Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 06:28 PM EDT

PDB ID	:	4O02
Title	:	AlphaVBeta3 integrin in complex with monoclonal antibody FAB fragment.
Authors	:	Mahalingam, B.; van Agthoven, J.; Xiong, J.; Arnaout, M.A.
Deposited on	:	2013-12-13
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

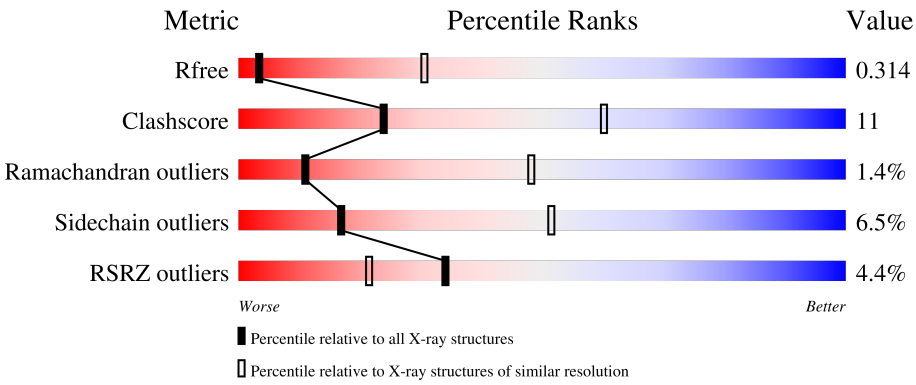
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	962	5%; 77%; 17%; • 5%
2	B	692	5%; 75%; 22%; • •
3	L	214	%; 73%; 24%; • •
4	H	218	3%; 72%; 25%; • •
5	C	6	33%; 67%

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Mol	Chain	Length	Quality of chain
6	D	3	100%
7	E	6	50% 50%
8	F	2	100%
8	I	2	50% 50%
8	J	2	100%
9	G	6	83% 17%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 13526 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	915	5875	3627	1033	1192	23	0	0	0

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	687	4364	2657	771	871	65	0	0	0

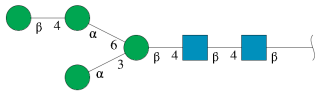
- Molecule 3 is a protein called 17E6 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	214	1453	887	253	307	6	0	0	0

- Molecule 4 is a protein called 17E6 heavy chain.

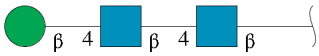
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	H	218	1440	891	247	293	9	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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.



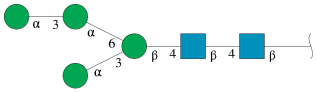
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	6	72	40	2	30	0	0	0

- Molecule 6 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			
6	D	3	39	22	2	15	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.

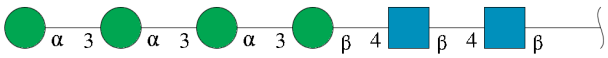


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	E	6	72	40	2	30	0	0	0

- Molecule 8 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

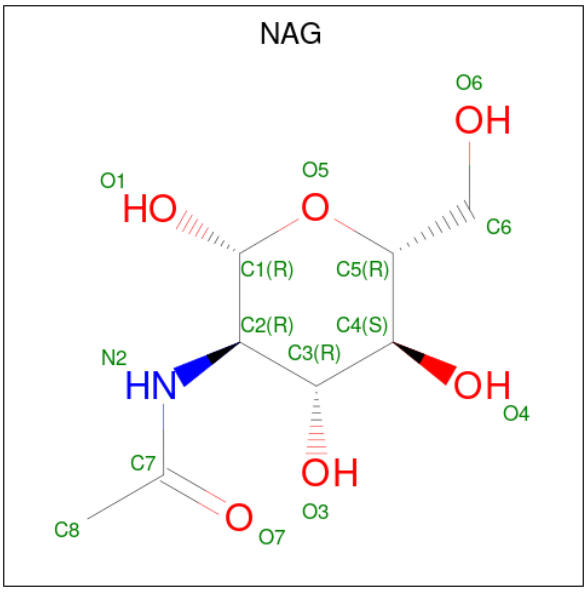
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	F	2	28	16	2	10	0	0	0
8	I	2	28	16	2	10	0	0	0
8	J	2	28	16	2	10	0	0	0

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-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			
9	G	6	72	40	2	30	0	0	0

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

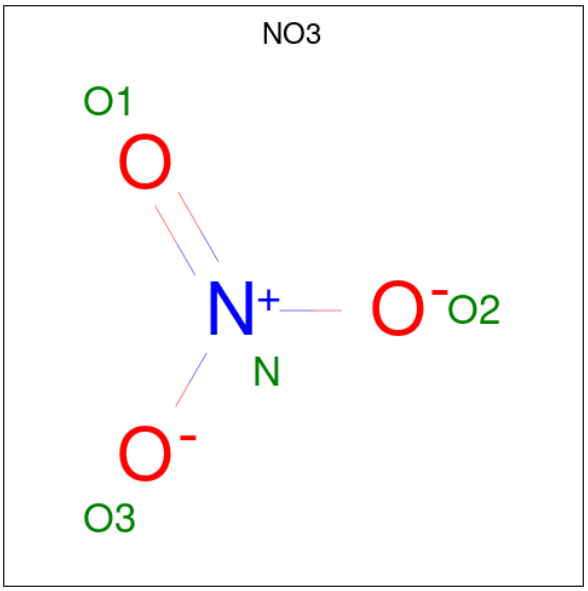


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
10	A	1	14	8	1	5	0	0
			Total	C	N	O		
10	B	1	14	8	1	5	0	0
			Total	C	N	O		
10	B	1	14	8	1	5	0	0

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
11	A	4	4	4	0	0
			Total	Mn		
11	B	1	1	1	0	0

- Molecule 12 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



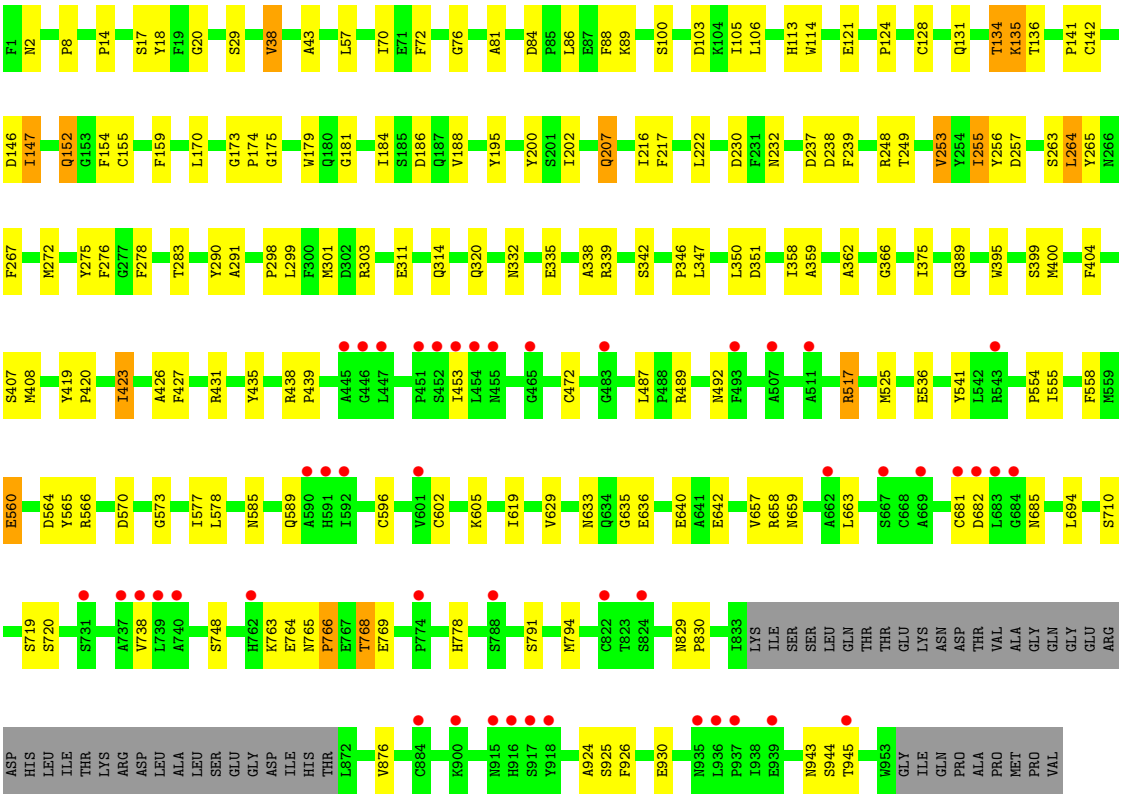
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	N	O		
12	A	1	4	1	3	0	0
			Total	N	O		
12	A	1	4	1	3	0	0

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.

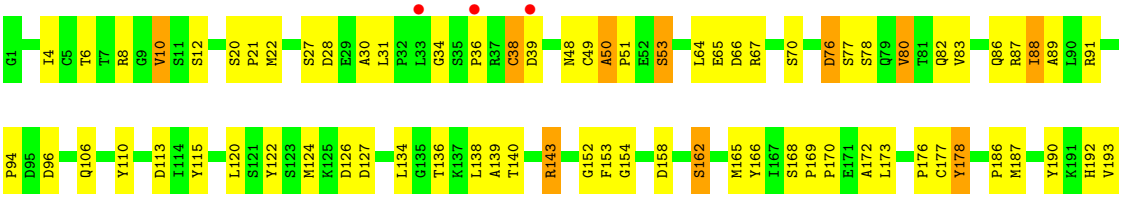
- Molecule 1: Integrin alpha-V

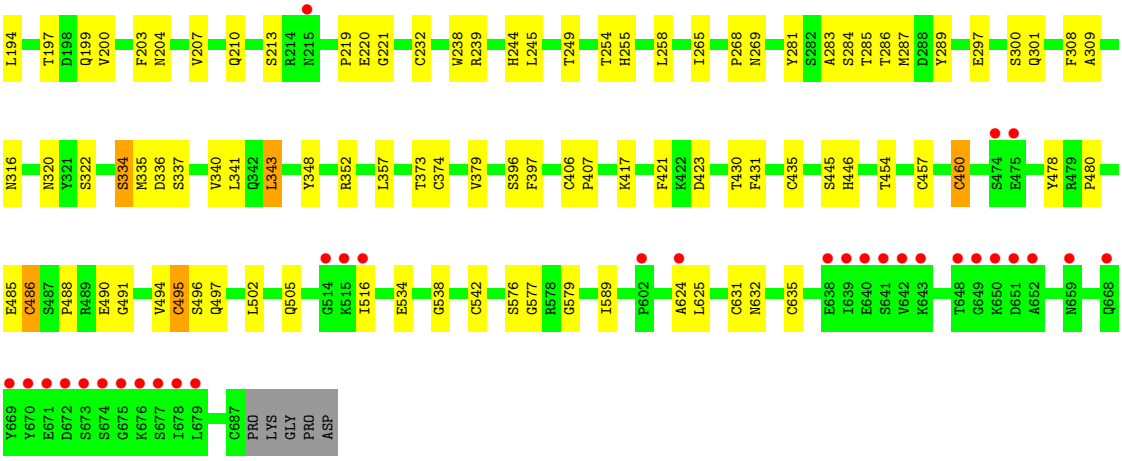
Chain A:



