



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:37 AM BST

PDB ID : 4F7C
Title : Crystal structure of bovine CD1d with bound C12-di-sulfatide
Authors : Wang, J.; Zajonc, D.M.
Deposited on : 2012-05-15
Resolution : 2.86 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
buster-report : 1.1.7 (2018)
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

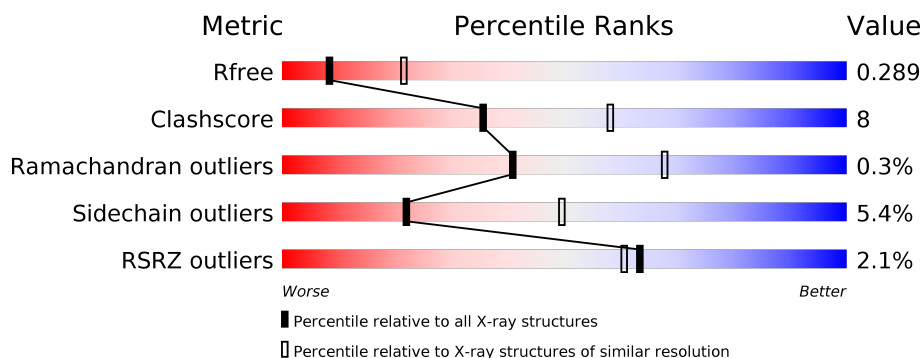
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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.



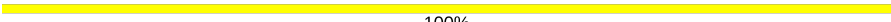
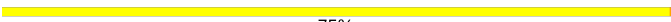

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	283	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 77% 14% • 5% </div> </div>
1	C	283	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 4% 74% 16% • 7% </div> </div>
2	B	98	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 80% 16% • • </div> </div>
2	D	98	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green, yellow, orange, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 81% 15% • • </div> </div>
3	E	2	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 100% </div> </div>
4	F	3	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 100% </div> </div>

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Mol	Chain	Length	Quality of chain
4	G	3	 100%
5	H	4	 75%  25%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6216 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 CD1D antigen, d polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2176	1397	375	397	7			
1	C	263	Total	C	N	O	S	0	0	0
			2131	1370	368	386	7			

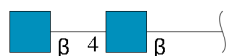
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	HIS	-	expression tag	UNP A1L565
A	279	HIS	-	expression tag	UNP A1L565
A	280	HIS	-	expression tag	UNP A1L565
A	281	HIS	-	expression tag	UNP A1L565
A	282	HIS	-	expression tag	UNP A1L565
A	283	HIS	-	expression tag	UNP A1L565
C	278	HIS	-	expression tag	UNP A1L565
C	279	HIS	-	expression tag	UNP A1L565
C	280	HIS	-	expression tag	UNP A1L565
C	281	HIS	-	expression tag	UNP A1L565
C	282	HIS	-	expression tag	UNP A1L565
C	283	HIS	-	expression tag	UNP A1L565

- Molecule 2 is a protein called Beta-2-microglobulin.

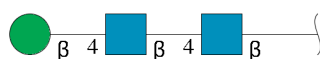
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	97	Total	C	N	O	S	0	0	0
			811	520	141	148	2			
2	D	97	Total	C	N	O	S	0	0	0
			807	517	140	148	2			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



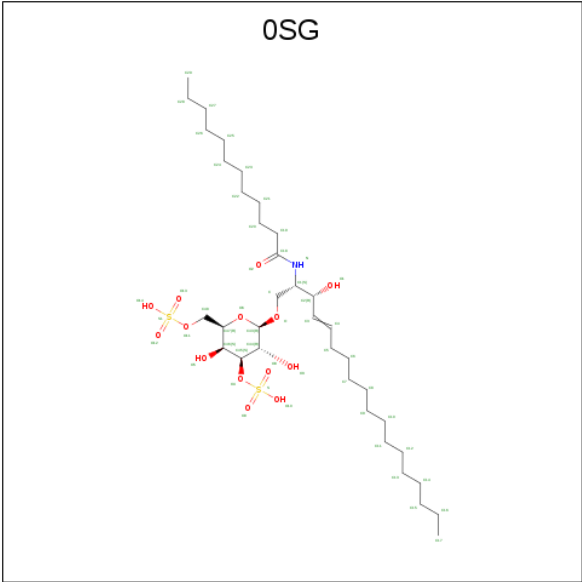
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	3	Total	C	N	O	0	0	0
			39	22	2	15			
4	G	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	H	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 6 is N-[(2S,3R,4E)-1-[(3,6-di-O-sulfo-beta-D-galactopyranosyl)oxy]-3-hydroxyocta-4-en-2-yl]dodecanamide (three-letter code: OSG) (formula: C₃₆H₆₉NO₁₄S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			53	36	1	14	2		
6	C	1	Total	C	N	O	S	0	0
			53	36	1	14	2		

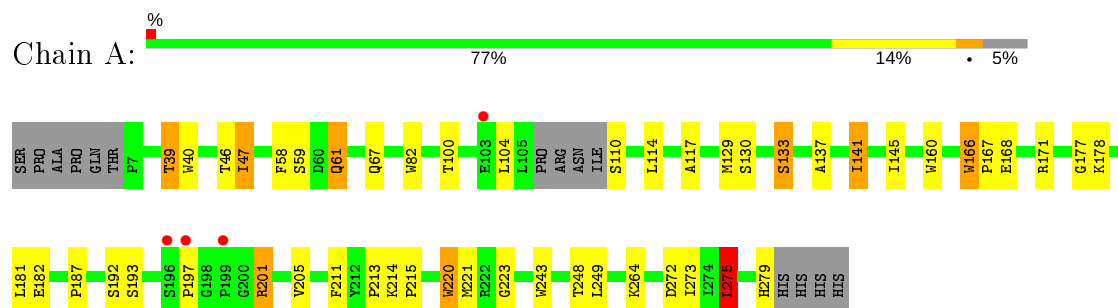
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	10	Total	O	0	0
			10	10		
7	B	6	Total	O	0	0
			6	6		
7	C	4	Total	O	0	0
			4	4		
7	D	9	Total	O	0	0
			9	9		

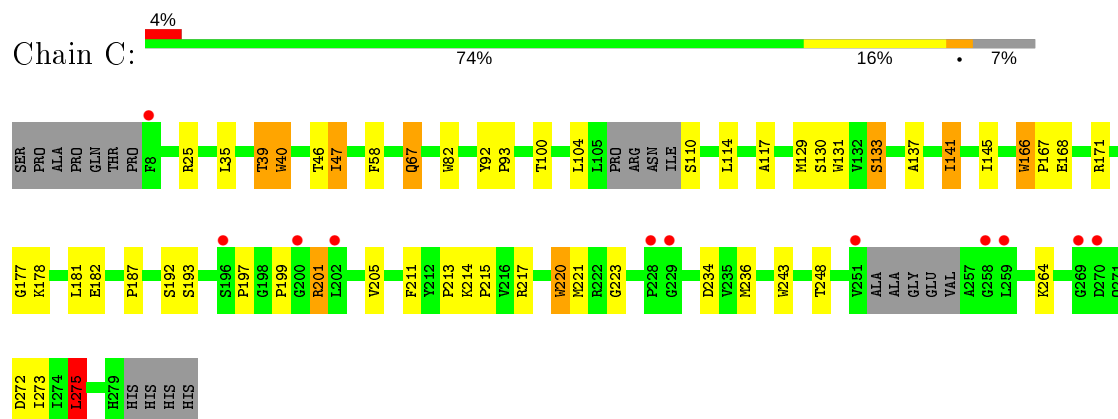
3 Residue-property plots [i](#)

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.

