Full wwPDB X-ray Structure Validation Report ⓘ

Dec 4, 2023 – 12:29 PM EST

PDB ID	:	8D50
Title	:	Crystal Structure of Mosaic HIV-1 Envelope (MosM3.1) in Complex with antibodies PGT124 and 35O22 at 4.3 Angstrom
Authors	:	Xian, Y.; Wilson, A.
Deposited on	:	2022-06-03
Resolution	:	4.32 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

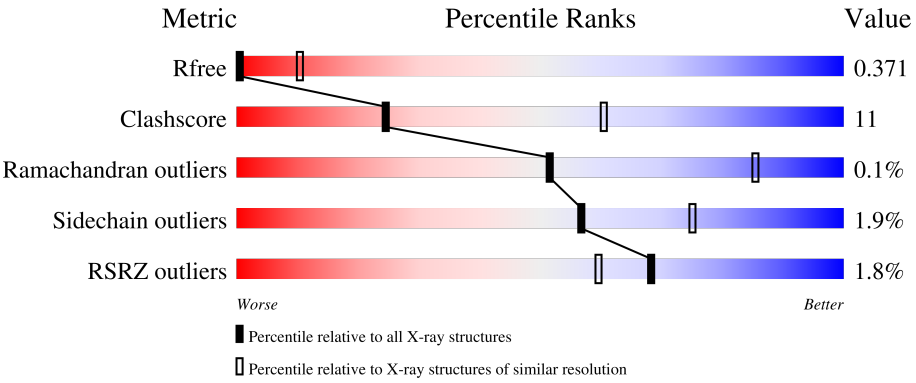
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.32 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	1018 (4.84-3.80)
Clashscore	141614	1081 (4.84-3.80)
Ramachandran outliers	138981	1033 (4.84-3.80)
Sidechain outliers	138945	1016 (4.84-3.80)
RSRZ outliers	127900	1078 (4.92-3.70)

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	G	431	% 70% 30%
2	B	137	% 66% 34%
3	D	141	8% 82% 18%
4	E	107	88% 12%
5	L	210	75% 24%

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Mol	Chain	Length	Quality of chain
6	H	226	3% 71% 29%
7	P	5	100%
8	A	2	50% 50%
8	K	2	100%
8	M	2	50% 50%
9	C	6	33% 67%
10	F	4	75% 25%
11	I	3	67% 33%
11	J	3	100%
11	N	3	33% 33% 33%

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
11	NAG	I	2	-	-	-	X
8	NAG	K	2	-	-	-	X
8	NAG	M	2	-	-	-	X

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 10251 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	431	Total	C	N	O	S	0	0	0
			3426	2155	610	634	27			

- Molecule 2 is a protein called Envelope glycoprotein gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1102	696	189	210	7			

- Molecule 3 is a protein called 35O22 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	141	Total	C	N	O	S	0	0	0
			1097	706	181	204	6			

- Molecule 4 is a protein called 35O22 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	107	Total	C	N	O	S	0	0	0
			818	514	135	163	6			

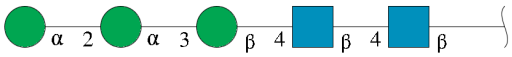
- Molecule 5 is a protein called PGT124 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	210	Total	C	N	O	S	0	0	0
			1595	1005	270	315	5			

- Molecule 6 is a protein called PGT124 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	226	Total	C	N	O	S	0	0	0
			1720	1093	287	335	5			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.

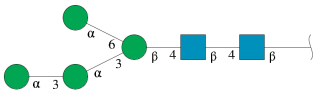


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	P	5	Total	C	N	O	0	0	0
			61	34	2	25			

- 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
8	A	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
8	M	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

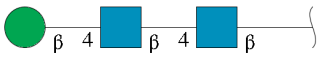


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	C	6	Total	C	N	O	0	0	0
			72	40	2	30			

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

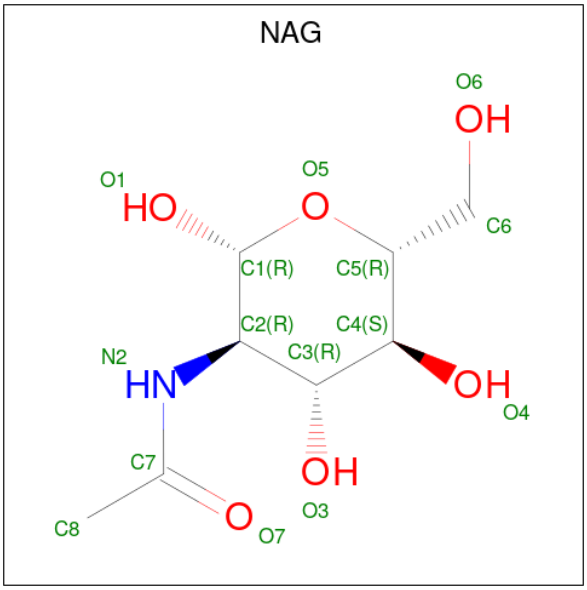
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	F	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 11 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.



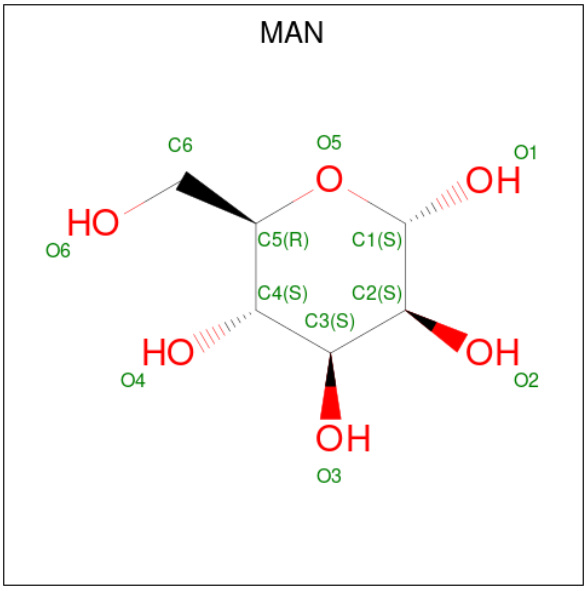
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	3	Total	C	N	O	0	0	0
			39	22	2	15			
11	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
11	N	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 13 is alpha-D-mannopyranose (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



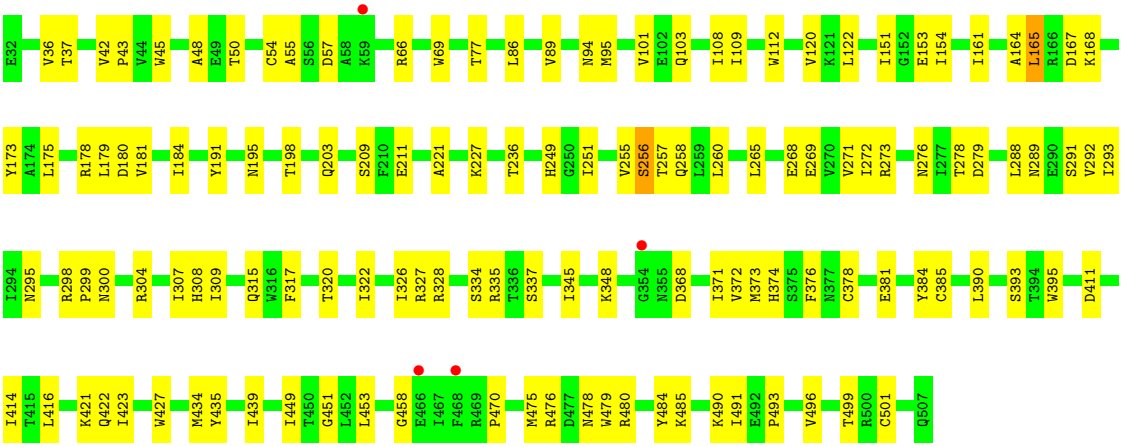
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	G	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

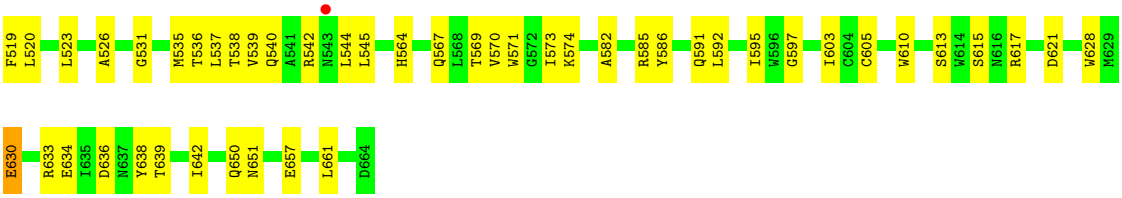
• Molecule 1: Envelope glycoprotein gp120

Chain G:



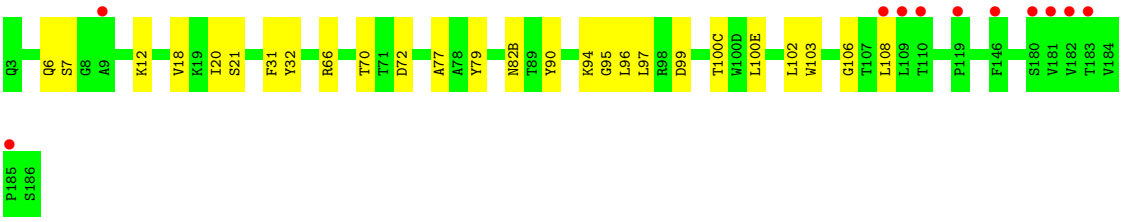
• Molecule 2: Envelope glycoprotein gp41

Chain B:



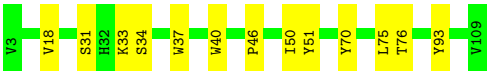
• Molecule 3: 35O22 Fab heavy chain

Chain D:



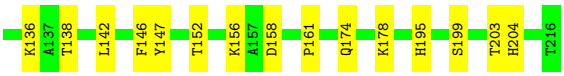
• Molecule 4: 35O22 Fab light chain

Chain E:



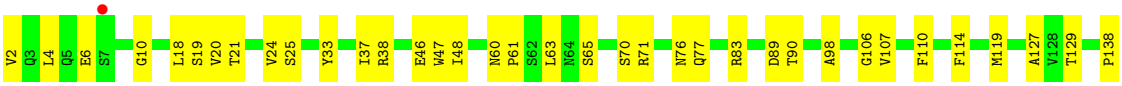
• Molecule 5: PGT124 Fab light chain

Chain L:



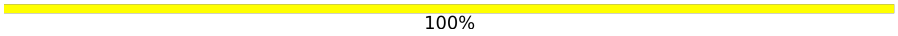
• Molecule 6: PGT124 Fab heavy chain

Chain H:



• Molecule 7: alpha-D-mannopyranose-(1-2)-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 P:

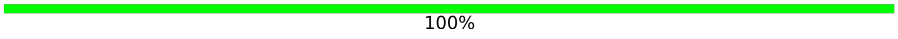


• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A:

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

Chain K:

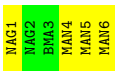


• Molecule 8: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:

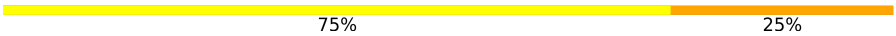
• Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:



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

Chain F:



• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

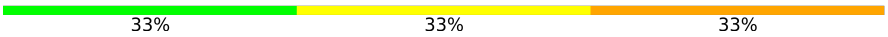
Chain I:

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

• Molecule 11: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	132.19Å 132.19Å 315.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.27 – 4.32 50.27 – 4.32	Depositor EDS
% Data completeness (in resolution range)	94.1 (50.27-4.32) 94.4 (50.27-4.32)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 4.29Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.323 , 0.369 0.323 , 0.371	Depositor DCC
R_{free} test set	975 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	113.8	Xtriage
Anisotropy	0.690	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 105.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	0.196 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	10251	wwPDB-VP
Average B, all atoms (Å^2)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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

5.1 Standard geometry

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

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	G	0.25	0/3495	0.51	0/4745
2	B	0.32	0/1121	0.51	0/1519
3	D	0.30	0/1125	0.55	0/1526
4	E	0.35	0/842	0.55	0/1151
5	L	0.32	0/1638	0.62	0/2238
6	H	0.36	0/1763	0.66	0/2407
All	All	0.31	0/9984	0.57	0/13586

