Full wwPDB X-ray Structure Validation Report (i)

Jun 25, 2024 – 10:22 AM EDT

PDB ID	:	6MTJ
Title	:	Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound to Small Molecule HIV-1 Entry Inhibitor BMS-378806 in Complex with Human Antibodies 3H109L and 35O22 at 2.9 Angstrom
Authors	:	Lai, Y.-T.; Kwong, P.D.
Deposited on	:	2018-10-19
Resolution	:	2.34 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 (i) 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 (i)) were used in the production of this report:

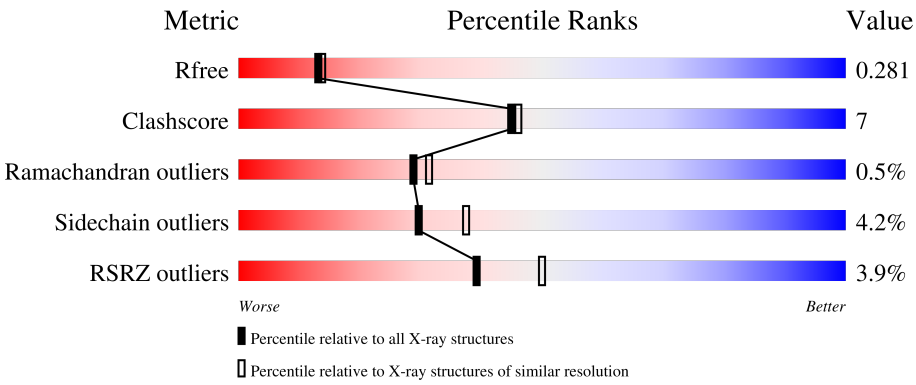
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 <=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	B	153	3%, 79%, 7%, •, 13%
2	D	134	10%, 70%, 25%, •
3	E	114	6%, 79%, 12%, •, 8%
4	G	481	3%, 71%, 19%, •, 9%

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Mol	Chain	Length	Quality of chain
5	H	244	3% 72% 19% 7%
6	L	217	% 81% 15%
7	A	6	17% 67% 17%
8	C	3	100%
8	F	3	67% 33%
9	I	2	100%
9	J	2	100%
9	M	2	50% 50%
10	K	10	10% 70% 20%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10263 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	133	1056	673	182	195	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called 35O22 scFv heavy chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	128	994	628	169	192	5	0	0	0

- Molecule 3 is a protein called 35O22 scFv light chain portion.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	105	805	506	133	160	6	0	0	0

- Molecule 4 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	G	440	3465	2177	614	646	28	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	137	ALA	ASN	engineered mutation	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	501	CYS	ALA	conflict	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6

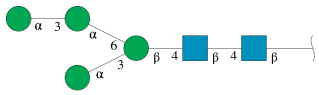
- Molecule 5 is a protein called 3H109L Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	H	226	1715	1093	278	338	6	0	0	0

- Molecule 6 is a protein called 3H109L Fab light chain.

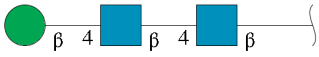
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	L	211	1604	1009	276	312	7	0	0	0

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-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
			Total	C	N	O			
7	A	6	72	40	2	30	0	0	0

- Molecule 8 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
			Total	C	N	O			
8	C	3	39	22	2	15	0	0	0

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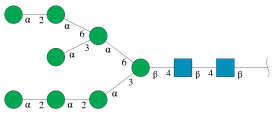
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	F	3	39	22	2	15	0	0	0

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

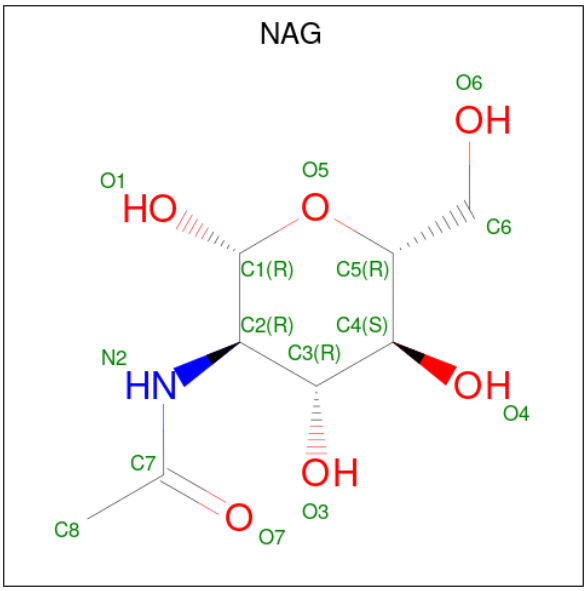
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	I	2	28	16	2	10	0	0	0
9	J	2	28	16	2	10	0	0	0
9	M	2	28	16	2	10	0	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



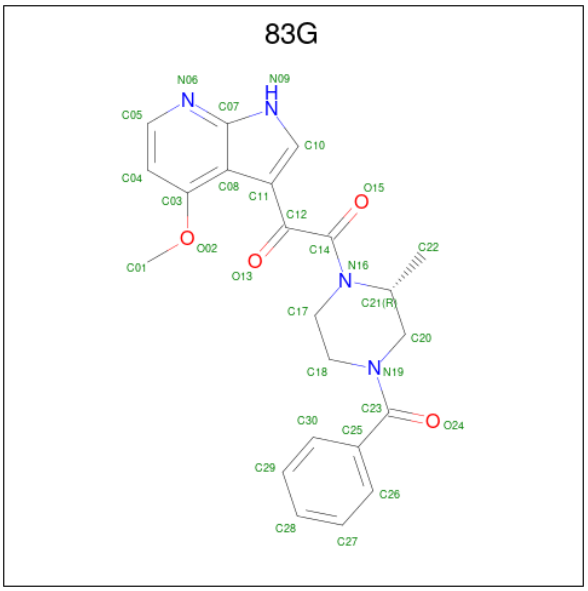
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	K	10	116	64	2	50	0	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
11	B	1	14	8	1	5	0	0
			Total	C	N	O		
11	B	1	14	8	1	5	0	0
			Total	C	N	O		
11	B	1	14	8	1	5	0	0
			Total	C	N	O		
11	D	1	14	8	1	5	0	0
			Total	C	N	O		
11	G	1	14	8	1	5	0	0
			Total	C	N	O		
11	G	1	14	8	1	5	0	0
			Total	C	N	O		
11	G	1	14	8	1	5	0	0
			Total	C	N	O		
11	G	1	14	8	1	5	0	0
			Total	C	N	O		
11	G	1	14	8	1	5	0	0
			Total	C	N	O		
11	G	1	14	8	1	5	0	0
			Total	C	N	O		
11	G	1	14	8	1	5	0	0
			Total	C	N	O		
11	G	1	14	8	1	5	0	0

- Molecule 12 is 1-[(2R)-4-(benzenecarbonyl)-2-methylpiperazin-1-yl]-2-(4-methoxy-1H-pyrrolo[2,3-b]pyridin-3-yl)ethane-1,2-dione (three-letter code: 83G) (formula: $C_{22}H_{22}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
12	G	1	30	22	4	4	0	0

- Molecule 13 is water.

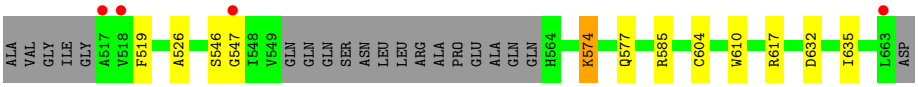
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	B	8	8	8	0	0
			Total	O		
13	D	7	7	7	0	0
			Total	O		
13	E	4	4	4	0	0
			Total	O		
13	G	29	29	29	0	0
			Total	O		
13	H	12	12	12	0	0
			Total	O		
13	L	16	16	16	0	0

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.

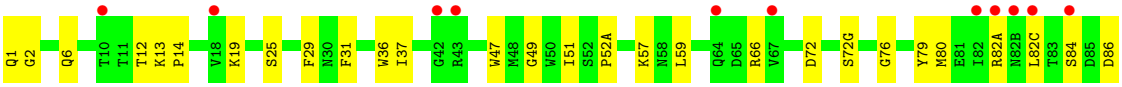
- Molecule 1: Envelope glycoprotein gp160

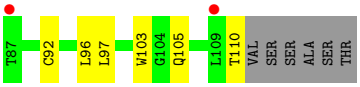
Chain B:



- Molecule 2: 35O22 scFv heavy chain portion

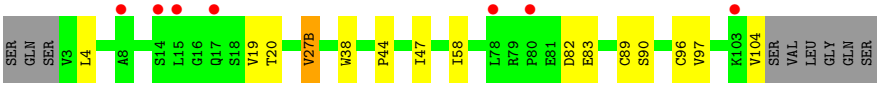
Chain D:





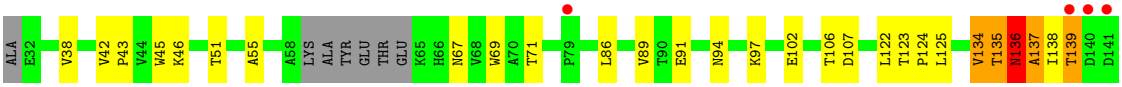
- Molecule 3: 35O22 scFv light chain portion

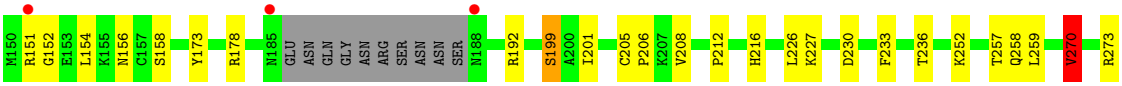
Chain E:

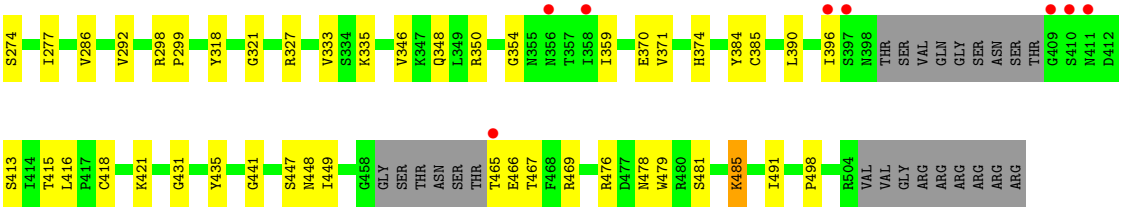


- Molecule 4: Envelope glycoprotein gp160

Chain G:

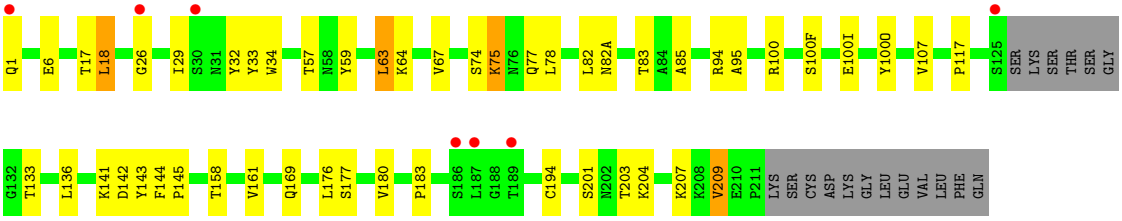






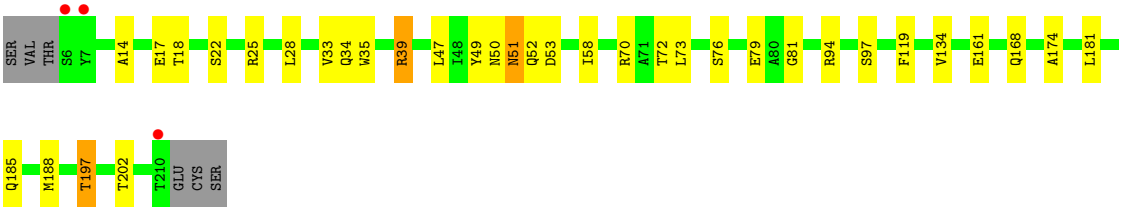
• Molecule 5: 3H109L Fab heavy chain

Chain H:



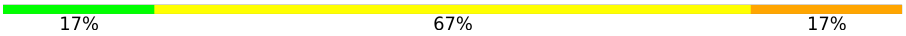
• Molecule 6: 3H109L Fab light chain

Chain L:



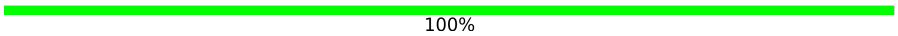
• Molecule 7: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:



• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

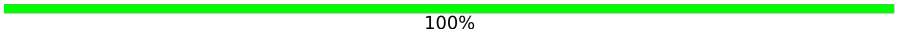
Chain C:



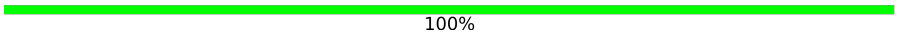
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 

• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	132.18Å 132.18Å 316.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.27 – 2.34 43.27 – 2.34	Depositor EDS
% Data completeness (in resolution range)	38.9 (43.27-2.34) 38.9 (43.27-2.34)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.233 , 0.281 0.233 , 0.281	Depositor DCC
R_{free} test set	2544 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.032 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	10263	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, MAN, 83G, BMA

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	B	0.23	0/1075	0.39	0/1458
2	D	0.24	0/1021	0.47	0/1390
3	E	0.24	0/829	0.44	0/1133
4	G	0.25	0/3536	0.45	0/4797
5	H	0.25	0/1758	0.47	0/2397
6	L	0.25	0/1647	0.46	0/2247
All	All	0.25	0/9866	0.45	0/13422

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	B	1056	0	1049	9	0
2	D	994	0	952	19	0
3	E	805	0	752	6	0
4	G	3465	0	3406	59	0
5	H	1715	0	1685	25	0
6	L	1604	0	1553	20	0
7	A	72	0	61	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	C	39	0	34	0	0
8	F	39	0	34	1	0
9	I	28	0	25	0	0
9	J	28	0	25	0	0
9	M	28	0	25	0	0
10	K	116	0	97	2	0
11	B	42	0	39	1	0
11	D	14	0	13	0	0
11	G	112	0	104	1	0
12	G	30	0	0	0	0
13	B	8	0	0	0	0
13	D	7	0	0	0	0
13	E	4	0	0	0	0
13	G	29	0	0	0	0
13	H	12	0	0	0	0
13	L	16	0	0	0	0
All	All	10263	0	9854	131	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 7.

All (131) 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)
5:H:136:LEU:HD13	5:H:209:VAL:HG21	1.67	0.76
6:L:34:GLN:HG3	6:L:49:TYR:HA	1.68	0.75
4:G:136:ASN:HD22	6:L:94:ARG:HD2	1.57	0.70
4:G:137:ALA:HA	4:G:151:ARG:HD3	1.75	0.69
4:G:298:ARG:NH2	4:G:441:GLY:O	2.27	0.68
4:G:138:ILE:HG12	4:G:139:THR:H	1.61	0.66
6:L:50:ASN:O	6:L:52:GLN:N	2.28	0.66
2:D:96:LEU:HG	2:D:97:LEU:HG	1.79	0.64
6:L:34:GLN:NE2	6:L:49:TYR:O	2.30	0.63
4:G:274:SER:HB3	4:G:277:ILE:HG12	1.81	0.62
6:L:39:ARG:NH1	6:L:81:GLY:O	2.33	0.62
5:H:18:LEU:HD22	5:H:82:LEU:HB3	1.82	0.61
5:H:117:PRO:HB3	5:H:143:TYR:HB3	1.83	0.60
4:G:292:VAL:HG13	4:G:449:ILE:HB	1.83	0.60
5:H:63:LEU:HD13	5:H:67:VAL:HG21	1.83	0.60
6:L:50:ASN:O	6:L:53:ASP:N	2.35	0.59
1:B:546:SER:OG	1:B:547:GLY:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:201:ILE:HD11	4:G:435:TYR:HB2	1.83	0.59
4:G:270:VAL:HG13	4:G:348:GLN:HG3	1.84	0.59
5:H:29:ILE:HD11	5:H:78:LEU:HB3	1.83	0.58
4:G:230:ASP:HB3	4:G:233:PHE:HB2	1.86	0.58
4:G:257:THR:HG22	4:G:258:GLN:HG3	1.86	0.57
7:A:2:NAG:H3	7:A:2:NAG:H83	1.87	0.57
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.41	0.56
4:G:346:VAL:HG13	4:G:359:ILE:HD11	1.87	0.56
4:G:359:ILE:HG22	4:G:466:GLU:HB2	1.87	0.55
2:D:6:GLN:H	2:D:105:GLN:HE22	1.53	0.54
5:H:17:THR:HA	5:H:82(A):ASN:HA	1.90	0.53
5:H:83:THR:HG23	5:H:85:ALA:H	1.73	0.53
3:E:4:LEU:HD11	3:E:90:SER:HB3	1.92	0.52
3:E:47:ILE:HD13	3:E:58:ILE:HD12	1.91	0.52
4:G:122:LEU:HD13	4:G:125:LEU:HD12	1.92	0.52
1:B:617:ARG:HH22	11:B:702:NAG:H4	1.75	0.52
5:H:100(O):TYR:HB3	6:L:34:GLN:HG2	1.91	0.51
4:G:257:THR:O	4:G:259:LEU:N	2.43	0.51
6:L:119:PHE:HB2	6:L:134:VAL:HG22	1.93	0.51
5:H:161:VAL:HA	5:H:180:VAL:HG12	1.92	0.51
4:G:233:PHE:O	4:G:273:ARG:NH1	2.43	0.51
2:D:19:LYS:HD2	2:D:79:TYR:HB3	1.93	0.50
3:E:38:TRP:CE2	3:E:44:PRO:HG3	2.47	0.50
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.94	0.50
2:D:51:ILE:HG13	2:D:57:LYS:HB3	1.93	0.50
4:G:94:ASN:HA	4:G:236:THR:HG22	1.94	0.50
2:D:36:TRP:CZ3	2:D:92:CYS:HB3	2.46	0.49
4:G:122:LEU:HB2	4:G:201:ILE:HG23	1.94	0.49
3:E:27(B):VAL:HG11	3:E:97:VAL:HG11	1.94	0.49
2:D:72:ASP:OD1	2:D:72:ASP:N	2.37	0.49
5:H:6:GLU:N	5:H:6:GLU:OE1	2.46	0.49
4:G:67:ASN:HD21	4:G:71:THR:HG23	1.77	0.49
4:G:205:CYS:O	4:G:208:VAL:HG22	2.13	0.49
6:L:14:ALA:HB3	6:L:17:GLU:HG3	1.94	0.49
1:B:585:ARG:NH2	4:G:491:ILE:O	2.46	0.48
4:G:134:VAL:HB	4:G:156:ASN:HB2	1.95	0.48
2:D:29:PHE:CE2	2:D:52(A):PRO:HB3	2.48	0.48
4:G:136:ASN:O	4:G:138:ILE:N	2.47	0.48
5:H:59:TYR:HB2	5:H:64:LYS:HD2	1.95	0.48
5:H:74:SER:OG	5:H:75:LYS:NZ	2.42	0.47
1:B:577:GLN:HG2	4:G:51:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:370:GLU:HG3	4:G:384:TYR:HE2	1.79	0.47
1:B:610:TRP:CD2	4:G:498:PRO:HB3	2.49	0.47
6:L:18:THR:HG22	6:L:76:SER:HA	1.96	0.47
6:L:197:THR:HA	6:L:202:THR:HA	1.97	0.47
4:G:158:SER:HA	4:G:173:TYR:HA	1.97	0.47
6:L:185:GLN:HA	6:L:188:MET:HG2	1.97	0.47
4:G:259:LEU:HB2	4:G:374:HIS:CE1	2.50	0.46
6:L:168:GLN:OE1	6:L:174:ALA:HB2	2.15	0.46
2:D:47:TRP:CZ2	2:D:49:GLY:HA2	2.51	0.46
4:G:91:GLU:HG3	4:G:226:LEU:HD13	1.97	0.46
6:L:70:ARG:HG3	6:L:72:THR:HG23	1.97	0.46
4:G:45:TRP:O	4:G:46:LYS:HD2	2.16	0.45
4:G:299:PRO:HG2	4:G:327:ARG:HB2	1.99	0.45
2:D:19:LYS:HA	2:D:80:MET:O	2.16	0.45
4:G:384:TYR:CE1	4:G:421:LYS:HB2	2.52	0.45
4:G:102:GLU:OE2	4:G:476:ARG:NH1	2.50	0.45
4:G:478:ASN:O	4:G:481:SER:OG	2.27	0.45
5:H:169:GLN:HG2	6:L:161:GLU:HG3	1.98	0.45
4:G:333:VAL:HG11	4:G:390:LEU:HD21	1.98	0.45
4:G:385:CYS:HA	4:G:418:CYS:HA	1.99	0.45
4:G:86:LEU:HB3	4:G:89:VAL:HG21	1.99	0.44
1:B:632:ASP:HA	1:B:635:ILE:HG22	1.99	0.44
4:G:206:PRO:HG3	4:G:318:TYR:CE2	2.52	0.44
1:B:526:ALA:HA	4:G:43:PRO:HB2	2.00	0.44
2:D:13:LYS:HD2	2:D:13:LYS:HA	1.68	0.44
2:D:31:PHE:HA	7:A:1:NAG:H62	1.99	0.43
5:H:176:LEU:HG	5:H:177:SER:H	1.83	0.43
6:L:22:SER:HA	6:L:72:THR:HG22	1.99	0.43
1:B:574:LYS:HE3	4:G:107:ASP:OD1	2.19	0.43
4:G:123:THR:N	4:G:124:PRO:HD2	2.33	0.43
2:D:37:ILE:HG13	2:D:103:TRP:CH2	2.53	0.43
5:H:18:LEU:HD12	5:H:107:VAL:HG11	2.01	0.43
6:L:28:LEU:HB2	6:L:94:ARG:HB2	2.00	0.43
6:L:47:LEU:HA	6:L:58:ILE:HD13	1.99	0.43
10:K:1:NAG:H83	10:K:1:NAG:H3	2.01	0.43
4:G:45:TRP:NE1	4:G:91:GLU:OE2	2.34	0.43
5:H:33:TYR:HB2	5:H:95:ALA:O	2.18	0.43
2:D:82(A):ARG:O	2:D:82(C):LEU:N	2.52	0.43
3:E:19:VAL:HG12	3:E:20:THR:H	1.82	0.43
4:G:227:LYS:HA	4:G:485:LYS:O	2.20	0.42
6:L:33:VAL:HG12	6:L:51:ASN:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:447:SER:HB3	8:F:1:NAG:HN2	1.85	0.42
2:D:86:ASP:N	2:D:86:ASP:OD1	2.53	0.42
6:L:35:TRP:CD2	6:L:73:LEU:HB2	2.55	0.42
4:G:42:VAL:HA	4:G:43:PRO:HD3	1.89	0.42
5:H:100:ARG:NH2	10:K:4:MAN:O6	2.52	0.42
2:D:29:PHE:CG	2:D:76:GLY:HA3	2.54	0.42
5:H:34:TRP:CZ3	5:H:94:ARG:HB2	2.54	0.42
4:G:212:PRO:HB2	4:G:252:LYS:HB3	2.01	0.42
4:G:277:ILE:HG13	11:G:613:NAG:H81	2.01	0.41
5:H:141:LYS:NZ	5:H:142:ASP:OD2	2.52	0.41
4:G:390:LEU:HG	4:G:416:LEU:HD21	2.02	0.41
5:H:133:THR:HG22	5:H:183:PRO:HA	2.01	0.41
4:G:199:SER:HA	4:G:431:GLY:HA2	2.03	0.41
4:G:152:GLY:O	4:G:178:ARG:HB2	2.20	0.41
4:G:335:LYS:H	4:G:413:SER:HA	1.85	0.41
1:B:604:CYS:SG	4:G:38:VAL:HB	2.60	0.41
2:D:66:ARG:O	2:D:82(A):ARG:N	2.54	0.41
5:H:1:GLN:O	5:H:26:GLY:HA3	2.20	0.41
5:H:144:PHE:HA	5:H:145:PRO:HA	1.78	0.41
4:G:94:ASN:HD22	4:G:97:LYS:HD3	1.85	0.41
5:H:32:TYR:CD1	5:H:94:ARG:HD2	2.56	0.41
5:H:207:LYS:HA	5:H:207:LYS:HD3	1.92	0.41
2:D:1:GLN:HB3	2:D:2:GLY:H	1.75	0.40
4:G:350:ARG:HD3	4:G:354:GLY:O	2.21	0.40
4:G:259:LEU:HB2	4:G:374:HIS:ND1	2.36	0.40
2:D:57:LYS:HB3	2:D:57:LYS:HE2	1.96	0.40
4:G:67:ASN:HD22	4:G:69:TRP:HD1	1.68	0.40
4:G:257:THR:HG21	4:G:371:VAL:HA	2.02	0.40
5:H:201:SER:O	5:H:203:THR:HG23	2.21	0.40
4:G:94:ASN:HB3	4:G:97:LYS:HG2	2.03	0.40
2:D:14:PRO:HG3	2:D:84:SER:HB3	2.02	0.40
3:E:83:GLU:HA	3:E:104:VAL: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	B	129/153 (84%)	119 (92%)	10 (8%)	0	100	100
2	D	126/134 (94%)	113 (90%)	13 (10%)	0	100	100
3	E	103/114 (90%)	85 (82%)	18 (18%)	0	100	100
4	G	430/481 (89%)	402 (94%)	23 (5%)	5 (1%)	13	11
5	H	222/244 (91%)	205 (92%)	17 (8%)	0	100	100
6	L	209/217 (96%)	199 (95%)	9 (4%)	1 (0%)	29	31
All	All	1219/1343 (91%)	1123 (92%)	90 (7%)	6 (0%)	29	31

