



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:27 AM UTC

PDB ID : 1F31 / pdb_00001f31
Title : CRYSTAL STRUCTURE OF CLOSTRIDIUM BOTULINUM NEURO-TOXIN B COMPLEXED WITH A TRISACCHARIDE
Authors : Swaminathan, S.; Eswaramoorthy, S.
Deposited on : 2000-05-31
Resolution : 2.60 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

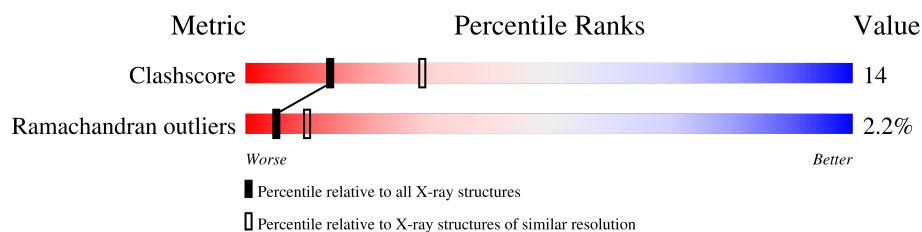
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1290	 67% 30% ..
2	B	3	 33% 67%

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	GLA	B	2	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10584 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	1280	Total	C	N	O	S	0	0	0
			10437	6728	1687	1989	33			

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-alpha-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			43	23	1	19			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 5 is water.

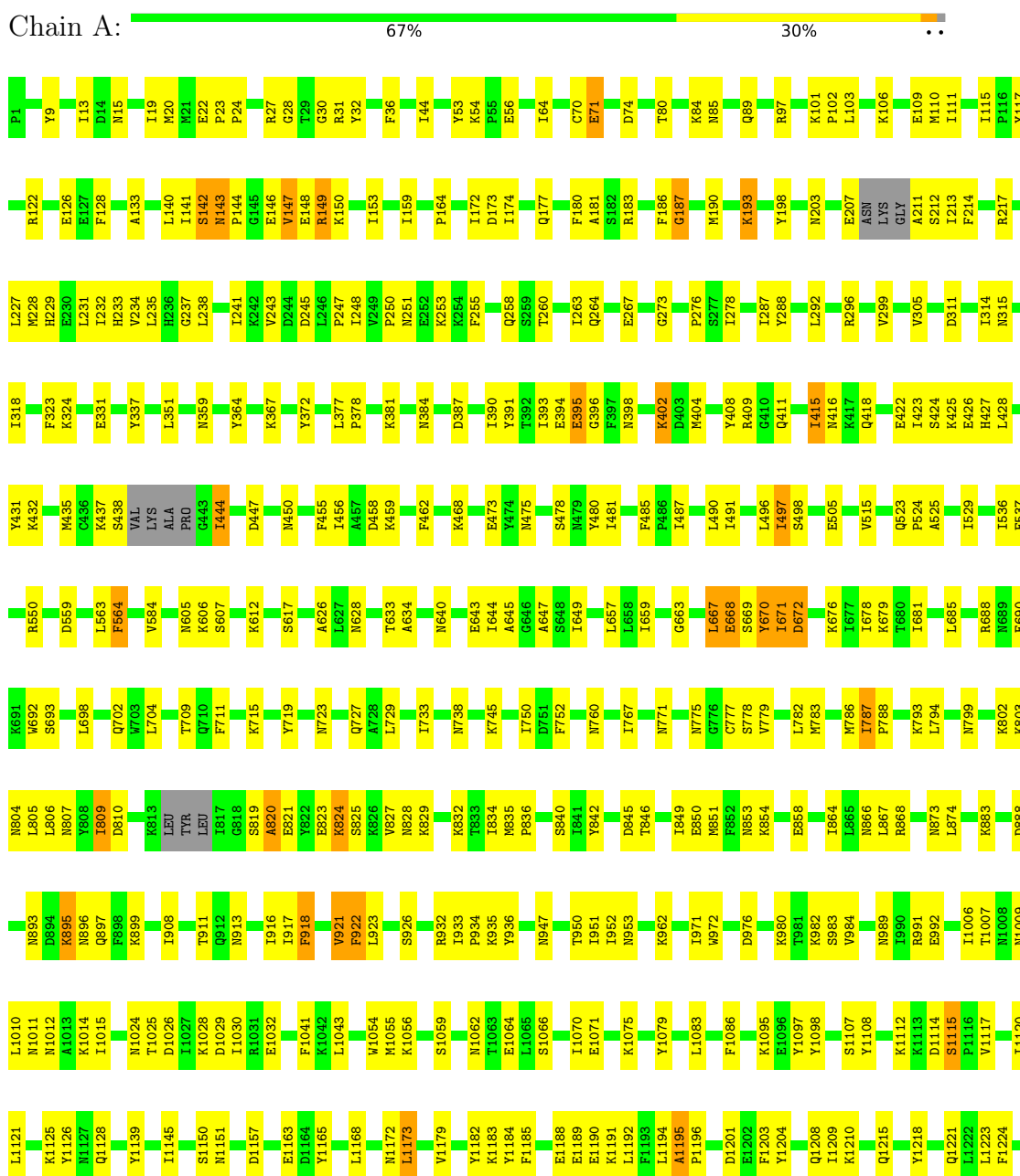
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	98	Total	O	0	0
			98	98		

