Full wwPDB X-ray Structure Validation Report

Aug 6, 2020 – 01:21 PM BST

PDB ID	:	6CH7
Title	:	XFEL crystal structure of a natively-glycosylated BG505 SOSIP.664 HIV-1 Envelope Trimer in complex with the broadly-neutralizing antibodies BG18 and 35O22
Authors	:	Barnes, C.O.; Bjorkman, P.J.
Deposited on	:	2018-02-22
Resolution	:	3.80 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 following versions of software and data (see references (1)) were used in the production of this report:

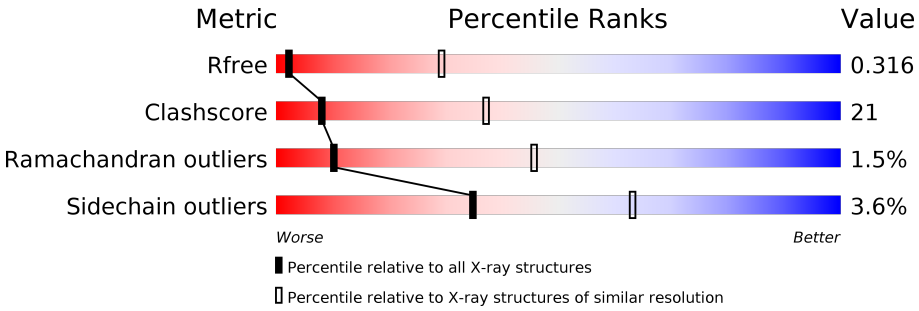
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	B	153	63% 23% • 12%
2	D	243	58% 33% • 7%
3	E	216	63% 32% • •
4	G	479	59% 33% • 6%
5	Q	241	65% 27% • •
6	R	215	58% 36% • •
7	A	5	60% 40%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	C	8	13% 63% 25%
9	F	8	88% 13%
10	H	3	33% 33% 33%
10	J	3	67% 33%
10	M	3	33% 67%
11	I	4	75% 25%
12	K	7	71% 29%
13	L	6	33% 17% 50%
14	N	2	50% 50%
15	O	7	57% 43%
16	P	7	57% 29% 14%
17	S	6	33% 33% 33%
18	T	9	22% 44% 33%

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 12160 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 gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	134	Total	C	N	O	S	0	0	0
			1068	675	186	201	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	engineered mutation	UNP Q2N0S7

- Molecule 2 is a protein called 35O22 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	226	Total	C	N	O	S	0	0	0
			1708	1086	287	328	7			

- Molecule 3 is a protein called 35O22 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	213	Total	C	N	O	S	0	0	0
			1615	1012	267	328	8			

- Molecule 4 is a protein called Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	452	Total	C	N	O	S	0	0	0
			3546	2224	628	667	27			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	152	THR	GLY	conflict	UNP Q2N0S6
G	332	ASN	THR	conflict	UNP Q2N0S6
G	501	CYS	ALA	conflict	UNP Q2N0S6

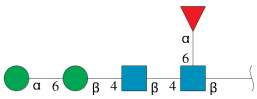
- Molecule 5 is a protein called BG18 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	231	Total	C	N	O	S	0	0	0
			1709	1077	291	333	8			

- Molecule 6 is a protein called BG18 Light Chain.

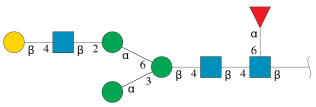
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	211	Total	C	N	O	S	0	0	0
			1527	958	255	308	6			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



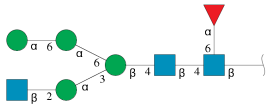
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	A	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 8 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



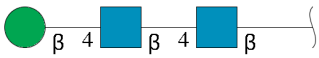
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	C	8	Total	C	N	O	0	0	0
			96	54	3	39			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	F	8	Total	C	N	O	0	0	0
			96	54	3	39			

- Molecule 10 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.

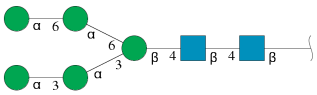


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	H	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	J	3	Total	C	N	O	0	0	0
			39	22	2	15			
10	M	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 11 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.

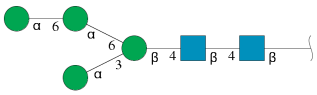
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	4	Total	C	N	O	0	0	0
			50	28	2	20			

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-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
12	K	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

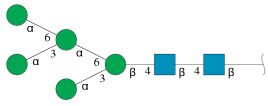


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 14 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
14	N	2	Total	C	N	O	0	0	0
			28	16	2	10			

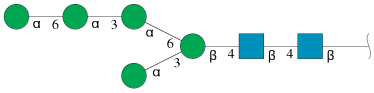
- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

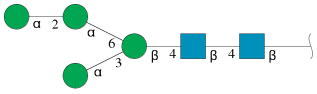
- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl

ucopyranose.



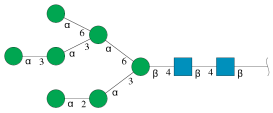
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



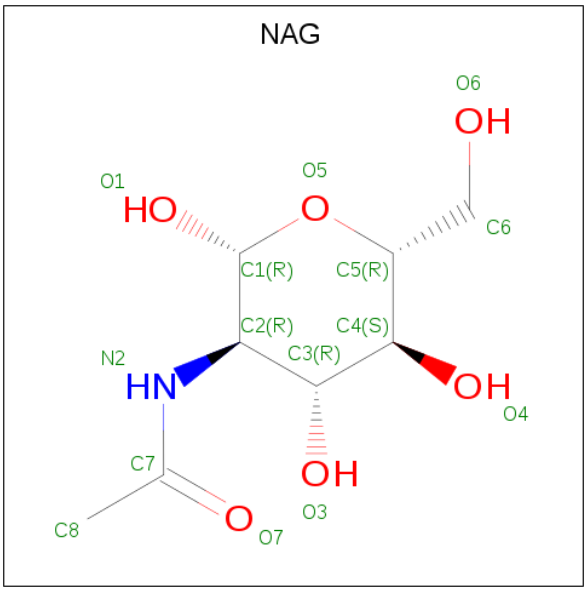
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	S	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 18 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
18	T	9	Total	C	N	O	0	0	0
			105	58	2	45			

- Molecule 19 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



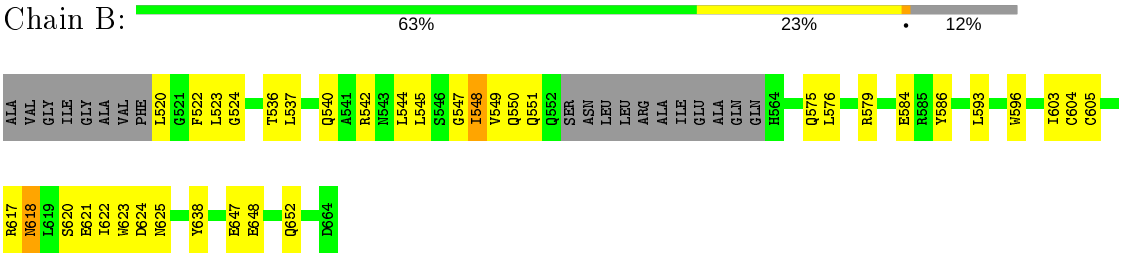
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
19	B	1	Total C N O 14 8 1 5	0	0
19	G	1	Total C N O 14 8 1 5	0	0
19	G	1	Total C N O 14 8 1 5	0	0

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. 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. 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.

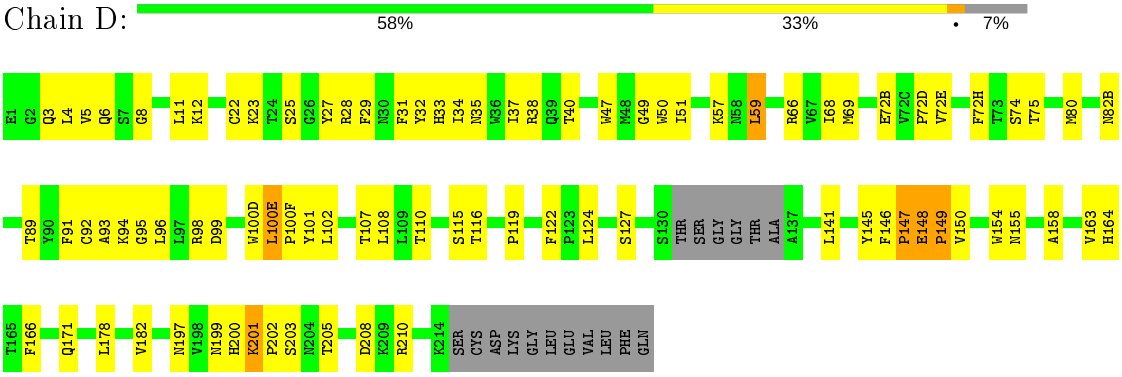
- Molecule 1: Envelope glycoprotein gp41

Chain B:



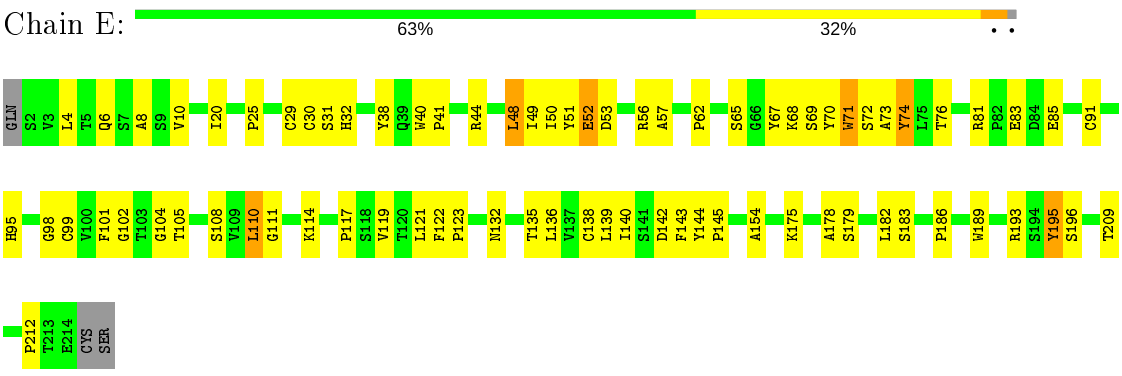
- Molecule 2: 35O22 Heavy Chain

Chain D:



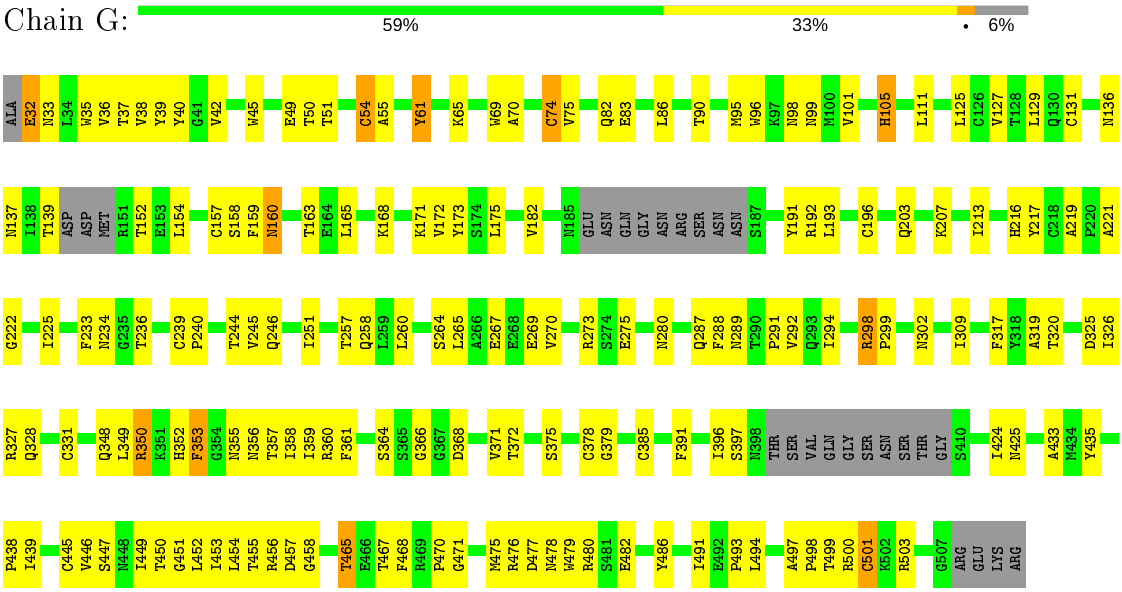
- Molecule 3: 35O22 Light Chain

Chain E:



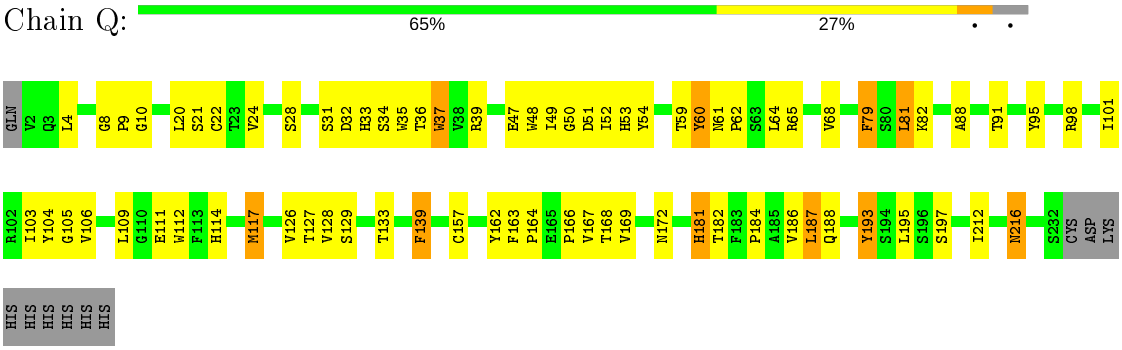
- Molecule 4: Envelope glycoprotein gp120

Chain G:



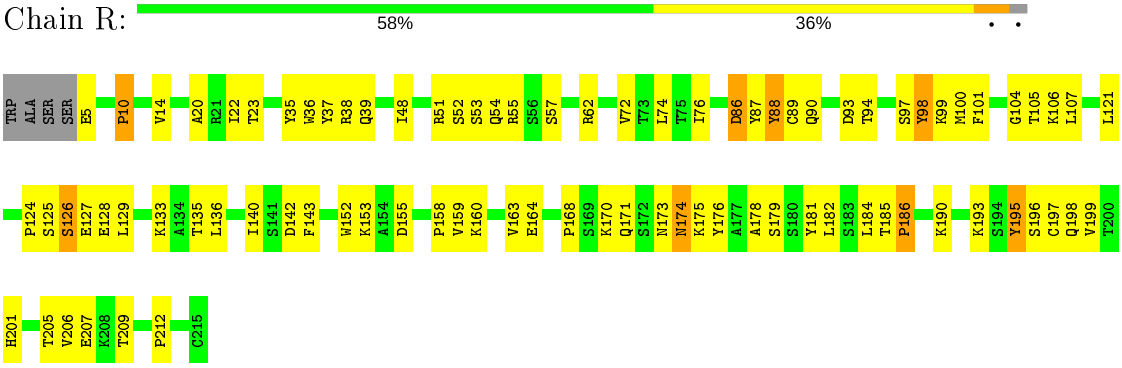
• Molecule 5: BG18 Heavy Chain

Chain Q:



• Molecule 6: BG18 Light Chain

Chain R:



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

Chain A:

• Molecule 8: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

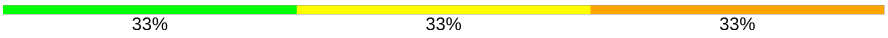
Chain C:

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

Chain F:

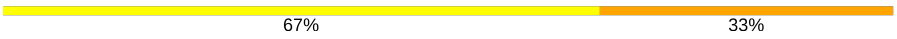
• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:



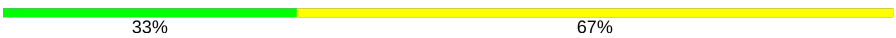
• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:



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

Chain M:

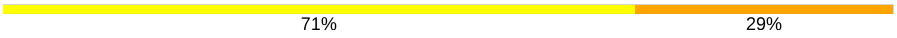


• Molecule 11: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

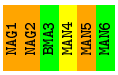
• Molecule 12: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 13: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



• Molecule 14: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

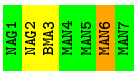
Chain N:

• Molecule 15: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:

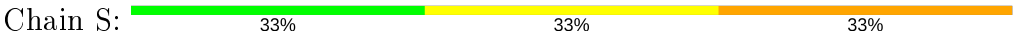
• Molecule 16: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:



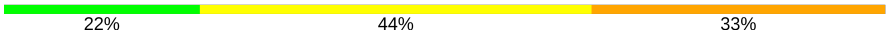
• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:



• Molecule 18: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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 T:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	238.94Å 238.94Å 354.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.03 – 3.80 24.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	93.9 (24.03-3.80) 93.9 (24.00-3.80)	Depositor EDS
R_{merge}	0.54	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.84Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.232 , 0.262 0.298 , 0.316	Depositor DCC
R_{free} test set	1809 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	175.6	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 103.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.30$, $< L^2 > = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12160	wwPDB-VP
Average B, all atoms (Å^2)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: FUC, GAL, NAG, BMA, 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	B	0.33	0/1086	0.51	0/1472
2	D	0.27	0/1752	0.52	0/2385
3	E	0.27	0/1659	0.48	0/2269
4	G	0.28	0/3619	0.50	0/4914
5	Q	0.26	0/1753	0.49	0/2397
6	R	0.26	0/1567	0.58	1/2149 (0.0%)
All	All	0.28	0/11436	0.51	1/15586 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	126	SER	N-CA-C	5.82	126.70	111.00

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	B	1068	0	1055	74	0
2	D	1708	0	1682	80	0
3	E	1615	0	1548	55	0
4	G	3546	0	3468	144	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Q	1709	0	1639	69	0
6	R	1527	0	1428	110	0
7	A	60	0	52	0	0
8	C	96	0	81	3	0
9	F	96	0	82	2	0
10	H	39	0	34	2	0
10	J	39	0	34	3	0
10	M	39	0	34	0	0
11	I	50	0	43	3	0
12	K	83	0	70	1	0
13	L	72	0	61	3	0
14	N	28	0	25	3	0
15	O	83	0	70	4	0
16	P	83	0	70	2	0
17	S	72	0	61	1	0
18	T	105	0	86	3	0
19	B	14	0	13	1	0
19	G	28	0	26	0	0
All	All	12160	0	11662	508	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 21.

