



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:00 PM UTC

PDB ID : 1FV2 / pdb_00001fv2
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

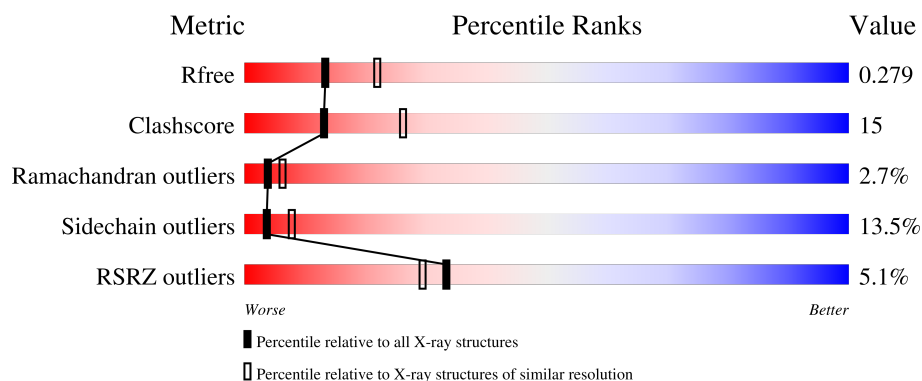
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	472	5% 61% 27% 8% .
2	B	7	29% 71%

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	GAL	B	4	-	-	X	-
2	SLB	B	6	X	-	-	-
4	CEQ	A	8[A]	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3893 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.

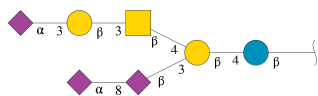
- Molecule 1 is a protein called TETANUS TOXIN HEAVY CHAIN.

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:

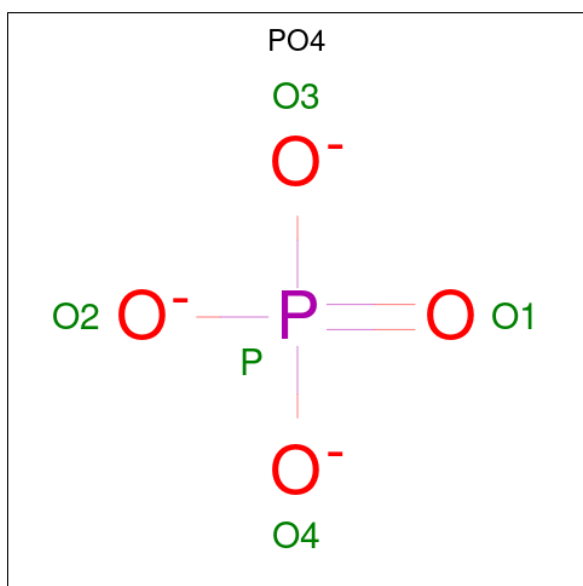
Chain	Residue	Modelled	Actual	Comment	Reference
A	844	MET	-	see remark 999	? P04958
A	845	GLY	-	see remark 999	? P04958
A	846	SER	-	see remark 999	? P04958
A	847	SER	-	see remark 999	? P04958
A	848	HIS	-	see remark 999	? P04958
A	849	HIS	-	see remark 999	? P04958
A	850	HIS	-	see remark 999	? P04958
A	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 an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



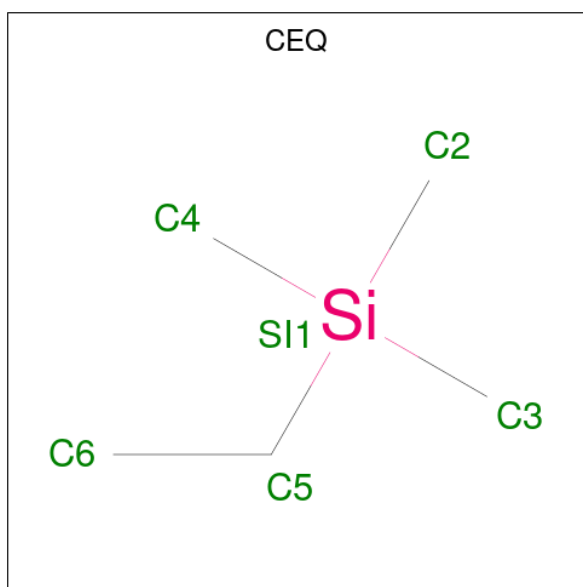
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			108	59	4	45			

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is ETHYL-TRIMETHYL-SILANE (CCD ID: CEQ) (formula: $C_5H_{14}Si$).