- Molecule 2: Integrin beta-3

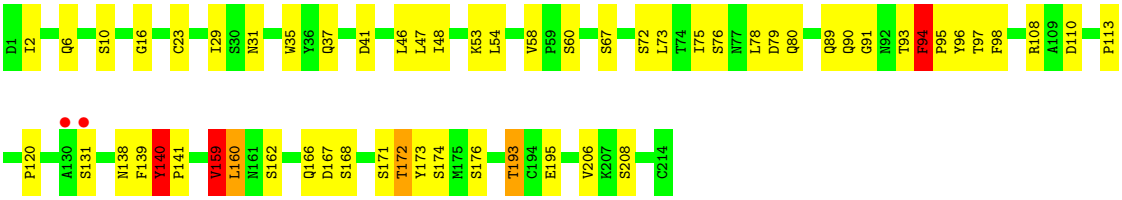
Chain B:





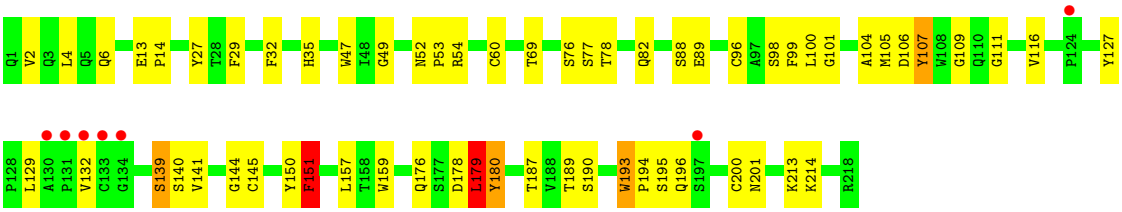
• Molecule 3: 17E6 light chain

Chain L:



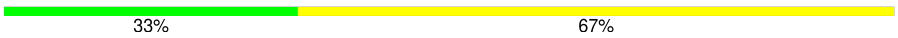
• Molecule 4: 17E6 heavy chain

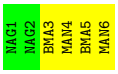
Chain H:



• Molecule 5: beta-D-mannopyranose-(1-4)-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

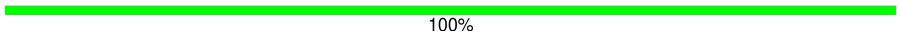
Chain C:





• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

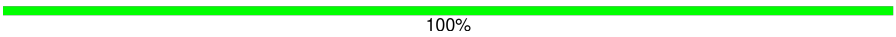
Chain D:



• 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 E:

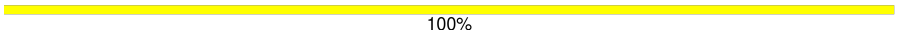
• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F: 

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

Chain I:

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

Chain J: 

• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-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 G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	110.46Å 266.99Å 102.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 3.60 49.86 – 3.61	Depositor EDS
% Data completeness (in resolution range)	87.6 (49.86-3.60) 87.7 (49.86-3.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	3.06 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.246 , 0.312 0.254 , 0.314	Depositor DCC
R_{free} test set	1563 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	112.3	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 122.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13526	wwPDB-VP
Average B, all atoms (Å^2)	155.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: MAN, NO3, NAG, MN, 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	A	0.28	0/5981	0.62	1/8211 (0.0%)
2	B	0.32	1/4438 (0.0%)	0.65	0/6091
3	L	0.29	0/1483	0.62	0/2037
4	H	0.29	0/1475	0.69	1/2027 (0.0%)
All	All	0.30	1/13377 (0.0%)	0.64	2/18366 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	4
3	L	0	3
4	H	0	4
All	All	0	13