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	G	3426	0	3367	96	0
2	B	1102	0	1077	35	0
3	D	1097	0	1071	20	0
4	E	818	0	768	10	0
5	L	1595	0	1541	33	0
6	H	1720	0	1686	44	0
7	P	61	0	52	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	28	0	25	2	0
8	K	28	0	25	0	0
8	M	28	0	25	0	0
9	C	72	0	61	1	0
10	F	50	0	43	2	0
11	I	39	0	34	2	0
11	J	39	0	34	4	0
11	N	39	0	34	3	0
12	B	28	0	26	0	0
12	G	70	0	65	2	0
13	G	11	0	10	1	0
All	All	10251	0	9944	220	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 (220) 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)
6:H:171:VAL:HA	6:H:217:VAL:HG12	1.45	0.98
6:H:138:PRO:HB3	6:H:164:TYR:HB3	1.60	0.82
1:G:300:ASN:HB2	1:G:322:ILE:HD11	1.65	0.77
3:D:96:LEU:HB3	3:D:100(E):LEU:HB3	1.68	0.76
2:B:539:VAL:HA	2:B:542:ARG:HE	1.52	0.75
1:G:265:LEU:HD11	11:N:1:NAG:H81	1.71	0.73
6:H:214:ILE:HD11	6:H:227:ASP:HB3	1.70	0.73
2:B:539:VAL:HG22	2:B:542:ARG:HH21	1.54	0.72
1:G:43:PRO:HD2	2:B:628:TRP:HB2	1.72	0.72
1:G:491:ILE:O	2:B:585:ARG:NH2	2.24	0.71
3:D:94:LYS:HD2	3:D:102:LEU:HB2	1.72	0.71
1:G:299:PRO:HB2	1:G:327:ARG:HD2	1.72	0.71
1:G:57:ASP:H	1:G:77:THR:HG22	1.57	0.70
1:G:390:LEU:HD13	1:G:470:PRO:HG3	1.74	0.68
1:G:122:LEU:HD13	1:G:203:GLN:HB2	1.75	0.68
5:L:50:ASN:HB3	5:L:53:ASP:HB2	1.76	0.68
3:D:12:LYS:HG3	3:D:18:VAL:HB	1.75	0.68
1:G:151:ILE:HG22	1:G:153:GLU:H	1.59	0.67
1:G:272:ILE:HG12	1:G:348:LYS:HD3	1.77	0.67
5:L:66(B):ILE:HG13	5:L:66(C):ASN:H	1.58	0.66
5:L:174:GLN:N	5:L:178:LYS:O	2.23	0.65
1:G:288:LEU:HD21	1:G:345:ILE:HD11	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:VAL:HG12	2:B:610:TRP:HE3	1.61	0.64
5:L:90:TYR:CZ	5:L:107:ALA:HB2	2.34	0.62
6:H:90:THR:HG23	6:H:129:THR:HA	1.82	0.62
1:G:154:ILE:HG12	1:G:328:ARG:HH22	1.64	0.61
1:G:179:LEU:HB3	1:G:421:LYS:HD3	1.82	0.61
5:L:37:GLN:HB2	5:L:47:LEU:HD11	1.80	0.61
1:G:300:ASN:HB3	1:G:327:ARG:H	1.65	0.61
1:G:227:LYS:HG3	1:G:485:LYS:HD3	1.82	0.61
11:J:2:NAG:H61	11:J:3:BMA:H2	1.82	0.61
1:G:108:ILE:HG22	1:G:427:TRP:CH2	2.36	0.61
6:H:187:ALA:HB2	6:H:197:LEU:HD23	1.82	0.60
1:G:37:THR:HG22	2:B:605:CYS:HA	1.83	0.60
5:L:46:LEU:HD21	5:L:49:TYR:HB3	1.83	0.60
6:H:46:GLU:OE1	6:H:60:ASN:ND2	2.35	0.60
13:G:606:MAN:H2	11:J:3:BMA:H4	1.84	0.60
6:H:182:VAL:HG23	6:H:201:VAL:HG22	1.84	0.60
1:G:54:CYS:HB3	2:B:571:TRP:CZ2	2.38	0.59
1:G:279:ASP:HB2	1:G:458:GLY:HA2	1.85	0.59
5:L:33:VAL:HG21	5:L:74:ALA:HB2	1.84	0.59
6:H:176:GLY:O	6:H:179:THR:HG23	2.03	0.59
1:G:48:ALA:HB2	1:G:490:LYS:HZ2	1.68	0.58
6:H:138:PRO:HD3	6:H:219:HIS:CD2	2.38	0.58
1:G:271:VAL:HA	1:G:348:LYS:HZ2	1.68	0.58
4:E:37:TRP:HB2	4:E:50:ILE:HB	1.84	0.58
6:H:60:ASN:HB3	6:H:63:LEU:HD23	1.84	0.58
6:H:38:ARG:HG3	6:H:48:ILE:HD11	1.86	0.57
1:G:260:LEU:HB2	1:G:451:GLY:HA3	1.87	0.57
6:H:216:ASN:HB2	6:H:225:LYS:HZ1	1.69	0.57
1:G:54:CYS:SG	1:G:55:ALA:N	2.77	0.57
1:G:491:ILE:HG22	1:G:493:PRO:HD3	1.87	0.57
1:G:291:SER:OG	11:N:1:NAG:H83	2.05	0.57
6:H:6:GLU:N	6:H:6:GLU:OE1	2.38	0.56
1:G:109:ILE:HA	1:G:427:TRP:CZ3	2.41	0.56
5:L:52:GLN:HG3	5:L:66:PRO:HB3	1.87	0.56
1:G:161:ILE:HG12	1:G:309:ILE:HG22	1.89	0.55
1:G:385:CYS:HB3	1:G:416:LEU:CD1	2.35	0.55
5:L:115:GLN:N	5:L:116:PRO:HD3	2.22	0.55
1:G:195:ASN:HB2	1:G:423:ILE:HD12	1.89	0.55
6:H:216:ASN:HB2	6:H:225:LYS:NZ	2.21	0.55
1:G:256:SER:O	1:G:478:ASN:ND2	2.39	0.55
6:H:2:VAL:N	6:H:25:SER:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:537:LEU:HD13	2:B:603:ILE:HD11	1.90	0.54
4:E:31:SER:HB3	4:E:70:TYR:HA	1.90	0.54
3:D:99:ASP:H	3:D:100(C):THR:HG22	1.72	0.54
2:B:536:THR:O	2:B:540:GLN:NE2	2.40	0.54
6:H:33:TYR:HB2	6:H:98:ALA:O	2.08	0.53
1:G:180:ASP:OD1	1:G:422:GLN:N	2.41	0.53
1:G:268:GLU:O	1:G:289:ASN:ND2	2.41	0.53
2:B:540:GLN:O	2:B:544:LEU:HG	2.08	0.53
1:G:322:ILE:HG12	1:G:326:ILE:HG12	1.91	0.53
1:G:95:MET:SD	1:G:273:ARG:HD3	2.48	0.52
1:G:101:VAL:HG11	1:G:480:ARG:HG3	1.91	0.52
5:L:115:GLN:O	5:L:117:LYS:NZ	2.41	0.52
1:G:42:VAL:HB	1:G:43:PRO:HD3	1.90	0.52
6:H:106:GLY:HA2	7:P:2:NAG:H61	1.92	0.52
5:L:120:PRO:HB3	5:L:146:PHE:HB3	1.92	0.52
1:G:269:GLU:HG2	11:I:1:NAG:H83	1.91	0.52
1:G:292:VAL:HG22	1:G:337:SER:HB3	1.92	0.52
5:L:49:TYR:HD1	5:L:55:PRO:HG3	1.75	0.51
1:G:269:GLU:HA	11:I:1:NAG:H83	1.92	0.51
6:H:119:MET:SD	6:H:119:MET:N	2.83	0.51
3:D:96:LEU:HG	3:D:97:LEU:H	1.75	0.51
1:G:95:MET:SD	1:G:484:TYR:HB2	2.51	0.51
1:G:269:GLU:OE1	1:G:348:LYS:HD2	2.11	0.51
5:L:146:PHE:HB2	5:L:204:HIS:CE1	2.46	0.51
11:N:1:NAG:H61	11:N:2:NAG:H82	1.91	0.51
1:G:45:TRP:CH2	1:G:491:ILE:HG12	2.45	0.51
5:L:152:THR:HB	5:L:203:THR:HB	1.92	0.51
1:G:153:GLU:HA	1:G:178:ARG:HB2	1.92	0.51
5:L:39:LYS:HG2	5:L:87:ALA:HB2	1.93	0.51
1:G:209:SER:HB2	1:G:211:GLU:HG2	1.93	0.50
5:L:32:ALA:HB3	5:L:94:TRP:HB2	1.93	0.50
3:D:72:ASP:HB2	3:D:77:ALA:HB3	1.94	0.50
6:H:107:VAL:HG12	6:H:110:PHE:H	1.76	0.50
1:G:423:ILE:HA	1:G:434:MET:O	2.11	0.50
6:H:192:SER:OG	6:H:194:LEU:HD13	2.12	0.50
2:B:657:GLU:O	2:B:661:LEU:HB2	2.12	0.49
6:H:214:ILE:HD11	6:H:227:ASP:CB	2.41	0.49
3:D:100(E):LEU:HD11	4:E:51:TYR:HB2	1.94	0.49
6:H:10:GLY:HA2	6:H:127:ALA:O	2.12	0.49
3:D:66:ARG:HD2	3:D:82(B):ASN:HB2	1.94	0.49
6:H:187:ALA:HA	6:H:197:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:130:GLU:O	5:L:133:GLN:HG2	2.13	0.49
1:G:260:LEU:HD11	1:G:453:LEU:HD21	1.94	0.48
1:G:94:ASN:HA	1:G:236:THR:HA	1.94	0.48
5:L:27:ALA:HB2	5:L:93:MET:SD	2.54	0.48
2:B:650:GLN:HG3	2:B:651:ASN:H	1.77	0.48
1:G:36:VAL:HG12	2:B:610:TRP:CE3	2.46	0.48
1:G:184:ILE:HD12	12:G:602:NAG:H82	1.96	0.48
1:G:50:THR:O	1:G:103:GLN:NE2	2.38	0.48
1:G:307:ILE:HD11	1:G:317:PHE:HD2	1.79	0.47
5:L:131:GLU:HG2	5:L:136:LYS:HB2	1.96	0.47
5:L:115:GLN:HA	5:L:147:TYR:HE1	1.79	0.47
10:F:3:BMA:H62	10:F:4:MAN:H2	1.66	0.47
1:G:258:GLN:NE2	1:G:372:VAL:O	2.48	0.47
5:L:102:TRP:CD1	6:H:61:PRO:HD2	2.50	0.47
2:B:569:THR:O	2:B:573:ILE:HG12	2.15	0.47
4:E:33:LYS:HB3	4:E:93:TYR:O	2.14	0.47
6:H:220:LYS:HB2	6:H:221:PRO:HD3	1.97	0.47
3:D:6:GLN:HB2	3:D:106:GLY:HA3	1.96	0.46
5:L:142:LEU:HB3	6:H:185:PHE:CZ	2.50	0.46
1:G:151:ILE:HG22	1:G:153:GLU:N	2.29	0.46
1:G:203:GLN:HG3	1:G:435:TYR:HD2	1.81	0.46
1:G:167:ASP:OD1	1:G:168:LYS:N	2.48	0.46
2:B:591:GLN:O	2:B:595:ILE:HG12	2.16	0.46
5:L:158:ASP:CG	5:L:195:HIS:HB3	2.37	0.46
6:H:65:SER:O	6:H:83:ARG:NH1	2.49	0.46
1:G:54:CYS:H	2:B:571:TRP:HZ2	1.64	0.45
2:B:531:GLY:O	2:B:535:MET:HG3	2.17	0.45
1:G:86:LEU:HD21	2:B:523:LEU:HB3	1.98	0.45
1:G:86:LEU:HB3	1:G:89:VAL:HG21	1.99	0.45
2:B:519:PHE:HD2	2:B:520:LEU:HD22	1.81	0.45
3:D:20:ILE:HD13	3:D:108:LEU:HD11	1.98	0.45
2:B:570:VAL:O	2:B:574:LYS:NZ	2.49	0.45
3:D:70:THR:HB	3:D:79:TYR:HB2	1.99	0.45
4:E:34:SER:HB2	4:E:93:TYR:CE1	2.51	0.45
4:E:37:TRP:CE2	4:E:75:LEU:HB2	2.52	0.45
1:G:276:ASN:OD1	1:G:278:THR:HG23	2.17	0.45
6:H:163:ASP:HB3	6:H:194:LEU:HD23	1.99	0.45
3:D:31:PHE:HB2	8:A:1:NAG:C8	2.47	0.45
2:B:650:GLN:HG3	2:B:651:ASN:N	2.32	0.44
1:G:257:THR:O	1:G:453:LEU:HD12	2.17	0.44
1:G:292:VAL:O	1:G:449:ILE:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:102:LEU:HD23	3:D:102:LEU:HA	1.83	0.44
1:G:221:ALA:HB1	2:B:544:LEU:O	2.18	0.44
1:G:249:HIS:O	1:G:251:ILE:HG13	2.18	0.44
6:H:169:VAL:HG12	6:H:219:HIS:ND1	2.33	0.44
2:B:597:GLY:HA3	2:B:651:ASN:HD21	1.82	0.44
3:D:32:TYR:HB3	3:D:95:GLY:H	1.82	0.44
1:G:45:TRP:HE1	2:B:523:LEU:HD21	1.81	0.44
1:G:373:MET:SD	1:G:384:TYR:HB3	2.57	0.44
1:G:421:LYS:HG2	1:G:423:ILE:O	2.18	0.44
5:L:156:LYS:HG2	5:L:161:PRO:HA	2.00	0.44
1:G:173:TYR:CE2	9:C:1:NAG:H3	2.53	0.43
4:E:40:TRP:CG	4:E:46:PRO:HB3	2.53	0.43
1:G:66:ARG:O	1:G:69:TRP:NE1	2.51	0.43
1:G:164:ALA:HB2	1:G:308:HIS:HD2	1.83	0.43
1:G:295:ASN:HB3	7:P:1:NAG:H81	1.99	0.43
6:H:219:HIS:HE2	6:H:221:PRO:HB2	1.81	0.43
5:L:156:LYS:HE3	5:L:199:SER:OG	2.18	0.43
3:D:31:PHE:HA	8:A:1:NAG:O3	2.17	0.43
3:D:103:TRP:CD2	4:E:46:PRO:HG2	2.53	0.43
6:H:178:LEU:HD23	6:H:178:LEU:HA	1.90	0.43
1:G:368:ASP:OD1	1:G:371:ILE:HG12	2.18	0.43
3:D:7:SER:HB3	3:D:21:SER:OG	2.18	0.43
5:L:129:SER:HA	5:L:132:LEU:HD12	2.00	0.43
1:G:181:VAL:CG1	1:G:191:TYR:HB3	2.49	0.43
6:H:38:ARG:HH12	6:H:89:ASP:HA	1.83	0.43
1:G:43:PRO:HG3	2:B:526:ALA:HA	2.01	0.43
1:G:334:SER:HB2	11:J:1:NAG:H81	2.01	0.42
1:G:496:VAL:HG11	2:B:642:ILE:HG21	2.00	0.42
3:D:103:TRP:CE2	4:E:46:PRO:HG2	2.54	0.42
1:G:476:ARG:HA	1:G:479:TRP:CD1	2.54	0.42
3:D:90:TYR:CD1	3:D:108:LEU:HD12	2.54	0.42
6:H:165:PHE:HA	6:H:166:PRO:HA	1.84	0.42
1:G:499:THR:HG22	1:G:501:CYS:H	1.85	0.42
1:G:381:GLU:HG2	1:G:439:ILE:HG12	2.01	0.42
1:G:211:GLU:OE1	10:F:2:NAG:H83	2.20	0.42
1:G:335:ARG:HG3	1:G:414:ILE:HD11	2.01	0.42
2:B:545:LEU:HD11	2:B:586:TYR:CD2	2.55	0.42
2:B:592:LEU:HD23	2:B:595:ILE:HD11	2.02	0.42
1:G:293:ILE:HB	11:J:1:NAG:H83	2.02	0.42
6:H:138:PRO:HD3	6:H:219:HIS:NE2	2.35	0.42
1:G:112:TRP:HB2	1:G:427:TRP:CH2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:13:VAL:N	5:L:111:THR:O	2.44	0.42
5:L:128:SER:OG	6:H:142:PRO:O	2.24	0.42
1:G:298:ARG:NH1	1:G:300:ASN:OD1	2.52	0.41
2:B:630:GLU:HA	2:B:633:ARG:HD2	2.02	0.41
1:G:411:ASP:OD2	7:P:1:NAG:H2	2.20	0.41
5:L:66(B):ILE:HG13	5:L:66(C):ASN:N	2.30	0.41
5:L:86:GLU:OE2	5:L:111:THR:HA	2.19	0.41
1:G:373:MET:HB2	1:G:385:CYS:O	2.20	0.41
6:H:216:ASN:HB3	6:H:227:ASP:CG	2.41	0.41
6:H:214:ILE:CD1	6:H:227:ASP:HB3	2.45	0.41
1:G:120:VAL:HG11	1:G:315:GLN:HB3	2.03	0.41
1:G:255:VAL:HG13	1:G:475:MET:SD	2.61	0.41
2:B:564:HIS:ND1	2:B:567:GLN:HG2	2.35	0.41
1:G:175:LEU:HB2	1:G:320:THR:HB	2.03	0.41
2:B:617:ARG:HB3	2:B:621:ASP:HB2	2.03	0.41
2:B:638:TYR:O	2:B:642:ILE:HG13	2.21	0.41
5:L:11:LEU:O	5:L:111:THR:N	2.42	0.41
1:G:304:ARG:HH21	1:G:439:ILE:HA	1.85	0.41
2:B:538:THR:O	2:B:542:ARG:HG2	2.20	0.41
5:L:94:TRP:HB3	6:H:114:PHE:HE2	1.86	0.41
6:H:47:TRP:O	6:H:60:ASN:HB2	2.19	0.41
6:H:140:VAL:O	6:H:228:LYS:HE2	2.21	0.41
1:G:198:THR:CG2	12:G:602:NAG:H62	2.51	0.41
5:L:138:THR:HG21	6:H:162:LYS:NZ	2.36	0.41
6:H:4:LEU:HD22	6:H:24:VAL:HG12	2.03	0.41
1:G:165:LEU:HD22	1:G:167:ASP:OD1	2.21	0.41
1:G:221:ALA:HB3	2:B:582:ALA:HB1	2.03	0.41
6:H:220:LYS:H	6:H:220:LYS:HG2	1.64	0.41
1:G:272:ILE:H	1:G:348:LYS:HZ3	1.69	0.40
1:G:45:TRP:NE1	2:B:523:LEU:HD21	2.36	0.40
3:D:32:TYR:CD1	3:D:94:LYS:HE2	2.56	0.40
6:H:157:LEU:HD11	6:H:230:VAL:HB	2.02	0.40
1:G:374:HIS:NE2	1:G:376:PHE:HB3	2.36	0.40
4:E:18:VAL:O	4:E:76:THR:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	G	417/431 (97%)	391 (94%)	26 (6%)	0	100 100
2	B	133/137 (97%)	127 (96%)	6 (4%)	0	100 100
3	D	131/141 (93%)	122 (93%)	9 (7%)	0	100 100
4	E	105/107 (98%)	98 (93%)	7 (7%)	0	100 100
5	L	208/210 (99%)	199 (96%)	8 (4%)	1 (0%)	29 68
6	H	222/226 (98%)	210 (95%)	12 (5%)	0	100 100
All	All	1216/1252 (97%)	1147 (94%)	68 (6%)	1 (0%)	51 85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	L	115	GLN

