



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 05:47 AM BST

PDB ID : 4KBB
Title : Structure of Botulinum neurotoxin B binding domain in complex with both synaptotagmin II and GD1a
Authors : Berntsson, R.P.A.; Peng, L.; Dong, M.; Stenmark, P.
Deposited on : 2013-04-23
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

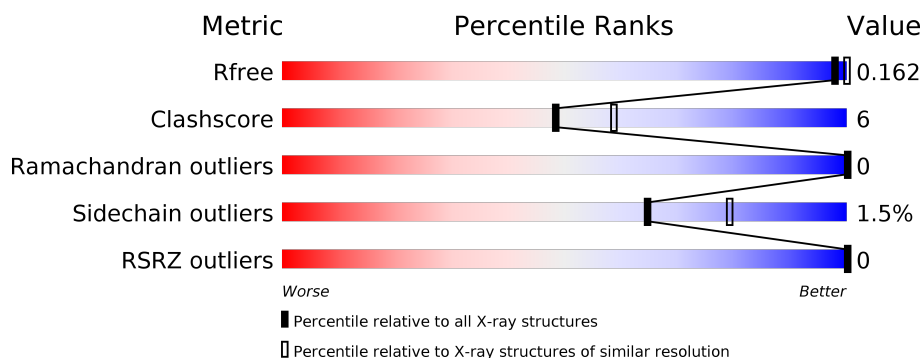
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	459	<div> <div>78%</div> <div>13%</div> <div>9%</div> </div>
1	B	459	<div> <div>76%</div> <div>14%</div> <div>9%</div> </div>
2	C	68	<div> <div>21%</div> <div>78%</div> </div>
2	D	68	<div> <div>21%</div> <div>6%</div> <div>74%</div> </div>
3	E	6	<div> <div>17%</div> <div>83%</div> </div>
3	F	6	<div> <div>50%</div> <div>50%</div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7875 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 Botulinum neurotoxin type B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	2	0
			3582	2317	587	670	8			
1	B	417	Total	C	N	O	S	0	0	0
			3564	2307	583	666	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	833	MET	-	expression tag	UNP P10844
A	834	GLY	-	expression tag	UNP P10844
A	835	SER	-	expression tag	UNP P10844
A	836	SER	-	expression tag	UNP P10844
A	837	HIS	-	expression tag	UNP P10844
A	838	HIS	-	expression tag	UNP P10844
A	839	HIS	-	expression tag	UNP P10844
A	840	HIS	-	expression tag	UNP P10844
A	841	HIS	-	expression tag	UNP P10844
A	842	HIS	-	expression tag	UNP P10844
A	843	SER	-	expression tag	UNP P10844
A	844	SER	-	expression tag	UNP P10844
A	845	GLY	-	expression tag	UNP P10844
A	846	LEU	-	expression tag	UNP P10844
A	847	VAL	-	expression tag	UNP P10844
A	848	PRO	-	expression tag	UNP P10844
A	849	ARG	-	expression tag	UNP P10844
A	850	GLY	-	expression tag	UNP P10844
A	851	SER	-	expression tag	UNP P10844
A	852	HIS	-	expression tag	UNP P10844
A	853	MET	-	expression tag	UNP P10844
A	854	ALA	-	expression tag	UNP P10844
A	855	SER	-	expression tag	UNP P10844
A	856	MET	-	expression tag	UNP P10844
B	833	MET	-	expression tag	UNP P10844

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	834	GLY	-	expression tag	UNP P10844
B	835	SER	-	expression tag	UNP P10844
B	836	SER	-	expression tag	UNP P10844
B	837	HIS	-	expression tag	UNP P10844
B	838	HIS	-	expression tag	UNP P10844
B	839	HIS	-	expression tag	UNP P10844
B	840	HIS	-	expression tag	UNP P10844
B	841	HIS	-	expression tag	UNP P10844
B	842	HIS	-	expression tag	UNP P10844
B	843	SER	-	expression tag	UNP P10844
B	844	SER	-	expression tag	UNP P10844
B	845	GLY	-	expression tag	UNP P10844
B	846	LEU	-	expression tag	UNP P10844
B	847	VAL	-	expression tag	UNP P10844
B	848	PRO	-	expression tag	UNP P10844
B	849	ARG	-	expression tag	UNP P10844
B	850	GLY	-	expression tag	UNP P10844
B	851	SER	-	expression tag	UNP P10844
B	852	HIS	-	expression tag	UNP P10844
B	853	MET	-	expression tag	UNP P10844
B	854	ALA	-	expression tag	UNP P10844
B	855	SER	-	expression tag	UNP P10844
B	856	MET	-	expression tag	UNP P10844

- Molecule 2 is a protein called Synaptotagmin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	S	7	0	0
			131	87	20	23	1			
2	D	18	Total	C	N	O	S	7	0	0
			155	100	24	30	1			

There are 28 discrepancies between the modelled and reference sequences:

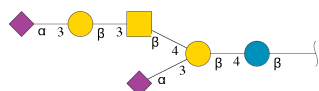
Chain	Residue	Modelled	Actual	Comment	Reference
C	3	GLU	-	expression tag	UNP P46097
C	4	GLY	-	expression tag	UNP P46097
C	5	TRP	-	expression tag	UNP P46097
C	6	THR	-	expression tag	UNP P46097
C	7	GLU	-	expression tag	UNP P46097
C	62	VAL	-	expression tag	UNP P46097
C	63	LEU	-	expression tag	UNP P46097

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	64	GLU	-	expression tag	UNP P46097
C	65	HIS	-	expression tag	UNP P46097
C	66	HIS	-	expression tag	UNP P46097
C	67	HIS	-	expression tag	UNP P46097
C	68	HIS	-	expression tag	UNP P46097
C	69	HIS	-	expression tag	UNP P46097
C	70	HIS	-	expression tag	UNP P46097
D	3	GLU	-	expression tag	UNP P46097
D	4	GLY	-	expression tag	UNP P46097
D	5	TRP	-	expression tag	UNP P46097
D	6	THR	-	expression tag	UNP P46097
D	7	GLU	-	expression tag	UNP P46097
D	62	VAL	-	expression tag	UNP P46097
D	63	LEU	-	expression tag	UNP P46097
D	64	GLU	-	expression tag	UNP P46097
D	65	HIS	-	expression tag	UNP P46097
D	66	HIS	-	expression tag	UNP P46097
D	67	HIS	-	expression tag	UNP P46097
D	68	HIS	-	expression tag	UNP P46097
D	69	HIS	-	expression tag	UNP P46097
D	70	HIS	-	expression tag	UNP P46097