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	335	MET	C-O	5.78	1.34	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	GLY	N-CA-C	-5.39	99.62	113.10
4	H	179	LEU	N-CA-C	5.25	125.16	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	THR	Peptide
1	A	768	THR	Peptide
2	B	50	ALA	Peptide
2	B	53	SER	Peptide
2	B	624	ALA	Peptide
2	B	8	ARG	Peptide
4	H	139	SER	Peptide
4	H	151	PHE	Peptide
4	H	178	ASP	Peptide
4	H	179	LEU	Peptide
3	L	140	TYR	Peptide
3	L	168	SER	Peptide
3	L	94	PHE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5875	0	4346	96	0
2	B	4364	0	3235	104	0
3	L	1453	0	1128	33	0
4	H	1440	0	1084	36	0
5	C	72	0	61	0	0
6	D	39	0	34	0	0
7	E	72	0	61	2	0
8	F	28	0	25	0	0
8	I	28	0	25	1	0
8	J	28	0	25	0	0
9	G	72	0	61	1	0
10	A	14	0	13	0	0
10	B	28	0	26	0	0
11	A	4	0	0	0	0
11	B	1	0	0	0	0
12	A	8	0	0	0	0
All	All	13526	0	10124	263	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 11.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG23	1:A:267:PHE:HB2	1.50	0.94
1:A:560:GLU:HG3	1:A:585:ASN:HB3	1.53	0.89
1:A:121:GLU:HA	2:B:169:PRO:HB3	1.57	0.85
1:A:100:SER:HB3	1:A:105:ILE:HG22	1.59	0.83
2:B:31:LEU:HG	2:B:34:GLY:HA3	1.67	0.77
2:B:579:GLY:HA2	2:B:589:ILE:HG13	1.67	0.76
1:A:232:ASN:HB3	1:A:264:LEU:HD13	1.67	0.76
2:B:488:PRO:HG2	2:B:491:GLY:HA3	1.73	0.70
1:A:195:TYR:HA	1:A:202:ILE:HD13	1.73	0.70
3:L:47:LEU:HA	3:L:58:VAL:HG11	1.74	0.70
4:H:193:TRP:CG	4:H:194:PRO:HD3	2.28	0.68
2:B:94:PRO:HB3	2:B:406:CYS:HB2	1.75	0.67
4:H:140:SER:O	4:H:190:SER:HB2	1.95	0.67
2:B:373:THR:HG22	2:B:379:VAL:HB	1.77	0.66
4:H:213:LYS:NZ	4:H:214:LYS:O	2.25	0.66
1:A:124:PRO:HG2	1:A:154:PHE:HA	1.76	0.66
2:B:126:ASP:OD2	2:B:127:ASP:N	2.28	0.66
3:L:46:LEU:HD11	4:H:104:ALA:HB1	1.77	0.65
1:A:657:VAL:HG22	1:A:659:ASN:H	1.60	0.65
1:A:131:GLN:HG3	1:A:136:THR:HG22	1.78	0.64
2:B:168:SER:HB2	2:B:173:LEU:HB3	1.79	0.64
3:L:162:SER:HB3	3:L:176:SER:HB3	1.80	0.64
2:B:127:ASP:HA	2:B:336:ASP:O	1.98	0.64
4:H:140:SER:HA	4:H:189:THR:HA	1.80	0.64
1:A:346:PRO:HA	1:A:358:ILE:HG12	1.80	0.63
1:A:88:PHE:HB2	1:A:113:HIS:HB2	1.80	0.63
3:L:29:ILE:HG21	3:L:90:GLN:HG3	1.81	0.63
1:A:14:PRO:HG2	1:A:17:SER:HB3	1.80	0.62
2:B:83:VAL:O	2:B:86:GLN:NE2	2.33	0.62
1:A:290:TYR:HB3	1:A:320:GLN:HB3	1.82	0.61
2:B:30:ALA:O	2:B:48:ASN:ND2	2.33	0.61
4:H:2:VAL:HG21	4:H:107:TYR:CD2	2.36	0.60
3:L:138:ASN:HA	3:L:172:THR:HB	1.82	0.60
3:L:110:ASP:HA	3:L:140:TYR:HB3	1.84	0.60
1:A:791:SER:OG	1:A:930:GLU:O	2.20	0.59
2:B:534:GLU:O	2:B:538:GLY:N	2.35	0.59
4:H:150:TYR:HB3	4:H:180:TYR:HB2	1.83	0.59
4:H:35:HIS:CD2	4:H:99:PHE:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLU:OE2	1:A:366:GLY:N	2.30	0.58
1:A:175:GLY:HA2	1:A:179:TRP:CD1	2.39	0.57
1:A:472:CYS:HA	1:A:541:TYR:HA	1.86	0.57
2:B:158:ASP:OD1	2:B:289:TYR:OH	2.22	0.57
4:H:69:THR:OG1	4:H:82:GLN:HB2	2.05	0.57
3:L:96:TYR:HB2	4:H:47:TRP:CG	2.40	0.57
1:A:395:TRP:CE2	1:A:431:ARG:HG2	2.40	0.57
2:B:486:CYS:HB3	2:B:494:VAL:O	2.03	0.57
2:B:64:LEU:HD11	2:B:89:ALA:HB2	1.86	0.57
4:H:35:HIS:HD2	4:H:99:PHE:HB2	1.69	0.57
1:A:350:LEU:HA	1:A:420:PRO:HD2	1.87	0.56
2:B:245:LEU:HD11	2:B:348:TYR:HD1	1.70	0.56
4:H:6:GLN:HG3	4:H:111:GLY:H	1.70	0.56
2:B:178:TYR:H	2:B:178:TYR:HD1	1.53	0.56
4:H:141:VAL:O	4:H:187:THR:HA	2.06	0.56
1:A:924:ALA:O	1:A:945:THR:N	2.32	0.55
1:A:925:SER:HA	1:A:944:SER:HA	1.88	0.55
1:A:570:ASP:HB3	1:A:573:GLY:HA2	1.87	0.55
2:B:27:SER:HA	2:B:457:CYS:HB3	1.88	0.55
1:A:100:SER:CB	1:A:105:ILE:HG22	2.35	0.55
3:L:166:GLN:HB2	3:L:173:TYR:CZ	2.41	0.55
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.87	0.55
1:A:399:SER:OG	1:A:400:MET:N	2.40	0.54
2:B:49:CYS:HA	2:B:51:PRO:HD2	1.88	0.54
2:B:194:LEU:HD22	2:B:203:PHE:HA	1.89	0.54
2:B:221:GLY:HA2	2:B:289:TYR:HE2	1.72	0.54
3:L:16:GLY:H	3:L:78:LEU:HB3	1.73	0.54
1:A:141:PRO:HB2	1:A:184:ILE:HD13	1.89	0.54
9:G:1:NAG:H61	9:G:2:NAG:H2	1.90	0.54
2:B:106:GLN:HG2	2:B:352:ARG:HG3	1.90	0.54
2:B:340:VAL:HA	2:B:343:LEU:HD23	1.88	0.54
1:A:633:ASN:ND2	1:A:636:GLU:O	2.40	0.54
1:A:256:TYR:CD1	1:A:263:SER:HB3	2.42	0.53
2:B:334:SER:OG	2:B:336:ASP:OD2	2.25	0.53
2:B:445:SER:OG	2:B:446:HIS:N	2.41	0.53
1:A:255:ILE:HD12	1:A:265:TYR:HB2	1.90	0.53
1:A:2:ASN:ND2	1:A:438:ARG:O	2.40	0.53
2:B:454:THR:O	2:B:460:CYS:HB3	2.07	0.53
1:A:17:SER:HB2	1:A:43:ALA:HB2	1.91	0.53
3:L:167:ASP:O	3:L:171:SER:HA	2.09	0.53
1:A:301:MET:HA	1:A:311:GLU:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:495:CYS:O	2:B:497:GLN:N	2.43	0.52
1:A:38:VAL:HG23	1:A:57:LEU:HB2	1.91	0.52
2:B:197:THR:HG22	2:B:199:GLN:H	1.74	0.52
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.45	0.52
1:A:253:VAL:HG22	1:A:276:PHE:HE2	1.75	0.51
4:H:13:GLU:HG3	4:H:14:PRO:HD2	1.91	0.51
1:A:338:ALA:HB1	1:A:362:ALA:HB1	1.93	0.51
2:B:122:TYR:N	2:B:213:SER:O	2.44	0.51
3:L:93:THR:OG1	3:L:94:PHE:N	2.44	0.51
2:B:169:PRO:HG2	2:B:170:PRO:HD3	1.92	0.51
4:H:151:PHE:HB2	4:H:179:LEU:CB	2.41	0.51
2:B:190:TYR:HB3	2:B:281:TYR:HB2	1.92	0.51
2:B:113:ASP:OD1	2:B:239:ARG:NE	2.42	0.50
1:A:114:TRP:HZ3	1:A:147:ILE:HG21	1.77	0.50
2:B:70:SER:HB2	2:B:80:VAL:O	2.11	0.50
1:A:76:GLY:O	1:A:89:LYS:NZ	2.44	0.50
1:A:86:LEU:HD11	1:A:200:TYR:CE1	2.47	0.50
2:B:407:PRO:HD2	2:B:431:PHE:CD1	2.47	0.50
3:L:48:ILE:HA	3:L:53:LYS:O	2.12	0.50
1:A:283:THR:CG2	1:A:358:ILE:HD11	2.42	0.49
1:A:339:ARG:HH12	2:B:268:PRO:HB3	1.77	0.49
1:A:159:PHE:HB3	1:A:174:PRO:HD3	1.92	0.49
1:A:314:GLN:OE1	1:A:332:ASN:ND2	2.46	0.49
1:A:640:GLU:HA	1:A:685:ASN:HA	1.95	0.49
3:L:54:LEU:HD11	3:L:60:SER:HA	1.94	0.49
1:A:299:LEU:HD11	2:B:258:LEU:HG	1.94	0.49
1:A:272:MET:HE1	2:B:320:ASN:HD22	1.78	0.49
1:A:487:LEU:O	1:A:489:ARG:N	2.40	0.49
2:B:165:MET:HG2	2:B:166:TYR:H	1.77	0.48
2:B:283:ALA:HB1	2:B:287:MET:HB2	1.94	0.48
4:H:29:PHE:CD2	4:H:77:SER:HA	2.48	0.48
3:L:159:VAL:O	3:L:160:LEU:HG	2.13	0.48
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.94	0.48
1:A:765:ASN:N	1:A:766:PRO:HD3	2.29	0.48
2:B:88:ILE:HG13	2:B:88:ILE:O	2.12	0.48
3:L:31:ASN:OD1	3:L:67:SER:HA	2.13	0.48
4:H:76:SER:OG	4:H:78:THR:OG1	2.30	0.48
1:A:404:PHE:HA	1:A:426:ALA:HB2	1.95	0.47
4:H:88:SER:HA	4:H:116:VAL:HB	1.96	0.47
2:B:64:LEU:HB2	2:B:87:ARG:HG3	1.95	0.47
2:B:134:LEU:HD11	2:B:341:LEU:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:144:GLY:HA2	4:H:159:TRP:CH2	2.49	0.47
2:B:143:ARG:HD3	2:B:143:ARG:HA	1.40	0.47
2:B:495:CYS:C	2:B:497:GLN:H	2.18	0.47
1:A:339:ARG:NH1	2:B:268:PRO:HB3	2.30	0.47
1:A:566:ARG:HA	1:A:566:ARG:HD3	1.73	0.47
1:A:186:ASP:OD1	1:A:207:GLN:HB2	2.15	0.47
1:A:395:TRP:CZ2	1:A:431:ARG:HG2	2.50	0.47
2:B:49:CYS:C	2:B:51:PRO:HD2	2.35	0.47
2:B:82:GLN:N	2:B:423:ASP:OD2	2.48	0.47
2:B:154:GLY:HA2	2:B:193:VAL:HG23	1.97	0.47
4:H:193:TRP:O	4:H:195:SER:N	2.47	0.47
1:A:230:ASP:HA	1:A:238:ASP:OD2	2.15	0.47
1:A:408:MET:HA	1:A:423:ILE:O	2.13	0.47
2:B:110:TYR:HB3	2:B:352:ARG:HH22	1.79	0.47
1:A:18:TYR:CD1	1:A:427:PHE:HD1	2.32	0.47
3:L:120:PRO:HG3	3:L:131:SER:O	2.15	0.46
1:A:577:ILE:HG22	1:A:578:LEU:O	2.14	0.46
2:B:139:ALA:O	2:B:143:ARG:HG2	2.16	0.46
3:L:2:ILE:O	3:L:97:THR:HG21	2.15	0.46
3:L:75:ILE:HG22	3:L:76:SER:O	2.16	0.46
1:A:20:GLY:O	1:A:407:SER:OG	2.31	0.46
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.96	0.46
2:B:153:PHE:HE2	2:B:210:GLN:HG3	1.79	0.46
2:B:200:VAL:O	2:B:203:PHE:HB3	2.15	0.46
1:A:517:ARG:CG	1:A:517:ARG:HH11	2.29	0.46
1:A:657:VAL:HG13	1:A:658:ARG:H	1.79	0.46
2:B:158:ASP:HA	2:B:221:GLY:N	2.30	0.46
2:B:139:ALA:HB2	2:B:200:VAL:HG21	1.96	0.46
4:H:4:LEU:HB2	4:H:109:GLY:HA2	1.97	0.46
4:H:100:LEU:HG	4:H:101:GLY:H	1.79	0.46
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.50	0.46
2:B:66:ASP:N	2:B:66:ASP:OD1	2.49	0.46
3:L:108:ARG:HD2	3:L:171:SER:O	2.16	0.46
3:L:91:GLY:HA2	3:L:96:TYR:CE1	2.50	0.46
1:A:106:LEU:HD11	1:A:128:CYS:HB3	1.98	0.46
1:A:146:ASP:OD2	4:H:54:ARG:NE	2.41	0.46
1:A:216:ILE:HG13	1:A:217:PHE:N	2.31	0.45
1:A:492:ASN:ND2	1:A:564:ASP:OD2	2.49	0.45
4:H:127:TYR:O	4:H:129:LEU:N	2.49	0.45
1:A:257:ASP:HB2	1:A:264:LEU:HD21	1.98	0.45
4:H:100:LEU:HB2	4:H:106:ASP:CG	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:35:TRP:CE2	3:L:73:LEU:HB2	2.52	0.45
3:L:110:ASP:OD2	3:L:141:PRO:HD3	2.17	0.45
1:A:170:LEU:HD22	1:A:239:PHE:CD1	2.52	0.45
1:A:278:PHE:CD2	1:A:298:PRO:HG3	2.51	0.45
3:L:89:GLN:HB2	3:L:98:PHE:CD2	2.52	0.45
1:A:375:ILE:HD12	1:A:389:GLN:HB3	1.98	0.45
2:B:21:PRO:HG2	2:B:96:ASP:HB2	1.98	0.45
2:B:204:ASN:HA	2:B:207:VAL:HG12	1.99	0.45
2:B:221:GLY:HA2	2:B:289:TYR:CE2	2.51	0.44
4:H:49:GLY:HA3	4:H:60:CYS:HA	1.99	0.44
1:A:663:LEU:HA	1:A:694:LEU:O	2.16	0.44
2:B:20:SER:HB3	2:B:22:MET:HG2	1.98	0.44
2:B:245:LEU:HD11	2:B:348:TYR:CD1	2.51	0.44
1:A:605:LYS:H	1:A:635:GLY:HA3	1.82	0.44
2:B:120:LEU:HD12	2:B:120:LEU:HA	1.68	0.44
2:B:169:PRO:CG	2:B:170:PRO:HD3	2.48	0.44
1:A:719:SER:OG	1:A:720:SER:N	2.51	0.44
2:B:30:ALA:HB1	2:B:49:CYS:HB3	1.99	0.44
2:B:176:PRO:CG	2:B:186:PRO:HA	2.47	0.44
7:E:4:MAN:H3	7:E:5:MAN:H2	1.52	0.44
1:A:642:GLU:HG2	1:A:682:ASP:HA	1.99	0.44
1:A:81:ALA:HB3	1:A:84:ASP:HB3	1.99	0.44
2:B:27:SER:HB2	2:B:53:SER:OG	2.18	0.44
2:B:297:GLU:OE1	2:B:301:GLN:NE2	2.51	0.44
3:L:48:ILE:HG23	3:L:53:LYS:H	1.83	0.44
4:H:52:ASN:HD22	4:H:53:PRO:HD2	1.83	0.44
1:A:8:PRO:HB3	1:A:435:TYR:HD2	1.83	0.44
1:A:70:ILE:HB	1:A:72:PHE:CE1	2.53	0.44
2:B:158:ASP:HA	2:B:221:GLY:H	1.83	0.44
3:L:79:ASP:OD1	3:L:80:GLN:N	2.39	0.44
4:H:98:SER:O	4:H:106:ASP:N	2.50	0.44
2:B:67:ARG:NH1	2:B:86:GLN:HG2	2.33	0.43
3:L:46:LEU:HD12	4:H:105:MET:O	2.17	0.43
3:L:195:GLU:HG3	3:L:206:VAL:HG22	2.00	0.43
1:A:283:THR:HG21	1:A:358:ILE:HD11	2.00	0.43
2:B:220:GLU:H	2:B:254:THR:HA	1.84	0.43
4:H:159:TRP:CZ3	4:H:200:CYS:HB2	2.53	0.43
1:A:554:PRO:HB2	1:A:589:GLN:HB3	1.99	0.43
2:B:30:ALA:CB	2:B:49:CYS:HB3	2.49	0.43
2:B:136:THR:HA	2:B:200:VAL:HG11	2.00	0.43
2:B:136:THR:O	2:B:140:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:ALA:O	2:B:287:MET:N	2.48	0.43
1:A:239:PHE:O	1:A:255:ILE:HA	2.18	0.43
3:L:113:PRO:HB3	3:L:139:PHE:CD2	2.54	0.43
2:B:357:LEU:HD11	2:B:397:PHE:CD2	2.53	0.43
1:A:763:LYS:O	1:A:766:PRO:HG3	2.19	0.43
2:B:28:ASP:N	2:B:457:CYS:O	2.52	0.43
2:B:91:ARG:HA	2:B:430:THR:O	2.19	0.43
2:B:265:ILE:HG23	2:B:286:THR:O	2.18	0.43
1:A:347:LEU:HD11	1:A:359:ALA:HB2	2.00	0.42
2:B:38:CYS:HB3	2:B:39:ASP:H	1.53	0.42
2:B:168:SER:HB2	2:B:173:LEU:CB	2.48	0.42
1:A:134:THR:OG1	1:A:135:LYS:N	2.53	0.42
1:A:152:GLN:HB3	1:A:155:CYS:HB2	2.02	0.42
1:A:829:ASN:HA	1:A:830:PRO:HD3	1.69	0.42
2:B:138:LEU:HA	2:B:341:LEU:HD13	2.01	0.42
1:A:525:MET:HE3	1:A:536:GLU:HG2	2.01	0.42
2:B:336:ASP:O	2:B:337:SER:CB	2.68	0.42
1:A:596:CYS:HB3	1:A:602:CYS:HB3	1.92	0.42
2:B:219:PRO:HG2	2:B:255:HIS:CE1	2.55	0.42
1:A:339:ARG:HB3	1:A:342:SER:OG	2.20	0.42
2:B:316:ASN:HB3	8:I:1:NAG:HN2	1.85	0.42
4:H:100:LEU:HG	4:H:101:GLY:N	2.34	0.42
2:B:115:TYR:OH	2:B:192:HIS:ND1	2.49	0.42
2:B:170:PRO:HG2	2:B:172:ALA:HB3	2.01	0.42
4:H:47:TRP:CH2	4:H:49:GLY:HA2	2.55	0.42
1:A:419:TYR:HA	1:A:420:PRO:HD3	1.77	0.41
2:B:152:GLY:HA2	2:B:194:LEU:HD23	2.02	0.41
3:L:139:PHE:CE2	3:L:174:SER:HA	2.54	0.41
2:B:65:GLU:HG3	2:B:87:ARG:HG2	2.02	0.41
3:L:96:TYR:HD1	3:L:96:TYR:HA	1.75	0.41
1:A:248:ARG:O	1:A:249:THR:OG1	2.32	0.41
1:A:629:VAL:O	1:A:694:LEU:HA	2.20	0.41
2:B:49:CYS:HB2	2:B:50:ALA:H	1.74	0.41
4:H:144:GLY:HA2	4:H:159:TRP:HH2	1.86	0.41
2:B:165:MET:HG3	2:B:187:MET:HE3	2.01	0.41
3:L:54:LEU:HD22	3:L:58:VAL:HG23	2.03	0.41
1:A:8:PRO:HB3	1:A:435:TYR:CD2	2.56	0.41
1:A:748:SER:HA	1:A:778:HIS:HA	2.02	0.41
2:B:124:MET:O	2:B:127:ASP:HB2	2.21	0.41
2:B:478:TYR:C	2:B:480:PRO:HD3	2.41	0.41
1:A:291:ALA:O	1:A:320:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:MET:HG2	2:B:166:TYR:N	2.35	0.41
1:A:794:MET:O	1:A:926:PHE:HA	2.21	0.41
2:B:76:ASP:O	2:B:78:SER:N	2.50	0.41
2:B:269:ASN:HA	2:B:287:MET:SD	2.60	0.41
3:L:193:THR:HG22	3:L:208:SER:HA	2.02	0.41
4:H:27:TYR:HE2	4:H:32:PHE:HB2	1.86	0.41
2:B:10:VAL:C	2:B:12:SER:H	2.24	0.41
2:B:502:LEU:O	2:B:505:GLN:O	2.39	0.41
4:H:157:LEU:HA	4:H:201:ASN:O	2.21	0.41
1:A:768:THR:OG1	1:A:769:GLU:N	2.54	0.40
1:A:298:PRO:O	1:A:339:ARG:HA	2.22	0.40
2:B:407:PRO:HD2	2:B:431:PHE:CE1	2.56	0.40
2:B:49:CYS:CA	2:B:51:PRO:HD2	2.50	0.40
2:B:249:THR:HA	2:B:309:ALA:O	2.21	0.40
2:B:485:GLU:CB	2:B:490:GLU:H	2.34	0.40
7:E:1:NAG:H61	7:E:2:NAG:H82	2.02	0.40
1:A:764:GLU:C	1:A:766:PRO:HD3	2.42	0.40
2:B:4:ILE:C	2:B:6:THR:H	2.24	0.40
2:B:238:TRP:CE3	2:B:244:HIS:HD2	2.39	0.40
4:H:139:SER:HA	4:H:190:SER:HB3	2.02	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	911/962 (95%)	815 (90%)	88 (10%)	8 (1%)	17 57
2	B	685/692 (99%)	595 (87%)	79 (12%)	11 (2%)	9 46
3	L	212/214 (99%)	196 (92%)	12 (6%)	4 (2%)	8 42
4	H	216/218 (99%)	190 (88%)	20 (9%)	6 (3%)	5 34
All	All	2024/2086 (97%)	1796 (89%)	199 (10%)	29 (1%)	11 48

