Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 06:35 AM EDT

PDB ID	:	5CJX
Title	:	Crystal structure of 8ANC195 Fab in complex with BG505 SOSIP.664 HIV-1 Env trimer
Authors	:	Scharf, L.; Bjorkman, P.J.
Deposited on	:	2015-07-15
Resolution	:	3.58 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:

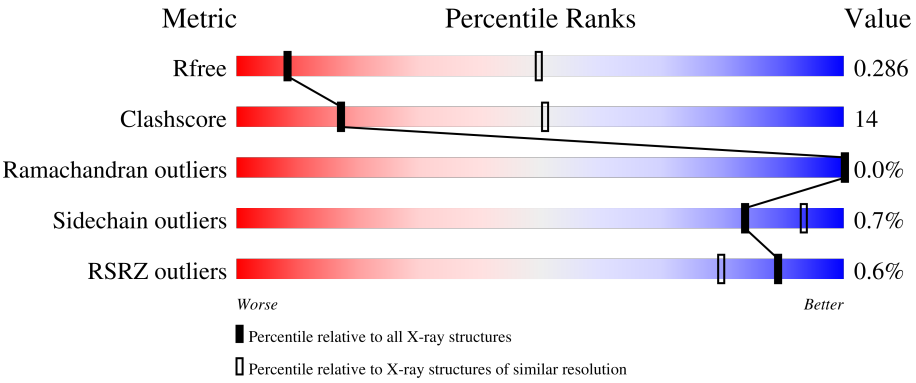
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.58 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	244	70% 22% 8%
1	D	244	74% 18% 8%
1	H	244	70% 23% • 7%
2	B	153	% 50% 31% 19%
2	J	153	55% 25% • 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	X	153	% 57% 22% 21%
3	C	215	% 86% 14%
3	E	215	85% 14%
3	L	215	83% 16%
4	G	479	62% 20% 17%
4	K	479	61% 23% 15%
4	Y	479	% 56% 27% 17%
5	F	5	80% 20%
5	b	5	20% 80%
6	I	2	50% 50%
6	M	2	100%
6	P	2	50% 50%
6	Q	2	100%
6	V	2	50% 50%
7	N	10	10% 60% 30%
7	S	10	70% 30%
7	Z	10	20% 40% 40%
8	O	6	100%
8	U	6	50% 50%
9	R	4	25% 75%
9	W	4	25% 50% 25%
10	T	3	67% 33%
10	a	3	67% 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	A	1000	-	-	-	X
11	NAG	K	1040	-	-	-	X
5	MAN	F	4	-	-	-	X
5	MAN	F	5	-	-	-	X
6	NAG	P	2	-	-	-	X
6	NAG	Q	2	-	-	-	X
7	MAN	Z	10	-	-	-	X
7	MAN	Z	9	-	-	X	-
8	NAG	O	1	-	-	X	-
9	MAN	W	4	-	-	-	X

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 22299 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 8ANC195 G52K5 heavy chain, IG gamma-1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1655	1049	278	323	5			
1	D	224	Total	C	N	O	S	0	0	0
			1614	1022	269	318	5			
1	H	227	Total	C	N	O	S	0	0	0
			1675	1063	282	325	5			

- Molecule 2 is a protein called BG505 Env gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	124	Total	C	N	O	S	0	0	0
			956	602	164	184	6			
2	J	124	Total	C	N	O	S	0	0	0
			957	605	163	183	6			
2	X	121	Total	C	N	O	S	0	0	0
			945	596	165	178	6			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called 8ANC195 G52K5 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1593	996	267	325	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1560	976	260	319	5			
3	L	214	Total	C	N	O	S	0	0	0
			1540	962	255	318	5			

- Molecule 4 is a protein called BG505 Env gp120.

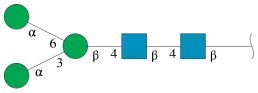
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	398	Total	C	N	O	S	0	0	0
			2857	1807	480	546	24			
4	K	405	Total	C	N	O	S	0	0	0
			2984	1891	502	564	27			
4	Y	397	Total	C	N	O	S	0	0	0
			2947	1864	501	556	26			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	320M	ASN	THR	engineered mutation	UNP Q2N0S6
G	501	CYS	ALA	engineered mutation	UNP Q2N0S6
G	509	ARG	-	expression tag	UNP Q2N0S6
G	510	ARG	-	expression tag	UNP Q2N0S6
G	511	ARG	-	expression tag	UNP Q2N0S6
G	512	ARG	-	expression tag	UNP Q2N0S6
G	513	ARG	-	expression tag	UNP Q2N0S6
K	332	ASN	THR	engineered mutation	UNP Q2N0S6
K	501	CYS	ALA	engineered mutation	UNP Q2N0S6
K	509	ARG	-	expression tag	UNP Q2N0S6
K	510	ARG	-	expression tag	UNP Q2N0S6
K	511	ARG	-	expression tag	UNP Q2N0S6
K	512	ARG	-	expression tag	UNP Q2N0S6
K	513	ARG	-	expression tag	UNP Q2N0S6
Y	320M	ASN	THR	engineered mutation	UNP Q2N0S6
Y	501	CYS	ALA	engineered mutation	UNP Q2N0S6
Y	509	ARG	-	expression tag	UNP Q2N0S6
Y	510	ARG	-	expression tag	UNP Q2N0S6
Y	511	ARG	-	expression tag	UNP Q2N0S6
Y	512	ARG	-	expression tag	UNP Q2N0S6
Y	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 5 is an oligosaccharide called 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-a

cetamido-2-deoxy-beta-D-glucopyranose.

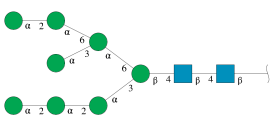


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	F	5	Total	C	N	O	0	0	0
			61	34	2	25			
5	b	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	M	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	P	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	Q	2	Total	C	N	O	0	0	0
			28	16	2	10			
6	V	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyran ose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyra nose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyra nose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-gl ucopyranose.



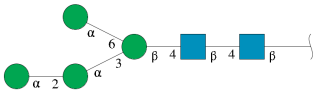
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	N	10	Total	C	N	O	0	0	0
			116	64	2	50			

Continued on next page...

Continued from previous page...

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

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.

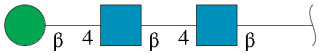


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	O	6	Total C N O 72 40 2 30	0	0	0
8	U	6	Total C N O 72 40 2 30	0	0	0

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

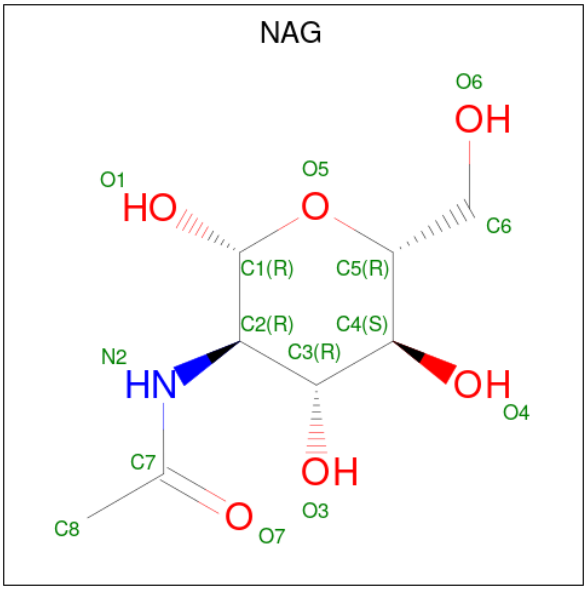
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	R	4	Total C N O 50 28 2 20	0	0	0
9	W	4	Total C N O 50 28 2 20	0	0	0

- 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	T	3	Total C N O 39 22 2 15	0	0	0
10	a	3	Total C N O 39 22 2 15	0	0	0

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



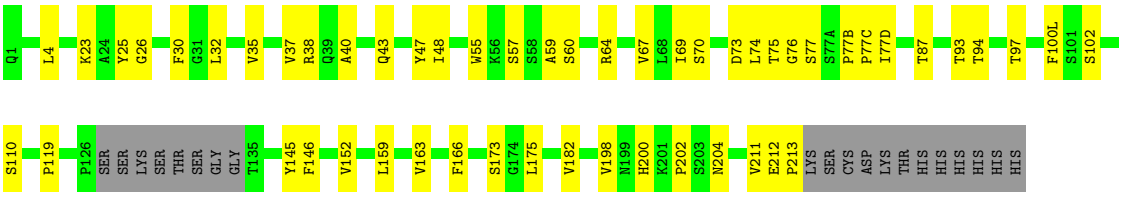
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total C N O 14 8 1 5	0	0
11	B	1	Total C N O 14 8 1 5	0	0
11	J	1	Total C N O 14 8 1 5	0	0
11	K	1	Total C N O 14 8 1 5	0	0
11	Y	1	Total C N O 14 8 1 5	0	0
11	Y	1	Total C N O 14 8 1 5	0	0

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 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.

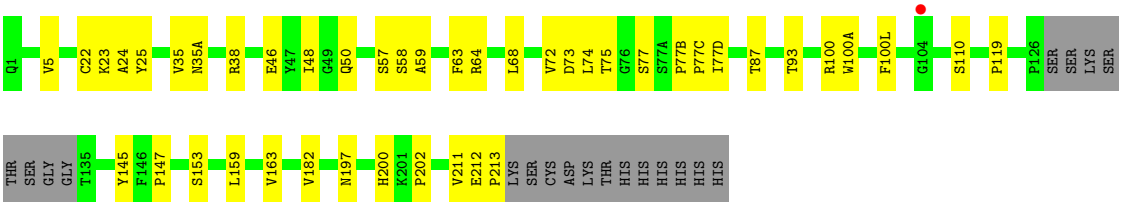
• Molecule 1: 8ANC195 G52K5 heavy chain, IG gamma-1 chain

Chain A:



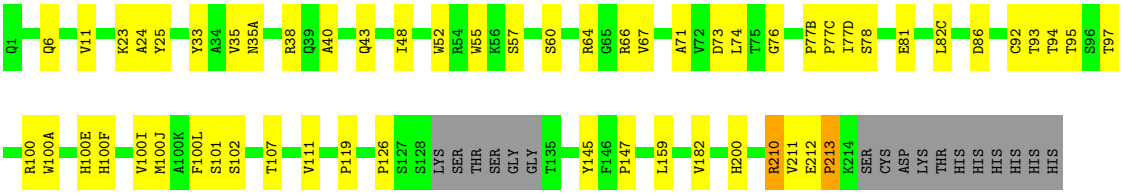
• Molecule 1: 8ANC195 G52K5 heavy chain, IG gamma-1 chain

Chain D:



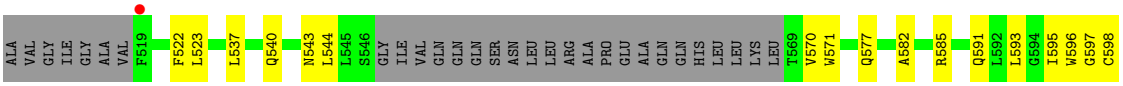
• Molecule 1: 8ANC195 G52K5 heavy chain, IG gamma-1 chain

Chain H:



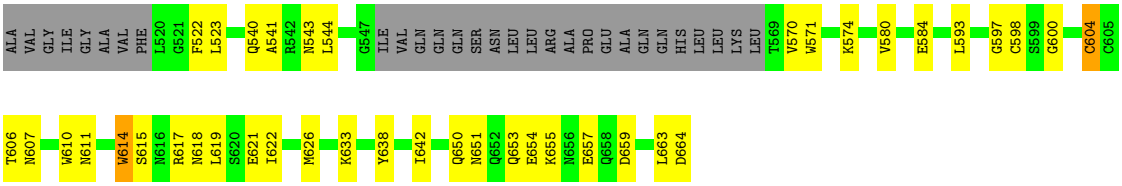
• Molecule 2: BG505 Env gp41

Chain B:



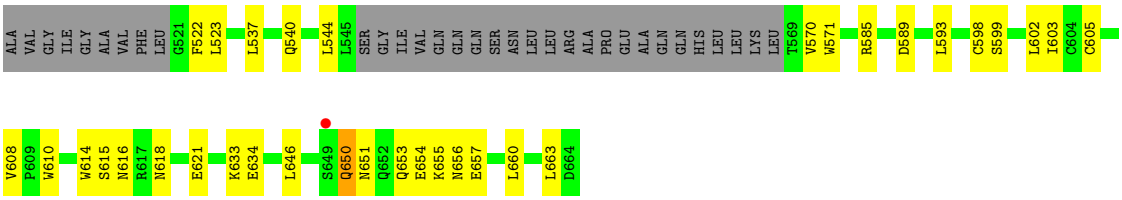
• Molecule 2: BG505 Env gp41

Chain J:



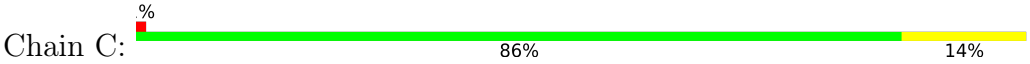
• Molecule 2: BG505 Env gp41

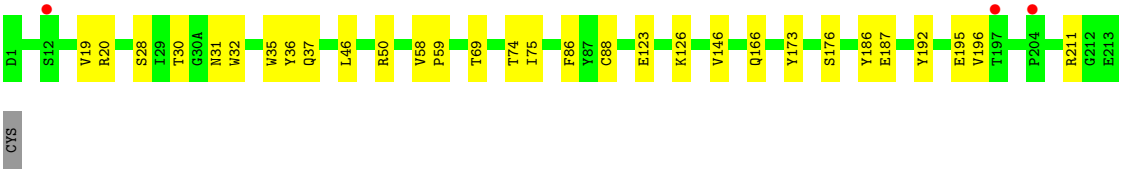
Chain X:



• Molecule 3: 8ANC195 G52K5 light chain

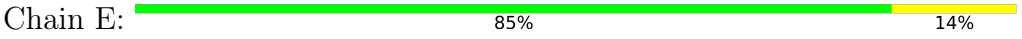
Chain C:

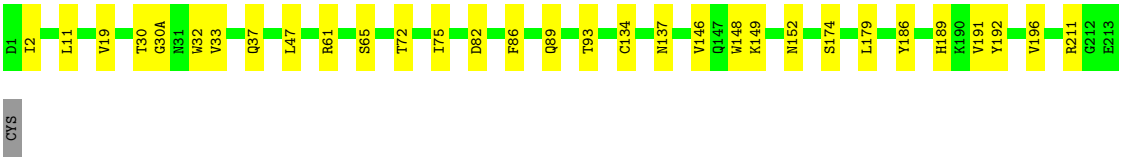




• Molecule 3: 8ANC195 G52K5 light chain

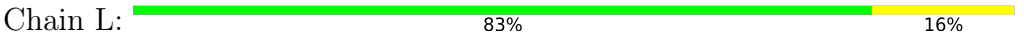
Chain E:

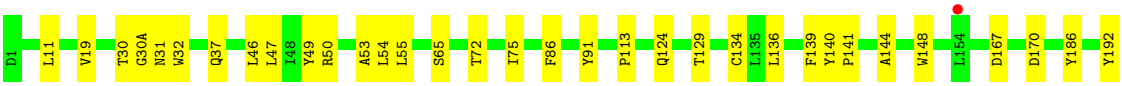


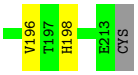


• Molecule 3: 8ANC195 G52K5 light chain

Chain L:

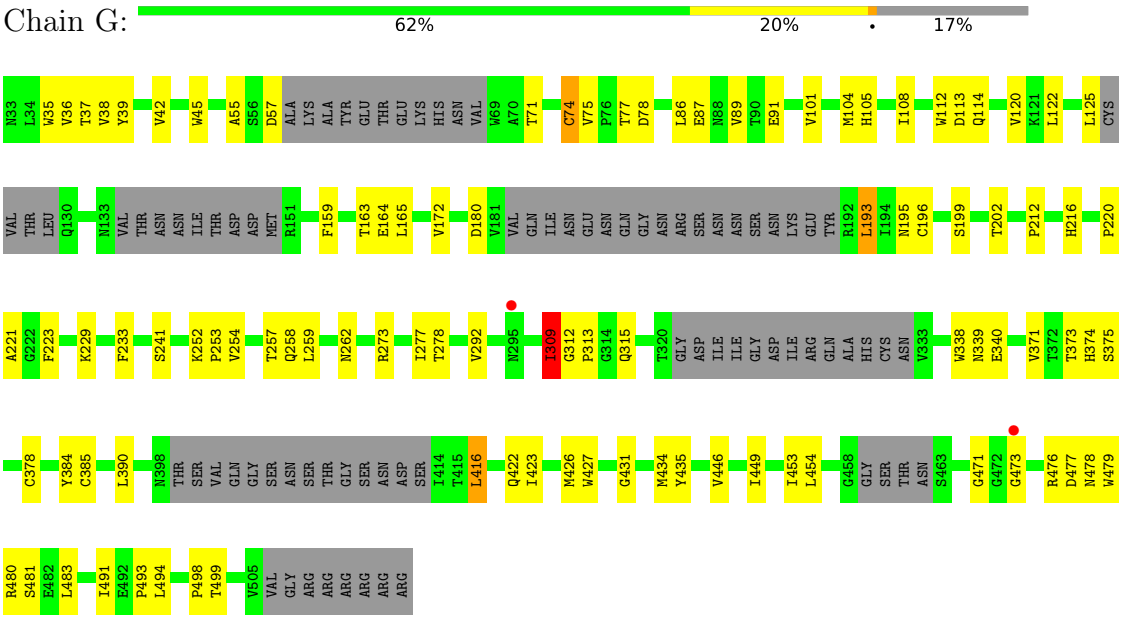






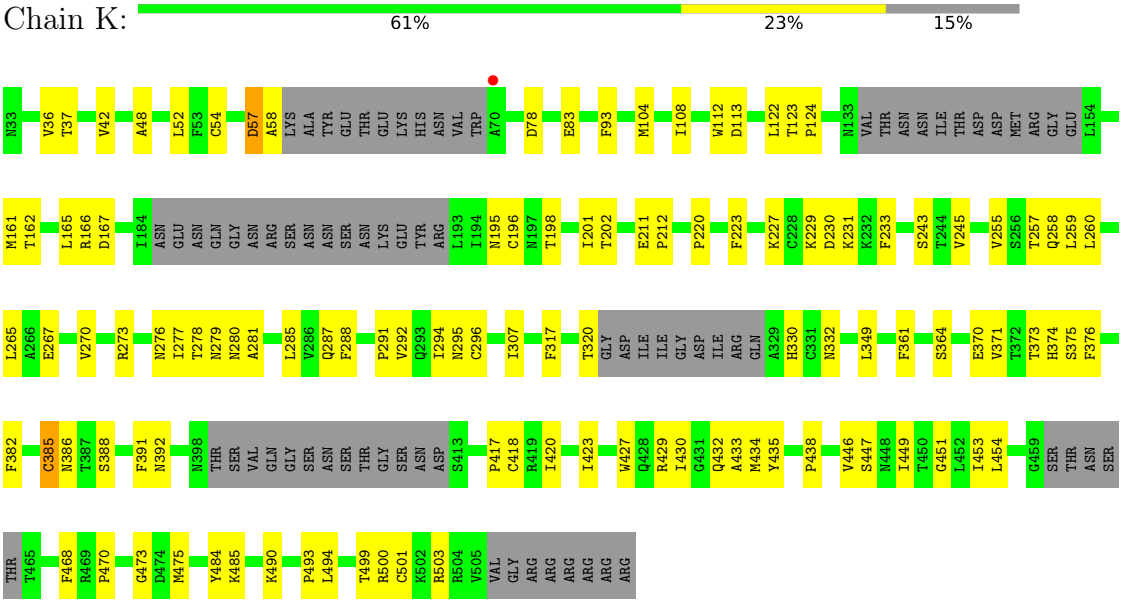
• Molecule 4: BG505 Env gp120

Chain G:



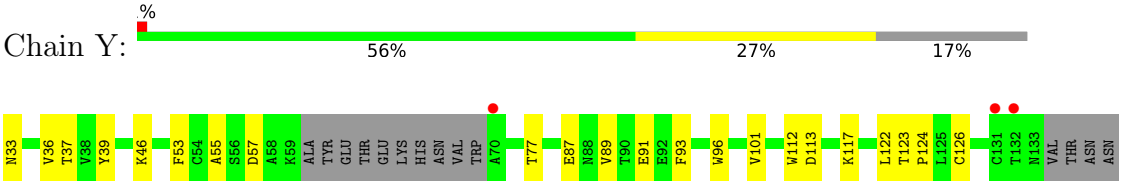
• Molecule 4: BG505 Env gp120

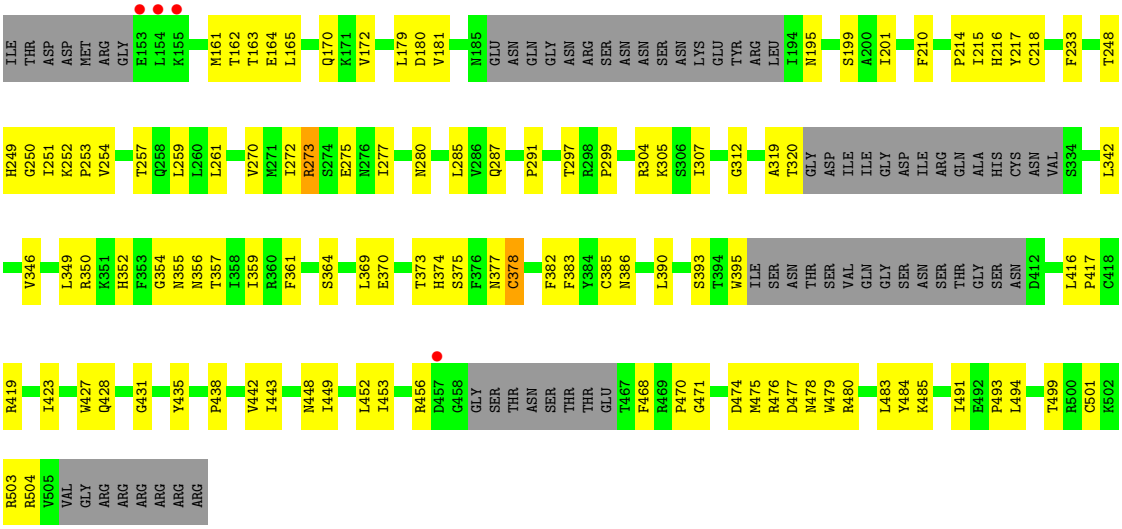
Chain K:



• Molecule 4: BG505 Env gp120

Chain Y:





• Molecule 5: 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 F:

• Molecule 5: 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

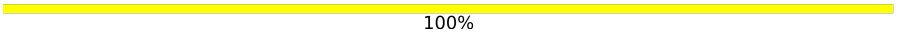
Chain b:

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

Chain I:

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

Chain M:

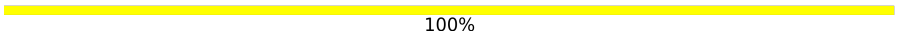


• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

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

Chain Q:

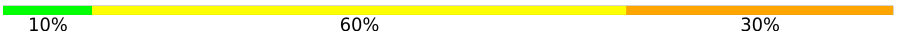


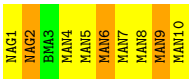
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:

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

Chain N:



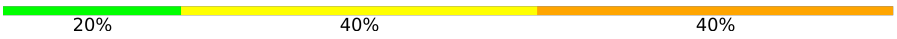


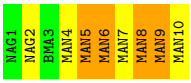
• Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

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

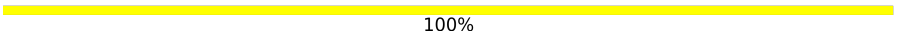
Chain Z:





• Molecule 8: alpha-D-mannopyranose-(1-2)-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 O:

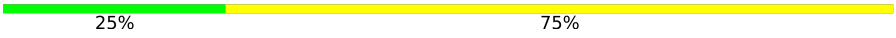


• Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:

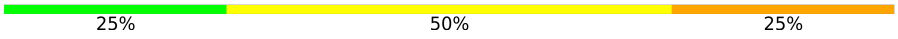
• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 9: 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 W:



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

Chain T:

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

Chain a:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	117.74Å 195.22Å 119.09Å 90.00° 101.60° 90.00°	Depositor
Resolution (Å)	29.73 – 3.58 29.73 – 3.58	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.73-3.58) 99.1 (29.73-3.58)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 3.55Å)	Xtriage
Refinement program	PHENIX (1.10pre_2100: ???)	Depositor
R, R_{free}	0.239 , 0.286 0.239 , 0.286	Depositor DCC
R_{free} test set	2015 reflections (3.29%)	wwPDB-VP
Wilson B-factor (Å^2)	130.2	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 76.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	22299	wwPDB-VP
Average B, all atoms (Å^2)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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	A	0.30	1/1700 (0.1%)	0.50	1/2334 (0.0%)
1	D	0.31	1/1656 (0.1%)	0.50	1/2280 (0.0%)
1	H	0.32	1/1720 (0.1%)	0.50	1/2359 (0.0%)
2	B	0.29	0/973	0.52	0/1327
2	J	0.28	0/974	0.51	0/1325
2	X	0.29	0/962	0.47	0/1309
3	C	0.26	0/1628	0.47	0/2221
3	E	0.26	0/1594	0.46	0/2181
3	L	0.26	0/1574	0.46	0/2159
4	G	0.33	1/2916 (0.0%)	0.49	0/4002
4	K	0.33	1/3047 (0.0%)	0.52	0/4172
4	Y	0.30	1/3009 (0.0%)	0.49	1/4119 (0.0%)
All	All	0.30	6/21753 (0.0%)	0.49	4/29788 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	G	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	309	ILE	C-N	9.34	1.49	1.33
4	K	385	CYS	CB-SG	-8.54	1.67	1.82
4	Y	378	CYS	CB-SG	-5.71	1.72	1.81
1	H	213	PRO	N-CD	5.22	1.55	1.47
1	D	213	PRO	N-CD	5.21	1.55	1.47
1	A	213	PRO	N-CD	5.02	1.54	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	GLU	C-N-CD	5.82	140.62	128.40
4	Y	273	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	H	212	GLU	C-N-CD	5.71	140.38	128.40
1	D	212	GLU	C-N-CD	5.68	140.33	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	309	ILE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1655	0	1577	35	0
1	D	1614	0	1511	45	0
1	H	1675	0	1600	52	0
2	B	956	0	898	70	0
2	J	957	0	915	38	0
2	X	945	0	905	36	0
3	C	1593	0	1489	19	0
3	E	1560	0	1438	22	0
3	L	1540	0	1382	24	0
4	G	2857	0	2565	79	0
4	K	2984	0	2763	105	0
4	Y	2947	0	2734	124	0
5	F	61	0	52	4	0
5	b	61	0	52	0	0
6	I	28	0	25	0	0
6	M	28	0	25	2	0
6	P	28	0	25	0	0
6	Q	28	0	25	1	0
6	V	28	0	25	0	0
7	N	116	0	97	7	0
7	S	116	0	96	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	Z	116	0	96	13	0
8	O	72	0	61	9	0
8	U	72	0	61	5	0
9	R	50	0	43	1	0
9	W	50	0	43	3	0
10	T	39	0	34	1	0
10	a	39	0	34	0	0
11	A	14	0	13	0	0
11	B	14	0	13	0	0
11	J	14	0	13	0	0
11	K	14	0	13	0	0
11	Y	28	0	26	1	0
All	All	22299	0	20649	595	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 14.