- Molecule 3 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-(2-3)]beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	6	Total	C	N	O	0	0	0
			88	48	3	37			
3	F	6	Total	C	N	O	0	0	0
			88	48	3	37			

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

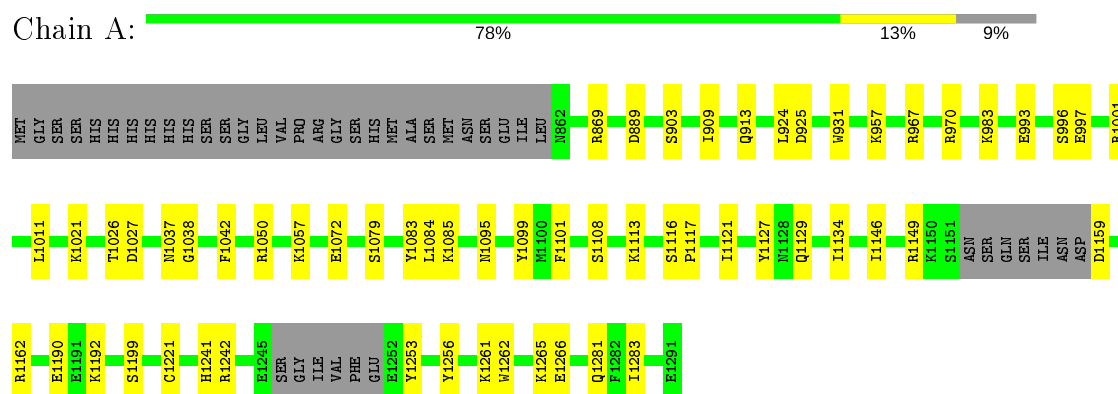
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	136	Total	O	0	0
			136	136		
6	B	118	Total	O	0	0
			118	118		
6	C	4	Total	O	0	0
			4	4		
6	D	6	Total	O	0	0
			6	6		

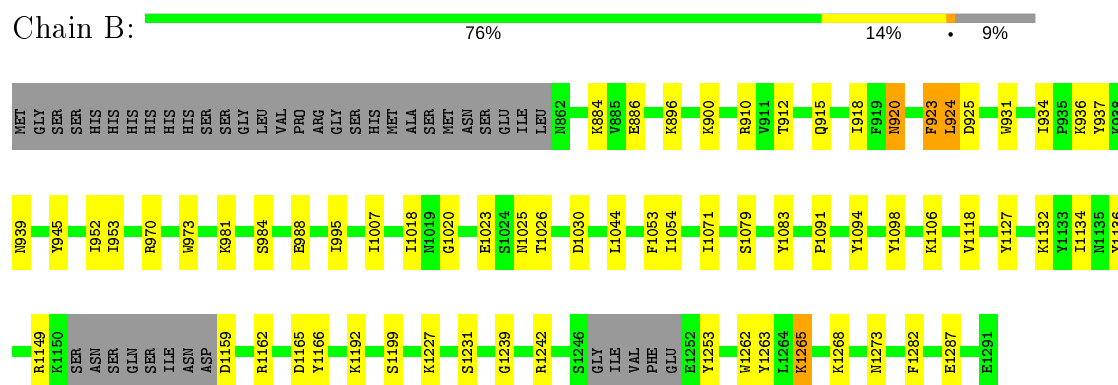
3 Residue-property plots

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.

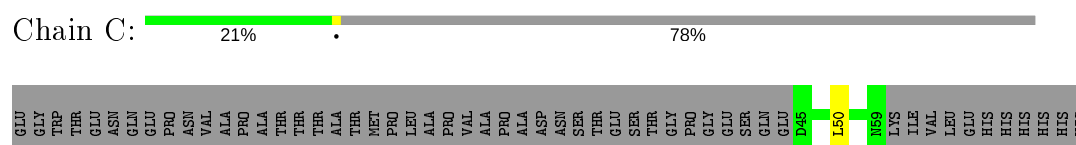
• Molecule 1: Botulinum neurotoxin type B



• Molecule 1: Botulinum neurotoxin type B



• Molecule 2: Synaptotagmin-2



• Molecule 2: Synaptotagmin-2





HIS

- Molecule 3: 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-(2-3)]beta-D-galactopyranos e-(1-4)-beta-D-glucopyranose



- Molecule 3: 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-(2-3)]beta-D-galactopyranos e-(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	47.16Å 158.24Å 75.24Å 90.00° 108.44° 90.00°	Depositor
Resolution (Å)	44.82 – 2.30 44.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (44.82-2.30) 99.2 (44.82-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.156 , 0.189 0.146 , 0.162	Depositor DCC
R_{free} test set	2346 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.397 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.380 for h,-k,-h-l	Depositor
Outliers	0 of 46354 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7875	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/3667	0.58	0/4941
1	B	0.43	0/3649	0.58	0/4917
2	C	0.37	0/133	0.51	0/174
2	D	0.73	0/157	0.64	0/206
All	All	0.43	0/7606	0.58	0/10238

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3582	0	3494	39	1
1	B	3564	0	3480	45	1
2	C	131	0	129	1	0
2	D	155	0	148	3	0
3	E	88	0	72	8	0
3	F	88	0	74	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	136	0	0	7	0
6	B	118	0	0	4	0
6	C	4	0	0	0	0
6	D	6	0	0	0	0
All	All	7875	0	7397	89	1

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 6.