All (508) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:LEU:HD12	1:B:586:TYR:CE2	1.25	1.61
1:B:545:LEU:HD12	1:B:586:TYR:CD2	1.42	1.52
6:R:142:ASP:CG	6:R:175:LYS:HZ1	1.04	1.50
1:B:545:LEU:CD1	1:B:586:TYR:CE2	1.94	1.47
6:R:98:TYR:CE2	6:R:100:MET:HG2	1.54	1.42
1:B:545:LEU:CD1	1:B:586:TYR:CD2	2.05	1.38
5:Q:48:TRP:CE2	6:R:99:LYS:HG3	1.63	1.33
1:B:550:GLN:OE1	1:B:579:ARG:HD2	1.28	1.30
6:R:142:ASP:CG	6:R:175:LYS:NZ	1.89	1.23
1:B:547:GLY:O	1:B:548:ILE:CG2	1.87	1.22
6:R:98:TYR:HE2	6:R:100:MET:CG	1.57	1.18
2:D:148:GLU:HB3	2:D:149:PRO:CD	1.76	1.15
6:R:163:VAL:HG11	6:R:182:LEU:HD22	1.24	1.15
1:B:536:THR:O	1:B:540:GLN:NE2	1.81	1.14
1:B:547:GLY:O	1:B:548:ILE:HG23	0.98	1.13

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:GLN:OE1	1:B:579:ARG:CD	2.00	1.08
4:G:391:PHE:CE2	4:G:470:PRO:HG3	1.90	1.07
2:D:148:GLU:HB3	2:D:149:PRO:HD3	1.35	1.05
6:R:142:ASP:CB	6:R:175:LYS:NZ	2.20	1.04
6:R:142:ASP:HA	6:R:175:LYS:CE	1.92	0.97
6:R:163:VAL:HG11	6:R:182:LEU:CD2	1.93	0.97
5:Q:48:TRP:NE1	6:R:99:LYS:HG3	1.79	0.97
1:B:545:LEU:CD1	1:B:586:TYR:HE2	1.77	0.96
6:R:142:ASP:CB	6:R:175:LYS:HZ1	1.76	0.95
1:B:547:GLY:C	1:B:548:ILE:HG23	1.83	0.94
1:B:545:LEU:HD11	1:B:586:TYR:CD2	2.03	0.93
2:D:148:GLU:CB	2:D:149:PRO:CD	2.46	0.92
5:Q:168:THR:H	5:Q:216:ASN:HB2	1.35	0.91
3:E:6:GLN:HG3	3:E:104:GLY:H	1.36	0.91
1:B:537:LEU:HA	1:B:540:GLN:NE2	1.87	0.89
4:G:391:PHE:HE2	4:G:470:PRO:HG3	1.33	0.89
4:G:391:PHE:HE2	4:G:470:PRO:CG	1.87	0.88
2:D:146:PHE:HB3	2:D:147:PRO:HD3	1.58	0.84
6:R:142:ASP:OD1	6:R:175:LYS:NZ	1.98	0.84
4:G:236:THR:H	10:J:1:NAG:H81	1.42	0.83
5:Q:91:THR:HB	5:Q:127:THR:HA	1.61	0.83
1:B:545:LEU:HD11	1:B:586:TYR:CE2	2.09	0.83
5:Q:48:TRP:CE2	6:R:99:LYS:CG	2.55	0.83
2:D:110:THR:OG1	2:D:148:GLU:OE2	1.97	0.81
1:B:548:ILE:O	1:B:549:VAL:HG12	1.81	0.80
6:R:36:TRP:HB2	6:R:48:ILE:HG21	1.63	0.80
4:G:298:ARG:NH2	4:G:439:ILE:O	2.14	0.79
5:Q:50:GLY:HA3	5:Q:60:TYR:HA	1.63	0.79
4:G:391:PHE:CE2	4:G:470:PRO:CG	2.62	0.79
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.64	0.79
6:R:198:GLN:HA	6:R:207:GLU:HB3	1.65	0.79
2:D:116:THR:HA	2:D:146:PHE:HD2	1.48	0.78
2:D:148:GLU:HB3	2:D:149:PRO:HD2	1.61	0.78
5:Q:48:TRP:CZ2	6:R:99:LYS:HG3	2.19	0.78
1:B:537:LEU:HA	1:B:540:GLN:CD	2.04	0.77
6:R:142:ASP:CB	6:R:175:LYS:HZ3	1.94	0.77
1:B:536:THR:C	1:B:540:GLN:HE22	1.89	0.76
4:G:33:ASN:O	4:G:500:ARG:HG2	1.86	0.76
6:R:52:SER:O	18:T:9:MAN:O3	2.03	0.76
4:G:90:THR:HG22	4:G:240:PRO:HA	1.68	0.76
6:R:173:ASN:C	6:R:174:ASN:ND2	2.40	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:201:LYS:H	2:D:202:PRO:CD	1.99	0.75
2:D:124:LEU:HB2	2:D:141:LEU:HB2	1.67	0.75
4:G:270:VAL:HG12	4:G:289:ASN:H	1.49	0.74
6:R:142:ASP:HB2	6:R:175:LYS:HZ3	1.52	0.74
1:B:537:LEU:C	1:B:540:GLN:OE1	2.26	0.74
1:B:540:GLN:OE1	1:B:540:GLN:N	2.19	0.74
4:G:35:TRP:HD1	4:G:501:CYS:H	1.33	0.73
6:R:98:TYR:HE2	6:R:100:MET:HG2	0.67	0.73
1:B:544:LEU:HG	4:G:222:GLY:HA2	1.68	0.73
4:G:129:LEU:HD23	4:G:159:PHE:HB3	1.71	0.73
6:R:142:ASP:HA	6:R:175:LYS:HE3	1.71	0.73
4:G:258:GLN:NE2	4:G:371:VAL:O	2.21	0.72
6:R:155:ASP:HA	6:R:193:LYS:HG2	1.73	0.71
1:B:545:LEU:O	1:B:545:LEU:HD23	1.89	0.71
4:G:475:MET:SD	4:G:478:ASN:ND2	2.64	0.70
4:G:70:ALA:HB2	4:G:213:ILE:HD11	1.73	0.70
4:G:98:ASN:ND2	4:G:486:TYR:O	2.24	0.70
1:B:625:ASN:OD1	2:D:32:TYR:OH	2.09	0.69
2:D:37:ILE:HG22	2:D:47:TRP:HA	1.72	0.69
1:B:545:LEU:CD1	1:B:586:TYR:HD2	1.95	0.69
2:D:163:VAL:HG12	2:D:182:VAL:HG23	1.73	0.69
1:B:540:GLN:CD	1:B:540:GLN:H	1.97	0.68
1:B:548:ILE:HD11	1:B:550:GLN:HB3	1.74	0.68
4:G:265:LEU:HD12	4:G:287:GLN:HB3	1.76	0.68
4:G:258:GLN:HG2	4:G:470:PRO:HB2	1.75	0.68
2:D:146:PHE:CB	2:D:147:PRO:HD3	2.21	0.68
5:Q:112:TRP:HH2	16:P:6:MAN:H2	1.58	0.67
5:Q:48:TRP:HB2	6:R:101:PHE:CE1	2.29	0.67
2:D:200:HIS:HD2	2:D:205:THR:HB	1.60	0.67
4:G:500:ARG:O	4:G:501:CYS:HB2	1.94	0.67
1:B:550:GLN:OE1	1:B:579:ARG:NH1	2.28	0.67
3:E:196:SER:HA	3:E:209:THR:HG23	1.77	0.67
6:R:152:TRP:CD1	6:R:163:VAL:HG21	2.30	0.66
1:B:544:LEU:C	1:B:544:LEU:HD23	2.16	0.66
4:G:264:SER:O	4:G:287:GLN:NE2	2.29	0.66
2:D:66:ARG:HD2	2:D:82(B):ASN:HB2	1.78	0.65
2:D:72(D):PRO:HG3	4:G:240:PRO:HG3	1.78	0.65
1:B:548:ILE:O	1:B:549:VAL:CG1	2.44	0.65
2:D:66:ARG:NH2	2:D:82(B):ASN:O	2.29	0.65
6:R:88:TYR:HA	6:R:104:GLY:HA3	1.78	0.65
4:G:269:GLU:HB2	4:G:348:GLN:HG3	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:142:ASP:OD1	6:R:175:LYS:CE	2.45	0.65
1:B:550:GLN:HB2	1:B:579:ARG:HD3	1.78	0.64
4:G:325:ASP:HA	6:R:54:GLN:HE22	1.62	0.64
4:G:360:ARG:O	4:G:467:THR:OG1	2.14	0.64
3:E:41:PRO:HB2	3:E:44:ARG:HB2	1.77	0.64
4:G:273:ARG:NH1	4:G:287:GLN:OE1	2.31	0.64
4:G:219:ALA:HB2	4:G:225:ILE:HG13	1.80	0.64
6:R:142:ASP:CA	6:R:175:LYS:NZ	2.60	0.63
6:R:142:ASP:HA	6:R:175:LYS:NZ	2.13	0.63
6:R:163:VAL:CG1	6:R:182:LEU:CD2	2.74	0.63
6:R:10:PRO:HA	6:R:105:THR:HA	1.80	0.63
4:G:455:THR:HG22	4:G:456:ARG:H	1.64	0.63
5:Q:166:PRO:O	5:Q:216:ASN:ND2	2.32	0.63
2:D:201:LYS:H	2:D:202:PRO:HD3	1.64	0.62
4:G:125:LEU:HG	4:G:193:LEU:HD11	1.82	0.62
4:G:391:PHE:CD2	4:G:470:PRO:HD3	2.34	0.62
4:G:454:LEU:HB3	4:G:468:PHE:HB3	1.80	0.62
6:R:22:ILE:HB	6:R:74:LEU:HB3	1.81	0.62
4:G:391:PHE:CD2	4:G:470:PRO:HG3	2.32	0.62
6:R:90:GLN:HG2	6:R:101:PHE:CE1	2.35	0.62
1:B:544:LEU:CG	4:G:222:GLY:HA2	2.30	0.61
2:D:6:GLN:HE21	2:D:92:CYS:H	1.47	0.61
6:R:160:LYS:O	6:R:163:VAL:HG22	1.99	0.61
3:E:4:LEU:HB3	3:E:102:GLY:HA2	1.82	0.61
4:G:49:GLU:HG2	4:G:99:ASN:HB3	1.82	0.61
1:B:545:LEU:C	1:B:545:LEU:HD23	2.21	0.61
1:B:550:GLN:HB2	1:B:579:ARG:CD	2.29	0.61
6:R:196:SER:HB2	6:R:209:THR:HG23	1.80	0.61
4:G:236:THR:N	10:J:1:NAG:H81	2.14	0.61
6:R:93:ASP:OD1	6:R:94:THR:N	2.33	0.61
6:R:153:LYS:HA	6:R:158:PRO:HA	1.83	0.60
6:R:152:TRP:CD2	6:R:182:LEU:HD21	2.36	0.60
6:R:153:LYS:NZ	6:R:196:SER:O	2.35	0.60
5:Q:28:SER:HB2	18:T:7:MAN:H61	1.83	0.60
2:D:37:ILE:HD11	2:D:91:PHE:HB2	1.84	0.60
1:B:549:VAL:HG13	1:B:549:VAL:O	2.02	0.60
2:D:146:PHE:CD2	2:D:147:PRO:HG3	2.37	0.60
3:E:195:TYR:HB2	3:E:212:PRO:HD3	1.84	0.60
5:Q:33:HIS:HA	5:Q:101:ILE:HG22	1.83	0.60
3:E:31:SER:O	3:E:32:HIS:ND1	2.35	0.60
4:G:39:TYR:HE2	4:G:497:ALA:HB3	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:175:LYS:HG3	6:R:175:LYS:O	2.01	0.60
5:Q:133:THR:OG1	5:Q:163:PHE:HB3	2.02	0.59
5:Q:32:ASP:O	5:Q:53:HIS:NE2	2.34	0.59
2:D:201:LYS:N	2:D:202:PRO:CD	2.64	0.59
4:G:95:MET:H	4:G:236:THR:HG21	1.67	0.59
2:D:37:ILE:HD13	3:E:40:TRP:HH2	1.67	0.59
4:G:325:ASP:OD1	4:G:326:ILE:N	2.33	0.59
4:G:350:ARG:HH22	4:G:397:SER:H	1.49	0.59
5:Q:22:CYS:HB2	5:Q:37:TRP:HZ2	1.68	0.58
5:Q:88:ALA:HA	5:Q:128:VAL:HG11	1.85	0.58
1:B:547:GLY:O	1:B:548:ILE:CB	2.51	0.58
6:R:90:GLN:HG2	6:R:101:PHE:CZ	2.39	0.58
4:G:292:VAL:O	4:G:449:ILE:HG22	2.04	0.58
5:Q:187:LEU:HA	5:Q:193:TYR:HD1	1.69	0.58
2:D:171:GLN:OE1	3:E:183:SER:OG	2.20	0.58
3:E:122:PHE:HE2	3:E:139:LEU:HB2	1.68	0.58
4:G:358:ILE:HB	4:G:465:THR:HG22	1.86	0.58
6:R:206:VAL:HG12	6:R:207:GLU:H	1.68	0.58
2:D:5:VAL:HG13	2:D:23:LYS:HB2	1.85	0.57
4:G:171:LYS:HE2	10:H:1:NAG:H2	1.85	0.57
5:Q:61:ASN:ND2	6:R:98:TYR:HE1	2.01	0.57
1:B:547:GLY:C	1:B:548:ILE:CG2	2.57	0.57
1:B:648:GLU:HA	1:B:652:GLN:HB3	1.85	0.57
4:G:359:ILE:H	4:G:396:ILE:CG2	2.18	0.57
2:D:47:TRP:HB2	3:E:101:PHE:HE2	1.69	0.57
4:G:74:CYS:SG	4:G:75:VAL:N	2.78	0.57
5:Q:114:HIS:NE2	16:P:6:MAN:O3	2.33	0.57
4:G:291:PRO:HB3	4:G:450:THR:HG22	1.85	0.57
5:Q:48:TRP:CZ2	6:R:99:LYS:CG	2.86	0.57
1:B:605:CYS:O	4:G:503:ARG:HG3	2.05	0.57
4:G:328:GLN:HB3	5:Q:109:LEU:HD21	1.87	0.57
3:E:6:GLN:HB3	3:E:105:THR:HG23	1.87	0.57
3:E:6:GLN:HG3	3:E:104:GLY:N	2.15	0.57
5:Q:39:ARG:HG2	5:Q:47:GLU:HB3	1.87	0.57
4:G:357:THR:OG1	4:G:465:THR:N	2.37	0.56
2:D:116:THR:HA	2:D:146:PHE:CD2	2.35	0.56
4:G:160:ASN:N	4:G:160:ASN:OD1	2.39	0.56
1:B:550:GLN:CD	1:B:579:ARG:HD2	2.20	0.56
4:G:82:GLN:HG2	4:G:246:GLN:HB2	1.87	0.56
4:G:476:ARG:HA	4:G:479:TRP:CE3	2.40	0.56
2:D:47:TRP:HZ2	2:D:50:TRP:HD1	1.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:110:LEU:HD23	3:E:111:GLY:H	1.69	0.56
4:G:391:PHE:HE2	4:G:470:PRO:CB	2.18	0.56
5:Q:181:HIS:O	5:Q:197:SER:OG	2.20	0.56
6:R:142:ASP:HA	6:R:175:LYS:HE2	1.85	0.56
2:D:122:PHE:HB2	2:D:141:LEU:HD22	1.86	0.56
6:R:168:PRO:HA	6:R:178:ALA:HB2	1.87	0.56
2:D:89:THR:HA	2:D:108:LEU:HA	1.88	0.56
4:G:368:ASP:H	4:G:371:VAL:HG12	1.71	0.56
3:E:48:LEU:HD12	3:E:49:ILE:H	1.70	0.56
4:G:95:MET:N	4:G:236:THR:HG21	2.21	0.56
2:D:197:ASN:HB2	2:D:208:ASP:HB3	1.88	0.55
6:R:98:TYR:CE2	6:R:100:MET:CG	2.49	0.55
5:Q:104:TYR:CZ	5:Q:111:GLU:HA	2.41	0.55
6:R:5:GLU:N	6:R:100:MET:SD	2.80	0.55
2:D:96:LEU:HA	2:D:101:TYR:HB2	1.88	0.55
2:D:150:VAL:HG22	2:D:178:LEU:HD21	1.88	0.55
4:G:173:TYR:CG	9:F:1:NAG:H62	2.42	0.55
5:Q:167:VAL:HG21	5:Q:195:LEU:HD23	1.88	0.55
6:R:142:ASP:HB2	6:R:175:LYS:NZ	2.11	0.55
1:B:537:LEU:HA	1:B:540:GLN:OE1	2.06	0.55
1:B:545:LEU:CG	1:B:586:TYR:CD2	2.87	0.55
3:E:135:THR:HA	3:E:182:LEU:HB3	1.88	0.55
2:D:108:LEU:HD21	2:D:149:PRO:HG3	1.89	0.55
4:G:298:ARG:NH1	4:G:302:ASN:OD1	2.40	0.55
4:G:137:ASN:ND2	6:R:55:ARG:O	2.40	0.54
4:G:101:VAL:HG21	4:G:480:ARG:HG2	1.89	0.54
10:J:3:BMA:H5	13:L:1:NAG:H81	1.90	0.54
4:G:317:PHE:CE2	4:G:319:ALA:HB2	2.43	0.54
4:G:45:TRP:HB3	4:G:491:ILE:HD13	1.90	0.54
5:Q:62:PRO:HA	5:Q:65:ARG:HG3	1.89	0.54
6:R:51:ARG:HA	6:R:57:SER:OG	2.08	0.54
3:E:51:TYR:O	3:E:53:ASP:N	2.40	0.54
6:R:121:LEU:HD11	6:R:140:ILE:HG23	1.89	0.54
4:G:129:LEU:O	4:G:191:TYR:N	2.37	0.54
5:Q:36:THR:OG1	5:Q:49:ILE:O	2.26	0.54
6:R:98:TYR:CE2	6:R:100:MET:HA	2.42	0.54
5:Q:168:THR:N	5:Q:216:ASN:HB2	2.15	0.53
4:G:165:LEU:HD22	4:G:168:LYS:HE3	1.91	0.53
4:G:83:GLU:HA	4:G:245:VAL:HG12	1.90	0.53
4:G:158:SER:HB2	4:G:173:TYR:CD2	2.43	0.53
4:G:359:ILE:HA	4:G:467:THR:HG23	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:55:ALA:HA	4:G:75:VAL:O	2.09	0.53
2:D:115:SER:O	2:D:146:PHE:CD2	2.62	0.53
5:Q:81:LEU:HD23	5:Q:82:LYS:H	1.72	0.53
6:R:98:TYR:CE2	6:R:100:MET:CA	2.91	0.53
1:B:620:SER:OG	1:B:624:ASP:OD2	2.25	0.53
3:E:189:TRP:HE1	3:E:212:PRO:HB2	1.74	0.53
4:G:61:TYR:O	4:G:65:LYS:HB3	2.09	0.53
2:D:110:THR:HG23	2:D:148:GLU:OE2	2.09	0.53
3:E:69:SER:OG	3:E:72:SER:OG	2.27	0.53
5:Q:129:SER:HB3	5:Q:163:PHE:HZ	1.74	0.53
6:R:86:ASP:N	6:R:86:ASP:OD1	2.33	0.52
2:D:98:ARG:HB2	8:C:1:NAG:H83	1.91	0.52
5:Q:9:PRO:HD2	5:Q:20:LEU:CD1	2.40	0.52
6:R:152:TRP:CE2	6:R:182:LEU:HD21	2.43	0.52
4:G:101:VAL:HG11	4:G:480:ARG:HE	1.75	0.52
6:R:163:VAL:HB	6:R:182:LEU:HD23	1.92	0.52
2:D:119:PRO:HG3	2:D:145:TYR:HB2	1.92	0.52
4:G:453:ILE:HG22	4:G:471:GLY:O	2.09	0.52
1:B:545:LEU:HD11	1:B:586:TYR:HD2	1.61	0.52
6:R:97:SER:O	6:R:98:TYR:HB3	2.09	0.52
4:G:175:LEU:HB2	4:G:320:THR:OG1	2.10	0.51
13:L:4:MAN:H62	13:L:5:MAN:H3	1.92	0.51
6:R:86:ASP:HA	6:R:106:LYS:HA	1.91	0.51
6:R:126:SER:OG	6:R:126:SER:O	2.22	0.51
2:D:200:HIS:HB3	2:D:202:PRO:HD2	1.93	0.51
5:Q:61:ASN:ND2	6:R:98:TYR:CE1	2.79	0.51
2:D:110:THR:CG2	2:D:148:GLU:OE2	2.58	0.51
1:B:603:ILE:HG12	4:G:39:TYR:HD1	1.76	0.51
4:G:193:LEU:HB2	4:G:196:CYS:SG	2.50	0.51
1:B:593:LEU:HD21	4:G:40:TYR:HB2	1.92	0.51
6:R:133:LYS:HA	6:R:186:PRO:HG3	1.92	0.51
4:G:391:PHE:CD2	4:G:470:PRO:CD	2.93	0.50
4:G:96:TRP:CD1	4:G:275:GLU:HB2	2.46	0.50
6:R:155:ASP:HB2	6:R:193:LYS:HE3	1.92	0.50
5:Q:50:GLY:CA	5:Q:60:TYR:HA	2.39	0.50
6:R:201:HIS:H	6:R:205:THR:HG21	1.76	0.50
1:B:537:LEU:CA	1:B:540:GLN:OE1	2.58	0.50
4:G:172:VAL:HG11	4:G:309:ILE:HG12	1.93	0.50