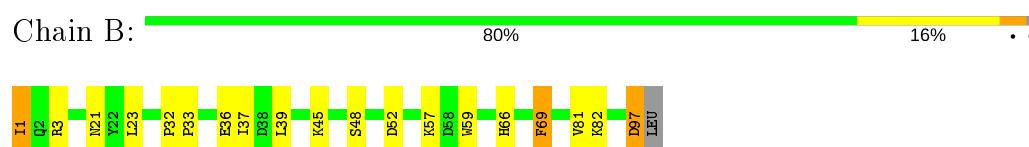
- Molecule 1: CD1D antigen, d polypeptide



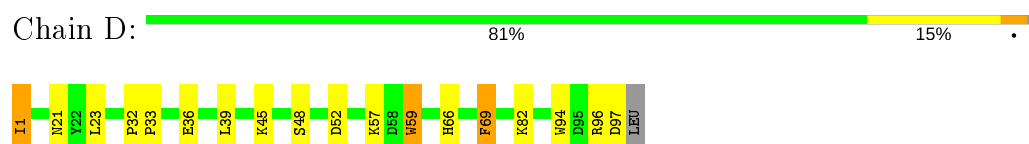
- Molecule 1: CD1D antigen, d polypeptide



- Molecule 2: Beta-2-microglobulin



- Molecule 2: Beta-2-microglobulin



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%

UAG1
UAG2

- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%


UAG1
UAG2
BMA3

- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%

UAG1
UAG2
BMA3

- Molecule 5: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  75% 25%

UAG1
UAG2
BMA3
BMA4

4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	168.55Å 168.55Å 41.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.75 – 2.86 46.75 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.75-2.86) 98.4 (46.75-2.87)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	235.84 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0104	Depositor
R, R_{free}	0.222 , 0.291 0.220 , 0.289	Depositor DCC
R_{free} test set	1112 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6216	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.81	3/2242 (0.1%)	0.71	1/3052 (0.0%)
1	C	0.80	5/2195 (0.2%)	0.70	1/2987 (0.0%)
2	B	0.75	0/837	0.73	0/1135
2	D	0.74	2/833 (0.2%)	0.72	0/1131
All	All	0.79	10/6107 (0.2%)	0.71	2/8305 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	82	TRP	CD2-CE2	7.14	1.50	1.41
1	A	82	TRP	CD2-CE2	6.98	1.49	1.41
1	A	220	TRP	CD2-CE2	5.48	1.48	1.41
1	A	160	TRP	CD2-CE2	5.44	1.47	1.41
2	D	94	TRP	CD2-CE2	5.42	1.47	1.41
1	C	243	TRP	CD2-CE2	5.33	1.47	1.41
1	C	131	TRP	CD2-CE2	5.31	1.47	1.41
2	D	59	TRP	CD2-CE2	5.26	1.47	1.41
1	C	220	TRP	CD2-CE2	5.21	1.47	1.41
1	C	40	TRP	CD2-CE2	5.04	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	LEU	CA-CB-CG	5.99	129.08	115.30
1	A	275	LEU	CA-CB-CG	5.67	128.34	115.30

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	2176	0	2098	36	0
1	C	2131	0	2051	37	0
2	B	811	0	786	16	0
2	D	807	0	775	17	0
3	E	28	0	25	0	0
4	F	39	0	34	0	0
4	G	39	0	34	0	0
5	H	50	0	43	1	0
6	A	53	0	69	0	0
6	C	53	0	69	0	0
7	A	10	0	0	2	0
7	B	6	0	0	0	0
7	C	4	0	0	0	0
7	D	9	0	0	0	0
All	All	6216	0	5984	98	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 8.

All (98) 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:C:39:THR:HG21	2:D:52:ASP:OD2	1.55	1.05
1:A:39:THR:HG21	2:B:52:ASP:OD2	1.65	0.96
1:C:133:SER:HB2	1:C:141:ILE:HD11	1.51	0.93
2:D:1:ILE:N	2:D:1:ILE:HD12	1.95	0.80
1:C:40:TRP:CE3	1:C:47:ILE:HG22	2.18	0.79
2:B:1:ILE:HD12	2:B:1:ILE:N	1.97	0.78
1:A:133:SER:HB2	1:A:141:ILE:HD11	1.66	0.78
1:A:40:TRP:CE3	1:A:47:ILE:HG22	2.21	0.75
1:C:168:GLU:HG3	1:C:171:ARG:HH22	1.53	0.74
2:D:1:ILE:H3	2:D:1:ILE:HD12	1.54	0.71
2:B:1:ILE:H3	2:B:1:ILE:HD12	1.57	0.69
2:D:39:LEU:HD12	2:D:48:SER:HB2	1.75	0.68
1:C:273:ILE:HG22	1:C:275:LEU:CD2	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:THR:CG2	2:B:52:ASP:OD2	2.42	0.66
1:A:205:VAL:HG22	1:A:248:THR:HG22	1.77	0.65
2:D:36:GLU:HB2	2:D:82:LYS:HB2	1.78	0.65
1:C:40:TRP:CZ3	1:C:47:ILE:HG22	2.31	0.64
1:A:40:TRP:CZ3	1:A:47:ILE:HG22	2.34	0.63
1:A:178:LYS:O	1:A:182:GLU:HG2	1.99	0.63
2:B:36:GLU:HB2	2:B:82:LYS:HB2	1.80	0.62
1:A:168:GLU:HG3	1:A:171:ARG:HH22	1.66	0.60
1:C:133:SER:HB2	1:C:141:ILE:CD1	2.29	0.60
2:D:32:PRO:HB2	2:D:33:PRO:CD	2.33	0.59
1:A:214:LYS:N	1:A:215:PRO:CD	2.65	0.59
1:C:39:THR:CG2	2:D:52:ASP:OD2	2.41	0.59
1:A:182:GLU:HA	7:A:408:HOH:O	2.01	0.58
1:A:100:THR:HG22	1:A:114:LEU:HG	1.85	0.57
1:C:205:VAL:HG22	1:C:248:THR:HG22	1.86	0.57
2:D:96:ARG:O	2:D:97:ASP:HB2	2.07	0.55
1:A:187:PRO:HB3	1:A:211:PHE:HB3	1.87	0.55
2:B:39:LEU:HD12	2:B:48:SER:HB2	1.88	0.55
1:C:214:LYS:N	1:C:215:PRO:CD	2.70	0.54
1:A:273:ILE:HG22	1:A:275:LEU:CD2	2.38	0.54
1:C:192:SER:OG	2:D:97:ASP:HB3	2.08	0.54
1:A:166:TRP:HB2	1:A:167:PRO:HD3	1.92	0.52
1:C:100:THR:HG22	1:C:114:LEU:HG	1.91	0.52
1:C:141:ILE:O	1:C:145:ILE:HG12	2.09	0.52
1:C:166:TRP:HB2	1:C:167:PRO:HD3	1.92	0.51
1:C:234:ASP:O	1:C:236:MET:HG3	2.10	0.51
1:C:187:PRO:HB3	1:C:211:PHE:HB3	1.91	0.50
1:A:192:SER:HB2	2:B:97:ASP:HB3	1.93	0.50
2:B:23:LEU:HD23	2:B:39:LEU:HD22	1.92	0.50
2:D:1:ILE:H1	2:D:1:ILE:HD12	1.73	0.49
2:B:32:PRO:HB2	2:B:33:PRO:CD	2.43	0.49
2:B:1:ILE:HD12	2:B:1:ILE:H1	1.74	0.49
1:A:46:THR:HB	1:A:67:GLN:HE21	1.77	0.49
1:C:117:ALA:HB2	2:D:59:TRP:CE2	2.48	0.49
1:C:178:LYS:O	1:C:182:GLU:HG2	2.12	0.48
1:C:177:GLY:O	1:C:181:LEU:HB2	2.14	0.48
1:C:46:THR:HB	1:C:67:GLN:HE21	1.78	0.48
2:B:21:ASN:HB3	2:B:69:PHE:CE1	2.50	0.47
1:C:214:LYS:N	1:C:215:PRO:HD3	2.29	0.47
2:D:1:ILE:H3	2:D:1:ILE:CD1	2.26	0.47
1:C:220:TRP:C	1:C:221:MET:HG2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:SER:HB2	1:A:141:ILE:CD1	2.40	0.47
2:D:1:ILE:N	2:D:1:ILE:CD1	2.68	0.47
1:C:213:PRO:HB2	1:C:215:PRO:HD2	1.97	0.47
1:A:214:LYS:H	1:A:215:PRO:HD3	1.81	0.46
1:A:137:ALA:HB1	1:A:141:ILE:HG12	1.96	0.46
1:A:213:PRO:HB2	1:A:215:PRO:HD2	1.97	0.46
1:C:220:TRP:O	1:C:221:MET:HG2	2.15	0.46
1:C:35:LEU:HD12	1:C:181:LEU:HD12	1.97	0.46
1:A:275:LEU:HD23	1:A:275:LEU:N	2.30	0.46
1:C:137:ALA:HB1	1:C:141:ILE:HG12	1.98	0.46
2:D:23:LEU:O	2:D:66:HIS:HA	2.16	0.46
1:A:177:GLY:O	1:A:181:LEU:HB2	2.16	0.45
2:D:32:PRO:CB	2:D:33:PRO:CD	2.95	0.45
1:A:214:LYS:N	1:A:215:PRO:HD3	2.31	0.45
2:D:32:PRO:HB2	2:D:33:PRO:HD2	1.99	0.44
1:A:117:ALA:HB2	2:B:59:TRP:CE2	2.52	0.44
2:B:1:ILE:CD1	2:B:1:ILE:N	2.70	0.44
2:B:32:PRO:HB2	2:B:33:PRO:HD2	2.00	0.43
1:C:197:PRO:HG2	1:C:201:ARG:HB3	2.00	0.43
1:A:46:THR:HB	1:A:67:GLN:NE2	2.34	0.43
1:C:264:LYS:HG2	1:C:272:ASP:OD2	2.19	0.43
1:C:46:THR:HB	1:C:67:GLN:NE2	2.34	0.43
1:A:214:LYS:HG3	1:A:243:TRP:CE2	2.53	0.42
1:C:275:LEU:HD23	1:C:275:LEU:N	2.35	0.42
2:B:37:ILE:HG12	2:B:81:VAL:HG22	2.01	0.42
1:A:141:ILE:O	1:A:145:ILE:HG12	2.19	0.42
1:A:213:PRO:HG3	7:A:408:HOH:O	2.17	0.42
1:C:40:TRP:CE3	1:C:47:ILE:CG2	2.96	0.42
1:A:201:ARG:HD2	1:A:201:ARG:HA	1.89	0.41
1:A:104:LEU:HA	1:A:110:SER:HA	2.02	0.41
1:A:264:LYS:HG2	1:A:272:ASP:OD2	2.20	0.41
1:A:59:SER:OG	1:A:61:GLN:HG3	2.21	0.41
2:D:21:ASN:HB3	2:D:69:PHE:CE1	2.56	0.41
1:A:40:TRP:CE3	1:A:47:ILE:CG2	2.98	0.41
1:C:104:LEU:HA	1:C:110:SER:HA	2.03	0.41
1:C:25:ARG:HB3	5:H:1:NAG:H82	2.02	0.41
1:C:217:ARG:HE	1:C:264:LYS:HD2	1.86	0.41
1:C:199:PRO:C	1:C:201:ARG:H	2.24	0.41
1:A:220:TRP:C	1:A:221:MET:HG2	2.41	0.41
1:C:92:TYR:HB3	1:C:93:PRO:HA	2.03	0.41
1:A:197:PRO:HG2	1:A:201:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:ILE:HD13	1:C:47:ILE:HG21	1.91	0.40
1:A:220:TRP:CD1	1:A:249:LEU:HB2	2.57	0.40
2:B:23:LEU:O	2:B:66:HIS:HA	2.20	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	265/283 (94%)	253 (96%)	11 (4%)	1 (0%)	34	62
1	C	257/283 (91%)	247 (96%)	9 (4%)	1 (0%)	34	62
2	B	95/98 (97%)	91 (96%)	4 (4%)	0	100	100
2	D	95/98 (97%)	90 (95%)	5 (5%)	0	100	100
All	All	712/762 (93%)	681 (96%)	29 (4%)	2 (0%)	41	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	223	GLY
1	A	223	GLY