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	51	ASN
4	G	137	ALA
4	G	135	THR
4	G	136	ASN
4	G	321	GLY
4	G	270	VAL

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	B	114/129 (88%)	112 (98%)	2 (2%)	59	70
2	D	107/112 (96%)	102 (95%)	5 (5%)	26	33
3	E	92/100 (92%)	88 (96%)	4 (4%)	29	36
4	G	392/427 (92%)	375 (96%)	17 (4%)	29	36
5	H	196/212 (92%)	185 (94%)	11 (6%)	21	24
6	L	175/181 (97%)	169 (97%)	6 (3%)	37	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1076/1161 (93%)	1031 (96%)	45 (4%)	30 37

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	519	PHE
1	B	574	LYS
2	D	12	THR
2	D	25	SER
2	D	59	LEU
2	D	72(G)	SER
2	D	110	THR
3	E	27(B)	VAL
3	E	82	ASP
3	E	89	CYS
3	E	96	CYS
4	G	106	THR
4	G	134	VAL
4	G	135	THR
4	G	136	ASN
4	G	139	THR
4	G	154	LEU
4	G	192	ARG
4	G	199	SER
4	G	270	VAL
4	G	286	VAL
4	G	396	ILE
4	G	415	THR
4	G	448	ASN
4	G	465	THR
4	G	467	THR
4	G	469	ARG
4	G	485	LYS
5	H	18	LEU
5	H	57	THR
5	H	63	LEU
5	H	75	LYS
5	H	77	GLN
5	H	100(F)	SER
5	H	100(I)	GLU
5	H	158	THR
5	H	194	CYS

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Mol	Chain	Res	Type
5	H	204	LYS
5	H	209	VAL
6	L	25	ARG
6	L	39	ARG
6	L	79	GLU
6	L	97	SER
6	L	181	LEU
6	L	197	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

28 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	$\#\|Z\| > 2$
7	NAG	A	1	7,4	14,14,15	0.26	0	17,19,21	0.48	0
7	NAG	A	2	7	14,14,15	0.39	0	17,19,21	1.28	2 (11%)
7	BMA	A	3	7	11,11,12	0.80	0	15,15,17	0.85	0
7	MAN	A	4	7	11,11,12	1.30	2 (18%)	15,15,17	1.77	4 (26%)
7	MAN	A	5	7	11,11,12	1.66	2 (18%)	15,15,17	2.25	4 (26%)
7	MAN	A	6	7	11,11,12	0.68	0	15,15,17	0.97	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	NAG	C	1	8,4	14,14,15	0.40	0	17,19,21	0.45	0
8	NAG	C	2	8	14,14,15	0.23	0	17,19,21	0.46	0
8	BMA	C	3	8	11,11,12	0.66	0	15,15,17	0.70	0
8	NAG	F	1	8,4	14,14,15	0.24	0	17,19,21	0.62	1 (5%)
8	NAG	F	2	8	14,14,15	0.28	0	17,19,21	0.59	0
8	BMA	F	3	8	11,11,12	0.67	0	15,15,17	0.72	0
9	NAG	I	1	4,9	14,14,15	0.34	0	17,19,21	0.42	0
9	NAG	I	2	9	14,14,15	0.25	0	17,19,21	0.42	0
9	NAG	J	1	4,9	14,14,15	0.20	0	17,19,21	0.48	0
9	NAG	J	2	9	14,14,15	0.22	0	17,19,21	0.51	0
10	NAG	K	1	10,4	14,14,15	0.35	0	17,19,21	1.48	2 (11%)
10	MAN	K	10	10	11,11,12	1.08	0	15,15,17	1.10	1 (6%)
10	NAG	K	2	10	14,14,15	0.32	0	17,19,21	0.40	0
10	BMA	K	3	10	11,11,12	0.69	0	15,15,17	1.16	2 (13%)
10	MAN	K	4	10	11,11,12	0.77	1 (9%)	15,15,17	1.28	2 (13%)
10	MAN	K	5	10	11,11,12	0.70	0	15,15,17	0.91	1 (6%)
10	MAN	K	6	10	11,11,12	0.93	1 (9%)	15,15,17	0.94	1 (6%)
10	MAN	K	7	10	11,11,12	0.76	0	15,15,17	0.96	1 (6%)
10	MAN	K	8	10	11,11,12	0.58	0	15,15,17	1.10	1 (6%)
10	MAN	K	9	10	11,11,12	0.80	0	15,15,17	1.42	2 (13%)
9	NAG	M	1	9	14,14,15	0.97	1 (7%)	17,19,21	0.75	0
9	NAG	M	2	9	14,14,15	0.26	0	17,19,21	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	1	7,4	-	0/6/23/26	0/1/1/1
7	NAG	A	2	7	-	5/6/23/26	0/1/1/1
7	BMA	A	3	7	-	2/2/19/22	0/1/1/1
7	MAN	A	4	7	-	1/2/19/22	0/1/1/1
7	MAN	A	5	7	-	1/2/19/22	0/1/1/1
7	MAN	A	6	7	-	0/2/19/22	0/1/1/1
8	NAG	C	1	8,4	-	1/6/23/26	0/1/1/1
8	NAG	C	2	8	-	0/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	NAG	F	1	8,4	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
8	BMA	F	3	8	-	2/2/19/22	0/1/1/1
9	NAG	I	1	4,9	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	2/6/23/26	0/1/1/1
9	NAG	J	1	4,9	-	2/6/23/26	0/1/1/1
9	NAG	J	2	9	-	2/6/23/26	0/1/1/1
10	NAG	K	1	10,4	-	4/6/23/26	0/1/1/1
10	MAN	K	10	10	-	0/2/19/22	0/1/1/1
10	NAG	K	2	10	-	2/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	MAN	K	4	10	-	2/2/19/22	0/1/1/1
10	MAN	K	5	10	-	0/2/19/22	0/1/1/1
10	MAN	K	6	10	-	1/2/19/22	0/1/1/1
10	MAN	K	7	10	-	0/2/19/22	0/1/1/1
10	MAN	K	8	10	-	0/2/19/22	0/1/1/1
10	MAN	K	9	10	-	2/2/19/22	0/1/1/1
9	NAG	M	1	9	-	0/6/23/26	0/1/1/1
9	NAG	M	2	9	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	5	MAN	C1-C2	4.00	1.61	1.52
9	M	1	NAG	O5-C1	-3.33	1.38	1.43
7	A	5	MAN	O5-C1	3.28	1.49	1.43
7	A	4	MAN	C1-C2	2.92	1.58	1.52
7	A	4	MAN	C2-C3	2.80	1.56	1.52
10	K	4	MAN	C1-C2	2.37	1.57	1.52
10	K	6	MAN	O5-C1	-2.19	1.40	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	5	MAN	C1-O5-C5	6.93	121.58	112.19
7	A	4	MAN	C1-C2-C3	4.90	115.68	109.67
10	K	1	NAG	C2-N2-C7	4.56	129.40	122.90
10	K	9	MAN	C1-O5-C5	4.47	118.25	112.19
7	A	2	NAG	C2-N2-C7	4.31	129.05	122.90
10	K	4	MAN	C1-O5-C5	3.11	116.41	112.19
7	A	5	MAN	O5-C1-C2	3.07	115.51	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	8	MAN	C1-O5-C5	2.72	115.87	112.19
10	K	1	NAG	C1-C2-N2	2.72	115.13	110.49
7	A	5	MAN	C1-C2-C3	2.69	112.98	109.67
10	K	3	BMA	C1-O5-C5	2.46	115.53	112.19
10	K	10	MAN	O2-C2-C3	-2.43	105.27	110.14
10	K	5	MAN	O2-C2-C3	-2.39	105.36	110.14
10	K	4	MAN	O2-C2-C3	-2.32	105.49	110.14
7	A	6	MAN	C1-O5-C5	2.31	115.33	112.19
7	A	4	MAN	C1-O5-C5	2.29	115.29	112.19
7	A	5	MAN	O2-C2-C3	-2.25	105.62	110.14
10	K	9	MAN	O2-C2-C3	-2.25	105.62	110.14
7	A	4	MAN	O2-C2-C3	-2.18	105.76	110.14
10	K	6	MAN	O2-C2-C3	-2.17	105.80	110.14
7	A	6	MAN	O2-C2-C3	-2.16	105.81	110.14
7	A	4	MAN	C2-C3-C4	2.15	114.61	110.89
8	F	1	NAG	C1-O5-C5	2.13	115.07	112.19
10	K	3	BMA	C1-C2-C3	2.08	112.22	109.67
10	K	7	MAN	O2-C2-C3	-2.06	106.02	110.14
7	A	2	NAG	C1-C2-N2	2.01	113.92	110.49

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	1	NAG	O5-C5-C6-O6
7	A	2	NAG	O5-C5-C6-O6
9	I	1	NAG	O5-C5-C6-O6
10	K	2	NAG	O5-C5-C6-O6
10	K	4	MAN	O5-C5-C6-O6
10	K	9	MAN	O5-C5-C6-O6
7	A	3	BMA	O5-C5-C6-O6
8	F	2	NAG	O5-C5-C6-O6
7	A	3	BMA	C4-C5-C6-O6
9	J	2	NAG	O5-C5-C6-O6
10	K	9	MAN	C4-C5-C6-O6
8	F	2	NAG	C4-C5-C6-O6
8	F	1	NAG	C4-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
7	A	2	NAG	O7-C7-N2-C2
10	K	1	NAG	C8-C7-N2-C2
10	K	1	NAG	O7-C7-N2-C2
9	I	1	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	J	2	NAG	C4-C5-C6-O6
10	K	4	MAN	C4-C5-C6-O6
7	A	2	NAG	C4-C5-C6-O6
10	K	2	NAG	C4-C5-C6-O6
9	I	2	NAG	O5-C5-C6-O6
9	J	1	NAG	O5-C5-C6-O6
7	A	5	MAN	O5-C5-C6-O6
10	K	6	MAN	O5-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
8	F	3	BMA	C4-C5-C6-O6
7	A	4	MAN	O5-C5-C6-O6
9	I	2	NAG	C4-C5-C6-O6
7	A	2	NAG	C3-C2-N2-C7
10	K	1	NAG	C3-C2-N2-C7
9	J	1	NAG	C4-C5-C6-O6
8	F	3	BMA	O5-C5-C6-O6
10	K	1	NAG	C1-C2-N2-C7

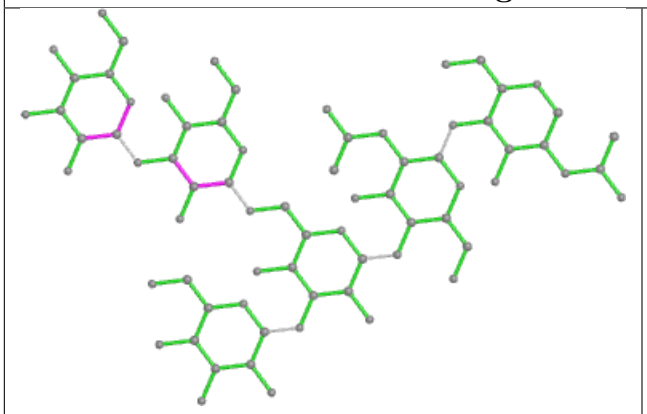
There are no ring outliers.