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	G	389/389 (100%)	384 (99%)	5 (1%)	69 82
2	B	120/120 (100%)	114 (95%)	6 (5%)	24 51
3	D	120/120 (100%)	120 (100%)	0	100 100
4	E	94/94 (100%)	94 (100%)	0	100 100
5	L	176/176 (100%)	175 (99%)	1 (1%)	86 92
6	H	194/194 (100%)	185 (95%)	9 (5%)	27 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1093/1093 (100%)	1072 (98%)	21 (2%)	57 75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	165	LEU
1	G	256	SER
1	G	378	CYS
1	G	393	SER
1	G	395	TRP
2	B	613	SER
2	B	615	SER
2	B	630	GLU
2	B	634	GLU
2	B	636	ASP
2	B	639	THR
5	L	70	PHE
6	H	18	LEU
6	H	19	SER
6	H	20	VAL
6	H	21	THR
6	H	37	ILE
6	H	70	SER
6	H	71	ARG
6	H	76	ASN
6	H	77	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	564	HIS
2	B	567	GLN
6	H	76	ASN

5.3.3 RNA

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)

30 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	$\#\|Z\| > 2$
8	NAG	A	1	1,8	14,14,15	0.95	1 (7%)	17,19,21	0.92	0
8	NAG	A	2	8	14,14,15	0.33	0	17,19,21	0.43	0
9	NAG	C	1	1,9	14,14,15	0.46	0	17,19,21	0.61	0
9	NAG	C	2	9	14,14,15	0.35	0	17,19,21	0.64	0
9	BMA	C	3	9	11,11,12	0.71	0	15,15,17	0.81	0
9	MAN	C	4	9	11,11,12	0.80	0	15,15,17	0.95	2 (13%)
9	MAN	C	5	9	11,11,12	0.84	1 (9%)	15,15,17	1.30	2 (13%)
9	MAN	C	6	9	11,11,12	0.87	0	15,15,17	1.11	2 (13%)
10	NAG	F	1	10,1	14,14,15	0.68	1 (7%)	17,19,21	0.68	0
10	NAG	F	2	10	14,14,15	0.19	0	17,19,21	0.50	0
10	BMA	F	3	10	11,11,12	0.68	0	15,15,17	0.82	0
10	MAN	F	4	10	11,11,12	0.93	1 (9%)	15,15,17	0.92	1 (6%)
11	NAG	I	1	11	14,14,15	0.37	0	17,19,21	0.58	0
11	NAG	I	2	11	14,14,15	0.31	0	17,19,21	0.42	0
11	BMA	I	3	11	11,11,12	0.64	0	15,15,17	0.70	0
11	NAG	J	1	11,1	14,14,15	1.32	1 (7%)	17,19,21	1.29	3 (17%)
11	NAG	J	2	11	14,14,15	0.53	0	17,19,21	1.10	1 (5%)
11	BMA	J	3	11	11,11,12	1.27	2 (18%)	15,15,17	1.24	1 (6%)
8	NAG	K	1	1,8	14,14,15	0.24	0	17,19,21	0.41	0
8	NAG	K	2	8	14,14,15	0.23	0	17,19,21	0.41	0
8	NAG	M	1	1,8	14,14,15	1.00	1 (7%)	17,19,21	1.08	1 (5%)
8	NAG	M	2	8	14,14,15	0.24	0	17,19,21	0.67	0
11	NAG	N	1	11,1	14,14,15	0.88	1 (7%)	17,19,21	1.17	1 (5%)
11	NAG	N	2	11	14,14,15	0.25	0	17,19,21	0.52	0
11	BMA	N	3	11	11,11,12	0.57	0	15,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	P	1	1,7	14,14,15	0.25	0	17,19,21	0.50	0
7	NAG	P	2	7	14,14,15	0.23	0	17,19,21	0.63	0
7	BMA	P	3	7	11,11,12	0.57	0	15,15,17	0.86	1 (6%)
7	MAN	P	4	7	11,11,12	1.62	3 (27%)	15,15,17	2.43	4 (26%)
7	MAN	P	5	7	11,11,12	0.72	0	15,15,17	0.99	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	1	1,8	-	1/6/23/26	0/1/1/1
8	NAG	A	2	8	-	0/6/23/26	0/1/1/1
9	NAG	C	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	C	2	9	-	1/6/23/26	0/1/1/1
9	BMA	C	3	9	-	1/2/19/22	0/1/1/1
9	MAN	C	4	9	-	2/2/19/22	0/1/1/1
9	MAN	C	5	9	-	1/2/19/22	0/1/1/1
9	MAN	C	6	9	-	0/2/19/22	1/1/1/1
10	NAG	F	1	10,1	-	0/6/23/26	0/1/1/1
10	NAG	F	2	10	-	0/6/23/26	0/1/1/1
10	BMA	F	3	10	-	0/2/19/22	0/1/1/1
10	MAN	F	4	10	-	1/2/19/22	0/1/1/1
11	NAG	I	1	11	-	1/6/23/26	0/1/1/1
11	NAG	I	2	11	-	0/6/23/26	0/1/1/1
11	BMA	I	3	11	-	0/2/19/22	0/1/1/1
11	NAG	J	1	11,1	-	2/6/23/26	0/1/1/1
11	NAG	J	2	11	-	0/6/23/26	0/1/1/1
11	BMA	J	3	11	-	1/2/19/22	0/1/1/1
8	NAG	K	1	1,8	-	0/6/23/26	0/1/1/1
8	NAG	K	2	8	-	0/6/23/26	0/1/1/1
8	NAG	M	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	M	2	8	-	1/6/23/26	0/1/1/1
11	NAG	N	1	11,1	-	3/6/23/26	0/1/1/1
11	NAG	N	2	11	-	2/6/23/26	0/1/1/1
11	BMA	N	3	11	-	0/2/19/22	0/1/1/1
7	NAG	P	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	P	2	7	-	1/6/23/26	0/1/1/1
7	BMA	P	3	7	-	0/2/19/22	0/1/1/1
7	MAN	P	4	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	P	5	7	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	J	1	NAG	O5-C1	-4.75	1.36	1.43
7	P	4	MAN	C1-C2	3.70	1.60	1.52
8	A	1	NAG	O5-C1	-3.32	1.38	1.43
11	N	1	NAG	O5-C1	-3.12	1.38	1.43
8	M	1	NAG	O5-C1	-3.00	1.38	1.43
7	P	4	MAN	O5-C1	2.88	1.48	1.43
9	C	5	MAN	C1-C2	2.53	1.58	1.52
11	J	3	BMA	O5-C1	-2.45	1.39	1.43
10	F	1	NAG	O5-C1	-2.31	1.40	1.43
7	P	4	MAN	O5-C5	2.21	1.47	1.43
10	F	4	MAN	C1-C2	2.15	1.57	1.52
11	J	3	BMA	O5-C5	-2.02	1.39	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	P	4	MAN	C1-O5-C5	7.41	122.23	112.19
11	J	3	BMA	C3-C4-C5	3.78	116.99	110.24
7	P	4	MAN	O5-C1-C2	3.52	116.20	110.77
11	J	1	NAG	C3-C4-C5	3.35	116.21	110.24
9	C	5	MAN	C1-O5-C5	3.21	116.55	112.19
11	J	2	NAG	C3-C4-C5	3.14	115.85	110.24
11	J	1	NAG	C4-C3-C2	3.08	115.53	111.02
9	C	6	MAN	C1-O5-C5	3.08	116.36	112.19
8	M	1	NAG	C3-C4-C5	3.07	115.71	110.24
11	N	1	NAG	C3-C4-C5	2.81	115.25	110.24
7	P	4	MAN	O2-C2-C3	-2.56	105.01	110.14
11	J	1	NAG	C1-O5-C5	-2.44	108.88	112.19
7	P	4	MAN	C1-C2-C3	2.43	112.66	109.67
9	C	5	MAN	O2-C2-C3	-2.23	105.68	110.14
10	F	4	MAN	O2-C2-C3	-2.22	105.70	110.14
9	C	4	MAN	O2-C2-C3	-2.22	105.70	110.14
7	P	3	BMA	O2-C2-C3	-2.20	105.73	110.14
9	C	6	MAN	O2-C2-C3	-2.19	105.75	110.14
7	P	5	MAN	O2-C2-C3	-2.18	105.77	110.14
9	C	4	MAN	C1-O5-C5	2.08	115.02	112.19
7	P	5	MAN	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (22) torsion outliers are listed below:

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

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	6	MAN	C1-C2-C3-C4-C5-O5

13 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	I	1	NAG	2	0
10	F	4	MAN	1	0
11	N	2	NAG	1	0
9	C	1	NAG	1	0
10	F	3	BMA	1	0
8	A	1	NAG	2	0
7	P	2	NAG	1	0
11	J	3	BMA	2	0
11	J	1	NAG	2	0

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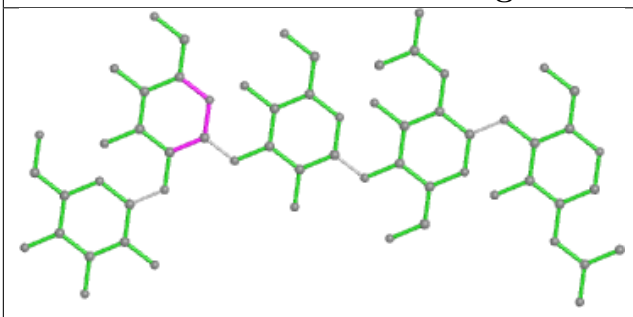
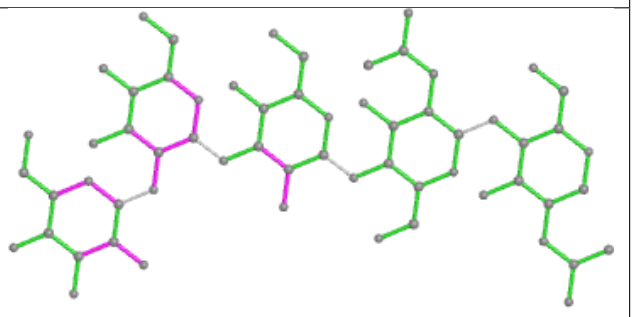
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	F	2	NAG	1	0
7	P	1	NAG	2	0
11	N	1	NAG	3	0
11	J	2	NAG	1	0

