ASN:N	1:A:1183:ASN:OD1	2.43	0.52
1:A:1271:HIS:ND1	2:A:4:GAL:O6	2.41	0.52
1:A:937:LYS:HD3	1:A:1070:ILE:HD11	1.90	0.52
1:A:1211:TYR:CD1	1:A:1223:ARG:HB3	2.46	0.51
1:A:943:TYR:O	1:A:945:ASP:N	2.45	0.50
1:A:1183:ASN:ND2	5:A:1423:HOH:O	2.45	0.50
1:A:1271:HIS:HA	2:A:4:GAL:O4	2.12	0.49
1:A:1111:ILE:HD12	1:A:1111:ILE:N	2.29	0.48
1:A:1130:LEU:HG	1:A:1175:PHE:CD1	2.48	0.48
1:A:1256:LYS:HD3	1:A:1258:TYR:CZ	2.48	0.48
1:A:924:HIS:HD2	1:A:1085:SER:OG	1.97	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1191:LYS:O	1:A:1194:ASP:HB2	2.12	0.48
1:A:951:THR:HB	1:A:1092:PHE:HB2	1.95	0.47
2:A:3:NGA:H1	2:A:6:SLB:O1A	2.14	0.47
1:A:1271:HIS:CG	2:A:4:GAL:O6	2.68	0.46
1:A:922:ALA:HB1	1:A:1087:ASP:HB2	1.96	0.46
1:A:1051:VAL:O	1:A:1053:MET:HG2	2.16	0.46
1:A:1039:ASP:O	1:A:1041:LEU:N	2.44	0.46
1:A:1123:ARG:HB2	1:A:1126:THR:HG21	1.97	0.46
1:A:939:MET:HA	1:A:942:GLU:CG	2.46	0.45
2:A:7:SIA:H7	2:A:7:SIA:H113	1.93	0.45
1:A:1097:ASN:O	1:A:1101:ILE:HD12	2.16	0.45
1:A:1130:LEU:HG	1:A:1175:PHE:CE1	2.51	0.45
1:A:1195:PHE:CE1	1:A:1258:TYR:CE1	3.01	0.44
1:A:1278:ASP:HB3	1:A:1279:PRO:CD	2.47	0.44
2:A:7:SIA:C7	2:A:7:SIA:C11	2.76	0.43
1:A:1112:THR:O	1:A:1191:LYS:HB3	2.18	0.43
1:A:890:ASP:OD1	1:A:891:ILE:N	2.51	0.43
1:A:945:ASP:OD1	1:A:1066:GLU:OE1	2.36	0.43
1:A:1271:HIS:HA	2:A:4:GAL:HO4	1.83	0.43
1:A:932:GLU:OE2	1:A:934:ILE:HD11	2.18	0.43
1:A:943:TYR:CZ	1:A:946:MET:HB3	2.54	0.43
1:A:866:ASN:HB3	1:A:867:LEU:H	1.72	0.43
1:A:932:GLU:HG2	1:A:934:ILE:HD12	2.01	0.42
1:A:1094:LYS:HD2	1:A:1095:ALA:O	2.19	0.42
1:A:915:VAL:HB	1:A:916:PRO:HD2	2.01	0.42
1:A:1185:GLU:O	1:A:1186:ILE:HG12	2.19	0.42
1:A:1224:ILE:HD13	1:A:1275:ILE:HD11	2.01	0.42
1:A:1111:ILE:H	1:A:1111:ILE:HD12	1.82	0.42
1:A:1085:SER:C	1:A:1086:ILE:HG13	2.39	0.42
1:A:1039:ASP:C	1:A:1041:LEU:H	2.23	0.42
1:A:939:MET:HA	1:A:942:GLU:HG3	2.02	0.42
1:A:1016:PHE:CE1	1:A:1053:MET:HE2	2.55	0.42
1:A:1123:ARG:NE	1:A:1189:PHE:HE1	2.13	0.42
1:A:867:LEU:H	1:A:867:LEU:HG	1.67	0.42
1:A:1231:ALA:HB3	1:A:1234:ILE:HB	2.00	0.41
1:A:975:SER:HA	1:A:994:SER:HB3	2.01	0.41
1:A:989:SER:HB2	1:A:1005:LYS:O	2.20	0.41
1:A:1145:ILE:O	1:A:1146:THR:OG1	2.25	0.41
1:A:1231:ALA:CB	1:A:1232:PRO:HD2	2.44	0.41
1:A:969:TYR:CD2	1:A:1079:ASN:HB2	2.56	0.41
1:A:1156:SER:OG	5:A:1399:HOH:O	2.22	0.41
1:A:1018:ASP:OD2	1:A:1025:ALA:HB1	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:937:LYS:HE3	1:A:1067:ASP:O	2.21	0.41
2:A:3:NGA:H1	2:A:6:SLB:C1	2.51	0.41
1:A:875:GLU:H	1:A:875:GLU:HG2	1.71	0.41
1:A:921:LYS:HE2	5:A:1424:HOH:O	2.20	0.41
1:A:886:ILE:HG13	1:A:941:ILE:HG21	2.03	0.41
1:A:1245:LEU:HA	1:A:1245:LEU:HD12	1.85	0.41
2:A:6:SLB:O10	2:A:6:SLB:H7	2.21	0.40