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	LYS
1	A	619	ILE
1	A	710	SER
4	H	180	TYR
1	A	453	ILE
1	A	738	VAL
1	A	876	VAL
2	B	516	ILE
2	B	632	ASN
3	L	159	VAL
2	B	36	PRO
2	B	80	VAL
2	B	496	SER
3	L	94	PHE
3	L	140	TYR
4	H	151	PHE
2	B	10	VAL
2	B	76	ASP
2	B	625	LEU
4	H	107	TYR
4	H	193	TRP
1	A	555	ILE
2	B	577	GLY
4	H	196	GLN
2	B	77	SER
1	A	766	PRO
3	L	95	PRO
2	B	162	SER
4	H	132	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	A	400/816 (49%)	378 (94%)	22 (6%)	21 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	334/614 (54%)	308 (92%)	26 (8%)	12	44
3	L	125/192 (65%)	115 (92%)	10 (8%)	12	43
4	H	107/183 (58%)	102 (95%)	5 (5%)	26	61
All	All	966/1805 (54%)	903 (94%)	63 (6%)	17	51

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	38	VAL
1	A	103	ASP
1	A	142	CYS
1	A	147	ILE
1	A	152	GLN
1	A	188	VAL
1	A	207	GLN
1	A	237	ASP
1	A	253	VAL
1	A	255	ILE
1	A	264	LEU
1	A	275	TYR
1	A	303	ARG
1	A	351	ASP
1	A	423	ILE
1	A	517	ARG
1	A	558	PHE
1	A	560	GLU
1	A	565	TYR
1	A	681	CYS
1	A	943	ASN
2	B	38	CYS
2	B	88	ILE
2	B	143	ARG
2	B	162	SER
2	B	177	CYS
2	B	178	TYR
2	B	232	CYS
2	B	284	SER
2	B	285	THR
2	B	300	SER
2	B	308	PHE

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Mol	Chain	Res	Type
2	B	322	SER
2	B	334	SER
2	B	343	LEU
2	B	374	CYS
2	B	396	SER
2	B	417	LYS
2	B	421	PHE
2	B	435	CYS
2	B	460	CYS
2	B	486	CYS
2	B	495	CYS
2	B	542	CYS
2	B	576	SER
2	B	631	CYS
2	B	635	CYS
3	L	6	GLN
3	L	10	SER
3	L	23	CYS
3	L	41	ASP
3	L	72	SER
3	L	94	PHE
3	L	159	VAL
3	L	160	LEU
3	L	172	THR
3	L	193	THR
4	H	89	GLU
4	H	96	CYS
4	H	145	CYS
4	H	151	PHE
4	H	176	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	310	GLN
1	A	314	GLN
1	A	332	ASN
2	B	313	ASN
3	L	138	ASN
4	H	52	ASN

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)

27 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	$\#\|Z\| > 2$
5	NAG	C	1	5,1	14,14,15	0.30	0	17,19,21	0.50	0
5	NAG	C	2	5	14,14,15	0.42	0	17,19,21	0.79	0
5	BMA	C	3	5	11,11,12	1.02	0	15,15,17	1.09	1 (6%)
5	MAN	C	4	5	11,11,12	0.97	1 (9%)	15,15,17	0.88	1 (6%)
5	BMA	C	5	5	11,11,12	0.59	0	15,15,17	0.96	1 (6%)
5	MAN	C	6	5	11,11,12	0.68	0	15,15,17	1.08	2 (13%)
6	NAG	D	1	6,1	14,14,15	0.40	0	17,19,21	0.45	0
6	NAG	D	2	6	14,14,15	0.40	0	17,19,21	0.51	0
6	BMA	D	3	6	11,11,12	0.70	0	15,15,17	0.83	0
7	NAG	E	1	7,1	14,14,15	0.50	0	17,19,21	1.00	1 (5%)
7	NAG	E	2	7	14,14,15	0.42	0	17,19,21	0.44	0
7	BMA	E	3	7	11,11,12	0.65	0	15,15,17	0.96	1 (6%)
7	MAN	E	4	7	11,11,12	0.85	0	15,15,17	1.48	2 (13%)
7	MAN	E	5	7	11,11,12	0.84	0	15,15,17	1.35	2 (13%)
7	MAN	E	6	7	11,11,12	0.53	0	15,15,17	1.05	2 (13%)
8	NAG	F	1	8,1	14,14,15	0.39	0	17,19,21	0.48	0
8	NAG	F	2	8	14,14,15	0.32	0	17,19,21	0.34	0
9	NAG	G	1	9,1	14,14,15	0.25	0	17,19,21	0.55	0
9	NAG	G	2	9	14,14,15	0.64	1 (7%)	17,19,21	0.80	1 (5%)
9	BMA	G	3	9	11,11,12	1.13	1 (9%)	15,15,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	MAN	G	4	9	11,11,12	1.21	1 (9%)	15,15,17	1.69	2 (13%)
9	MAN	G	5	9	11,11,12	1.29	2 (18%)	15,15,17	1.57	4 (26%)
9	MAN	G	6	9	11,11,12	0.77	1 (9%)	15,15,17	1.46	2 (13%)
8	NAG	I	1	2,8	14,14,15	0.75	1 (7%)	17,19,21	1.03	1 (5%)
8	NAG	I	2	8	14,14,15	0.38	0	17,19,21	0.93	1 (5%)
8	NAG	J	1	2,8	14,14,15	1.27	1 (7%)	17,19,21	1.61	1 (5%)
8	NAG	J	2	8	14,14,15	0.43	0	17,19,21	0.64	1 (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
5	NAG	C	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	C	2	5	-	4/6/23/26	0/1/1/1
5	BMA	C	3	5	-	0/2/19/22	0/1/1/1
5	MAN	C	4	5	-	1/2/19/22	0/1/1/1
5	BMA	C	5	5	-	0/2/19/22	0/1/1/1
5	MAN	C	6	5	-	2/2/19/22	0/1/1/1
6	NAG	D	1	6,1	-	2/6/23/26	0/1/1/1
6	NAG	D	2	6	-	0/6/23/26	0/1/1/1
6	BMA	D	3	6	-	2/2/19/22	0/1/1/1
7	NAG	E	1	7,1	-	4/6/23/26	0/1/1/1
7	NAG	E	2	7	-	2/6/23/26	0/1/1/1
7	BMA	E	3	7	-	2/2/19/22	0/1/1/1
7	MAN	E	4	7	-	1/2/19/22	1/1/1/1
7	MAN	E	5	7	-	1/2/19/22	1/1/1/1
7	MAN	E	6	7	-	0/2/19/22	0/1/1/1
8	NAG	F	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	F	2	8	-	2/6/23/26	0/1/1/1
9	NAG	G	1	9,1	-	2/6/23/26	0/1/1/1
9	NAG	G	2	9	-	2/6/23/26	0/1/1/1
9	BMA	G	3	9	-	2/2/19/22	0/1/1/1
9	MAN	G	4	9	-	1/2/19/22	1/1/1/1
9	MAN	G	5	9	-	0/2/19/22	0/1/1/1
9	MAN	G	6	9	-	0/2/19/22	0/1/1/1
8	NAG	I	1	2,8	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	I	2	8	-	2/6/23/26	0/1/1/1
8	NAG	J	1	2,8	-	2/6/23/26	0/1/1/1
8	NAG	J	2	8	-	2/6/23/26	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	1	NAG	O5-C1	4.64	1.51	1.43
9	G	5	MAN	C1-C2	2.75	1.58	1.52
8	I	1	NAG	O5-C1	2.61	1.48	1.43
5	C	4	MAN	O5-C1	-2.51	1.39	1.43
9	G	5	MAN	C2-C3	2.46	1.56	1.52
9	G	4	MAN	O3-C3	2.36	1.48	1.43
9	G	3	BMA	C2-C3	2.35	1.56	1.52
9	G	6	MAN	C1-C2	2.14	1.57	1.52
9	G	2	NAG	O5-C1	2.08	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	J	1	NAG	C1-O5-C5	5.94	120.14	112.19
9	G	4	MAN	C1-O5-C5	5.16	119.10	112.19
7	E	4	MAN	C1-O5-C5	4.64	118.41	112.19
7	E	5	MAN	C1-O5-C5	4.27	117.91	112.19
9	G	6	MAN	C1-O5-C5	3.85	117.35	112.19
8	I	1	NAG	C1-O5-C5	3.76	117.22	112.19
9	G	5	MAN	C1-O5-C5	3.32	116.64	112.19
8	I	2	NAG	C1-O5-C5	3.29	116.59	112.19
5	C	6	MAN	C1-O5-C5	3.10	116.34	112.19
9	G	2	NAG	C1-O5-C5	3.06	116.28	112.19
7	E	3	BMA	C1-O5-C5	3.00	116.21	112.19
7	E	6	MAN	C1-O5-C5	2.79	115.92	112.19
9	G	5	MAN	C1-C2-C3	2.74	113.63	109.64
7	E	4	MAN	O2-C2-C3	-2.45	105.08	110.15
5	C	3	BMA	C1-C2-C3	-2.41	106.14	109.64
7	E	1	NAG	C1-O5-C5	2.34	115.32	112.19
9	G	6	MAN	O2-C2-C3	-2.24	105.52	110.15
9	G	5	MAN	O2-C2-C3	-2.23	105.53	110.15
9	G	5	MAN	O5-C1-C2	2.18	116.00	110.79
7	E	6	MAN	O2-C2-C3	-2.17	105.66	110.15
5	C	4	MAN	O2-C2-C3	-2.17	105.67	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	5	BMA	C1-O5-C5	2.17	115.09	112.19
5	C	6	MAN	O2-C2-C3	-2.15	105.69	110.15
9	G	4	MAN	O2-C2-C3	-2.10	105.80	110.15
8	J	2	NAG	C1-O5-C5	2.07	114.97	112.19
7	E	5	MAN	O2-C2-C3	-2.06	105.88	110.15