5 monomers are involved in 5 short contacts:

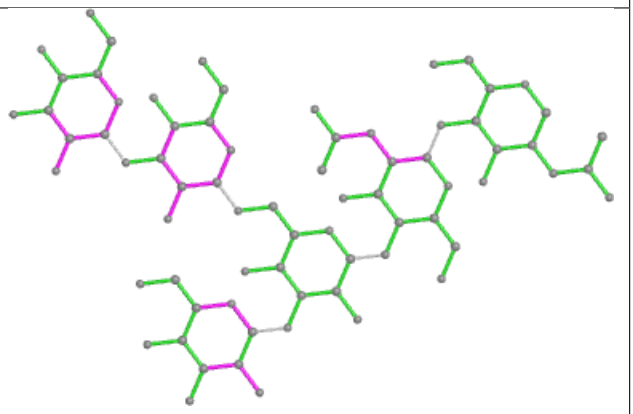
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	K	1	NAG	1	0
7	A	2	NAG	1	0
7	A	1	NAG	1	0
10	K	4	MAN	1	0
8	F	1	NAG	1	0

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

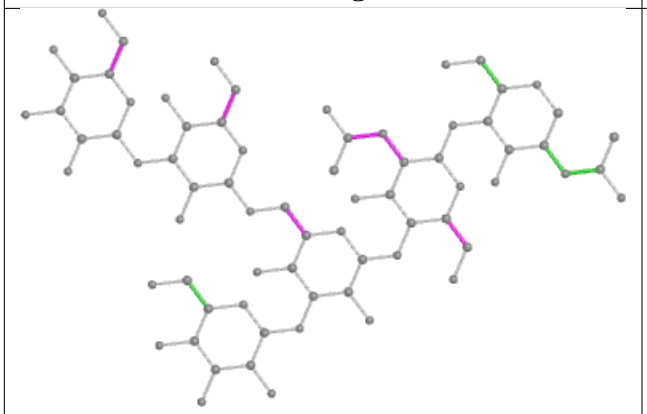
Oligosaccharide Chain A



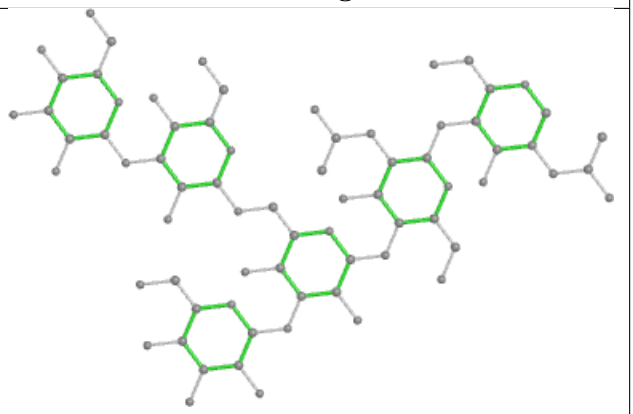
Bond lengths



Bond angles

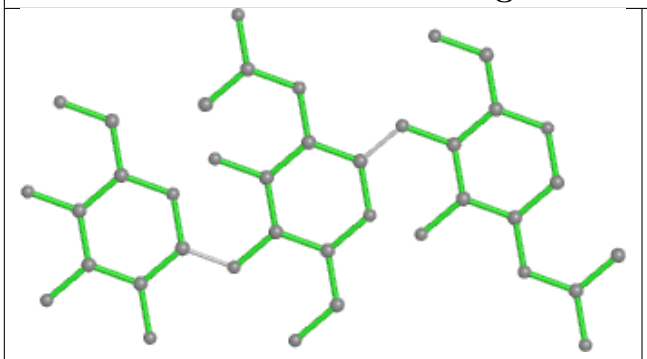


Torsions

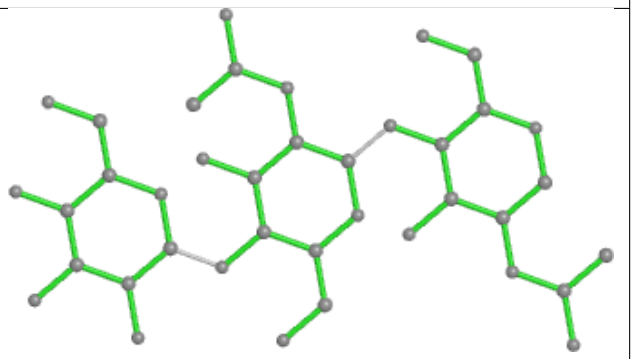


Rings

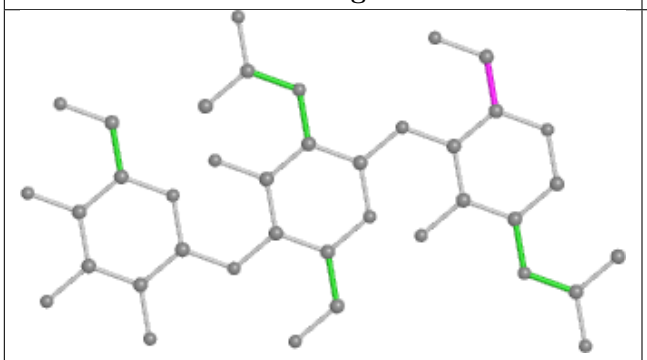
Oligosaccharide Chain C



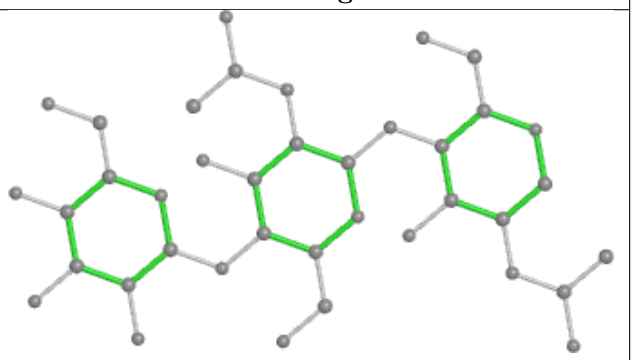
Bond lengths



Bond angles

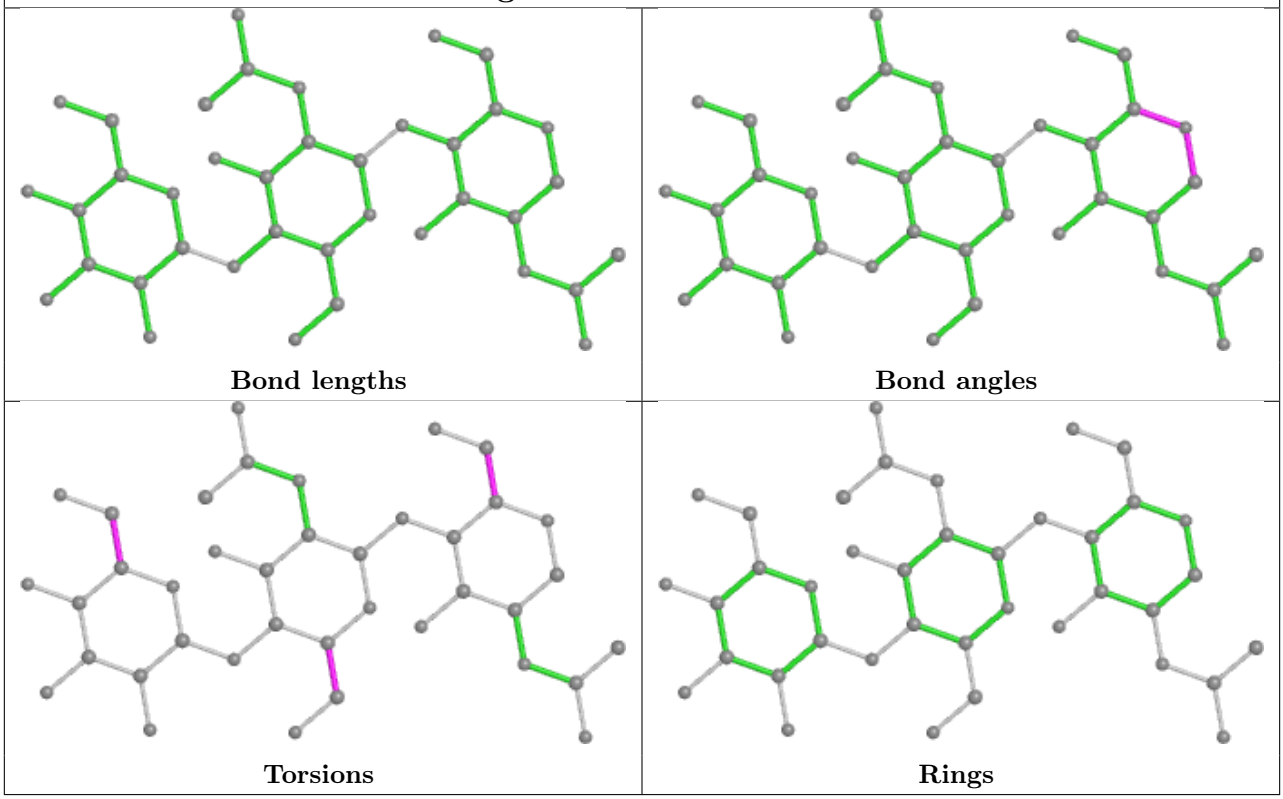


Torsions

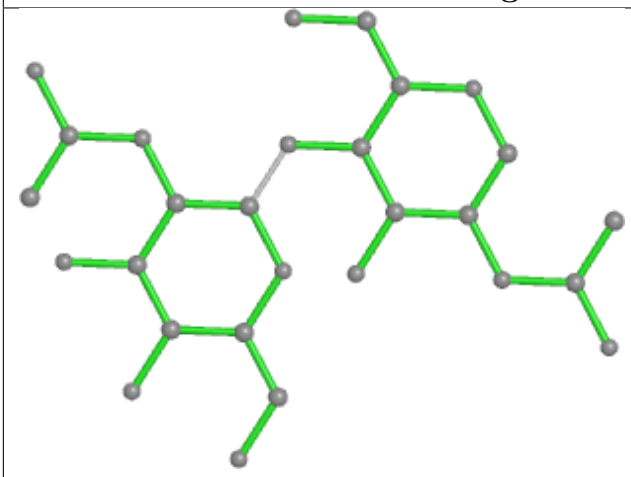


Rings

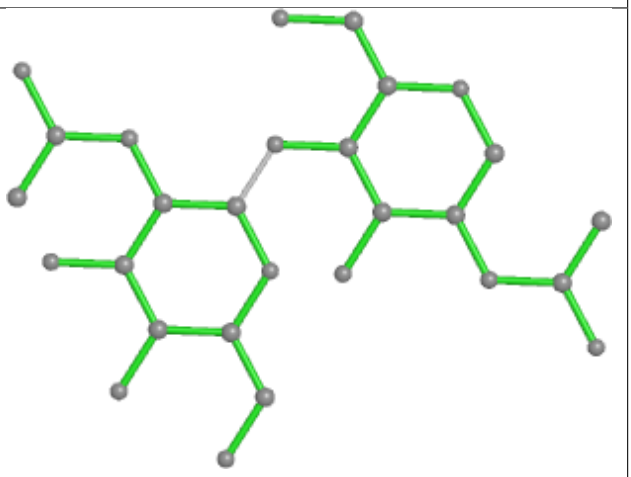
Oligosaccharide Chain F



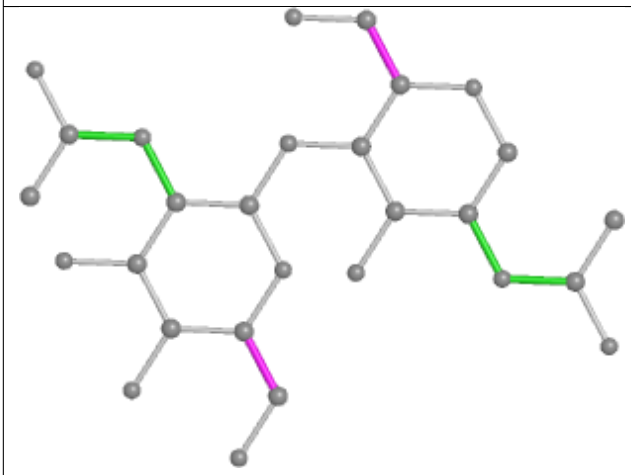
Oligosaccharide Chain I



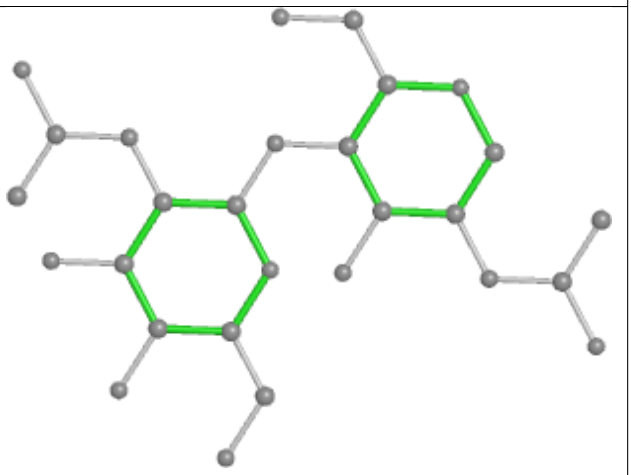
Bond lengths



Bond angles

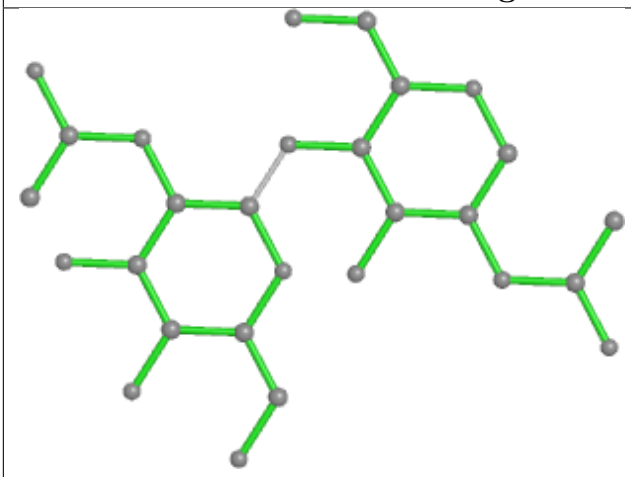


Torsions

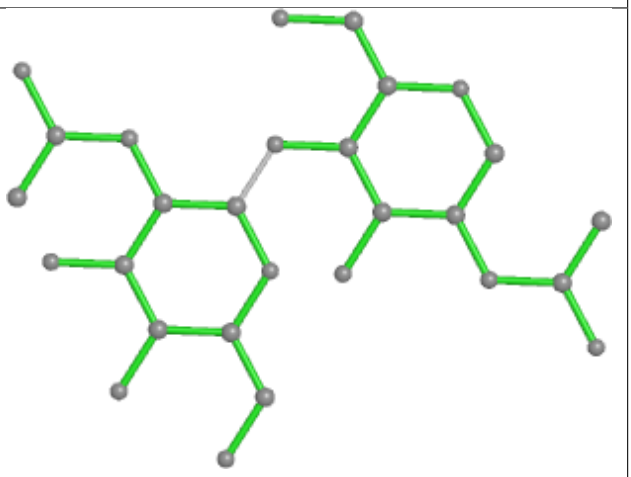


Rings

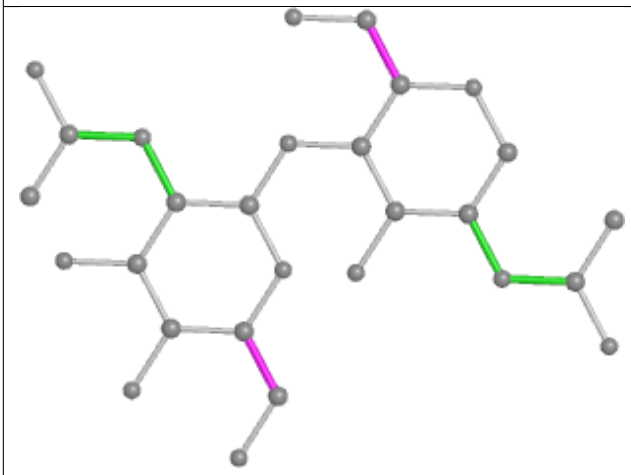
Oligosaccharide Chain J



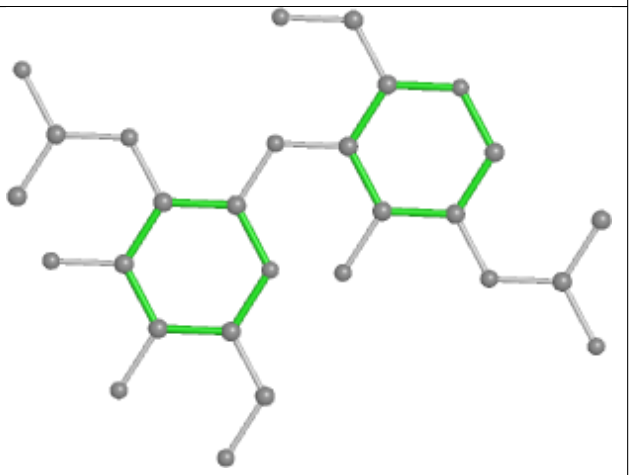
Bond lengths



Bond angles

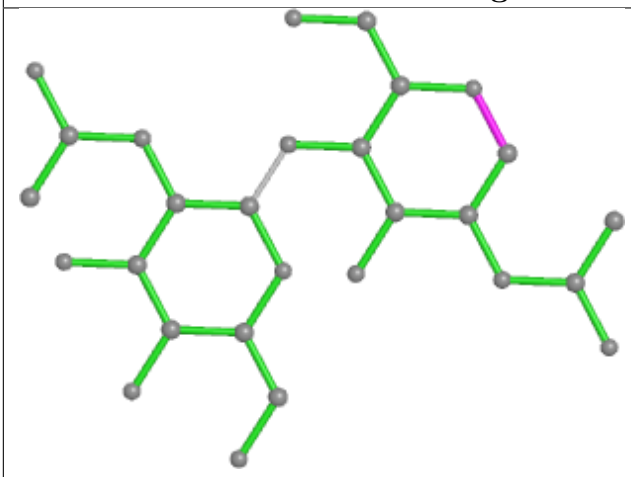


Torsions

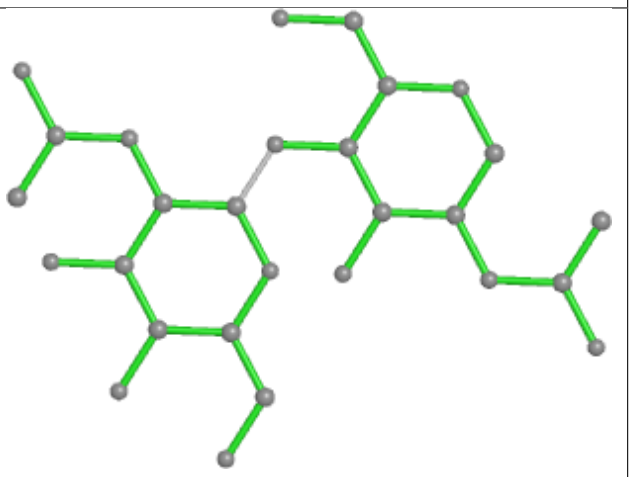


Rings

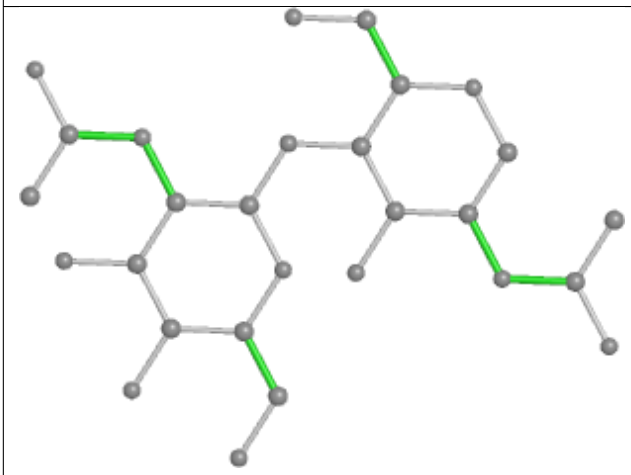
Oligosaccharide Chain M



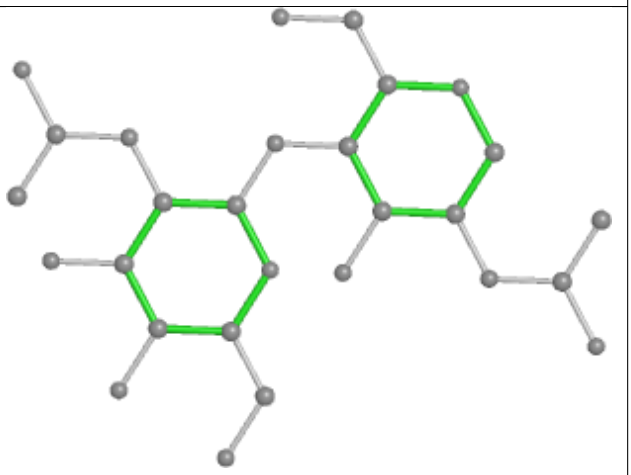
Bond lengths



Bond angles

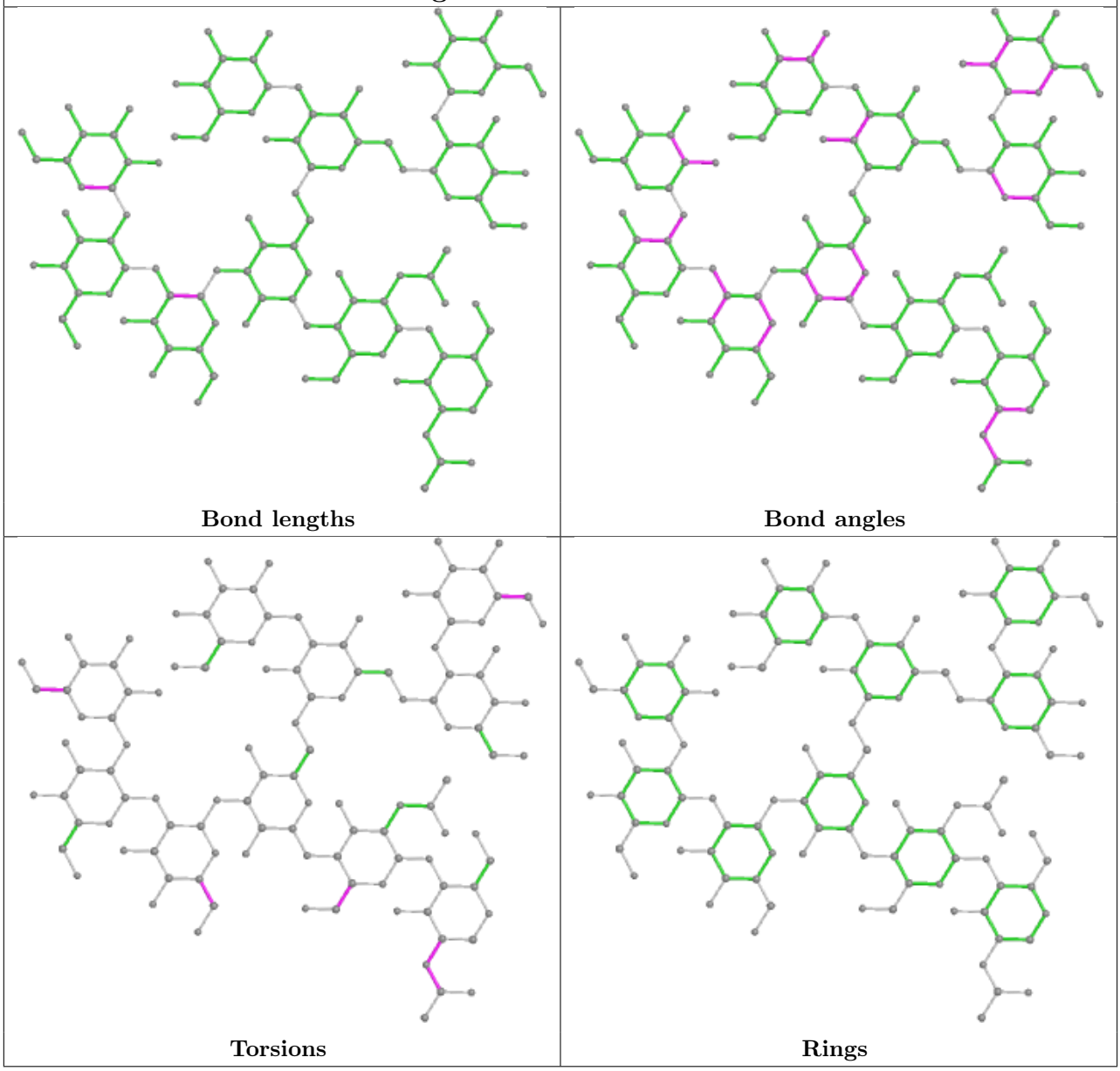


Torsions



Rings

Oligosaccharide Chain K



5.6 Ligand geometry (i)

13 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	$\#\|Z\| > 2$
11	NAG	G	611	4	14,14,15	0.33	0	17,19,21	0.46	0
11	NAG	B	702	1	14,14,15	0.35	0	17,19,21	0.50	0
11	NAG	B	703	1	14,14,15	0.28	0	17,19,21	0.45	0
11	NAG	G	612	4	14,14,15	0.29	0	17,19,21	0.52	0
11	NAG	G	634	4	14,14,15	0.31	0	17,19,21	0.61	1 (5%)
11	NAG	D	201	2	14,14,15	0.38	0	17,19,21	0.52	0
11	NAG	B	701	1	14,14,15	0.34	0	17,19,21	0.54	0
11	NAG	G	617	4	14,14,15	0.26	0	17,19,21	0.43	0