All (595) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:LEU:O	2:B:649:SER:HB2	1.16	1.32
4:K:231:LYS:HD2	4:K:267:GLU:CD	1.61	1.21
2:B:645:LEU:O	2:B:649:SER:CB	1.88	1.19
4:G:278:THR:HG22	8:O:1:NAG:O6	1.40	1.15
2:B:650:GLN:O	2:B:654:GLU:N	1.77	1.15
2:B:598:CYS:SG	2:B:604:CYS:SG	1.26	1.15
4:Y:216:HIS:CE1	4:Y:250:GLY:HA3	1.81	1.14
2:B:597:GLY:N	2:B:651:ASN:HD21	1.42	1.14
2:J:604:CYS:O	4:K:37:THR:HG23	1.51	1.11
2:B:598:CYS:SG	2:B:604:CYS:CB	2.39	1.10
1:D:59:ALA:HB2	7:Z:9:MAN:H4	1.30	1.09
2:B:601:LYS:O	2:X:655:LYS:NZ	1.92	1.03
4:Y:257:THR:HG21	4:Y:370:GLU:O	1.59	1.02
4:Y:216:HIS:CE1	4:Y:250:GLY:CA	2.43	1.01
2:B:608:VAL:HG22	2:B:649:SER:OG	1.61	1.00
4:Y:257:THR:CG2	4:Y:370:GLU:O	2.09	1.00
4:K:386:ASN:OD1	4:K:388:SER:N	2.00	0.93
2:J:597:GLY:HA3	4:K:503:ARG:HH12	1.39	0.88
2:J:618:ASN:HB3	2:J:621:GLU:HB2	1.55	0.88
2:B:597:GLY:N	2:B:651:ASN:ND2	2.21	0.87
1:D:59:ALA:HB2	7:Z:9:MAN:C4	2.05	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:231:LYS:CD	4:K:267:GLU:CD	2.44	0.86
4:Y:216:HIS:CD2	4:Y:250:GLY:N	2.44	0.86
1:D:38:ARG:HB2	1:D:48:ILE:HD11	1.58	0.85
4:Y:216:HIS:NE2	4:Y:250:GLY:N	2.26	0.83
2:B:597:GLY:CA	2:B:651:ASN:HD21	1.92	0.83
2:B:601:LYS:C	2:X:655:LYS:HZ1	1.81	0.82
2:X:605:CYS:HA	4:Y:37:THR:HG22	1.61	0.81
4:K:259:LEU:HB2	4:K:374:HIS:CE1	2.15	0.81
1:D:59:ALA:CB	7:Z:9:MAN:H4	2.10	0.81
1:H:210:ARG:HH11	1:H:210:ARG:HG2	1.45	0.81
1:A:74:LEU:HD23	1:A:77(B):PRO:HA	1.63	0.80
2:B:601:LYS:CB	2:B:602:LEU:HD13	2.10	0.80
4:Y:249:HIS:CD2	4:Y:251:ILE:HG12	2.16	0.80
4:G:278:THR:OG1	1:H:74:LEU:HD11	1.82	0.80
8:U:3:BMA:HO4	8:U:5:MAN:HO6	1.30	0.80
1:H:11:VAL:HG21	1:H:147:PRO:HG3	1.64	0.79
2:B:602:LEU:HD22	2:X:655:LYS:HZ3	1.48	0.79
2:B:544:LEU:HD21	4:G:493:PRO:HG3	1.66	0.78
4:Y:304:ARG:NH1	4:Y:320:THR:OG1	2.18	0.77
1:D:57:SER:OG	7:Z:8:MAN:H2	1.85	0.77
1:H:57:SER:HG	7:N:9:MAN:HO6	1.31	0.76
4:G:477:ASP:OD1	4:G:480:ARG:NH1	2.18	0.76
1:H:38:ARG:HB3	1:H:48:ILE:HD11	1.66	0.76
4:K:231:LYS:HD2	4:K:267:GLU:OE2	1.87	0.75
2:X:593:LEU:HD11	4:Y:494:LEU:HD21	1.68	0.75
2:J:664:ASP:O	4:Y:504:ARG:NH2	2.20	0.75
2:B:650:GLN:O	2:B:654:GLU:CB	2.35	0.75
4:K:233:PHE:O	4:K:273:ARG:NH2	2.18	0.75
4:K:113:ASP:OD1	4:K:429:ARG:NH2	2.21	0.74
4:Y:386:ASN:HB3	4:Y:417:PRO:HG2	1.69	0.73
4:K:231:LYS:HD2	4:K:267:GLU:OE1	1.88	0.73
1:H:6:GLN:HE21	1:H:107:THR:HG23	1.52	0.73
4:G:292:VAL:HB	4:G:449:ILE:HB	1.72	0.72
4:G:278:THR:CG2	8:O:1:NAG:O6	2.30	0.72
2:J:593:LEU:HD11	4:K:494:LEU:HD21	1.71	0.72
2:J:598:CYS:O	2:J:600:GLY:N	2.20	0.72
4:Y:257:THR:HG23	4:Y:370:GLU:O	1.87	0.72
2:X:544:LEU:HD21	4:Y:493:PRO:HG3	1.72	0.71
2:B:602:LEU:HB2	2:X:655:LYS:NZ	2.04	0.71
2:B:608:VAL:CG2	2:B:649:SER:OG	2.36	0.71
4:Y:215:ILE:O	4:Y:251:ILE:N	2.23	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:55:ALA:HB3	4:Y:216:HIS:HB2	1.71	0.71
1:A:159:LEU:HD21	1:A:182:VAL:HG11	1.73	0.71
2:B:631:TRP:CE2	2:B:635:ILE:HD11	2.26	0.70
4:G:278:THR:CG2	8:O:1:NAG:H5	2.21	0.70
4:K:295:ASN:HA	4:K:446:VAL:HG12	1.72	0.70
1:D:74:LEU:HB3	1:D:77(C):PRO:HD3	1.72	0.70
2:J:610:TRP:HE3	4:K:36:VAL:HG12	1.56	0.70
4:Y:257:THR:HB	4:Y:375:SER:H	1.58	0.69
1:D:38:ARG:NH2	1:D:46:GLU:OE1	2.23	0.69
4:G:385:CYS:HB3	4:G:416:LEU:HD13	1.74	0.69
1:H:66:ARG:NH1	1:H:86:ASP:OD2	2.25	0.69
1:A:76:GLY:HA2	4:K:278:THR:HA	1.73	0.68
3:E:186:TYR:O	3:E:192:TYR:OH	2.11	0.68
4:Y:101:VAL:HG11	4:Y:480:ARG:HG2	1.75	0.68
1:D:74:LEU:HD11	4:Y:277:ILE:HB	1.74	0.68
2:J:544:LEU:HD21	4:K:493:PRO:HG3	1.74	0.68
3:L:30(A):GLY:O	3:L:50:ARG:NH1	2.26	0.68
4:Y:304:ARG:NH2	4:Y:435:TYR:OH	2.26	0.68
4:Y:257:THR:HG21	4:Y:373:THR:O	1.94	0.68
4:G:476:ARG:HA	4:G:479:TRP:CD1	2.28	0.68
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.76	0.68
4:Y:249:HIS:HD2	4:Y:251:ILE:HG12	1.60	0.67
4:K:37:THR:OG1	4:K:499:THR:HG21	1.95	0.67
4:K:231:LYS:CD	4:K:267:GLU:OE2	2.41	0.67
4:K:201:ILE:HD11	4:K:435:TYR:HB2	1.75	0.66
2:B:598:CYS:O	2:B:599:SER:OG	2.12	0.66
4:Y:249:HIS:O	4:Y:251:ILE:HG13	1.95	0.66
1:H:74:LEU:HD13	1:H:77(C):PRO:HD3	1.78	0.66
4:Y:257:THR:OG1	4:Y:375:SER:OG	2.13	0.66
2:B:603:ILE:C	2:B:603:ILE:HD12	2.16	0.66
4:Y:161:MET:SD	4:Y:162:THR:N	2.69	0.66
4:G:163:THR:HG23	4:G:165:LEU:H	1.60	0.66
4:K:231:LYS:CE	4:K:267:GLU:OE2	2.44	0.66
1:H:52:TRP:NE1	1:H:97:THR:HG21	2.11	0.65
4:G:278:THR:HG22	8:O:1:NAG:C6	2.26	0.65
4:K:292:VAL:HB	4:K:449:ILE:HB	1.79	0.65
4:G:71:THR:O	4:G:74:CYS:HB3	1.97	0.65
2:B:631:TRP:CZ2	2:B:635:ILE:HD11	2.31	0.65
1:H:73:ASP:OD1	1:H:74:LEU:N	2.26	0.65
1:H:94:THR:HB	1:H:102:SER:HB2	1.78	0.65
1:A:23:LYS:HA	1:A:77(D):ILE:HG12	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:186:TYR:O	3:E:211:ARG:NH2	2.29	0.64
4:G:278:THR:HG21	8:O:1:NAG:H5	1.80	0.64
1:D:100:ARG:NH1	4:Y:91:GLU:OE1	2.30	0.64
2:B:623:TRP:HZ2	4:G:499:THR:HG22	1.61	0.64
1:A:25:TYR:CD1	8:U:2:NAG:H2	2.33	0.64
4:K:361:PHE:C	4:K:391:PHE:O	2.36	0.64
4:Y:215:ILE:N	4:Y:251:ILE:O	2.28	0.64
4:Y:257:THR:CG2	4:Y:373:THR:O	2.46	0.64
3:L:136:LEU:HD21	3:L:196:VAL:HG21	1.79	0.64
4:K:165:LEU:HD23	4:K:167:ASP:H	1.62	0.63
1:H:25:TYR:CD1	8:O:2:NAG:H2	2.33	0.63
2:X:651:ASN:ND2	2:X:655:LYS:HD2	2.14	0.63
4:Y:216:HIS:ND1	4:Y:250:GLY:CA	2.60	0.63
4:K:231:LYS:CD	4:K:267:GLU:OE1	2.45	0.63
1:A:57:SER:OG	7:S:9:MAN:O6	2.13	0.63
1:D:68:LEU:HD23	7:Z:6:MAN:C6	2.29	0.63
1:H:23:LYS:HA	1:H:77(D):ILE:HG12	1.81	0.63
2:X:610:TRP:CE3	4:Y:36:VAL:HG12	2.34	0.63
4:K:231:LYS:HE3	4:K:267:GLU:OE2	1.99	0.62
2:B:570:VAL:HG12	2:B:571:TRP:H	1.63	0.62
2:X:610:TRP:HE3	4:Y:36:VAL:HG12	1.64	0.62
9:W:1:NAG:H62	9:W:2:NAG:C7	2.29	0.62
4:Y:216:HIS:CG	4:Y:250:GLY:HA2	2.35	0.62
4:Y:112:TRP:CH2	4:Y:210:PHE:HE2	2.18	0.62
4:K:391:PHE:HD2	4:K:470:PRO:HD3	1.64	0.62
5:F:1:NAG:H62	5:F:2:NAG:C7	2.29	0.62
4:Y:254:VAL:HG11	4:Y:261:LEU:O	2.00	0.61
4:Y:57:ASP:O	4:Y:77:THR:HG22	2.00	0.61
2:X:585:ARG:NH2	4:Y:491:ILE:O	2.34	0.61
4:Y:216:HIS:NE2	4:Y:250:GLY:CA	2.62	0.61
2:B:623:TRP:CZ2	4:G:499:THR:HG22	2.35	0.61
1:D:159:LEU:HD21	1:D:182:VAL:HG11	1.83	0.61
4:K:273:ARG:HB2	4:K:285:LEU:HG	1.83	0.61
2:J:650:GLN:O	2:J:654:GLU:HB2	2.00	0.61
2:X:650:GLN:O	2:X:654:GLU:N	2.33	0.61
2:B:650:GLN:O	2:B:654:GLU:HB3	2.01	0.60
4:K:122:LEU:HB2	4:K:201:ILE:HG23	1.80	0.60
3:E:30:THR:HG21	2:X:616:ASN:H	1.65	0.60
4:K:265:LEU:HD21	4:K:291:PRO:HD3	1.82	0.60
4:K:361:PHE:HB3	4:K:391:PHE:O	2.01	0.60
1:A:211:VAL:HG12	1:A:211:VAL:O	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:GLN:NE2	2:J:541:ALA:O	2.36	0.59
4:Y:359:ILE:HD13	4:Y:361:PHE:HE1	1.68	0.59
4:K:223:PHE:CE1	4:K:490:LYS:HG2	2.37	0.59
1:A:25:TYR:HD1	8:U:2:NAG:H2	1.66	0.59
4:Y:259:LEU:HB2	4:Y:374:HIS:CE1	2.37	0.59
4:Y:475:MET:SD	4:Y:478:ASN:ND2	2.75	0.59
1:D:93:THR:HG21	1:D:100(L):PHE:CD1	2.38	0.59
4:Y:216:HIS:ND1	4:Y:250:GLY:HA2	2.17	0.59
2:B:593:LEU:HG	2:B:599:SER:H	1.66	0.59
4:G:253:PRO:HA	4:G:479:TRP:HZ3	1.68	0.59