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
6	D	3	BMA	O5-C5-C6-O6
8	F	2	NAG	O5-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
8	I	2	NAG	C4-C5-C6-O6
5	C	6	MAN	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6
6	D	3	BMA	C4-C5-C6-O6
9	G	3	BMA	O5-C5-C6-O6
8	F	2	NAG	C4-C5-C6-O6
7	E	3	BMA	O5-C5-C6-O6
9	G	1	NAG	O5-C5-C6-O6
5	C	1	NAG	O5-C5-C6-O6
6	D	1	NAG	O5-C5-C6-O6
8	I	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C8-C7-N2-C2
5	C	2	NAG	O7-C7-N2-C2
8	I	1	NAG	C8-C7-N2-C2
8	I	1	NAG	O7-C7-N2-C2
8	J	1	NAG	C8-C7-N2-C2
8	J	1	NAG	O7-C7-N2-C2
7	E	2	NAG	O5-C5-C6-O6
9	G	2	NAG	O5-C5-C6-O6
5	C	6	MAN	C4-C5-C6-O6
7	E	3	BMA	C4-C5-C6-O6
9	G	1	NAG	C4-C5-C6-O6
8	J	2	NAG	O5-C5-C6-O6
8	J	2	NAG	C4-C5-C6-O6
9	G	4	MAN	O5-C5-C6-O6
7	E	4	MAN	O5-C5-C6-O6
7	E	1	NAG	C4-C5-C6-O6
9	G	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	D	1	NAG	C4-C5-C6-O6
7	E	1	NAG	C1-C2-N2-C7
7	E	1	NAG	O5-C5-C6-O6
7	E	2	NAG	C4-C5-C6-O6
9	G	2	NAG	C4-C5-C6-O6
7	E	1	NAG	C3-C2-N2-C7
7	E	5	MAN	C4-C5-C6-O6
5	C	4	MAN	O5-C5-C6-O6

All (3) ring outliers are listed below:

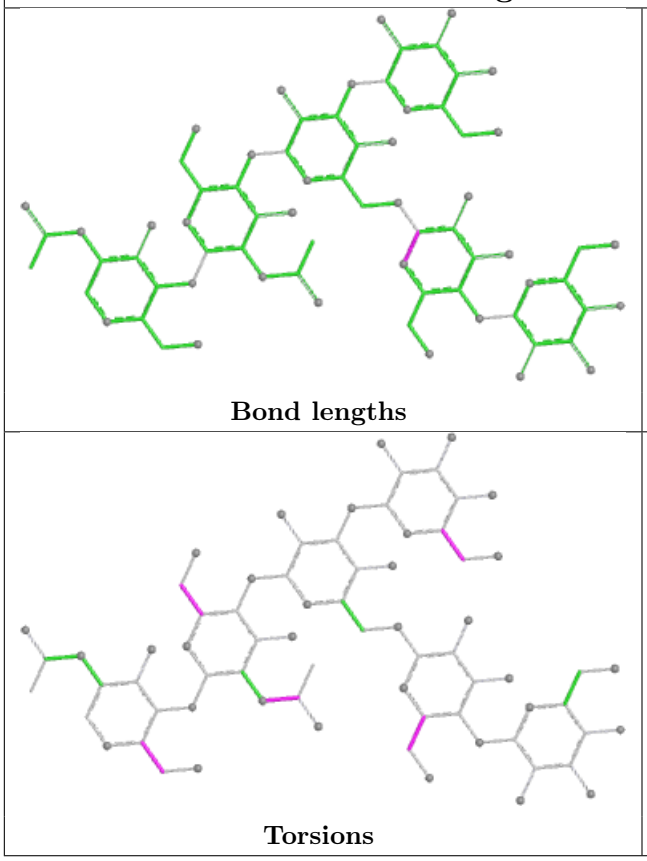
Mol	Chain	Res	Type	Atoms
9	G	4	MAN	C1-C2-C3-C4-C5-O5
7	E	4	MAN	C1-C2-C3-C4-C5-O5
7	E	5	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 4 short contacts:

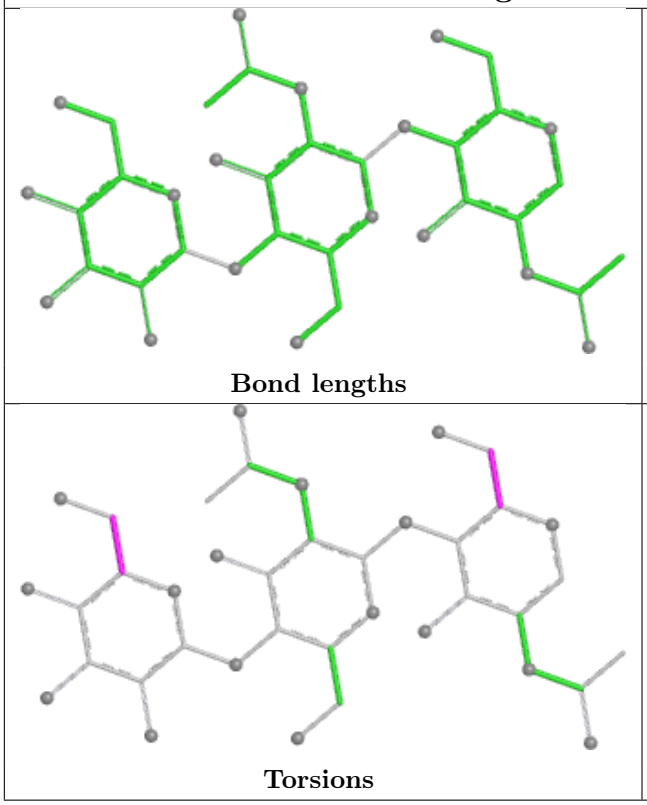
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	1	NAG	1	0
7	E	5	MAN	1	0
8	I	1	NAG	1	0
9	G	1	NAG	1	0
9	G	2	NAG	1	0
7	E	4	MAN	1	0
7	E	2	NAG	1	0

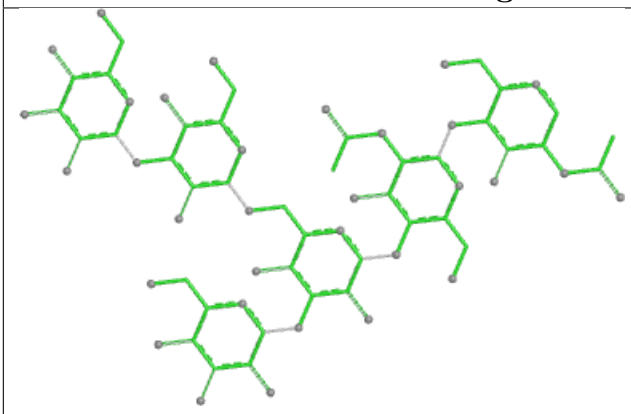
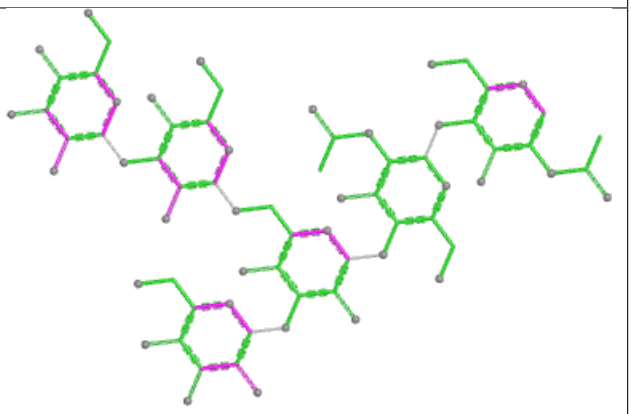
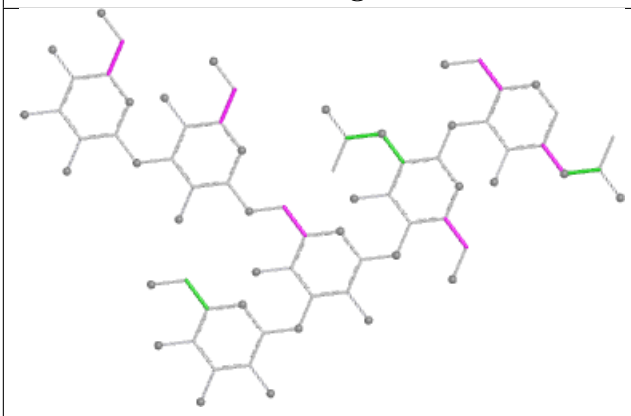
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C

