Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 05:03 PM EDT

PDB ID	:	6MSL
Title	:	Integrin AlphaVBeta3 ectodomain bound to EETI-II 2.5D
Authors	:	van Agthoven, J.F.; Arnaout, M.A.
Deposited on	:	2018-10-16
Resolution	:	3.10 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:

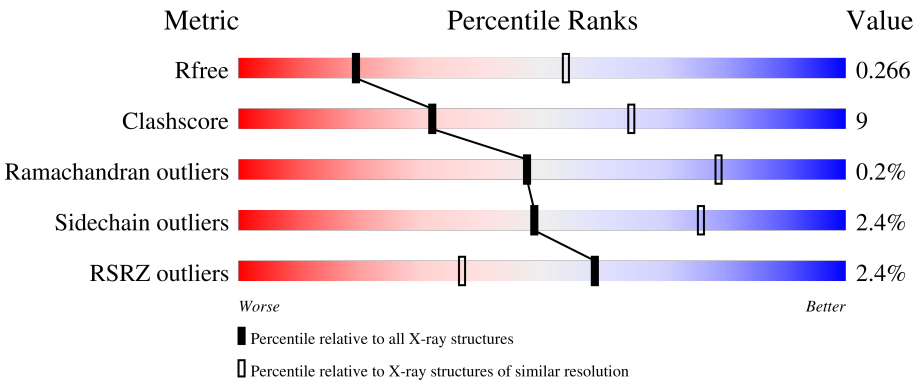
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	967	76% 19% • •
2	B	695	4% 76% 22% ••
3	C	32	34% 72% 28%
4	D	4	50% 50%
4	G	4	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	2	50% 50%
5	H	2	100%
5	I	2	50% 50%
5	J	2	50% 50%
5	K	2	50% 50%
6	F	6	33% 17% 50%
7	L	3	33% 67%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	E	2	-	-	-	X
8	NAG	B	701	-	-	-	X
9	MN	B	710	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 13129 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	924	7196	4556	1221	1384	35	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	690	5294	3250	904	1070	70	0	0	0

- Molecule 3 is a protein called Cystine Knot Protein 2.5D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	32	220	130	40	44	6	0	0	0

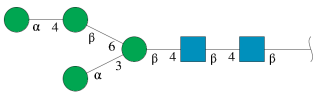
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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

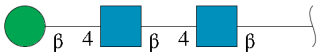
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	E	2	28	16	2	10	0	0	0
5	H	2	28	16	2	10	0	0	0
5	I	2	28	16	2	10	0	0	0
5	J	2	28	16	2	10	0	0	0
5	K	2	28	16	2	10	0	0	0

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-beta-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.



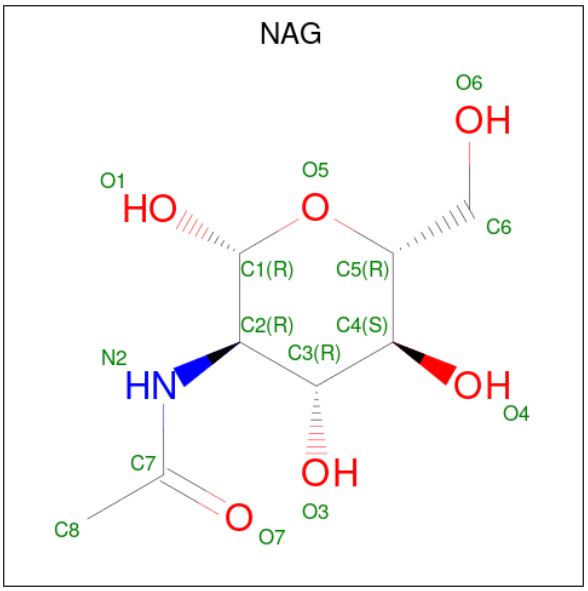
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
6	F	6	72	40	2	30	0	0	0

- Molecule 7 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			
7	L	3	39	22	2	15	0	0	0

- Molecule 8 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		
8	A	1	14	8	1	5	0	0
			Total	C	N	O		
8	A	1	14	8	1	5	0	0
			Total	C	N	O		
8	B	1	14	8	1	5	0	0
			Total	C	N	O		
8	B	1	14	8	1	5	0	0

- Molecule 9 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
9	A	5	5	5	0	0
			Total	Mn		
9	B	3	3	3	0	0

- Molecule 10 is water.

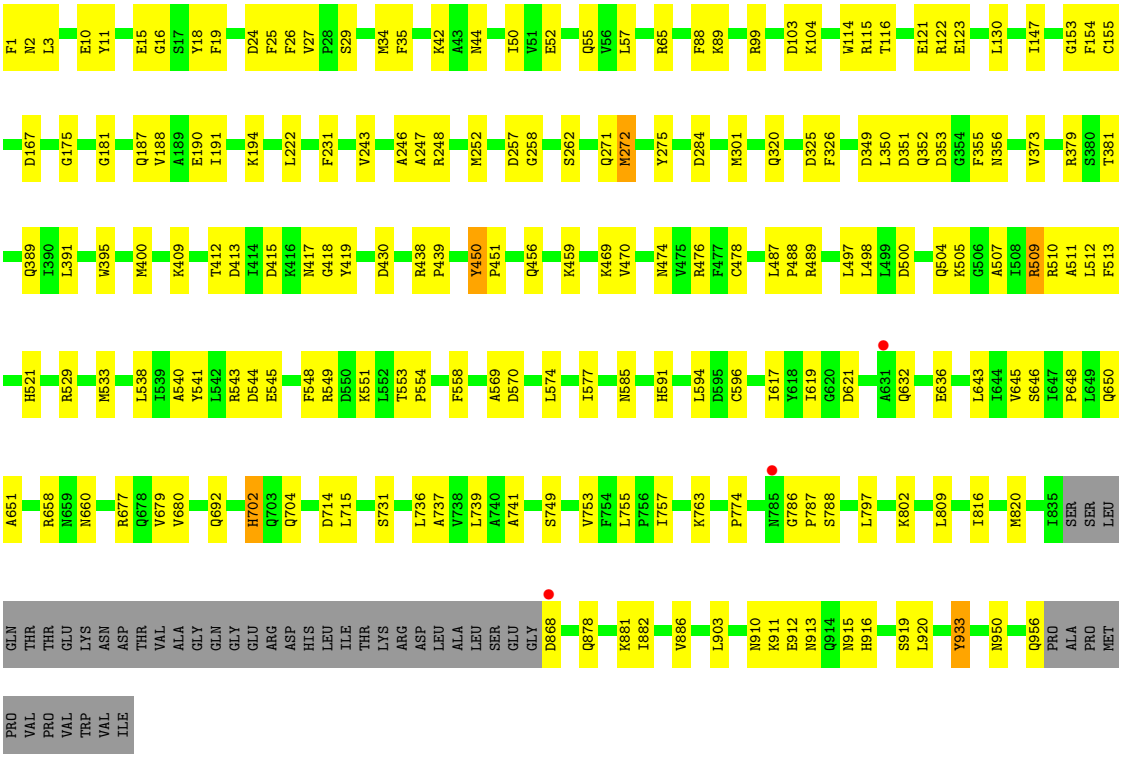
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	1	1	1	0	0
			Total	O		
10	B	3	3	3	0	0

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.

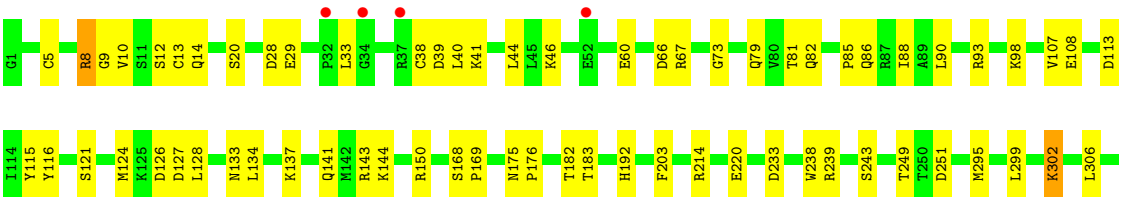
• Molecule 1: Integrin alpha-V

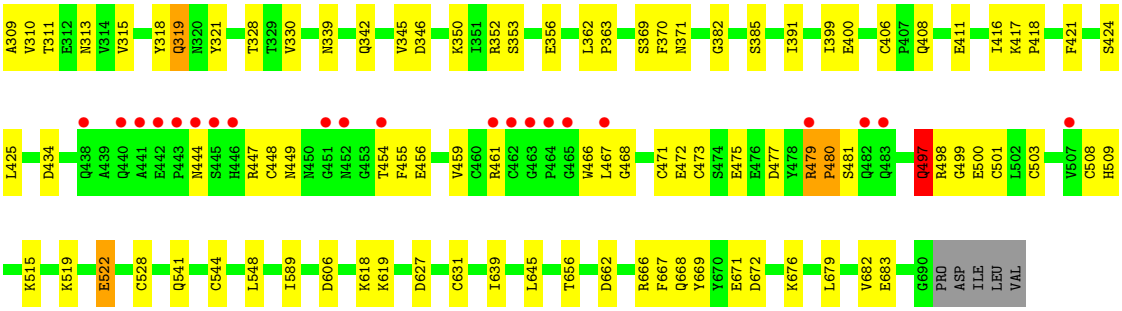
Chain A:



• Molecule 2: Integrin beta-3

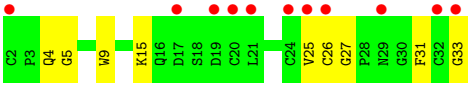
Chain B:





• Molecule 3: Cystine Knot Protein 2.5D

Chain C: 34% 72% 28%



• Molecule 4: 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 D: 50% 50%

• Molecule 4: 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: 100%

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

Chain E: 50% 50%

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

Chain H: 100%

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

Chain I:

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

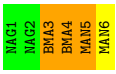
Chain J:

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

Chain K:

• Molecule 6: alpha-D-mannopyranose-(1-4)-beta-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 F:



• Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.76Å 129.76Å 305.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.21 – 3.10 49.47 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.7 (49.21-3.10) 89.7 (49.47-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.222 , 0.266 0.222 , 0.266	Depositor DCC
R_{free} test set	2601 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13129	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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, 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	0.35	0/7352	0.55	0/9967
2	B	0.35	0/5390	0.55	0/7289
3	C	0.34	0/225	0.58	0/304
All	All	0.35	0/12967	0.55	0/17560

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	1
2	B	0	2
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	450	TYR	Peptide
2	B	479	ARG	Peptide
2	B	497	GLN	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	7196	0	7014	117	0
2	B	5294	0	5024	107	0
3	C	220	0	188	5	0
4	D	50	0	43	0	0
4	G	50	0	43	1	0
5	E	28	0	25	2	0
5	H	28	0	25	0	0
5	I	28	0	25	0	0
5	J	28	0	25	0	0
5	K	28	0	25	1	0
6	F	72	0	61	2	0
7	L	39	0	34	0	0
8	A	28	0	26	0	0
8	B	28	0	26	2	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
10	A	1	0	0	0	0
10	B	3	0	0	0	0
All	All	13129	0	12584	228	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 9.