5:Q:188:GLN:HA	6:R:164:GLU:OE1	2.11	0.50
6:R:142:ASP:OD1	6:R:175:LYS:HE3	2.11	0.50
3:E:121:LEU:HD11	3:E:136:LEU:HD21	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:320:THR:HG23	4:G:438:PRO:HG3	1.94	0.50
1:B:548:ILE:C	1:B:549:VAL:HG12	2.31	0.50
2:D:119:PRO:HG2	2:D:200:HIS:ND1	2.27	0.50
4:G:129:LEU:HB3	4:G:157:CYS:SG	2.52	0.50
4:G:158:SER:HB2	4:G:173:TYR:CG	2.47	0.50
6:R:174:ASN:ND2	6:R:174:ASN:N	2.60	0.50
3:E:30:CYS:SG	3:E:73:ALA:HB2	2.51	0.50
5:Q:48:TRP:CH2	6:R:98:TYR:HA	2.47	0.50
4:G:445:CYS:C	4:G:446:VAL:HG22	2.32	0.49
5:Q:4:LEU:HD13	5:Q:24:VAL:HB	1.92	0.49
4:G:267:GLU:HA	4:G:267:GLU:OE1	2.11	0.49
5:Q:31:SER:HA	5:Q:54:TYR:CD1	2.47	0.49
2:D:38:ARG:NH1	2:D:40:THR:OG1	2.45	0.49
2:D:72(E):VAL:HG23	2:D:74:SER:HA	1.95	0.49
2:D:93:ALA:HB3	2:D:100(F):PRO:HB3	1.94	0.49
4:G:96:TRP:HZ2	4:G:273:ARG:HB3	1.77	0.49
6:R:152:TRP:O	6:R:159:VAL:N	2.30	0.49
5:Q:103:ILE:HD11	18:T:3:BMA:H5	1.94	0.49
4:G:96:TRP:CZ2	4:G:273:ARG:HB3	2.48	0.49
11:I:1:NAG:H3	11:I:2:NAG:H2	1.94	0.49
5:Q:172:ASN:HA	5:Q:212:ILE:HG13	1.95	0.49
6:R:163:VAL:CB	6:R:182:LEU:HD23	2.43	0.49
4:G:299:PRO:HB2	4:G:327:ARG:HB2	1.93	0.49
4:G:203:GLN:HG3	4:G:435:TYR:HD2	1.77	0.49
4:G:361:PHE:HB3	4:G:391:PHE:O	2.13	0.48
1:B:522:PHE:CD2	1:B:523:LEU:HG	2.48	0.48
3:E:70:TYR:HB3	3:E:71:TRP:CE3	2.48	0.48
3:E:67:TYR:HB3	3:E:74:TYR:HE1	1.78	0.48
6:R:170:LYS:HE3	6:R:176:TYR:CZ	2.48	0.48
2:D:100(E):LEU:HD23	2:D:100(E):LEU:H	1.79	0.48
6:R:129:LEU:HD12	6:R:129:LEU:H	1.79	0.48
1:B:545:LEU:HD13	1:B:586:TYR:CE2	2.30	0.48
6:R:133:LYS:HD3	6:R:186:PRO:HD3	1.96	0.48
2:D:108:LEU:HG	2:D:148:GLU:OE1	2.14	0.48
5:Q:51:ASP:OD2	5:Q:52:ILE:N	2.47	0.48
5:Q:48:TRP:CZ3	6:R:98:TYR:HA	2.48	0.48
15:O:1:NAG:H62	15:O:2:NAG:H82	1.95	0.48
2:D:25:SER:HA	2:D:75:THR:HG22	1.95	0.48
4:G:182:VAL:HG23	4:G:192:ARG:NH1	2.29	0.48
2:D:93:ALA:CB	2:D:100(F):PRO:HB3	2.44	0.48
4:G:54:CYS:SG	4:G:55:ALA:N	2.87	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:136:LEU:HD11	6:R:184:LEU:HB2	1.96	0.48
1:B:622:ILE:HG13	1:B:623:TRP:CD1	2.49	0.47
2:D:127:SER:HB2	3:E:123:PRO:HD3	1.95	0.47
4:G:391:PHE:HE2	4:G:470:PRO:HB3	1.79	0.47
6:R:23:THR:HA	6:R:72:VAL:O	2.14	0.47
6:R:36:TRP:CD2	6:R:74:LEU:HD22	2.49	0.47
1:B:520:LEU:HA	1:B:524:GLY:HA3	1.95	0.47
1:B:617:ARG:NH1	1:B:621:GLU:OE1	2.48	0.47
3:E:65:SER:HB2	3:E:76:THR:HB	1.96	0.47
5:Q:162:TYR:CE2	5:Q:195:LEU:HD13	2.49	0.47
1:B:550:GLN:O	1:B:551:GLN:C	2.52	0.47
4:G:152:THR:O	4:G:154:LEU:N	2.46	0.47
4:G:359:ILE:H	4:G:396:ILE:HG21	1.79	0.47
5:Q:162:TYR:CE2	5:Q:193:TYR:HB2	2.49	0.47
4:G:391:PHE:CE2	4:G:470:PRO:HD3	2.49	0.47
15:O:1:NAG:O6	15:O:2:NAG:N2	2.44	0.47
6:R:153:LYS:HD3	6:R:198:GLN:HE22	1.80	0.47
2:D:199:ASN:HA	2:D:205:THR:HG21	1.96	0.47
4:G:331:CYS:HB2	4:G:385:CYS:SG	2.55	0.47
3:E:85:GLU:HG3	3:E:108:SER:HA	1.97	0.47
6:R:128:GLU:HG3	6:R:135:THR:H	1.79	0.47
5:Q:21:SER:HA	5:Q:79:PHE:O	2.15	0.46
6:R:51:ARG:HH11	6:R:54:GLN:HA	1.79	0.46
3:E:10:VAL:HG21	3:E:20:ILE:HG13	1.96	0.46
4:G:265:LEU:HD13	4:G:288:PHE:O	2.15	0.46
2:D:31:PHE:HD2	8:C:1:NAG:HN2	1.62	0.46
2:D:34:ILE:HD11	2:D:92:CYS:HB2	1.97	0.46
1:B:544:LEU:CD1	4:G:222:GLY:HA2	2.45	0.46
14:N:1:NAG:H61	14:N:2:NAG:O5	2.15	0.46
6:R:38:ARG:HB3	6:R:87:TYR:CE1	2.49	0.46
2:D:102:LEU:HA	2:D:102:LEU:HD23	1.73	0.46
3:E:140:ILE:HD11	3:E:178:ALA:HB3	1.97	0.46
1:B:548:ILE:CD1	1:B:550:GLN:HB3	2.43	0.46
3:E:91:CYS:HB3	3:E:101:PHE:HA	1.98	0.46
1:B:522:PHE:CE2	1:B:523:LEU:HG	2.51	0.46
2:D:35:ASN:ND2	2:D:100(D):TRP:O	2.49	0.46
3:E:56:ARG:HD2	3:E:62:PRO:HA	1.98	0.46
4:G:163:THR:HG23	4:G:165:LEU:H	1.81	0.46
1:B:544:LEU:HD23	1:B:544:LEU:O	2.15	0.46
2:D:155:ASN:ND2	2:D:208:ASP:OD2	2.49	0.46
2:D:94:LYS:O	2:D:101:TYR:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:391:PHE:CE2	4:G:470:PRO:CD	2.99	0.46
4:G:294:ILE:HG13	4:G:447:SER:O	2.15	0.46
3:E:132:ASN:HB3	3:E:186:PRO:HG3	1.98	0.46
4:G:105:HIS:CD2	4:G:476:ARG:HB3	2.51	0.46
6:R:163:VAL:CG1	6:R:182:LEU:HD23	2.46	0.46
2:D:8:GLY:HA2	2:D:107:THR:HB	1.98	0.45
14:N:1:NAG:H4	14:N:2:NAG:H2	1.65	0.45
5:Q:169:VAL:HG11	5:Q:182:THR:OG1	2.16	0.45
5:Q:49:ILE:HG22	5:Q:50:GLY:H	1.79	0.45
5:Q:98:ARG:O	5:Q:117:MET:HA	2.16	0.45
1:B:544:LEU:HG	4:G:222:GLY:CA	2.41	0.45
2:D:57:LYS:NZ	2:D:68:ILE:HG13	2.31	0.45
4:G:379:GLY:O	4:G:439:ILE:HG13	2.16	0.45
5:Q:186:VAL:HG22	5:Q:187:LEU:H	1.81	0.45
6:R:152:TRP:CD1	6:R:163:VAL:CG2	2.98	0.45
6:R:35:TYR:HB2	6:R:90:GLN:HB2	1.99	0.45
17:S:3:BMA:H3	17:S:6:MAN:H2	1.81	0.45
1:B:604:CYS:HB2	4:G:38:VAL:CG2	2.47	0.45
1:B:604:CYS:HB2	4:G:38:VAL:HG22	1.98	0.45
1:B:622:ILE:HG13	1:B:623:TRP:HD1	1.81	0.45
4:G:182:VAL:HG21	11:I:1:NAG:H82	1.98	0.45
6:R:98:TYR:CZ	6:R:100:MET:HA	2.52	0.45
6:R:62:ARG:H	6:R:62:ARG:HG2	1.48	0.45
2:D:146:PHE:CD1	2:D:146:PHE:O	2.70	0.45
5:Q:101:ILE:HD11	5:Q:112:TRP:O	2.16	0.45
5:Q:10:GLY:HA2	5:Q:126:VAL:HG22	1.99	0.45
5:Q:50:GLY:HA3	5:Q:59:THR:O	2.17	0.45
1:B:545:LEU:C	1:B:545:LEU:CD2	2.86	0.45
1:B:604:CYS:O	4:G:37:THR:HG23	2.16	0.45
3:E:30:CYS:SG	3:E:68:LYS:HG3	2.57	0.45
2:D:47:TRP:CZ2	3:E:98:GLY:HA3	2.51	0.45
4:G:127:VAL:HG23	4:G:159:PHE:HB2	1.99	0.45
5:Q:8:GLY:HA3	5:Q:20:LEU:HD12	1.99	0.45
6:R:153:LYS:HG2	6:R:158:PRO:HA	1.97	0.45
6:R:171:GLN:O	6:R:175:LYS:HG2	2.16	0.45
1:B:596:TRP:HE1	1:B:647:GLU:HG3	1.82	0.44
2:D:201:LYS:H	2:D:202:PRO:HD2	1.81	0.44
3:E:20:ILE:O	3:E:74:TYR:HA	2.17	0.44
5:Q:163:PHE:N	5:Q:164:PRO:CD	2.80	0.44
6:R:37:TYR:H	6:R:48:ILE:HB	1.82	0.44
5:Q:48:TRP:HB2	6:R:101:PHE:CD1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:121:LEU:HD21	3:E:136:LEU:HD21	1.98	0.44
4:G:350:ARG:HG3	4:G:355:ASN:HA	1.99	0.44
4:G:349:LEU:O	4:G:353:PHE:N	2.50	0.44
6:R:173:ASN:N	6:R:173:ASN:OD1	2.51	0.44
1:B:537:LEU:HA	1:B:540:GLN:HE22	1.65	0.44
2:D:3:GLN:N	2:D:3:GLN:OE1	2.50	0.44
5:Q:64:LEU:O	5:Q:68:VAL:HG22	2.18	0.44
6:R:152:TRP:CE3	6:R:182:LEU:HD11	2.53	0.44
4:G:36:VAL:HA	4:G:498:PRO:HA	2.00	0.44
5:Q:139:PHE:CZ	6:R:128:GLU:HB3	2.53	0.44
1:B:586:TYR:HE1	4:G:40:TYR:HH	1.64	0.44
3:E:8:ALA:N	3:E:105:THR:HG22	2.32	0.44
9:F:4:MAN:H2	9:F:5:NAG:H2	1.58	0.44
4:G:260:LEU:HD12	4:G:451:GLY:HA3	1.99	0.44
5:Q:101:ILE:HD12	5:Q:114:HIS:HA	1.98	0.44
6:R:128:GLU:HB2	6:R:133:LYS:O	2.17	0.44
3:E:114:LYS:HA	3:E:144:TYR:HD2	1.83	0.44
4:G:366:GLY:O	4:G:372:THR:HG21	2.18	0.44
4:G:494:LEU:HD23	4:G:494:LEU:HA	1.82	0.44
1:B:544:LEU:C	1:B:544:LEU:CD2	2.86	0.44
4:G:265:LEU:CD1	4:G:287:GLN:HB3	2.45	0.44
5:Q:186:VAL:HG22	5:Q:187:LEU:HD23	2.00	0.44
6:R:133:LYS:HE3	6:R:185:THR:HG22	1.99	0.44
5:Q:34:SER:O	5:Q:35:TRP:HD1	2.00	0.43
3:E:25:PRO:C	3:E:29:CYS:HB3	2.39	0.43
4:G:32:GLU:HB2	4:G:33:ASN:H	1.68	0.43
5:Q:47:GLU:HG3	5:Q:48:TRP:H	1.83	0.43
1:B:550:GLN:OE1	1:B:579:ARG:HD3	2.06	0.43
3:E:38:TYR:CE2	3:E:48:LEU:HD22	2.53	0.43
4:G:257:THR:OG1	4:G:375:SER:OG	2.28	0.43
2:D:27:TYR:CD1	2:D:32:TYR:HD1	2.37	0.43
2:D:6:GLN:NE2	2:D:92:CYS:H	2.15	0.43
1:B:548:ILE:HG21	4:G:221:ALA:N	2.33	0.43
4:G:280:ASN:H	4:G:280:ASN:ND2	2.16	0.43
4:G:477:ASP:OD1	4:G:480:ARG:NH1	2.51	0.43
4:G:69:TRP:HA	4:G:111:LEU:HD21	2.01	0.43
6:R:140:ILE:O	6:R:179:SER:HA	2.19	0.43
2:D:31:PHE:CE1	2:D:98:ARG:HD3	2.53	0.43
3:E:140:ILE:HG12	3:E:178:ALA:O	2.19	0.43
5:Q:163:PHE:H	5:Q:164:PRO:CD	2.32	0.43
5:Q:187:LEU:HA	5:Q:193:TYR:CD1	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:LEU:HD12	1:B:579:ARG:HH21	1.84	0.43
2:D:148:GLU:CB	2:D:149:PRO:HD2	2.29	0.43
2:D:33:HIS:O	2:D:95:GLY:N	2.50	0.43
1:B:624:ASP:HB3	2:D:99:ASP:HB2	1.99	0.43
2:D:108:LEU:H	2:D:108:LEU:HD23	1.84	0.43
2:D:96:LEU:HD13	3:E:51:TYR:CE1	2.54	0.42
4:G:350:ARG:NH2	4:G:397:SER:H	2.16	0.42
4:G:425:ASN:HB3	4:G:433:ALA:HA	2.01	0.42
4:G:251:ILE:HG12	4:G:482:GLU:HG2	2.00	0.42
1:B:549:VAL:HG22	1:B:549:VAL:O	2.19	0.42
3:E:70:TYR:HB3	3:E:71:TRP:CZ3	2.54	0.42
15:O:4:MAN:H62	15:O:6:MAN:H2	1.76	0.42
6:R:14:VAL:HG12	6:R:107:LEU:HD21	2.01	0.42
12:K:4:MAN:H3	12:K:5:MAN:H5	2.01	0.42
4:G:265:LEU:HD23	4:G:267:GLU:H	1.85	0.42
5:Q:105:GLY:HA3	5:Q:111:GLU:OE1	2.19	0.42
6:R:199:VAL:O	6:R:205:THR:HB	2.20	0.42
2:D:110:THR:CB	2:D:148:GLU:OE2	2.67	0.42
3:E:144:TYR:CD1	3:E:145:PRO:HA	2.54	0.42
4:G:280:ASN:C	4:G:456:ARG:HG3	2.40	0.42
2:D:28:ARG:HG2	2:D:72(H):PHE:O	2.19	0.42
3:E:81:ARG:O	3:E:83:GLU:N	2.51	0.42
4:G:207:LYS:HG2	4:G:207:LYS:H	1.69	0.42
2:D:11:LEU:O	2:D:12:LYS:HD2	2.19	0.42
3:E:49:ILE:HG22	3:E:50:ILE:HG12	2.02	0.42
4:G:457:ASP:HB2	4:G:467:THR:O	2.20	0.42
3:E:51:TYR:CE2	3:E:57:ALA:HA	2.55	0.42
4:G:50:THR:OG1	4:G:51:THR:N	2.53	0.42
5:Q:187:LEU:HD23	5:Q:187:LEU:H	1.83	0.42
6:R:164:GLU:O	6:R:181:TYR:O	2.37	0.42
3:E:189:TRP:NE1	3:E:212:PRO:HB2	2.35	0.42
4:G:424:ILE:HA	4:G:424:ILE:HD12	1.88	0.42
4:G:105:HIS:HD2	4:G:476:ARG:HE	1.68	0.42
6:R:20:ALA:HB3	6:R:76:ILE:HG12	2.00	0.42
3:E:132:ASN:HB3	3:E:186:PRO:HB3	2.02	0.41
5:Q:139:PHE:HZ	6:R:128:GLU:HB3	1.86	0.41
4:G:233:PHE:CE1	4:G:239:CYS:HB2	2.55	0.41
4:G:86:LEU:HG	4:G:244:THR:HG22	2.03	0.41
6:R:125:SER:O	6:R:126:SER:HB3	2.21	0.41
6:R:170:LYS:HG3	6:R:176:TYR:CE1	2.55	0.41
1:B:618:ASN:OD1	19:B:701:NAG:N2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:172:VAL:HG21	4:G:309:ILE:HG21	2.02	0.41
4:G:456:ARG:HH21	4:G:458:GLY:HA2	1.84	0.41
10:H:2:NAG:O6	10:H:2:NAG:O4	2.32	0.41
11:I:1:NAG:H61	11:I:2:NAG:H83	2.02	0.41
13:L:1:NAG:H62	13:L:2:NAG:H82	2.02	0.41
5:Q:24:VAL:HG11	5:Q:35:TRP:HH2	1.84	0.41
4:G:69:TRP:O	4:G:111:LEU:HD21	2.21	0.41
6:R:124:PRO:HB3	6:R:135:THR:O	2.20	0.41
6:R:174:ASN:N	6:R:174:ASN:HD22	2.18	0.41
4:G:136:ASN:O	4:G:139:THR:HG22	2.21	0.41
4:G:207:LYS:HB3	4:G:207:LYS:HE2	1.96	0.41
4:G:42:VAL:HG12	4:G:493:PRO:C	2.41	0.41
5:Q:35:TRP:HE3	5:Q:79:PHE:CE2	2.38	0.41
6:R:121:LEU:HG	6:R:197:CYS:SG	2.61	0.41
1:B:537:LEU:HD21	1:B:603:ILE:HD11	2.02	0.41
2:D:49:GLY:HA3	2:D:59:LEU:HG	2.02	0.41
4:G:359:ILE:HG23	4:G:467:THR:HG21	2.02	0.41
4:G:348:GLN:O	4:G:352:HIS:ND1	2.54	0.41
4:G:158:SER:OG	4:G:159:PHE:N	2.54	0.41
5:Q:95:TYR:OH	6:R:39:GLN:NE2	2.53	0.41
2:D:200:HIS:HB2	2:D:203:SER:O	2.21	0.41
3:E:117:PRO:HG3	3:E:143:PHE:HB3	2.03	0.41
2:D:51:ILE:HD11	2:D:69:MET:HG3	2.03	0.41
3:E:142:ASP:OD1	3:E:175:LYS:HG3	2.21	0.41
4:G:233:PHE:HE2	4:G:236:THR:HG22	1.86	0.41
2:D:47:TRP:HB2	3:E:101:PHE:CE2	2.53	0.41
4:G:499:THR:O	4:G:500:ARG:C	2.55	0.41
2:D:29:PHE:HB3	2:D:72(B):GLU:OE1	2.21	0.40
2:D:4:LEU:HD11	2:D:22:CYS:HB3	2.03	0.40
3:E:154:ALA:HB2	3:E:195:TYR:CZ	2.56	0.40
4:G:288:PHE:CZ	4:G:452:LEU:HG	2.56	0.40
6:R:206:VAL:HG12	6:R:207:GLU:N	2.35	0.40
3:E:95:HIS:NE2	8:C:5:NAG:O6	2.48	0.40
15:O:4:MAN:O4	15:O:6:MAN:H3	2.21	0.40
2:D:154:TRP:HE1	2:D:158:ALA:H	1.69	0.40
3:E:138:CYS:O	3:E:179:SER:OG	2.27	0.40
5:Q:184:PRO:HA	5:Q:195:LEU:HG	2.04	0.40
1:B:575:GLN:O	1:B:579:ARG:HG3	2.22	0.40
3:E:119:VAL:HG22	3:E:140:ILE:HG22	2.03	0.40
3:E:6:GLN:HB3	3:E:105:THR:CG2	2.50	0.40
14:N:1:NAG:O3	14:N:2:NAG:N2	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:143:PHE:CE2	6:R:176:TYR:HB2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	130/153 (85%)	118 (91%)	11 (8%)	1 (1%)	19 57
2	D	222/243 (91%)	192 (86%)	26 (12%)	4 (2%)	8 42
3	E	211/216 (98%)	182 (86%)	26 (12%)	3 (1%)	11 46
4	G	444/479 (93%)	377 (85%)	62 (14%)	5 (1%)	14 51
5	Q	229/241 (95%)	194 (85%)	34 (15%)	1 (0%)	34 70
6	R	209/215 (97%)	156 (75%)	46 (22%)	7 (3%)	4 32
All	All	1445/1547 (93%)	1219 (84%)	205 (14%)	21 (2%)	10 46