12	83G	G	637	-	32,33,33	2.67	7 (21%)	38,47,47	2.27	16 (42%)
11	NAG	G	633	4	14,14,15	0.25	0	17,19,21	0.49	0
11	NAG	G	613	4	14,14,15	0.25	0	17,19,21	0.42	0
11	NAG	G	607	4	14,14,15	0.31	0	17,19,21	0.52	0
11	NAG	G	632	4	14,14,15	0.26	0	17,19,21	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	G	611	4	-	0/6/23/26	0/1/1/1
11	NAG	B	702	1	-	2/6/23/26	0/1/1/1
11	NAG	B	703	1	-	1/6/23/26	0/1/1/1
11	NAG	G	612	4	-	1/6/23/26	0/1/1/1
11	NAG	G	634	4	-	2/6/23/26	0/1/1/1
11	NAG	D	201	2	-	1/6/23/26	0/1/1/1
11	NAG	B	701	1	-	2/6/23/26	0/1/1/1
11	NAG	G	617	4	-	2/6/23/26	0/1/1/1
12	83G	G	637	-	-	2/18/35/35	0/4/4/4
11	NAG	G	633	4	-	2/6/23/26	0/1/1/1
11	NAG	G	613	4	-	1/6/23/26	0/1/1/1
11	NAG	G	607	4	-	0/6/23/26	0/1/1/1
11	NAG	G	632	4	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	637	83G	O13-C12	8.22	1.40	1.23
12	G	637	83G	C14-N16	8.00	1.47	1.34
12	G	637	83G	C23-N19	5.57	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	G	637	83G	C25-C23	3.22	1.55	1.50
12	G	637	83G	C18-N19	-3.21	1.41	1.47
12	G	637	83G	C11-C12	2.74	1.54	1.49
12	G	637	83G	C10-N09	-2.32	1.31	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	G	637	83G	C12-C14-N16	6.30	125.32	118.95
12	G	637	83G	O13-C12-C11	-4.55	109.22	123.45
12	G	637	83G	O02-C03-C08	4.24	122.12	115.89
12	G	637	83G	C05-N06-C07	4.20	121.78	116.60
12	G	637	83G	C10-C11-C12	-3.27	121.56	127.45
12	G	637	83G	C04-C05-N06	-3.23	119.58	124.58
12	G	637	83G	O02-C03-C04	-3.13	119.05	124.24
12	G	637	83G	C11-C08-C07	-3.05	105.10	107.54
12	G	637	83G	C01-O02-C03	-2.70	113.97	117.75
12	G	637	83G	C25-C23-N19	2.58	122.00	118.72
12	G	637	83G	C11-C12-C14	-2.44	115.11	118.61
12	G	637	83G	O24-C23-N19	-2.33	118.48	122.34
12	G	637	83G	O13-C12-C14	-2.33	114.36	117.74
12	G	637	83G	C21-N16-C14	2.27	126.59	120.65
12	G	637	83G	O15-C14-N16	-2.26	117.37	122.15
11	G	634	NAG	C1-O5-C5	2.14	115.09	112.19
12	G	637	83G	C05-C04-C03	2.05	120.42	118.06

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	637	83G	O13-C12-C14-N16
12	G	637	83G	O13-C12-C14-O15
11	G	633	NAG	C4-C5-C6-O6
11	B	702	NAG	O5-C5-C6-O6