5.3.2 Protein sidechains [i](#)

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	236/250 (94%)	223 (94%)	13 (6%)	21	49
1	C	231/250 (92%)	219 (95%)	12 (5%)	23	51
2	B	92/94 (98%)	86 (94%)	6 (6%)	17	41
2	D	91/94 (97%)	87 (96%)	4 (4%)	28	58
All	All	650/688 (94%)	615 (95%)	35 (5%)	22	49

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	47	ILE
1	A	58	PHE
1	A	61	GLN
1	A	129	MET
1	A	130	SER
1	A	133	SER
1	A	141	ILE
1	A	166	TRP
1	A	193	SER
1	A	201	ARG
1	A	275	LEU
1	A	279	HIS
2	B	1	ILE
2	B	3	ARG
2	B	45	LYS
2	B	57	LYS
2	B	69	PHE
2	B	97	ASP
1	C	39	THR
1	C	47	ILE
1	C	58	PHE
1	C	67	GLN
1	C	129	MET
1	C	130	SER
1	C	133	SER
1	C	141	ILE
1	C	166	TRP
1	C	193	SER
1	C	201	ARG
1	C	275	LEU
2	D	1	ILE
2	D	45	LYS

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Mol	Chain	Res	Type
2	D	57	LYS
2	D	69	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
2	B	2	GLN
1	C	67	GLN
2	D	2	GLN

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	NAG	E	1	1,3	14,14,15	0.63	0	17,19,21	1.41	1 (5%)
3	NAG	E	2	3	14,14,15	0.56	0	17,19,21	1.51	4 (23%)
4	NAG	F	1	1,4	14,14,15	0.90	1 (7%)	17,19,21	1.57	3 (17%)
4	NAG	F	2	4	14,14,15	0.65	0	17,19,21	1.61	4 (23%)
4	BMA	F	3	4	11,11,12	0.60	0	15,15,17	1.54	2 (13%)
4	NAG	G	1	1,4	14,14,15	0.64	0	17,19,21	1.52	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	G	2	4	14,14,15	0.57	0	17,19,21	1.08	1 (5%)
4	BMA	G	3	4	11,11,12	0.57	0	15,15,17	1.57	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.72	0	17,19,21	1.23	2 (11%)
5	NAG	H	2	5	14,14,15	0.67	0	17,19,21	1.38	2 (11%)
5	BMA	H	3	5	11,11,12	0.84	0	15,15,17	1.51	2 (13%)
5	BMA	H	4	5	11,11,12	0.68	0	15,15,17	1.76	2 (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
3	NAG	E	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
4	NAG	F	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1
4	BMA	F	3	4	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	0/6/23/26	0/1/1/1
4	NAG	G	2	4	-	0/6/23/26	0/1/1/1
4	BMA	G	3	4	-	2/2/19/22	0/1/1/1
5	NAG	H	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	5	-	2/6/23/26	0/1/1/1
5	BMA	H	3	5	-	1/2/19/22	0/1/1/1
5	BMA	H	4	5	-	1/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1	NAG	C2-N2	-2.39	1.42	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	4	BMA	C1-O5-C5	4.80	118.69	112.19
4	G	3	BMA	C1-O5-C5	4.60	118.42	112.19
4	F	1	NAG	C2-N2-C7	-4.16	116.97	122.90
5	H	3	BMA	C3-C4-C5	4.15	117.64	110.24
5	H	2	NAG	C4-C3-C2	4.15	117.10	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	3	BMA	C1-O5-C5	3.81	117.36	112.19
4	G	1	NAG	C4-C3-C2	3.42	116.03	111.02
5	H	4	BMA	C3-C4-C5	3.34	116.19	110.24
4	F	2	NAG	C4-C3-C2	3.28	115.82	111.02
4	F	2	NAG	C1-C2-N2	-3.28	104.89	110.49
3	E	2	NAG	C2-N2-C7	-3.25	118.27	122.90
4	F	3	BMA	C3-C4-C5	3.11	115.78	110.24
3	E	1	NAG	C2-N2-C7	-3.07	118.53	122.90
4	G	2	NAG	C4-C3-C2	3.05	115.49	111.02
4	G	1	NAG	O3-C3-C2	-2.97	103.32	109.47
4	G	1	NAG	C1-O5-C5	2.96	116.20	112.19
5	H	1	NAG	C2-N2-C7	-2.93	118.73	122.90
3	E	2	NAG	C1-C2-N2	-2.90	105.53	110.49
4	F	2	NAG	O5-C5-C6	2.81	111.61	107.20
4	F	1	NAG	C1-C2-N2	-2.76	105.78	110.49
5	H	2	NAG	C3-C4-C5	2.68	115.03	110.24
4	F	1	NAG	C3-C4-C5	-2.58	105.64	110.24
5	H	1	NAG	C3-C4-C5	-2.49	105.80	110.24
3	E	2	NAG	C4-C3-C2	2.46	114.62	111.02
3	E	2	NAG	C1-O5-C5	2.19	115.16	112.19
5	H	3	BMA	O3-C3-C2	2.06	113.93	109.99
4	G	3	BMA	O2-C2-C1	2.01	113.26	109.15
4	F	2	NAG	C1-O5-C5	-2.00	109.48	112.19

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	3	BMA	O5-C5-C6-O6
5	H	2	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	G	3	BMA	C4-C5-C6-O6
5	H	2	NAG	O5-C5-C6-O6
4	F	3	BMA	C4-C5-C6-O6
4	F	1	NAG	C4-C5-C6-O6
5	H	4	BMA	O5-C5-C6-O6
5	H	3	BMA	O5-C5-C6-O6
4	F	1	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6