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

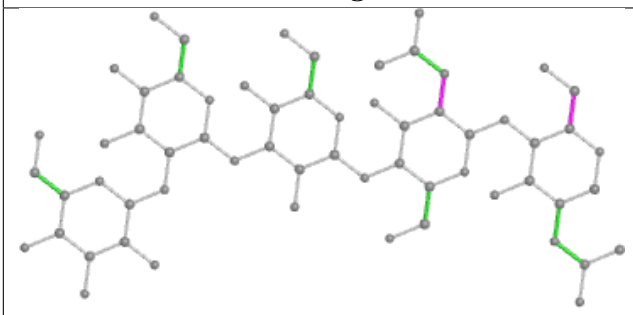
Oligosaccharide Chain P



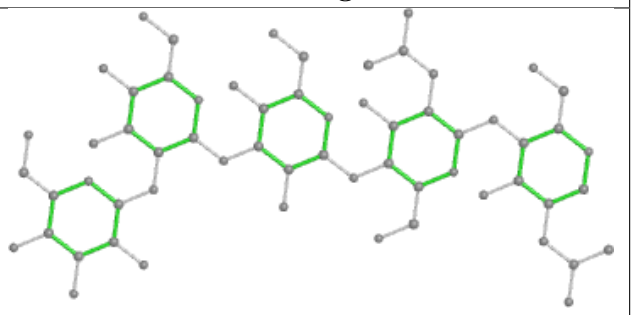
Bond lengths



Bond angles

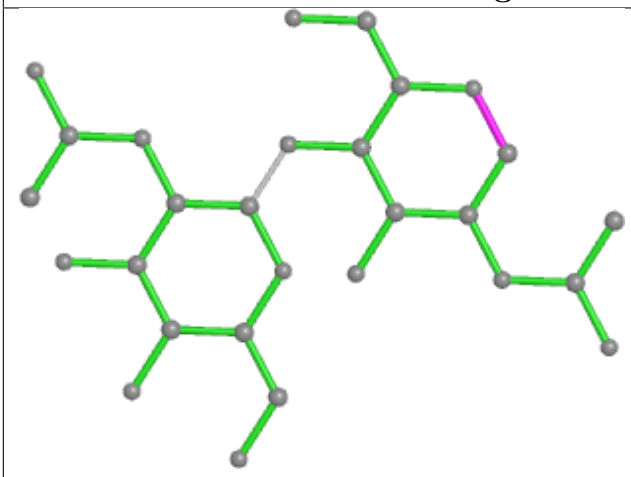


Torsions

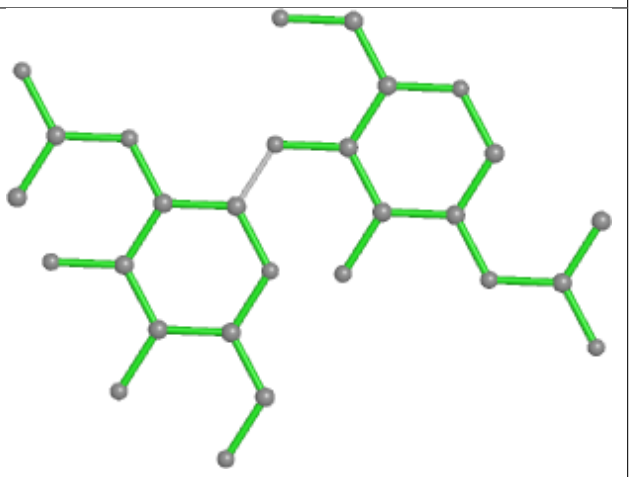


Rings

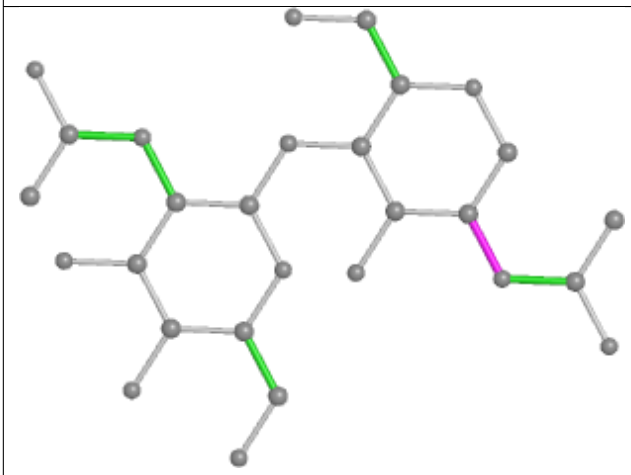
Oligosaccharide Chain A



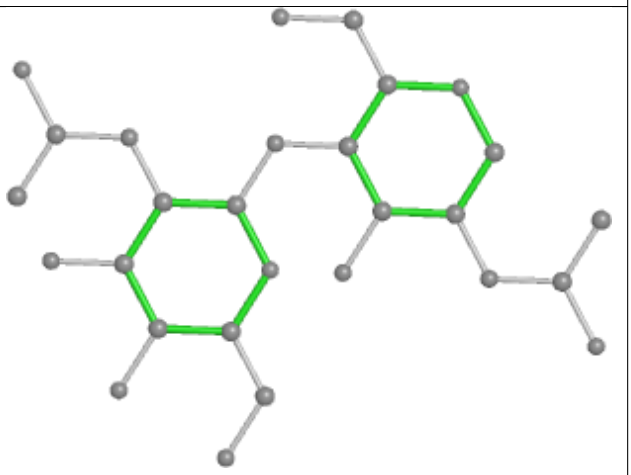
Bond lengths



Bond angles

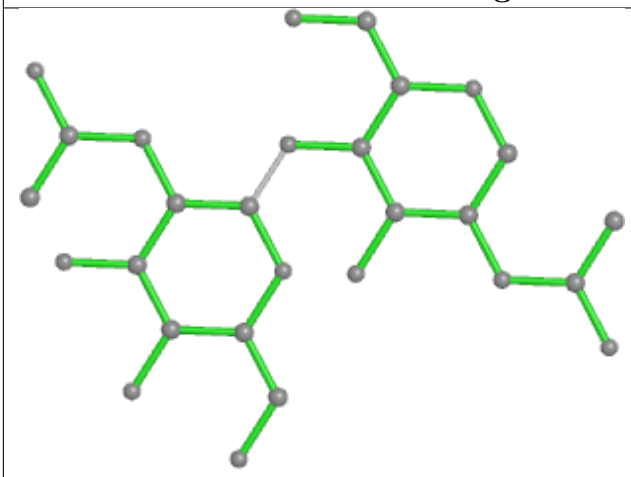


Torsions

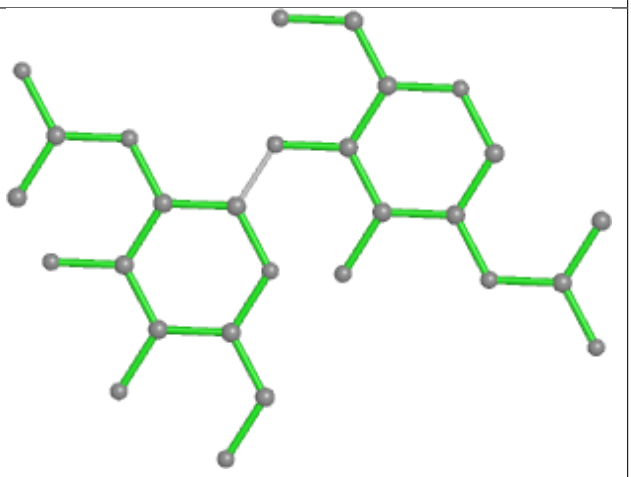


Rings

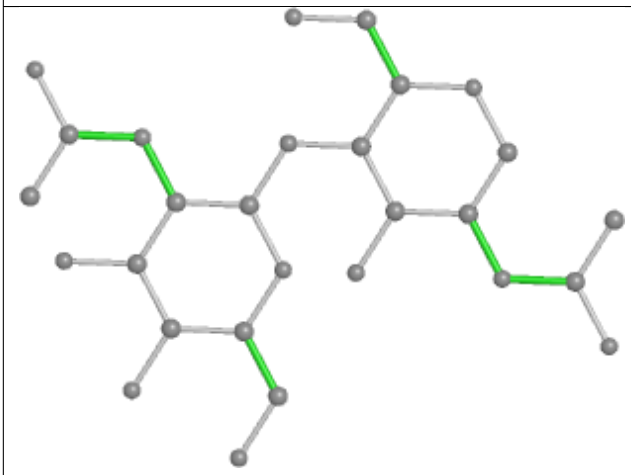
Oligosaccharide Chain K



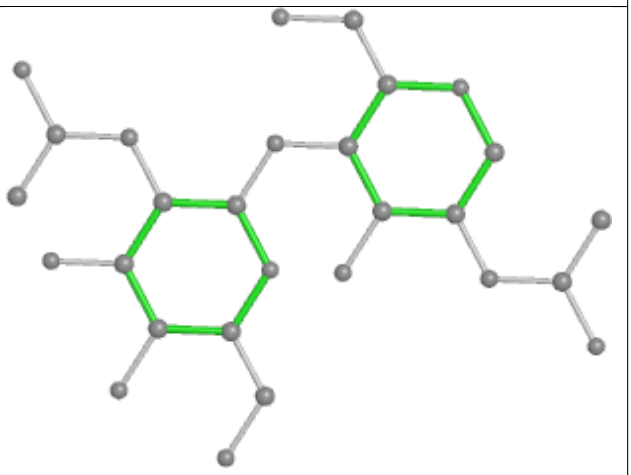
Bond lengths



Bond angles

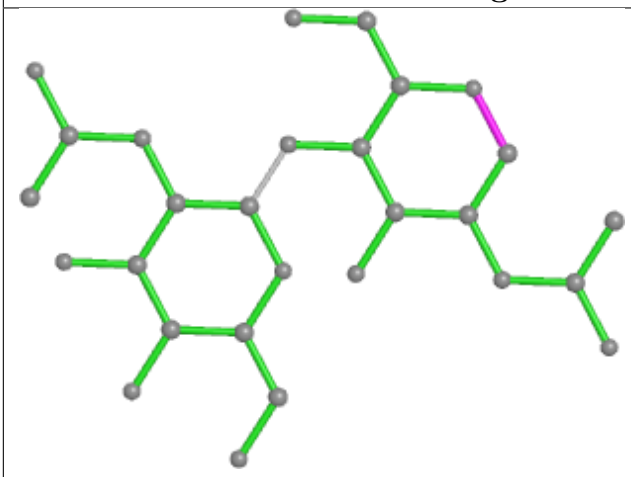


Torsions

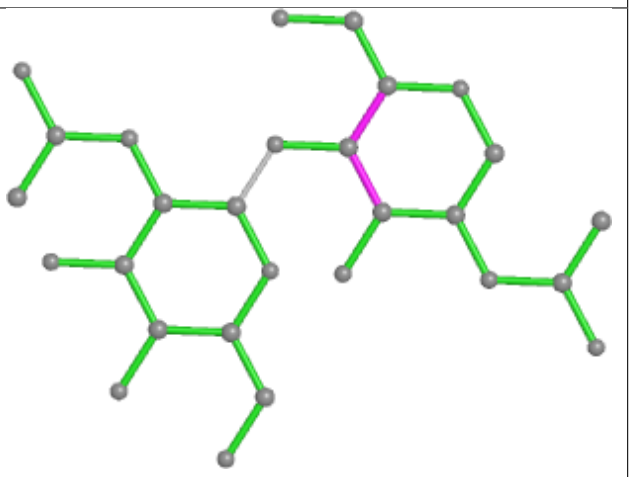


Rings

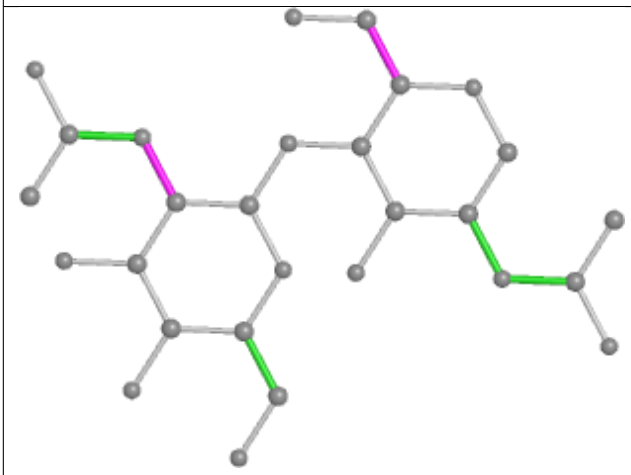
Oligosaccharide Chain M



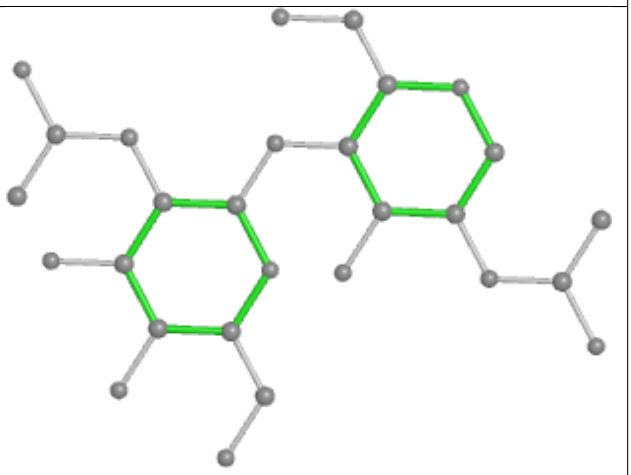
Bond lengths



Bond angles

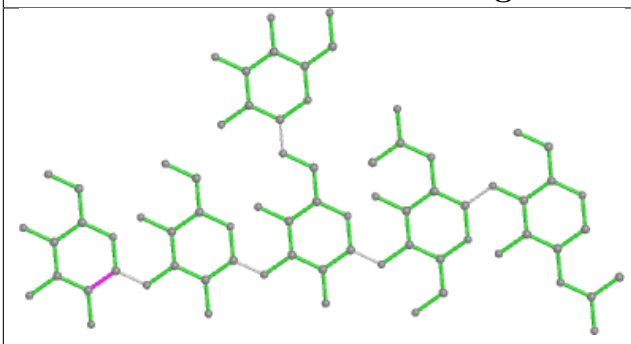


Torsions

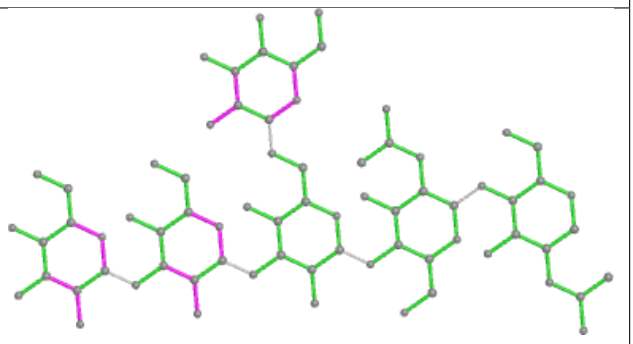


Rings

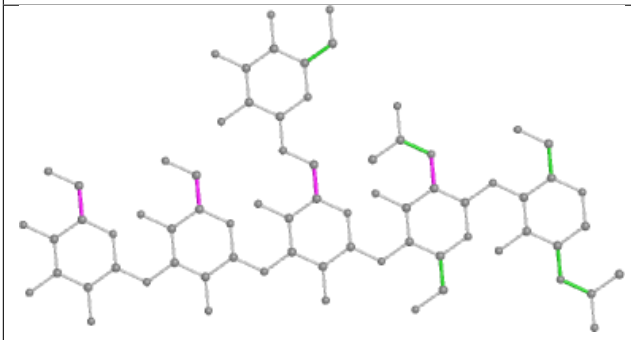
Oligosaccharide Chain C



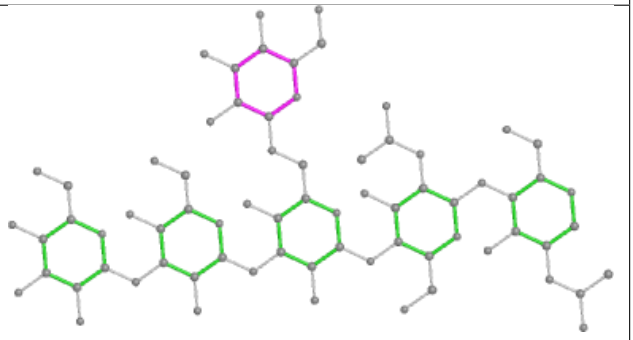
Bond lengths



Bond angles

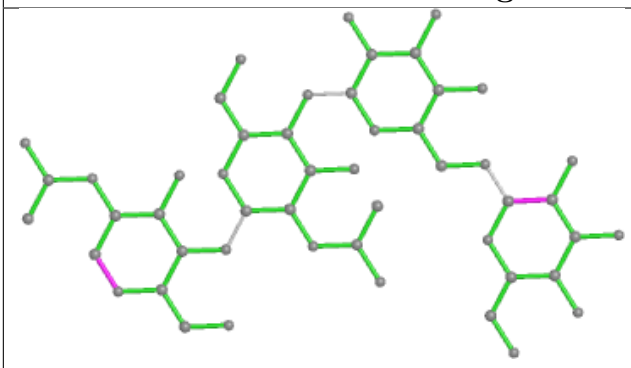


Torsions

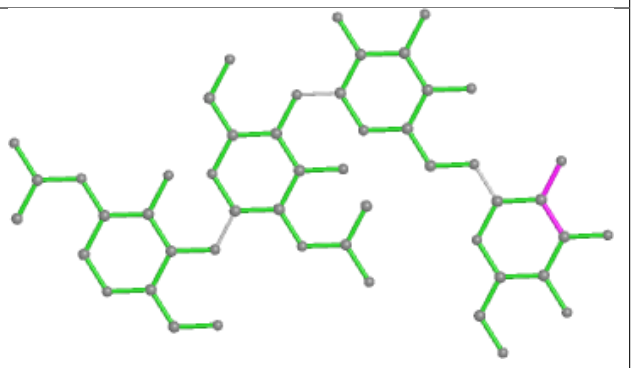


Rings

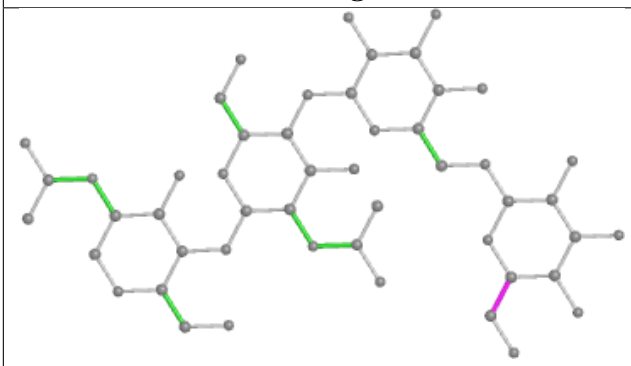
Oligosaccharide Chain F



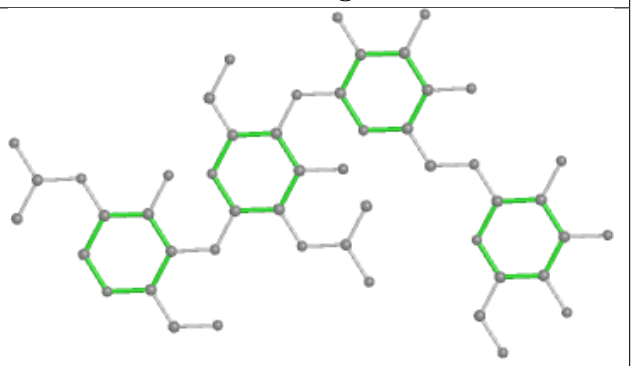
Bond lengths



Bond angles

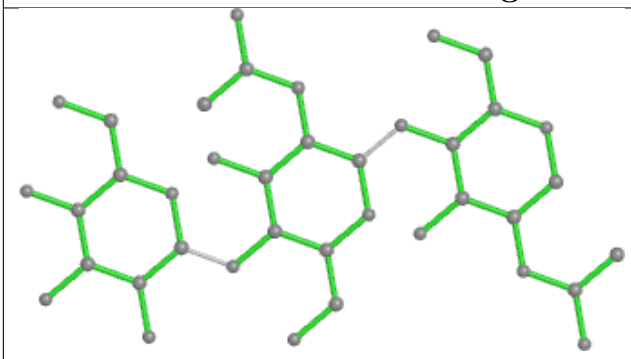


Torsions

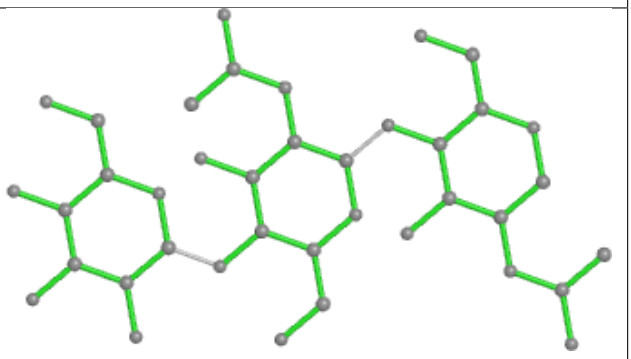


Rings

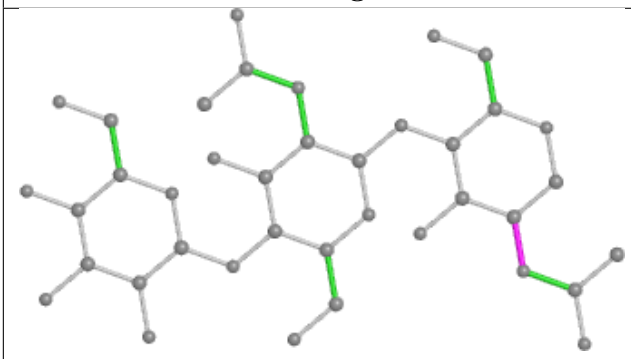
Oligosaccharide Chain I



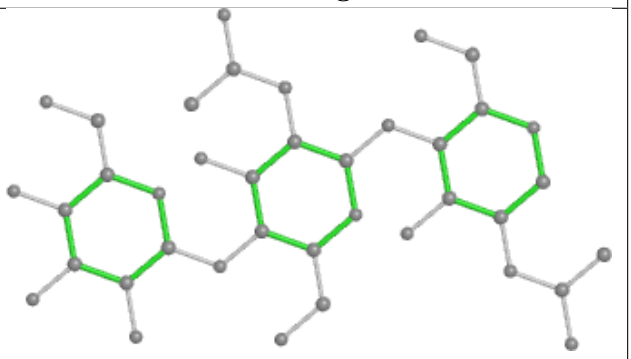
Bond lengths



Bond angles

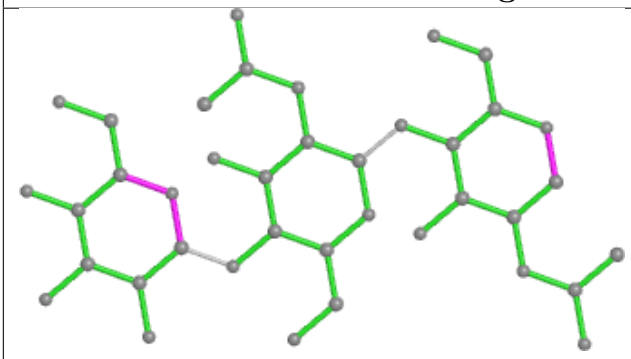


Torsions

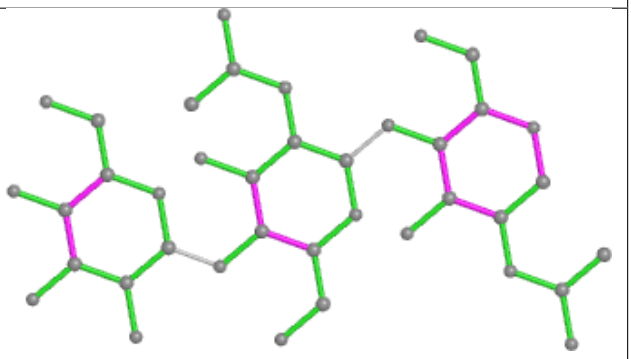


Rings

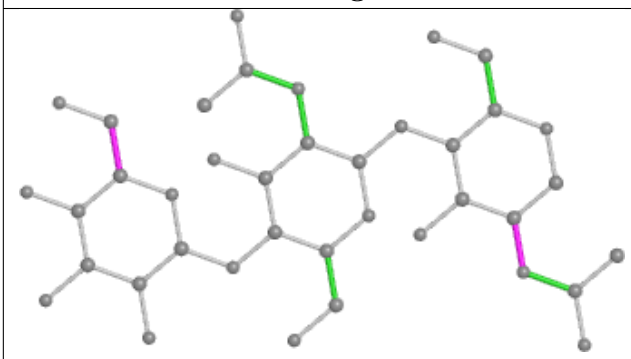
Oligosaccharide Chain J



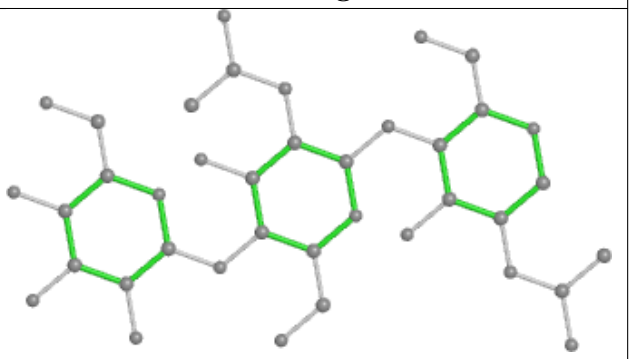
Bond lengths