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

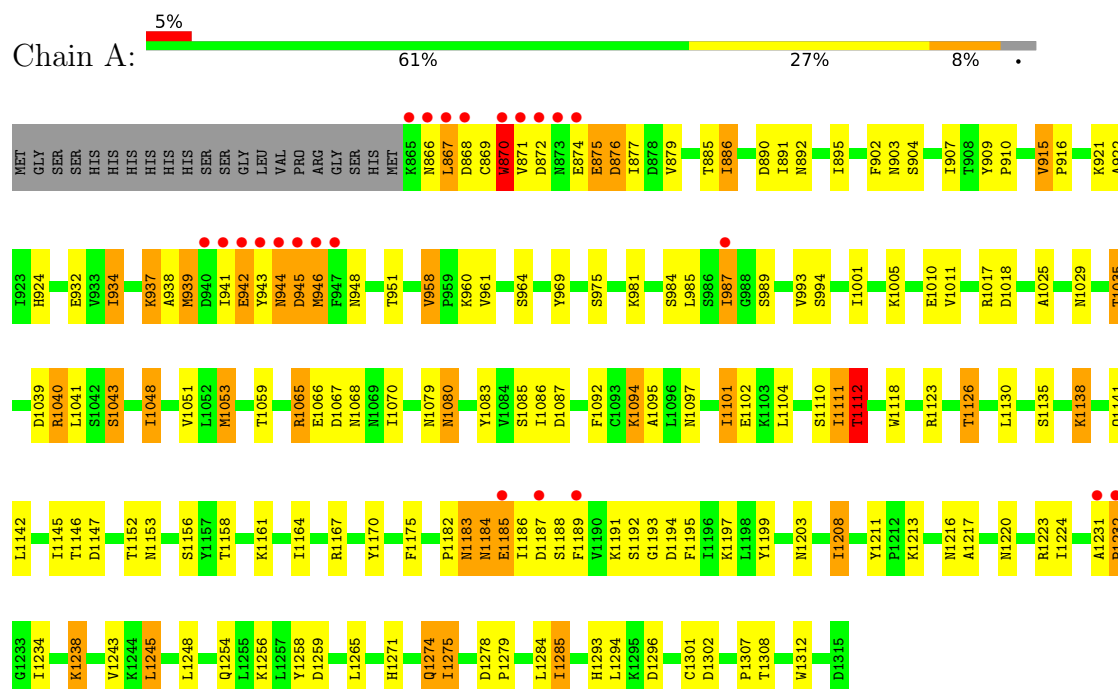
- Molecule 5 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: TETANUS TOXIN HEAVY CHAIN



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-8)-N-acetyl-beta-neuraminic acid-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose



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 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.50) 99.3 (40.00-2.50)	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 5.0	Depositor
R, R_{free}	0.224 , 0.276 0.231 , 0.279	Depositor DCC
R_{free} test set	583 reflections (3.05%)	wwPDB-VP
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 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.038 for h,-k,-h-l	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.