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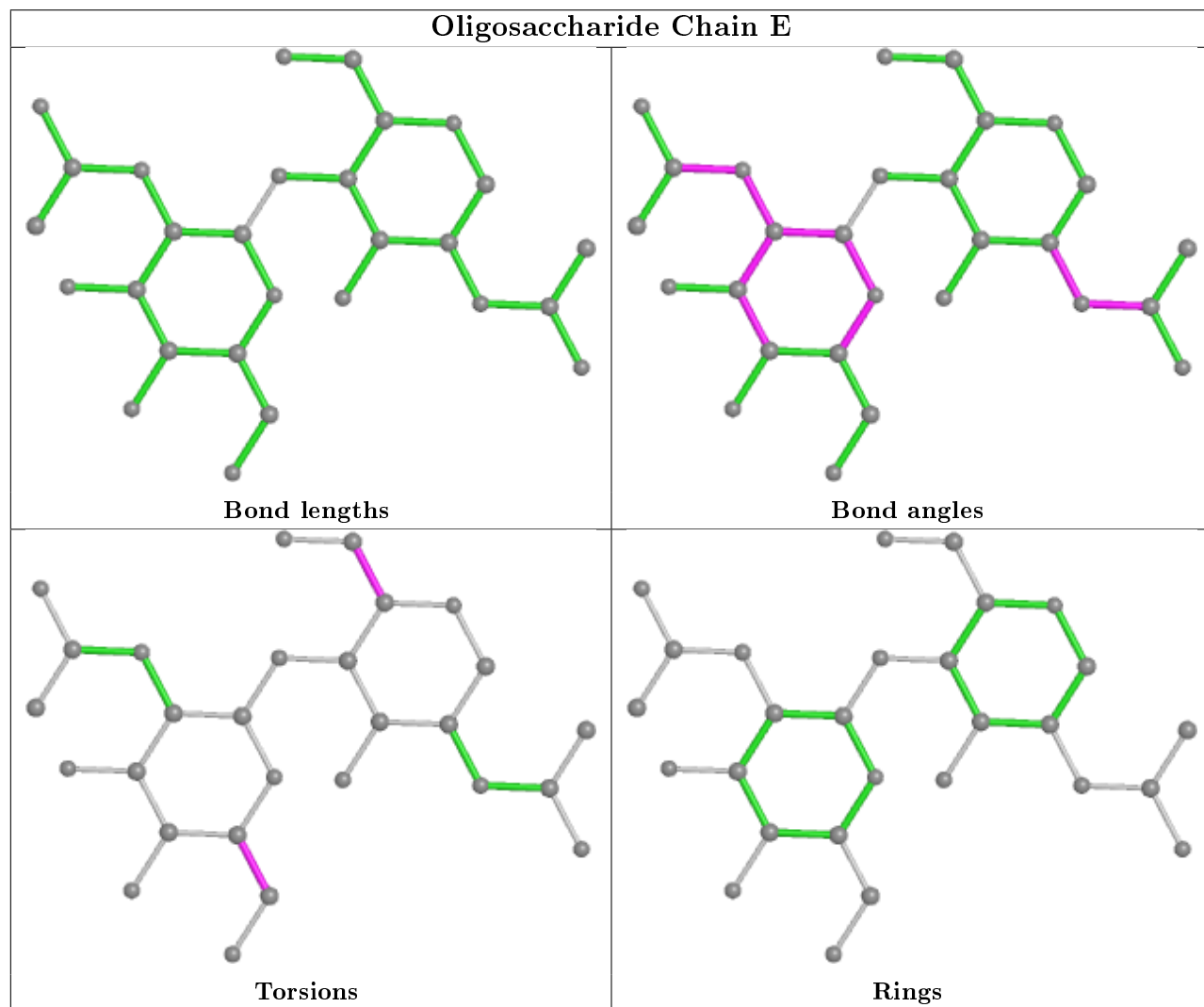
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6

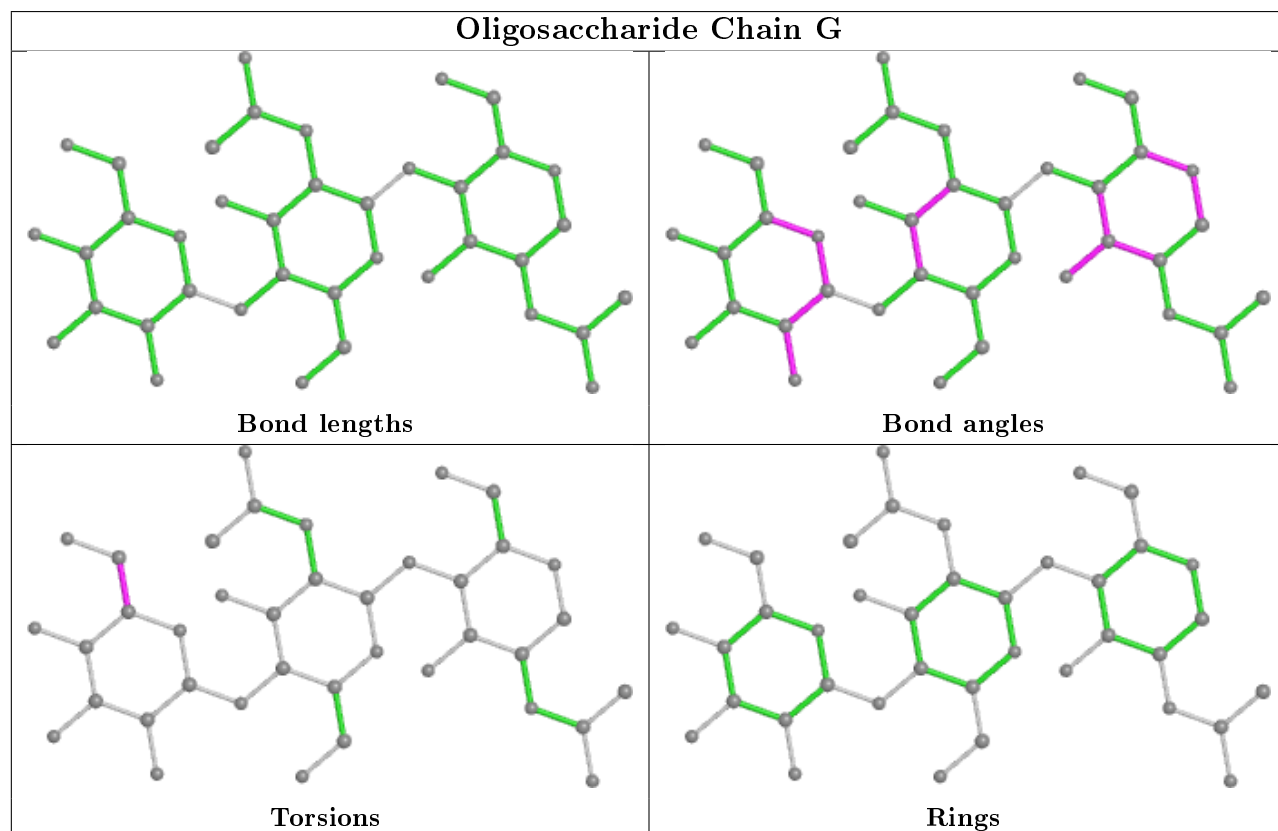
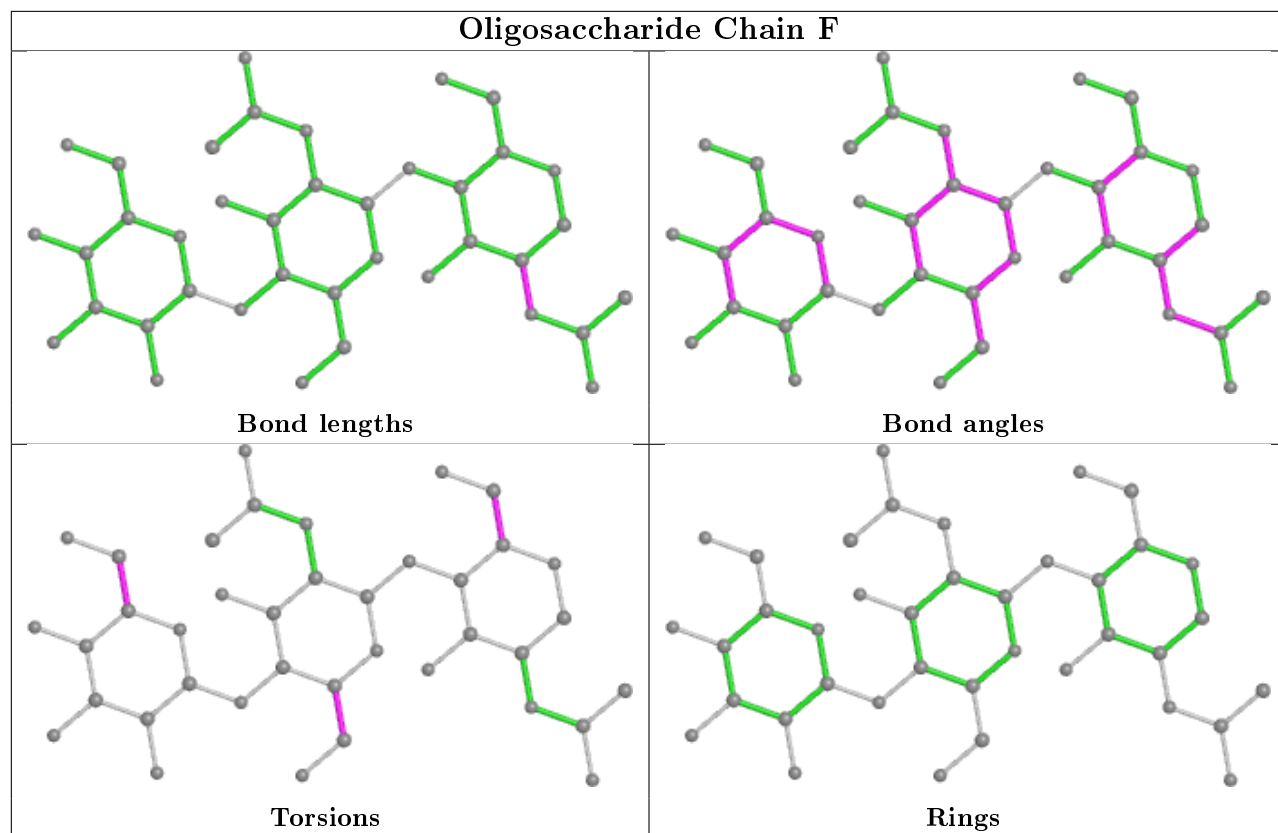
There are no ring outliers.