All (228) 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)
2:B:39:ASP:HB3	2:B:44:LEU:HD12	1.63	0.79
2:B:10:VAL:HG21	2:B:519:LYS:HD2	1.65	0.78
3:C:25:VAL:HG12	3:C:33:GLY:HA2	1.67	0.75
2:B:8:ARG:NH1	2:B:544:CYS:SG	2.61	0.74
2:B:121:SER:CB	2:B:220:GLU:OE1	2.35	0.74
2:B:233:ASP:OD2	2:B:302:LYS:NZ	2.19	0.71
1:A:510:ARG:NH2	1:A:553:THR:O	2.14	0.71
2:B:447:ARG:HB3	2:B:455:PHE:HE2	1.55	0.71
2:B:417:LYS:NZ	2:B:421:PHE:O	2.21	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:GLU:HG3	2:B:385:SER:HB3	1.74	0.69
2:B:449:ASN:ND2	2:B:471:CYS:SG	2.62	0.68
2:B:479:ARG:O	2:B:481:SER:N	2.28	0.67
2:B:645:LEU:HB2	2:B:682:VAL:HG22	1.77	0.67
1:A:415:ASP:OD1	1:A:417:ASN:OD1	2.13	0.66
1:A:741:ALA:H	1:A:786:GLY:HA3	1.60	0.66
1:A:121:GLU:HA	2:B:168:SER:HB2	1.77	0.65
3:C:26:CYS:SG	3:C:27:GLY:N	2.69	0.65
1:A:248:ARG:NH1	1:A:272:MET:SD	2.70	0.64
2:B:168:SER:OG	2:B:169:PRO:HD3	1.96	0.64
2:B:417:LYS:NZ	2:B:418:PRO:O	2.31	0.64
2:B:479:ARG:HB3	2:B:480:PRO:HD3	1.80	0.64
1:A:27:VAL:HG12	1:A:34:MET:HG2	1.81	0.63
2:B:447:ARG:HG3	2:B:456:GLU:OE2	1.98	0.63
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.81	0.63
1:A:651:ALA:O	1:A:677:ARG:NH2	2.31	0.63
1:A:487:LEU:O	1:A:529:ARG:NH2	2.32	0.63
2:B:656:THR:HG22	2:B:666:ARG:HG3	1.81	0.63
1:A:498:LEU:HD23	1:A:558:PHE:HD2	1.64	0.62
1:A:50:ILE:HD12	1:A:89:LYS:HB2	1.80	0.62
1:A:130:LEU:HD21	1:A:188:VAL:HG13	1.81	0.62
2:B:28:ASP:OD1	2:B:29:GLU:N	2.30	0.62
2:B:150:ARG:HE	2:B:239:ARG:HD3	1.65	0.62
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.81	0.62
1:A:757:ILE:HD13	1:A:774:PRO:HD3	1.82	0.62
1:A:505:LYS:HG2	2:B:509:HIS:HB2	1.82	0.61
1:A:915:ASN:ND2	1:A:956:GLN:O	2.33	0.61
2:B:39:ASP:O	2:B:44:LEU:HD13	2.01	0.61
2:B:249:THR:HA	2:B:309:ALA:O	2.01	0.61
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.84	0.60
2:B:175:ASN:HD21	2:B:183:THR:HA	1.68	0.59
1:A:114:TRP:HZ3	1:A:147:ILE:HG21	1.67	0.59
1:A:478:CYS:HB3	1:A:533:MET:HG3	1.83	0.59
1:A:271:GLN:NE2	1:A:301:MET:O	2.35	0.59
1:A:25:PHE:CD2	1:A:412:THR:HB	2.38	0.59
1:A:147:ILE:HD12	1:A:147:ILE:O	2.03	0.58
2:B:39:ASP:HB3	2:B:44:LEU:CD1	2.32	0.58
2:B:133:ASN:O	2:B:137:LYS:HG2	2.04	0.58
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.38	0.57
1:A:243:VAL:HG22	1:A:246:ALA:HB2	1.85	0.57
1:A:154:PHE:O	1:A:175:GLY:HA3	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:5:CYS:HB3	2:B:38:CYS:O	2.06	0.56
2:B:79:GLN:NE2	2:B:81:THR:OG1	2.33	0.56
2:B:369:SER:HB2	2:B:400:GLU:HB3	1.88	0.56
2:B:417:LYS:HG3	2:B:424:SER:HB3	1.88	0.56
2:B:339:ASN:ND2	2:B:342:GLN:OE1	2.39	0.56
2:B:669:TYR:HB3	2:B:679:LEU:HD13	1.88	0.55
1:A:352:GLN:NE2	1:A:418:GLY:O	2.36	0.55
2:B:589:ILE:HD12	2:B:589:ILE:O	2.06	0.55
1:A:413:ASP:OD1	1:A:415:ASP:OD1	2.24	0.55
2:B:311:THR:HB	2:B:313:ASN:OD1	2.07	0.54
1:A:19:PHE:HE2	1:A:57:LEU:HD12	1.72	0.54
1:A:820:MET:HG3	1:A:886:VAL:HG22	1.88	0.54
1:A:24:ASP:OD1	1:A:25:PHE:N	2.39	0.54
1:A:816:ILE:HG21	1:A:820:MET:HB3	1.90	0.54
1:A:44:ASN:O	1:A:55:GLN:NE2	2.40	0.53
2:B:447:ARG:HB3	2:B:455:PHE:CE2	2.40	0.53
1:A:500:ASP:OD2	1:A:510:ARG:HD3	2.09	0.53
1:A:450:TYR:CD2	1:A:474:ASN:HB2	2.44	0.53
1:A:646:SER:OG	1:A:714:ASP:HB2	2.08	0.53
2:B:444:ASN:HB2	2:B:454:THR:HG23	1.90	0.53
2:B:115:TYR:OH	2:B:192:HIS:ND1	2.33	0.53
2:B:182:THR:HG22	2:B:183:THR:H	1.74	0.53
1:A:18:TYR:CE2	1:A:42:LYS:HD2	2.43	0.53
5:E:1:NAG:H3	5:E:1:NAG:H83	1.91	0.53
1:A:116:THR:HG21	1:A:147:ILE:HD13	1.91	0.53
1:A:658:ARG:NH2	2:B:528:CYS:O	2.42	0.53
1:A:262:SER:HB2	5:E:1:NAG:H82	1.91	0.53
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.91	0.53
1:A:558:PHE:HZ	1:A:585:ASN:HD22	1.57	0.53
2:B:481:SER:HB2	2:B:501:CYS:SG	2.49	0.53
2:B:362:LEU:HD12	2:B:363:PRO:HD2	1.90	0.52
1:A:247:ALA:O	1:A:248:ARG:HG2	2.08	0.52
2:B:391:ILE:HD12	2:B:391:ILE:H	1.73	0.52
1:A:325:ASP:OD1	1:A:326:PHE:N	2.42	0.52
1:A:911:LYS:C	1:A:913:ASN:H	2.11	0.52
2:B:339:ASN:HB3	2:B:342:GLN:HB2	1.93	0.51
2:B:606:ASP:N	2:B:606:ASP:OD1	2.42	0.51
2:B:667:PHE:CD2	2:B:679:LEU:HD11	2.45	0.51
1:A:438:ARG:HH11	1:A:577:ILE:HB	1.75	0.51
2:B:82:GLN:HG2	2:B:107:VAL:HG13	1.93	0.51
1:A:549:ARG:NH1	2:B:500:GLU:OE2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:MET:O	2:B:128:LEU:HD13	2.11	0.51
1:A:648:PRO:O	1:A:677:ARG:NH2	2.41	0.51
1:A:104:LYS:HB3	1:A:130:LEU:HD11	1.93	0.51
1:A:913:ASN:HB3	1:A:916:HIS:ND1	2.26	0.51
1:A:459:LYS:HB3	1:A:469:LYS:O	2.11	0.50
2:B:541:GLN:HE21	2:B:548:LEU:HD12	1.77	0.50
1:A:645:VAL:HG22	1:A:715:LEU:HD13	1.92	0.50
2:B:466:TRP:O	2:B:473:CYS:HB2	2.10	0.50
2:B:66:ASP:HB3	2:B:85:PRO:HB3	1.94	0.50
1:A:42:LYS:NZ	1:A:52:GLU:OE1	2.44	0.50
1:A:351:ASP:OD1	1:A:351:ASP:N	2.42	0.50
2:B:126:ASP:OD1	2:B:127:ASP:OD1	2.30	0.50
1:A:521:HIS:ND1	1:A:538:LEU:HD11	2.27	0.50
2:B:408:GLN:NE2	2:B:434:ASP:OD2	2.44	0.50
2:B:455:PHE:HB2	2:B:459:VAL:O	2.12	0.50
2:B:497:GLN:OE1	2:B:497:GLN:N	2.45	0.49
2:B:306:LEU:HB3	2:B:328:THR:HG22	1.94	0.49
2:B:666:ARG:O	2:B:682:VAL:HG23	2.13	0.49
1:A:596:CYS:C	1:A:636:GLU:OE1	2.49	0.49
3:C:4:GLN:HG2	3:C:9:TRP:CH2	2.48	0.49
2:B:121:SER:HB2	2:B:220:GLU:OE1	2.07	0.49
2:B:134:LEU:HB3	2:B:203:PHE:HE1	1.77	0.49
1:A:913:ASN:HB3	1:A:916:HIS:CG	2.48	0.49
2:B:88:ILE:HG13	2:B:425:LEU:HD11	1.94	0.49
1:A:569:ALA:HB3	1:A:574:LEU:HB3	1.94	0.48
2:B:150:ARG:NE	2:B:239:ARG:HD3	2.26	0.48
2:B:475:GLU:OE1	2:B:475:GLU:N	2.43	0.48
1:A:349:ASP:OD1	1:A:355:PHE:O	2.32	0.48
1:A:621:ASP:HB2	1:A:787:PRO:HB3	1.96	0.48
1:A:456:GLN:HB3	1:A:545:GLU:HG2	1.96	0.48
1:A:650:GLN:HE21	1:A:704:GLN:H	1.61	0.48
1:A:645:VAL:HB	1:A:679:VAL:HB	1.96	0.48
1:A:99:ARG:HA	1:A:99:ARG:HD3	1.62	0.48
2:B:671:GLU:HG3	2:B:672:ASP:H	1.79	0.48
1:A:487:LEU:HB3	1:A:529:ARG:HH21	1.79	0.47
1:A:510:ARG:HG2	1:A:548:PHE:CD2	2.49	0.47
1:A:788:SER:HB3	1:A:933:TYR:HE2	1.79	0.47
2:B:477:ASP:HB3	2:B:479:ARG:HG3	1.96	0.47
1:A:2:ASN:OD1	1:A:2:ASN:N	2.46	0.47
1:A:881:LYS:HE2	1:A:881:LYS:HB3	1.68	0.47
2:B:295:MET:O	2:B:299:LEU:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ALA:HB2	1:A:252:MET:HE2	1.97	0.47
1:A:919:SER:OG	1:A:950:ASN:OD1	2.18	0.47
1:A:284:ASP:O	1:A:356:ASN:HB2	2.14	0.47
1:A:167:ASP:O	1:A:188:VAL:HG23	2.14	0.47
1:A:554:PRO:HB3	1:A:591:HIS:CD2	2.51	0.46
1:A:498:LEU:HB2	1:A:558:PHE:HB3	1.96	0.46
2:B:176:PRO:HB2	2:B:214:ARG:HB3	1.96	0.46
2:B:447:ARG:HA	2:B:447:ARG:HD3	1.61	0.46
1:A:739:LEU:O	1:A:787:PRO:HD2	2.15	0.46
1:A:26:PHE:HB3	1:A:35:PHE:HB2	1.97	0.46
2:B:299:LEU:HD21	2:B:306:LEU:HB2	1.97	0.46
1:A:379:ARG:NE	1:A:381:THR:OG1	2.48	0.45
1:A:248:ARG:HD2	8:B:702:NAG:H2	1.99	0.45
2:B:144:LYS:HE2	2:B:345:VAL:HG21	1.97	0.45
1:A:231:PHE:HA	1:A:320:GLN:HE22	1.82	0.45
1:A:868:ASP:OD1	1:A:868:ASP:N	2.49	0.45
1:A:123:GLU:HB3	1:A:153:GLY:O	2.17	0.45
1:A:643:LEU:O	1:A:680:VAL:HA	2.17	0.45
2:B:481:SER:O	2:B:481:SER:OG	2.34	0.45
2:B:113:ASP:OD1	2:B:239:ARG:NH2	2.49	0.45
2:B:318:TYR:HA	2:B:321:TYR:HB2	1.99	0.45
1:A:450:TYR:HB3	1:A:451:PRO:HD3	1.98	0.45
1:A:632:GLN:HB3	1:A:692:GLN:HG2	1.98	0.45
1:A:809:LEU:HG	1:A:920:LEU:HD13	1.99	0.45
1:A:788:SER:HB3	1:A:933:TYR:CE2	2.52	0.44
2:B:667:PHE:HD2	2:B:679:LEU:HD11	1.81	0.44
1:A:802:LYS:HB2	1:A:878:GLN:HB3	2.00	0.44
2:B:9:GLY:HA3	2:B:38:CYS:SG	2.58	0.44
2:B:20:SER:O	2:B:93:ARG:NH2	2.51	0.44
2:B:399:ILE:HD13	2:B:416:ILE:HD13	2.00	0.44
2:B:682:VAL:HG12	2:B:683:GLU:O	2.17	0.44
1:A:349:ASP:OD1	1:A:353:ASP:OD1	2.35	0.44
2:B:645:LEU:HD11	2:B:668:GLN:HG2	1.98	0.44
1:A:507:ALA:O	1:A:509:ARG:NH1	2.50	0.44
2:B:618:LYS:HG2	2:B:631:CYS:SG	2.58	0.44
2:B:39:ASP:C	2:B:44:LEU:HD13	2.38	0.44
2:B:627:ASP:N	2:B:627:ASP:OD1	2.50	0.44
1:A:617:ILE:HG13	1:A:736:LEU:HD23	2.00	0.43
2:B:73:GLY:N	2:B:108:GLU:O	2.51	0.43
1:A:470:VAL:HG11	1:A:541:TYR:CD2	2.53	0.43
1:A:551:LYS:HB2	1:A:594:LEU:HD22	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ASP:OD1	2:B:40:LEU:N	2.45	0.43
2:B:461:ARG:HG3	2:B:467:LEU:HG	2.00	0.43
6:F:3:BMA:H62	6:F:4:BMA:H2	1.54	0.43
1:A:797:LEU:HB3	1:A:882:ILE:HB	1.99	0.43
1:A:11:TYR:CE2	1:A:65:ARG:HD3	2.54	0.43
2:B:468:GLY:HA2	2:B:473:CYS:SG	2.59	0.43
1:A:3:LEU:HG	1:A:350:LEU:HD21	2.00	0.43
1:A:513:PHE:HA	1:A:540:ALA:HA	1.99	0.43
2:B:126:ASP:HA	3:C:31:PHE:CE2	2.54	0.43
2:B:175:ASN:ND2	2:B:183:THR:HG23	2.33	0.43
2:B:522:GLU:H	2:B:522:GLU:CD	2.21	0.43
1:A:181:GLY:HA3	1:A:222:LEU:HB3	2.00	0.43
1:A:187:GLN:O	1:A:191:ILE:HG13	2.18	0.43
1:A:487:LEU:HB3	1:A:529:ARG:NH2	2.34	0.42
2:B:471:CYS:SG	2:B:472:GLU:N	2.92	0.42
1:A:10:GLU:CD	1:A:395:TRP:HZ2	2.22	0.42
2:B:619:LYS:HE3	2:B:639:ILE:HG22	2.01	0.42
2:B:350:LYS:O	2:B:353:SER:OG	2.35	0.42
2:B:371:ASN:HD22	5:K:1:NAG:C7	2.33	0.42
1:A:497:LEU:O	1:A:498:LEU:HD13	2.19	0.42
1:A:548:PHE:HD2	1:A:549:ARG:H	1.64	0.42
1:A:910:ASN:C	1:A:912:GLU:H	2.22	0.42
2:B:299:LEU:HD12	2:B:299:LEU:HA	1.90	0.42
1:A:16:GLY:N	1:A:430:ASP:OD2	2.48	0.42
1:A:543:ARG:HB2	1:A:548:PHE:HD1	1.85	0.42
2:B:67:ARG:HB2	2:B:86:GLN:HE22	1.85	0.41
1:A:248:ARG:HD2	8:B:702:NAG:O7	2.20	0.41
1:A:753:VAL:HG11	1:A:903:LEU:HD22	2.01	0.41
1:A:511:ALA:O	1:A:512:LEU:HD23	2.21	0.41
1:A:257:ASP:OD1	1:A:258:GLY:N	2.54	0.41
2:B:60:GLU:HA	2:B:98:LYS:HE3	2.01	0.41
2:B:233:ASP:HB3	2:B:238:TRP:HD1	1.85	0.41
2:B:499:GLY:HA3	2:B:508:CYS:HB2	2.01	0.41
2:B:672:ASP:HA	2:B:676:LYS:O	2.21	0.41
1:A:190:GLU:O	1:A:194:LYS:HB2	2.20	0.41
2:B:12:SER:OG	2:B:13:CYS:N	2.54	0.41
6:F:4:BMA:H4	6:F:5:MAN:H2	1.40	0.41
1:A:650:GLN:HB3	1:A:702:HIS:O	2.21	0.41
2:B:243:SER:OG	2:B:352:ARG:NH2	2.52	0.41
1:A:15:GLU:HA	1:A:430:ASP:OD2	2.21	0.41
1:A:487:LEU:HD12	1:A:488:PRO:HD2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:LEU:HD23	1:A:757:ILE:HG13	2.02	0.41
2:B:310:VAL:HG23	2:B:315:VAL:HG22	2.03	0.41
2:B:370:PHE:O	2:B:382:GLY:N	2.53	0.41
3:C:5:GLY:HA3	3:C:9:TRP:CD1	2.55	0.41
1:A:619:ILE:HG13	1:A:737:ALA:O	2.21	0.41
2:B:141:GLN:HG3	2:B:345:VAL:HG11	2.02	0.41
1:A:29:SER:OG	1:A:103:ASP:OD2	2.31	0.40
1:A:714:ASP:OD2	1:A:731:SER:OG	2.39	0.40
2:B:444:ASN:O	2:B:454:THR:OG1	2.28	0.40
2:B:141:GLN:HG2	2:B:342:GLN:HA	2.04	0.40
4:G:1:NAG:O6	4:G:2:NAG:O7	2.39	0.40
1:A:88:PHE:CE1	1:A:122:ARG:HG2	2.57	0.40
2:B:33:LEU:HD12	2:B:33:LEU:HA	1.90	0.40
2:B:479:ARG:HB3	2:B:480:PRO:CD	2.50	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	920/967 (95%)	838 (91%)	82 (9%)	0	100	100
2	B	688/695 (99%)	605 (88%)	79 (12%)	4 (1%)	25	59
3	C	30/32 (94%)	17 (57%)	13 (43%)	0	100	100
All	All	1638/1694 (97%)	1460 (89%)	174 (11%)	4 (0%)	47	79