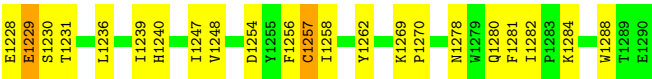
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: BOTULINUM NEUROTOXIN TYPE B





- Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-alpha-D-galactopyranose-(1-4)-alpha-D-glucopyranose



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.30Å 123.65Å 95.56Å 90.00° 113.38° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	75.5 (50.00-2.60)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10584	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLA, SO4, GLC, ZN, SIA

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	0.48	1/10660 (0.0%)	0.97	43/14404 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	787	ILE	CA-CB	5.42	1.57	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	LYS	N-CA-C	-9.94	101.72	114.04
1	A	497	ILE	N-CA-C	7.63	119.29	109.30
1	A	1195	ALA	N-CA-C	7.35	114.61	108.07
1	A	1231	THR	N-CA-C	-7.34	104.36	112.72
1	A	559	ASP	N-CA-C	7.24	119.25	111.36
1	A	584	VAL	N-CA-C	7.12	117.50	108.82
1	A	804	ASN	N-CA-C	-6.87	103.72	111.07
1	A	1257	CYS	N-CA-C	6.60	120.37	110.14
1	A	626	ALA	N-CA-C	6.28	118.13	111.28
1	A	783	MET	N-CA-C	6.28	119.11	111.82
1	A	1184	TYR	N-CA-C	6.24	120.50	112.26
1	A	187	GLY	N-CA-C	-6.17	103.68	112.81
1	A	667	LEU	N-CA-C	-6.12	105.10	113.30
1	A	71	GLU	N-CA-C	6.12	118.61	109.25
1	A	1114	ASP	N-CA-C	6.05	119.70	112.93
1	A	1098	TYR	N-CA-C	-6.00	101.11	110.42
1	A	462	PHE	N-CA-C	6.00	119.25	109.59
1	A	971	ILE	N-CA-C	5.92	117.01	108.48
1	A	248	ILE	N-CA-C	-5.84	100.17	108.58
1	A	233	HIS	N-CA-C	-5.83	104.92	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1012	ASN	N-CA-C	5.72	117.97	108.99
1	A	809	ILE	N-CA-C	-5.69	105.33	113.07
1	A	174	ILE	N-CA-C	5.62	116.67	108.58
1	A	193	LYS	N-CA-C	-5.57	99.34	108.41
1	A	1125	LYS	N-CA-C	5.42	116.88	109.18
1	A	1115	SER	N-CA-C	5.41	115.09	108.11
1	A	229	HIS	N-CA-C	-5.40	105.47	111.36
1	A	644	ILE	N-CA-C	5.39	116.46	111.45
1	A	895	LYS	N-CA-C	-5.35	106.33	112.92
1	A	1173	LEU	CB-CA-C	-5.34	110.43	116.63
1	A	415	ILE	N-CA-C	5.33	116.73	111.67
1	A	70	CYS	N-CA-C	-5.25	99.20	108.23
1	A	606	LYS	N-CA-C	-5.24	106.86	113.20
1	A	402	LYS	N-CA-C	-5.21	106.78	112.72
1	A	395	GLU	N-CA-C	5.20	120.48	113.72
1	A	422	GLU	N-CA-C	-5.18	103.19	110.50
1	A	1079	TYR	N-CA-C	5.18	117.74	110.23
1	A	633	THR	N-CA-C	5.10	119.13	113.01
1	A	947	ASN	N-CA-C	5.08	117.03	109.25
1	A	1009	ASN	N-CA-C	-5.08	102.38	109.69
1	A	251	ASN	N-CA-C	-5.04	101.75	109.76
1	A	888	ASP	N-CA-C	5.01	118.17	111.75
1	A	564	PHE	N-CA-C	5.01	116.69	108.52

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	10437	0	10201	295	0
2	B	43	0	37	15	0
3	A	1	0	0	0	0
4	A	5	0	0	1	0
5	A	98	0	0	2	0
All	All	10584	0	10238	299	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 14.