All (89) 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:1262:TRP:CE3	3:E:4:GAL:H5	2.19	0.78
1:B:1262:TRP:CD1	3:F:3:NGA:H62	2.19	0.77
1:A:1149:ARG:HH21	1:A:1159:ASP:HB3	1.54	0.73
1:A:869:ARG:NH1	6:A:1523:HOH:O	2.16	0.72
1:A:1050:ARG:NH1	6:A:1509:HOH:O	2.26	0.69
1:A:993:GLU:OE1	6:A:1483:HOH:O	2.11	0.69
1:B:1149:ARG:HH21	1:B:1159:ASP:HB3	1.60	0.66
1:A:1011:LEU:HD23	1:A:1011:LEU:H	1.61	0.65
1:B:1242:ARG:HG2	1:B:1253:TYR:HB3	1.77	0.64
1:A:1149:ARG:NH2	1:A:1159:ASP:HB3	2.15	0.62
1:A:1127:TYR:CZ	1:A:1129:GLN:HB2	2.37	0.59
1:A:931:TRP:HB2	1:A:1057:LYS:HG2	1.85	0.58
1:A:1262:TRP:CZ3	3:E:4:GAL:H5	2.40	0.57
1:A:1021:LYS:NZ	1:A:1072:GLU:OE1	2.35	0.56
3:E:5:SIA:O9	3:E:5:SIA:O7	2.16	0.55
1:B:1149:ARG:NH2	1:B:1159:ASP:HB3	2.22	0.55
1:B:952:ILE:HG22	1:B:1044:LEU:HD22	1.89	0.54
1:B:1026:THR:OG1	3:E:1:BGC:H5	2.08	0.53
1:A:913:GLN:NE2	1:A:1038:GLY:O	2.41	0.52
1:A:967:ARG:NH1	1:A:970:ARG:HH11	2.07	0.52
1:B:920:ASN:OD1	6:B:1502:HOH:O	2.19	0.51
1:B:896:LYS:HD2	1:B:1091:PRO:HG2	1.93	0.51
1:B:981:LYS:NZ	1:B:1030:ASP:HB3	2.25	0.50
1:B:1118:VAL:HG11	2:D:57:GLU:HG2	1.94	0.50
1:A:1190:GLU:HG3	1:A:1241:HIS:CG	2.47	0.50
1:B:973:TRP:CD2	1:B:1007:ILE:HG21	2.47	0.49
1:A:1242:ARG:HG2	1:A:1253:TYR:HB3	1.95	0.49
1:A:957:LYS:HE3	1:A:1037:ASN:HD21	1.78	0.49
1:B:1127:TYR:CE1	1:B:1134:ILE:HD11	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1442:HOH:O	3:E:6:SIA:H111	2.12	0.48
1:A:903:SER:OG	1:A:1050:ARG:HD2	2.14	0.48
3:E:1:BGC:H6C1	3:E:2:GAL:O5	2.13	0.48
1:B:952:ILE:HG13	1:B:953:ILE:HG13	1.96	0.47
1:A:1099:TYR:HB2	1:A:1283:ILE:HB	1.96	0.47
1:B:884:LYS:HB3	1:B:912:THR:HB	1.96	0.47
1:B:984:SER:O	3:E:1:BGC:H1	2.14	0.47
1:A:1084:LEU:HD22	1:A:1221:CYS:HB3	1.96	0.47
1:A:1190:GLU:HG3	1:A:1241:HIS:CD2	2.50	0.46
1:B:970:ARG:HB2	1:B:988:GLU:HG3	1.98	0.46
1:B:1273:ASN:ND2	3:F:5:SIA:H92	2.31	0.45
1:A:1127:TYR:CZ	1:A:1134:ILE:HD11	2.52	0.45
1:B:886:GLU:OE2	1:B:910:ARG:HD2	2.17	0.45
1:B:924:LEU:HG	1:B:925:ASP:H	1.81	0.45
1:B:923:PHE:CD1	1:B:923:PHE:N	2.85	0.45
1:A:909:ILE:HB	1:A:1042:PHE:HB2	1.99	0.45
1:A:1113:LYS:HB3	1:A:1116:SER:HB3	1.98	0.45
2:D:46:MET:O	2:D:50:LEU:HD12	2.17	0.45
1:B:1094:TYR:OH	1:B:1165:ASP:OD2	2.30	0.45
1:A:1011:LEU:CD2	1:A:1011:LEU:H	2.27	0.44
1:B:1098:TYR:CG	1:B:1282:PHE:HB3	2.53	0.44
1:B:915:GLN:HB3	6:B:1503:HOH:O	2.18	0.44
1:A:1162:ARG:NH2	6:A:1529:HOH:O	2.31	0.44
1:A:996:SER:HB2	6:A:1404:HOH:O	2.18	0.44
1:A:1101:PHE:HB2	1:A:1283:ILE:HD11	1.98	0.44
1:B:1192:LYS:NZ	2:D:57:GLU:HG3	2.32	0.44
1:B:1262:TRP:CE3	3:F:4:GAL:H5	2.53	0.44
1:B:900:LYS:HE3	1:B:1053:PHE:CG	2.53	0.43
1:B:1020:GLY:HA2	1:B:1071:ILE:HG22	2.00	0.43
1:B:1018:ILE:HG12	1:B:1023:GLU:HG3	2.00	0.43
1:A:983:LYS:HD2	1:A:1026:THR:HG21	2.01	0.43
1:B:939:ASN:ND2	1:B:1136:TYR:OH	2.40	0.43
1:A:1026:THR:HG22	1:A:1027:ASP:O	2.19	0.43
1:B:995:ILE:HG13	1:B:1106:LYS:HB3	2.00	0.43
1:A:1192:LYS:HE2	1:A:1256:TYR:CD1	2.54	0.42
1:B:1239:GLY:HA3	1:B:1263:TYR:HE2	1.83	0.42
1:B:934:ILE:HG23	1:B:1054:ILE:HD11	2.01	0.42
1:B:973:TRP:CE3	1:B:1007:ILE:HD13	2.55	0.42
1:B:1227:LYS:HD3	1:B:1231:SER:OG	2.20	0.42
1:B:931:TRP:HH2	1:B:1079:SER:HG	1.68	0.42
1:B:937:TYR:HB3	1:B:945:TYR:CD1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:SER:O	1:A:1085:LYS:NZ	2.52	0.41
1:B:1054:ILE:HA	1:B:1054:ILE:HD13	1.95	0.41
1:B:937:TYR:HB3	1:B:945:TYR:CG	2.56	0.41
1:A:1108:SER:HB3	1:A:1121:ILE:CG2	2.50	0.41
1:A:1095:ASN:HA	1:A:1146:ILE:HD11	2.02	0.41
1:B:1132:LYS:HD2	1:B:1132:LYS:HA	1.76	0.41
1:B:900:LYS:NZ	1:B:1287:GLU:OE2	2.42	0.41
1:A:1265:LYS:NZ	1:A:1266:GLU:OE2	2.53	0.41
1:B:936:LYS:HE2	1:B:937:TYR:CE1	2.56	0.41
1:A:1281:GLN:HA	6:A:1419:HOH:O	2.21	0.40
1:A:1083:TYR:HA	1:A:1162:ARG:HA	2.04	0.40
1:A:1117:PRO:HG3	2:C:50:LEU:O	2.22	0.40
1:A:993:GLU:HB2	6:A:1404:HOH:O	2.20	0.40
1:A:997:GLU:HA	1:A:1001:ARG:NH1	2.35	0.40
1:B:937:TYR:CE1	1:B:1134:ILE:HD13	2.56	0.40
1:B:1083:TYR:HA	1:B:1162:ARG:HA	2.03	0.40
1:B:1265:LYS:HA	1:B:1268:LYS:HD2	2.03	0.40
1:B:937:TYR:OH	6:B:1459:HOH:O	2.17	0.40
3:E:5:SIA:C6	3:E:5:SIA:O1B	2.70	0.40