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: SLB, BGC, CEQ, SIA, NGA, GAL, PO4

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	1.10	6/3731 (0.2%)	1.34	26/5064 (0.5%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1053	MET	SD-CE	-6.79	1.62	1.79
1	A	946	MET	SD-CE	6.28	1.95	1.79
1	A	1308	THR	CA-CB	5.32	1.62	1.53
1	A	958	VAL	CA-C	-5.26	1.47	1.52
1	A	1301	CYS	C-O	-5.18	1.17	1.24
1	A	1001	ILE	C-O	-5.13	1.18	1.24

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1183	ASN	N-CA-C	14.12	126.37	110.97
1	A	1043	SER	N-CA-C	8.78	122.22	108.79
1	A	1065	ARG	N-CA-C	-8.43	99.66	110.53
1	A	1265	LEU	N-CA-C	-7.63	104.00	113.38
1	A	1011	VAL	N-CA-C	6.90	117.78	108.11
1	A	1035	THR	CB-CA-C	6.30	122.17	109.38
1	A	1274	GLN	N-CA-C	6.19	118.38	107.61
1	A	981	LYS	N-CA-C	6.08	119.16	110.10
1	A	1118	TRP	N-CA-C	-5.99	105.97	113.28
1	A	1193	GLY	N-CA-C	-5.95	106.87	114.37
1	A	942	GLU	N-CA-C	5.87	119.71	112.54
1	A	1001	ILE	N-CA-C	5.73	116.19	108.17
1	A	877	ILE	N-CA-C	-5.72	105.16	110.53
1	A	1182	PRO	CA-C-N	5.68	128.14	120.65
1	A	1182	PRO	C-N-CA	5.68	128.14	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1285	ILE	N-CA-C	5.59	116.75	108.65
1	A	1197	LYS	N-CA-C	-5.58	99.92	109.24
1	A	1307	PRO	CA-C-O	-5.54	115.31	122.13
1	A	993	VAL	CB-CA-C	-5.53	102.89	110.96
1	A	902	PHE	N-CA-C	-5.46	103.70	110.41
1	A	1238	LYS	N-CA-C	5.32	120.95	113.02
1	A	904	SER	N-CA-C	-5.27	98.99	108.48
1	A	1170	TYR	N-CA-C	5.26	118.99	112.58
1	A	915	VAL	CB-CA-C	-5.22	104.25	109.89
1	A	964	SER	CB-CA-C	-5.11	102.16	110.85
1	A	1275	ILE	N-CA-C	5.02	116.18	108.71

There are no chirality outliers.

There are no planarity outliers.

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	3648	0	3588	98	0
2	B	108	0	87	18	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	3675	110	0

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 15.