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	548	ILE
2	D	147	PRO
3	E	52	GLU
4	G	61	TYR
2	D	148	GLU
4	G	501	CYS
3	E	193	ARG
4	G	364	SER
4	G	465	THR
6	R	10	PRO
6	R	98	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	R	127	GLU
5	Q	216	ASN
6	R	88	TYR
2	D	149	PRO
2	D	201	LYS
3	E	71	TRP
4	G	356	ASN
6	R	53	SER
6	R	195	TYR
6	R	212	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	116/129 (90%)	112 (97%)	4 (3%)	37	64
2	D	190/206 (92%)	184 (97%)	6 (3%)	39	65
3	E	186/189 (98%)	180 (97%)	6 (3%)	39	65
4	G	401/427 (94%)	389 (97%)	12 (3%)	41	66
5	Q	187/208 (90%)	176 (94%)	11 (6%)	19	51
6	R	163/182 (90%)	157 (96%)	6 (4%)	34	62
All	All	1243/1341 (93%)	1198 (96%)	45 (4%)	35	63

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

Mol	Chain	Res	Type
1	B	542	ARG
1	B	584	GLU
1	B	618	ASN
1	B	638	TYR
2	D	59	LEU
2	D	80	MET
2	D	100(E)	LEU
2	D	164	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	166	PHE
2	D	210	ARG
3	E	48	LEU
3	E	52	GLU
3	E	74	TYR
3	E	99	CYS
3	E	110	LEU
3	E	195	TYR
4	G	32	GLU
4	G	54	CYS
4	G	74	CYS
4	G	105	HIS
4	G	131	CYS
4	G	160	ASN
4	G	217	TYR
4	G	234	ASN
4	G	298	ARG
4	G	350	ARG
4	G	353	PHE
4	G	378	CYS
5	Q	37	TRP
5	Q	60	TYR
5	Q	79	PHE
5	Q	81	LEU
5	Q	106	VAL
5	Q	117	MET
5	Q	139	PHE
5	Q	157	CYS
5	Q	181	HIS
5	Q	187	LEU
5	Q	193	TYR
6	R	86	ASP
6	R	89	CYS
6	R	174	ASN
6	R	186	PRO
6	R	190	LYS
6	R	195	TYR

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

Mol	Chain	Res	Type
1	B	551	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	552	GLN
2	D	200	HIS
6	R	174	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

78 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	1	1,7	14,14,15	0.37	0	17,19,21	0.64	0
7	NAG	A	2	7	14,14,15	0.41	0	17,19,21	0.78	0
7	BMA	A	3	7	11,11,12	0.34	0	15,15,17	1.00	2 (13%)
7	MAN	A	4	7	11,11,12	0.28	0	15,15,17	0.91	1 (6%)
7	FUC	A	5	7	10,10,11	0.75	0	14,14,16	0.87	0
8	NAG	C	1	8,4	14,14,15	0.33	0	17,19,21	1.63	4 (23%)
8	NAG	C	2	8	14,14,15	0.30	0	17,19,21	1.22	2 (11%)
8	BMA	C	3	8	11,11,12	0.46	0	15,15,17	1.75	4 (26%)
8	MAN	C	4	8,2	11,11,12	0.68	0	15,15,17	2.08	4 (26%)
8	NAG	C	5	8	14,14,15	0.38	0	17,19,21	1.31	1 (5%)
8	GAL	C	6	8	11,11,12	0.54	0	15,15,17	1.04	1 (6%)
8	MAN	C	7	8	11,11,12	0.22	0	15,15,17	0.87	0
8	FUC	C	8	8	10,10,11	1.06	1 (10%)	14,14,16	1.22	3 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	F	1	9,4	14,14,15	0.30	0	17,19,21	0.67	0
9	NAG	F	2	9	14,14,15	0.35	0	17,19,21	0.95	1 (5%)
9	BMA	F	3	9	11,11,12	0.41	0	15,15,17	1.63	2 (13%)
9	MAN	F	4	9	11,11,12	0.58	0	15,15,17	1.16	1 (6%)
9	NAG	F	5	9	14,14,15	0.32	0	17,19,21	0.63	0
9	MAN	F	6	9	11,11,12	0.30	0	15,15,17	0.89	1 (6%)
9	MAN	F	7	9	11,11,12	0.28	0	15,15,17	0.86	1 (6%)
9	FUC	F	8	9	10,10,11	0.97	0	14,14,16	1.10	2 (14%)
10	NAG	H	1	10,4	14,14,15	0.40	0	17,19,21	0.90	0
10	NAG	H	2	10	14,14,15	0.43	0	17,19,21	1.16	3 (17%)
10	BMA	H	3	10	11,11,12	0.26	0	15,15,17	0.80	0
11	NAG	I	1	11,4	14,14,15	0.52	0	17,19,21	1.12	2 (11%)
11	NAG	I	2	11	14,14,15	0.65	0	17,19,21	0.74	0
11	BMA	I	3	11	11,11,12	0.30	0	15,15,17	0.80	1 (6%)
11	MAN	I	4	11	11,11,12	0.27	0	15,15,17	0.84	1 (6%)
10	NAG	J	1	10,4	14,14,15	0.28	0	17,19,21	0.84	1 (5%)
10	NAG	J	2	10	14,14,15	0.35	0	17,19,21	0.94	1 (5%)
10	BMA	J	3	10	11,11,12	0.28	0	15,15,17	0.82	0
12	NAG	K	1	12,4	14,14,15	0.29	0	17,19,21	1.14	1 (5%)
12	NAG	K	2	12	14,14,15	0.57	0	17,19,21	1.29	2 (11%)
12	BMA	K	3	12	11,11,12	0.36	0	15,15,17	1.39	4 (26%)
12	MAN	K	4	12	11,11,12	0.38	0	15,15,17	0.93	1 (6%)
12	MAN	K	5	12	11,11,12	0.92	2 (18%)	15,15,17	1.99	3 (20%)
12	MAN	K	6	12	11,11,12	0.27	0	15,15,17	0.85	1 (6%)
12	MAN	K	7	12	11,11,12	0.23	0	15,15,17	0.93	2 (13%)
13	NAG	L	1	13,4	14,14,15	0.37	0	17,19,21	1.32	1 (5%)
13	NAG	L	2	13	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
13	BMA	L	3	13	11,11,12	0.23	0	15,15,17	0.85	0
13	MAN	L	4	13	11,11,12	0.27	0	15,15,17	0.77	0
13	MAN	L	5	13	11,11,12	0.92	1 (9%)	15,15,17	1.94	3 (20%)
13	MAN	L	6	13	11,11,12	0.25	0	15,15,17	0.84	0
10	NAG	M	1	10,4	14,14,15	0.25	0	17,19,21	0.72	0
10	NAG	M	2	10	14,14,15	0.46	0	17,19,21	1.18	1 (5%)
10	BMA	M	3	10	11,11,12	0.58	0	15,15,17	1.13	1 (6%)
14	NAG	N	1	4,14	14,14,15	0.34	0	17,19,21	1.16	1 (5%)
14	NAG	N	2	4,14	14,14,15	0.49	0	17,19,21	0.75	0
15	NAG	O	1	15,4	14,14,15	0.34	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	NAG	O	2	15	14,14,15	0.35	0	17,19,21	1.01	2 (11%)
15	BMA	O	3	15	11,11,12	0.70	0	15,15,17	1.65	4 (26%)
15	MAN	O	4	15	11,11,12	0.71	0	15,15,17	2.59	8 (53%)
15	MAN	O	5	15	11,11,12	0.34	0	15,15,17	1.01	2 (13%)
15	MAN	O	6	15	11,11,12	0.50	0	15,15,17	1.43	3 (20%)
15	MAN	O	7	15	11,11,12	0.26	0	15,15,17	0.94	1 (6%)
16	NAG	P	1	4,16	14,14,15	0.38	0	17,19,21	0.76	0
16	NAG	P	2	16	14,14,15	0.45	0	17,19,21	1.44	3 (17%)
16	BMA	P	3	16	11,11,12	0.50	0	15,15,17	1.98	4 (26%)
16	MAN	P	4	16	11,11,12	0.29	0	15,15,17	1.03	0
16	MAN	P	5	16	11,11,12	0.27	0	15,15,17	0.64	0
16	MAN	P	6	16	11,11,12	0.19	0	15,15,17	0.91	1 (6%)
16	MAN	P	7	16	11,11,12	0.24	0	15,15,17	0.84	0
17	NAG	S	1	4,17	14,14,15	0.35	0	17,19,21	1.17	2 (11%)
17	NAG	S	2	17	14,14,15	0.49	0	17,19,21	0.76	0
17	BMA	S	3	17	11,11,12	0.33	0	15,15,17	1.44	3 (20%)
17	MAN	S	4	17	11,11,12	0.25	0	15,15,17	1.04	1 (6%)
17	MAN	S	5	17	11,11,12	0.26	0	15,15,17	0.72	0
17	MAN	S	6	17	11,11,12	0.28	0	15,15,17	0.83	1 (6%)
18	NAG	T	1	18,4	14,14,15	0.30	0	17,19,21	1.79	3 (17%)
18	NAG	T	2	18,5	14,14,15	0.85	1 (7%)	17,19,21	1.71	4 (23%)
18	BMA	T	3	18	11,11,12	0.30	0	15,15,17	0.93	1 (6%)
18	MAN	T	4	18	11,11,12	0.32	0	15,15,17	0.74	0
18	MAN	T	5	18	11,11,12	0.45	0	15,15,17	1.31	3 (20%)
18	MAN	T	6	18	11,11,12	0.26	0	15,15,17	0.85	0
18	MAN	T	7	18	11,11,12	0.34	0	15,15,17	0.97	1 (6%)
18	MAN	T	8	18	11,11,12	0.72	0	15,15,17	1.81	3 (20%)
18	MAN	T	9	18	11,11,12	0.34	0	15,15,17	1.08	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
7	NAG	A	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	A	2	7	-	4/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	A	3	7	-	0/2/19/22	0/1/1/1
7	MAN	A	4	7	-	0/2/19/22	0/1/1/1
7	FUC	A	5	7	-	-	0/1/1/1
8	NAG	C	1	8,4	-	6/6/23/26	0/1/1/1
8	NAG	C	2	8	-	3/6/23/26	0/1/1/1
8	BMA	C	3	8	-	0/2/19/22	0/1/1/1
8	MAN	C	4	8,2	-	0/2/19/22	0/1/1/1
8	NAG	C	5	8	-	3/6/23/26	0/1/1/1
8	GAL	C	6	8	-	0/2/19/22	0/1/1/1
8	MAN	C	7	8	-	0/2/19/22	0/1/1/1
8	FUC	C	8	8	-	-	0/1/1/1
9	NAG	F	1	9,4	-	5/6/23/26	0/1/1/1
9	NAG	F	2	9	-	4/6/23/26	0/1/1/1
9	BMA	F	3	9	-	2/2/19/22	0/1/1/1
9	MAN	F	4	9	-	0/2/19/22	0/1/1/1
9	NAG	F	5	9	-	3/6/23/26	0/1/1/1
9	MAN	F	6	9	-	1/2/19/22	0/1/1/1
9	MAN	F	7	9	-	0/2/19/22	0/1/1/1
9	FUC	F	8	9	-	-	0/1/1/1
10	NAG	H	1	10,4	-	3/6/23/26	0/1/1/1
10	NAG	H	2	10	-	4/6/23/26	0/1/1/1
10	BMA	H	3	10	-	2/2/19/22	0/1/1/1
11	NAG	I	1	11,4	-	3/6/23/26	0/1/1/1
11	NAG	I	2	11	-	4/6/23/26	0/1/1/1
11	BMA	I	3	11	-	1/2/19/22	0/1/1/1
11	MAN	I	4	11	-	0/2/19/22	0/1/1/1
10	NAG	J	1	10,4	-	3/6/23/26	0/1/1/1
10	NAG	J	2	10	-	4/6/23/26	0/1/1/1
10	BMA	J	3	10	-	0/2/19/22	0/1/1/1
12	NAG	K	1	12,4	-	5/6/23/26	0/1/1/1
12	NAG	K	2	12	-	4/6/23/26	0/1/1/1
12	BMA	K	3	12	-	1/2/19/22	0/1/1/1
12	MAN	K	4	12	-	0/2/19/22	0/1/1/1
12	MAN	K	5	12	-	0/2/19/22	0/1/1/1
12	MAN	K	6	12	-	2/2/19/22	0/1/1/1
12	MAN	K	7	12	-	1/2/19/22	0/1/1/1
13	NAG	L	1	13,4	-	4/6/23/26	0/1/1/1
13	NAG	L	2	13	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BMA	L	3	13	-	2/2/19/22	0/1/1/1
13	MAN	L	4	13	-	2/2/19/22	0/1/1/1
13	MAN	L	5	13	-	1/2/19/22	0/1/1/1
13	MAN	L	6	13	-	0/2/19/22	0/1/1/1
10	NAG	M	1	10,4	-	3/6/23/26	0/1/1/1
10	NAG	M	2	10	-	4/6/23/26	0/1/1/1
10	BMA	M	3	10	-	0/2/19/22	0/1/1/1
14	NAG	N	1	4,14	-	6/6/23/26	0/1/1/1
14	NAG	N	2	4,14	-	5/6/23/26	0/1/1/1
15	NAG	O	1	15,4	-	3/6/23/26	0/1/1/1
15	NAG	O	2	15	-	5/6/23/26	0/1/1/1
15	BMA	O	3	15	-	2/2/19/22	0/1/1/1
15	MAN	O	4	15	-	2/2/19/22	0/1/1/1
15	MAN	O	5	15	-	0/2/19/22	0/1/1/1
15	MAN	O	6	15	-	2/2/19/22	0/1/1/1
15	MAN	O	7	15	-	0/2/19/22	0/1/1/1
16	NAG	P	1	4,16	-	1/6/23/26	0/1/1/1
16	NAG	P	2	16	-	4/6/23/26	0/1/1/1
16	BMA	P	3	16	-	0/2/19/22	0/1/1/1
16	MAN	P	4	16	-	0/2/19/22	0/1/1/1
16	MAN	P	5	16	-	2/2/19/22	0/1/1/1
16	MAN	P	6	16	-	0/2/19/22	0/1/1/1
16	MAN	P	7	16	-	0/2/19/22	0/1/1/1
17	NAG	S	1	4,17	-	0/6/23/26	0/1/1/1
17	NAG	S	2	17	-	3/6/23/26	0/1/1/1
17	BMA	S	3	17	-	1/2/19/22	0/1/1/1
17	MAN	S	4	17	-	1/2/19/22	0/1/1/1
17	MAN	S	5	17	-	0/2/19/22	0/1/1/1
17	MAN	S	6	17	-	1/2/19/22	0/1/1/1
18	NAG	T	1	18,4	-	2/6/23/26	0/1/1/1
18	NAG	T	2	18,5	-	2/6/23/26	0/1/1/1
18	BMA	T	3	18	-	2/2/19/22	0/1/1/1
18	MAN	T	4	18	-	2/2/19/22	0/1/1/1
18	MAN	T	5	18	-	1/2/19/22	0/1/1/1
18	MAN	T	6	18	-	0/2/19/22	0/1/1/1
18	MAN	T	7	18	-	1/2/19/22	0/1/1/1
18	MAN	T	8	18	-	2/2/19/22	0/1/1/1
18	MAN	T	9	18	-	2/2/19/22	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	2	NAG	C1-C2	2.47	1.56	1.52
13	L	5	MAN	O5-C1	2.12	1.47	1.43
12	K	5	MAN	O5-C1	2.11	1.47	1.43
8	C	8	FUC	C1-C2	2.09	1.57	1.52
12	K	5	MAN	C1-C2	2.02	1.56	1.52