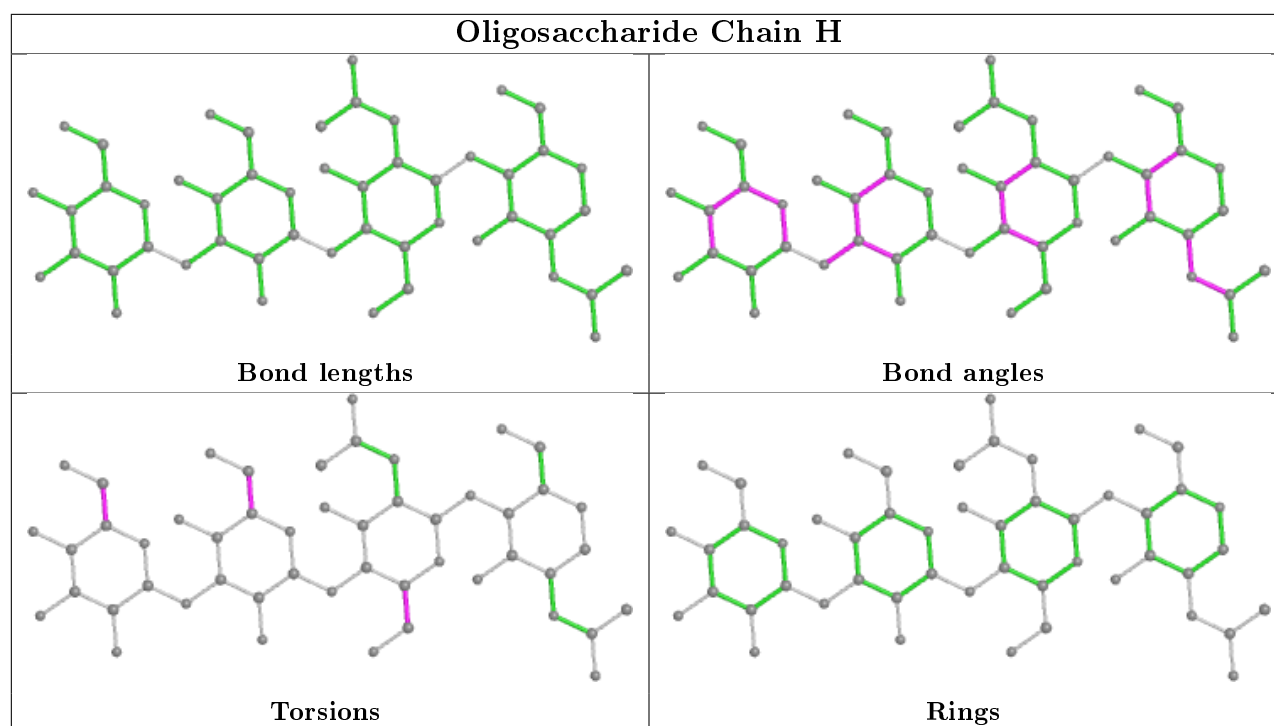
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1	NAG	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](#)

2 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
6	0SG	C	308	-	52,53,53	1.34	5 (9%)	58,67,67	1.69	8 (13%)
6	0SG	A	306	-	52,53,53	1.26	3 (5%)	58,67,67	1.38	3 (5%)

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
6	0SG	C	308	-	-	25/50/70/70	0/1/1/1
6	0SG	A	306	-	-	18/50/70/70	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	306	0SG	C3-C4	5.08	1.53	1.31
6	C	308	0SG	C3-C4	5.05	1.53	1.31
6	C	308	0SG	C19-C18	3.60	1.58	1.51
6	A	306	0SG	C19-C18	2.94	1.56	1.51
6	C	308	0SG	O13-S1	2.33	1.55	1.45
6	A	306	0SG	O4-C45	-2.21	1.41	1.46
6	C	308	0SG	O12-S1	2.19	1.54	1.45
6	C	308	0SG	O9-S	2.17	1.54	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	308	0SG	C2-C3-C4	-6.87	109.46	124.79
6	A	306	0SG	C2-C3-C4	-6.35	110.63	124.79
6	C	308	0SG	C-O-C43	-5.48	103.04	113.74
6	A	306	0SG	C-O-C43	-4.64	104.67	113.74
6	A	306	0SG	C5-C4-C3	-3.91	107.90	125.39
6	C	308	0SG	C5-C4-C3	-3.68	108.96	125.39
6	C	308	0SG	O6-C47-C48	-3.63	99.34	106.67
6	C	308	0SG	O-C43-C44	3.23	113.34	108.30
6	C	308	0SG	C43-C44-C45	-2.94	104.90	110.07
6	C	308	0SG	C43-O6-C47	-2.72	108.35	113.69
6	C	308	0SG	C45-O4-S	2.06	122.85	118.88

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	308	0SG	O-C-C1-C2
6	C	308	0SG	O-C-C1-N
6	C	308	0SG	C44-C45-O4-S
6	C	308	0SG	C45-O4-S-O10
6	C	308	0SG	O6-C47-C48-O11
6	C	308	0SG	C46-C47-C48-O11
6	A	306	0SG	O-C-C1-C2
6	A	306	0SG	O-C-C1-N
6	C	308	0SG	C18-C19-C20-C21
6	A	306	0SG	C18-C19-C20-C21
6	A	306	0SG	C7-C8-C9-C10
6	A	306	0SG	C13-C14-C15-C16
6	A	306	0SG	C9-C10-C11-C12