All (299) 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:1240:HIS:HB2	2:B:3:SIA:H92	1.20	1.11
1:A:989:ASN:HD22	1:A:992:GLU:HG2	1.27	0.98
1:A:1189:GLU:HG3	2:B:2:GLA:H5	1.47	0.96
1:A:367:LYS:H	1:A:411:GLN:HE22	1.17	0.93
1:A:1240:HIS:HB2	2:B:3:SIA:C9	2.04	0.82
1:A:409:ARG:NH1	1:A:415:ILE:HD13	2.00	0.76
1:A:147:VAL:HA	1:A:150:LYS:HZ2	1.50	0.75
1:A:247:PRO:HB3	1:A:264:GLN:NE2	2.00	0.75
1:A:1071:GLU:OE2	1:A:1075:LYS:HE3	1.86	0.75
1:A:692:TRP:CH2	1:A:834:ILE:HB	2.22	0.74
1:A:1112:LYS:HD3	1:A:1115:SER:OG	1.87	0.74
1:A:550:ARG:HG2	1:A:550:ARG:HH11	1.53	0.74
1:A:1011:ASN:CG	1:A:1028:LYS:HE2	2.13	0.73
1:A:1075:LYS:HE2	1:A:1215:GLN:HE22	1.55	0.72
1:A:1221:GLN:HE21	1:A:1278:ASN:HD22	1.36	0.72
1:A:980:LYS:HE2	1:A:1029:ASP:OD1	1.87	0.72
1:A:1126:TYR:CZ	1:A:1128:GLN:HB2	2.25	0.71
1:A:423:ILE:HD11	1:A:428:LEU:HD21	1.74	0.70
1:A:377:LEU:HB3	1:A:378:PRO:HD2	1.73	0.70
1:A:1185:PHE:HB3	1:A:1190:GLU:OE1	1.92	0.69
1:A:1221:GLN:HE21	1:A:1278:ASN:ND2	1.90	0.69
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.57	0.68
1:A:228:MET:O	1:A:232:ILE:HG13	1.93	0.68
1:A:126:GLU:H	1:A:126:GLU:CD	2.01	0.68
1:A:147:VAL:HA	1:A:150:LYS:NZ	2.10	0.67
1:A:473:GLU:HG3	1:A:475:ASN:HB2	1.78	0.66
1:A:953:ASN:HD22	1:A:962:LYS:HG3	1.61	0.66
1:A:1188:GLU:HG2	2:B:2:GLA:O2	1.96	0.65
1:A:825:SER:HA	1:A:828:ASN:HD22	1.60	0.65
1:A:1188:GLU:HB3	2:B:2:GLA:C5	2.27	0.64
1:A:468:LYS:O	1:A:663:GLY:HA3	1.97	0.64
1:A:142:SER:HB2	1:A:148:GLU:O	1.97	0.64
1:A:143:ASN:HB2	1:A:144:PRO:CD	2.28	0.64
1:A:1011:ASN:ND2	1:A:1028:LYS:HG2	2.13	0.64
2:B:3:SIA:H113	2:B:3:SIA:H7	1.80	0.64
1:A:235:LEU:HD21	1:A:351:LEU:HD22	1.80	0.63
1:A:536:ILE:HG23	1:A:537:PHE:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1240:HIS:HA	2:B:3:SIA:H111	1.80	0.63
1:A:893:ASN:HD21	1:A:897:GLN:HB2	1.62	0.62
1:A:550:ARG:HG2	1:A:550:ARG:NH1	2.14	0.62
1:A:668:GLU:O	1:A:670:TYR:N	2.33	0.62
1:A:1240:HIS:O	1:A:1254:ASP:HA	2.00	0.62
1:A:64:ILE:HD12	1:A:64:ILE:O	2.00	0.62
1:A:425:LYS:C	1:A:427:HIS:H	2.05	0.62
1:A:952:ILE:HD11	1:A:1055:MET:HE1	1.82	0.62
1:A:213:ILE:CB	1:A:760:ASN:HD22	2.13	0.61
1:A:805:LEU:O	1:A:807:ASN:N	2.32	0.61
1:A:715:LYS:HD2	1:A:771:ASN:OD1	2.00	0.61
1:A:153:ILE:HA	1:A:505:GLU:O	2.01	0.61
1:A:485:PHE:HE2	1:A:490:LEU:HB2	1.66	0.60
1:A:787:ILE:HB	1:A:788:PRO:HD3	1.83	0.60
1:A:143:ASN:HB2	1:A:144:PRO:HD3	1.82	0.60
1:A:873:ASN:ND2	1:A:874:LEU:H	2.00	0.60
1:A:473:GLU:HG3	1:A:475:ASN:H	1.66	0.60
1:A:681:ILE:HG23	1:A:805:LEU:HD22	1.82	0.60
1:A:1126:TYR:OH	1:A:1128:GLN:HB2	2.02	0.59
1:A:1172:ASN:OD1	1:A:1173:LEU:HD13	2.02	0.59
1:A:1192:LEU:HD21	1:A:1258:ILE:HB	1.85	0.59
1:A:827:VAL:HG12	1:A:827:VAL:O	2.03	0.58
1:A:950:THR:HG21	1:A:953:ASN:HB2	1.85	0.58
1:A:394:GLU:HG2	1:A:395:GLU:HG3	1.83	0.58
1:A:1188:GLU:HG2	2:B:2:GLA:H4	1.84	0.58
1:A:22:GLU:HB2	1:A:32:TYR:CE2	2.38	0.58
1:A:296:ARG:O	1:A:299:VAL:HG12	2.04	0.58
1:A:1188:GLU:HB3	2:B:2:GLA:H5	1.85	0.57
1:A:253:LYS:HD2	5:A:2083:HOH:O	2.04	0.57
1:A:1007:THR:HB	1:A:1064:GLU:HG3	1.86	0.57
1:A:922:PHE:O	1:A:923:LEU:HB3	2.05	0.57
1:A:15:ASN:HA	1:A:19:ILE:HG22	1.87	0.56
1:A:212:SER:CB	1:A:217:ARG:HB3	2.35	0.56
1:A:437:LYS:O	1:A:438:SER:HB2	2.06	0.56
1:A:367:LYS:H	1:A:411:GLN:NE2	1.96	0.56
1:A:685:LEU:O	1:A:688:ARG:HB3	2.06	0.56
1:A:1195:ALA:HB1	1:A:1196:PRO:HD2	1.88	0.56