4:G:478:ASN:OD1	4:G:479:TRP:N	2.35	0.59
4:K:195:ASN:HB3	4:K:423:ILE:HD12	1.85	0.59
1:H:210:ARG:HH11	1:H:210:ARG:CG	2.16	0.59
4:K:257:THR:HG21	4:K:370:GLU:O	2.03	0.58
4:K:391:PHE:CD2	4:K:470:PRO:HD3	2.37	0.58
4:G:259:LEU:HB2	4:G:374:HIS:CE1	2.38	0.58
3:C:30:THR:HG21	2:J:615:SER:HA	1.86	0.58
2:J:650:GLN:O	2:J:654:GLU:CB	2.51	0.58
4:Y:53:PHE:CZ	4:Y:218:CYS:HB2	2.37	0.58
2:J:597:GLY:N	2:J:651:ASN:OD1	2.37	0.58
2:B:650:GLN:O	2:B:654:GLU:CA	2.50	0.58
4:G:423:ILE:HG22	4:G:435:TYR:HA	1.84	0.58
4:G:309:ILE:HG23	4:G:309:ILE:O	2.04	0.57
2:X:608:VAL:N	2:X:650:GLN:OE1	2.37	0.57
1:A:87:THR:HG23	1:A:110:SER:HA	1.85	0.57
1:H:93:THR:HG21	1:H:100(L):PHE:CD1	2.39	0.57
1:H:25:TYR:CE1	1:H:77(B):PRO:HG3	2.39	0.57
4:K:276:ASN:HB3	4:K:279:ASN:HB3	1.84	0.57
2:B:602:LEU:HB2	2:X:655:LYS:HZ3	1.68	0.57
1:H:6:GLN:OE1	1:H:92:CYS:N	2.37	0.57
2:X:610:TRP:NE1	2:X:614:TRP:O	2.34	0.57
4:Y:428:GLN:O	4:Y:428:GLN:HG3	2.05	0.57
1:A:93:THR:HG21	1:A:100(L):PHE:CD1	2.40	0.57
1:H:126:PRO:HG2	1:H:213:PRO:HB3	1.86	0.57
4:Y:233:PHE:O	4:Y:273:ARG:NH2	2.38	0.57
2:B:523:LEU:HA	2:B:540:GLN:HE21	1.70	0.57
1:H:81:GLU:OE1	7:N:6:MAN:H62	2.05	0.57
1:A:75:THR:HG22	1:A:77:SER:H	1.69	0.56
4:Y:350:ARG:O	4:Y:354:GLY:N	2.36	0.56
4:Y:215:ILE:HD12	4:Y:253:PRO:HG3	1.87	0.56
1:D:73:ASP:HA	1:D:77(C):PRO:HB3	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:31:ASN:O	3:L:50:ARG:HA	2.05	0.56
1:D:68:LEU:CD2	7:Z:6:MAN:O6	2.53	0.56
2:J:655:LYS:HZ3	2:X:602:LEU:H	1.54	0.56
4:Y:484:TYR:CE1	4:Y:485:LYS:HG2	2.41	0.56
4:G:212:PRO:HG2	6:M:1:NAG:O7	2.06	0.56
4:G:373:THR:HG21	4:G:384:TYR:HB3	1.86	0.56
4:K:373:THR:OG1	4:K:385:CYS:N	2.38	0.56
4:G:45:TRP:O	1:H:100(A):TRP:HH2	1.88	0.56
2:J:663:LEU:HD12	2:J:664:ASP:HB2	1.88	0.56
2:B:663:LEU:HD11	4:K:500:ARG:HE	1.72	0.55
1:D:5:VAL:O	1:D:23:LYS:N	2.36	0.55
1:H:52:TRP:HE1	1:H:97:THR:HG21	1.69	0.55
4:Y:257:THR:O	4:Y:259:LEU:N	2.34	0.55
4:K:392:ASN:OD1	4:K:392:ASN:O	2.24	0.55
4:K:211:GLU:OE1	4:K:211:GLU:N	2.37	0.55
4:Y:257:THR:HG1	4:Y:375:SER:HG	1.42	0.55
4:Y:305:LYS:N	4:Y:319:ALA:O	2.39	0.55
4:Y:291:PRO:HG3	11:Y:1041:NAG:H82	1.89	0.55
2:J:617:ARG:NH1	2:J:626:MET:SD	2.79	0.55
4:Y:217:TYR:O	4:Y:248:THR:HG23	2.05	0.55
2:B:617:ARG:NH1	2:B:634:GLU:OE2	2.34	0.55
3:E:65:SER:OG	3:E:72:THR:OG1	2.20	0.55
4:G:453:ILE:O	4:G:471:GLY:N	2.39	0.55
3:L:49:TYR:O	3:L:53:ALA:HB3	2.06	0.55
2:X:618:ASN:OD1	2:X:621:GLU:N	2.39	0.55
4:G:426:MET:HG3	4:G:427:TRP:CD2	2.42	0.55
4:K:195:ASN:HD22	4:K:201:ILE:HB	1.71	0.55
4:K:220:PRO:HG2	4:K:223:PHE:CD2	2.42	0.55
4:G:257:THR:O	4:G:259:LEU:N	2.37	0.55
1:H:57:SER:OG	7:N:9:MAN:O6	2.11	0.55
2:J:618:ASN:O	2:J:622:ILE:HG13	2.07	0.55
4:K:257:THR:O	4:K:258:GLN:HB2	2.05	0.55
2:X:537:LEU:HD11	4:Y:39:TYR:HD2	1.72	0.55
2:B:614:TRP:HA	2:B:638:TYR:CD2	2.42	0.54
4:G:55:ALA:HA	4:G:75:VAL:O	2.08	0.54
3:C:37:GLN:HB2	3:C:86:PHE:CE1	2.42	0.54
4:G:57:ASP:HA	4:G:77:THR:HG22	1.89	0.54
2:B:585:ARG:NH2	4:G:491:ILE:O	2.41	0.54
2:B:645:LEU:C	2:B:649:SER:HB2	2.13	0.54
1:D:100(A):TRP:O	9:W:2:NAG:H81	2.08	0.54
4:K:257:THR:O	4:K:374:HIS:ND1	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:122:LEU:HB2	4:Y:201:ILE:HG23	1.88	0.54
4:G:252:LYS:HB3	4:G:254:VAL:HG23	1.89	0.54
1:A:25:TYR:CD1	1:A:77(B):PRO:HG3	2.43	0.54
1:H:159:LEU:HD21	1:H:182:VAL:HG11	1.89	0.54
3:L:53:ALA:HA	5:F:2:NAG:C6	2.38	0.54
4:G:202:THR:O	4:G:434:MET:HA	2.08	0.53
4:K:104:MET:O	4:K:108:ILE:HG12	2.07	0.53
4:K:48:ALA:HB3	4:K:490:LYS:HG3	1.90	0.53
2:X:585:ARG:NH1	2:X:589:ASP:OD2	2.39	0.53
2:J:653:GLN:O	2:J:657:GLU:HB2	2.09	0.53
2:B:608:VAL:HG22	2:B:649:SER:HG	1.71	0.53
4:K:112:TRP:CE3	4:K:427:TRP:HZ3	2.26	0.53
2:B:603:ILE:HD12	2:B:603:ILE:O	2.08	0.53
4:Y:280:ASN:HB3	4:Y:456:ARG:HB3	1.90	0.53
2:B:537:LEU:HD11	4:G:39:TYR:HD2	1.73	0.53
4:G:164:GLU:OE1	4:G:313:PRO:HA	2.09	0.53
2:B:601:LYS:CB	2:B:602:LEU:CD1	2.85	0.53
2:J:597:GLY:HA3	4:K:503:ARG:NH1	2.18	0.53
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.90	0.53
4:K:257:THR:HB	4:K:375:SER:H	1.73	0.53
2:X:523:LEU:HA	2:X:540:GLN:HE21	1.73	0.53
4:Y:161:MET:N	4:Y:170:GLN:O	2.42	0.53
4:Y:273:ARG:NH1	4:Y:484:TYR:CG	2.77	0.53
1:H:211:VAL:HG12	1:H:211:VAL:O	2.08	0.52
1:A:4:LEU:HD11	1:A:94:THR:HG22	1.90	0.52
1:D:24:ALA:HB3	1:D:77(C):PRO:O	2.08	0.52
4:K:48:ALA:CB	4:K:490:LYS:HG3	2.40	0.52
4:K:161:MET:SD	4:K:162:THR:N	2.82	0.52
4:Y:172:VAL:HG11	4:Y:307:ILE:HD13	1.92	0.52
4:Y:216:HIS:CD2	4:Y:250:GLY:CA	2.92	0.52
4:Y:377:ASN:HA	4:Y:382:PHE:HA	1.92	0.52
1:A:35:VAL:HA	1:A:93:THR:O	2.10	0.52
1:A:40:ALA:HB3	1:A:43:GLN:HB2	1.91	0.52
1:A:55:TRP:CZ3	7:S:2:NAG:H61	2.44	0.52
1:A:163:VAL:HG22	1:A:182:VAL:HG22	1.91	0.52
2:B:602:LEU:CD1	2:B:602:LEU:N	2.73	0.52
2:X:570:VAL:HG22	2:X:571:TRP:H	1.74	0.52
4:K:223:PHE:CD1	4:K:490:LYS:HG2	2.44	0.52
4:Y:217:TYR:N	4:Y:248:THR:HG1	2.07	0.52
2:B:601:LYS:O	2:X:655:LYS:CE	2.58	0.52
3:L:186:TYR:HA	3:L:192:TYR:OH	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Y:123:THR:N	4:Y:124:PRO:CD	2.73	0.52
4:Y:216:HIS:CG	4:Y:250:GLY:CA	2.92	0.52
4:Y:364:SER:HB2	4:Y:470:PRO:HG2	1.91	0.52
4:K:260:LEU:HD12	4:K:451:GLY:HA3	1.91	0.52
4:K:296:CYS:SG	4:K:376:PHE:HZ	2.33	0.52
2:B:645:LEU:O	2:B:649:SER:CA	2.57	0.52
4:K:349:LEU:HD21	4:K:468:PHE:CE2	2.45	0.52
2:J:574:LYS:HE3	4:K:52:LEU:O	2.10	0.52
1:D:25:TYR:CD1	1:D:77(B):PRO:HG3	2.45	0.51
3:E:37:GLN:CB	3:E:47:LEU:HD11	2.39	0.51
4:K:295:ASN:N	4:K:332:ASN:O	2.36	0.51
4:K:349:LEU:HD21	4:K:468:PHE:HE2	1.75	0.51
4:K:364:SER:HB2	4:K:470:PRO:HG2	1.92	0.51
3:E:37:GLN:HB2	3:E:86:PHE:CE1	2.45	0.51
4:K:212:PRO:HG2	10:T:1:NAG:O7	2.10	0.51
1:D:100(A):TRP:CZ2	4:Y:46:LYS:HE2	2.45	0.51
3:L:19:VAL:HG12	3:L:75:ILE:HB	1.92	0.51
1:D:100:ARG:O	2:X:633:LYS:NZ	2.39	0.51
2:J:607:ASN:OD1	2:J:607:ASN:N	2.44	0.51
4:Y:217:TYR:H	4:Y:248:THR:HG1	1.59	0.51
2:B:647:GLU:CG	2:B:648:GLU:N	2.73	0.51
4:Y:304:ARG:HD2	4:Y:320:THR:HA	1.92	0.51
3:C:186:TYR:O	3:C:192:TYR:OH	2.23	0.51
2:J:606:THR:OG1	4:K:36:VAL:O	2.29	0.51
1:A:152:VAL:HG22	1:A:198:VAL:HG22	1.93	0.50
1:H:100(I):VAL:HG12	3:L:91:TYR:HB2	1.93	0.50
4:G:55:ALA:HB3	4:G:216:HIS:HB2	1.93	0.50
4:G:112:TRP:CD2	4:G:427:TRP:HZ3	2.29	0.50
4:Y:499:THR:HG23	4:Y:501:CYS:H	1.75	0.50
1:D:68:LEU:HD23	7:Z:6:MAN:H62	1.91	0.50
1:D:68:LEU:HD23	7:Z:6:MAN:O6	2.11	0.50
4:K:280:ASN:OD1	4:K:281:ALA:N	2.44	0.50
4:Y:299:PRO:HA	4:Y:442:VAL:HG13	1.93	0.50
1:A:204:ASN:O	1:A:204:ASN:ND2	2.44	0.50
2:B:645:LEU:O	2:B:649:SER:N	2.45	0.50
1:D:35(A):ASN:O	1:D:93:THR:HB	2.12	0.50
2:J:610:TRP:CE3	4:K:36:VAL:HG12	2.43	0.50
1:H:25:TYR:HD1	8:O:2:NAG:H2	1.75	0.50
2:B:598:CYS:O	2:B:600:GLY:N	2.42	0.50
2:J:638:TYR:O	2:J:642:ILE:HG13	2.11	0.50
1:D:50:GLN:N	1:D:58:SER:OG	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ARG:HD2	7:Z:9:MAN:O3	2.12	0.50
3:E:189:HIS:NE2	3:E:191:VAL:HG22	2.27	0.50
2:J:570:VAL:HG22	2:J:571:TRP:H	1.77	0.50