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	448	CYS
2	B	480	PRO
2	B	497	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	498	ARG

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	784/821 (96%)	768 (98%)	16 (2%)	55	80
2	B	612/617 (99%)	595 (97%)	17 (3%)	43	73
3	C	24/24 (100%)	23 (96%)	1 (4%)	30	62
All	All	1420/1462 (97%)	1386 (98%)	34 (2%)	49	76

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	ARG
1	A	155	CYS
1	A	272	MET
1	A	275	TYR
1	A	400	MET
1	A	476	ARG
1	A	489	ARG
1	A	504	GLN
1	A	509	ARG
1	A	544	ASP
1	A	570	ASP
1	A	660	ASN
1	A	702	HIS
1	A	749	SER
1	A	763	LYS
1	A	933	TYR
2	B	8	ARG
2	B	14	GLN
2	B	41	LYS
2	B	46	LYS
2	B	90	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	116	TYR
2	B	143	ARG
2	B	251	ASP
2	B	302	LYS
2	B	319	GLN
2	B	346	ASP
2	B	406	CYS
2	B	411	GLU
2	B	503	CYS
2	B	515	LYS
2	B	522	GLU
2	B	662	ASP
3	C	15	LYS

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	623	ASN
1	A	927	ASN
2	B	106	GLN
2	B	141	GLN
2	B	339	ASN
2	B	440	GLN
2	B	541	GLN

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	$\#\|Z\| > 2$
4	NAG	D	1	1,4	14,14,15	0.45	0	17,19,21	0.75	0
4	NAG	D	2	4	14,14,15	0.32	0	17,19,21	0.38	0
4	BMA	D	3	4	11,11,12	1.19	1 (9%)	15,15,17	1.22	2 (13%)
4	MAN	D	4	4	11,11,12	1.54	2 (18%)	15,15,17	1.08	1 (6%)
5	NAG	E	1	1,5	14,14,15	0.29	0	17,19,21	1.42	2 (11%)
5	NAG	E	2	5	14,14,15	0.61	0	17,19,21	0.67	1 (5%)
6	NAG	F	1	1,6	14,14,15	0.20	0	17,19,21	0.61	0
6	NAG	F	2	6	14,14,15	0.51	0	17,19,21	0.59	0
6	BMA	F	3	6	11,11,12	0.66	0	15,15,17	1.06	1 (6%)
6	BMA	F	4	6	11,11,12	1.78	3 (27%)	15,15,17	1.24	3 (20%)
6	MAN	F	5	6	11,11,12	1.80	2 (18%)	15,15,17	1.62	3 (20%)
6	MAN	F	6	6	11,11,12	1.27	1 (9%)	15,15,17	1.09	0
4	NAG	G	1	1,4	14,14,15	0.48	0	17,19,21	0.68	0
4	NAG	G	2	4	14,14,15	0.61	0	17,19,21	0.42	0
4	BMA	G	3	4	11,11,12	1.37	3 (27%)	15,15,17	1.22	2 (13%)
4	MAN	G	4	4	11,11,12	1.24	1 (9%)	15,15,17	1.24	2 (13%)
5	NAG	H	1	1,5	14,14,15	0.44	0	17,19,21	0.62	0
5	NAG	H	2	5	14,14,15	0.50	0	17,19,21	0.62	0
5	NAG	I	1	1,5	14,14,15	0.43	0	17,19,21	0.47	0
5	NAG	I	2	5	14,14,15	0.82	1 (7%)	17,19,21	1.26	1 (5%)
5	NAG	J	1	1,5	14,14,15	0.52	0	17,19,21	0.63	1 (5%)
5	NAG	J	2	5	14,14,15	0.52	0	17,19,21	0.52	0
5	NAG	K	1	5,2	14,14,15	0.42	0	17,19,21	0.79	1 (5%)
5	NAG	K	2	5	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
7	NAG	L	1	7,2	14,14,15	0.22	0	17,19,21	0.48	0
7	NAG	L	2	7	14,14,15	0.80	1 (7%)	17,19,21	1.30	1 (5%)
7	BMA	L	3	7	11,11,12	1.90	4 (36%)	15,15,17	1.41	1 (6%)

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
4	NAG	D	1	1,4	-	1/6/23/26	0/1/1/1
4	NAG	D	2	4	-	4/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	1,5	-	5/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
6	NAG	F	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2	6	-	0/6/23/26	0/1/1/1
6	BMA	F	3	6	-	1/2/19/22	0/1/1/1
6	BMA	F	4	6	-	2/2/19/22	0/1/1/1
6	MAN	F	5	6	-	0/2/19/22	0/1/1/1
6	MAN	F	6	6	-	2/2/19/22	0/1/1/1
4	NAG	G	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	BMA	G	3	4	-	0/2/19/22	0/1/1/1
4	MAN	G	4	4	-	1/2/19/22	1/1/1/1
5	NAG	H	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	H	2	5	-	0/6/23/26	0/1/1/1
5	NAG	I	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	I	2	5	-	4/6/23/26	0/1/1/1
5	NAG	J	1	1,5	-	0/6/23/26	0/1/1/1
5	NAG	J	2	5	-	0/6/23/26	0/1/1/1
5	NAG	K	1	5,2	-	1/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
7	NAG	L	1	7,2	-	2/6/23/26	0/1/1/1
7	NAG	L	2	7	-	1/6/23/26	0/1/1/1
7	BMA	L	3	7	-	1/2/19/22	1/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	3	BMA	O5-C5	3.82	1.51	1.43
6	F	5	MAN	C1-C2	3.75	1.60	1.52
6	F	5	MAN	C2-C3	3.57	1.57	1.52
6	F	4	BMA	C4-C5	3.24	1.59	1.53
5	I	2	NAG	O5-C1	2.90	1.48	1.43
7	L	2	NAG	O5-C1	2.89	1.48	1.43
6	F	4	BMA	C4-C3	2.73	1.59	1.52
7	L	3	BMA	C4-C5	2.56	1.58	1.53
4	D	3	BMA	C2-C3	2.56	1.56	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	4	BMA	C2-C3	2.53	1.56	1.52
4	D	4	MAN	C4-C5	2.37	1.58	1.53
6	F	6	MAN	C4-C3	2.34	1.58	1.52
7	L	3	BMA	C1-C2	2.32	1.57	1.52
4	D	4	MAN	C4-C3	2.26	1.58	1.52
7	L	3	BMA	C6-C5	2.17	1.59	1.51
4	G	3	BMA	O3-C3	2.12	1.48	1.43
4	G	3	BMA	C2-C3	2.09	1.55	1.52
4	G	4	MAN	O5-C5	2.04	1.47	1.43
4	G	3	BMA	C4-C3	2.03	1.57	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	2	NAG	C1-O5-C5	4.84	118.75	112.19
7	L	2	NAG	C1-O5-C5	4.79	118.68	112.19
5	E	1	NAG	C2-N2-C7	4.65	129.52	122.90
6	F	5	MAN	C1-C2-C3	3.73	114.25	109.67
7	L	3	BMA	C1-O5-C5	3.48	116.90	112.19
4	G	4	MAN	C1-O5-C5	3.35	116.72	112.19
6	F	3	BMA	C1-O5-C5	2.56	115.67	112.19
4	G	3	BMA	O3-C3-C2	2.48	114.73	109.99
6	F	5	MAN	O5-C1-C2	2.46	114.56	110.77
4	D	3	BMA	C1-O5-C5	2.44	115.50	112.19
5	E	1	NAG	C1-C2-N2	2.39	114.58	110.49
5	K	1	NAG	C1-O5-C5	2.38	115.42	112.19
4	G	3	BMA	C1-C2-C3	-2.36	106.77	109.67
5	E	2	NAG	C1-O5-C5	2.29	115.30	112.19
6	F	4	BMA	O3-C3-C2	2.19	114.19	109.99
6	F	4	BMA	C1-O5-C5	2.17	115.13	112.19
4	D	3	BMA	O3-C3-C2	2.13	114.07	109.99
5	J	1	NAG	C1-O5-C5	2.11	115.05	112.19
4	G	4	MAN	O2-C2-C3	-2.11	105.92	110.14
6	F	4	BMA	C3-C4-C5	2.07	113.93	110.24
4	D	4	MAN	C1-O5-C5	2.04	114.96	112.19
5	K	2	NAG	C3-C4-C5	2.02	113.83	110.24
6	F	5	MAN	O2-C2-C3	-2.01	106.12	110.14