All (1) 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:889:ASP:OD2	1:B:1166:TYR:OH[1_454]	2.18	0.02

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	413/459 (90%)	399 (97%)	14 (3%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	411/459 (90%)	399 (97%)	12 (3%)	0	100	100
2	C	13/68 (19%)	13 (100%)	0	0	100	100
2	D	16/68 (24%)	16 (100%)	0	0	100	100
All	All	853/1054 (81%)	827 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	395/430 (92%)	391 (99%)	4 (1%)	76	87
1	B	393/430 (91%)	386 (98%)	7 (2%)	59	75
2	C	14/58 (24%)	14 (100%)	0	100	100
2	D	17/58 (29%)	16 (94%)	1 (6%)	19	27
All	All	819/976 (84%)	807 (98%)	12 (2%)	65	79

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	924	LEU
1	A	925	ASP
1	A	1199	SER
1	A	1261	LYS
1	B	918	ILE
1	B	920	ASN
1	B	923	PHE
1	B	924	LEU
1	B	1025	ASN
1	B	1199	SER
1	B	1265	LYS
2	D	52	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1105	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 ⓘ

12 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$
3	BGC	E	1	3	12,12,12	1.14	1 (8%)	17,17,17	2.66	6 (35%)
3	GAL	E	2	3	11,11,12	1.20	1 (9%)	15,15,17	1.37	2 (13%)
3	NGA	E	3	3	14,14,15	1.72	3 (21%)	17,19,21	1.78	4 (23%)
3	GAL	E	4	3	11,11,12	1.64	3 (27%)	15,15,17	1.97	3 (20%)
3	SIA	E	5	3	17,20,21	2.53	6 (35%)	21,28,31	2.88	12 (57%)
3	SIA	E	6	3	17,20,21	1.04	1 (5%)	21,28,31	3.74	13 (61%)
3	BGC	F	1	3	12,12,12	1.22	1 (8%)	17,17,17	1.58	6 (35%)
3	GAL	F	2	3	11,11,12	3.12	6 (54%)	15,15,17	2.83	4 (26%)
3	NGA	F	3	3	14,14,15	1.66	4 (28%)	17,19,21	2.21	3 (17%)
3	GAL	F	4	3	11,11,12	1.63	3 (27%)	15,15,17	1.66	3 (20%)
3	SIA	F	5	3	17,20,21	1.62	2 (11%)	21,28,31	2.02	9 (42%)
3	SIA	F	6	3	17,20,21	1.77	4 (23%)	21,28,31	1.77	6 (28%)

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	BGC	E	1	3	-	2/2/22/22	0/1/1/1
3	GAL	E	2	3	-	1/2/19/22	0/1/1/1
3	NGA	E	3	3	-	2/6/23/26	0/1/1/1
3	GAL	E	4	3	-	0/2/19/22	0/1/1/1
3	SIA	E	5	3	-	8/14/34/38	0/1/1/1
3	SIA	E	6	3	-	12/14/34/38	0/1/1/1
3	BGC	F	1	3	-	0/2/22/22	0/1/1/1
3	GAL	F	2	3	-	1/2/19/22	0/1/1/1
3	NGA	F	3	3	-	1/6/23/26	0/1/1/1
3	GAL	F	4	3	-	0/2/19/22	0/1/1/1
3	SIA	F	5	3	-	4/14/34/38	0/1/1/1
3	SIA	F	6	3	-	1/14/34/38	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2	GAL	O5-C1	6.23	1.53	1.43
3	E	5	SIA	C7-C6	-5.35	1.46	1.53
3	E	5	SIA	C4-C5	-5.33	1.48	1.53
3	E	5	SIA	C8-C7	-4.45	1.45	1.53
3	F	6	SIA	C3-C4	-4.22	1.45	1.52
3	F	2	GAL	C2-C3	-4.05	1.46	1.52
3	F	2	GAL	C4-C5	-4.00	1.44	1.53
3	F	5	SIA	C7-C6	-3.97	1.47	1.53
3	F	5	SIA	C4-C5	-3.86	1.49	1.53
3	E	3	NGA	O5-C1	-3.81	1.37	1.43
3	F	2	GAL	C4-C3	-3.76	1.42	1.52
3	F	3	NGA	C7-N2	3.44	1.46	1.34
3	E	4	GAL	O5-C1	-3.36	1.38	1.43
3	F	4	GAL	C2-C3	-3.18	1.47	1.52
3	E	5	SIA	O10-C10	-3.16	1.16	1.23
3	F	4	GAL	C4-C3	-3.12	1.44	1.52
3	F	3	NGA	C3-C2	-2.96	1.46	1.52
3	F	6	SIA	C10-N5	2.91	1.44	1.34
3	E	5	SIA	C3-C2	2.91	1.57	1.52
3	F	2	GAL	O4-C4	2.85	1.49	1.43
3	F	6	SIA	O6-C2	2.78	1.50	1.43
3	F	2	GAL	O3-C3	2.62	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3	NGA	C2-N2	-2.60	1.41	1.46
3	F	6	SIA	O8-C8	-2.52	1.38	1.43
3	F	3	NGA	C4-C3	-2.48	1.46	1.52
3	E	4	GAL	O5-C5	-2.43	1.38	1.43
3	F	3	NGA	O3-C3	2.35	1.48	1.43
3	E	2	GAL	O5-C1	-2.32	1.40	1.43
3	F	4	GAL	O3-C3	2.26	1.48	1.43
3	F	1	BGC	O5-C5	-2.20	1.39	1.44
3	E	3	NGA	O7-C7	-2.14	1.18	1.23
3	E	4	GAL	O4-C4	-2.10	1.38	1.43
3	E	6	SIA	C8-C7	-2.09	1.49	1.53
3	E	1	BGC	O4-C4	-2.08	1.38	1.43
3	E	5	SIA	O4-C4	-2.00	1.39	1.43