All (110) 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:987:ILE:H	1:A:987:ILE:HD12	1.18	1.03
2:B:7:SIA:H112	2:B:7:SIA:H7	1.39	1.00
1:A:1271:HIS:HB2	2:B:4:GAL:O6	1.64	0.95
2:B:7:SIA:H7	2:B:7:SIA:C11	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:SIA:H112	2:B:7:SIA:C7	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	0.77
2:B:4:GAL:O3	2:B: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:B:4:GAL:O6	2.41	0.69
1:A:1048:ILE:HG13	1:A:1053:MET:HG3	1.73	0.69
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:870:TRP:CD1	1:A:870:TRP:H	2.12	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:B:4:GAL:O3	2:B:5:SIA:O6	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:B:4:GAL:O3	2:B: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:B:4:GAL:C6	2.29	0.61
1:A:909:TYR:HB3	1:A:910:PRO:HD2	1.83	0.61
2:B:7:SIA:H112	2:B: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:B:5:SIA:H7	2:B:5:SIA:C10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1145:ILE:O	1:A:1146:THR:OG1	2.25	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:937:LYS:HD3	1:A:1070:ILE:HD11	1.90	0.52
1:A:1271:HIS:ND1	2:B:4:GAL:O6	2.41	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:B: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
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
1:A:1039:ASP:C	1:A:1041:LEU:H	2.23	0.47
1:A:1085:SER:C	1:A:1086:ILE:HG13	2.39	0.47
1:A:922:ALA:HB1	1:A:1087:ASP:HB2	1.96	0.46
1:A:1271:HIS:CG	2:B:4:GAL:O6	2.68	0.46
1:A:1039:ASP:O	1:A:1041:LEU:N	2.44	0.46
1:A:1051:VAL:O	1:A:1053:MET:HG2	2.16	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
1:A:1097:ASN:O	1:A:1101:ILE:HD12	2.16	0.45
2:B:7:SIA:H7	2:B:7:SIA:H113	1.93	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:1312:TRP:CD1	1:A:1312:TRP:C	2.95	0.44
1:A:1278:ASP:HB3	1:A:1279:PRO:CD	2.47	0.44
1:A:1112:THR:O	1:A:1191:LYS:HB3	2.18	0.43
1:A:1285:ILE:C	1:A:1285:ILE:HD12	2.43	0.43
2:B:7:SIA:C11	2:B:7:SIA:C7	2.76	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:932:GLU:OE2	1:A:934:ILE:HD11	2.18	0.43
1:A:866:ASN:HB3	1:A:867:LEU:H	1.72	0.43
1:A:943:TYR:CZ	1:A:946:MET:HB3	2.54	0.43
1:A:869:CYS:O	1:A:870:TRP:C	2.61	0.42
1:A:932:GLU:HG2	1:A:934:ILE:HD12	2.01	0.42
1:A:915:VAL:HB	1:A:916:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:LYS:HD2	1:A:1095:ALA:O	2.19	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:1259:ASP:OD1	1:A:1259:ASP:C	2.62	0.42
1:A:1111:ILE:HD12	1:A:1111:ILE:H	1.82	0.42
1:A:939:MET:HA	1:A:942:GLU:HG3	2.02	0.42
1:A:867:LEU:H	1:A:867:LEU:HG	1.67	0.42
1:A:1123:ARG:NE	1:A:1189:PHE:HE1	2.13	0.42
1:A:1083:TYR:CD1	1:A:1083:TYR:C	2.98	0.41
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
2:B:2:GAL:H3	2:B:6:SLB:H31	1.74	0.41
1:A:1184:ASN:O	1:A:1185:GLU:C	2.59	0.41
1:A:969:TYR:CD2	1:A:1079:ASN:HB2	2.56	0.41
1:A:1018:ASP:OD2	1:A:1025:ALA:HB1	2.21	0.41
1:A:1156:SER:OG	5:A:1399:HOH:O	2.22	0.41
1:A:1231:ALA:CB	1:A:1232:PRO:HD2	2.44	0.41
1:A:875:GLU:H	1:A:875:GLU:HG2	1.71	0.41
1:A:886:ILE:HG13	1:A:941:ILE:HG21	2.03	0.41
1:A:921:LYS:HE2	5:A:1424:HOH:O	2.20	0.41
1:A:937:LYS:HE3	1:A:1067:ASP:O	2.21	0.41
1:A:1245:LEU:HD12	1:A:1245:LEU:HA	1.85	0.41
2:B:6:SLB:H7	2:B:6:SLB:O10	2.21	0.40

There are no symmetry-related clashes.

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	449/472 (95%)	397 (88%)	40 (9%)	12 (3%)	4 6

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%)	352 (86%)	55 (14%)	4 8

All (55) 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	874	GLU
1	A	875	GLU
1	A	885	THR
1	A	886	ILE
1	A	892	ASN
1	A	895	ILE
1	A	907	ILE
1	A	934	ILE
1	A	937	LYS
1	A	939	MET

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Mol	Chain	Res	Type
1	A	945	ASP
1	A	958	VAL
1	A	960	LYS
1	A	961	VAL
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	1101	ILE
1	A	1102	GLU
1	A	1104	LEU
1	A	1111	ILE
1	A	1112	THR
1	A	1126	THR
1	A	1135	SER
1	A	1138	LYS
1	A	1147	ASP
1	A	1152	THR
1	A	1158	THR
1	A	1161	LYS
1	A	1164	ILE
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	1213	LYS
1	A	1238	LYS
1	A	1243	VAL
1	A	1245	LEU
1	A	1248	LEU
1	A	1274	GLN
1	A	1284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	HIS
1	A	998	ASN
1	A	999	ASN
1	A	1013	GLN
1	A	1029	ASN
1	A	1038	ASN
1	A	1080	ASN
1	A	1082	GLN
1	A	1205	ASN
1	A	1216	ASN
1	A	1219	ASN
1	A	1220	ASN
1	A	1280	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 ⓘ