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	F	3	BMA	O3-C3-C2	-5.54	99.38	109.99
8	C	4	MAN	O2-C2-C1	5.44	120.29	109.15
15	O	4	MAN	O5-C5-C6	5.36	115.61	107.20
18	T	1	NAG	O4-C4-C3	-5.19	98.34	110.35
13	L	5	MAN	C1-C2-C3	4.92	115.72	109.67
12	K	5	MAN	C1-C2-C3	4.81	115.58	109.67
18	T	8	MAN	O2-C2-C3	4.75	119.66	110.14
12	K	5	MAN	O5-C1-C2	-4.21	104.28	110.77
17	S	3	BMA	O5-C5-C6	4.12	113.67	107.20
13	L	5	MAN	O5-C1-C2	-3.98	104.63	110.77
15	O	4	MAN	C1-C2-C3	3.95	114.52	109.67
18	T	1	NAG	O4-C4-C5	-3.91	99.60	109.30
13	L	1	NAG	O4-C4-C5	-3.85	99.73	109.30
16	P	3	BMA	O3-C3-C2	-3.75	102.81	109.99
8	C	1	NAG	O4-C4-C5	-3.71	100.08	109.30
8	C	4	MAN	O3-C3-C4	3.69	118.87	110.35
8	C	5	NAG	C2-N2-C7	3.61	128.05	122.90
16	P	3	BMA	O5-C1-C2	-3.57	105.26	110.77
16	P	2	NAG	O4-C4-C3	3.55	118.56	110.35
18	T	2	NAG	O5-C1-C2	-3.53	105.72	111.29
10	M	2	NAG	O4-C4-C3	3.51	118.47	110.35
16	P	3	BMA	O3-C3-C4	3.49	118.41	110.35
8	C	3	BMA	O5-C5-C6	3.45	112.62	107.20
12	K	2	NAG	O5-C1-C2	-3.43	105.87	111.29
8	C	3	BMA	C1-O5-C5	-3.41	107.57	112.19
12	K	5	MAN	C1-O5-C5	3.38	116.77	112.19
15	O	6	MAN	C1-C2-C3	3.36	113.80	109.67
18	T	2	NAG	O4-C4-C3	-3.36	102.59	110.35
17	S	1	NAG	O4-C4-C3	-3.27	102.79	110.35
8	C	1	NAG	O4-C4-C3	-3.24	102.85	110.35
15	O	4	MAN	O6-C6-C5	-3.22	100.25	111.29
18	T	2	NAG	O4-C4-C5	-3.19	101.37	109.30
18	T	8	MAN	C1-C2-C3	-3.18	105.75	109.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	1	NAG	O4-C4-C3	-3.16	103.04	110.35
15	O	3	BMA	O3-C3-C4	3.15	117.64	110.35
15	O	4	MAN	C1-O5-C5	-3.14	107.94	112.19
17	S	4	MAN	O5-C1-C2	-3.10	105.98	110.77
8	C	2	NAG	O4-C4-C5	-3.09	101.62	109.30
15	O	4	MAN	O3-C3-C4	3.07	117.46	110.35
13	L	5	MAN	C1-O5-C5	3.05	116.32	112.19
8	C	2	NAG	O5-C1-C2	-3.01	106.53	111.29
18	T	8	MAN	O3-C3-C2	2.89	115.53	109.99
15	O	6	MAN	O5-C1-C2	-2.89	106.31	110.77
18	T	7	MAN	O5-C1-C2	-2.85	106.37	110.77
8	C	4	MAN	C1-C2-C3	-2.83	106.18	109.67
12	K	2	NAG	O4-C4-C5	-2.81	102.31	109.30
12	K	3	BMA	O3-C3-C2	2.81	115.37	109.99
15	O	6	MAN	O5-C5-C6	2.77	111.54	107.20
10	M	3	BMA	O5-C1-C2	-2.74	106.54	110.77
18	T	5	MAN	O3-C3-C4	2.74	116.67	110.35
15	O	4	MAN	C3-C4-C5	-2.69	105.45	110.24
14	N	1	NAG	C1-O5-C5	2.68	115.83	112.19
15	O	3	BMA	O5-C1-C2	-2.66	106.67	110.77
15	O	4	MAN	O4-C4-C3	2.59	116.33	110.35
9	F	8	FUC	O2-C2-C1	2.58	114.44	109.15
16	P	6	MAN	O5-C1-C2	-2.57	106.81	110.77
15	O	2	NAG	O4-C4-C5	-2.55	102.95	109.30
12	K	6	MAN	O5-C1-C2	-2.54	106.84	110.77
18	T	2	NAG	C1-O5-C5	-2.51	108.79	112.19
15	O	5	MAN	O5-C1-C2	-2.51	106.89	110.77
18	T	9	MAN	O5-C5-C6	2.50	111.13	107.20
8	C	1	NAG	C6-C5-C4	-2.47	107.22	113.00
15	O	4	MAN	O5-C1-C2	-2.46	106.97	110.77
16	P	2	NAG	C4-C3-C2	-2.44	107.44	111.02
15	O	3	BMA	O5-C5-C6	2.42	111.00	107.20
16	P	3	BMA	C1-O5-C5	-2.42	108.92	112.19
8	C	8	FUC	C1-C2-C3	2.41	112.63	109.67
17	S	1	NAG	O5-C1-C2	-2.41	107.49	111.29
7	A	3	BMA	O5-C1-C2	-2.36	107.12	110.77
11	I	1	NAG	C1-O5-C5	-2.36	109.00	112.19
15	O	2	NAG	O5-C1-C2	-2.35	107.57	111.29
8	C	4	MAN	C3-C4-C5	-2.34	106.06	110.24
8	C	3	BMA	O5-C1-C2	-2.33	107.17	110.77
16	P	2	NAG	C1-O5-C5	2.32	115.34	112.19
15	O	7	MAN	O5-C1-C2	-2.31	107.21	110.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	T	3	BMA	C1-O5-C5	-2.30	109.08	112.19
12	K	3	BMA	O5-C1-C2	-2.28	107.25	110.77
7	A	4	MAN	O5-C1-C2	-2.28	107.25	110.77
11	I	1	NAG	O4-C4-C3	2.27	115.61	110.35
11	I	3	BMA	O5-C1-C2	-2.27	107.27	110.77
13	L	2	NAG	C1-O5-C5	2.27	115.26	112.19
9	F	2	NAG	O4-C4-C5	-2.26	103.68	109.30
11	I	4	MAN	O5-C1-C2	-2.22	107.35	110.77
8	C	8	FUC	O5-C5-C4	2.20	113.47	109.52
8	C	8	FUC	C1-O5-C5	2.19	117.73	112.78
18	T	5	MAN	O5-C1-C2	-2.18	107.40	110.77
18	T	5	MAN	O3-C3-C2	-2.18	105.83	109.99
8	C	6	GAL	C1-O5-C5	2.16	115.11	112.19
15	O	3	BMA	C6-C5-C4	2.15	118.05	113.00
18	T	1	NAG	O5-C1-C2	-2.13	107.92	111.29
10	J	2	NAG	C2-N2-C7	2.12	125.92	122.90
10	J	1	NAG	C2-N2-C7	2.11	125.91	122.90
12	K	7	MAN	O5-C5-C6	2.11	110.50	107.20
17	S	6	MAN	O5-C1-C2	-2.11	107.52	110.77
8	C	3	BMA	O2-C2-C3	-2.10	105.93	110.14
15	O	5	MAN	O5-C5-C6	2.10	110.50	107.20
12	K	3	BMA	O3-C3-C4	-2.10	105.50	110.35
7	A	3	BMA	O5-C5-C6	2.08	110.46	107.20
12	K	7	MAN	O5-C1-C2	-2.08	107.56	110.77
10	H	2	NAG	O4-C4-C3	2.07	115.14	110.35
9	F	7	MAN	O5-C1-C2	-2.06	107.59	110.77
8	C	1	NAG	C1-O5-C5	-2.06	109.41	112.19
10	H	2	NAG	O4-C4-C5	-2.06	104.19	109.30
17	S	3	BMA	O5-C1-C2	-2.05	107.61	110.77
9	F	4	MAN	O2-C2-C1	2.04	113.34	109.15
10	H	2	NAG	O3-C3-C2	-2.04	105.24	109.47
9	F	3	BMA	C1-C2-C3	2.04	112.18	109.67
9	F	6	MAN	O5-C1-C2	-2.04	107.63	110.77
17	S	3	BMA	C1-O5-C5	-2.02	109.45	112.19
12	K	4	MAN	O5-C1-C2	-2.01	107.67	110.77
12	K	3	BMA	O4-C4-C3	-2.01	105.71	110.35
9	F	8	FUC	O5-C5-C4	2.01	113.12	109.52

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	1	NAG	C8-C7-N2-C2
8	C	1	NAG	O7-C7-N2-C2
17	S	2	NAG	C3-C2-N2-C7
17	S	2	NAG	C8-C7-N2-C2
17	S	2	NAG	O7-C7-N2-C2
11	I	1	NAG	C3-C2-N2-C7
11	I	1	NAG	C8-C7-N2-C2
11	I	1	NAG	O7-C7-N2-C2
13	L	1	NAG	C3-C2-N2-C7
13	L	1	NAG	C8-C7-N2-C2
13	L	1	NAG	O7-C7-N2-C2
8	C	2	NAG	C3-C2-N2-C7
8	C	2	NAG	C8-C7-N2-C2
8	C	2	NAG	O7-C7-N2-C2
8	C	5	NAG	C8-C7-N2-C2
8	C	5	NAG	O7-C7-N2-C2
10	H	1	NAG	C3-C2-N2-C7
10	H	1	NAG	C8-C7-N2-C2
10	H	1	NAG	O7-C7-N2-C2
12	K	2	NAG	C8-C7-N2-C2
12	K	2	NAG	O7-C7-N2-C2
9	F	5	NAG	C8-C7-N2-C2
9	F	5	NAG	O7-C7-N2-C2
9	F	2	NAG	C3-C2-N2-C7
9	F	2	NAG	C8-C7-N2-C2
9	F	2	NAG	O7-C7-N2-C2
10	J	1	NAG	C8-C7-N2-C2
10	J	1	NAG	O7-C7-N2-C2
14	N	1	NAG	C8-C7-N2-C2
14	N	1	NAG	O7-C7-N2-C2
12	K	1	NAG	C3-C2-N2-C7
12	K	1	NAG	C8-C7-N2-C2
12	K	1	NAG	O7-C7-N2-C2
15	O	2	NAG	C3-C2-N2-C7
15	O	2	NAG	C8-C7-N2-C2
15	O	2	NAG	O7-C7-N2-C2
10	M	1	NAG	C3-C2-N2-C7
10	M	1	NAG	C8-C7-N2-C2
10	M	1	NAG	O7-C7-N2-C2
16	P	2	NAG	C8-C7-N2-C2
16	P	2	NAG	O7-C7-N2-C2
15	O	3	BMA	C4-C5-C6-O6
9	F	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	F	1	NAG	O7-C7-N2-C2
18	T	9	MAN	C4-C5-C6-O6
14	N	1	NAG	O5-C5-C6-O6
7	A	2	NAG	C8-C7-N2-C2
14	N	2	NAG	C8-C7-N2-C2
16	P	5	MAN	O5-C5-C6-O6
14	N	1	NAG	C4-C5-C6-O6
13	L	3	BMA	O5-C5-C6-O6
15	O	3	BMA	O5-C5-C6-O6
7	A	2	NAG	O7-C7-N2-C2
18	T	1	NAG	C8-C7-N2-C2
15	O	1	NAG	C8-C7-N2-C2
14	N	2	NAG	O7-C7-N2-C2
15	O	4	MAN	C4-C5-C6-O6
7	A	2	NAG	C1-C2-N2-C7
18	T	2	NAG	C1-C2-N2-C7
8	C	5	NAG	C1-C2-N2-C7
14	N	1	NAG	C1-C2-N2-C7
16	P	2	NAG	C1-C2-N2-C7
7	A	1	NAG	O5-C5-C6-O6
7	A	1	NAG	C4-C5-C6-O6
18	T	1	NAG	O7-C7-N2-C2
15	O	1	NAG	O7-C7-N2-C2
18	T	4	MAN	O5-C5-C6-O6
8	C	1	NAG	C4-C5-C6-O6
12	K	2	NAG	C1-C2-N2-C7
10	J	1	NAG	C1-C2-N2-C7
11	I	2	NAG	C8-C7-N2-C2
11	I	2	NAG	O7-C7-N2-C2
18	T	3	BMA	O5-C5-C6-O6
11	I	3	BMA	O5-C5-C6-O6
12	K	1	NAG	O5-C5-C6-O6
15	O	2	NAG	O5-C5-C6-O6
15	O	2	NAG	C4-C5-C6-O6
18	T	9	MAN	O5-C5-C6-O6
13	L	4	MAN	O5-C5-C6-O6
12	K	6	MAN	O5-C5-C6-O6
10	H	3	BMA	O5-C5-C6-O6
16	P	5	MAN	C4-C5-C6-O6
10	H	3	BMA	C4-C5-C6-O6
15	O	6	MAN	C4-C5-C6-O6
10	M	2	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	N	2	NAG	C1-C2-N2-C7
8	C	1	NAG	O5-C5-C6-O6
12	K	6	MAN	C4-C5-C6-O6
13	L	1	NAG	O5-C5-C6-O6
11	I	2	NAG	C1-C2-N2-C7
9	F	1	NAG	C1-C2-N2-C7
13	L	4	MAN	C4-C5-C6-O6
18	T	4	MAN	C4-C5-C6-O6
10	M	2	NAG	O7-C7-N2-C2
11	I	2	NAG	O5-C5-C6-O6
16	P	2	NAG	O5-C5-C6-O6
17	S	3	BMA	O5-C5-C6-O6
13	L	2	NAG	O5-C5-C6-O6
12	K	3	BMA	O5-C5-C6-O6
13	L	5	MAN	O5-C5-C6-O6
18	T	5	MAN	O5-C5-C6-O6
15	O	1	NAG	O5-C5-C6-O6
15	O	4	MAN	O5-C5-C6-O6
13	L	2	NAG	C8-C7-N2-C2
10	H	2	NAG	O5-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
16	P	1	NAG	O5-C5-C6-O6
15	O	6	MAN	O5-C5-C6-O6
17	S	4	MAN	O5-C5-C6-O6
12	K	2	NAG	O5-C5-C6-O6
9	F	5	NAG	O5-C5-C6-O6
10	M	2	NAG	O5-C5-C6-O6
17	S	6	MAN	O5-C5-C6-O6
13	L	3	BMA	C4-C5-C6-O6
10	H	2	NAG	C3-C2-N2-C7
14	N	1	NAG	C3-C2-N2-C7
10	M	2	NAG	C3-C2-N2-C7
13	L	2	NAG	O7-C7-N2-C2
10	J	2	NAG	C4-C5-C6-O6
10	H	2	NAG	C8-C7-N2-C2
8	C	1	NAG	C1-C2-N2-C7
18	T	3	BMA	C4-C5-C6-O6
10	J	2	NAG	O5-C5-C6-O6
18	T	8	MAN	C4-C5-C6-O6
10	H	2	NAG	O7-C7-N2-C2
9	F	6	MAN	O5-C5-C6-O6
9	F	3	BMA	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	T	8	MAN	O5-C5-C6-O6
12	K	7	MAN	C4-C5-C6-O6
8	C	1	NAG	C3-C2-N2-C7
7	A	2	NAG	C3-C2-N2-C7
14	N	2	NAG	C3-C2-N2-C7
18	T	7	MAN	O5-C5-C6-O6
9	F	3	BMA	C4-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
10	J	2	NAG	C3-C2-N2-C7
18	T	2	NAG	C3-C2-N2-C7
9	F	1	NAG	C3-C2-N2-C7
10	J	2	NAG	C1-C2-N2-C7
12	K	1	NAG	C4-C5-C6-O6
14	N	2	NAG	C4-C5-C6-O6

There are no ring outliers.

29 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	4	MAN	1	0
8	C	1	NAG	2	0
10	J	3	BMA	1	0
10	H	2	NAG	1	0
15	O	6	MAN	2	0
11	I	2	NAG	2	0
13	L	4	MAN	1	0
18	T	7	MAN	1	0
9	F	1	NAG	1	0
12	K	5	MAN	1	0
11	I	1	NAG	3	0
13	L	1	NAG	2	0
15	O	1	NAG	2	0
18	T	9	MAN	1	0
13	L	2	NAG	1	0
18	T	3	BMA	1	0
17	S	3	BMA	1	0
15	O	4	MAN	2	0
13	L	5	MAN	1	0
8	C	5	NAG	1	0
14	N	2	NAG	3	0
10	H	1	NAG	1	0
12	K	4	MAN	1	0

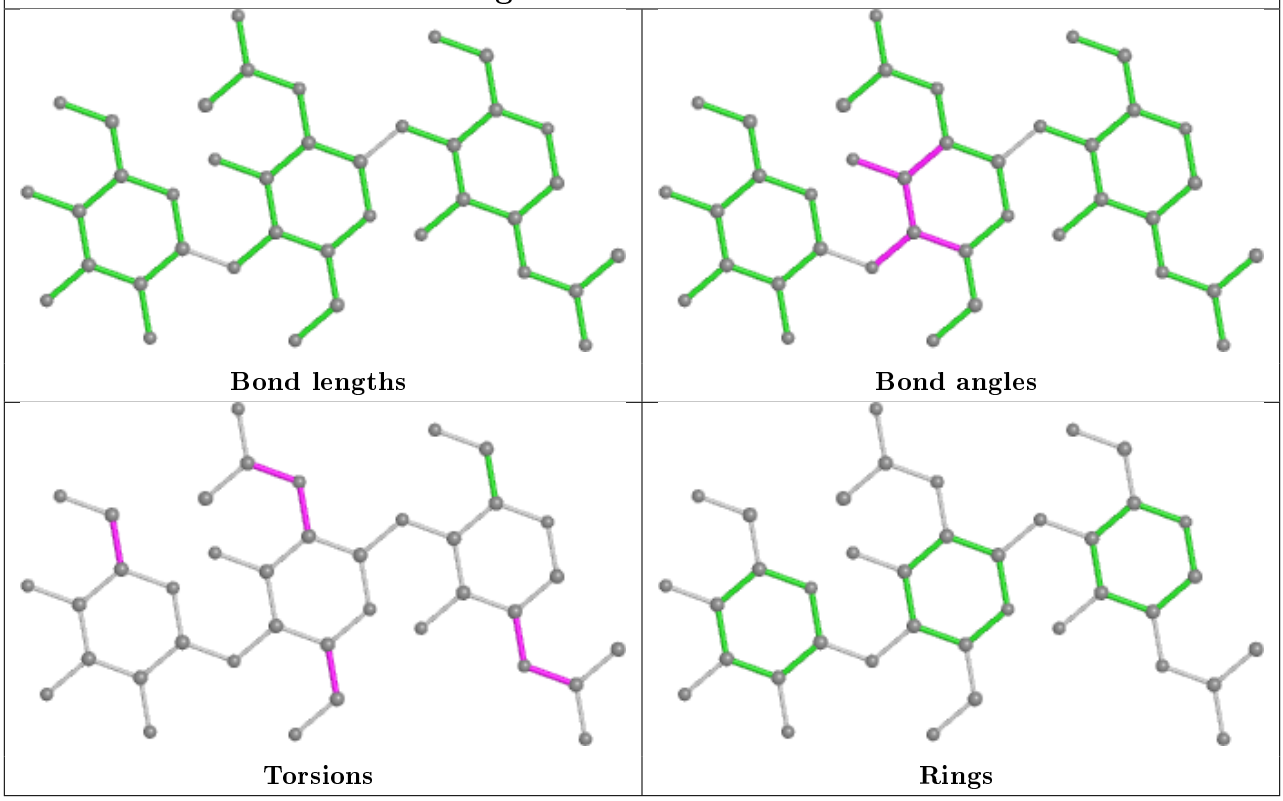
Continued on next page...

Continued from previous page...

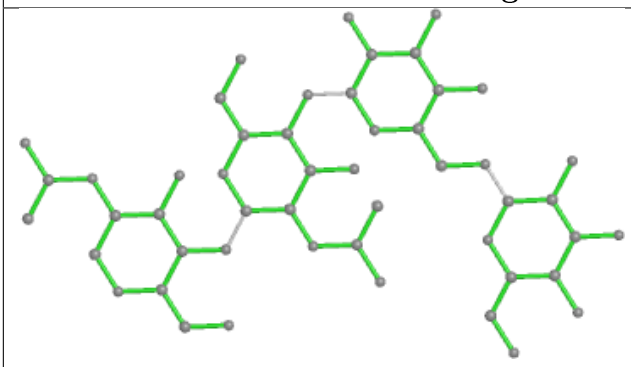
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	S	6	MAN	1	0
16	P	6	MAN	2	0
9	F	5	NAG	1	0
10	J	1	NAG	2	0
14	N	1	NAG	3	0
15	O	2	NAG	2	0