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	6	SIA	C8-C7-C6	9.81	131.63	113.03
3	F	2	GAL	C1-C2-C3	7.61	119.02	109.67
3	F	3	NGA	O5-C5-C6	6.59	117.53	107.20
3	E	5	SIA	C3-C4-C5	6.34	119.12	111.46
3	E	6	SIA	C4-C5-N5	-6.32	97.87	110.38
3	E	6	SIA	O7-C7-C8	-6.17	93.90	108.81
3	E	1	BGC	O4-C4-C5	6.07	124.37	109.30
3	E	5	SIA	C4-C5-N5	-5.97	98.57	110.38
3	E	4	GAL	O5-C1-C2	-5.70	101.97	110.77
3	F	2	GAL	O5-C1-C2	-5.65	102.05	110.77
3	E	5	SIA	O8-C8-C7	-5.20	96.45	109.10
3	F	6	SIA	C3-C2-C1	-4.58	101.93	111.93
3	E	6	SIA	O8-C8-C9	4.49	119.68	109.14
3	E	6	SIA	C6-C5-N5	4.42	118.25	110.91
3	E	1	BGC	C1-O5-C5	4.34	121.85	113.66
3	F	4	GAL	C1-C2-C3	4.18	114.81	109.67
3	E	1	BGC	O5-C5-C6	-4.01	96.47	106.44
3	E	6	SIA	C3-C4-C5	3.77	116.02	111.46
3	E	6	SIA	O9-C9-C8	-3.74	102.93	111.07
3	E	3	NGA	O3-C3-C2	-3.72	101.78	109.47
3	F	2	GAL	O3-C3-C2	-3.60	103.10	109.99
3	E	1	BGC	O4-C4-C3	-3.52	102.22	110.35
3	E	2	GAL	O3-C3-C2	3.49	116.68	109.99
3	E	1	BGC	C4-C3-C2	-3.45	104.81	110.82
3	F	6	SIA	C4-C3-C2	3.42	115.94	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	SIA	C8-C7-C6	-3.40	106.59	113.03
3	E	1	BGC	C3-C4-C5	-3.33	104.30	110.24
3	F	5	SIA	O7-C7-C6	-3.25	102.47	109.50
3	E	6	SIA	O4-C4-C3	-3.25	101.89	109.94
3	F	4	GAL	O5-C1-C2	3.18	115.68	110.77
3	E	5	SIA	O4-C4-C5	-3.09	102.65	109.77
3	E	5	SIA	C11-C10-N5	3.07	121.30	116.10
3	F	3	NGA	O5-C5-C4	3.02	118.18	110.83
3	E	5	SIA	C6-O6-C2	3.01	117.78	111.34
3	F	3	NGA	C6-C5-C4	3.01	120.05	113.00
3	F	5	SIA	O7-C7-C8	2.98	116.02	108.81
3	E	5	SIA	O8-C8-C9	2.93	116.01	109.14
3	F	1	BGC	O1-C1-O5	-2.88	101.72	110.38
3	F	5	SIA	C6-O6-C2	2.87	117.49	111.34
3	E	6	SIA	O8-C8-C7	-2.82	102.24	109.10
3	E	6	SIA	O4-C4-C5	2.81	116.24	109.77
3	E	5	SIA	C4-C3-C2	2.73	114.71	109.81
3	F	5	SIA	C3-C4-C5	2.72	114.75	111.46
3	E	3	NGA	O5-C1-C2	-2.64	107.11	111.29
3	F	1	BGC	O4-C4-C5	-2.63	102.78	109.30
3	F	6	SIA	C11-C10-N5	2.61	120.52	116.10
3	E	3	NGA	C1-C2-N2	2.60	114.92	110.49
3	F	1	BGC	O2-C2-C1	-2.55	103.25	109.16
3	E	6	SIA	O7-C7-C6	2.53	114.95	109.50
3	F	5	SIA	C4-C5-N5	-2.52	105.40	110.38
3	F	6	SIA	O9-C9-C8	2.50	116.53	111.07
3	E	5	SIA	C3-C2-C1	-2.48	106.52	111.93
3	F	6	SIA	O6-C2-C3	2.43	114.13	109.87
3	F	4	GAL	C2-C3-C4	2.41	115.06	110.89
3	E	4	GAL	O4-C4-C3	-2.41	104.79	110.35
3	E	2	GAL	O3-C3-C4	2.33	115.73	110.35
3	E	6	SIA	C5-N5-C10	2.29	128.74	123.18
3	F	5	SIA	O4-C4-C5	-2.27	104.55	109.77
3	E	5	SIA	C5-N5-C10	2.21	128.56	123.18
3	F	5	SIA	O6-C2-C3	-2.21	106.00	109.87
3	E	3	NGA	O5-C5-C4	-2.20	105.47	110.83
3	E	4	GAL	O5-C5-C4	-2.14	105.62	110.83
3	F	5	SIA	C9-C8-C7	2.14	117.04	112.41
3	F	1	BGC	C3-C4-C5	-2.10	106.49	110.24
3	E	6	SIA	C3-C2-C1	2.06	116.42	111.93
3	E	5	SIA	O10-C10-N5	-2.05	118.18	121.95
3	E	5	SIA	O7-C7-C6	-2.05	105.06	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	BGC	C4-C3-C2	2.03	114.36	110.82
3	F	6	SIA	O8-C8-C7	2.01	114.00	109.10
3	F	2	GAL	C1-O5-C5	2.00	114.91	112.19
3	F	1	BGC	O5-C1-C2	-2.00	106.72	110.28

There are no chirality outliers.