11	G	633	NAG	O5-C5-C6-O6
11	G	617	NAG	O5-C5-C6-O6
11	G	634	NAG	O5-C5-C6-O6
11	G	617	NAG	C4-C5-C6-O6
11	G	634	NAG	C4-C5-C6-O6
11	B	701	NAG	O5-C5-C6-O6
11	D	201	NAG	O5-C5-C6-O6
11	G	612	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
11	B	703	NAG	O5-C5-C6-O6
11	G	613	NAG	O5-C5-C6-O6
11	B	702	NAG	C4-C5-C6-O6
11	B	701	NAG	C4-C5-C6-O6

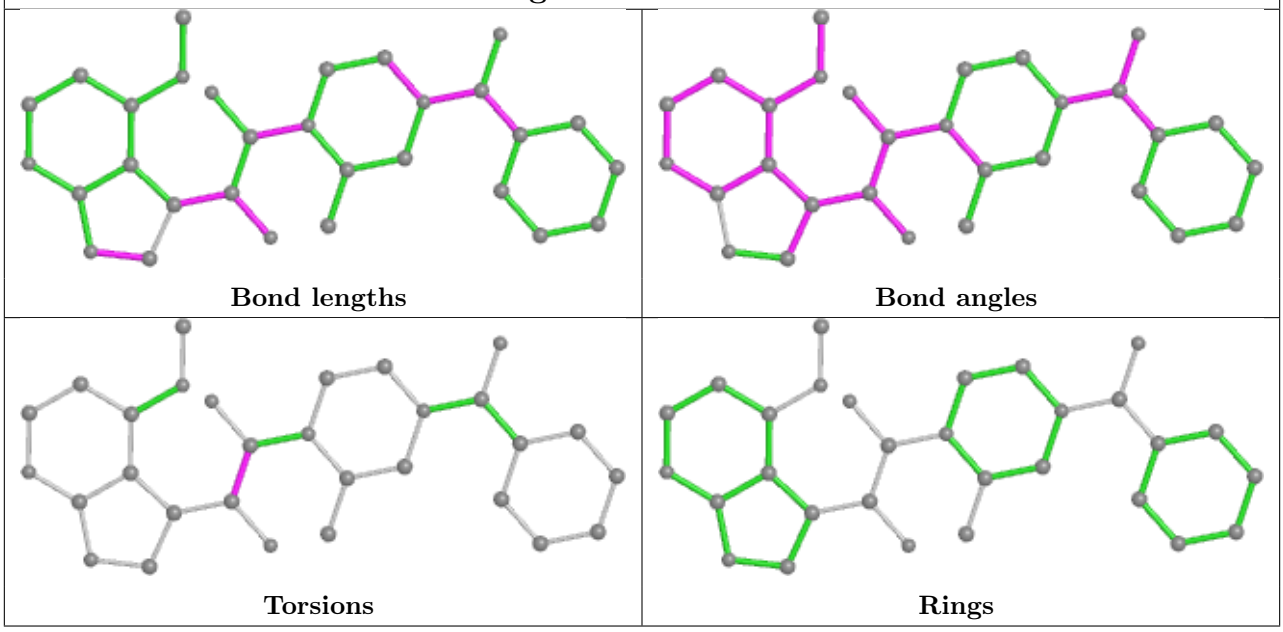
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	702	NAG	1	0
11	G	613	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 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 then 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.

Ligand 83G G 637



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	B	133/153 (86%)	-0.07	4 (3%) 50 60	5, 24, 60, 115	0
2	D	128/134 (95%)	0.50	13 (10%) 6 11	28, 62, 97, 104	0
3	E	105/114 (92%)	0.30	7 (6%) 17 25	27, 53, 88, 94	0
4	G	440/481 (91%)	-0.17	15 (3%) 45 55	6, 25, 76, 127	0
5	H	226/244 (92%)	0.10	7 (3%) 49 59	15, 45, 78, 106	0
6	L	211/217 (97%)	-0.41	3 (1%) 75 82	11, 29, 48, 105	0
All	All	1243/1343 (92%)	-0.04	49 (3%) 39 50	5, 35, 83, 127	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	517	ALA	8.7
5	H	187	LEU	8.2
1	B	518	VAL	6.9
4	G	141	ASP	5.7
4	G	409	GLY	5.7
5	H	26	GLY	5.7
4	G	396	ILE	5.6
6	L	7	TYR	5.4
1	B	663	LEU	5.1
2	D	18	VAL	5.0
4	G	465	THR	3.7
4	G	188	ASN	3.6
5	H	189	THR	3.6
2	D	82(C)	LEU	3.6
4	G	397	SER	3.5
3	E	15	LEU	3.5
3	E	8	ALA	3.4
5	H	125	SER	3.3
4	G	410	SER	3.2

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Mol	Chain	Res	Type	RSRZ
2	D	64	GLN	3.2
4	G	140	ASP	3.2
2	D	109	LEU	3.0
4	G	151	ARG	2.9
4	G	356	ASN	2.9
2	D	82(B)	ASN	2.9
2	D	43	ARG	2.8
6	L	210	THR	2.8
3	E	78	LEU	2.8
3	E	80	PRO	2.7
2	D	67	VAL	2.7
2	D	42	GLY	2.6
1	B	547	GLY	2.6
4	G	185	ASN	2.5
2	D	10	THR	2.5
5	H	30	SER	2.5
3	E	103	LYS	2.5
4	G	79	PRO	2.4
5	H	1	GLN	2.4
2	D	87	THR	2.4
2	D	82(A)	ARG	2.3
3	E	17	GLN	2.3
6	L	6	SER	2.3
3	E	14	SER	2.2
2	D	82	ILE	2.2
4	G	139	THR	2.1
4	G	358	ILE	2.1
4	G	411	ASN	2.1
5	H	186	SER	2.1
2	D	84	SER	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 (i)