There are no symmetry-related clashes.

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	449/472 (95%)	397 (88%)	40 (9%)	12 (3%)	8 10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	870	TRP
1	A	872	ASP
1	A	944	ASN
1	A	876	ASP
1	A	1110	SER
1	A	1112	THR
1	A	1040	ARG
1	A	1220	ASN
1	A	1294	LEU
1	A	1184	ASN
1	A	1232	PRO
1	A	1029	ASN

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	407/425 (96%)	359 (88%)	48 (12%)	8 14

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	867	LEU
1	A	870	TRP
1	A	871	VAL
1	A	875	GLU
1	A	886	ILE
1	A	907	ILE
1	A	937	LYS
1	A	939	MET
1	A	940	ASP
1	A	945	ASP
1	A	958	VAL
1	A	960	LYS
1	A	982	LYS
1	A	984	SER
1	A	985	LEU
1	A	987	ILE
1	A	1010	GLU
1	A	1017	ARG
1	A	1035	THR
1	A	1043	SER
1	A	1048	ILE
1	A	1059	THR
1	A	1068	ASN
1	A	1080	ASN
1	A	1094	LYS
1	A	1104	LEU
1	A	1111	ILE
1	A	1112	THR
1	A	1126	THR
1	A	1135	SER
1	A	1138	LYS

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Mol	Chain	Res	Type
1	A	1147	ASP
1	A	1152	THR
1	A	1158	THR
1	A	1161	LYS
1	A	1167	ARG
1	A	1185	GLU
1	A	1188	SER
1	A	1192	SER
1	A	1203	ASN
1	A	1208	ILE
1	A	1216	ASN
1	A	1238	LYS
1	A	1243	VAL
1	A	1245	LEU
1	A	1248	LEU
1	A	1274	GLN
1	A	1284	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	HIS
1	A	936	HIS
1	A	998	ASN
1	A	1029	ASN
1	A	1080	ASN
1	A	1216	ASN
1	A	1272	ASN
1	A	1280	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

7 carbohydrates 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	BGC	A	1	2,4	11,11,12	0.66	0	11,15,17	1.61	2 (18%)
2	GAL	A	2	2	10,10,12	1.63	3 (30%)	8,13,17	1.00	0
2	NGA	A	3	2	13,14,15	0.92	0	14,19,21	0.68	0
2	GAL	A	4	2	11,11,12	0.84	0	10,15,17	0.72	0
2	SIA	A	5	2	21,21,21	5.96	2 (9%)	31,31,31	3.87	11 (35%)
2	SLB	A	6	2	21,21,21	1.11	2 (9%)	31,31,31	2.49	4 (12%)
2	SIA	A	7	2	20,20,21	3.53	2 (10%)	23,28,31	2.13	3 (13%)