4:G:193:LEU:HD12	4:G:193:LEU:H	1.76	0.50
2:J:651:ASN:O	2:J:655:LYS:HG2	2.12	0.50
4:K:277:ILE:HD12	7:S:1:NAG:H81	1.94	0.50
4:Y:383:PHE:CZ	4:Y:385:CYS:SG	3.05	0.50
1:H:74:LEU:CD1	1:H:77(B):PRO:HA	2.42	0.49
3:C:28:SER:HA	3:C:69:THR:HG22	1.94	0.49
2:X:660:LEU:O	2:X:663:LEU:HG	2.12	0.49
4:K:255:VAL:HG13	4:K:475:MET:SD	2.51	0.49
3:L:54:LEU:HD11	5:F:3:BMA:H3	1.94	0.49
3:L:65:SER:OG	3:L:72:THR:OG1	2.29	0.49
4:Y:180:ASP:OD1	4:Y:181:VAL:HG13	2.12	0.49
2:B:610:TRP:HE3	4:G:36:VAL:HG22	1.77	0.49
3:C:166:GLN:HG3	3:C:173:TYR:CZ	2.47	0.49
2:B:614:TRP:O	3:L:30:THR:HG21	2.12	0.49
3:C:123:GLU:HA	3:C:126:LYS:HZ3	1.78	0.49
2:J:522:PHE:CD1	2:J:543:ASN:HB3	2.47	0.49
4:K:391:PHE:CE2	4:K:470:PRO:HB3	2.48	0.49
1:H:74:LEU:HB2	1:H:77(C):PRO:HG3	1.95	0.49
2:X:585:ARG:HH22	4:Y:493:PRO:HD3	1.77	0.49
4:Y:257:THR:HB	4:Y:375:SER:N	2.26	0.49
2:B:615:SER:HA	3:L:30:THR:HG21	1.93	0.49
4:G:78:ASP:OD1	4:G:78:ASP:N	2.46	0.49
4:K:123:THR:N	4:K:124:PRO:CD	2.76	0.49
3:C:30:THR:OG1	2:J:615:SER:N	2.31	0.48
1:D:147:PRO:O	1:D:200:HIS:NE2	2.37	0.48
4:G:104:MET:O	4:G:108:ILE:HG12	2.13	0.48
4:Y:195:ASN:HB3	4:Y:423:ILE:CD1	2.43	0.48
4:G:478:ASN:O	4:G:481:SER:OG	2.21	0.48
1:H:210:ARG:HG2	1:H:210:ARG:NH1	2.20	0.48
2:B:595:ILE:HG22	2:B:647:GLU:HB2	1.95	0.48
4:Y:96:TRP:CE3	4:Y:275:GLU:HB2	2.49	0.48
4:Y:285:LEU:HD21	4:Y:477:ASP:HB3	1.95	0.48
1:D:163:VAL:HG22	1:D:182:VAL:HG22	1.95	0.48
1:H:126:PRO:HD2	1:H:213:PRO:HA	1.95	0.48
1:D:23:LYS:HA	1:D:77(D):ILE:HG22	1.94	0.48
4:G:257:THR:OG1	4:G:375:SER:N	2.43	0.48
2:X:598:CYS:O	2:X:599:SER:HB3	2.13	0.48
4:Y:179:LEU:HD13	4:Y:369:LEU:HD21	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:645:LEU:O	2:B:649:SER:HB3	2.03	0.48
4:G:120:VAL:HG23	4:G:315:GLN:HB3	1.95	0.48
4:Y:259:LEU:HD13	4:Y:449:ILE:HD13	1.95	0.48
3:E:61:ARG:NH1	3:E:82:ASP:OD2	2.47	0.48
3:E:137:ASN:OD1	3:E:174:SER:HB3	2.13	0.48
2:B:610:TRP:HH2	2:B:635:ILE:HD13	1.79	0.48
1:D:35:VAL:HA	1:D:93:THR:O	2.14	0.48
4:K:270:VAL:HB	4:K:287:GLN:O	2.14	0.48
4:K:429:ARG:CZ	4:K:432:GLN:HG2	2.44	0.48
4:G:101:VAL:HG21	4:G:480:ARG:HG2	1.96	0.48
4:K:93:PHE:HB2	4:K:233:PHE:HZ	1.76	0.48
4:Y:427:TRP:O	4:Y:428:GLN:C	2.51	0.48
4:Y:427:TRP:O	4:Y:428:GLN:HG2	2.14	0.48
4:G:278:THR:CG2	8:O:1:NAG:C5	2.92	0.47
1:H:33:TYR:CD2	1:H:94:THR:HG22	2.49	0.47
1:A:146:PHE:HB2	1:A:175:LEU:HD12	1.96	0.47
3:C:35:TRP:CZ3	3:C:88:CYS:HB3	2.49	0.47
1:D:211:VAL:O	1:D:211:VAL:HG12	2.13	0.47
1:H:210:ARG:CG	1:H:210:ARG:NH1	2.75	0.47
4:K:57:ASP:HB3	4:K:58:ALA:H	1.49	0.47
3:E:19:VAL:HG12	3:E:75:ILE:HB	1.96	0.47
4:K:371:VAL:HG22	4:K:473:GLY:N	2.29	0.47
4:G:338:TRP:CZ2	4:G:390:LEU:HB3	2.50	0.47
1:D:23:LYS:HA	1:D:77(D):ILE:CG2	2.44	0.47
1:D:68:LEU:HD21	7:Z:6:MAN:O6	2.15	0.47
4:G:42:VAL:HG22	4:G:493:PRO:O	2.14	0.47
4:K:229:LYS:HE2	4:K:243:SER:OG	2.14	0.47
4:Y:346:VAL:O	4:Y:350:ARG:N	2.44	0.47
1:D:74:LEU:HB3	1:D:77(C):PRO:CD	2.43	0.47
4:K:330:HIS:HA	4:K:417:PRO:HA	1.95	0.47
4:K:386:ASN:OD1	4:K:388:SER:CB	2.63	0.47
4:K:484:TYR:CE2	4:K:485:LYS:HG3	2.50	0.47
1:H:35(A):ASN:O	1:H:93:THR:HB	2.14	0.47
2:J:523:LEU:H	2:J:540:GLN:HG3	1.79	0.47
1:A:166:PHE:CE2	3:C:176:SER:HB3	2.50	0.47
4:G:113:ASP:OD1	4:G:114:GLN:N	2.48	0.47
1:H:60:SER:O	1:H:64:ARG:N	2.47	0.47
1:H:67:VAL:O	7:N:9:MAN:H62	2.15	0.47
4:K:371:VAL:HG22	4:K:473:GLY:H	1.80	0.47
4:Y:259:LEU:HD22	4:Y:452:LEU:CD2	2.45	0.47
2:X:656:ASN:O	2:X:660:LEU:HG	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:259:LEU:H	4:K:374:HIS:HD1	1.63	0.46
1:A:59:ALA:HB3	7:S:9:MAN:H4	1.97	0.46
1:H:82(C):LEU:HB3	1:H:111:VAL:HG21	1.97	0.46
1:H:100(F):HIS:HB2	3:L:32:TRP:CE3	2.50	0.46
2:B:618:ASN:HB2	2:B:621:GLU:HG3	1.98	0.46
1:H:93:THR:HA	1:H:102:SER:O	2.15	0.46
1:A:30:PHE:CE2	1:A:77(C):PRO:HB2	2.51	0.46
2:B:602:LEU:N	2:B:602:LEU:HD12	2.30	0.46
4:G:229:LYS:O	4:G:241:SER:OG	2.33	0.46
4:K:202:THR:O	4:K:434:MET:HA	2.15	0.46
3:L:11:LEU:HD13	3:L:19:VAL:HG21	1.97	0.46
2:X:522:PHE:CE1	2:X:523:LEU:HG	2.50	0.46
1:D:119:PRO:HB3	1:D:145:TYR:HB3	1.97	0.46
1:H:24:ALA:O	1:H:77(B):PRO:HB2	2.16	0.46
1:A:67:VAL:O	7:S:9:MAN:H62	2.16	0.46
3:C:146:VAL:HG12	3:C:196:VAL:HG22	1.98	0.46
4:K:227:LYS:HA	4:K:485:LYS:O	2.16	0.46
4:Y:217:TYR:N	4:Y:248:THR:OG1	2.41	0.46
1:A:32:LEU:C	1:A:97:THR:HG22	2.36	0.45
3:C:19:VAL:HG12	3:C:75:ILE:HB	1.97	0.45
1:D:50:GLN:HG2	1:D:58:SER:OG	2.15	0.45
3:L:124:GLN:HG2	3:L:129:THR:O	2.17	0.45
3:L:134:CYS:HB2	3:L:148:TRP:CH2	2.51	0.45
3:L:144:ALA:HB2	3:L:198:HIS:HD2	1.81	0.45
3:E:134:CYS:HB2	3:E:148:TRP:CH2	2.51	0.45
4:G:494:LEU:HD23	4:G:494:LEU:HA	1.85	0.45
2:J:606:THR:HA	4:K:503:ARG:HE	1.82	0.45
4:K:270:VAL:HG12	4:K:288:PHE:HA	1.97	0.45
1:D:100(A):TRP:CH2	4:Y:46:LYS:HE2	2.52	0.45
2:J:580:VAL:O	2:J:584:GLU:HG2	2.16	0.45
4:K:122:LEU:O	4:K:123:THR:C	2.55	0.45
2:B:598:CYS:O	2:B:599:SER:CB	2.63	0.45
1:D:22:CYS:O	1:D:77(D):ILE:HB	2.16	0.45
4:Y:164:GLU:HG2	4:Y:312:GLY:HA3	1.98	0.45
4:Y:272:ILE:HD11	4:Y:352:HIS:ND1	2.32	0.45
3:L:53:ALA:HA	5:F:2:NAG:H62	1.98	0.45
4:Y:33:ASN:OD1	4:Y:33:ASN:N	2.50	0.45
1:D:64:ARG:NE	7:Z:9:MAN:O3	2.50	0.45
3:E:37:GLN:HB3	3:E:47:LEU:HD11	1.98	0.45
4:Y:113:ASP:O	4:Y:117:LYS:HD3	2.17	0.45
1:A:70:SER:HB2	7:S:3:BMA:O4	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:540:GLN:N	2:B:540:GLN:OE1	2.49	0.45
4:K:201:ILE:HA	4:K:433:ALA:HB3	1.99	0.45
4:K:257:THR:HB	4:K:375:SER:N	2.32	0.45
3:E:146:VAL:HG12	3:E:196:VAL:HG22	1.99	0.45
4:G:278:THR:HG22	8:O:1:NAG:C5	2.46	0.45
4:G:371:VAL:HG22	4:G:473:GLY:H	1.81	0.45
4:K:37:THR:OG1	4:K:499:THR:CG2	2.64	0.45
4:Y:359:ILE:HD13	4:Y:361:PHE:CE1	2.48	0.45
1:D:48:ILE:HG23	1:D:63:PHE:CD2	2.52	0.44
1:D:75:THR:HG22	1:D:77:SER:H	1.81	0.44
4:G:87:GLU:O	4:G:89:VAL:HG23	2.17	0.44
4:Y:477:ASP:OD1	4:Y:480:ARG:NH1	2.49	0.44
4:G:105:HIS:CG	4:G:476:ARG:HG2	2.52	0.44
4:K:78:ASP:OD1	4:K:78:ASP:N	2.50	0.44
2:X:615:SER:OG	2:X:634:GLU:HG2	2.18	0.44
2:B:604:CYS:HB3	4:G:38:VAL:HB	1.99	0.44
2:J:611:ASN:HB3	2:J:614:TRP:CD2	2.52	0.44
4:Y:249:HIS:CD2	4:Y:251:ILE:CG1	2.95	0.44
4:Y:474:ASP:OD1	4:Y:476:ARG:HG3	2.18	0.44
1:D:87:THR:HG23	1:D:110:SER:HA	1.99	0.44
1:H:147:PRO:O	1:H:200:HIS:NE2	2.38	0.44
4:Y:494:LEU:HD23	4:Y:494:LEU:HA	1.66	0.44
2:B:596:TRP:C	2:B:651:ASN:ND2	2.71	0.44
4:G:180:ASP:CG	4:G:422:GLN:H	2.21	0.44
4:K:278:THR:CG2	8:U:1:NAG:H62	2.48	0.44
4:K:361:PHE:CB	4:K:391:PHE:O	2.66	0.44
4:Y:356:ASN:OD1	4:Y:357:THR:N	2.51	0.44
4:G:163:THR:OG1	4:G:164:GLU:N	2.50	0.44
4:G:476:ARG:HA	4:G:479:TRP:HD1	1.77	0.44
3:L:37:GLN:HB2	3:L:86:PHE:CE1	2.52	0.44
4:Y:304:ARG:NH1	4:Y:438:PRO:HG2	2.32	0.44
2:B:582:ALA:HB1	4:G:221:ALA:HB3	1.99	0.44
4:G:37:THR:HG21	4:G:499:THR:OG1	2.18	0.44
4:G:195:ASN:OD1	4:G:196:CYS:N	2.51	0.44
1:H:40:ALA:HB3	1:H:43:GLN:HB2	1.98	0.44
4:K:374:HIS:HD2	4:K:376:PHE:CE1	2.36	0.44
2:X:646:LEU:HD21	4:Y:36:VAL:HG21	2.00	0.44
4:Y:249:HIS:CD2	4:Y:249:HIS:O	2.70	0.44