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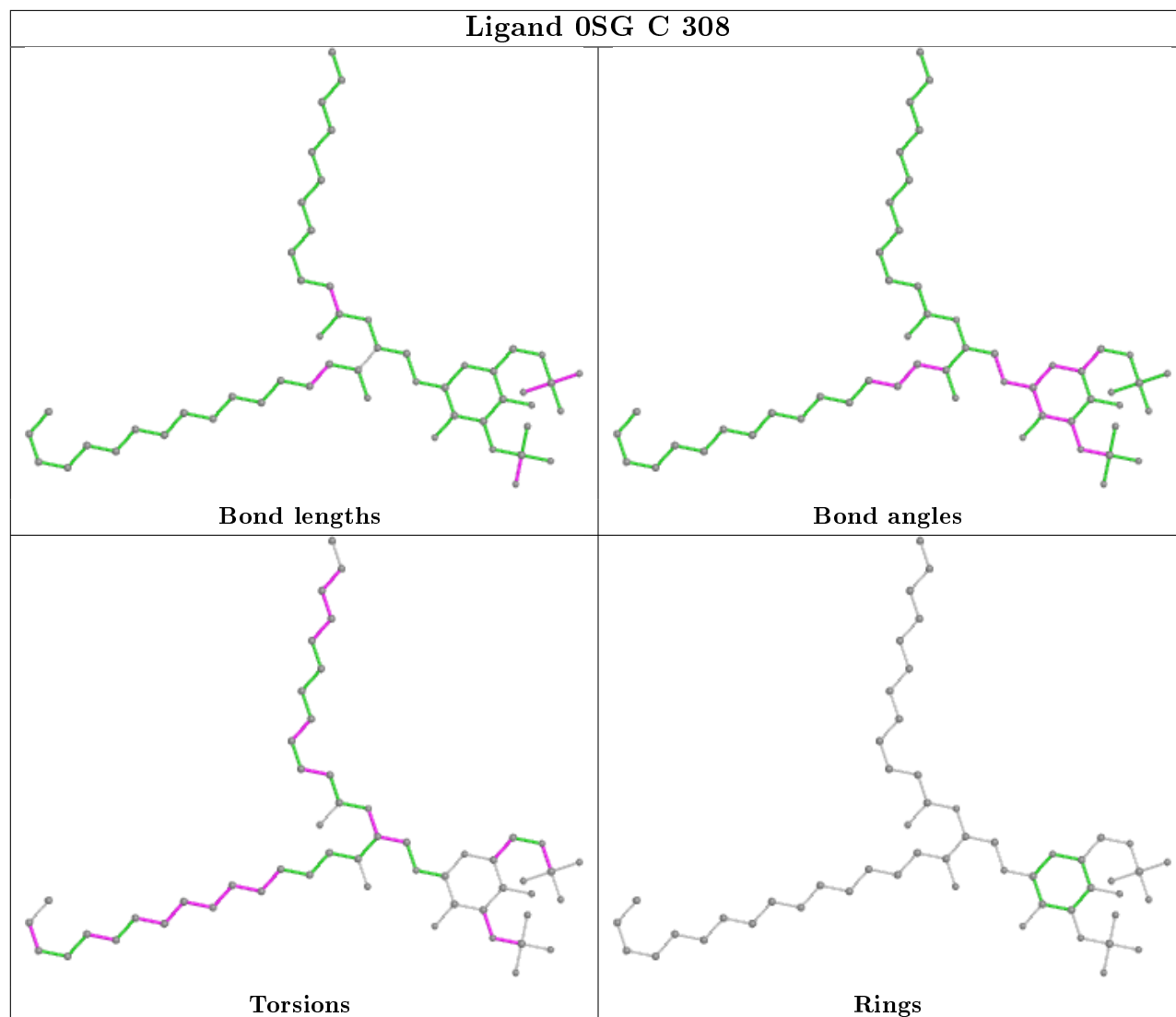
Mol	Chain	Res	Type	Atoms
6	C	308	0SG	C25-C26-C27-C28
6	C	308	0SG	C48-O11-S1-O13
6	C	308	0SG	C7-C8-C9-C10
6	C	308	0SG	C11-C10-C9-C8
6	A	306	0SG	C24-C25-C26-C27
6	C	308	0SG	C45-O4-S-O8
6	C	308	0SG	C11-C12-C13-C14
6	A	306	0SG	C25-C26-C27-C28
6	C	308	0SG	C4-C5-C6-C7
6	C	308	0SG	C20-C21-C22-C23
6	A	306	0SG	C14-C15-C16-C17
6	A	306	0SG	C26-C27-C28-C29
6	A	306	0SG	C11-C10-C9-C8
6	C	308	0SG	C48-O11-S1-O12
6	C	308	0SG	C14-C15-C16-C17
6	C	308	0SG	C24-C25-C26-C27
6	C	308	0SG	C6-C7-C8-C9
6	A	306	0SG	C2-C3-C4-C5
6	C	308	0SG	C5-C6-C7-C8
6	C	308	0SG	C45-O4-S-O9
6	C	308	0SG	C26-C27-C28-C29
6	A	306	0SG	C2-C1-N-C18
6	C	308	0SG	C9-C10-C11-C12
6	C	308	0SG	C46-C45-O4-S
6	A	306	0SG	C44-C45-O4-S
6	A	306	0SG	C46-C45-O4-S
6	C	308	0SG	C2-C1-N-C18
6	A	306	0SG	C22-C23-C24-C25
6	A	306	0SG	C-C1-N-C18
6	A	306	0SG	C6-C7-C8-C9

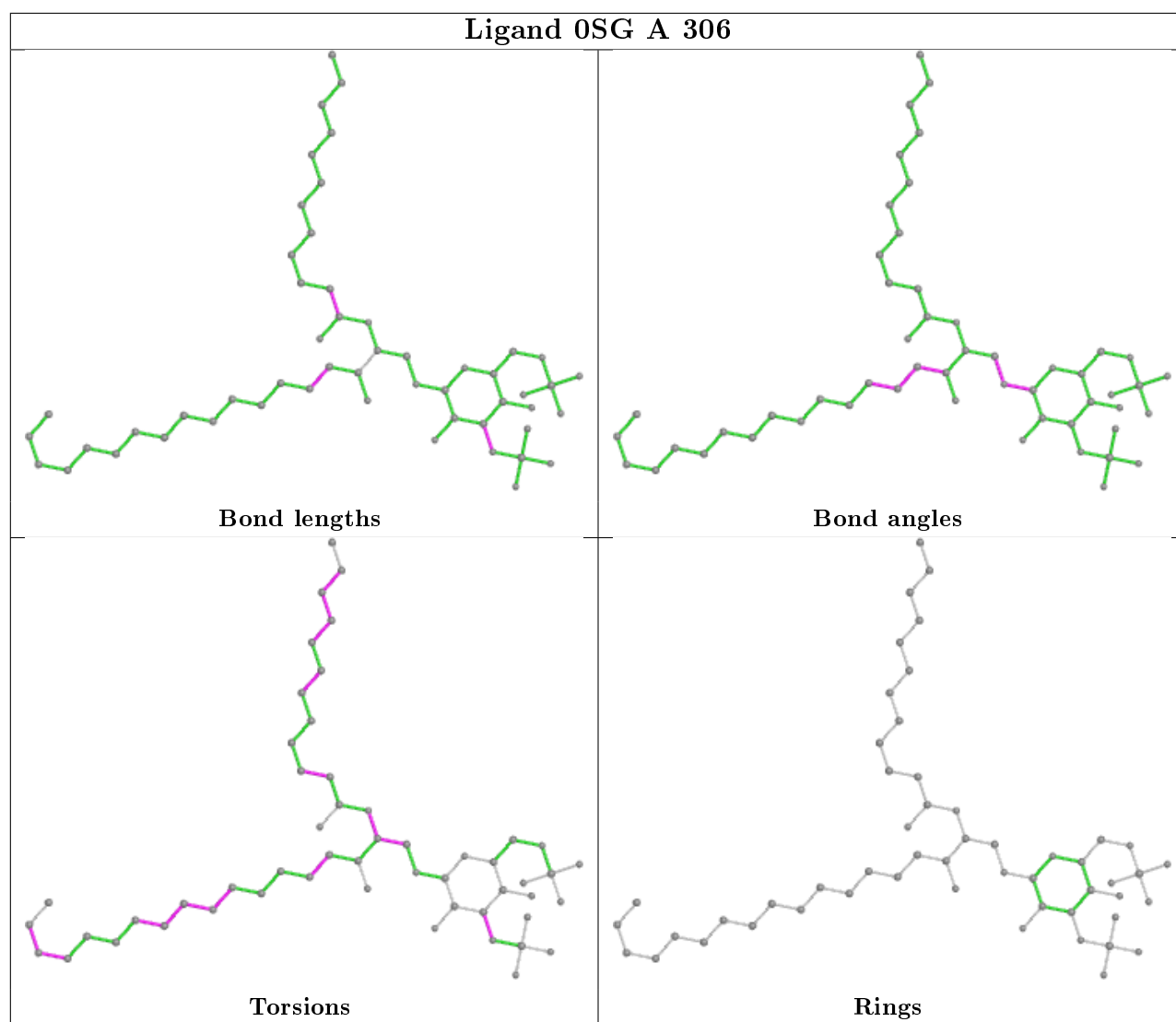
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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](#)