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	MAN	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
5	E	1	NAG	O5-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
4	D	4	MAN	C4-C5-C6-O6
4	G	2	NAG	C4-C5-C6-O6
4	G	1	NAG	O5-C5-C6-O6
6	F	6	MAN	C4-C5-C6-O6
6	F	4	BMA	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
5	I	2	NAG	O5-C5-C6-O6
5	I	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
5	E	1	NAG	C8-C7-N2-C2
5	E	1	NAG	O7-C7-N2-C2
5	E	2	NAG	C8-C7-N2-C2
5	E	2	NAG	O7-C7-N2-C2
5	I	2	NAG	C8-C7-N2-C2
5	I	2	NAG	O7-C7-N2-C2
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
4	D	2	NAG	O5-C5-C6-O6
6	F	6	MAN	O5-C5-C6-O6
6	F	4	BMA	C4-C5-C6-O6
5	I	1	NAG	O5-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
6	F	3	BMA	O5-C5-C6-O6
4	G	1	NAG	C4-C5-C6-O6
7	L	2	NAG	O5-C5-C6-O6
7	L	3	BMA	O5-C5-C6-O6
7	L	1	NAG	C4-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
7	L	1	NAG	O5-C5-C6-O6
5	E	2	NAG	C4-C5-C6-O6
5	H	1	NAG	C4-C5-C6-O6
5	E	1	NAG	C3-C2-N2-C7
5	H	1	NAG	O5-C5-C6-O6
4	G	4	MAN	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6

All (2) ring outliers are listed below:

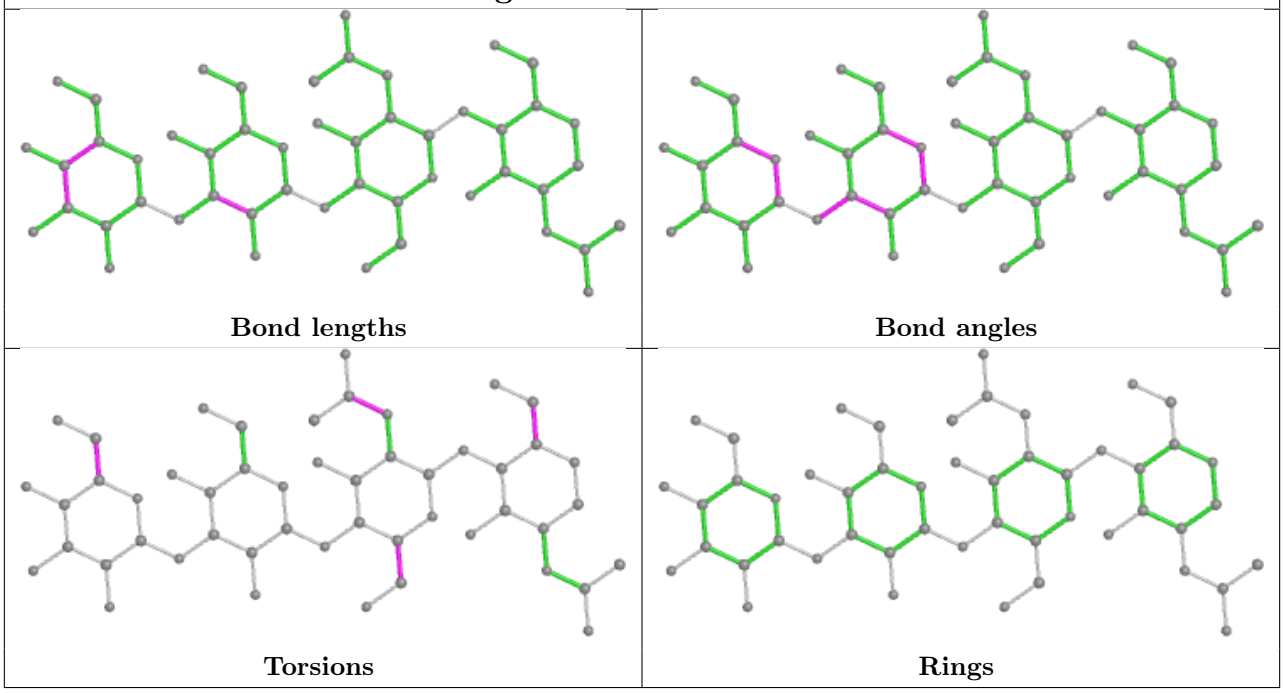
Mol	Chain	Res	Type	Atoms
7	L	3	BMA	C1-C2-C3-C4-C5-O5
4	G	4	MAN	C1-C2-C3-C4-C5-O5

7 monomers are involved in 6 short contacts:

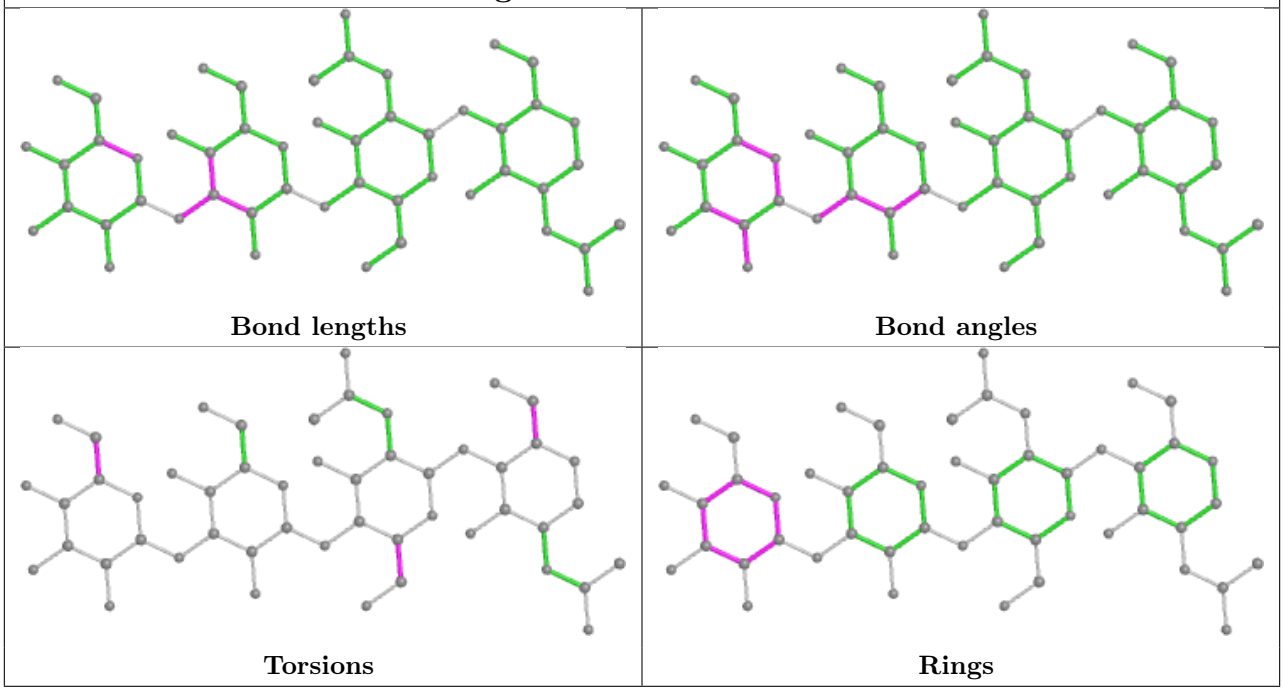
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
6	F	5	MAN	1	0
4	G	1	NAG	1	0
6	F	4	BMA	2	0
4	G	2	NAG	1	0
6	F	3	BMA	1	0
5	E	1	NAG	2	0