1:A:324:LYS:HD2	1:A:337:TYR:HE2	1.71	0.55
1:A:819:SER:O	1:A:821:GLU:N	2.39	0.55
1:A:263:ILE:HD13	1:A:372:TYR:HE2	1.71	0.55
1:A:1014:LYS:HE2	1:A:1024:ASN:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ILE:HD13	1:A:372:TYR:CE2	2.42	0.55
1:A:849:ILE:HG22	1:A:853:ASN:ND2	2.21	0.55
1:A:536:ILE:HG23	1:A:537:PHE:H	1.71	0.55
2:B:3:SIA:H7	2:B:3:SIA:C11	2.37	0.55
1:A:22:GLU:CD	1:A:28:GLY:HA2	2.32	0.55
1:A:117:TYR:HA	1:A:323:PHE:CZ	2.41	0.55
1:A:250:PRO:HG3	1:A:260:THR:HG23	1.87	0.55
1:A:775:ASN:CB	1:A:851:MET:HE3	2.37	0.55
1:A:44:ILE:HD13	1:A:159:ILE:HB	1.88	0.54
1:A:1195:ALA:HB1	1:A:1196:PRO:CD	2.37	0.54
1:A:667:LEU:N	1:A:667:LEU:HD12	2.23	0.54
1:A:97:ARG:HG3	1:A:97:ARG:HH11	1.72	0.54
1:A:103:LEU:HD22	1:A:487:ILE:HD11	1.88	0.54
1:A:1086:PHE:CB	1:A:1282:ILE:HG12	2.38	0.54
1:A:231:LEU:O	1:A:234:VAL:HB	2.08	0.53
1:A:1066:SER:O	1:A:1070:ILE:HG13	2.09	0.53
1:A:402:LYS:HE3	1:A:404:MET:HE2	1.90	0.53
1:A:983:SER:O	1:A:1025:THR:HG21	2.07	0.53
1:A:719:TYR:HA	1:A:767:ILE:HD11	1.91	0.53
1:A:1010:LEU:HD12	1:A:1011:ASN:N	2.24	0.53
1:A:1097:TYR:CG	1:A:1281:PHE:HB3	2.44	0.53
1:A:324:LYS:NZ	1:A:331:GLU:HB3	2.24	0.53
1:A:775:ASN:HB3	1:A:851:MET:HE3	1.91	0.53
1:A:802:LYS:NZ	1:A:828:ASN:OD1	2.41	0.53
1:A:404:MET:HE1	1:A:416:ASN:CG	2.34	0.52
1:A:404:MET:HE1	1:A:416:ASN:OD1	2.08	0.52
1:A:1026:ASP:OD1	1:A:1028:LYS:HG3	2.10	0.52
1:A:1189:GLU:HG3	2:B:2:GLA:C5	2.30	0.52
1:A:173:ASP:HB3	1:A:190:MET:HE1	1.90	0.52
1:A:1168:LEU:O	1:A:1179:VAL:HG23	2.09	0.52
1:A:659:ILE:HG22	1:A:793:LYS:HG3	1.91	0.52
1:A:1010:LEU:HD13	1:A:1011:ASN:CG	2.34	0.52
1:A:9:TYR:H	1:A:85:ASN:HD22	1.57	0.52
1:A:849:ILE:HG22	1:A:853:ASN:HD21	1.75	0.52
1:A:1086:PHE:CG	1:A:1282:ILE:HG12	2.45	0.52
1:A:402:LYS:O	1:A:404:MET:HG2	2.10	0.52
1:A:913:ASN:HB3	1:A:916:ILE:CD1	2.40	0.52
1:A:984:VAL:HG13	1:A:1015:ILE:HD11	1.92	0.51
1:A:97:ARG:HD3	1:A:391:TYR:OH	2.09	0.51
1:A:951:ILE:HG22	1:A:1043:LEU:HD22	1.92	0.51
1:A:198:TYR:CZ	1:A:381:LYS:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:ASN:O	1:A:802:LYS:N	2.42	0.51
1:A:896:ASN:O	1:A:1056:LYS:HG3	2.11	0.51
1:A:1229:GLU:O	1:A:1230:SER:C	2.54	0.51
1:A:126:GLU:CD	1:A:126:GLU:N	2.69	0.51
1:A:384:ASN:ND2	1:A:387:ASP:HB2	2.25	0.51
1:A:402:LYS:HB2	1:A:404:MET:HG3	1.93	0.51
1:A:384:ASN:HD22	1:A:387:ASP:HB2	1.76	0.50
1:A:1011:ASN:CB	1:A:1028:LYS:HE2	2.41	0.50
1:A:921:VAL:O	1:A:922:PHE:CB	2.59	0.50
1:A:1011:ASN:HB3	1:A:1028:LYS:HE2	1.92	0.50
1:A:146:GLU:O	1:A:148:GLU:N	2.40	0.50
1:A:612:LYS:HZ2	1:A:617:SER:CB	2.24	0.50
1:A:435:MET:HE2	1:A:529:ILE:HD11	1.92	0.50
1:A:1112:LYS:HD3	1:A:1115:SER:HG	1.74	0.50
1:A:13:ILE:HD13	1:A:20:MET:HG2	1.93	0.50
1:A:976:ASP:HB2	1:A:1032:GLU:O	2.12	0.50
1:A:106:LYS:O	1:A:110:MET:HG2	2.12	0.49
1:A:497:ILE:HD13	1:A:498:SER:H	1.77	0.49
1:A:1075:LYS:HE2	1:A:1215:GLN:NE2	2.24	0.49
1:A:122:ARG:HH11	1:A:177:GLN:NE2	2.10	0.49
1:A:497:ILE:HD13	1:A:498:SER:N	2.27	0.49
1:A:873:ASN:HD22	1:A:874:LEU:H	1.58	0.49
1:A:645:ALA:HB3	1:A:649:ILE:HG23	1.94	0.49
1:A:913:ASN:HB3	1:A:916:ILE:HD11	1.93	0.49
1:A:645:ALA:HB3	1:A:649:ILE:CG2	2.42	0.49
1:A:809:ILE:CD1	1:A:824:LYS:HA	2.43	0.49
1:A:180:PHE:HB2	1:A:183:ARG:HD2	1.94	0.48
1:A:227:LEU:O	1:A:231:LEU:HG	2.12	0.48
1:A:723:ASN:OD1	1:A:727:GLN:NE2	2.47	0.48
1:A:563:LEU:HD23	1:A:564:PHE:CE1	2.47	0.48
1:A:143:ASN:CB	1:A:144:PRO:CD	2.92	0.48