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	269/283 (95%)	0.04	4 (1%) 73 72	23, 41, 80, 107	0
1	C	263/283 (92%)	0.15	11 (4%) 36 31	25, 46, 90, 117	0
2	B	97/98 (98%)	-0.36	0 100 100	20, 33, 60, 78	0
2	D	97/98 (98%)	-0.35	0 100 100	24, 36, 67, 84	0
All	All	726/762 (95%)	-0.02	15 (2%) 63 60	20, 41, 82, 117	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	200	GLY	3.6
1	C	270	ASP	3.4
1	A	199	PRO	3.2
1	C	202	LEU	3.2
1	C	228	PRO	2.8
1	A	197	PRO	2.6
1	A	196	SER	2.6
1	C	229	GLY	2.4
1	C	269	GLY	2.4
1	C	8	PHE	2.3
1	C	196	SER	2.1
1	C	251	VAL	2.1
1	A	103	GLU	2.1
1	C	259	LEU	2.0
1	C	258	GLY	2.0

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

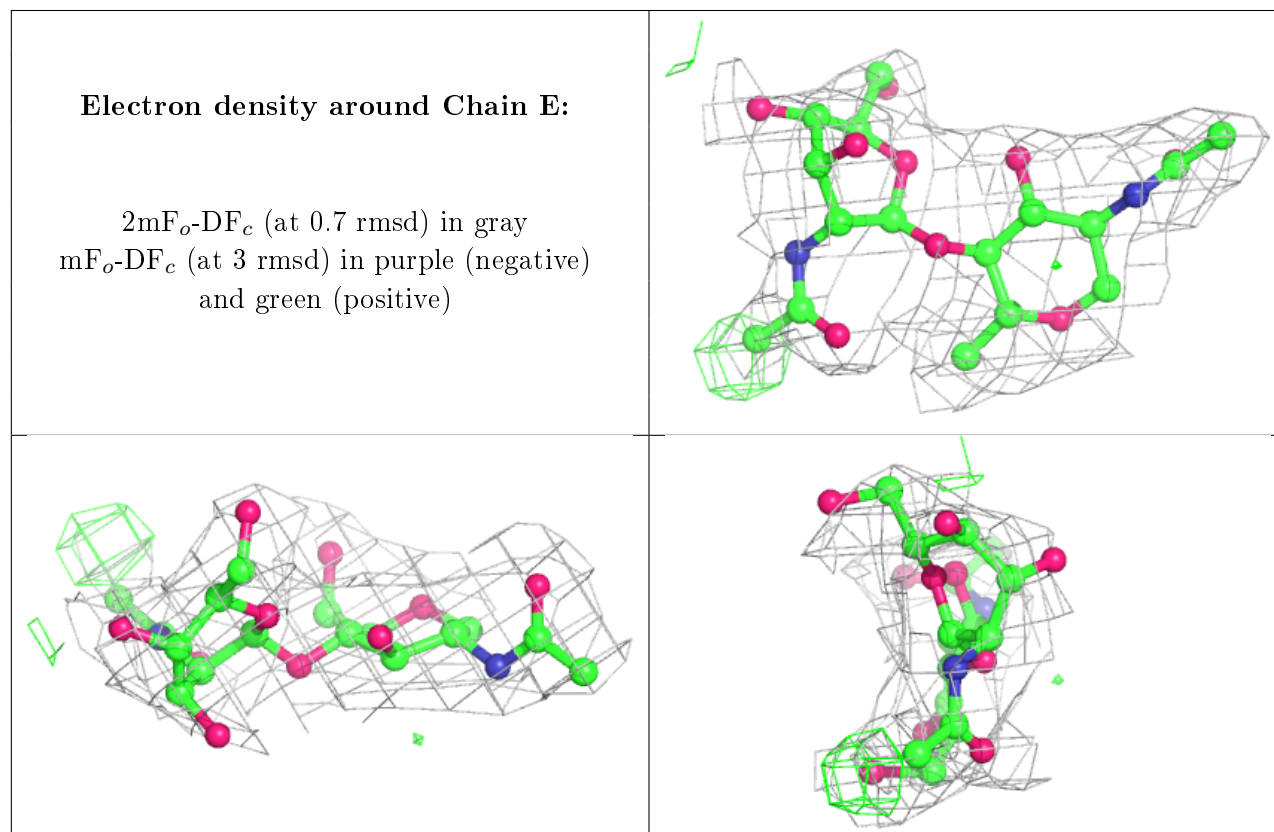
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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.

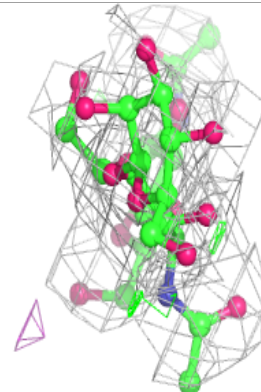
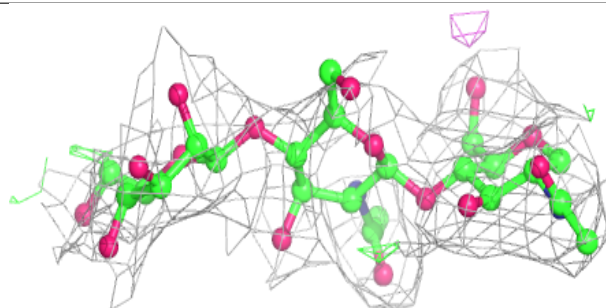
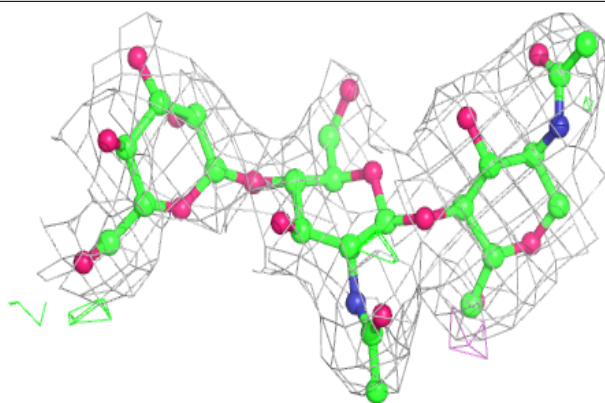
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	BMA	G	3	11/12	0.57	0.30	77,106,113,113	0
5	BMA	H	4	11/12	0.70	0.25	95,110,113,114	0
4	BMA	F	3	11/12	0.71	0.26	82,96,105,106	0
5	BMA	H	3	11/12	0.75	0.26	94,101,106,110	0
3	NAG	E	2	14/15	0.81	0.32	70,87,90,94	0
4	NAG	F	2	14/15	0.84	0.20	64,79,87,92	0
4	NAG	G	2	14/15	0.87	0.35	69,84,99,113	0
5	NAG	H	2	14/15	0.87	0.24	69,78,91,91	0
4	NAG	G	1	14/15	0.94	0.19	53,62,68,70	0
3	NAG	E	1	14/15	0.95	0.16	47,56,64,67	0
5	NAG	H	1	14/15	0.95	0.13	36,42,49,61	0
4	NAG	F	1	14/15	0.96	0.15	37,39,46,57	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.

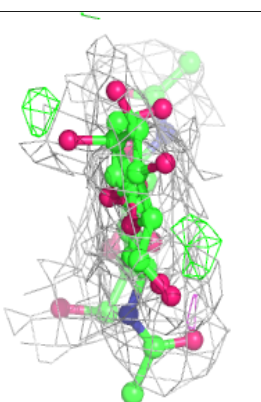
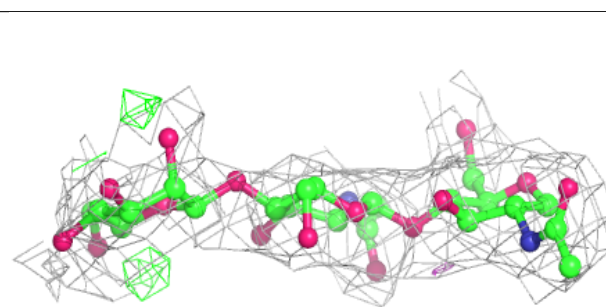
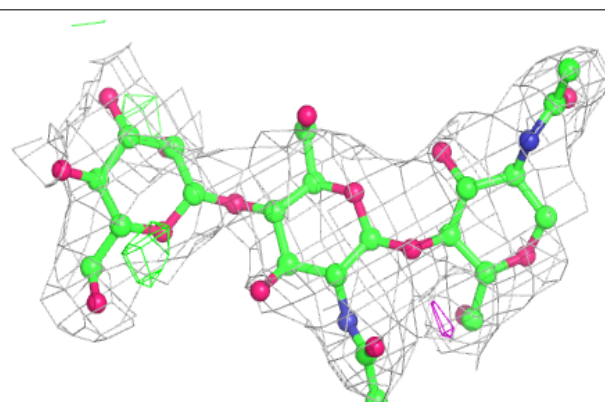