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

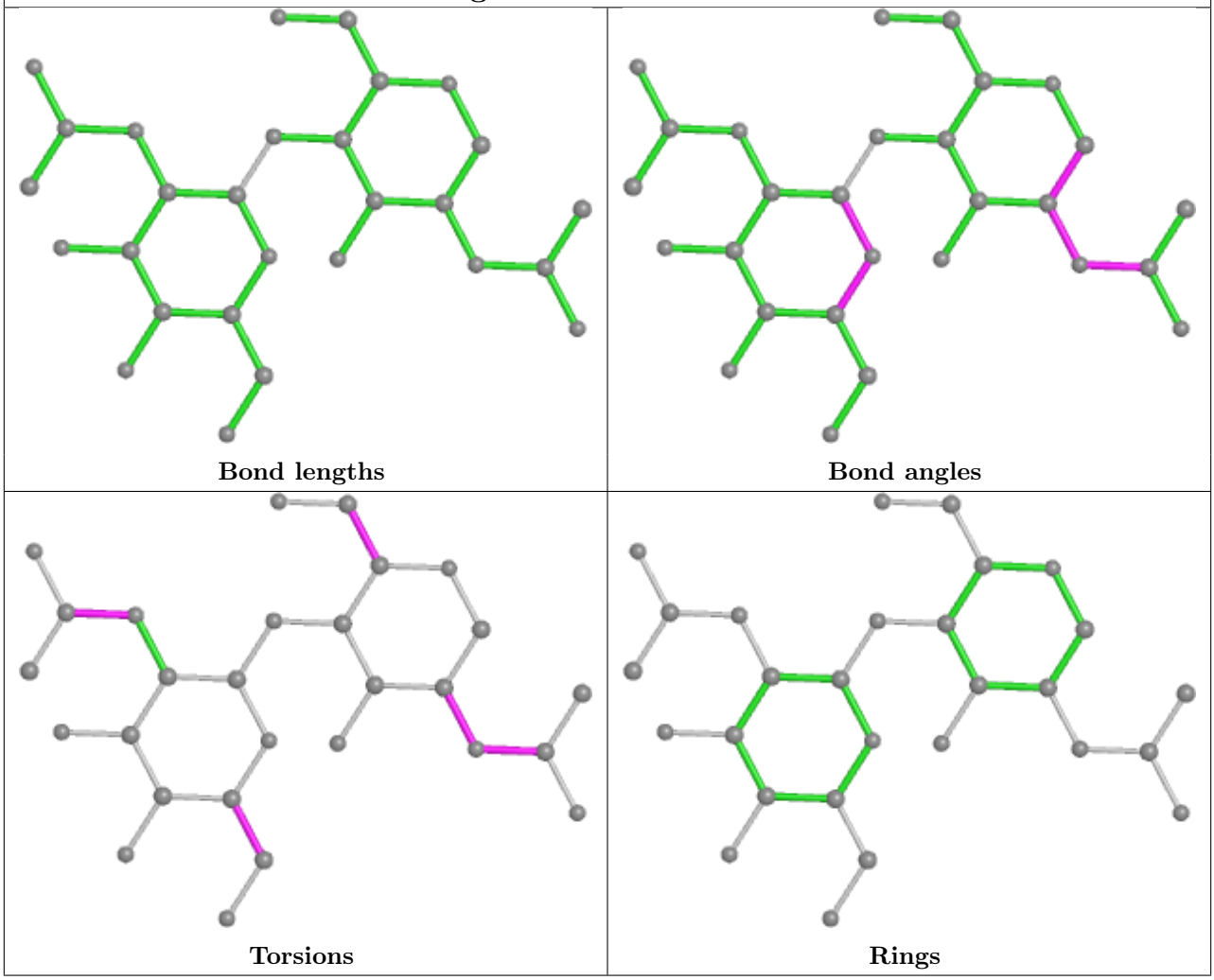
Oligosaccharide Chain D



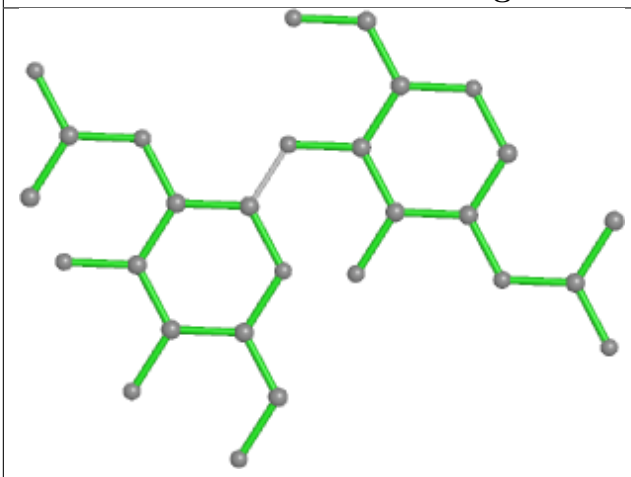
Oligosaccharide Chain G



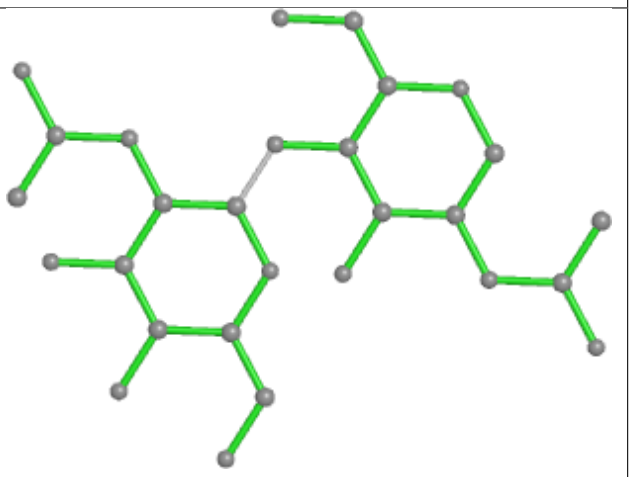
Oligosaccharide Chain E



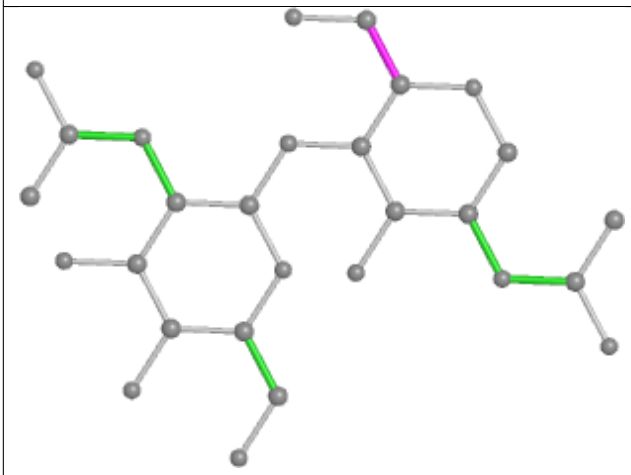
Oligosaccharide Chain H



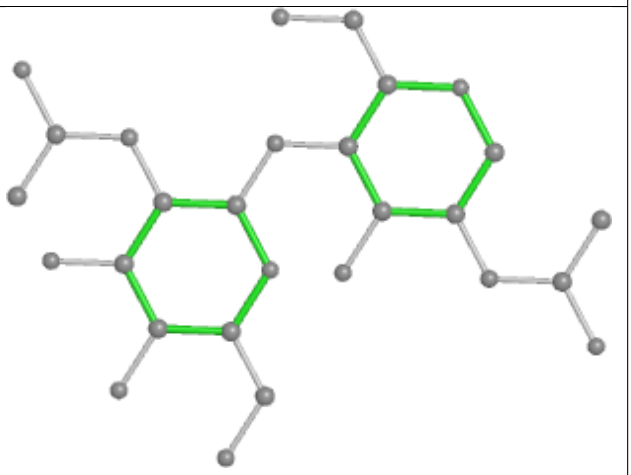
Bond lengths



Bond angles

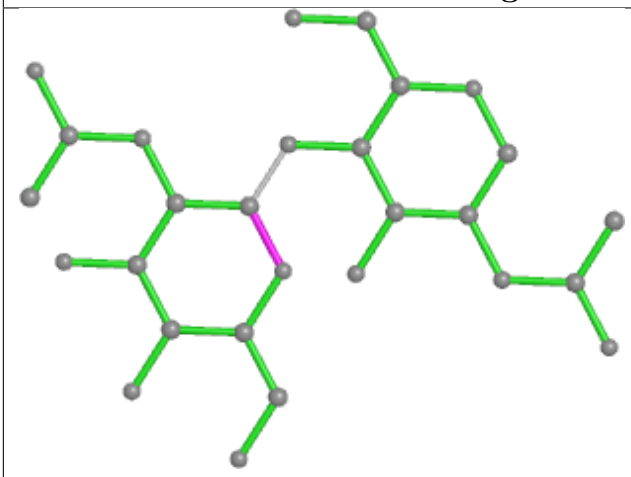


Torsions

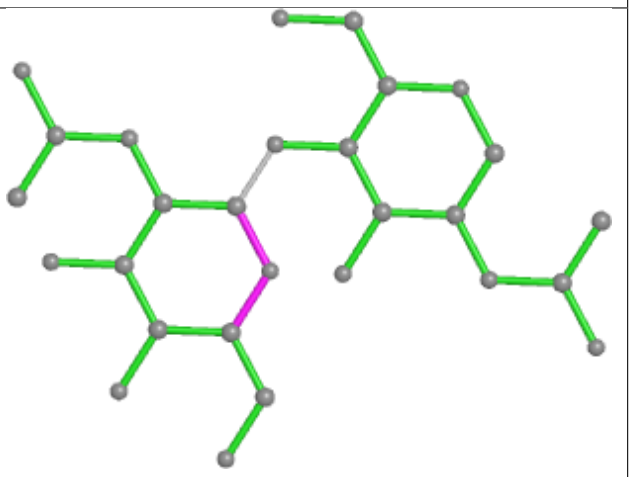


Rings

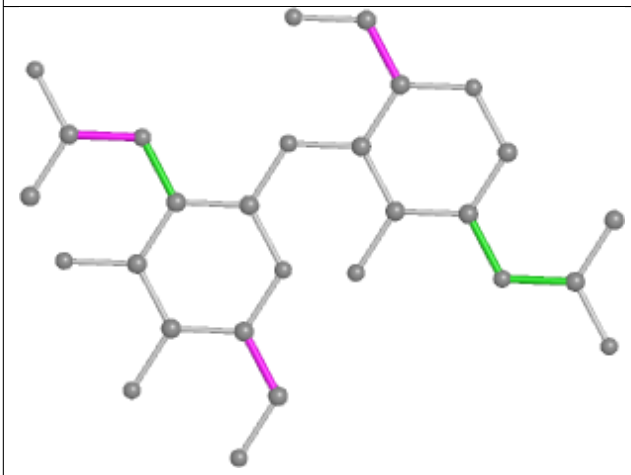
Oligosaccharide Chain I



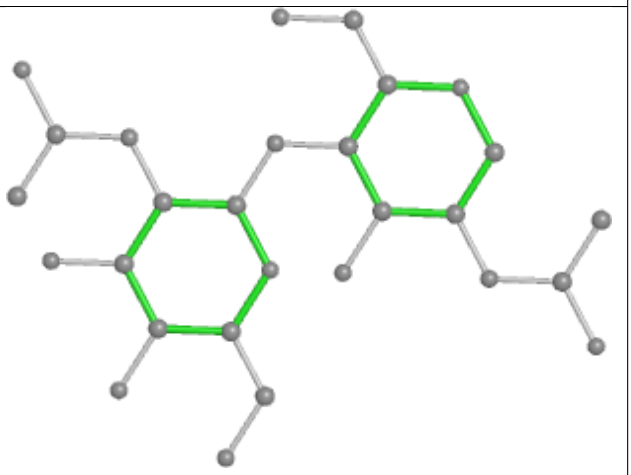
Bond lengths



Bond angles

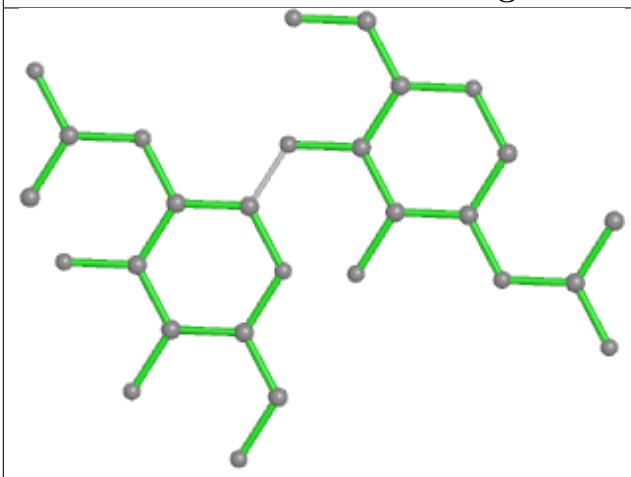


Torsions

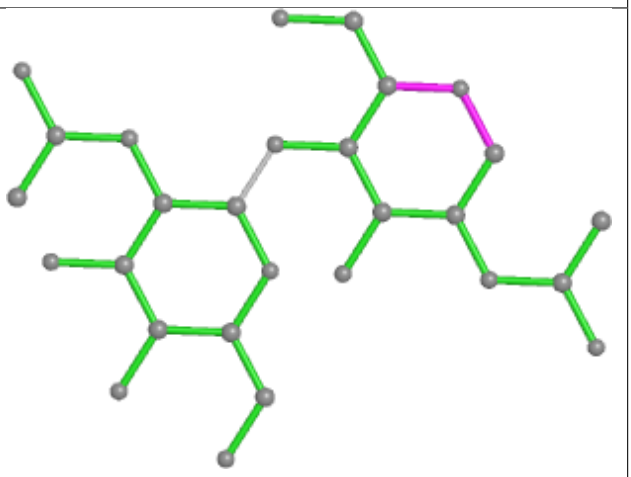


Rings

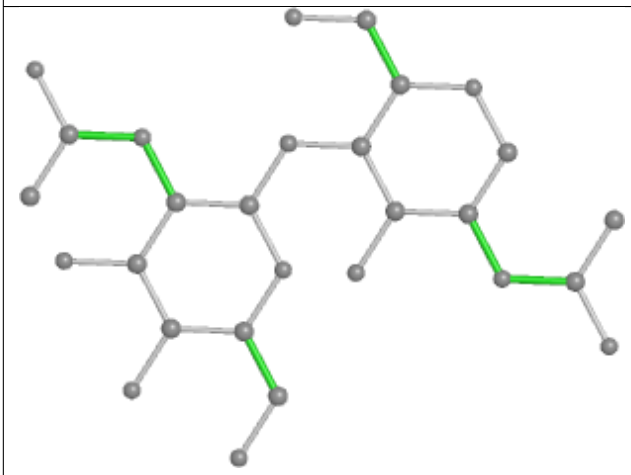
Oligosaccharide Chain J



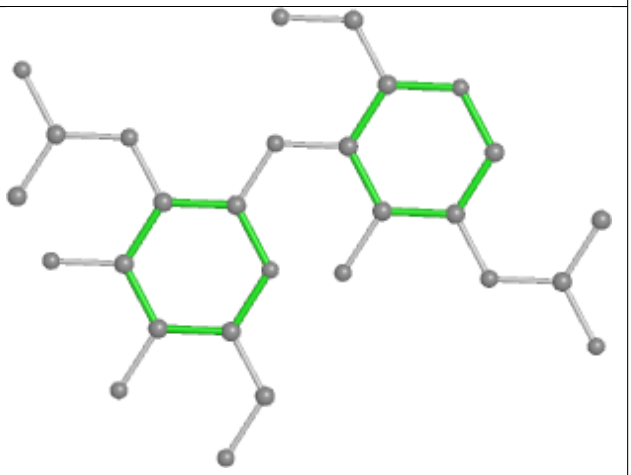
Bond lengths



Bond angles

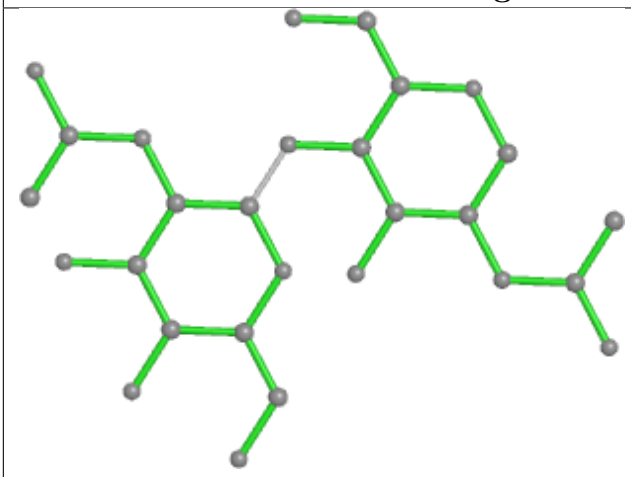


Torsions

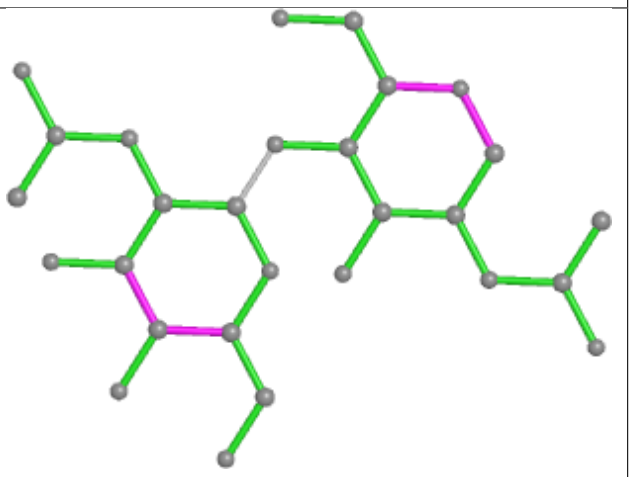


Rings

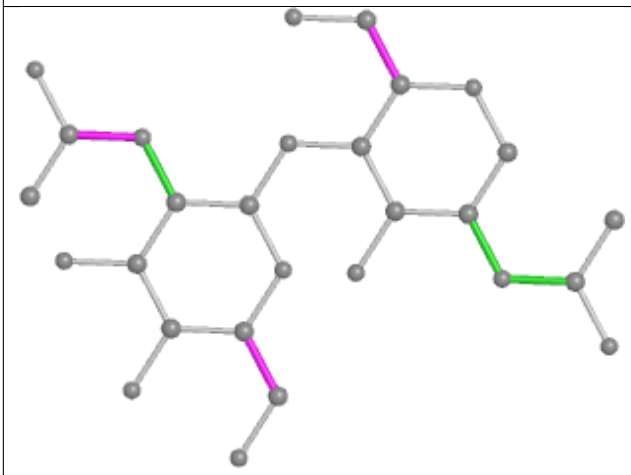
Oligosaccharide Chain K



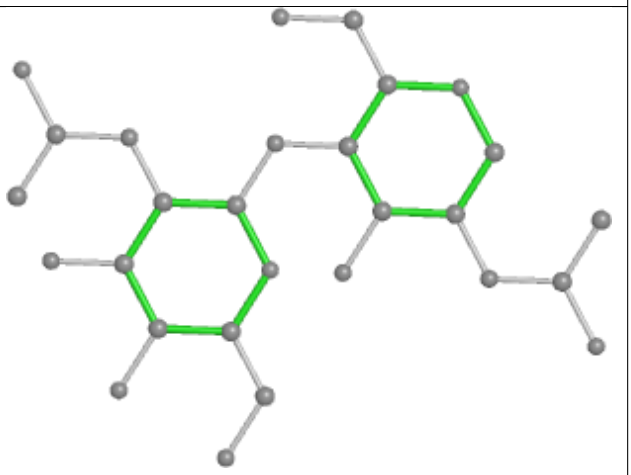
Bond lengths



Bond angles

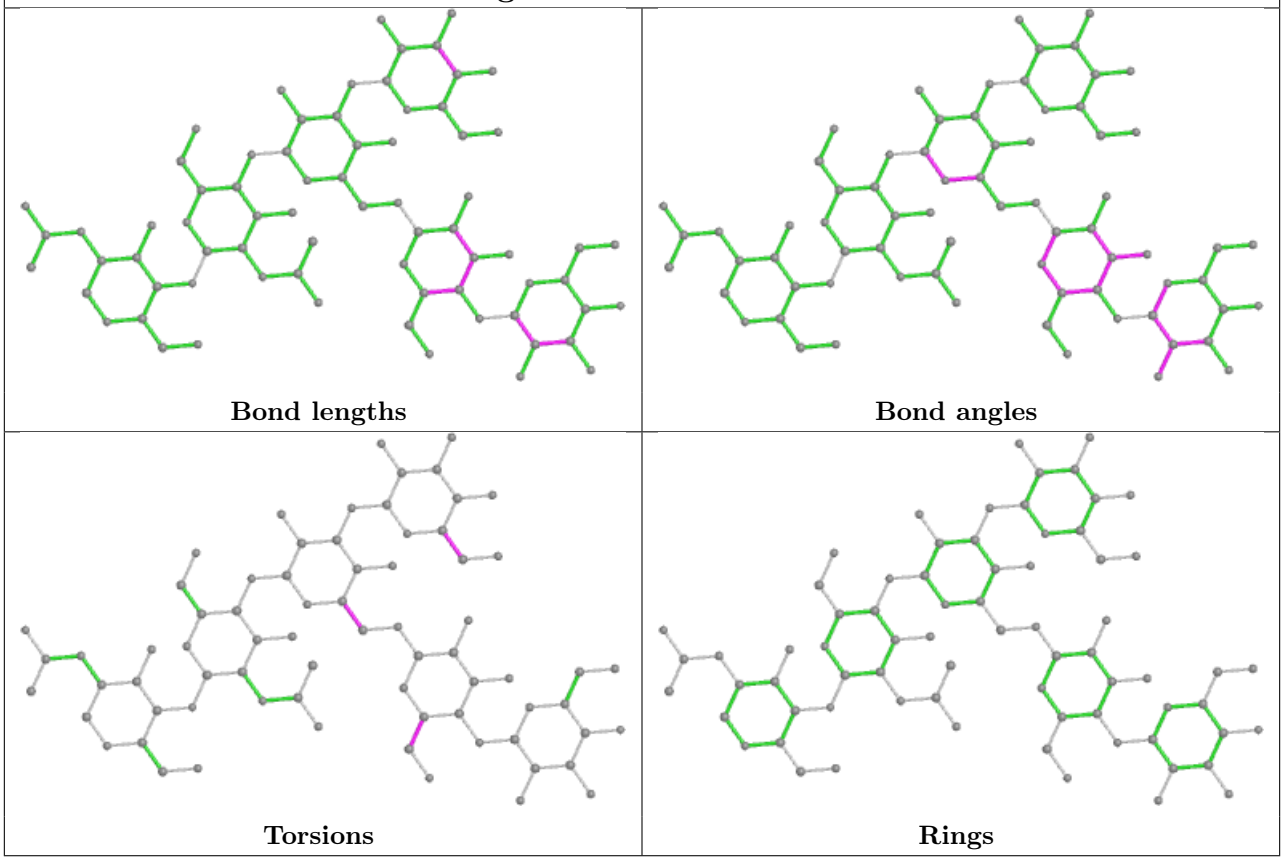


Torsions

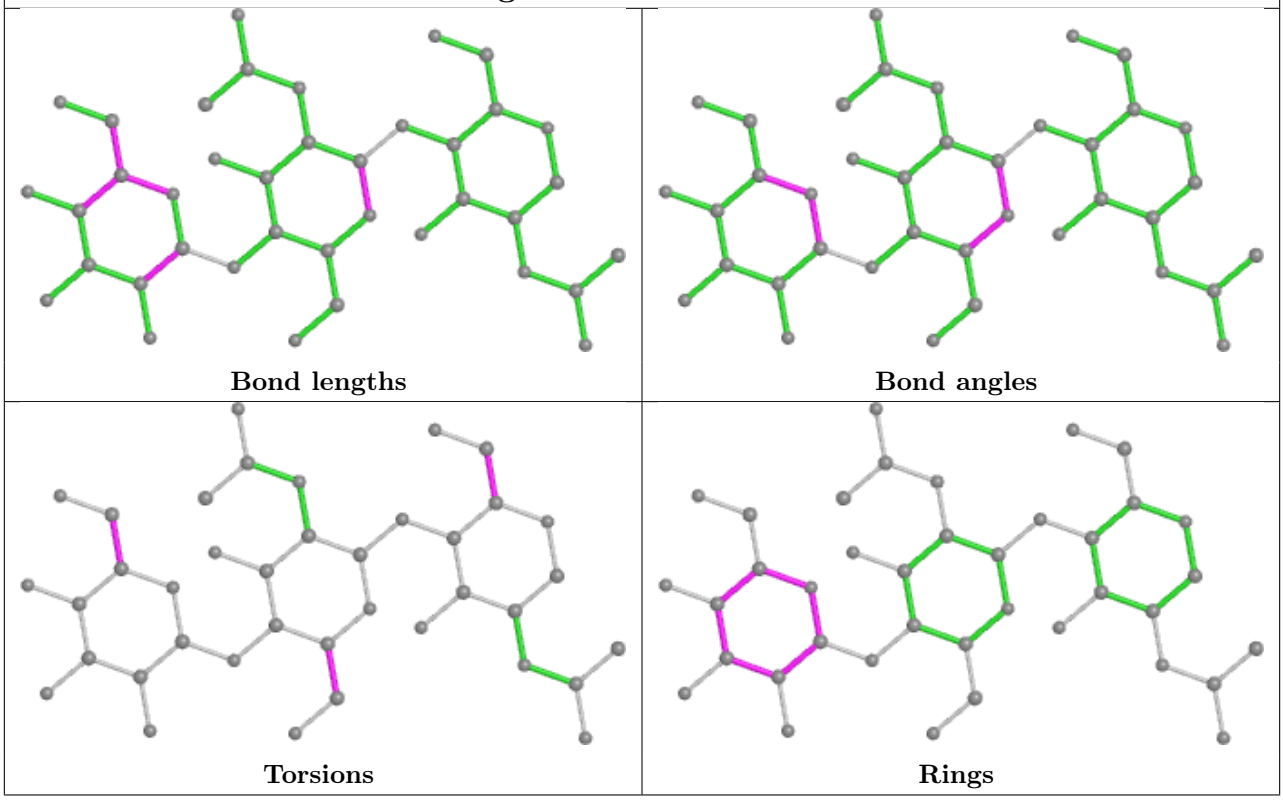


Rings

Oligosaccharide Chain F



Oligosaccharide Chain L



5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
8	NAG	A	1020	1	14,14,15	0.40	0	17,19,21	0.56	0
8	NAG	B	701	2	14,14,15	1.29	2 (14%)	17,19,21	1.09	1 (5%)
8	NAG	A	1017	1	14,14,15	0.32	0	17,19,21	0.56	0
8	NAG	B	702	2	14,14,15	0.49	0	17,19,21	0.65	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
8	NAG	A	1020	1	-	2/6/23/26	0/1/1/1