7 monosaccharides 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	B	1	2,4	12,12,12	1.18	1 (8%)	17,17,17	1.91	4 (23%)
2	GAL	B	2	2	11,11,12	1.08	1 (9%)	15,15,17	4.09	3 (20%)
2	NGA	B	3	2	14,14,15	1.06	1 (7%)	17,19,21	1.60	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GAL	B	4	2	11,11,12	1.66	1 (9%)	15,15,17	1.25	1 (6%)
2	SIA	B	5	2	20,20,21	3.43	2 (10%)	21,28,31	2.55	4 (19%)
2	SLB	B	6	2	20,20,21	0.98	2 (10%)	21,28,31	2.97	5 (23%)
2	SIA	B	7	2	20,20,21	3.77	2 (10%)	21,28,31	1.92	5 (23%)

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	B	1	2,4	-	0/2/22/22	0/1/1/1
2	GAL	B	2	2	-	2/2/19/22	0/1/1/1
2	NGA	B	3	2	-	3/6/23/26	0/1/1/1
2	GAL	B	4	2	-	2/2/19/22	0/1/1/1
2	SIA	B	5	2	-	9/18/34/38	0/1/1/1
2	SLB	B	6	2	1/1/8/9	11/18/34/38	0/1/1/1
2	SIA	B	7	2	-	8/18/34/38	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	SIA	C2-C1	-16.21	1.32	1.52
2	B	5	SIA	C2-C1	-14.62	1.34	1.52
2	B	4	GAL	O3-C3	4.79	1.54	1.43
2	B	1	BGC	O4-C4	-3.84	1.33	1.43
2	B	7	SIA	O1B-C1	-3.17	1.20	1.30
2	B	3	NGA	O3-C3	-2.96	1.35	1.43
2	B	6	SLB	O1B-C1	-2.78	1.21	1.30
2	B	2	GAL	O4-C4	-2.74	1.36	1.43
2	B	6	SLB	C4-C5	2.30	1.55	1.53
2	B	5	SIA	O1B-C1	-2.18	1.23	1.30

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	GAL	O4-C4-C5	13.55	142.68	109.32
2	B	6	SLB	O8-C8-C9	12.08	136.49	109.03
2	B	5	SIA	O9-C9-C8	-8.40	93.51	111.16
2	B	2	GAL	O3-C3-C4	6.65	126.04	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	SIA	O6-C2-C1	5.87	118.79	107.72
2	B	7	SIA	O6-C2-C1	4.26	115.76	107.72
2	B	1	BGC	O4-C4-C5	4.19	119.64	109.32
2	B	7	SIA	O1B-C1-O1A	-3.86	115.33	124.08
2	B	3	NGA	O3-C3-C4	3.85	119.44	110.38
2	B	7	SIA	O1B-C1-C2	3.55	121.96	112.71
2	B	1	BGC	O5-C1-C2	-3.50	104.15	110.30
2	B	3	NGA	O3-C3-C2	-3.46	102.22	109.40
2	B	4	GAL	O3-C3-C4	3.34	118.24	110.38
2	B	1	BGC	O4-C4-C3	-3.25	102.71	110.38
2	B	6	SLB	O1B-C1-O1A	-3.15	116.93	124.08
2	B	1	BGC	O5-C5-C4	-2.89	104.48	109.70
2	B	5	SIA	O6-C2-C3	2.82	114.35	110.56
2	B	2	GAL	C3-C4-C5	-2.75	105.24	110.23
2	B	7	SIA	O6-C2-C3	2.73	114.23	110.56
2	B	5	SIA	C6-C5-N5	2.67	115.16	110.91
2	B	7	SIA	O7-C7-C8	2.63	114.91	108.93
2	B	6	SLB	O6-C2-C1	-2.54	102.92	107.72
2	B	6	SLB	O1B-C1-C2	2.49	119.19	112.71
2	B	6	SLB	C5-N5-C10	-2.30	117.71	123.11
2	B	3	NGA	C4-C3-C2	-2.13	107.90	111.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	6	SLB	C8