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

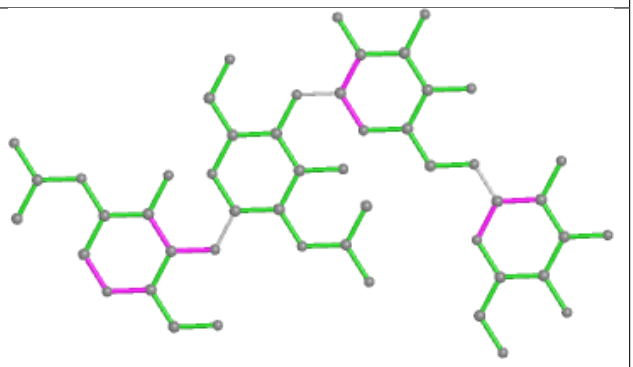
Oligosaccharide Chain H



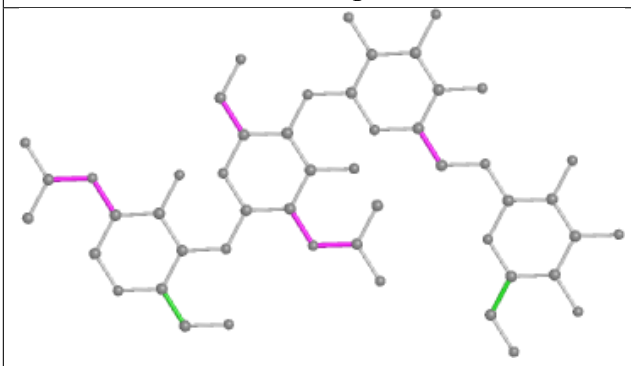
Oligosaccharide Chain I



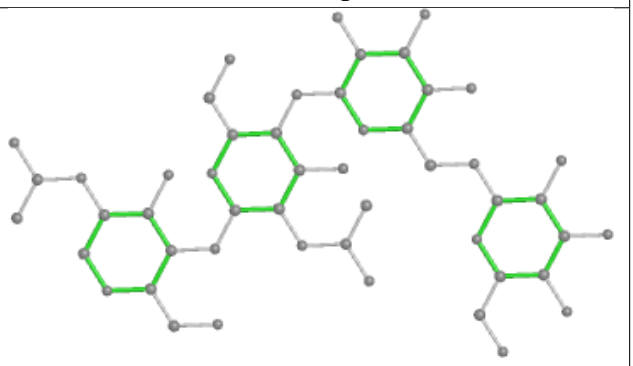
Bond lengths



Bond angles

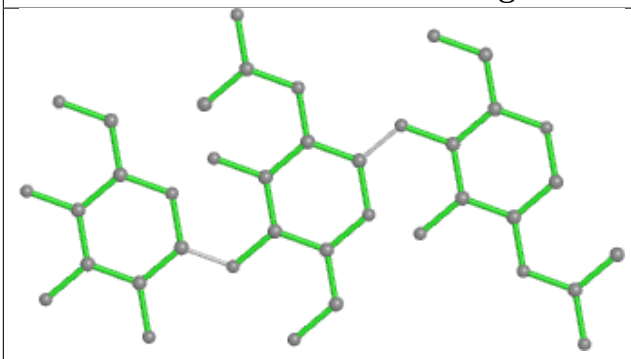


Torsions

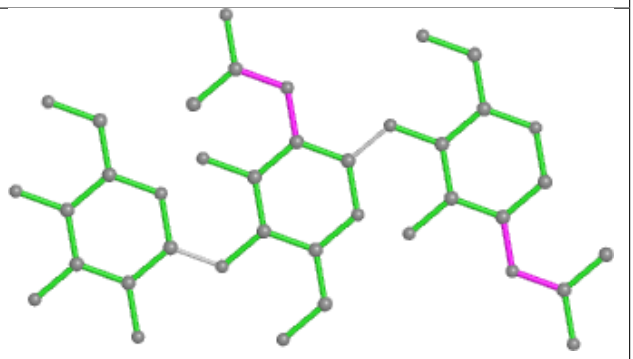


Rings

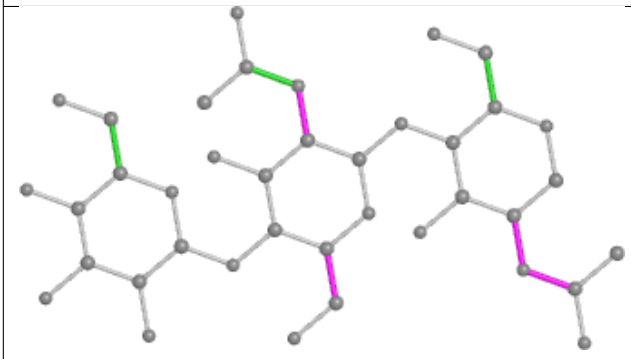
Oligosaccharide Chain J



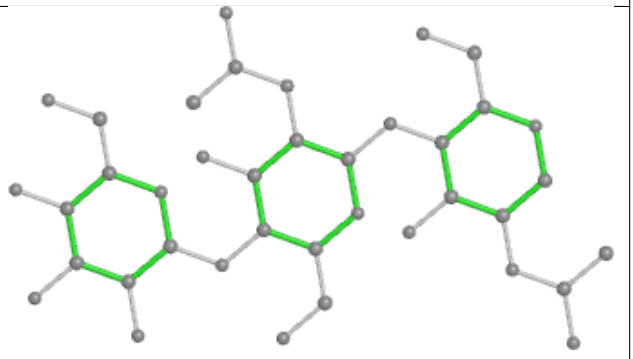
Bond lengths



Bond angles

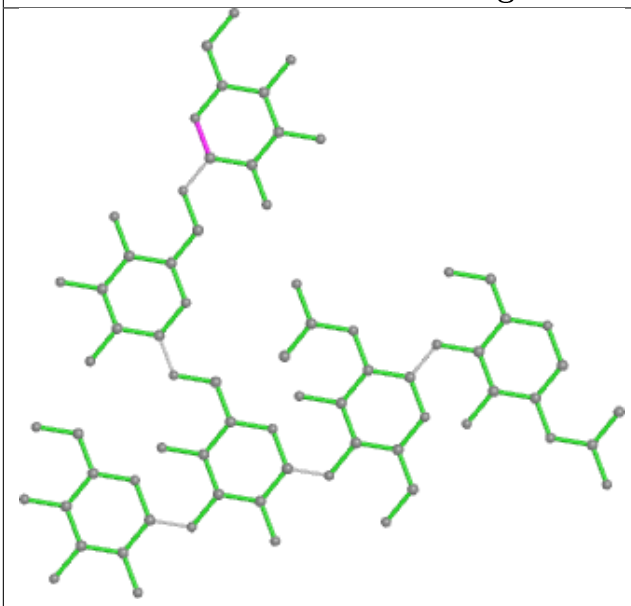


Torsions

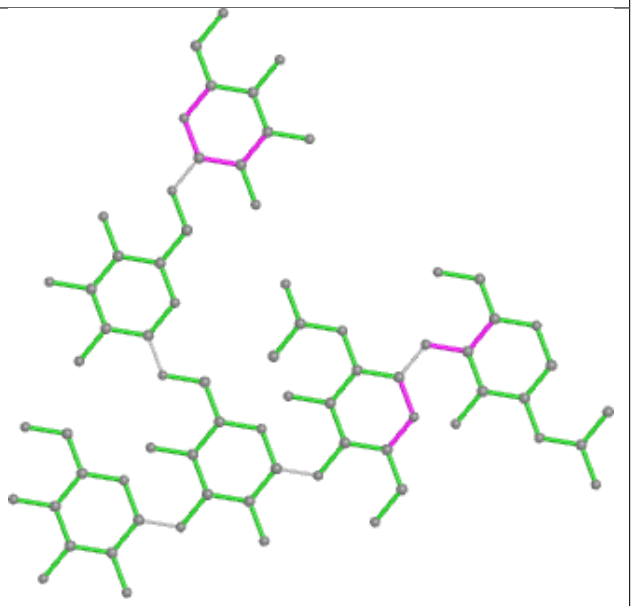


Rings

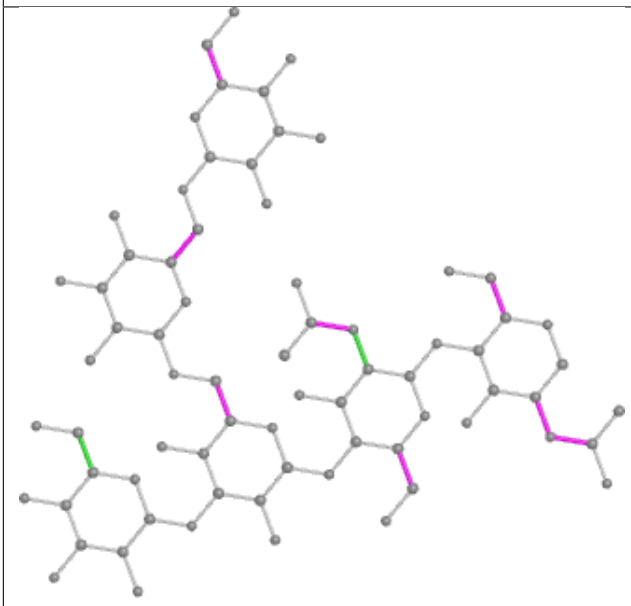
Oligosaccharide Chain L



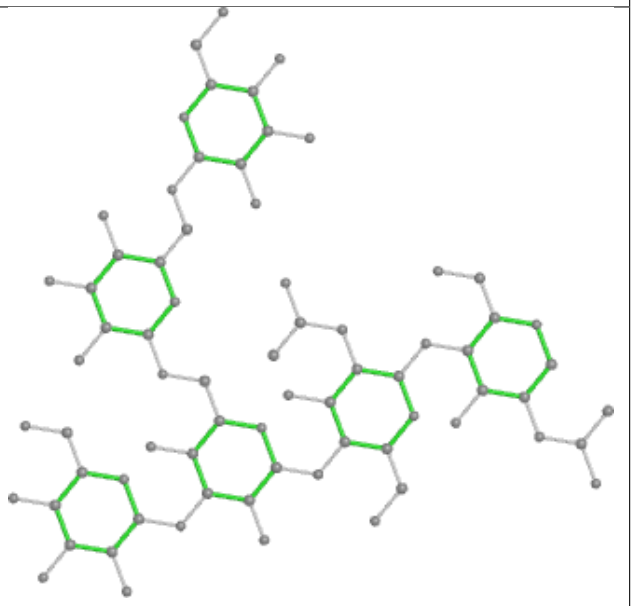
Bond lengths



Bond angles

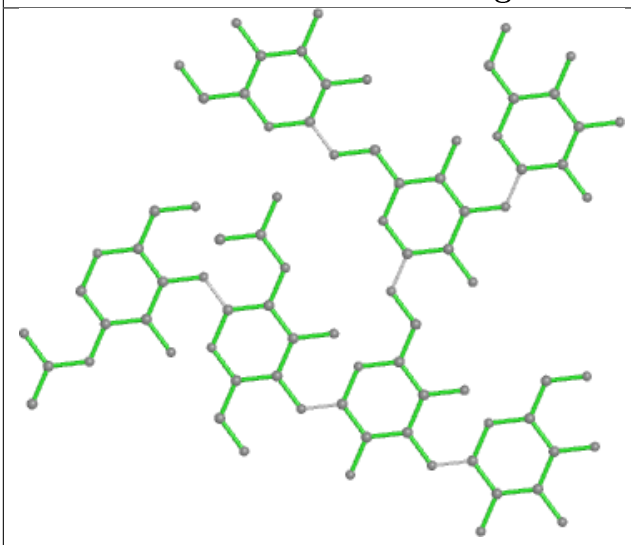


Torsions

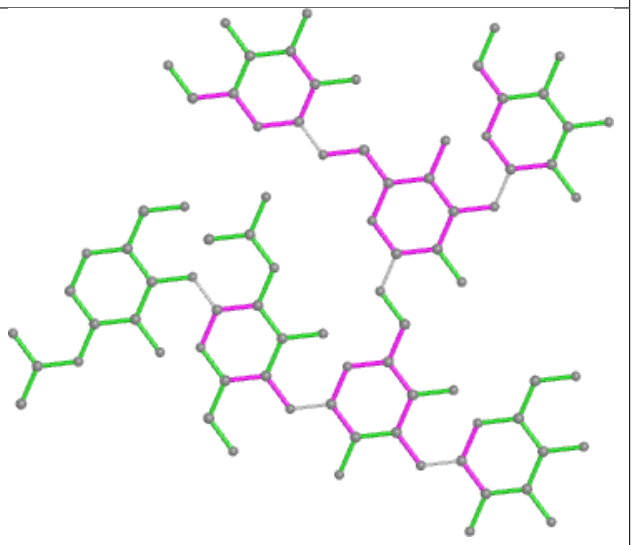


Rings

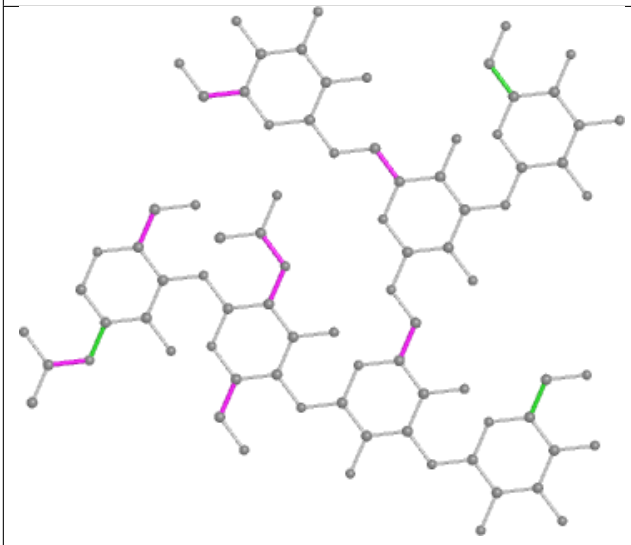
Oligosaccharide Chain O



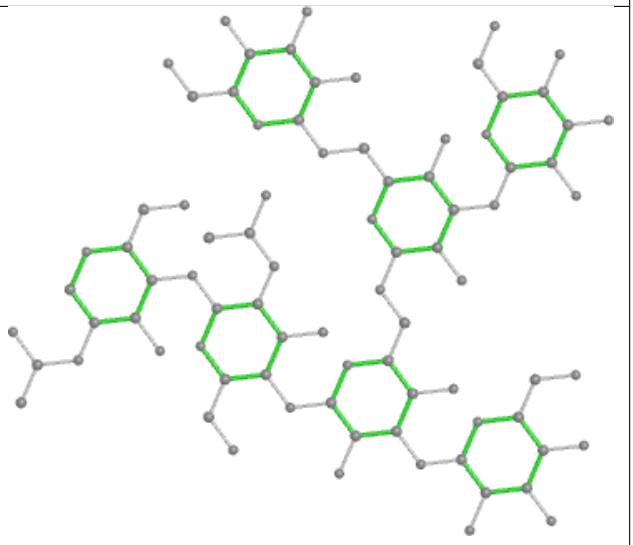
Bond lengths



Bond angles

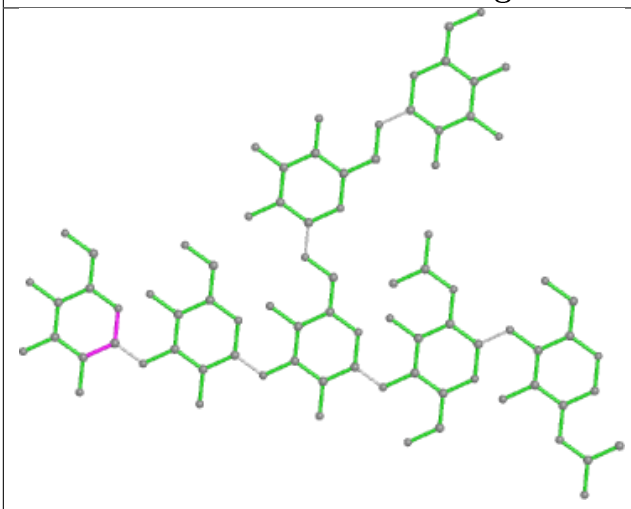


Torsions

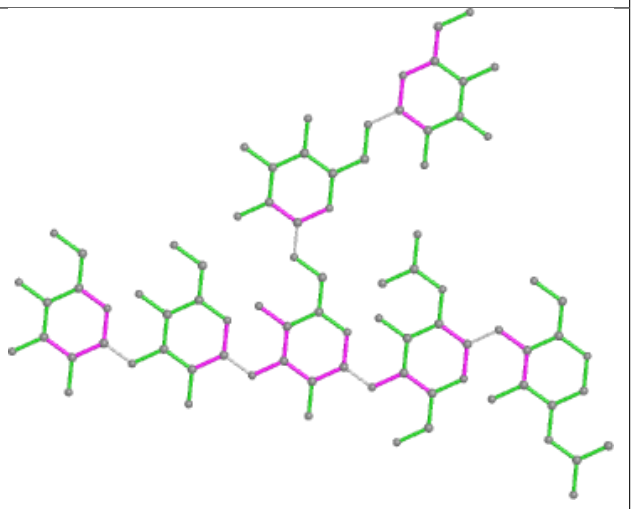


Rings

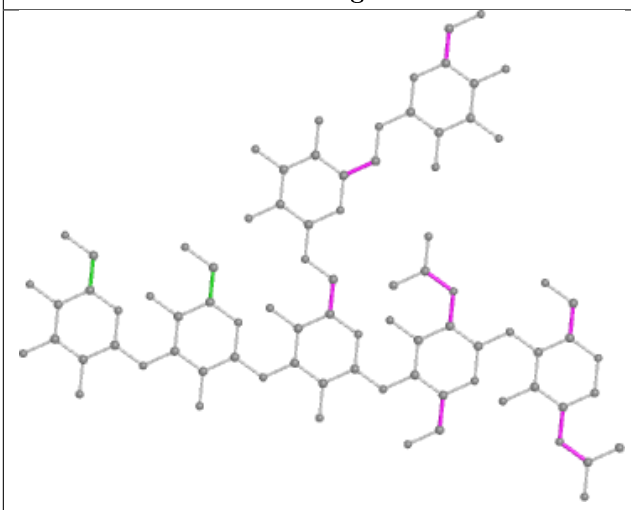
Oligosaccharide Chain K



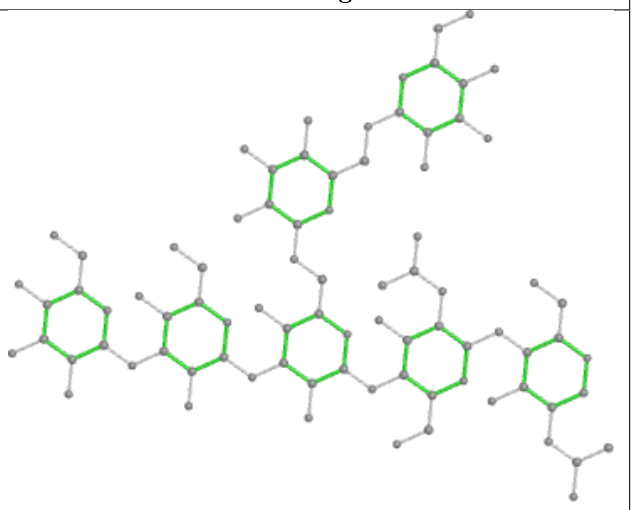
Bond lengths



Bond angles

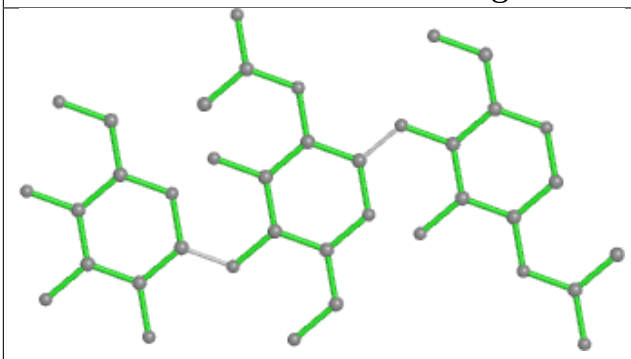


Torsions

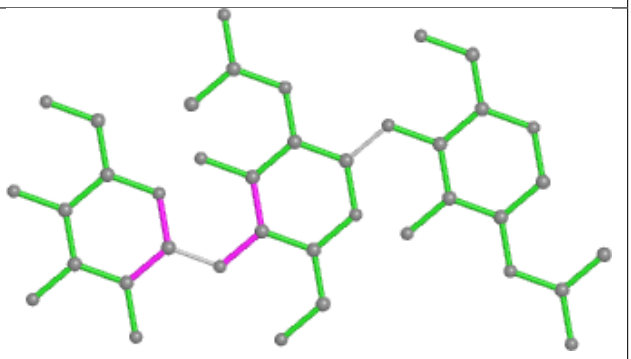


Rings

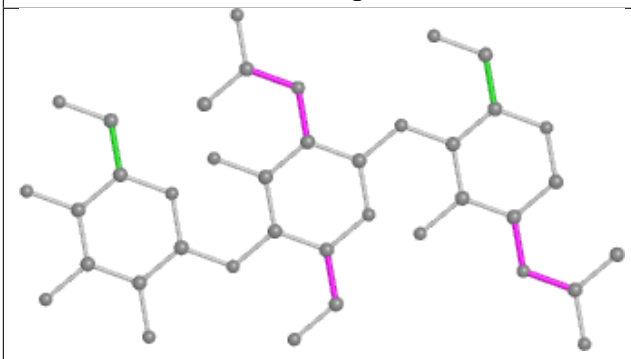
Oligosaccharide Chain M



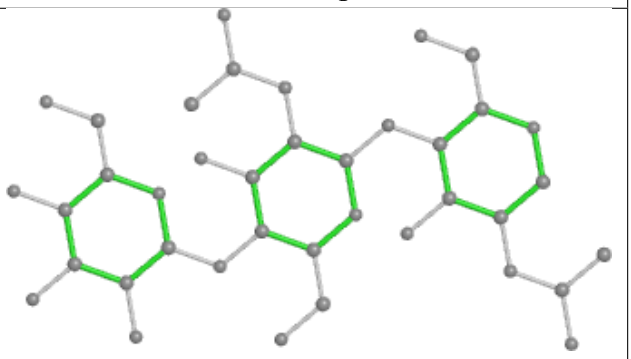
Bond lengths



Bond angles

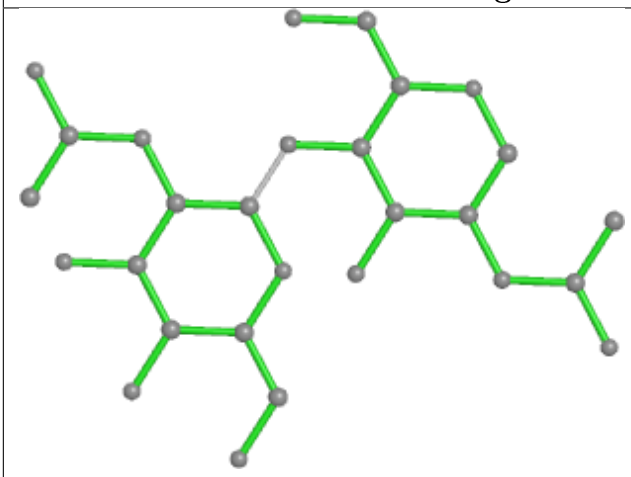


Torsions

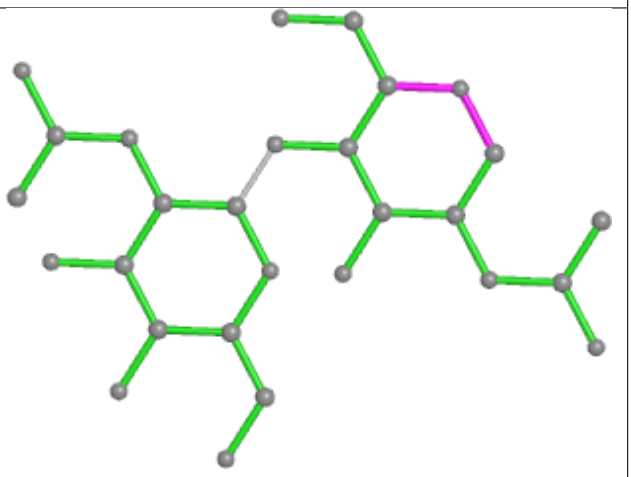


Rings

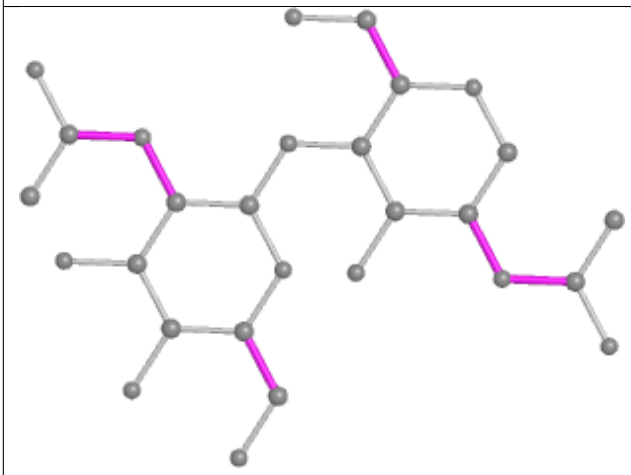