1:A:311:ASP:HB3	1:A:314:ILE:HG12	1.95	0.48
1:A:809:ILE:HD11	1:A:827:VAL:HG21	1.95	0.48
1:A:102:PRO:HB2	1:A:491:ILE:HG23	1.95	0.48
1:A:391:TYR:HA	1:A:396:GLY:O	2.14	0.48
1:A:1201:ASP:HB3	5:A:2094:HOH:O	2.13	0.48
1:A:213:ILE:N	1:A:760:ASN:ND2	2.62	0.48
1:A:628:ASN:HB2	1:A:634:ALA:HB2	1.96	0.48
1:A:657:LEU:HD21	1:A:786:MET:HE3	1.96	0.47
1:A:32:TYR:OH	1:A:150:LYS:HE3	2.14	0.47
1:A:444:ILE:HG23	1:A:444:ILE:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:HB2	1:A:408:TYR:CG	2.49	0.47
1:A:845:ASP:O	1:A:849:ILE:HG12	2.14	0.47
1:A:895:LYS:O	1:A:1056:LYS:HE3	2.15	0.47
1:A:647:ALA:HB1	1:A:777:CYS:HB3	1.95	0.47
1:A:245:ASP:O	1:A:247:PRO:HD3	2.14	0.47
1:A:425:LYS:C	1:A:427:HIS:N	2.72	0.47
1:A:1083:LEU:HD13	1:A:1209:ILE:HD13	1.97	0.47
1:A:172:ILE:HD11	1:A:193:LYS:HE3	1.97	0.47
1:A:491:ILE:O	1:A:491:ILE:HG22	2.13	0.47
1:A:455:PHE:C	1:A:456:ILE:HG13	2.40	0.47
1:A:1218:TYR:O	1:A:1280:GLN:HG2	2.15	0.47
1:A:1083:LEU:HD13	1:A:1209:ILE:CD1	2.45	0.46
1:A:867:LEU:O	1:A:868:ARG:HD3	2.16	0.46
1:A:832:LYS:O	1:A:832:LYS:HG3	2.14	0.46
1:A:437:LYS:O	1:A:438:SER:CB	2.63	0.46
1:A:390:ILE:HD11	1:A:418:GLN:HG3	1.98	0.46
1:A:1139:TYR:CD2	1:A:1284:LYS:HE3	2.51	0.46
1:A:85:ASN:ND2	1:A:89:GLN:HE21	2.13	0.46
1:A:149:ARG:HG2	1:A:149:ARG:NH1	2.28	0.46
1:A:750:ILE:HD13	1:A:752:PHE:CE1	2.51	0.46
1:A:866:ASN:OD1	1:A:1059:SER:HB3	2.16	0.46
1:A:36:PHE:CD1	1:A:36:PHE:N	2.84	0.46
1:A:989:ASN:ND2	1:A:991:ARG:H	2.14	0.46
1:A:109:GLU:HB3	1:A:497:ILE:HD11	1.98	0.45
1:A:523:GLN:O	1:A:524:PRO:C	2.60	0.45
1:A:782:LEU:O	1:A:786:MET:HB2	2.17	0.45
1:A:1224:PHE:CD1	1:A:1258:ILE:HD12	2.52	0.45
1:A:64:ILE:HD12	1:A:64:ILE:C	2.41	0.45
1:A:1107:SER:HB3	1:A:1120:ILE:CG2	2.47	0.45
1:A:1208:GLN:OE1	1:A:1210:LYS:HD3	2.17	0.45
1:A:149:ARG:HH11	1:A:149:ARG:CG	2.29	0.45
1:A:292:LEU:HD12	1:A:292:LEU:O	2.17	0.45
1:A:935:LYS:HD2	1:A:1288:TRP:CE3	2.52	0.45
2:B:3:SIA:H113	2:B:3:SIA:C7	2.45	0.45
1:A:487:ILE:O	1:A:491:ILE:HG13	2.16	0.45
1:A:1163:GLU:OE1	1:A:1210:LYS:HD2	2.17	0.45
1:A:738:ASN:HA	1:A:745:LYS:HE2	1.99	0.44
1:A:917:ILE:O	1:A:918:PHE:HB2	2.16	0.44
1:A:1182:TYR:HA	1:A:1203:PHE:CD1	2.52	0.44
1:A:846:THR:O	1:A:850:GLU:HG3	2.17	0.44
1:A:873:ASN:ND2	1:A:874:LEU:N	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:CB	1:A:760:ASN:ND2	2.80	0.44
1:A:893:ASN:OD1	1:A:895:LYS:HB2	2.18	0.44
1:A:241:ILE:C	1:A:243:VAL:H	2.25	0.44
1:A:679:LYS:HB2	1:A:679:LYS:HE2	1.78	0.44
1:A:398:ASN:HA	1:A:404:MET:O	2.17	0.44
1:A:982:LYS:HG3	1:A:1030:ILE:HG12	1.99	0.44
1:A:807:ASN:O	1:A:810:ASP:HB3	2.18	0.44
1:A:111:ILE:HG23	1:A:238:LEU:CD1	2.48	0.44
1:A:207:GLU:CB	1:A:211:ALA:HB3	2.48	0.44
1:A:287:ILE:O	1:A:288:TYR:C	2.60	0.44
1:A:278:ILE:O	1:A:278:ILE:HG22	2.18	0.44
1:A:809:ILE:HD12	1:A:824:LYS:HG3	2.00	0.44
1:A:972:TRP:CD2	1:A:1006:ILE:HG21	2.53	0.44
1:A:671:ILE:O	1:A:672:ASP:O	2.36	0.43
1:A:819:SER:C	1:A:821:GLU:N	2.76	0.43
1:A:27:ARG:HG2	1:A:27:ARG:HH11	1.83	0.43
1:A:53:TYR:CD2	1:A:164:PRO:HG2	2.53	0.43
1:A:932:ARG:HB3	1:A:1054:TRP:HB2	2.00	0.43
1:A:97:ARG:HA	1:A:393:ILE:HG23	2.00	0.43
1:A:431:TYR:HA	1:A:525:ALA:O	2.18	0.43
1:A:835:MET:HA	1:A:836:PRO:HD3	1.91	0.43
1:A:128:PHE:CZ	1:A:305:VAL:HG21	2.53	0.43
1:A:883:LYS:HB2	1:A:911:THR:HB	2.01	0.43
1:A:480:TYR:OH	1:A:690:GLU:HA	2.18	0.43
1:A:1188:GLU:HB3	2:B:2:GLA:O5	2.19	0.43