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	5	SIA	C11-C10-N5-C5
2	B	5	SIA	O10-C10-N5-C5
2	B	6	SLB	C5-C6-C7-C8
2	B	6	SLB	C5-C6-C7-O7
2	B	6	SLB	O6-C6-C7-C8
2	B	6	SLB	O6-C6-C7-O7
2	B	6	SLB	C6-C7-C8-O8
2	B	6	SLB	O7-C7-C8-O8
2	B	7	SIA	C6-C7-C8-C9
2	B	7	SIA	C6-C7-C8-O8
2	B	7	SIA	O7-C7-C8-C9
2	B	7	SIA	C11-C10-N5-C5

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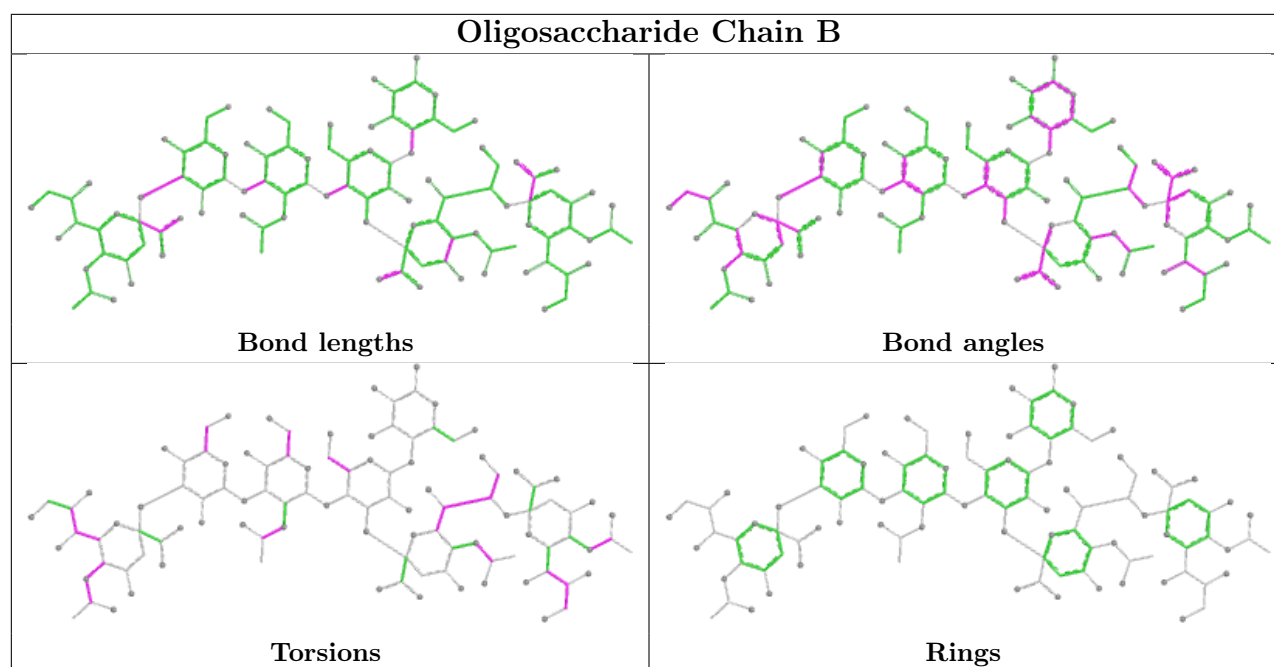
Mol	Chain	Res	Type	Atoms
2	B	7	SIA	O10-C10-N5-C5
2	B	6	SLB	C11-C10-N5-C5
2	B	2	GAL	O5-C5-C6-O6
2	B	6	SLB	O8-C8-C9-O9
2	B	6	SLB	C7-C8-C9-O9
2	B	4	GAL	O5-C5-C6-O6
2	B	7	SIA	O7-C7-C8-O8
2	B	2	GAL	C4-C5-C6-O6
2	B	6	SLB	O10-C10-N5-C5
2	B	5	SIA	O7-C7-C8-O8
2	B	4	GAL	C4-C5-C6-O6
2	B	3	NGA	C8-C7-N2-C2
2	B	3	NGA	O7-C7-N2-C2
2	B	5	SIA	O7-C7-C8-C9
2	B	5	SIA	C6-C7-C8-C9
2	B	5	SIA	C6-C7-C8-O8
2	B	7	SIA	C7-C8-C9-O9
2	B	7	SIA	O8-C8-C9-O9
2	B	3	NGA	O5-C5-C6-O6
2	B	5	SIA	O6-C6-C7-O7
2	B	6	SLB	C6-C7-C8-C9
2	B	5	SIA	C5-C6-C7-O7
2	B	5	SIA	C6-C5-N5-C10