8	NAG	B	701	2	-	2/6/23/26	0/1/1/1
8	NAG	A	1017	1	-	2/6/23/26	0/1/1/1
8	NAG	B	702	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)
8	B	701	NAG	O5-C1	4.12	1.50	1.43
8	B	701	NAG	C1-C2	2.43	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	701	NAG	C1-O5-C5	4.24	117.94	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1020	NAG	O5-C5-C6-O6
8	A	1017	NAG	O5-C5-C6-O6
8	A	1020	NAG	C4-C5-C6-O6
8	A	1017	NAG	C4-C5-C6-O6
8	B	701	NAG	O5-C5-C6-O6
8	B	702	NAG	O5-C5-C6-O6
8	B	701	NAG	C4-C5-C6-O6
8	B	702	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	702	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	924/967 (95%)	-0.07	3 (0%) 94 88	23, 53, 92, 109	0
2	B	690/695 (99%)	0.10	25 (3%) 42 22	23, 61, 120, 146	1 (0%)
3	C	32/32 (100%)	1.61	11 (34%) 0 0	33, 101, 127, 143	0
All	All	1646/1694 (97%)	0.03	39 (2%) 59 37	23, 57, 109, 146	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	452	ASN	7.2
2	B	446	HIS	6.9
3	C	33	GLY	6.8
3	C	20	CYS	5.0
2	B	444	ASN	4.9
2	B	37	ARG	4.3
3	C	17	ASP	4.1
2	B	445	SER	4.1
2	B	454	THR	4.1
2	B	465	GLY	4.1
2	B	464	PRO	3.9
2	B	443	PRO	3.8
3	C	21	LEU	3.6
2	B	442	GLU	3.5
2	B	441	ALA	3.4
3	C	24	CYS	3.3
2	B	461	ARG	3.3
3	C	2	CYS	3.2
3	C	25	VAL	3.2
2	B	34	GLY	3.1
2	B	462	CYS	2.8
2	B	451	GLY	2.8
2	B	482	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	26	CYS	2.7
3	C	29	ASN	2.7
1	A	631	ALA	2.7
2	B	438	GLN	2.6
2	B	440	GLN	2.6
3	C	32	CYS	2.5
3	C	19	ASP	2.5
2	B	479	ARG	2.5
2	B	507	VAL	2.5
2	B	467	LEU	2.3
2	B	52	GLU	2.3
2	B	483	GLN	2.3
1	A	868	ASP	2.2
2	B	463	GLY	2.2
2	B	32	PRO	2.2
1	A	785	ASN	2.1

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