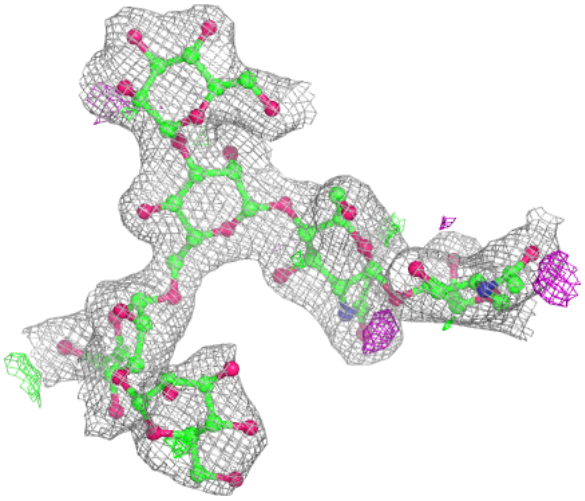
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

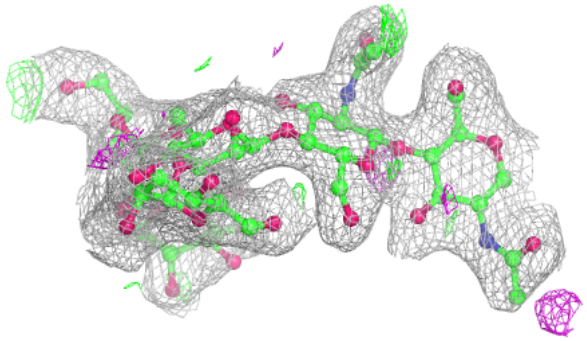
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
10	MAN	K	10	11/12	0.82	0.17	51,68,78,86	0
8	BMA	C	3	11/12	0.83	0.28	72,89,104,108	0
7	MAN	A	4	11/12	0.86	0.15	45,67,80,89	0
8	BMA	F	3	11/12	0.87	0.24	81,90,101,103	0
9	NAG	M	2	14/15	0.87	0.23	66,85,99,105	0
7	MAN	A	5	11/12	0.87	0.26	65,76,94,96	0
9	NAG	I	2	14/15	0.88	0.31	66,95,107,116	0
10	NAG	K	1	14/15	0.89	0.13	23,40,50,61	0
9	NAG	M	1	14/15	0.91	0.15	37,66,82,98	0
10	MAN	K	7	11/12	0.91	0.10	34,44,62,75	0
10	MAN	K	9	11/12	0.91	0.25	67,73,88,91	0
9	NAG	J	2	14/15	0.91	0.25	44,70,85,92	0
10	MAN	K	8	11/12	0.92	0.15	35,49,74,84	0
7	NAG	A	1	14/15	0.94	0.11	17,23,37,38	0
8	NAG	F	2	14/15	0.94	0.14	33,48,81,82	0
10	NAG	K	2	14/15	0.94	0.09	18,41,51,54	0
10	MAN	K	6	11/12	0.94	0.10	29,38,48,49	0
10	MAN	K	5	11/12	0.95	0.09	15,20,32,34	0
8	NAG	C	1	14/15	0.95	0.09	22,36,49,55	0
8	NAG	C	2	14/15	0.95	0.17	36,67,86,87	0
7	NAG	A	2	14/15	0.95	0.10	23,31,43,44	0
8	NAG	F	1	14/15	0.95	0.13	10,21,45,53	0
10	MAN	K	4	11/12	0.95	0.11	15,22,30,42	0
9	NAG	J	1	14/15	0.96	0.10	14,28,39,56	0
7	MAN	A	6	11/12	0.96	0.10	23,32,51,51	0
10	BMA	K	3	11/12	0.96	0.07	20,27,35,37	0
9	NAG	I	1	14/15	0.96	0.10	31,46,61,84	0
7	BMA	A	3	11/12	0.96	0.09	25,33,41,55	0

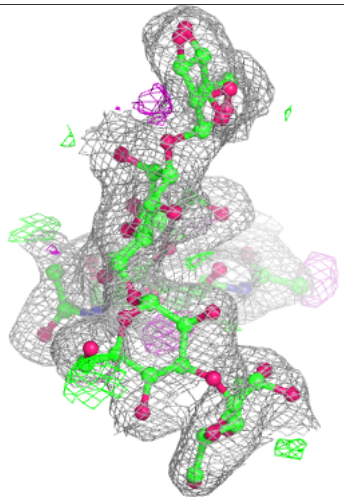
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain A:

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

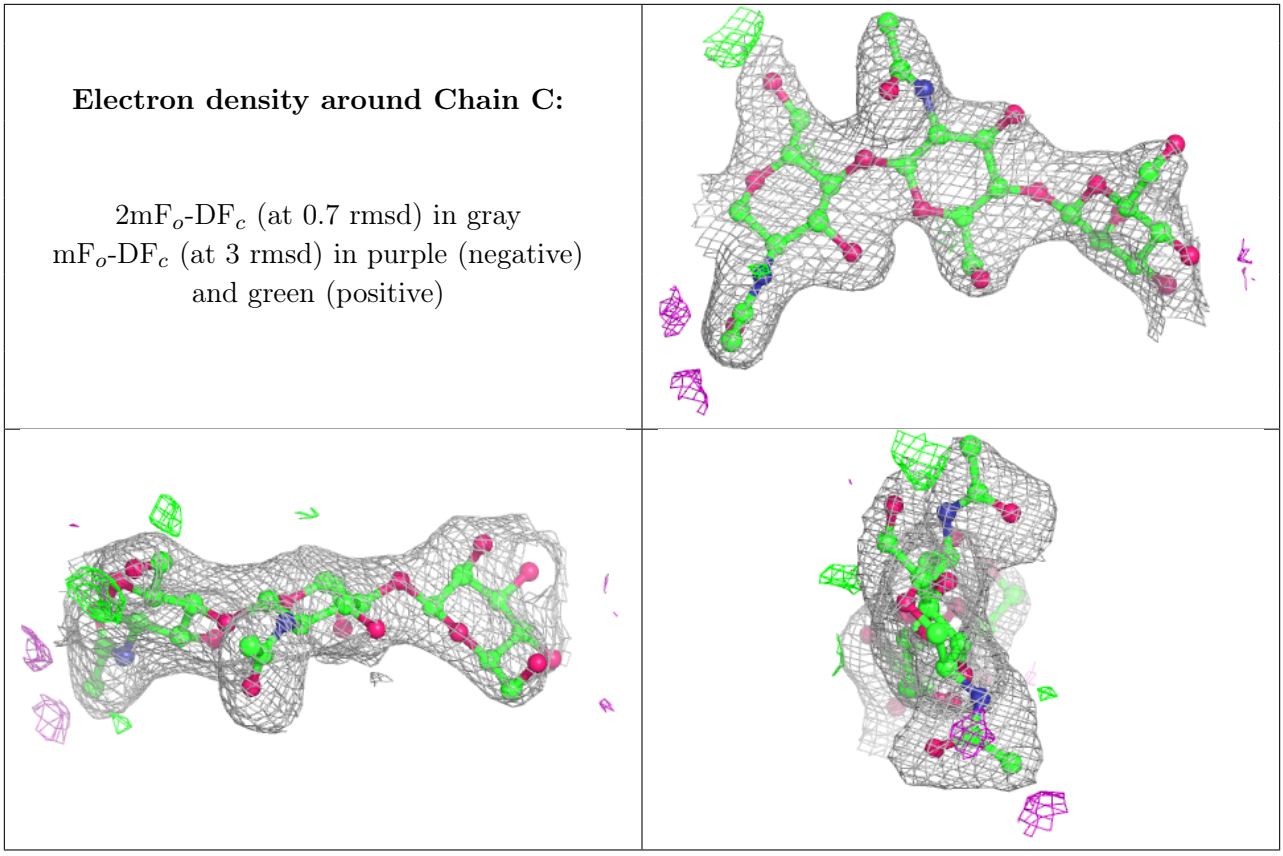






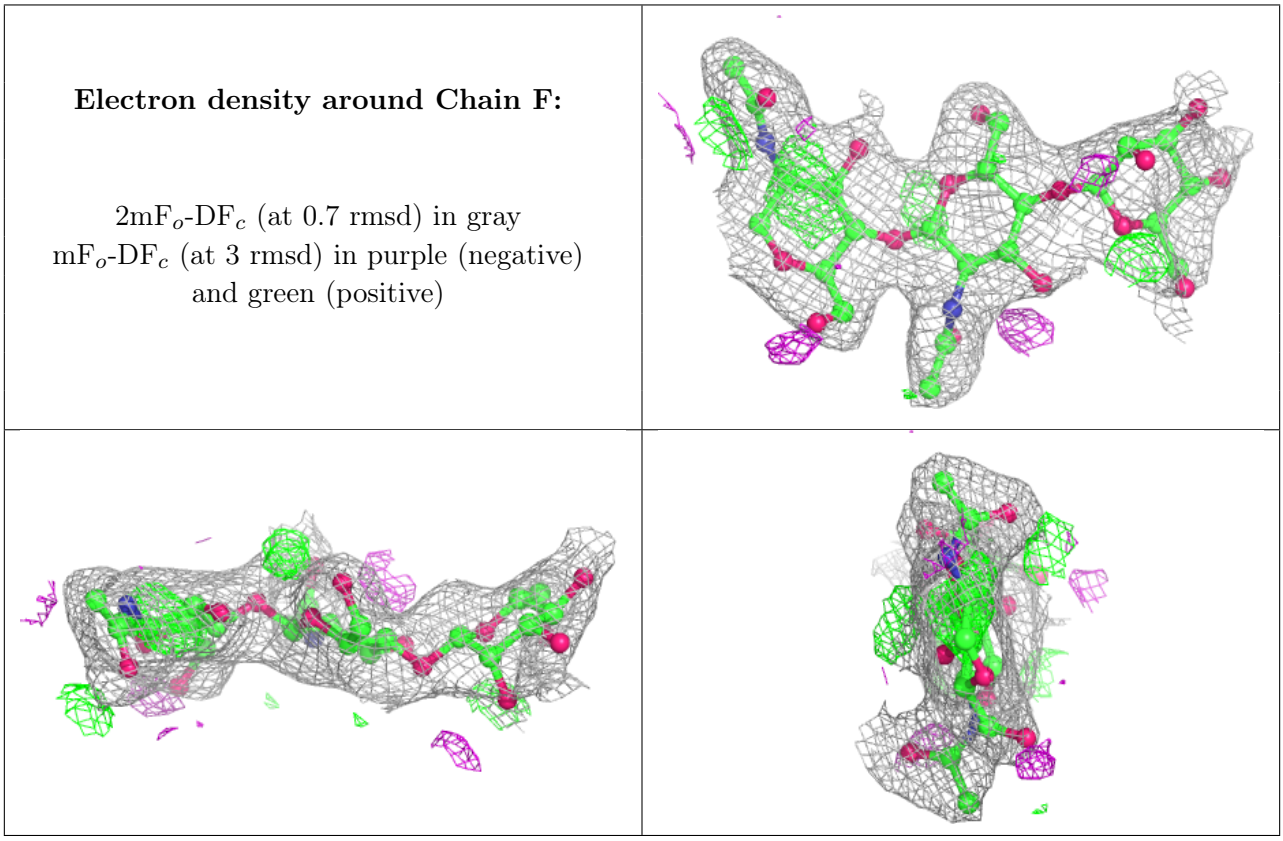
Electron density around Chain C:

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



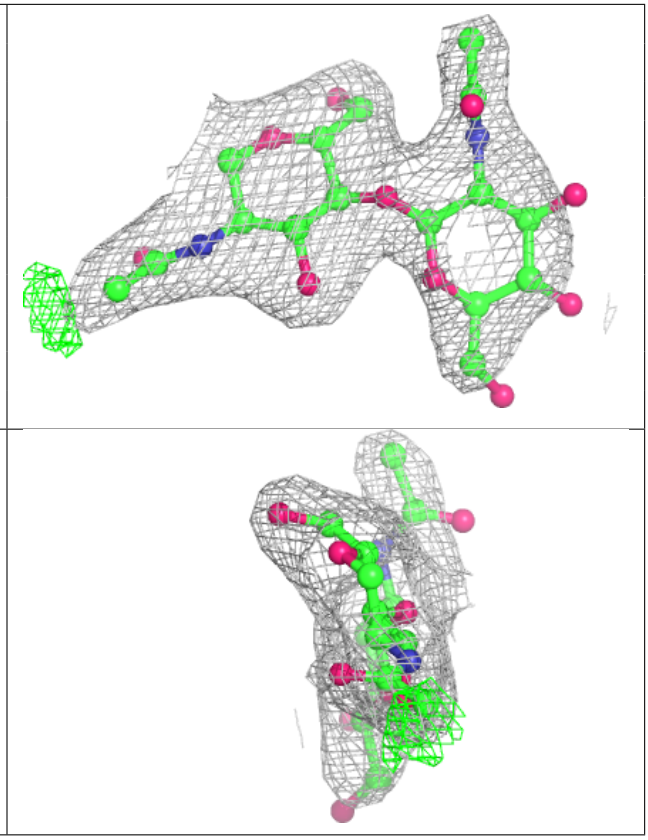
Electron density around Chain F:

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



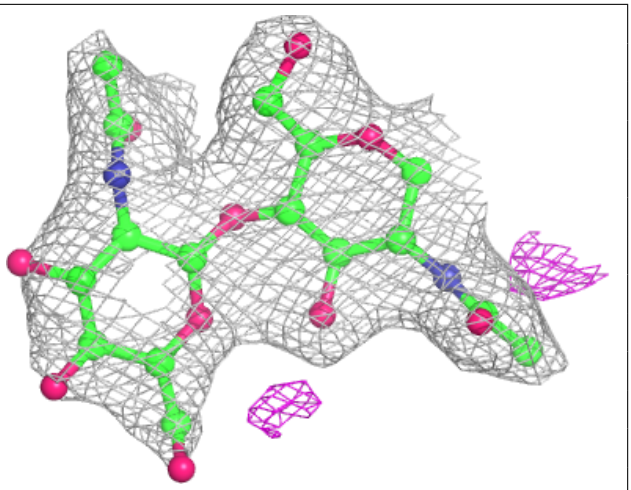
Electron density around Chain I:

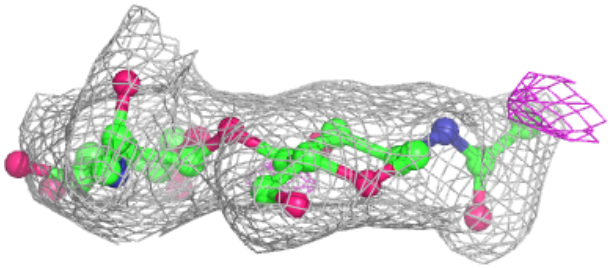
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

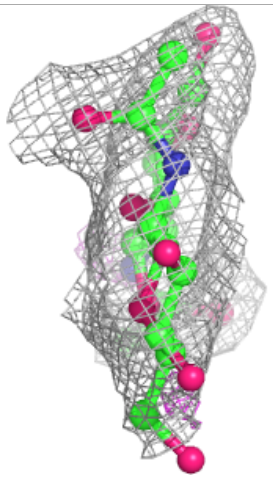


Electron density around Chain J:

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

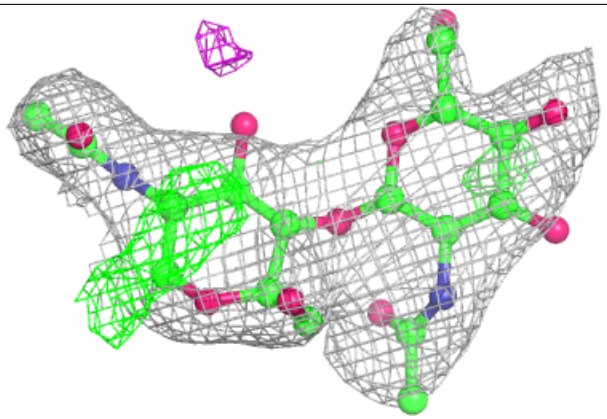


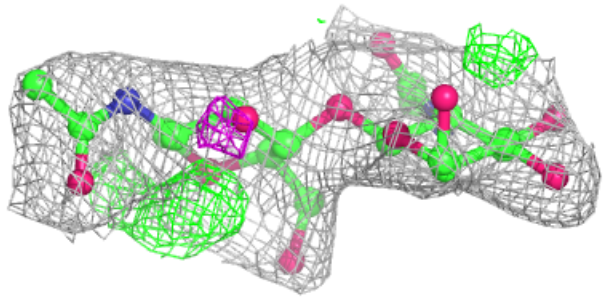


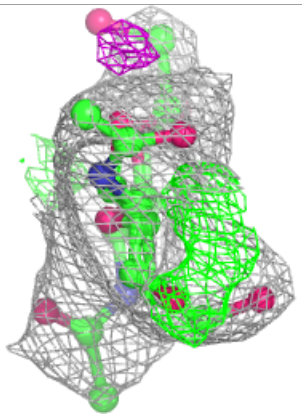


Electron density around Chain M:

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

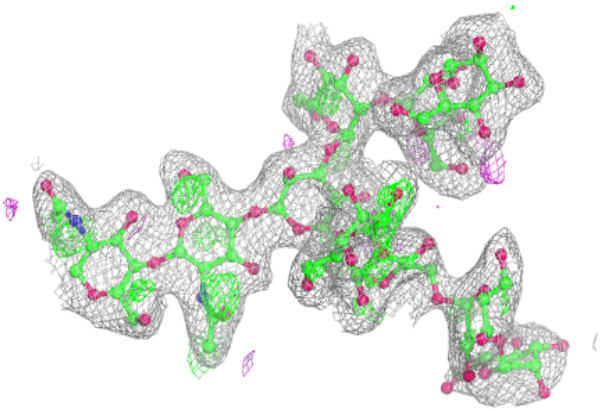


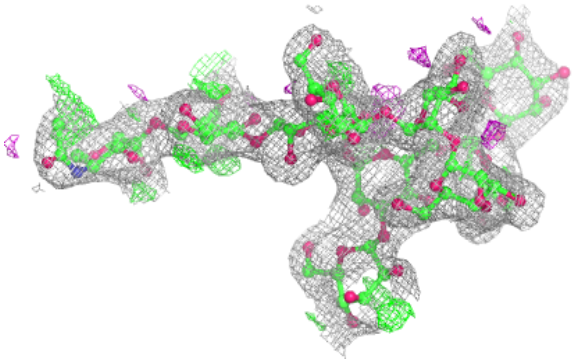


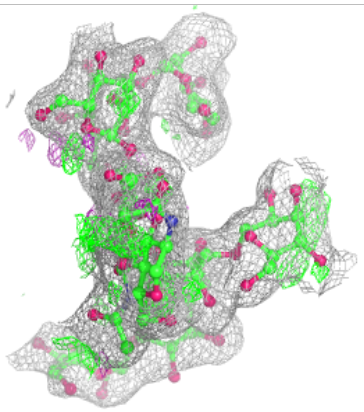


Electron density around Chain K:

$2mF_o$-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)

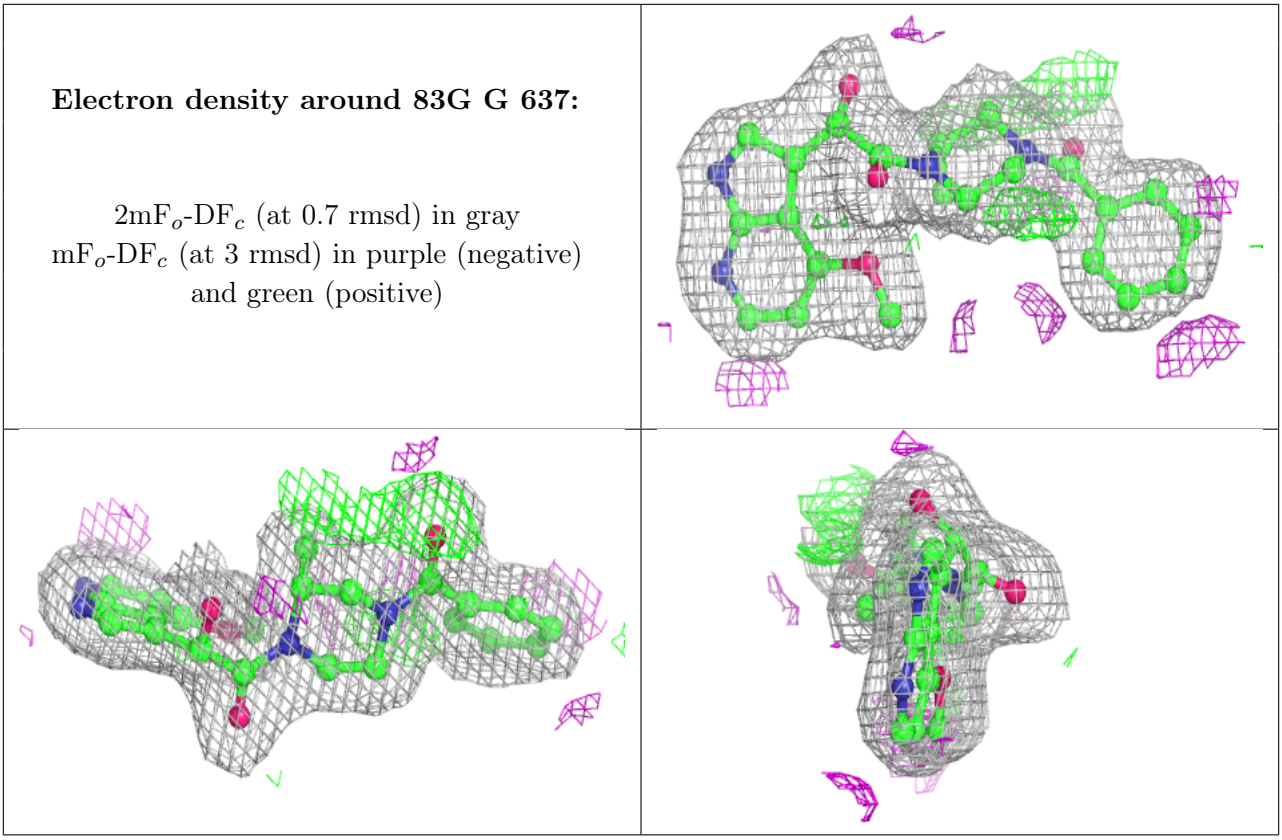
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	B	703	14/15	0.81	0.25	65,87,96,97	0
11	NAG	G	607	14/15	0.83	0.25	67,82,110,114	0
11	NAG	B	701	14/15	0.84	0.42	75,87,104,117	0
11	NAG	B	702	14/15	0.86	0.36	77,87,103,106	0
11	NAG	G	617	14/15	0.88	0.27	45,70,81,93	0
11	NAG	G	613	14/15	0.89	0.15	60,68,78,88	0
11	NAG	D	201	14/15	0.90	0.23	45,78,107,109	0
11	NAG	G	632	14/15	0.91	0.17	43,70,80,84	0
11	NAG	G	612	14/15	0.92	0.14	32,52,71,73	0
11	NAG	G	633	14/15	0.93	0.19	47,62,75,75	0
11	NAG	G	611	14/15	0.95	0.17	27,57,70,86	0
11	NAG	G	634	14/15	0.95	0.10	26,39,45,57	0
12	83G	G	637	30/30	0.95	0.12	4,12,20,21	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 83G G 637:

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.