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4	GAL	9	0
2	B	7	SIA	6	0
2	B	6	SLB	2	0
2	B	2	GAL	1	0
2	B	5	SIA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	CEQ	A	8[A]	2	5,5,5	2.53	4 (80%)	7,7,7	0.61	0
3	PO4	A	201	-	4,4,4	1.43	1 (25%)	6,6,6	0.90	0
4	CEQ	A	8[B]	2	5,5,5	2.60	4 (80%)	7,7,7	0.86	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
4	CEQ	A	8[A]	2	-	3/3/3/3	-
4	CEQ	A	8[B]	2	-	1/3/3/3	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8[B]	CEQ	SI1-C5	-3.81	1.79	1.87
4	A	8[A]	CEQ	SI1-C5	-3.78	1.79	1.87
4	A	8[B]	CEQ	SI1-C2	-2.56	1.79	1.87
4	A	8[A]	CEQ	SI1-C4	-2.53	1.79	1.87
4	A	8[B]	CEQ	SI1-C3	-2.53	1.79	1.87
4	A	8[B]	CEQ	SI1-C4	-2.48	1.79	1.87
4	A	8[A]	CEQ	SI1-C3	-2.46	1.79	1.87
4	A	8[A]	CEQ	SI1-C2	-2.25	1.80	1.87
3	A	201	PO4	P-O2	-2.03	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	8[A]	CEQ	C6-C5-SI1-C3
4	A	8[A]	CEQ	C6-C5-SI1-C2
4	A	8[A]	CEQ	C6-C5-SI1-C4
4	A	8[B]	CEQ	C6-C5-SI1-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.21	23 (5%)	33 29	19, 34, 66, 103	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	945	ASP	6.7
1	A	941	ILE	5.9
1	A	944	ASN	4.9
1	A	866	ASN	4.3
1	A	947	PHE	3.9
1	A	870	TRP	3.8
1	A	1185	GLU	3.4
1	A	943	TYR	3.3
1	A	865	LYS	3.3
1	A	872	ASP	3.2
1	A	873	ASN	2.9
1	A	867	LEU	2.7
1	A	987	ILE	2.7
1	A	871	VAL	2.7
1	A	946	MET	2.5
1	A	1187	ASP	2.4
1	A	942	GLU	2.4
1	A	940	ASP	2.3
1	A	874	GLU	2.3
1	A	1232	PRO	2.3
1	A	868	ASP	2.2
1	A	1189	PHE	2.2
1	A	1231	ALA	2.1