5	NAG	I	2	14/15	0.66	0.39	65,107,123,126	0
4	MAN	G	4	11/12	0.70	0.34	69,106,117,119	0
7	BMA	L	3	11/12	0.75	0.16	63,84,94,99	0
4	MAN	D	4	11/12	0.77	0.22	77,99,118,118	0
5	NAG	E	2	14/15	0.77	0.45	73,100,114,126	0
5	NAG	K	2	14/15	0.78	0.17	66,87,114,119	0
5	NAG	J	2	14/15	0.78	0.38	68,94,106,113	0
6	BMA	F	4	11/12	0.79	0.19	68,86,94,96	0
5	NAG	H	1	14/15	0.83	0.20	75,99,111,111	0
4	BMA	G	3	11/12	0.84	0.50	96,100,115,131	0
5	NAG	I	1	14/15	0.86	0.26	69,89,95,115	0
4	NAG	G	2	14/15	0.86	0.34	70,95,109,111	0

Continued on next page...

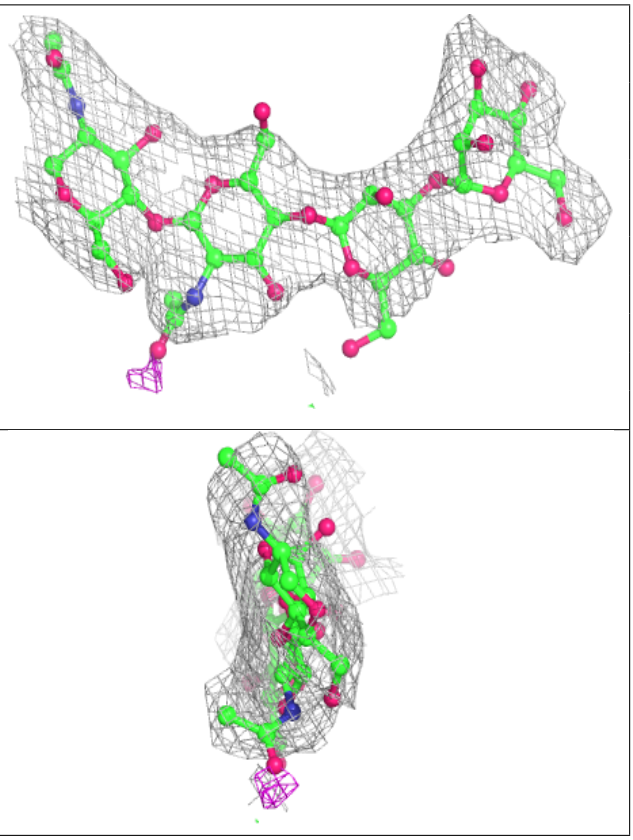
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	H	2	14/15	0.86	0.17	65,94,104,108	0
6	MAN	F	6	11/12	0.88	0.14	72,86,92,92	0
5	NAG	K	1	14/15	0.88	0.21	70,82,96,109	0
4	BMA	D	3	11/12	0.90	0.33	83,102,108,111	0
4	NAG	D	2	14/15	0.90	0.18	38,76,87,93	0
5	NAG	E	1	14/15	0.91	0.24	65,82,92,100	0
6	BMA	F	3	11/12	0.92	0.12	69,75,85,98	0
7	NAG	L	2	14/15	0.92	0.22	71,84,96,98	0
4	NAG	G	1	14/15	0.92	0.20	60,77,86,109	0
6	MAN	F	5	11/12	0.93	0.17	65,84,93,95	0
7	NAG	L	1	14/15	0.94	0.19	55,72,79,80	0
4	NAG	D	1	14/15	0.95	0.17	37,47,58,59	0
6	NAG	F	2	14/15	0.95	0.16	34,46,62,81	0
5	NAG	J	1	14/15	0.95	0.13	49,68,79,80	0
6	NAG	F	1	14/15	0.97	0.17	25,40,55,58	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.

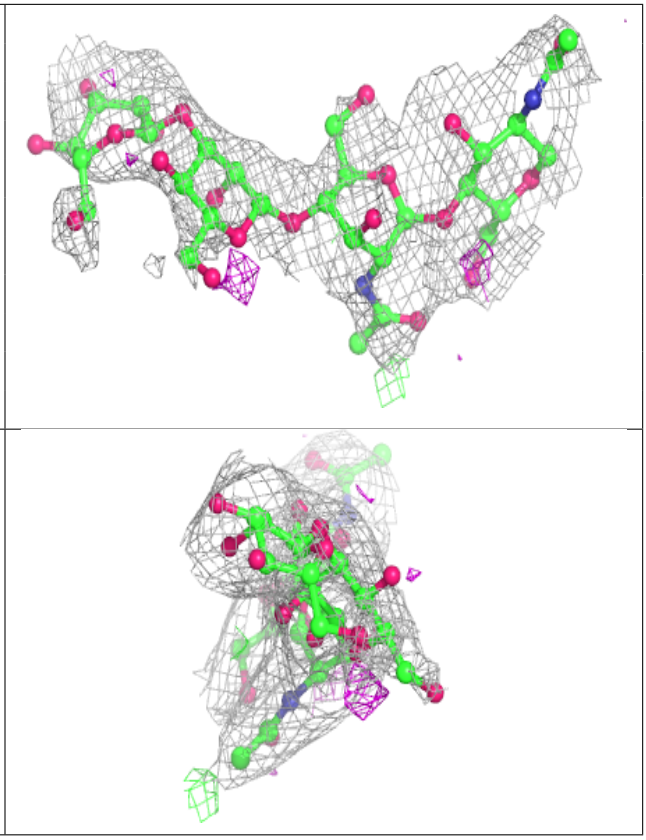
Electron density around Chain D:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



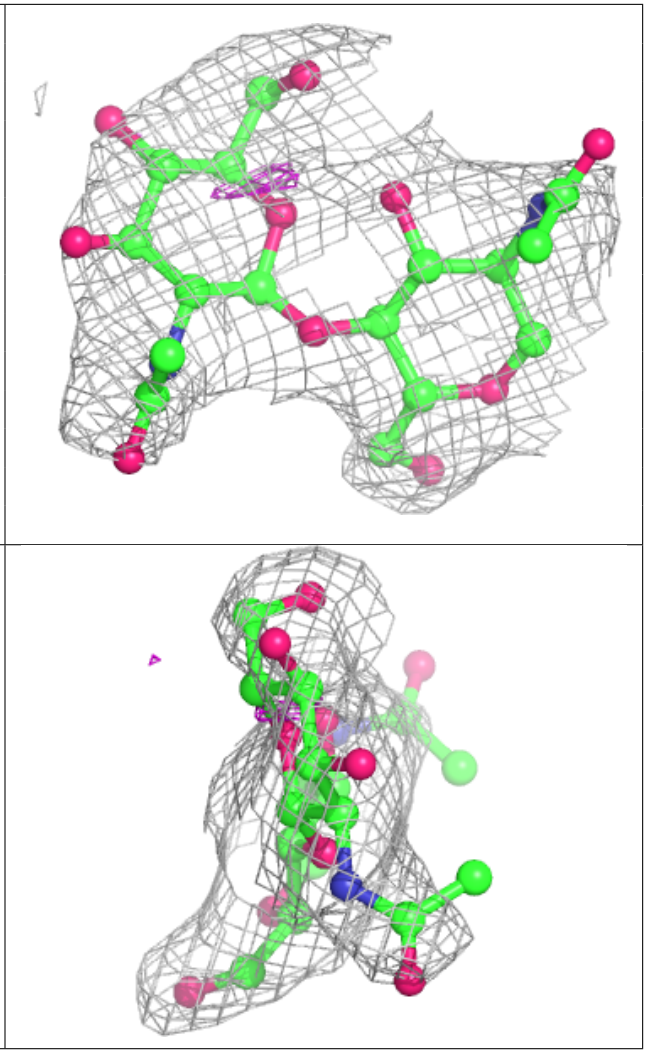
Electron density around Chain G:

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



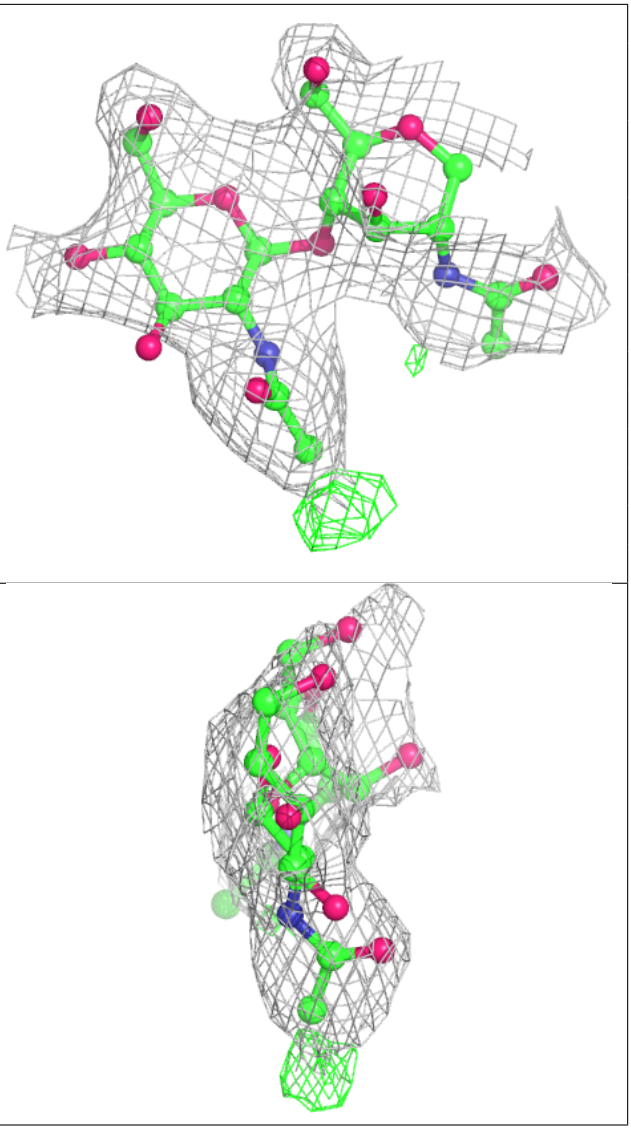
Electron density around Chain E:

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



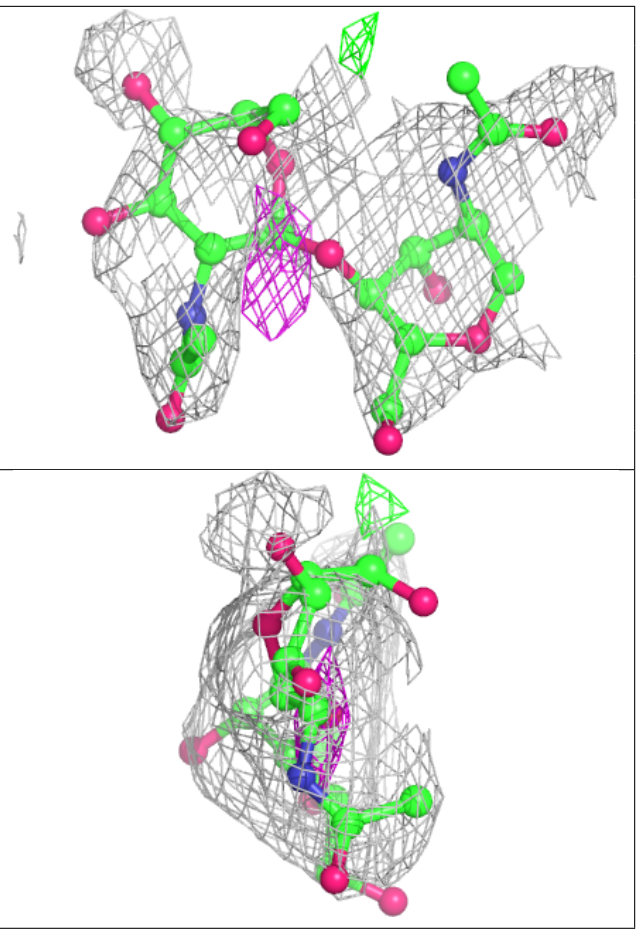
Electron density around Chain H:

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



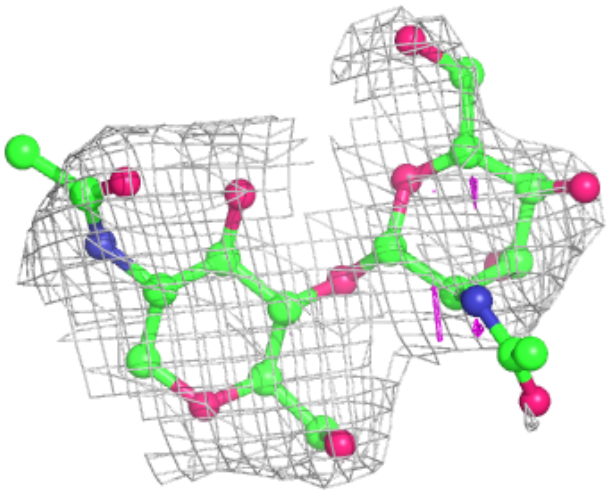
Electron density around Chain I:

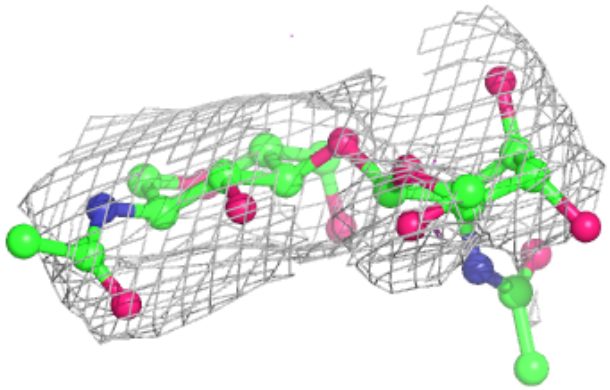
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

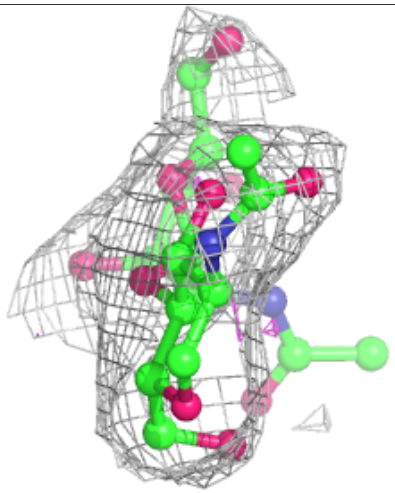


Electron density around Chain J:

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

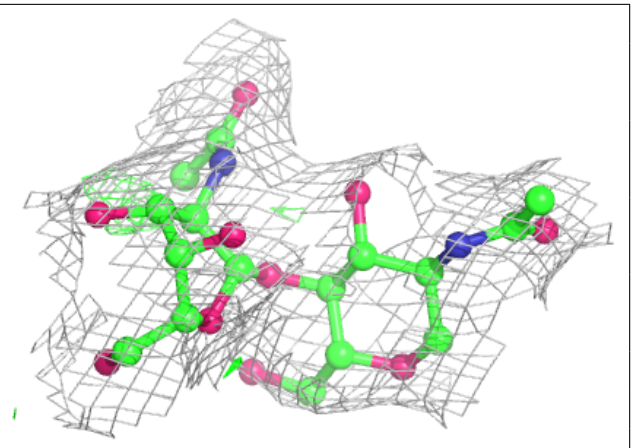


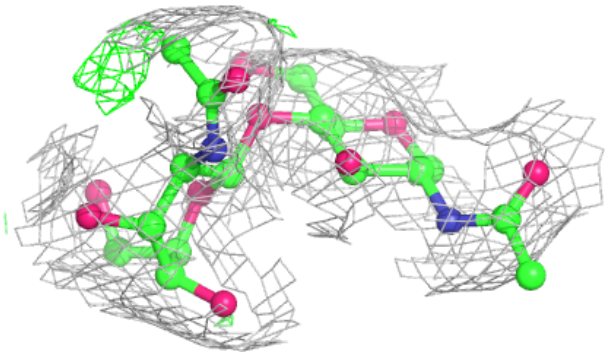


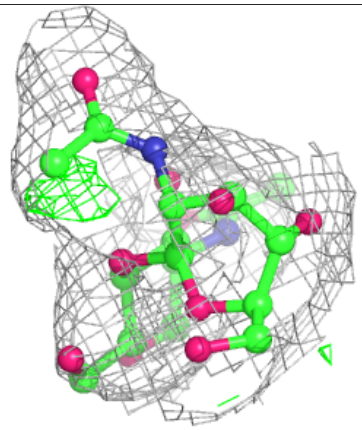


Electron density around Chain K:

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

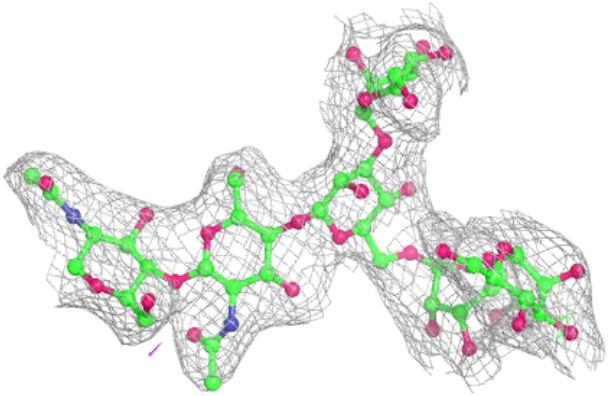


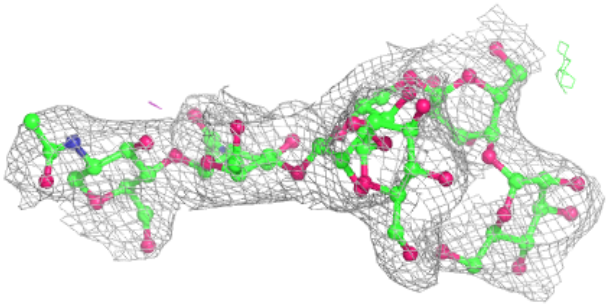


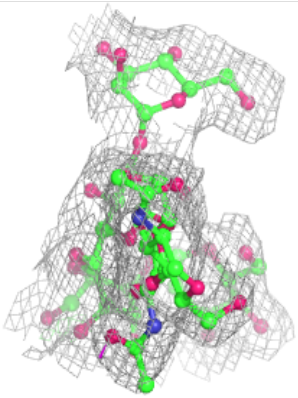


Electron density around Chain F:

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

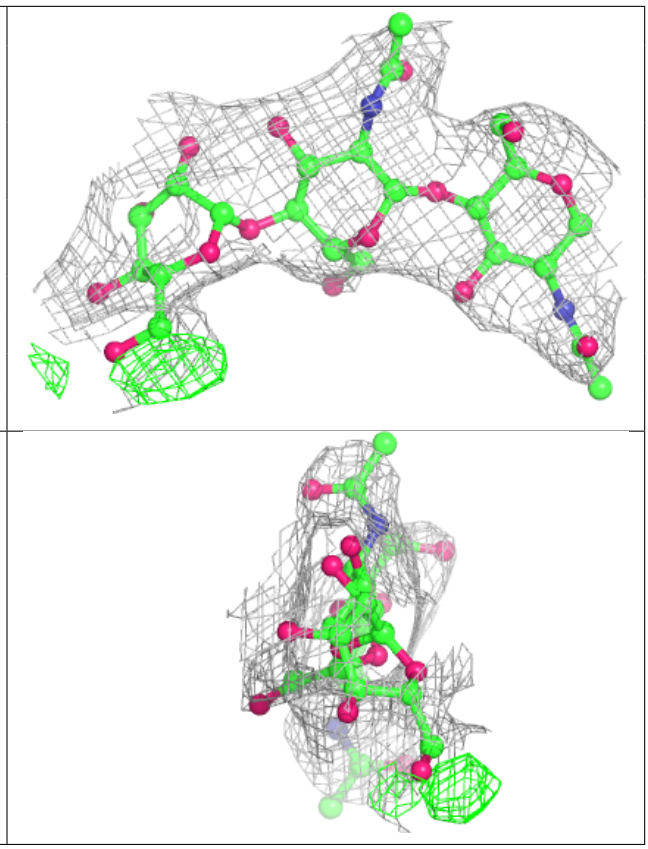






Electron density around Chain L:

$2mF_o$-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
8	NAG	B	701	14/15	0.62	0.41	75,107,123,124	0
9	MN	B	710	1/1	0.68	0.44	163,163,163,163	0
8	NAG	A	1017	14/15	0.80	0.39	75,93,110,112	0
8	NAG	A	1020	14/15	0.86	0.20	42,71,88,93	0
9	MN	A	1029	1/1	0.90	0.19	120,120,120,120	0
8	NAG	B	702	14/15	0.90	0.18	54,58,69,72	0
9	MN	B	709	1/1	0.92	0.28	86,86,86,86	0
9	MN	A	1025	1/1	0.93	0.21	202,202,202,202	0
9	MN	A	1028	1/1	0.96	0.08	64,64,64,64	0
9	MN	A	1026	1/1	0.97	0.14	69,69,69,69	0
9	MN	A	1027	1/1	0.98	0.09	74,74,74,74	0
9	MN	B	708	1/1	1.00	0.23	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.