4:Y:390:LEU:HG	4:Y:416:LEU:HD21	1.98	0.44
6:Q:1:NAG:H62	6:Q:2:NAG:C7	2.47	0.44
4:G:91:GLU:OE1	1:H:100:ARG:NH2	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:112:TRP:CE3	4:G:427:TRP:HZ3	2.36	0.44
4:K:499:THR:HG23	4:K:501:CYS:H	1.83	0.44
4:Y:252:LYS:HA	4:Y:253:PRO:HD2	1.90	0.44
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.99	0.43
2:B:598:CYS:C	2:B:600:GLY:H	2.20	0.43
3:E:30(A):GLY:HA3	3:E:32:TRP:CZ3	2.53	0.43
3:E:2:ILE:HG12	3:E:93:THR:HG22	1.99	0.43
4:G:233:PHE:O	4:G:273:ARG:NH2	2.44	0.43
1:H:55:TRP:CZ3	7:N:2:NAG:H61	2.53	0.43
1:H:71:ALA:HA	1:H:78:SER:HA	1.98	0.43
3:L:167:ASP:HB3	3:L:170:ASP:OD1	2.17	0.43
4:Y:259:LEU:HD22	4:Y:452:LEU:HD22	1.99	0.43
2:B:602:LEU:CD2	2:X:655:LYS:HZ3	2.25	0.43
4:K:374:HIS:CD2	4:K:376:PHE:CE1	3.07	0.43
4:Y:270:VAL:HG13	4:Y:287:GLN:O	2.19	0.43
4:G:35:TRP:O	4:G:498:PRO:HA	2.18	0.43
4:G:277:ILE:CD1	7:N:1:NAG:H81	2.49	0.43
2:X:653:GLN:O	2:X:657:GLU:HB2	2.17	0.43
1:A:38:ARG:HB3	1:A:48:ILE:HD11	2.00	0.43
1:A:94:THR:CG2	1:A:102:SER:HB2	2.48	0.43
4:G:446:VAL:HB	6:M:2:NAG:O7	2.18	0.43
1:H:35:VAL:HA	1:H:93:THR:O	2.17	0.43
4:Y:163:THR:OG1	4:Y:164:GLU:N	2.52	0.43
3:C:195:GLU:N	3:C:195:GLU:OE1	2.52	0.43
4:G:86:LEU:HB3	4:G:89:VAL:HG21	2.00	0.43
4:G:252:LYS:HG3	4:G:262:ASN:O	2.18	0.43
2:X:570:VAL:O	2:X:571:TRP:HB3	2.19	0.43
2:X:605:CYS:O	4:Y:503:ARG:HD3	2.18	0.43
3:C:31:ASN:O	3:C:50:ARG:HA	2.19	0.43
3:E:189:HIS:CD2	3:E:191:VAL:H	2.37	0.43
1:H:25:TYR:CD1	1:H:77(B):PRO:HG3	2.54	0.43
2:J:522:PHE:CD1	2:J:540:GLN:HA	2.54	0.43
2:B:577:GLN:N	2:B:577:GLN:OE1	2.51	0.43
2:B:650:GLN:C	2:B:654:GLU:HB3	2.39	0.43
4:Y:373:THR:HG22	4:Y:419:ARG:HH21	1.84	0.43
3:C:58:VAL:HG13	3:C:59:PRO:HD2	2.01	0.43
2:J:659:ASP:HB2	2:X:603:ILE:HD13	2.00	0.43
4:K:223:PHE:HE1	4:K:490:LYS:HG2	1.83	0.43
4:K:294:ILE:HG22	4:K:447:SER:O	2.19	0.43
3:E:11:LEU:HD13	3:E:19:VAL:HG21	2.01	0.42
3:E:37:GLN:NE2	3:E:82:ASP:O	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:382:PHE:O	4:K:420:ILE:HA	2.19	0.42
1:D:153:SER:O	1:D:197:ASN:N	2.39	0.42
4:Y:342:LEU:O	4:Y:346:VAL:HG23	2.19	0.42
2:B:522:PHE:CD1	2:B:543:ASN:HB2	2.55	0.42
3:C:32:TRP:HH2	2:J:633:LYS:HG2	1.85	0.42
4:G:277:ILE:HD11	7:N:1:NAG:H81	2.02	0.42
4:K:122:LEU:O	4:K:124:PRO:N	2.53	0.42
4:Y:453:ILE:O	4:Y:471:GLY:N	2.39	0.42
4:G:122:LEU:HD21	4:G:125:LEU:HD23	2.00	0.42
4:Y:172:VAL:HG11	4:Y:307:ILE:HG21	2.02	0.42
2:B:603:ILE:C	2:B:603:ILE:CD1	2.85	0.42
2:B:615:SER:O	2:B:616:ASN:HB3	2.20	0.42
3:C:36:TYR:CE1	3:C:46:LEU:HD13	2.54	0.42
4:Y:199:SER:HB3	4:Y:431:GLY:H	1.85	0.42
1:A:94:THR:HG23	1:A:102:SER:HB2	2.01	0.42
4:K:165:LEU:HD23	4:K:166:ARG:N	2.35	0.42
3:E:149:LYS:HD3	3:E:152:ASN:HA	2.01	0.42
1:H:33:TYR:HD2	1:H:94:THR:HG22	1.84	0.42
4:Y:93:PHE:HB2	4:Y:233:PHE:HZ	1.84	0.42
4:Y:297:THR:HG23	4:Y:443:ILE:O	2.19	0.42
4:Y:215:ILE:C	4:Y:251:ILE:H	2.20	0.42
9:R:1:NAG:H62	9:R:2:NAG:C7	2.50	0.42
1:A:26:GLY:HA2	8:U:1:NAG:O3	2.20	0.42
2:B:598:CYS:C	2:B:600:GLY:N	2.73	0.42
3:C:20:ARG:HG2	3:C:74:THR:HG22	2.02	0.42
3:C:187:GLU:OE2	3:C:211:ARG:NH1	2.52	0.42
4:Y:101:VAL:HG12	4:Y:483:LEU:HD12	2.02	0.42
1:D:72:VAL:HG23	7:Z:5:MAN:H62	2.02	0.41
4:K:42:VAL:HG22	4:K:493:PRO:O	2.20	0.41
3:E:189:HIS:CD2	3:E:191:VAL:HG22	2.55	0.41
4:G:101:VAL:HG22	4:G:483:LEU:HD12	2.02	0.41
4:G:339:ASN:OD1	4:G:340:GLU:N	2.53	0.41
4:K:112:TRP:CD2	4:K:427:TRP:HZ3	2.38	0.41
4:K:307:ILE:HD11	4:K:317:PHE:HD2	1.84	0.41
4:K:320:THR:OG1	4:K:438:PRO:HG2	2.20	0.41
1:A:200:HIS:CD2	1:A:202:PRO:HD2	2.55	0.41
4:Y:355:ASN:OD1	4:Y:356:ASN:N	2.53	0.41
9:W:1:NAG:H62	9:W:2:NAG:C8	2.50	0.41
4:K:231:LYS:HD3	4:K:267:GLU:OE1	2.19	0.41
3:L:113:PRO:HB3	3:L:139:PHE:HB3	2.02	0.41
4:Y:87:GLU:O	4:Y:89:VAL:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:HIS:CD2	1:D:202:PRO:HD2	2.55	0.41
4:G:165:LEU:HA	4:Y:126:CYS:O	2.20	0.41
4:K:198:THR:HG22	4:K:430:ILE:HG23	2.01	0.41
4:Y:214:PRO:HA	4:Y:251:ILE:O	2.20	0.41
4:Y:453:ILE:HD11	4:Y:478:ASN:OD1	2.20	0.41
2:B:608:VAL:HG21	2:B:646:LEU:HD23	2.01	0.41
4:K:257:THR:HG22	4:K:258:GLN:HG3	2.03	0.41
4:K:453:ILE:O	4:K:454:LEU:HD23	2.21	0.41
4:Y:195:ASN:HB3	4:Y:423:ILE:HD13	2.02	0.41
4:G:159:PHE:CZ	4:G:172:VAL:HG21	2.56	0.41
2:J:650:GLN:O	2:J:654:GLU:HB3	2.19	0.41
1:A:69:ILE:N	7:S:9:MAN:O6	2.54	0.41
1:D:64:ARG:CD	7:Z:9:MAN:O3	2.69	0.41
4:G:257:THR:O	4:G:258:GLN:HB2	2.21	0.41
4:G:277:ILE:HG22	1:H:76:GLY:HA2	2.02	0.41
4:G:453:ILE:O	4:G:454:LEU:HD23	2.20	0.41
4:K:83:GLU:HA	4:K:245:VAL:HG12	2.02	0.41
4:K:230:ASP:OD1	4:K:233:PHE:HB2	2.21	0.41
3:L:140:TYR:CD1	3:L:141:PRO:HA	2.55	0.41
4:Y:195:ASN:HD22	4:Y:201:ILE:HB	1.86	0.41
3:C:187:GLU:CD	3:C:211:ARG:HD2	2.40	0.41
4:G:220:PRO:HG2	4:G:223:PHE:CD2	2.56	0.41
4:Y:122:LEU:O	4:Y:123:THR:C	2.59	0.41
4:Y:163:THR:HG23	4:Y:165:LEU:H	1.84	0.41
2:B:599:SER:OG	2:B:600:GLY:N	2.54	0.40
2:B:611:ASN:OD1	2:B:614:TRP:CG	2.74	0.40
2:B:656:ASN:O	2:B:659:ASP:HB3	2.21	0.40
4:G:199:SER:HB3	4:G:431:GLY:H	1.86	0.40
1:H:6:GLN:NE2	1:H:107:THR:HG23	2.26	0.40
2:J:619:LEU:HD23	2:J:619:LEU:HA	1.86	0.40
3:L:46:LEU:HD23	3:L:55:LEU:HD22	2.02	0.40
1:A:37:VAL:HG22	1:A:47:TYR:HA	2.03	0.40
1:H:95:THR:HA	1:H:101:SER:OG	2.21	0.40
4:Y:253:PRO:HA	4:Y:479:TRP:HZ3	1.86	0.40
3:E:33:VAL:HA	3:E:89:GLN:O	2.20	0.40
1:H:100(E):HIS:HA	1:H:100(J):MET:HB3	2.03	0.40
4:Y:393:SER:HB3	4:Y:395:TRP:NE1	2.37	0.40
2:J:598:CYS:C	2:J:600:GLY:N	2.72	0.40
1:A:60:SER:O	1:A:64:ARG:N	2.55	0.40
3:E:148:TRP:CG	3:E:179:LEU:HD22	2.57	0.40
4:Y:349:LEU:HD21	4:Y:468:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/244 (90%)	212 (96%)	8 (4%)	0	100	100
1	D	220/244 (90%)	210 (96%)	10 (4%)	0	100	100
1	H	223/244 (91%)	214 (96%)	9 (4%)	0	100	100
2	B	120/153 (78%)	107 (89%)	13 (11%)	0	100	100
2	J	120/153 (78%)	112 (93%)	8 (7%)	0	100	100
2	X	117/153 (76%)	108 (92%)	9 (8%)	0	100	100
3	C	212/215 (99%)	210 (99%)	2 (1%)	0	100	100
3	E	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
3	L	212/215 (99%)	208 (98%)	4 (2%)	0	100	100
4	G	382/479 (80%)	358 (94%)	23 (6%)	1 (0%)	41	74
4	K	391/479 (82%)	372 (95%)	19 (5%)	0	100	100
4	Y	383/479 (80%)	367 (96%)	16 (4%)	0	100	100
All	All	2812/3273 (86%)	2687 (96%)	124 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	G	312	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	184/210 (88%)	182 (99%)	2 (1%)	73 88
1	D	175/210 (83%)	175 (100%)	0	100 100
1	H	185/210 (88%)	184 (100%)	1 (0%)	88 95
2	B	99/129 (77%)	99 (100%)	0	100 100
2	J	100/129 (78%)	98 (98%)	2 (2%)	55 79
2	X	99/129 (77%)	98 (99%)	1 (1%)	76 89
3	C	170/182 (93%)	170 (100%)	0	100 100
3	E	163/182 (90%)	163 (100%)	0	100 100
3	L	157/182 (86%)	157 (100%)	0	100 100
4	G	289/427 (68%)	285 (99%)	4 (1%)	67 85
4	K	315/427 (74%)	311 (99%)	4 (1%)	69 87
4	Y	312/427 (73%)	310 (99%)	2 (1%)	86 95
All	All	2248/2844 (79%)	2232 (99%)	16 (1%)	84 93