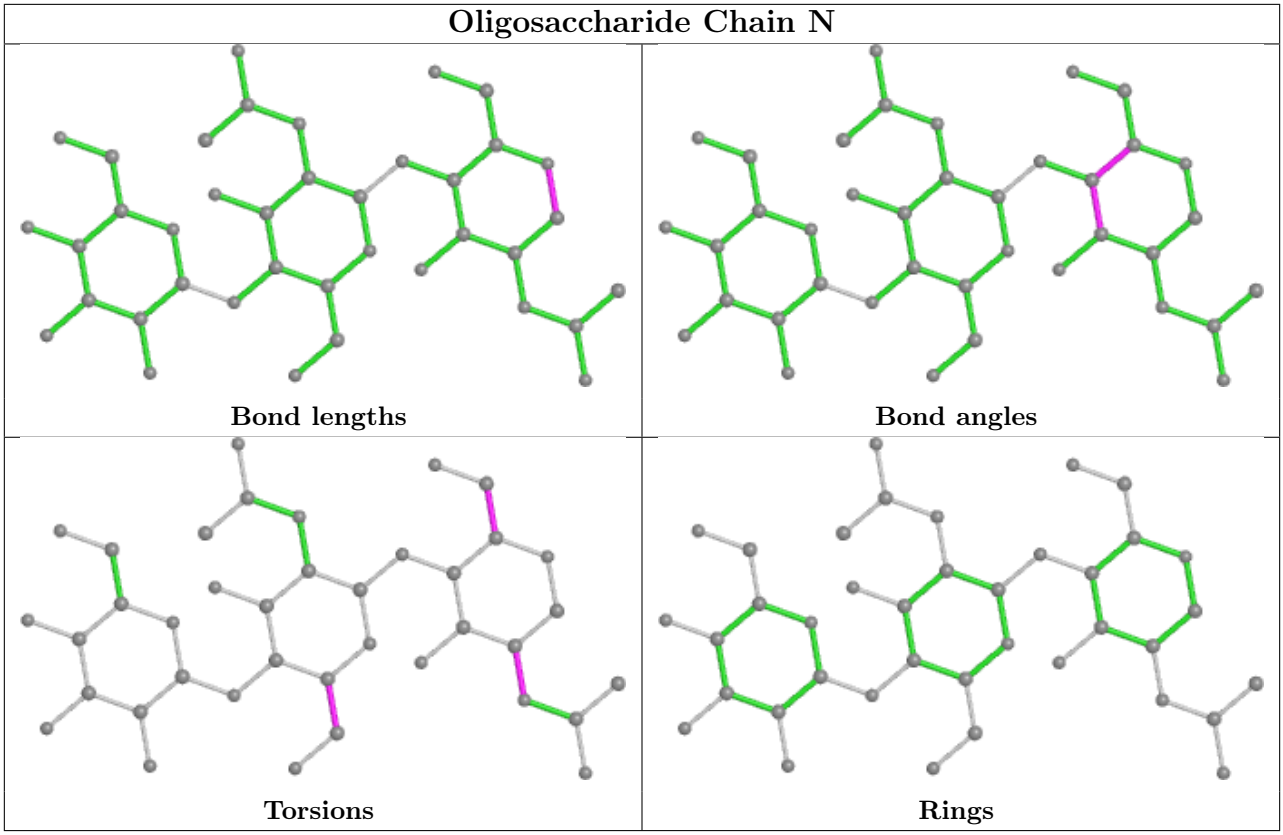
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	NAG	G	604	1	14,14,15	0.44	0	17,19,21	0.49	0
12	NAG	G	605	1	14,14,15	0.22	0	17,19,21	0.42	0
12	NAG	G	601	1	14,14,15	0.57	0	17,19,21	0.95	1 (5%)
13	MAN	G	606	-	11,11,12	1.72	3 (27%)	15,15,17	1.42	2 (13%)
12	NAG	B	702	2	14,14,15	0.30	0	17,19,21	0.57	0
12	NAG	G	602	-	14,14,15	0.16	0	17,19,21	0.64	0
12	NAG	G	603	1	14,14,15	0.20	0	17,19,21	0.40	0
12	NAG	B	701	2	14,14,15	0.27	0	17,19,21	0.48	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
12	NAG	G	604	1	-	2/6/23/26	0/1/1/1
12	NAG	G	605	1	-	0/6/23/26	0/1/1/1
12	NAG	G	601	1	-	2/6/23/26	0/1/1/1
13	MAN	G	606	-	-	0/2/19/22	0/1/1/1
12	NAG	B	702	2	-	0/6/23/26	0/1/1/1
12	NAG	G	602	-	-	2/6/23/26	0/1/1/1
12	NAG	G	603	1	-	2/6/23/26	0/1/1/1
12	NAG	B	701	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	G	606	MAN	O5-C1	-3.93	1.37	1.43
13	G	606	MAN	C2-C3	-2.69	1.48	1.52
13	G	606	MAN	C4-C5	2.42	1.58	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	G	606	MAN	O2-C2-C3	-3.65	102.83	110.14
12	G	601	NAG	C1-O5-C5	3.44	116.85	112.19
13	G	606	MAN	C1-O5-C5	2.30	115.31	112.19

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	603	NAG	C8-C7-N2-C2
12	G	603	NAG	O7-C7-N2-C2
12	G	604	NAG	C8-C7-N2-C2
12	G	604	NAG	O7-C7-N2-C2
12	G	601	NAG	O5-C5-C6-O6
12	G	601	NAG	C4-C5-C6-O6
12	G	602	NAG	C4-C5-C6-O6
12	G	602	NAG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	G	606	MAN	1	0
12	G	602	NAG	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	6
3	D	4
6	H	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	397:ALA	C	410:ALA	N	26.97
1	G	355:ASN	C	368:ASP	N	25.63
1	G	136:GLY	C	146:VAL	N	19.33
1	H	145:PRO	C	151:SER	N	16.96
1	D	54:SER	C	60:ALA	N	15.44
1	D	82(B):ASN	C	89:THR	N	15.27
1	D	119:PRO	C	140:CYS	N	12.75
1	G	60:SER	C	65:LYS	N	7.35
1	D	146:PHE	C	176:TYR	N	7.35
1	B	553:ASN	C	563:GLN	N	5.97
1	G	184:ILE	C	186:THR	N	5.48
1	G	458:GLY	C	466:GLU	N	4.90