All (32) torsion outliers are listed below:

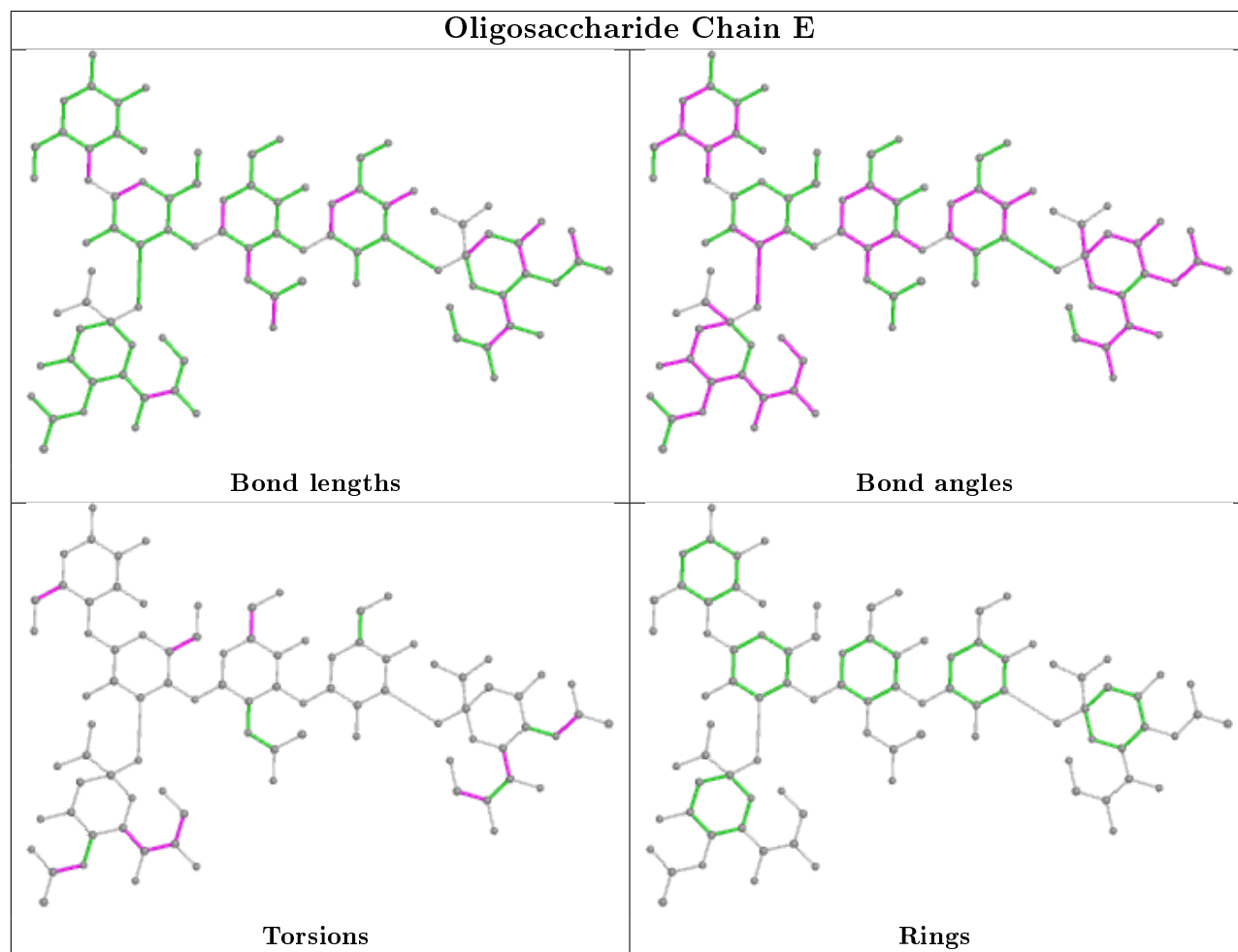
Mol	Chain	Res	Type	Atoms
3	E	5	SIA	C5-C6-C7-C8
3	E	5	SIA	C5-C6-C7-O7
3	E	5	SIA	O6-C6-C7-C8
3	E	5	SIA	O6-C6-C7-O7
3	E	5	SIA	C11-C10-N5-C5
3	E	5	SIA	O10-C10-N5-C5
3	E	6	SIA	C5-C6-C7-C8
3	E	6	SIA	C5-C6-C7-O7
3	E	6	SIA	O6-C6-C7-C8
3	E	6	SIA	O6-C6-C7-O7
3	E	6	SIA	C6-C7-C8-C9
3	E	6	SIA	O7-C7-C8-O8
3	E	1	BGC	O5-C5-C6-O6
3	F	5	SIA	C7-C8-C9-O9
3	E	6	SIA	C7-C8-C9-O9
3	F	3	NGA	O5-C5-C6-O6
3	E	6	SIA	O7-C7-C8-C9
3	E	3	NGA	C4-C5-C6-O6
3	E	3	NGA	O5-C5-C6-O6
3	E	1	BGC	C4-C5-C6-O6
3	E	6	SIA	C11-C10-N5-C5
3	E	6	SIA	O10-C10-N5-C5
3	E	5	SIA	O8-C8-C9-O9
3	E	6	SIA	O8-C8-C9-O9
3	E	6	SIA	C6-C7-C8-O8
3	F	6	SIA	O8-C8-C9-O9
3	E	5	SIA	C7-C8-C9-O9
3	F	5	SIA	O8-C8-C9-O9
3	F	5	SIA	O7-C7-C8-O8
3	F	2	GAL	O5-C5-C6-O6
3	F	5	SIA	O7-C7-C8-C9
3	E	2	GAL	O5-C5-C6-O6