Oligosaccharide Chain N



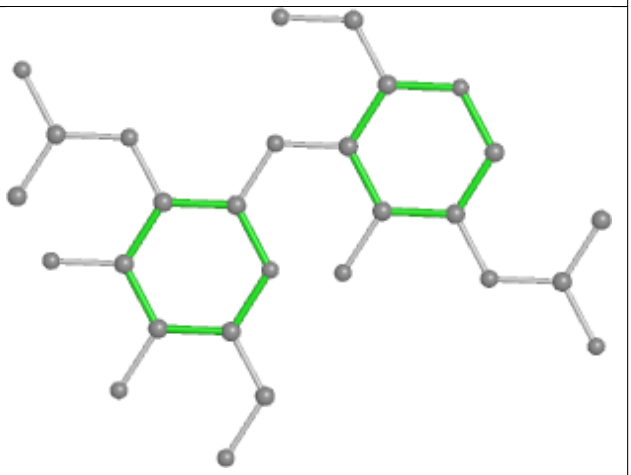
Bond lengths



Bond angles

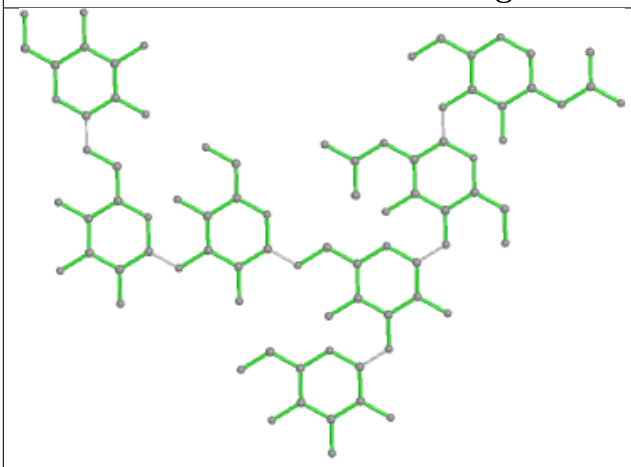


Torsions

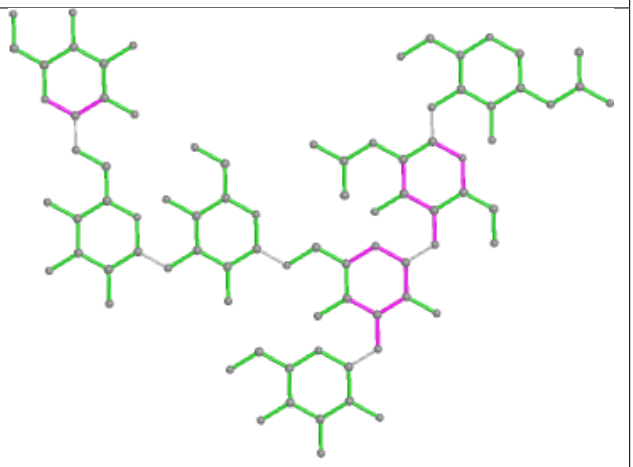


Rings

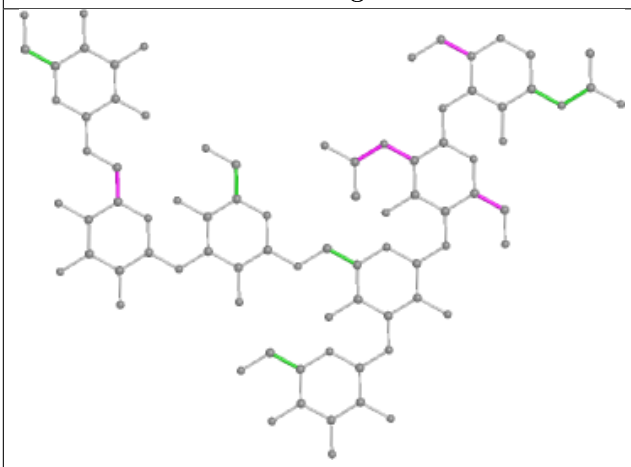
Oligosaccharide Chain P



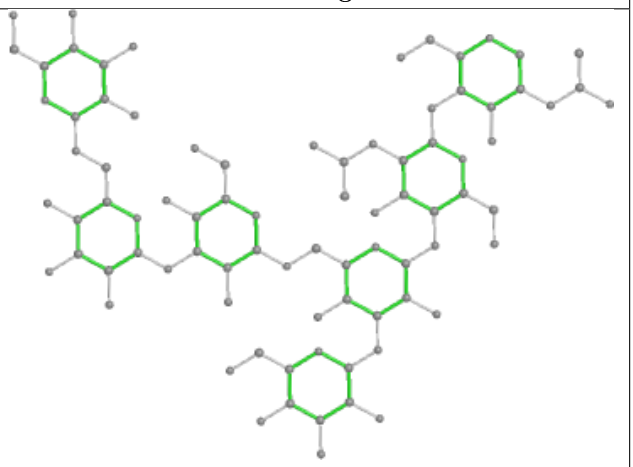
Bond lengths



Bond angles

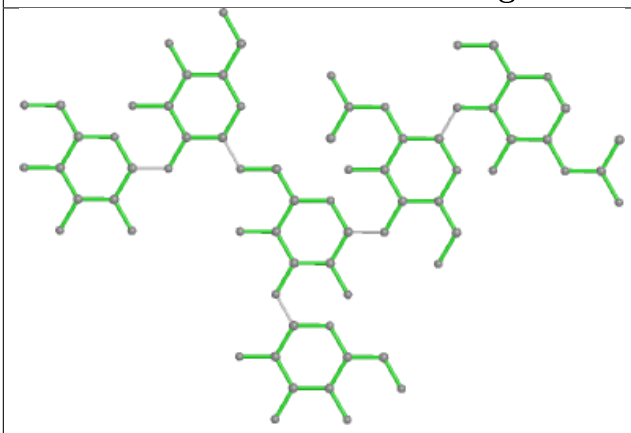


Torsions

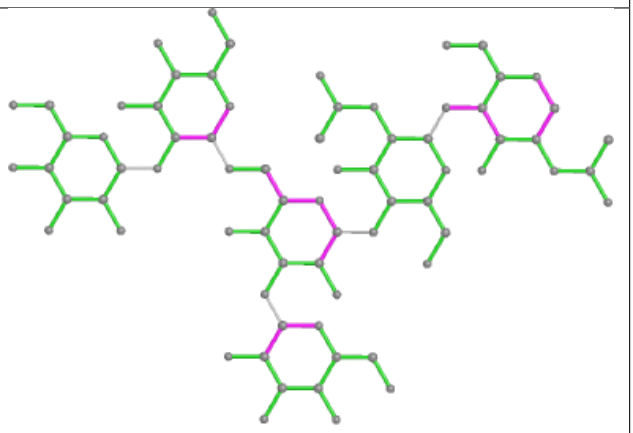


Rings

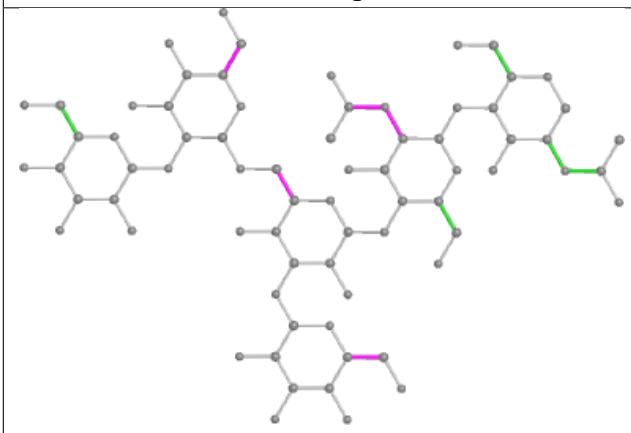
Oligosaccharide Chain S



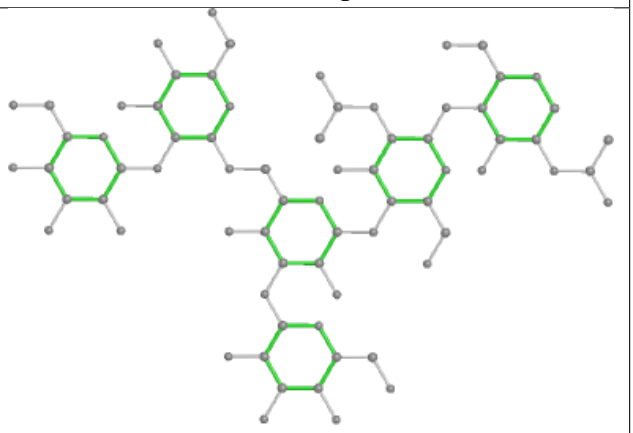
Bond lengths



Bond angles

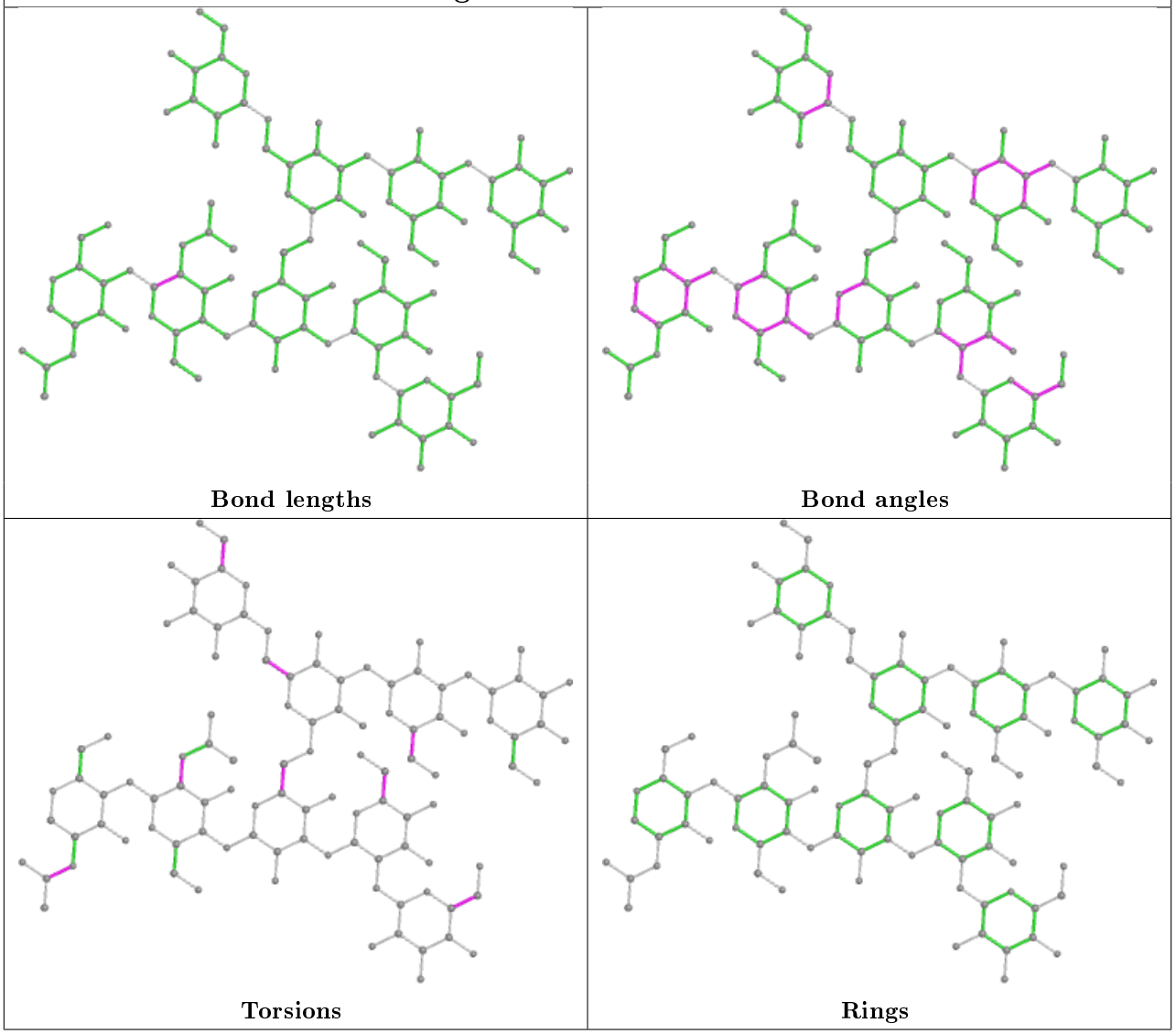


Torsions



Rings

Oligosaccharide Chain T



5.6 Ligand geometry (i)

3 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	$\#\|Z\| > 2$
19	NAG	G	633	4	14,14,15	0.29	0	17,19,21	0.75	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
19	NAG	B	701	1	14,14,15	0.38	0	17,19,21	0.76	0
19	NAG	G	601	4	14,14,15	0.29	0	17,19,21	0.66	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
19	NAG	G	633	4	-	3/6/23/26	0/1/1/1
19	NAG	B	701	1	-	2/6/23/26	0/1/1/1
19	NAG	G	601	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	G	633	NAG	C8-C7-N2-C2
19	G	633	NAG	O7-C7-N2-C2
19	B	701	NAG	C8-C7-N2-C2
19	B	701	NAG	O7-C7-N2-C2
19	G	601	NAG	O5-C5-C6-O6
19	G	633	NAG	O5-C5-C6-O6
19	G	601	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	701	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

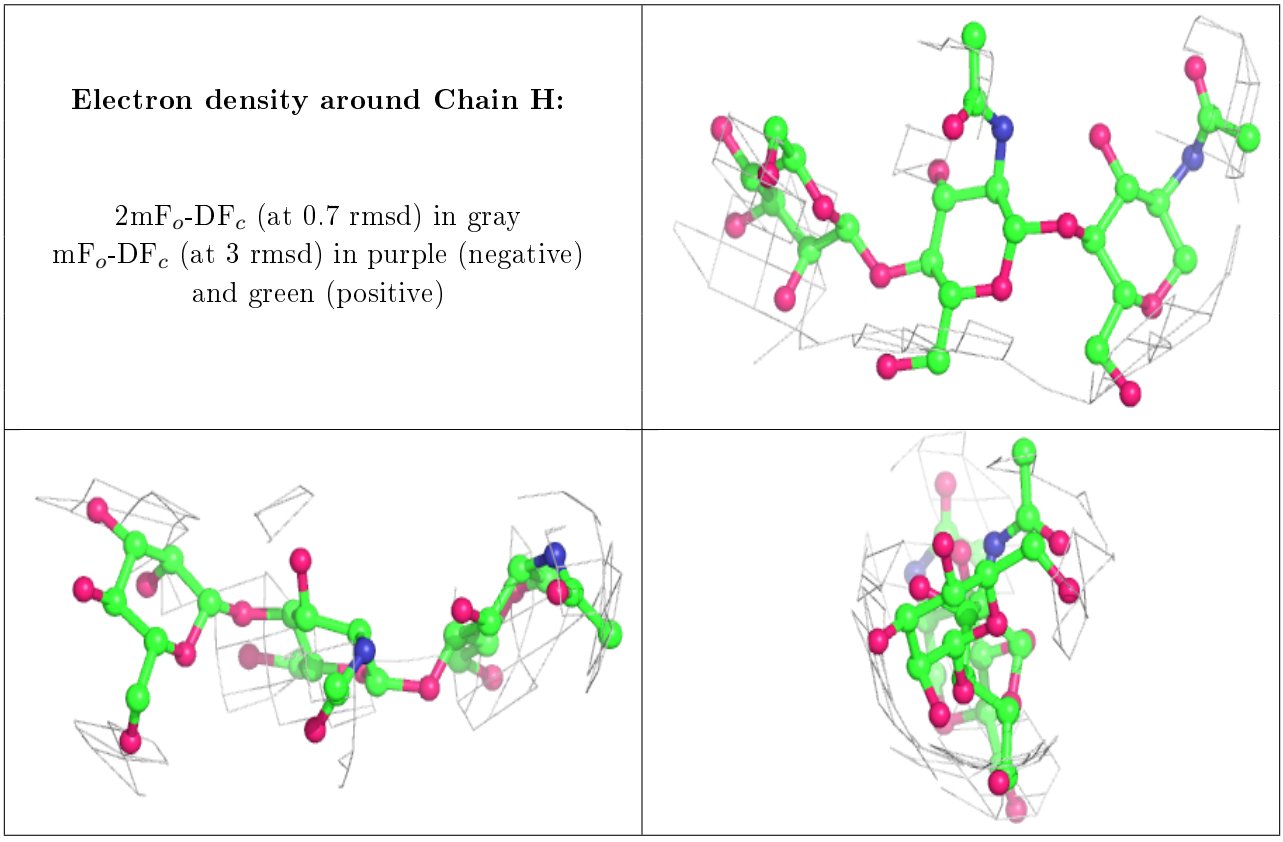
6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

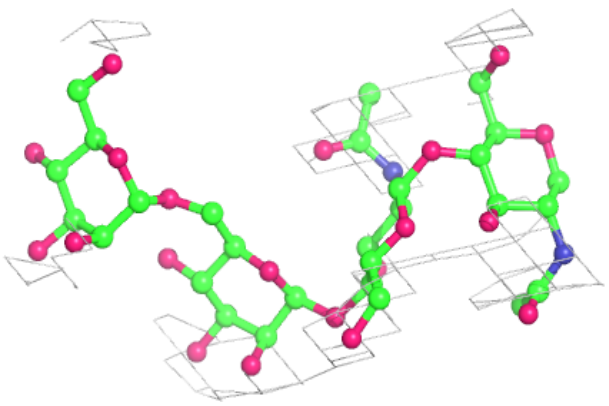
Unable to reproduce the depositors R factor - this section is therefore empty.