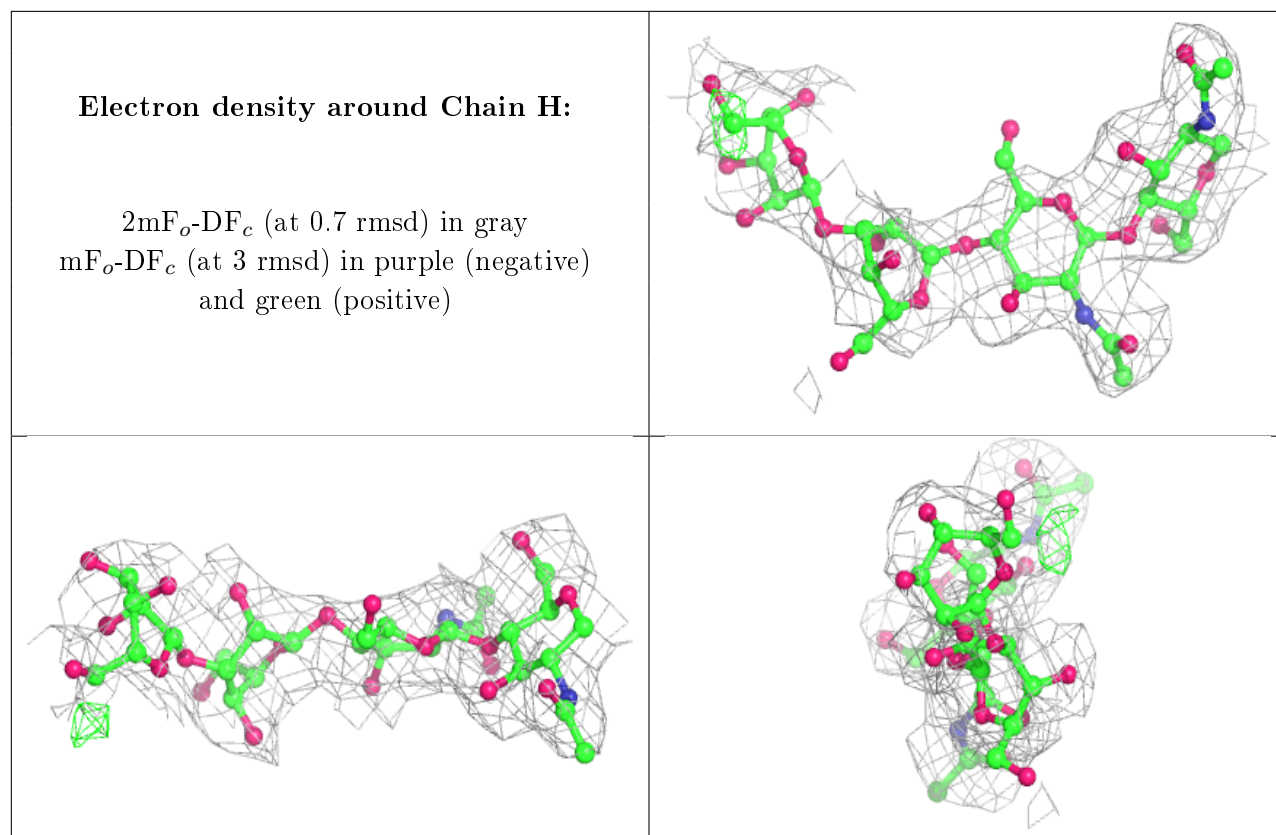
Electron density around Chain F:

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

**Electron density around Chain G:**

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





6.4 Ligands [i](#)

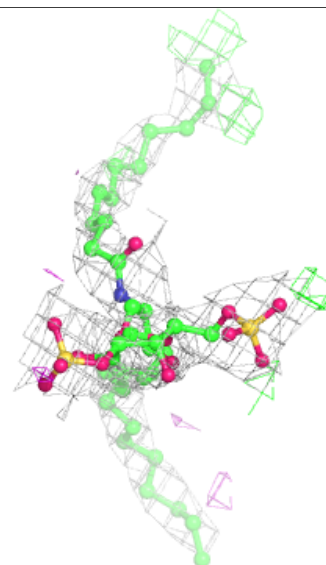
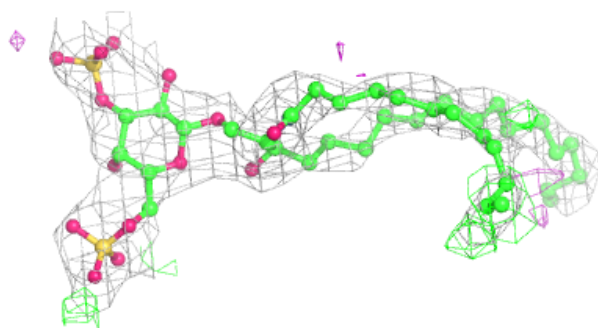
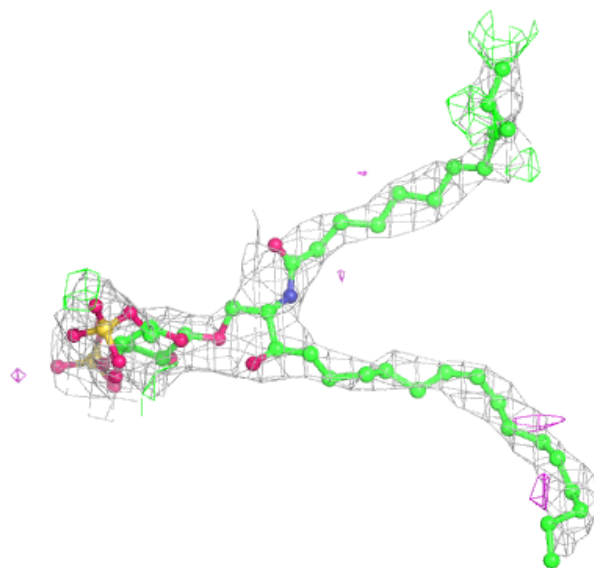
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	OSG	C	308	53/53	0.88	0.30	40,66,112,125	0
6	OSG	A	306	53/53	0.92	0.25	43,64,98,102	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

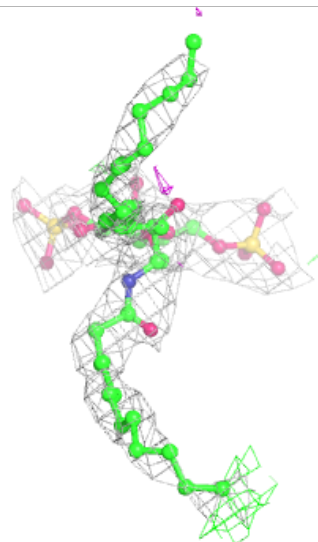
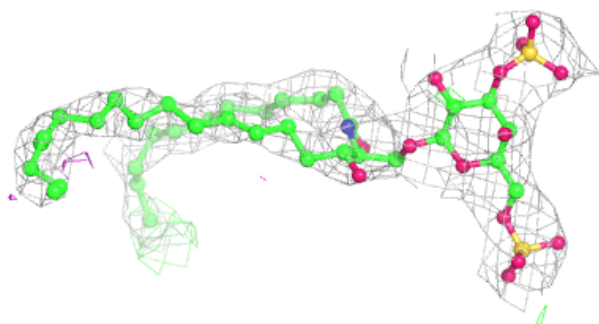
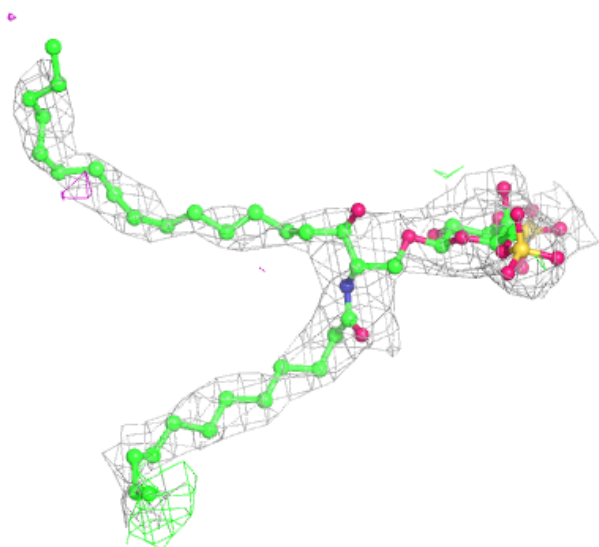
Electron density around 0SG C 308:

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



Electron density around OSG A 306:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.