1:A:423:ILE:CD1	1:A:428:LEU:HD21	2.46	0.43
1:A:458:ASP:OD1	1:A:459:LYS:N	2.51	0.43
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.95	0.43
1:A:31:ARG:HA	1:A:31:ARG:HD2	1.79	0.43
1:A:187:GLY:HA2	1:A:237:GLY:O	2.19	0.43
1:A:258:GLN:HG3	1:A:450:ASN:O	2.19	0.43
1:A:916:ILE:HG22	1:A:917:ILE:N	2.34	0.43
1:A:71:GLU:O	1:A:428:LEU:HA	2.18	0.43
1:A:80:THR:O	1:A:84:LYS:HG3	2.19	0.43
1:A:359:ASN:HB3	1:A:487:ILE:HD12	2.00	0.43
1:A:840:SER:HA	1:A:849:ILE:HD11	2.00	0.43
1:A:1108:TYR:CZ	1:A:1121:LEU:HB2	2.53	0.43
1:A:267:GLU:OE1	4:A:1292:SO4:O3	2.37	0.42
1:A:640:ASN:O	1:A:643:GLU:HB2	2.18	0.42
1:A:854:LYS:O	1:A:858:GLU:HG3	2.19	0.42
1:A:1086:PHE:HB2	1:A:1282:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1120:ILE:HG13	1:A:1239:ILE:HG23	2.00	0.42
1:A:1247:ILE:HG13	1:A:1248:VAL:HG23	2.00	0.42
2:B:3:SIA:H7	2:B:3:SIA:C10	2.49	0.42
1:A:9:TYR:CZ	1:A:84:LYS:HD3	2.54	0.42
1:A:478:SER:HB2	1:A:480:TYR:HE1	1.84	0.42
1:A:1145:ILE:O	1:A:1145:ILE:HG23	2.19	0.42
1:A:54:LYS:HB3	1:A:56:GLU:OE1	2.19	0.42
1:A:487:ILE:O	1:A:487:ILE:HG12	2.19	0.42
1:A:692:TRP:CE3	1:A:794:LEU:HD13	2.55	0.42
1:A:921:VAL:O	1:A:921:VAL:HG13	2.19	0.42
1:A:115:ILE:O	1:A:115:ILE:HG13	2.19	0.42
1:A:899:LYS:HD2	1:A:1054:TRP:CZ2	2.55	0.42
1:A:935:LYS:HG2	1:A:936:TYR:N	2.35	0.42
1:A:1240:HIS:HB3	1:A:1257:CYS:SG	2.60	0.42
1:A:273:GLY:O	1:A:276:PRO:HD2	2.20	0.42
1:A:676:LYS:O	1:A:678:ILE:HG22	2.20	0.42
1:A:819:SER:O	1:A:820:ALA:C	2.63	0.42
1:A:908:ILE:HB	1:A:1041:PHE:HB2	2.01	0.42
1:A:676:LYS:C	1:A:678:ILE:H	2.27	0.41
1:A:779:VAL:O	1:A:782:LEU:HB3	2.20	0.41
1:A:926:SER:OG	1:A:1007:THR:HG22	2.20	0.41
1:A:1117:VAL:C	1:A:1194:LEU:HD12	2.44	0.41
1:A:711:PHE:CE1	1:A:778:SER:HA	2.54	0.41
1:A:536:ILE:CG2	1:A:537:PHE:N	2.82	0.41
1:A:698:LEU:O	1:A:702:GLN:HG3	2.20	0.41
1:A:933:ILE:HA	1:A:934:PRO:HD2	1.90	0.41
1:A:315:ASN:ND2	1:A:318:ILE:HG12	2.36	0.41
1:A:678:ILE:HD11	1:A:823:GLU:HG3	2.01	0.41
1:A:825:SER:O	1:A:829:LYS:HG2	2.20	0.41
1:A:64:ILE:HD12	1:A:523:GLN:HG2	2.02	0.41
1:A:101:LYS:HB2	1:A:364:TYR:CZ	2.55	0.41
1:A:432:LYS:HD3	1:A:447:ASP:HB3	2.02	0.41
1:A:1223:LEU:HA	1:A:1236:LEU:HD23	2.03	0.41
1:A:1269:LYS:HA	1:A:1270:PRO:C	2.45	0.41
1:A:255:PHE:HD1	1:A:435:MET:HE1	1.86	0.41
1:A:1126:TYR:CE1	1:A:1128:GLN:HB2	2.55	0.41
1:A:140:LEU:C	1:A:141:ILE:HD13	2.45	0.41
1:A:181:ALA:HB1	1:A:186:PHE:HB2	2.03	0.41
1:A:235:LEU:HD21	1:A:351:LEU:CD2	2.49	0.41
1:A:864:ILE:CG2	1:A:1062:ASN:ND2	2.84	0.41
1:A:918:PHE:C	1:A:918:PHE:CD2	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:TYR:CE1	1:A:1228:GLU:HG3	2.56	0.41
1:A:1183:LYS:HA	1:A:1204:TYR:CE2	2.55	0.41
1:A:1240:HIS:CB	2:B:3:SIA:H92	2.15	0.41
1:A:288:TYR:HB2	1:A:481:ILE:CD1	2.51	0.40
1:A:976:ASP:C	1:A:976:ASP:OD1	2.64	0.40
1:A:203:ASN:HD21	1:A:217:ARG:HE	1.69	0.40
1:A:605:ASN:C	1:A:607:SER:H	2.29	0.40
1:A:729:LEU:O	1:A:733:ILE:HG13	2.22	0.40
1:A:1095:LYS:H	1:A:1145:ILE:HG13	1.87	0.40
1:A:1183:LYS:HG2	1:A:1204:TYR:CE2	2.56	0.40
1:A:1236:LEU:HD12	1:A:1262:TYR:HB3	2.03	0.40
1:A:693:SER:HA	1:A:842:TYR:OH	2.20	0.40
1:A:704:LEU:O	1:A:709:THR:HG23	2.22	0.40
1:A:1029:ASP:O	1:A:1029:ASP:OD2	2.39	0.40
1:A:803:LYS:NZ	1:A:803:LYS:HB2	2.36	0.40
1:A:1190:GLU:HG2	1:A:1191:LYS:O	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	1272/1290 (99%)	1144 (90%)	100 (8%)	28 (2%)	5 10