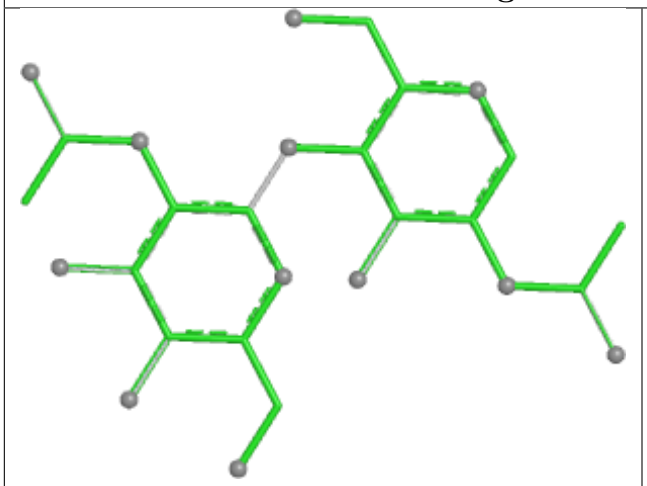


Oligosaccharide Chain D

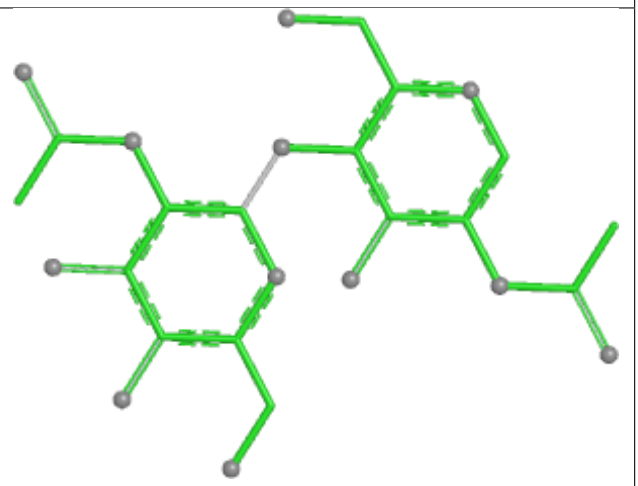


Oligosaccharide Chain E	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

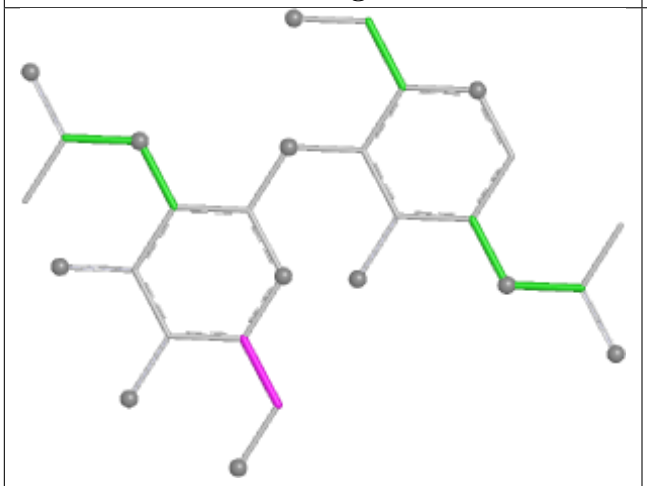
Oligosaccharide Chain F



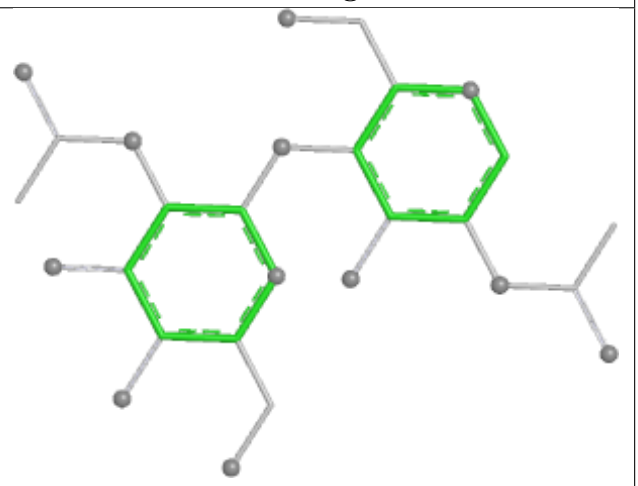
Bond lengths



Bond angles

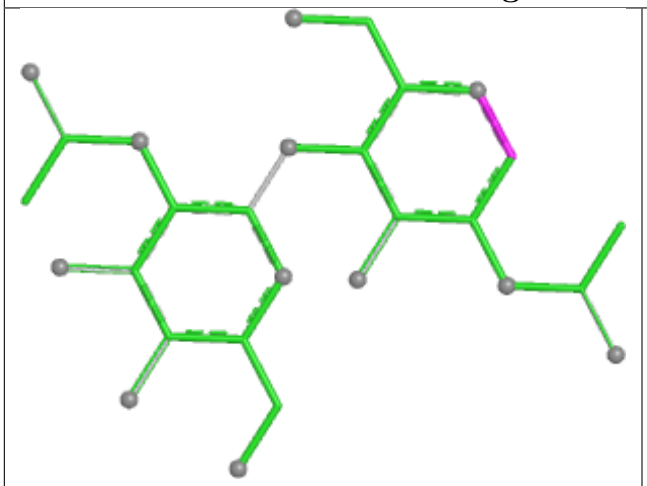


Torsions

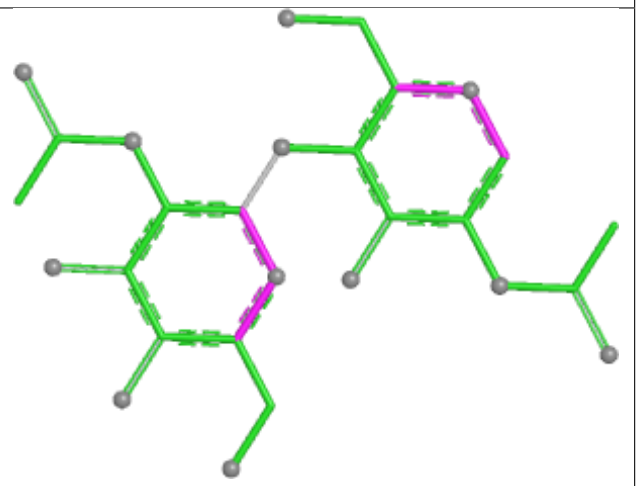


Rings

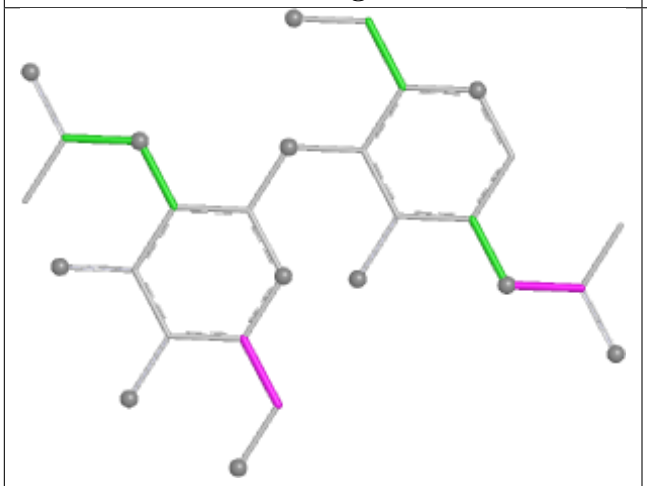
Oligosaccharide Chain I



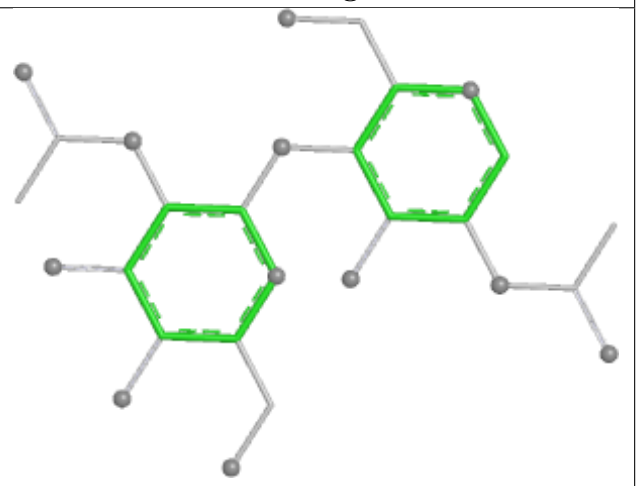
Bond lengths



Bond angles

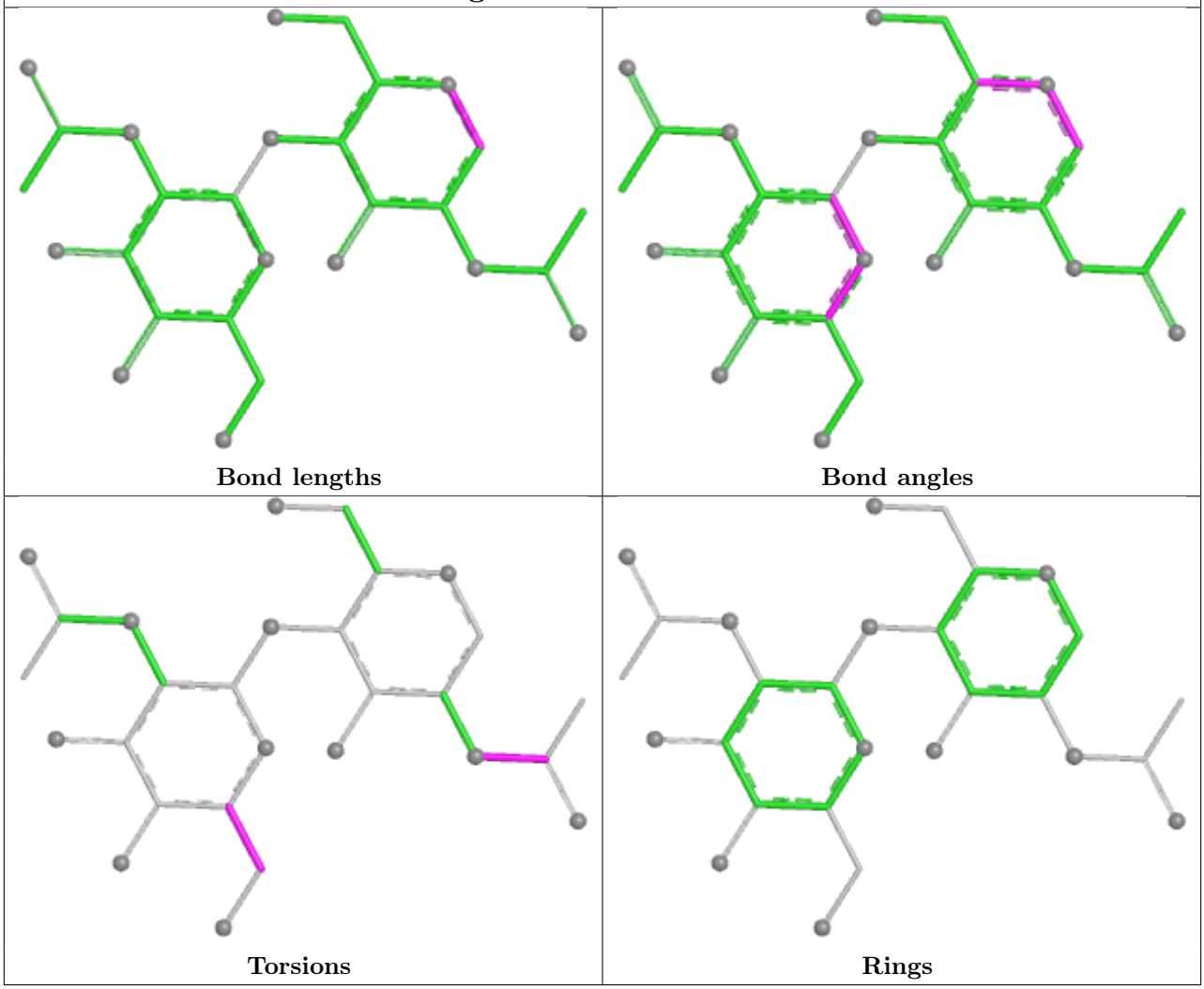


Torsions

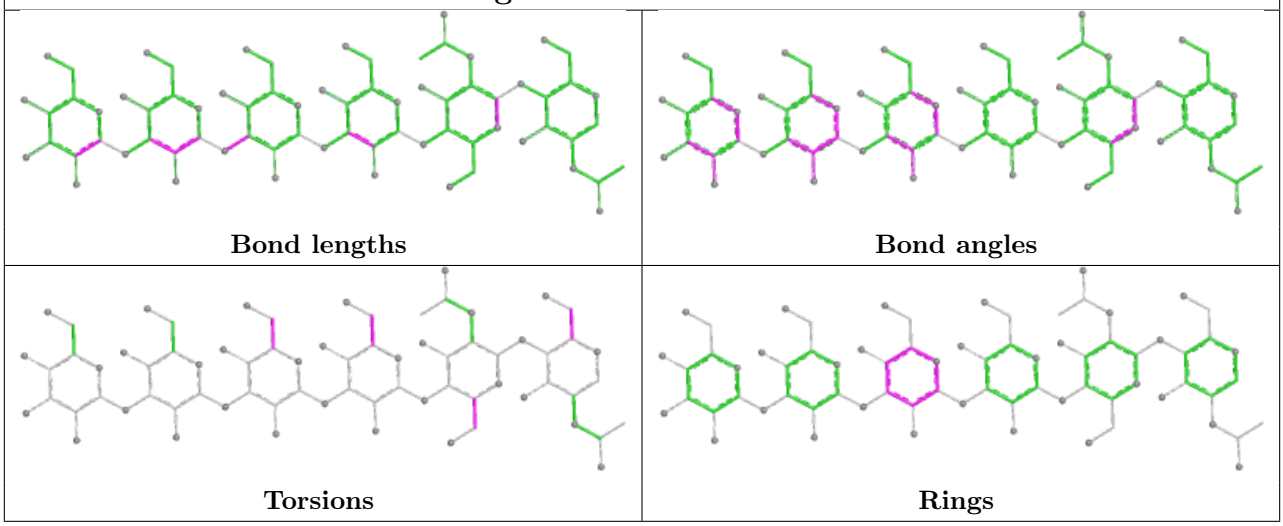


Rings

Oligosaccharide Chain J



Oligosaccharide Chain G



5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	NAG	B	706	2	14,14,15	0.33	0	17,19,21	0.56	0
10	NAG	A	1016	1	14,14,15	0.42	0	17,19,21	0.48	0
12	NO3	A	1030	-	1,3,3	3.21	1 (100%)	0,3,3	-	-
12	NO3	A	1029	-	1,3,3	3.36	1 (100%)	0,3,3	-	-
10	NAG	B	701	2	14,14,15	0.42	0	17,19,21	0.75	1 (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
10	NAG	B	706	2	-	0/6/23/26	0/1/1/1
10	NAG	A	1016	1	-	4/6/23/26	0/1/1/1
10	NAG	B	701	2	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	1029	NO3	O1-N	3.36	1.40	1.24
12	A	1030	NO3	O1-N	3.21	1.40	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	701	NAG	C1-O5-C5	2.73	115.85	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	1016	NAG	O5-C5-C6-O6
10	A	1016	NAG	C4-C5-C6-O6
10	B	701	NAG	C4-C5-C6-O6
10	B	701	NAG	O5-C5-C6-O6
10	A	1016	NAG	C3-C2-N2-C7
10	A	1016	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	915/962 (95%)	-0.02	46 (5%)	28	18	52, 165, 260, 296	0
2	B	687/692 (99%)	-0.10	35 (5%)	28	17	55, 145, 303, 428	0
3	L	214/214 (100%)	-0.36	2 (0%)	84	73	71, 127, 234, 297	0
4	H	218/218 (100%)	-0.08	7 (3%)	47	32	81, 154, 242, 329	0
All	All	2034/2086 (97%)	-0.09	90 (4%)	34	21	52, 149, 274, 428	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	515	LYS	10.5
2	B	678	ILE	9.7
2	B	670	TYR	9.3
2	B	650	LYS	9.2
4	H	133	CYS	9.0
1	A	683	LEU	8.9
1	A	454	LEU	7.7
2	B	672	ASP	7.4
4	H	131	PRO	7.4
2	B	651	ASP	7.4
1	A	452	SER	6.4
2	B	673	SER	6.2
1	A	455	ASN	6.2
1	A	822	CYS	6.1
2	B	668	GLN	6.1
4	H	130	ALA	5.9
2	B	638	GLU	5.9
2	B	669	TYR	5.7
4	H	132	VAL	5.5
2	B	639	ILE	5.3
2	B	659	ASN	5.3

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Mol	Chain	Res	Type	RSRZ
2	B	516	ILE	5.0
1	A	824	SER	4.8
1	A	739	LEU	4.6
2	B	677	SER	4.6
1	A	453	ILE	4.6
1	A	936	LEU	4.5
1	A	684	GLY	4.5
2	B	652	ALA	4.5
2	B	675	GLY	4.5
1	A	511	ALA	4.4
3	L	131	SER	4.3
2	B	649	GLY	4.2
1	A	937	PRO	4.1
1	A	917	SER	4.1
1	A	915	ASN	4.1