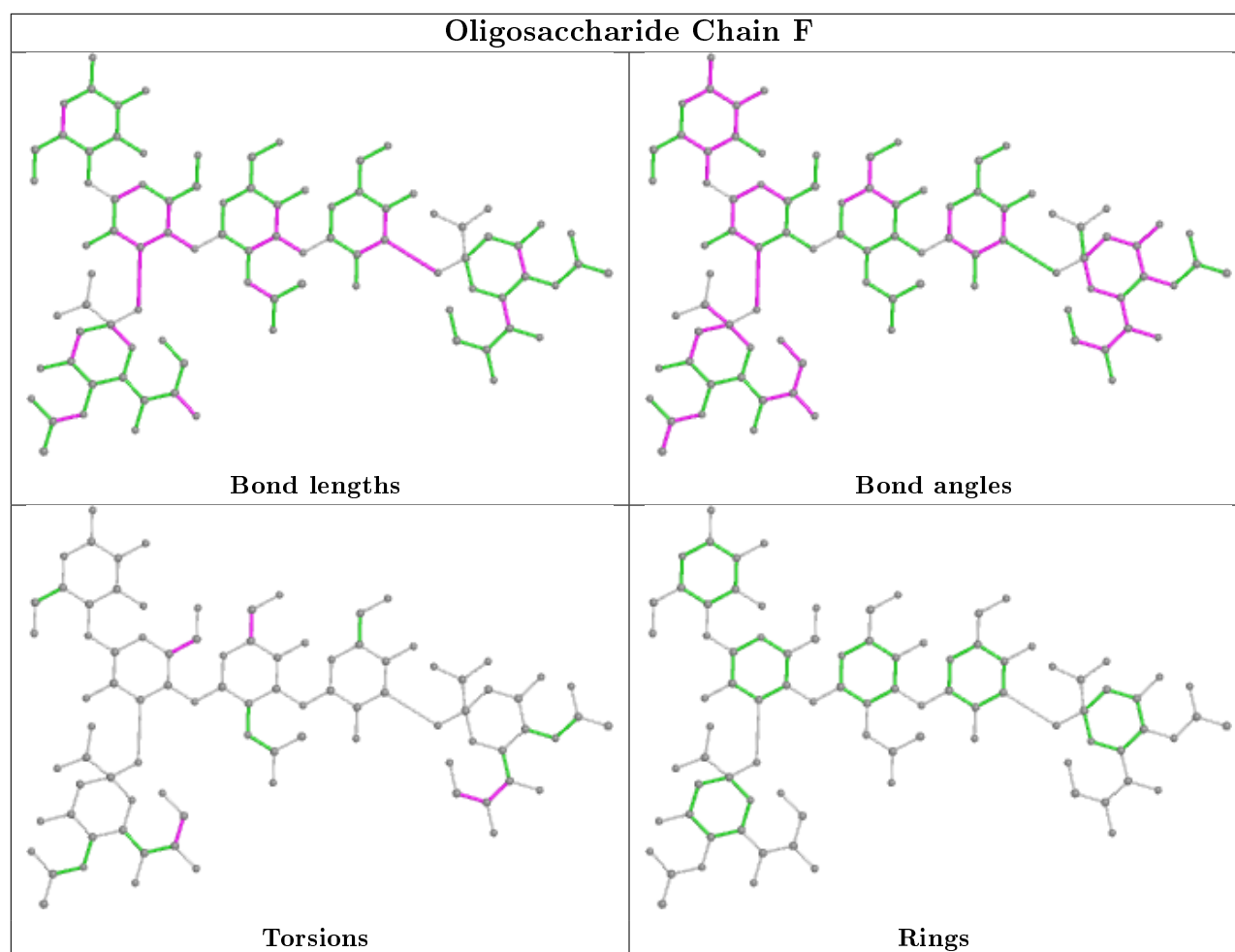
There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	5	SIA	2	0
3	E	1	BGC	3	0
3	E	4	GAL	2	0
3	F	3	NGA	1	0
3	E	2	GAL	1	0
3	F	5	SIA	1	0
3	F	4	GAL	1	0
3	E	6	SIA	1	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](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no chain breaks in this entry.

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	417/459 (90%)	-0.53	0 100 100	10, 21, 50, 80	0
1	B	417/459 (90%)	-0.56	0 100 100	9, 21, 49, 71	0
2	C	15/68 (22%)	-0.07	0 100 100	22, 29, 60, 68	2 (13%)
2	D	18/68 (26%)	-0.61	0 100 100	18, 25, 37, 56	2 (11%)
All	All	867/1054 (82%)	-0.54	0 100 100	9, 22, 50, 80	4 (0%)

There are no RSRZ outliers to report.

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](#)

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
3	NGA	E	3	14/15	0.92	0.11	14,28,34,35	0
3	BGC	E	1	12/12	0.94	0.11	29,38,43,44	0
3	SIA	E	6	20/21	0.95	0.09	18,29,36,38	0
3	NGA	F	3	14/15	0.96	0.11	13,23,25,28	0
3	SIA	E	5	20/21	0.96	0.10	23,33,42,44	0
3	GAL	E	4	11/12	0.97	0.09	20,24,32,36	0
3	GAL	E	2	11/12	0.97	0.07	18,26,32,34	0
3	SIA	F	5	20/21	0.97	0.10	16,23,36,37	0
3	GAL	F	4	11/12	0.97	0.08	16,23,28,28	0

Continued on next page...