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	BGC	A	1	2,4	-	0/2/18/22	0/1/1/1
2	GAL	A	2	2	-	0/2/15/22	0/1/1/1
2	NGA	A	3	2	-	0/6/22/26	0/1/1/1
2	GAL	A	4	2	-	0/2/18/22	0/1/1/1
2	SIA	A	5	2	-	0/20/38/38	0/1/1/1
2	SLB	A	6	2	1/1/8/9	0/20/38/38	0/1/1/1
2	SIA	A	7	2	-	1/15/34/38	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5	SIA	O2-C2	19.84	1.65	1.39
2	A	5	SIA	C2-C1	-18.29	1.34	1.53
2	A	7	SIA	O6-C2	14.88	1.42	1.28
2	A	2	GAL	C4-C3	3.22	1.54	1.38
2	A	7	SIA	O1B-C1	-3.14	1.20	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	GAL	C1-C2	-2.66	1.50	1.53
2	A	2	GAL	C6-C5	2.65	1.54	1.50
2	A	6	SLB	C4-C5	2.47	1.55	1.53
2	A	6	SLB	O1B-C1	-2.20	1.21	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5	SIA	O2-C2-O6	-12.87	87.65	109.95
2	A	6	SLB	O8-C8-C9	11.71	136.49	109.20
2	A	7	SIA	O6-C2-C3	-8.17	114.23	124.91
2	A	5	SIA	O2-C2-C3	-7.90	98.17	109.67
2	A	5	SIA	O9-C9-C8	-7.84	93.51	111.05
2	A	5	SIA	O6-C2-C3	7.00	114.35	110.22
2	A	5	SIA	C2-O6-C6	-6.99	103.28	113.93
2	A	6	SLB	O6-C6-C5	4.69	113.98	109.55
2	A	5	SIA	C3-C2-C1	4.60	121.29	113.58
2	A	1	BGC	O5-C1-C2	-3.69	104.15	109.86
2	A	7	SIA	O1B-C1-O1A	-3.53	115.33	123.35
2	A	5	SIA	O6-C2-C1	3.50	118.79	106.17
2	A	5	SIA	C2-C3-C4	-3.17	104.82	110.75
2	A	1	BGC	O6-C6-C5	-2.70	108.41	112.42
2	A	6	SLB	C7-C6-C5	-2.60	110.41	114.24
2	A	5	SIA	O6-C6-C7	2.45	109.49	106.34
2	A	7	SIA	O7-C7-C8	2.44	114.91	108.74
2	A	5	SIA	C6-C5-N5	2.39	115.16	110.99
2	A	5	SIA	O6-C6-C5	2.18	111.61	109.55
2	A	6	SLB	O1B-C1-O1A	-2.17	116.93	123.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	6	SLB	C8

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	7	SIA	O10-C10-N5-C5

There are no ring outliers.

5.6 Ligand geometry

3 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
3	PO4	A	201	-	4,4,4	0.68	0	6,6,6	0.31	0
4	CEQ	A	8[A]	2	5,5,5	2.28	4 (80%)	7,7,7	0.60	0
4	CEQ	A	8[B]	2	5,5,5	2.35	4 (80%)	7,7,7	0.88	0

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
3	PO4	A	201	-	-	0/0/0/0	0/0/0/0
4	CEQ	A	8[A]	2	-	0/3/3/3	0/0/0/0
4	CEQ	A	8[B]	2	-	0/3/3/3	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8[B]	CEQ	SI1-C5	-3.35	1.79	1.87
4	A	8[A]	CEQ	SI1-C5	-3.32	1.79	1.87
4	A	8[B]	CEQ	SI1-C2	-2.36	1.79	1.86
4	A	8[A]	CEQ	SI1-C4	-2.33	1.79	1.86
4	A	8[B]	CEQ	SI1-C3	-2.32	1.79	1.86
4	A	8[B]	CEQ	SI1-C4	-2.28	1.79	1.86
4	A	8[A]	CEQ	SI1-C3	-2.26	1.79	1.86
4	A	8[A]	CEQ	SI1-C2	-2.06	1.80	1.86

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	451/472 (95%)	0.01	17 (3%) 38 40	19, 34, 66, 103	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	945	ASP	6.6
1	A	944	ASN	6.2
1	A	873	ASN	5.8
1	A	942	GLU	5.4
1	A	872	ASP	5.4
1	A	866	ASN	5.1
1	A	941	ILE	4.5
1	A	940	ASP	4.3
1	A	865	LYS	4.1
1	A	1185	GLU	3.9
1	A	870	TRP	3.5
1	A	943	TYR	3.3
1	A	939	MET	3.0
1	A	867	LEU	2.5
1	A	869	CYS	2.5
1	A	947	PHE	2.2
1	A	938	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SIA	A	5	21/21	0.25	6.32	42,48,51,53	0
2	GAL	A	2	10/12	0.14	4.20	38,39,42,42	0
2	SLB	A	6	21/21	0.18	2.74	48,53,58,61	0
2	SIA	A	7	20/21	0.20	1.84	39,48,56,59	0
2	GAL	A	4	11/12	0.17	0.78	41,43,46,51	0
2	NGA	A	3	14/15	0.14	-0.12	37,41,46,46	0
2	BGC	A	1	11/12	0.11	-0.79	39,45,54,63	0

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CEQ	A	8[A]	6/6	0.32	8.06	80,87,88,88	6
4	CEQ	A	8[B]	6/6	0.32	7.35	73,76,77,77	6
3	PO4	A	201	5/5	0.15	0.39	48,49,50,52	0

6.5 Other polymers ⓘ

There are no such residues in this entry.