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

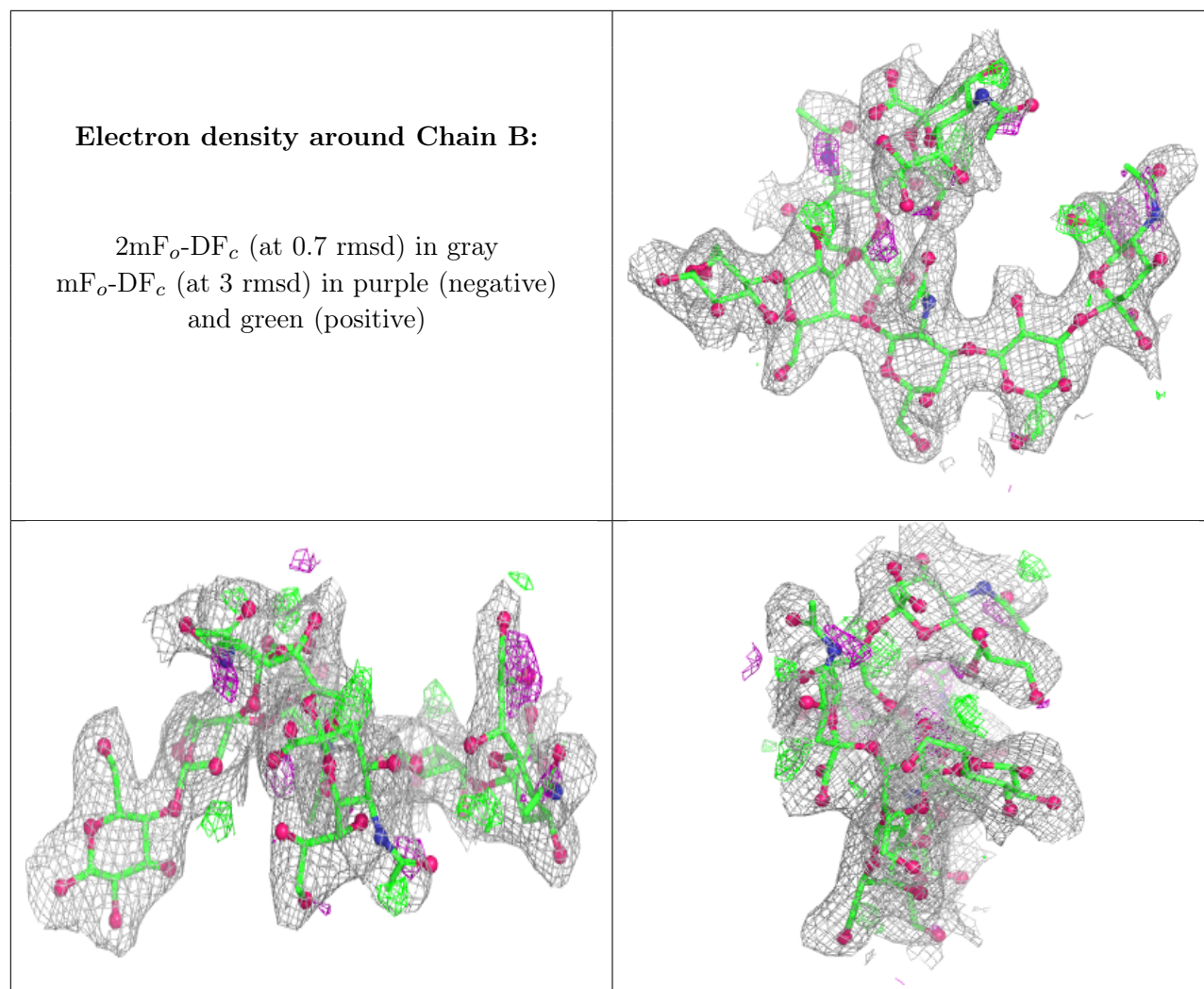
There are no non-standard protein/DNA/RNA residues in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	SIA	B	5	20/21	0.73	0.17	42,49,51,53	0
2	SLB	B	6	20/21	0.76	0.16	48,54,59,61	0
2	SIA	B	7	20/21	0.76	0.16	39,48,56,59	0
2	GAL	B	4	11/12	0.81	0.12	41,43,46,51	0
2	BGC	B	1	12/12	0.85	0.10	38,45,54,63	0
2	GAL	B	2	11/12	0.87	0.10	38,39,42,49	0
2	NGA	B	3	14/15	0.89	0.09	37,41,46,46	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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. 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	B-factors(Å ²)	Q<0.9
4	CEQ	A	8[A]	6/6	0.87	0.29	80,87,88,88	6
4	CEQ	A	8[B]	6/6	0.87	0.29	73,76,77,77	6
3	PO4	A	201	5/5	0.90	0.11	48,49,50,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.