2	B	679	LEU	3.9
2	B	36	PRO	3.8
2	B	641	SER	3.8
2	B	648	THR	3.7
3	L	130	ALA	3.6
1	A	446	GLY	3.6
2	B	674	SER	3.6
1	A	682	ASP	3.5
4	H	124	PRO	3.5
1	A	667	SER	3.5
1	A	451	PRO	3.3
1	A	483	GLY	3.3
2	B	474	SER	3.3
2	B	602	PRO	3.2
1	A	935	ASN	3.2
1	A	543	ARG	3.2
1	A	945	THR	3.2
1	A	939	GLU	3.2
4	H	197	SER	3.2
1	A	916	HIS	3.1
1	A	445	ALA	3.0
1	A	774	PRO	2.9
1	A	681	CYS	2.9
1	A	507	ALA	2.9
1	A	601	VAL	2.9
4	H	134	GLY	2.8
2	B	642	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	447	LEU	2.8
1	A	737	ALA	2.7
2	B	643	LYS	2.7
2	B	640	GLU	2.6
1	A	900	LYS	2.6
1	A	592	ILE	2.6
2	B	676	LYS	2.5
1	A	884	CYS	2.5
1	A	590	ALA	2.5
1	A	740	ALA	2.5
2	B	475	GLU	2.5
1	A	465	GLY	2.4
1	A	662	ALA	2.4
1	A	591	HIS	2.4
2	B	39	ASP	2.4
1	A	738	VAL	2.4
2	B	514	GLY	2.3
1	A	493	PHE	2.2
2	B	671	GLU	2.2
1	A	731	SER	2.2
1	A	918	TYR	2.2
1	A	788	SER	2.2
1	A	762	HIS	2.1
1	A	669	ALA	2.1
2	B	33	LEU	2.1
2	B	215	ASN	2.1
2	B	624	ALA	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
6	BMA	D	3	11/12	0.61	0.23	223,233,237,238	0

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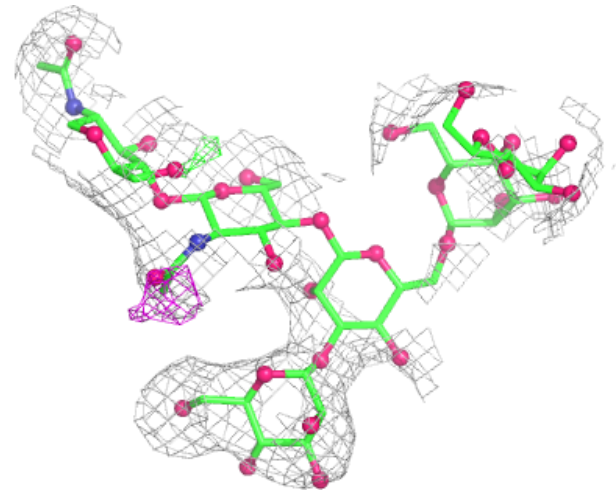
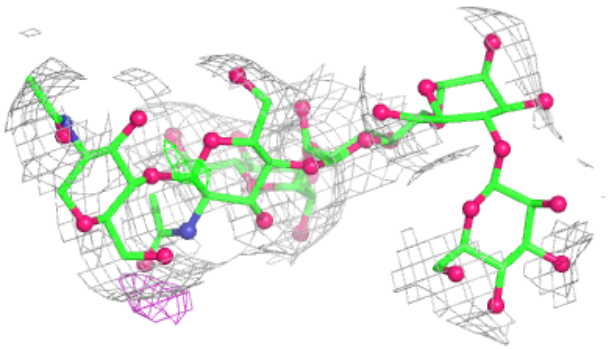
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MAN	C	6	11/12	0.67	0.29	184,196,205,209	0
9	BMA	G	3	11/12	0.75	0.20	225,229,266,267	0
9	MAN	G	6	11/12	0.75	0.18	229,231,239,245	0
5	BMA	C	3	11/12	0.80	0.16	161,174,187,190	0
9	MAN	G	4	11/12	0.80	0.18	253,259,264,264	0
8	NAG	J	2	14/15	0.80	0.16	175,184,186,188	0
9	MAN	G	5	11/12	0.81	0.24	242,256,261,263	0
9	NAG	G	1	14/15	0.81	0.16	170,191,197,202	0
6	NAG	D	2	14/15	0.82	0.22	198,212,220,228	0
5	MAN	C	4	11/12	0.84	0.14	172,188,221,223	0
7	MAN	E	5	11/12	0.86	0.18	170,178,183,185	0
9	NAG	G	2	14/15	0.86	0.14	207,215,221,224	0
7	MAN	E	4	11/12	0.86	0.16	147,158,173,174	0
8	NAG	F	1	14/15	0.87	0.18	146,165,175,177	0
8	NAG	I	2	14/15	0.88	0.20	139,147,159,160	0
5	NAG	C	2	14/15	0.89	0.21	110,131,145,149	0
6	NAG	D	1	14/15	0.89	0.13	132,150,165,181	0
7	MAN	E	6	11/12	0.89	0.13	150,152,158,164	0
5	BMA	C	5	11/12	0.90	0.10	212,215,218,219	0
8	NAG	F	2	14/15	0.91	0.19	178,183,190,192	0
8	NAG	J	1	14/15	0.92	0.11	104,130,146,163	0
7	BMA	E	3	11/12	0.93	0.14	112,127,139,141	0
7	NAG	E	1	14/15	0.93	0.19	73,83,91,95	0
8	NAG	I	1	14/15	0.93	0.23	101,128,141,146	0
5	NAG	C	1	14/15	0.94	0.20	57,77,88,91	0
7	NAG	E	2	14/15	0.96	0.17	66,95,109,116	0

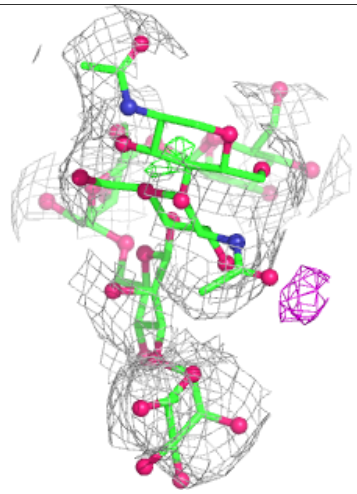
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

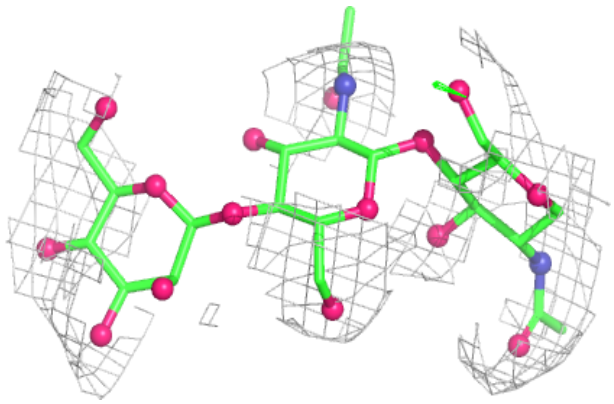


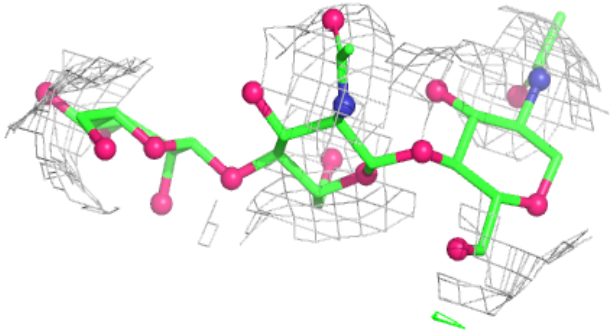


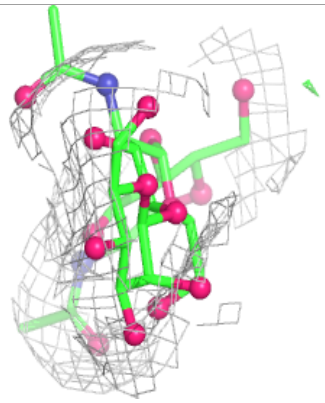


Electron density around Chain D:

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

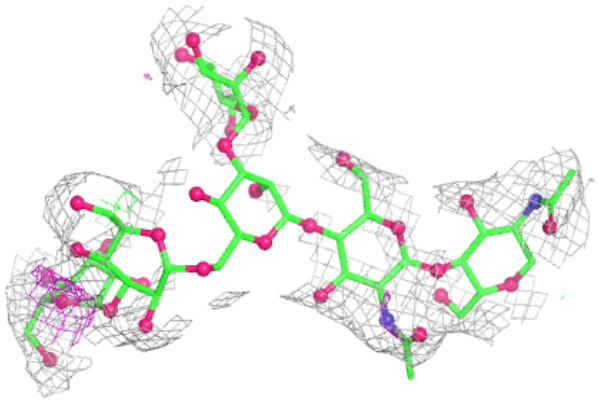


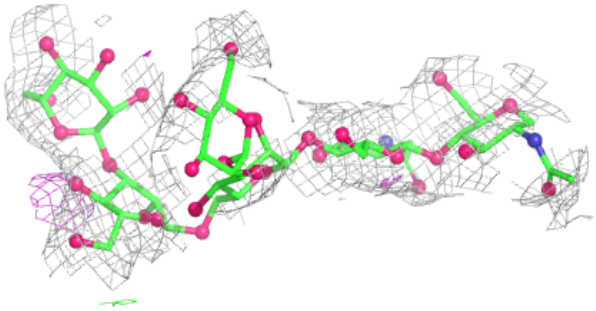


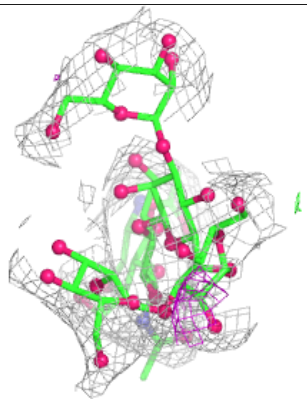


Electron density around Chain E:

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

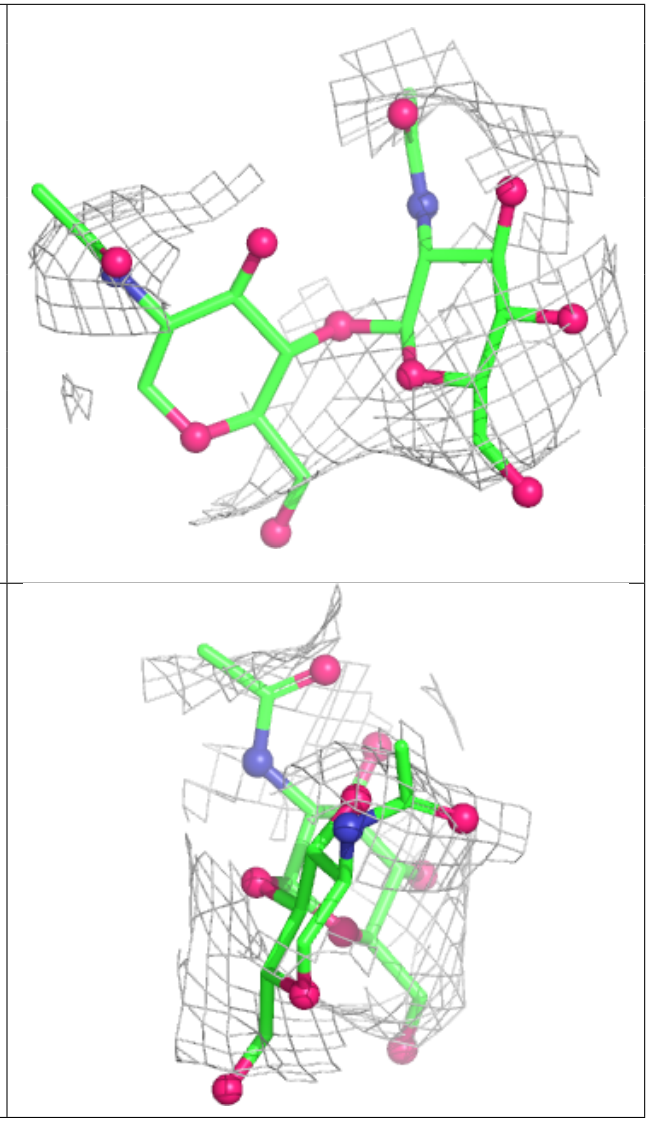






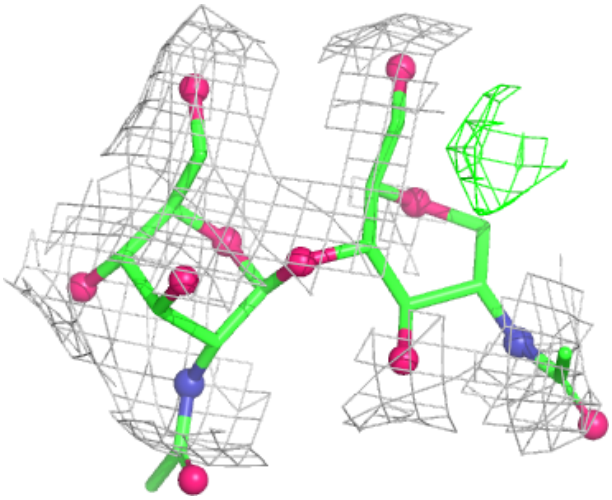
Electron density around Chain F:

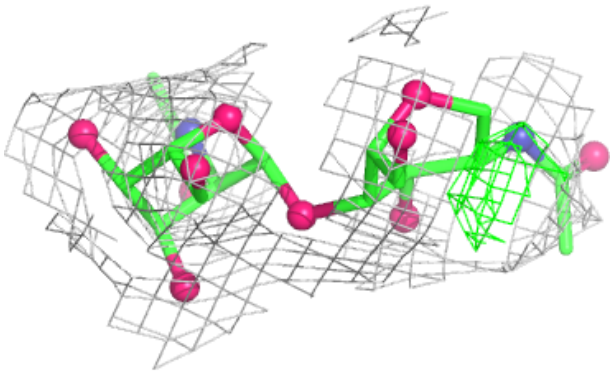
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

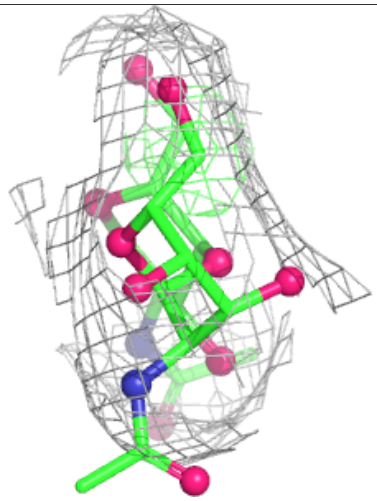


Electron density around Chain I:

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

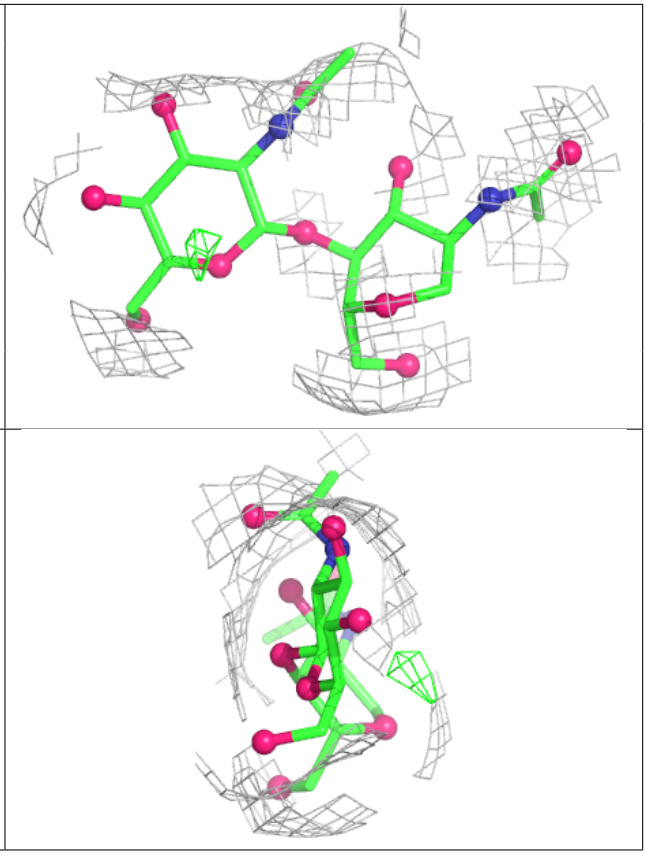






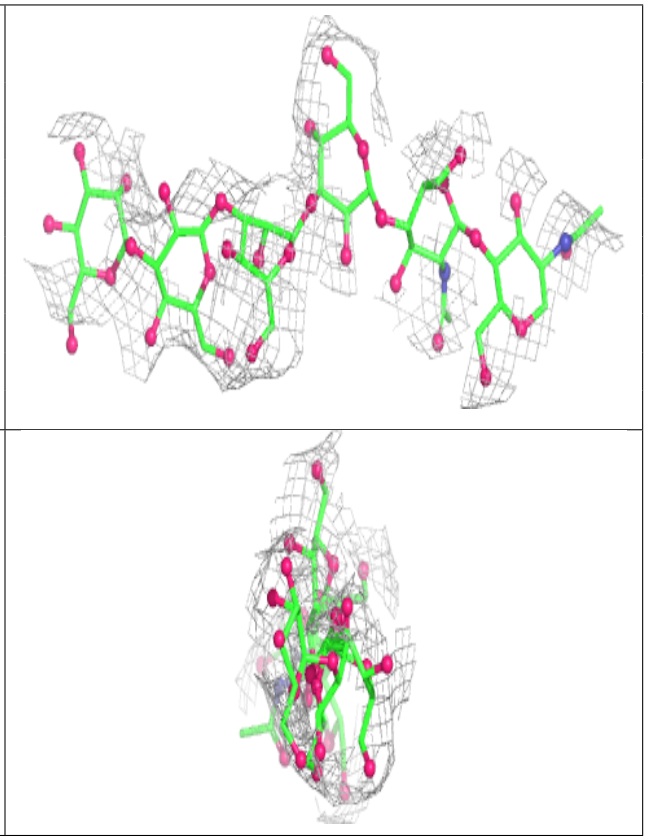
Electron density around Chain J:

$2mF_o$-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 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(Å^2)	Q<0.9
10	NAG	A	1016	14/15	0.51	0.38	190,203,212,212	0
11	MN	A	1027	1/1	0.75	0.16	187,187,187,187	0
11	MN	B	707	1/1	0.78	0.16	271,271,271,271	0
11	MN	A	1025	1/1	0.84	0.06	241,241,241,241	0
10	NAG	B	706	14/15	0.85	0.18	145,154,161,162	0
10	NAG	B	701	14/15	0.89	0.16	120,143,162,168	0
12	NO3	A	1029	4/4	0.94	0.30	95,98,100,103	0
11	MN	A	1026	1/1	0.96	0.07	181,181,181,181	0
12	NO3	A	1030	4/4	0.96	0.26	81,83,84,87	0
11	MN	A	1028	1/1	0.98	0.25	169,169,169,169	0

6.5 Other polymers (i)

There are no such residues in this entry.