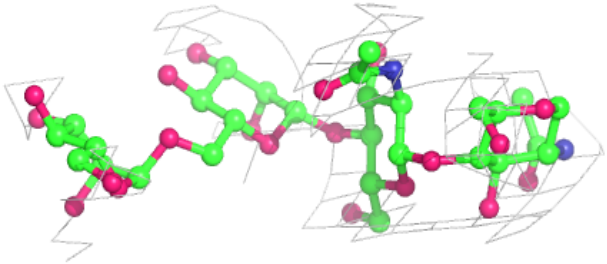
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

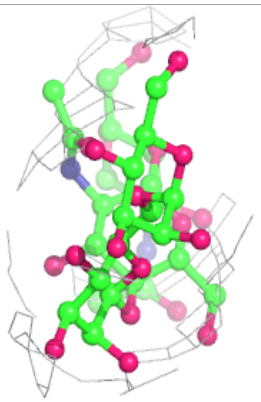


Electron density around Chain I:

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

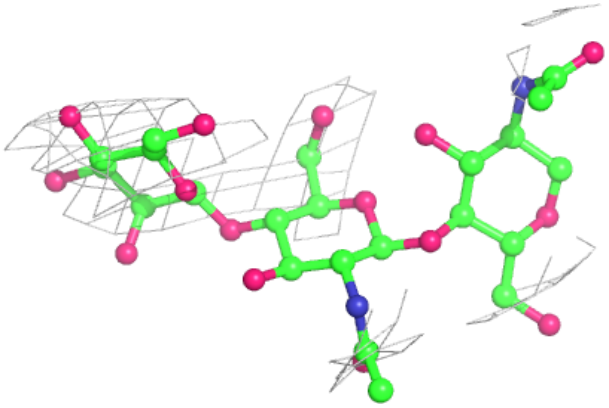


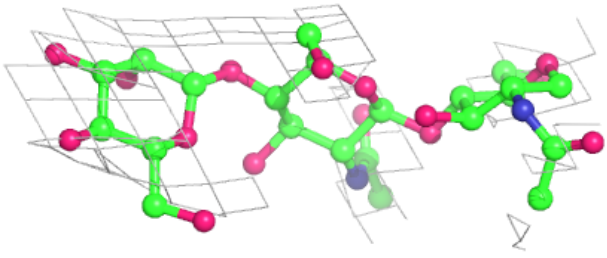


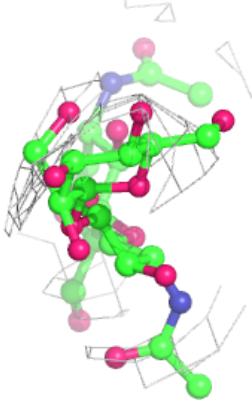


Electron density around Chain J:

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

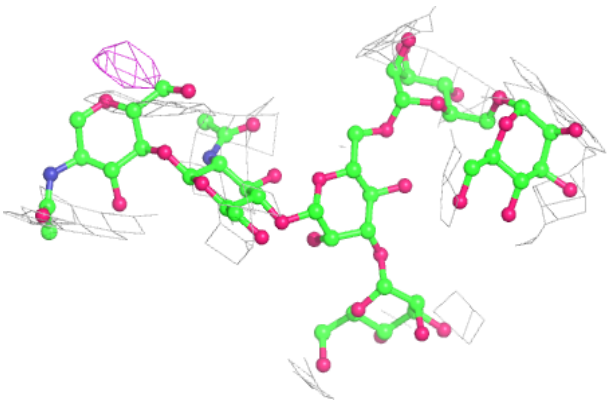


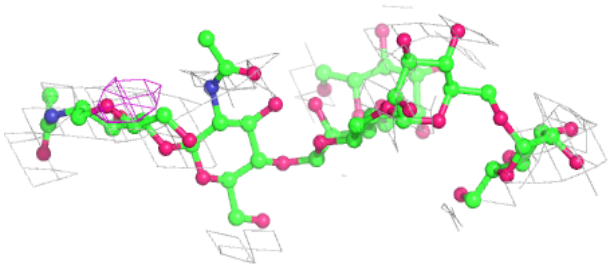


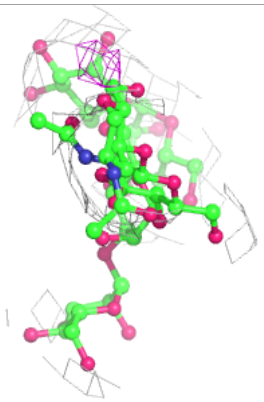


Electron density around Chain L:

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

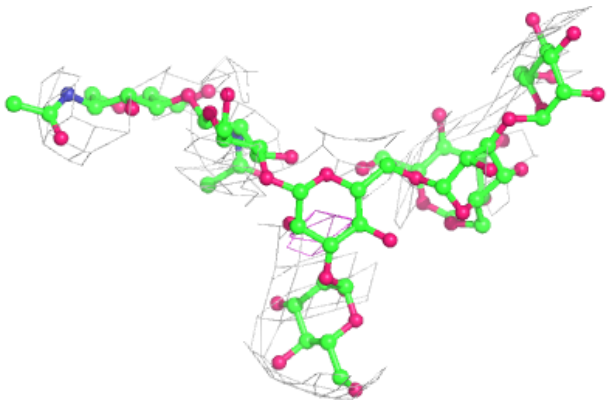


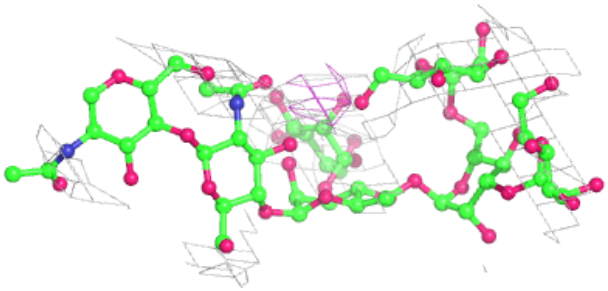


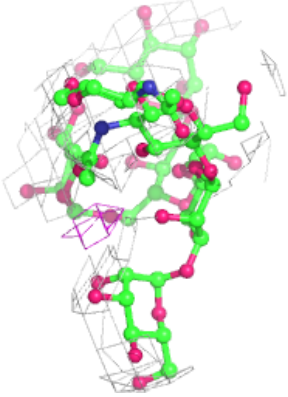


Electron density around Chain O:

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

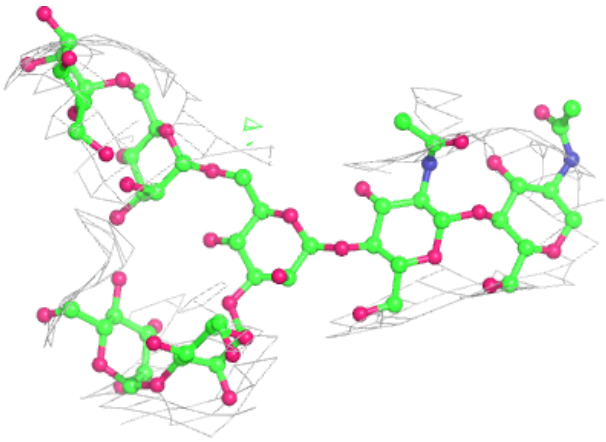


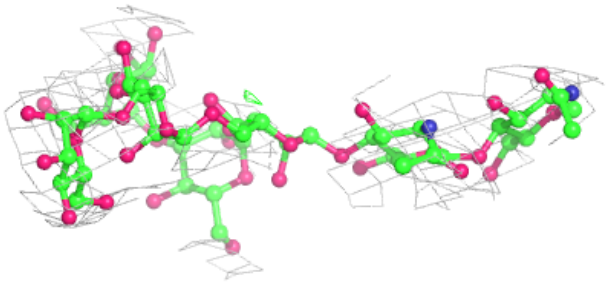


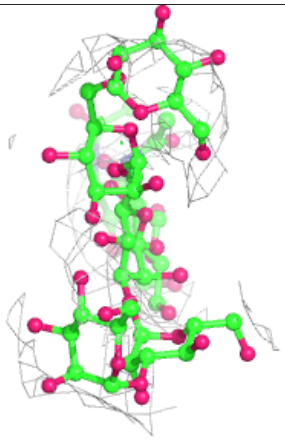


Electron density around Chain K:

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

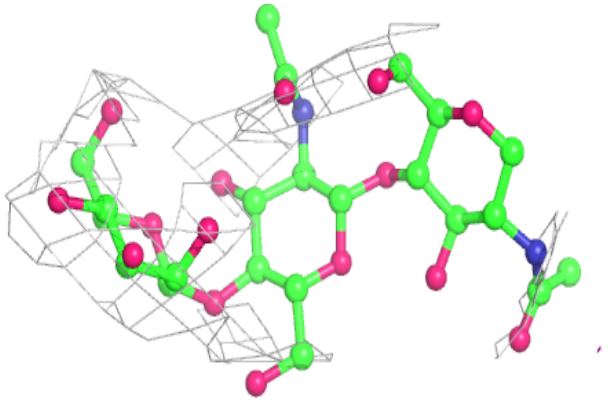


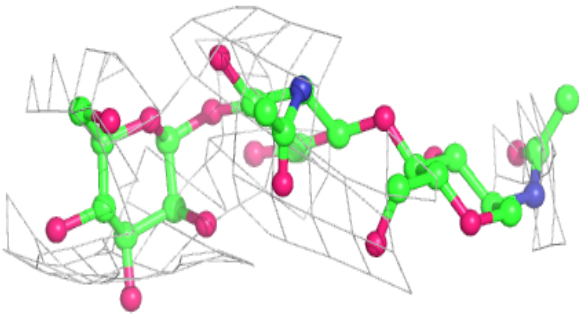


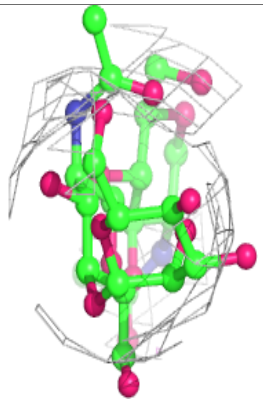


Electron density around Chain M:

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

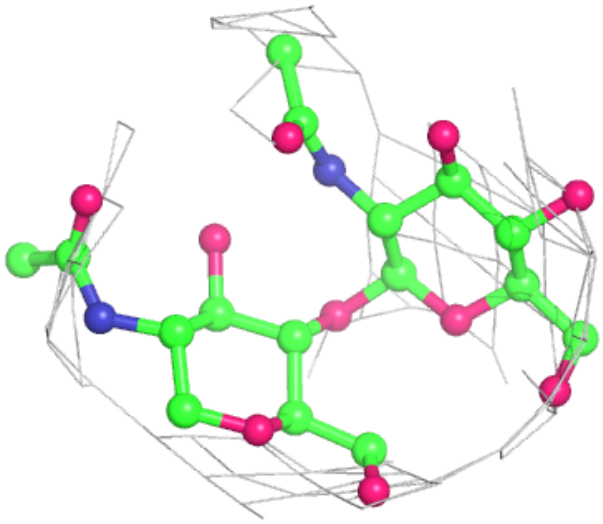


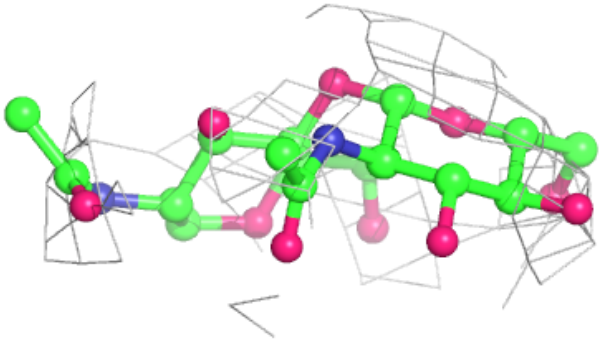


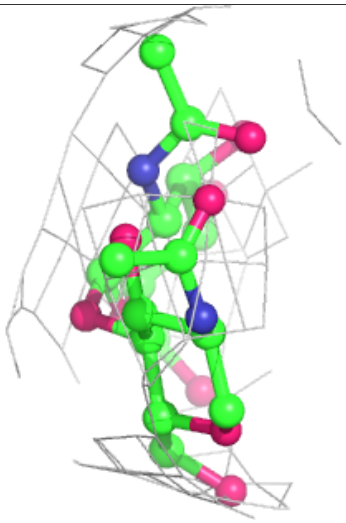


Electron density around Chain N:

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

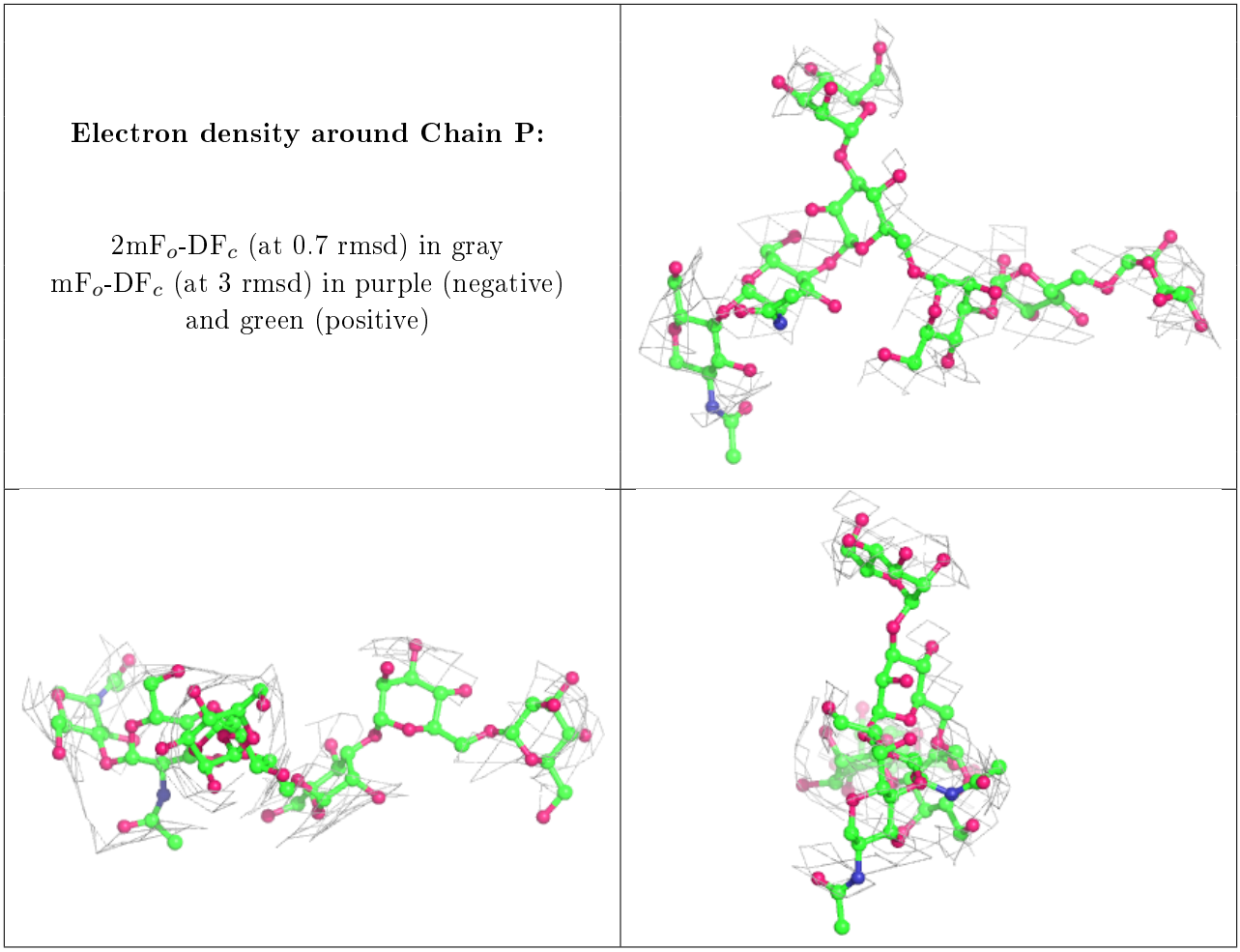






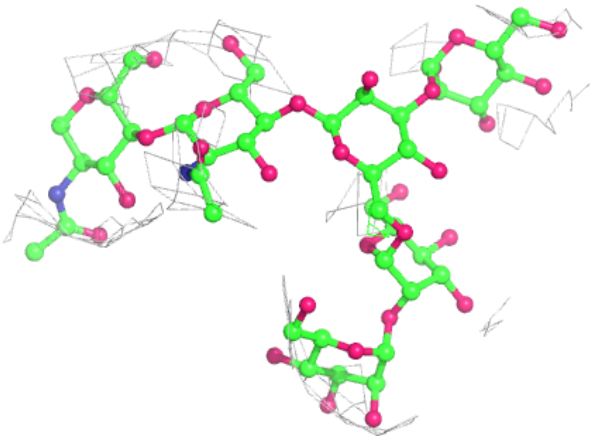
Electron density around Chain P:

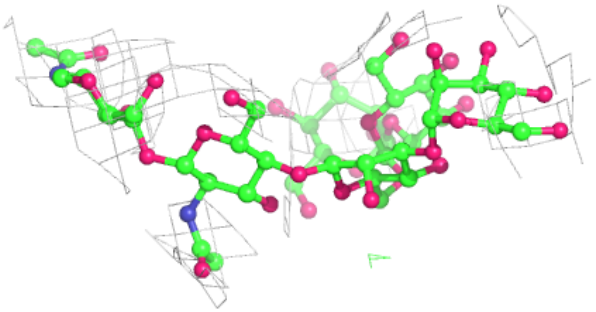
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

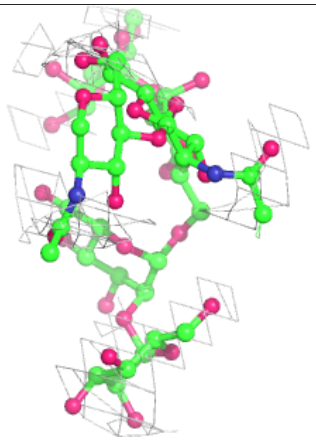


Electron density around Chain S:

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

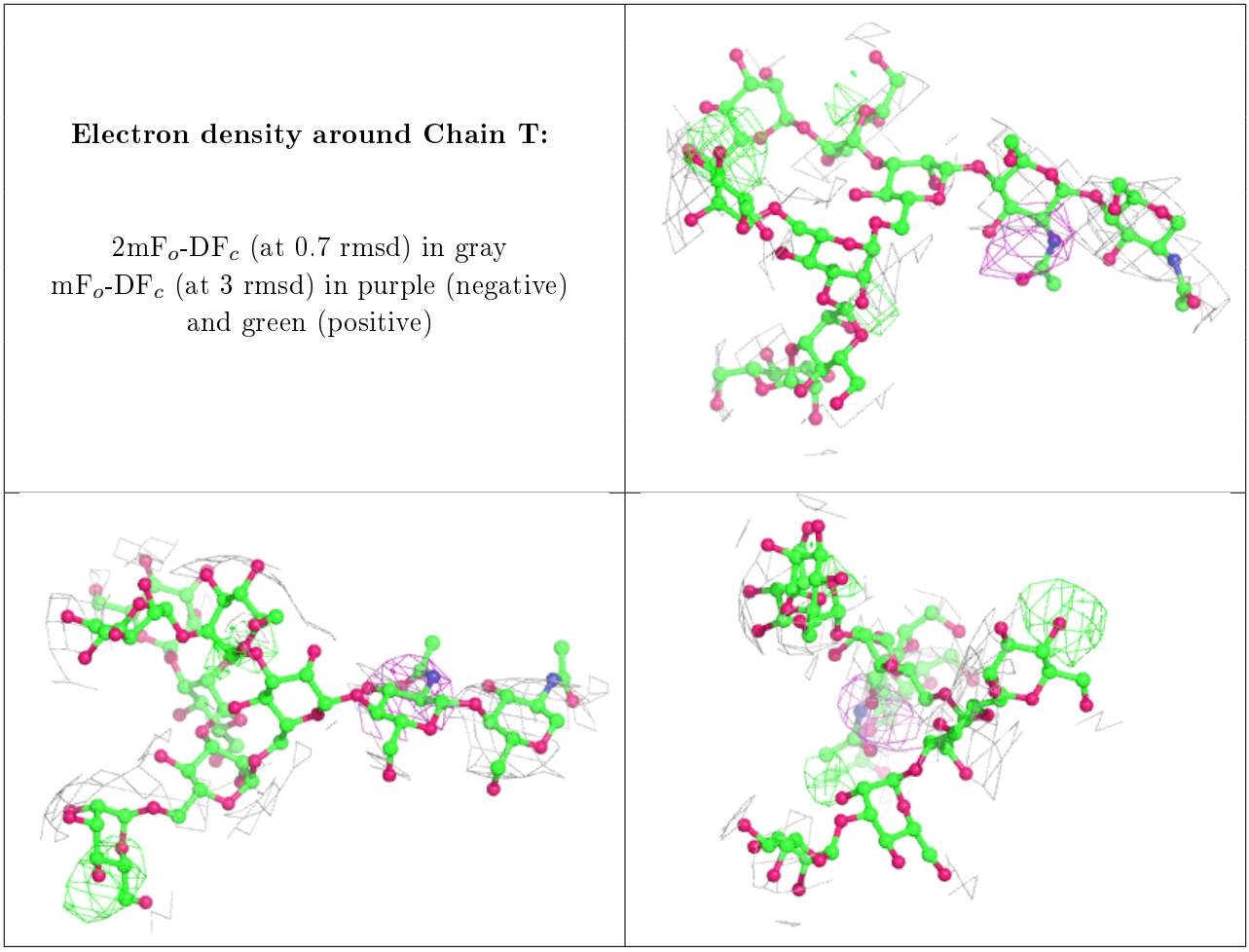






Electron density around Chain T:

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



6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.