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	ILE
1	A	496	LEU
1	A	669	SER
1	A	672	ASP
1	A	918	PHE

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Mol	Chain	Res	Type
1	A	1151	ASN
1	A	149	ARG
1	A	214	PHE
1	A	424	SER
1	A	668	GLU
1	A	670	TYR
1	A	820	ALA
1	A	922	PHE
1	A	1157	ASP
1	A	1229	GLU
1	A	143	ASN
1	A	30	GLY
1	A	133	ALA
1	A	806	LEU
1	A	1150	SER
1	A	142	SER
1	A	426	GLU
1	A	515	VAL
1	A	671	ILE
1	A	74	ASP
1	A	1256	PHE
1	A	147	VAL
1	A	921	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

3 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	GLC	B	1	2	12,12,12	0.89	0	17,17,17	0.69	0
2	GLA	B	2	2	11,11,12	1.23	1 (9%)	15,15,17	0.97	1 (6%)
2	SIA	B	3	2	20,20,21	1.34	4 (20%)	21,28,31	1.51	2 (9%)

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	GLC	B	1	2	-	0/2/22/22	0/1/1/1
2	GLA	B	2	2	-	2/2/19/22	0/1/1/1
2	SIA	B	3	2	-	6/18/34/38	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	SIA	C4-C5	2.78	1.55	1.53
2	B	3	SIA	C2-C1	2.47	1.55	1.52
2	B	3	SIA	C7-C6	2.45	1.56	1.52
2	B	2	GLA	C1-C2	2.18	1.57	1.52
2	B	3	SIA	C6-C5	2.07	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	SIA	O6-C2-C1	5.41	117.92	107.72
2	B	3	SIA	O1B-C1-C2	2.33	118.76	112.71
2	B	2	GLA	C2-C3-C4	-2.20	106.99	110.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