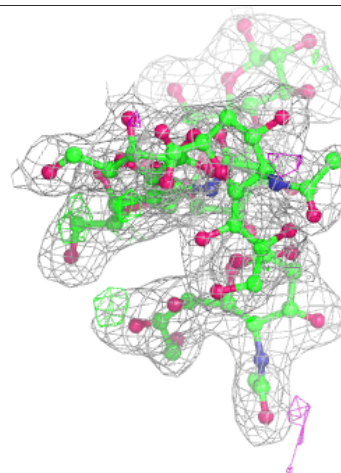
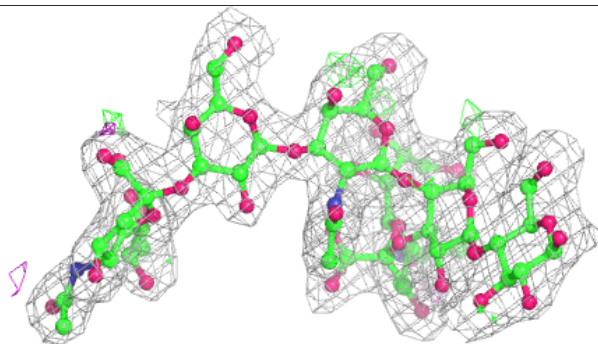
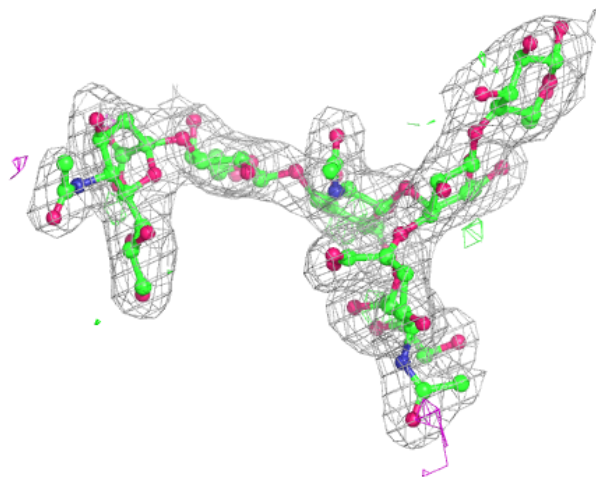
Continued from previous page...

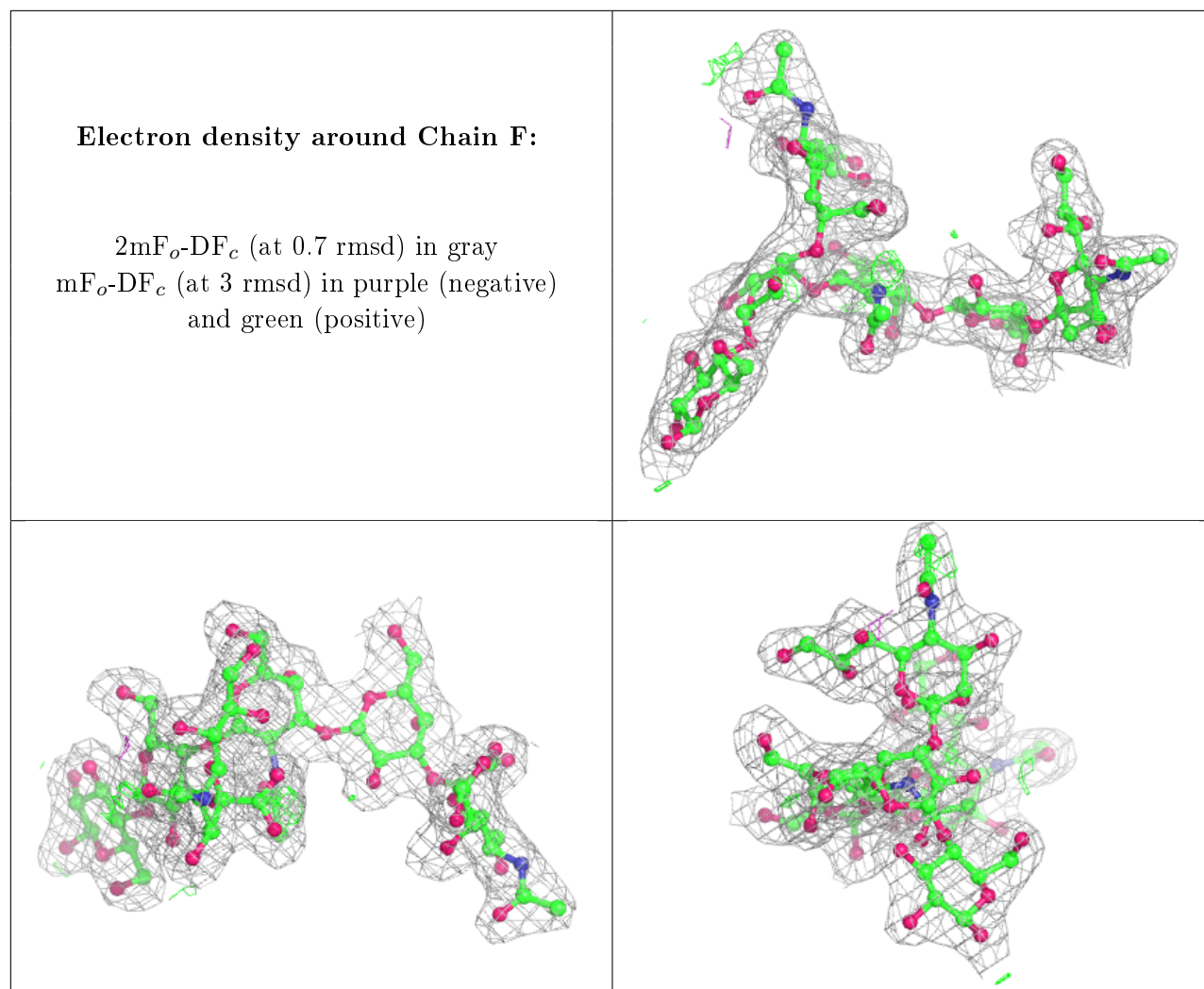
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SIA	F	6	20/21	0.97	0.09	9,20,29,36	0
3	BGC	F	1	12/12	0.97	0.08	19,25,28,31	0
3	GAL	F	2	11/12	0.98	0.08	13,17,24,27	0

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.

Electron density around Chain E:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
 and green (positive)





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(\AA^2)	Q<0.9
4	CL	A	1300	1/1	0.96	0.10	38,38,38,38	0
5	MG	B	1301	1/1	0.99	0.09	22,22,22,22	0
4	CL	B	1300	1/1	0.99	0.12	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.