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	G	431/431 (100%)	-0.29	4 (0%) 84 77	65, 165, 219, 301	0
2	B	137/137 (100%)	-0.30	1 (0%) 87 82	97, 167, 209, 251	0
3	D	141/141 (100%)	0.04	11 (7%) 13 11	130, 218, 268, 313	0
4	E	107/107 (100%)	-0.57	0 100 100	135, 195, 229, 245	0
5	L	210/210 (100%)	-0.44	1 (0%) 91 86	149, 201, 231, 248	0
6	H	226/226 (100%)	-0.32	6 (2%) 54 44	107, 206, 250, 262	0
All	All	1252/1252 (100%)	-0.31	23 (1%) 68 59	65, 188, 241, 313	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	182	VAL	7.7
1	G	466	GLU	6.6
3	D	181	VAL	5.2
6	H	157	LEU	4.0
3	D	109	LEU	3.4
1	G	468	PHE	3.2
3	D	108	LEU	3.1
6	H	158	GLY	3.1
3	D	119	PRO	2.9
3	D	110	THR	2.8
3	D	146	PHE	2.8
5	L	47	LEU	2.8
3	D	183	THR	2.6
3	D	180	SER	2.6
6	H	7	SER	2.6
1	G	354	GLY	2.4
2	B	543	ASN	2.4
3	D	185	PRO	2.3
6	H	169	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	59	LYS	2.2
6	H	198	SER	2.2
3	D	9	ALA	2.1
6	H	155	ALA	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, 95^{th} 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
9	MAN	C	6	11/12	0.12	0.40	297,297,297,297	0
9	BMA	C	3	11/12	0.53	0.15	274,274,274,274	0
11	NAG	I	2	14/15	0.64	0.46	199,199,199,199	0
10	MAN	F	4	11/12	0.68	0.20	234,234,234,234	0
8	NAG	K	2	14/15	0.70	0.43	235,235,235,235	0
11	NAG	J	2	14/15	0.70	0.24	260,260,260,260	0
11	NAG	I	1	14/15	0.72	0.24	180,180,180,180	0
8	NAG	M	2	14/15	0.73	0.58	266,266,266,266	0
9	NAG	C	2	14/15	0.73	0.23	244,244,244,244	0
11	NAG	J	1	14/15	0.74	0.18	229,229,229,229	0
8	NAG	A	2	14/15	0.75	0.24	195,195,195,195	0
10	NAG	F	2	14/15	0.76	0.23	218,218,218,218	0
9	NAG	C	1	14/15	0.76	0.29	222,222,222,222	0
8	NAG	A	1	14/15	0.79	0.15	185,185,185,185	0
11	BMA	J	3	11/12	0.79	0.13	262,262,262,262	0
9	MAN	C	4	11/12	0.80	0.17	270,270,270,270	0
10	BMA	F	3	11/12	0.80	0.14	232,232,232,232	0
10	NAG	F	1	14/15	0.81	0.20	208,208,208,208	0
11	BMA	N	3	11/12	0.81	0.25	251,251,251,251	0
8	NAG	M	1	14/15	0.84	0.28	217,217,217,217	0
9	MAN	C	5	11/12	0.86	0.15	273,273,273,273	0
11	NAG	N	1	14/15	0.88	0.23	228,228,228,228	0
7	MAN	P	4	11/12	0.89	0.22	146,146,146,146	0
11	BMA	I	3	11/12	0.90	0.54	211,211,211,211	0

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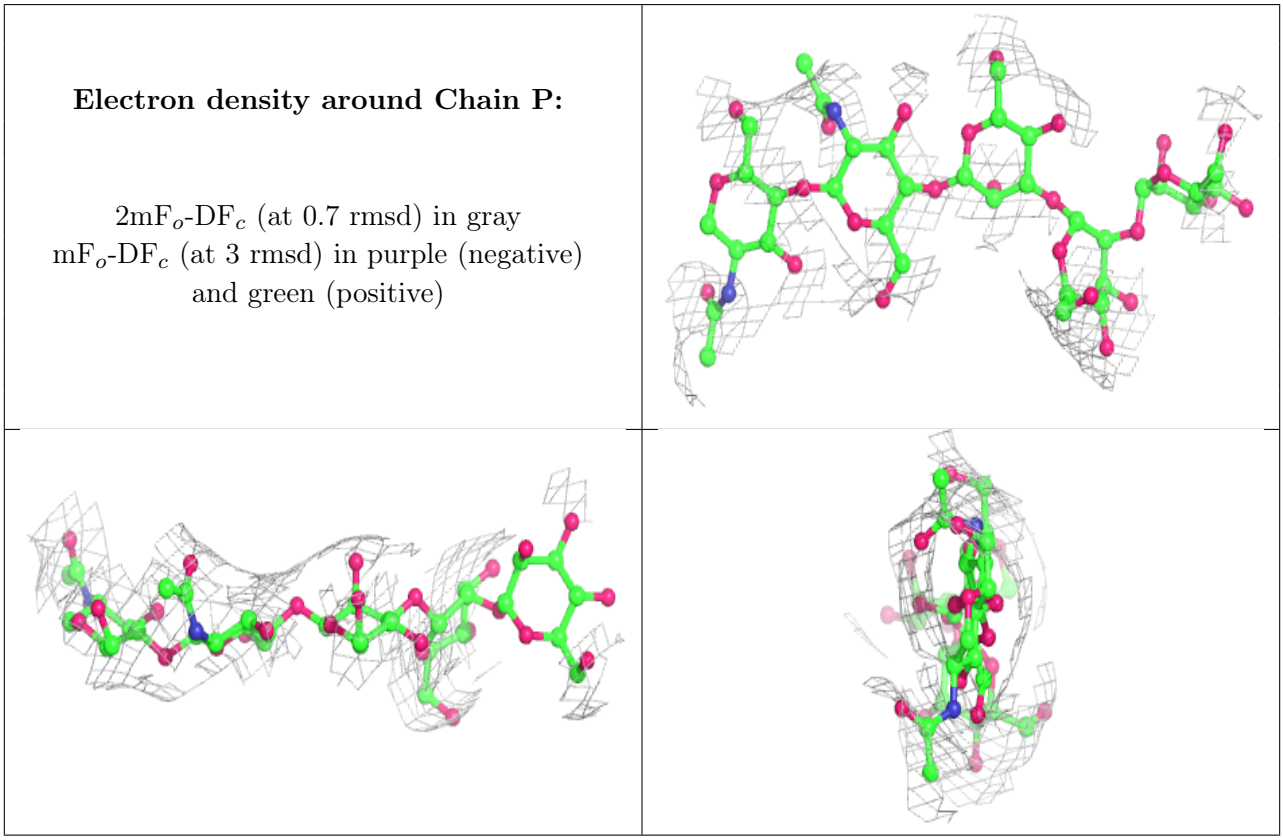
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	N	2	14/15	0.90	0.24	241,241,241,241	0
8	NAG	K	1	14/15	0.90	0.15	186,186,186,186	0
7	BMA	P	3	11/12	0.91	0.19	167,184,199,210	0
7	NAG	P	1	14/15	0.91	0.19	204,223,227,238	0
7	NAG	P	2	14/15	0.91	0.14	182,211,231,239	0
7	MAN	P	5	11/12	0.92	0.21	169,169,169,169	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.

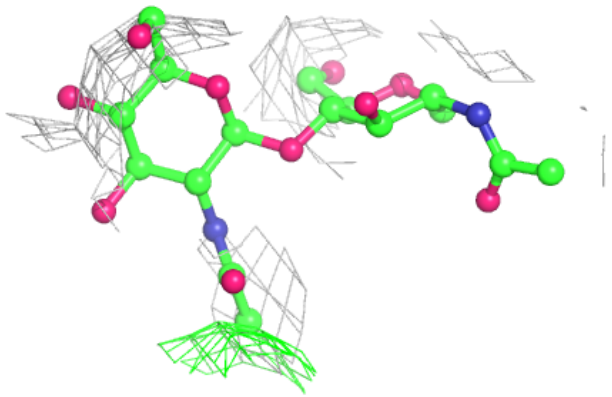
Electron density around Chain P:

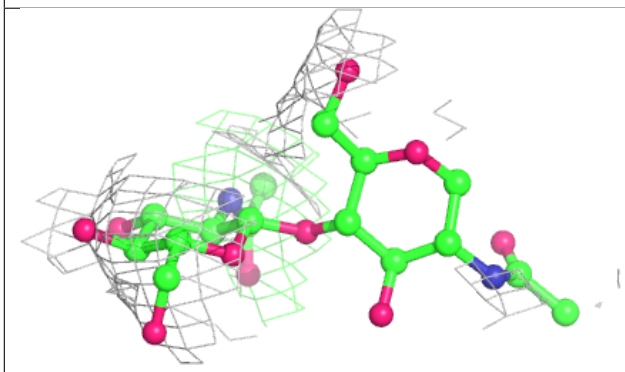
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

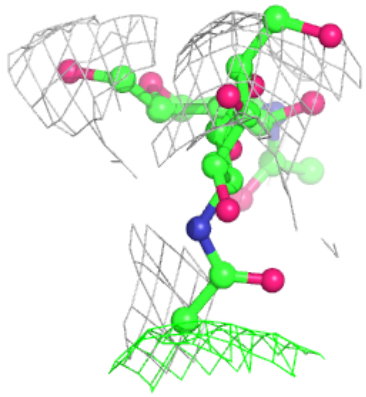


Electron density around Chain A:

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

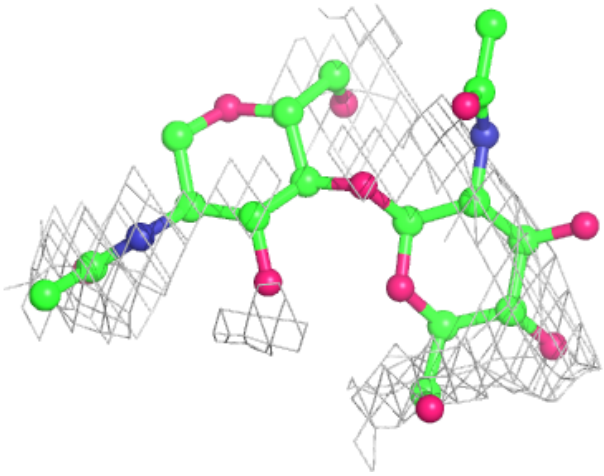


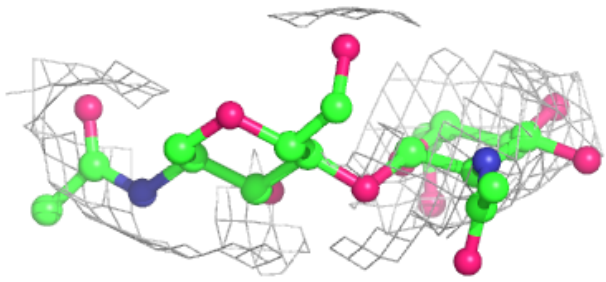


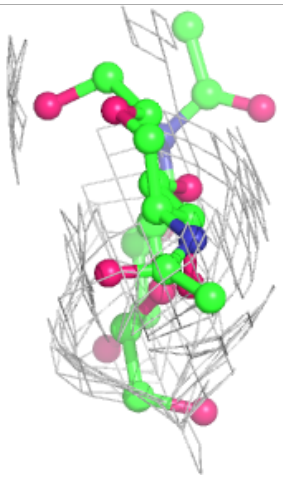


Electron density around Chain K:

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

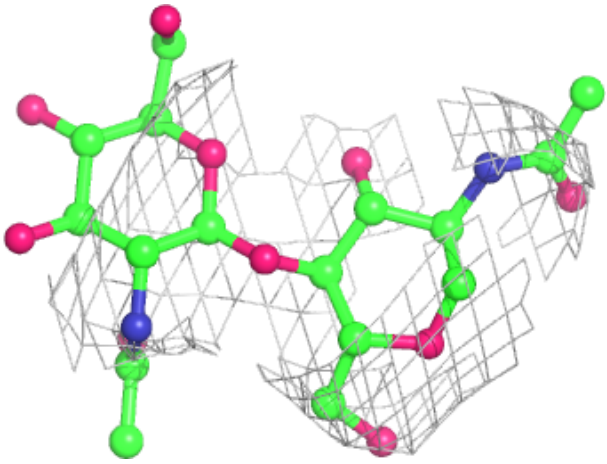


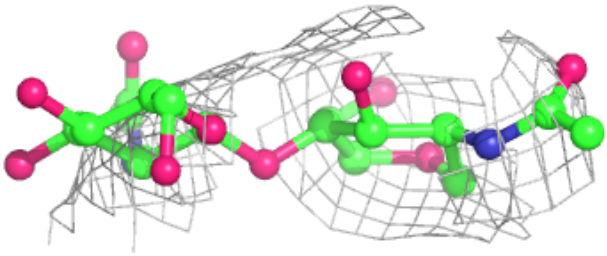


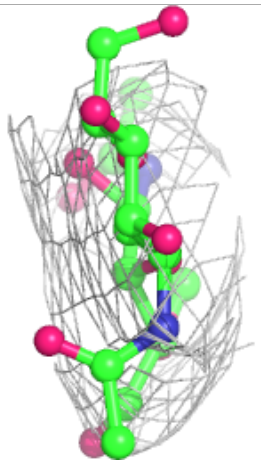


Electron density around Chain M:

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

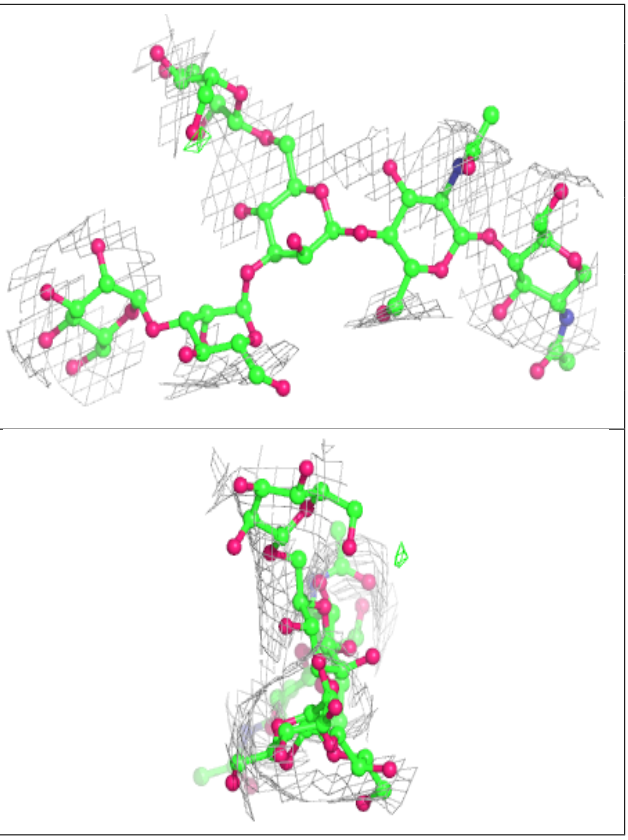






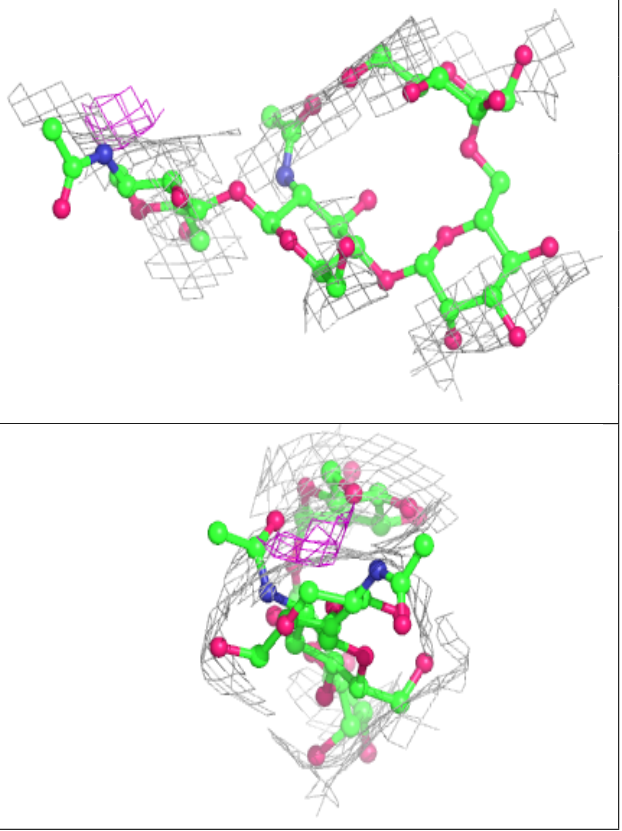
Electron density around Chain C:

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



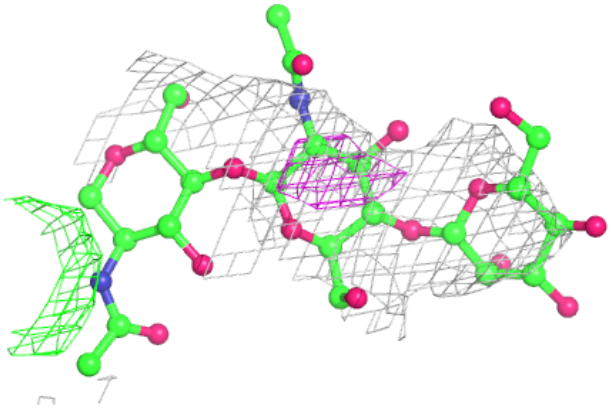
Electron density around Chain F:

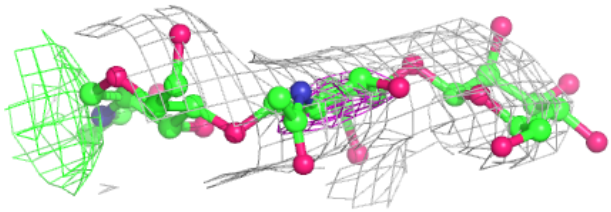
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

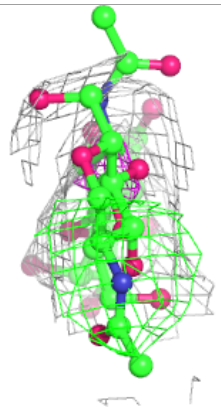


Electron density around Chain I:

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

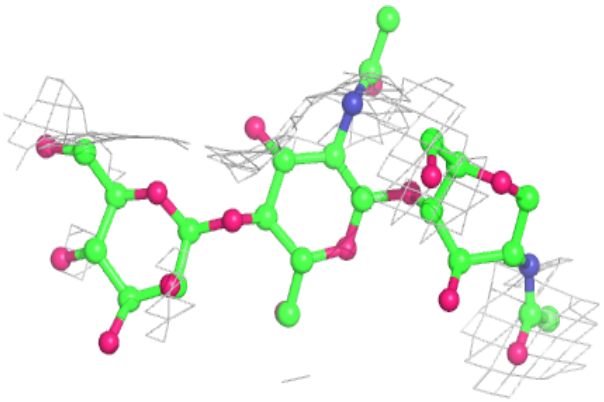


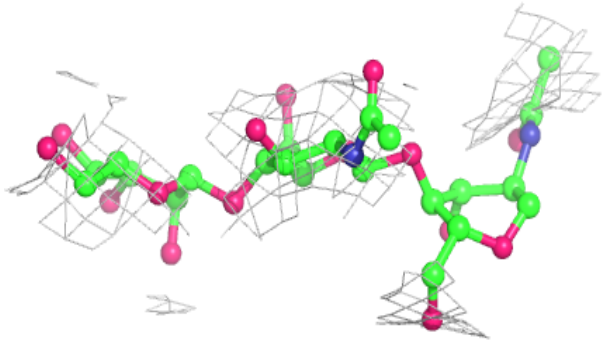


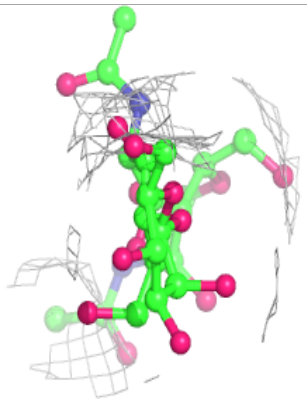


Electron density around Chain J:

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

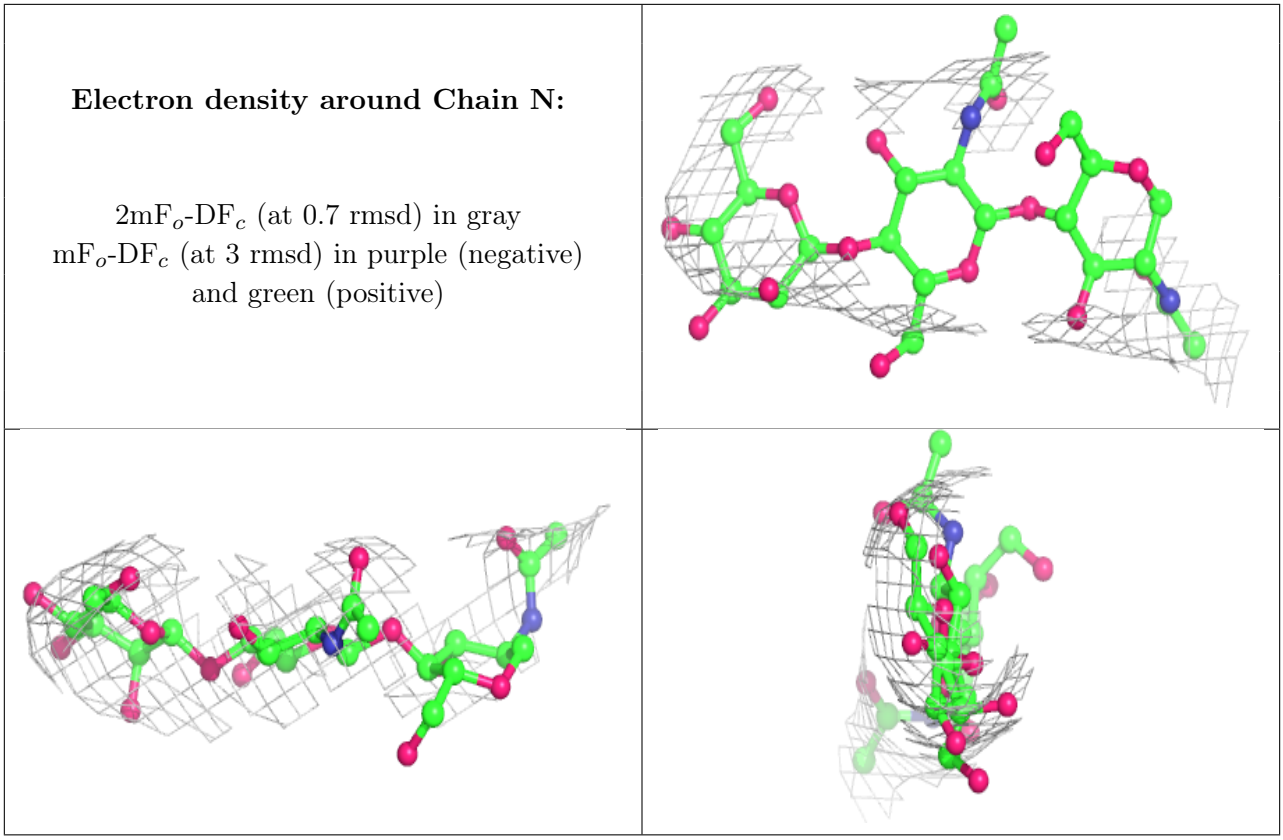






Electron density around Chain N:

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



6.4 Ligands

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, 95^{th} 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
12	NAG	G	603	14/15	0.76	0.21	180,180,180,180	0
13	MAN	G	606	11/12	0.76	0.22	264,264,264,264	0
12	NAG	G	601	14/15	0.79	0.21	204,204,204,204	0
12	NAG	B	702	14/15	0.81	0.34	227,227,227,227	0
12	NAG	G	604	14/15	0.83	0.21	183,183,183,183	0
12	NAG	G	602	14/15	0.86	0.48	195,195,195,195	0
12	NAG	B	701	14/15	0.87	0.25	226,226,226,226	0
12	NAG	G	605	14/15	0.94	0.13	192,192,192,192	0

6.5 Other polymers

There are no such residues in this entry.