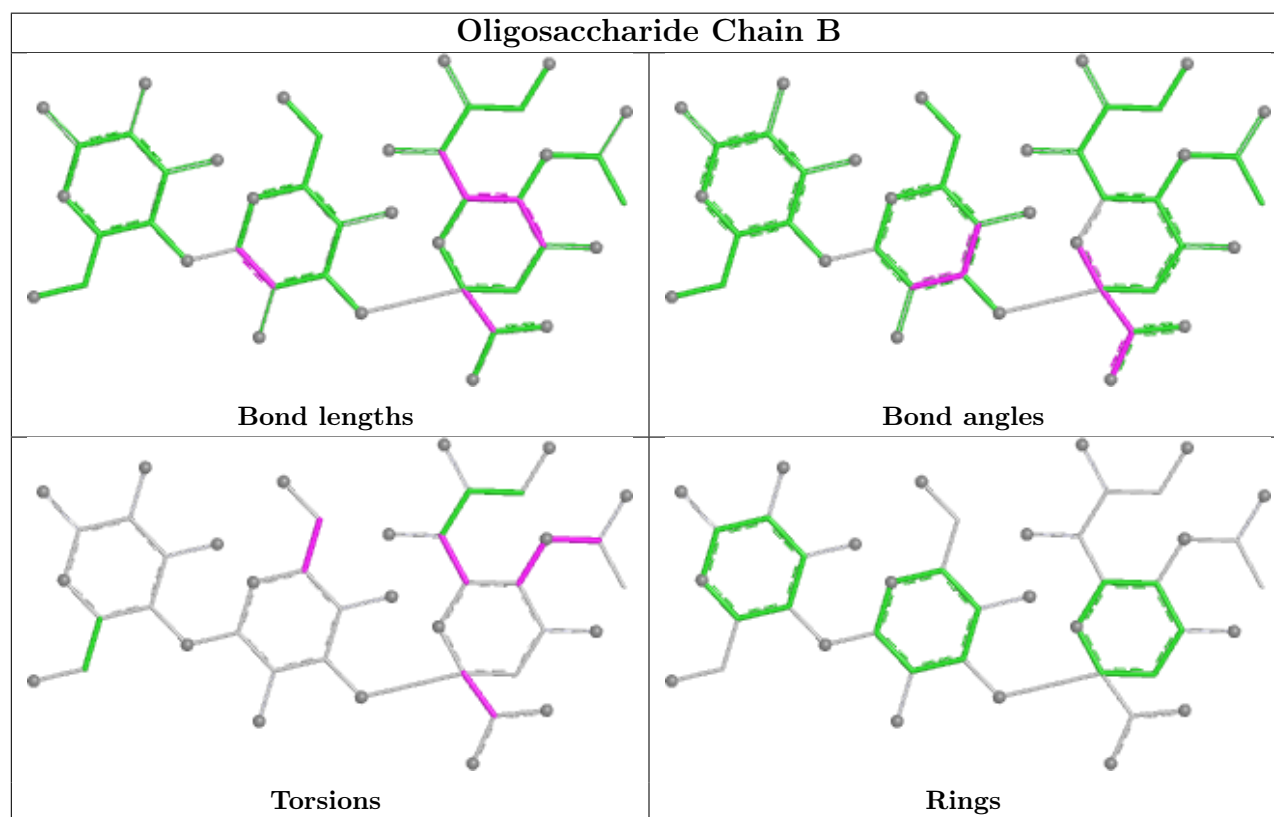
Mol	Chain	Res	Type	Atoms
2	B	3	SIA	C6-C5-N5-C10
2	B	3	SIA	O6-C6-C7-O7
2	B	3	SIA	C11-C10-N5-C5
2	B	3	SIA	O10-C10-N5-C5
2	B	2	GLA	C4-C5-C6-O6
2	B	2	GLA	O5-C5-C6-O6
2	B	3	SIA	O1A-C1-C2-O6
2	B	3	SIA	O6-C6-C7-C8

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	GLA	7	0
2	B	3	SIA	8	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	SO4	A	1292	3	4,4,4	0.73	0	6,6,6	0.38	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1292	SO4	1	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.