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ASP
1	A	173	SER
4	G	74	CYS
4	G	193	LEU
4	G	378	CYS
4	G	416	LEU
1	H	210	ARG
2	J	604	CYS
2	J	614	TRP
4	K	54	CYS
4	K	57	ASP
4	K	196	CYS
4	K	418	CYS
2	X	650	GLN
4	Y	378	CYS
4	Y	448	ASN

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	651	ASN
4	K	374	HIS
4	Y	33	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

76 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	F	1	2,5	14,14,15	0.59	0	17,19,21	0.58	0
5	NAG	F	2	5	14,14,15	0.39	0	17,19,21	0.61	0
5	BMA	F	3	5	11,11,12	0.98	1 (9%)	15,15,17	0.79	0
5	MAN	F	4	5	11,11,12	0.72	0	15,15,17	1.29	2 (13%)
5	MAN	F	5	5	11,11,12	0.75	0	15,15,17	1.08	2 (13%)
6	NAG	I	1	4,6	14,14,15	0.63	1 (7%)	17,19,21	0.56	0
6	NAG	I	2	6	14,14,15	0.17	0	17,19,21	0.39	0
6	NAG	M	1	4,6	14,14,15	0.46	0	17,19,21	0.39	0
6	NAG	M	2	6	14,14,15	0.15	0	17,19,21	0.37	0
7	NAG	N	1	7,4	14,14,15	0.34	0	17,19,21	0.54	0
7	MAN	N	10	7	11,11,12	0.76	0	15,15,17	0.91	1 (6%)
7	NAG	N	2	7	14,14,15	0.67	1 (7%)	17,19,21	0.52	0
7	BMA	N	3	7	11,11,12	0.75	0	15,15,17	0.80	0
7	MAN	N	4	7	11,11,12	0.40	0	15,15,17	1.17	1 (6%)
7	MAN	N	5	7	11,11,12	0.60	0	15,15,17	1.19	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	MAN	N	6	7	11,11,12	0.84	0	15,15,17	1.05	2 (13%)
7	MAN	N	7	7	11,11,12	0.58	0	15,15,17	1.17	2 (13%)
7	MAN	N	8	7	11,11,12	0.47	0	15,15,17	1.28	2 (13%)
7	MAN	N	9	7	11,11,12	0.68	0	15,15,17	1.02	2 (13%)
8	NAG	O	1	4,8	14,14,15	0.34	0	17,19,21	0.48	0
8	NAG	O	2	8	14,14,15	0.23	0	17,19,21	0.51	0
8	BMA	O	3	8	11,11,12	0.97	0	15,15,17	1.09	1 (6%)
8	MAN	O	4	8	11,11,12	0.84	1 (9%)	15,15,17	1.13	2 (13%)
8	MAN	O	5	8	11,11,12	0.67	0	15,15,17	1.04	2 (13%)
8	MAN	O	6	8	11,11,12	0.80	0	15,15,17	1.02	2 (13%)
6	NAG	P	1	6,1	14,14,15	0.71	1 (7%)	17,19,21	0.54	0
6	NAG	P	2	6	14,14,15	0.16	0	17,19,21	0.49	0
6	NAG	Q	1	2,6	14,14,15	0.42	0	17,19,21	0.69	0
6	NAG	Q	2	6	14,14,15	0.20	0	17,19,21	0.55	0
9	NAG	R	1	2,9	14,14,15	0.46	0	17,19,21	0.37	0
9	NAG	R	2	9	14,14,15	0.22	0	17,19,21	0.56	0
9	BMA	R	3	9	11,11,12	0.78	0	15,15,17	0.69	0
9	MAN	R	4	9	11,11,12	0.56	0	15,15,17	1.00	2 (13%)
7	NAG	S	1	7,4	14,14,15	1.11	1 (7%)	17,19,21	1.01	2 (11%)
7	MAN	S	10	7	11,11,12	0.88	1 (9%)	15,15,17	0.86	1 (6%)
7	NAG	S	2	7	14,14,15	0.84	1 (7%)	17,19,21	0.51	0
7	BMA	S	3	7	11,11,12	0.83	0	15,15,17	0.93	0
7	MAN	S	4	7	11,11,12	0.52	0	15,15,17	0.98	2 (13%)
7	MAN	S	5	7	11,11,12	0.73	0	15,15,17	0.92	1 (6%)
7	MAN	S	6	7	11,11,12	0.58	0	15,15,17	1.11	2 (13%)
7	MAN	S	7	7	11,11,12	1.01	1 (9%)	15,15,17	0.89	1 (6%)
7	MAN	S	8	7	11,11,12	0.62	0	15,15,17	1.09	2 (13%)
7	MAN	S	9	7	11,11,12	0.79	1 (9%)	15,15,17	0.90	0
10	NAG	T	1	4,10	14,14,15	0.62	1 (7%)	17,19,21	0.48	0
10	NAG	T	2	10	14,14,15	0.19	0	17,19,21	0.36	0
10	BMA	T	3	10	11,11,12	0.58	0	15,15,17	0.70	0
8	NAG	U	1	4,8	14,14,15	0.43	0	17,19,21	0.74	1 (5%)
8	NAG	U	2	8	14,14,15	0.40	0	17,19,21	0.48	0
8	BMA	U	3	8	11,11,12	1.00	1 (9%)	15,15,17	0.91	0
8	MAN	U	4	8	11,11,12	0.89	1 (9%)	15,15,17	1.15	2 (13%)
8	MAN	U	5	8	11,11,12	0.91	0	15,15,17	0.95	1 (6%)
8	MAN	U	6	8	11,11,12	0.75	0	15,15,17	1.06	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	V	1	2,6	14,14,15	0.58	1 (7%)	17,19,21	0.67	0
6	NAG	V	2	6	14,14,15	0.24	0	17,19,21	0.35	0
9	NAG	W	1	2,9	14,14,15	0.78	1 (7%)	17,19,21	0.75	1 (5%)
9	NAG	W	2	9	14,14,15	0.25	0	17,19,21	0.56	0
9	BMA	W	3	9	11,11,12	0.84	0	15,15,17	0.83	0
9	MAN	W	4	9	11,11,12	0.78	0	15,15,17	1.19	2 (13%)
7	NAG	Z	1	7,4	14,14,15	0.35	0	17,19,21	0.54	0
7	MAN	Z	10	7	11,11,12	0.75	0	15,15,17	0.91	1 (6%)
7	NAG	Z	2	7	14,14,15	0.68	1 (7%)	17,19,21	0.52	0
7	BMA	Z	3	7	11,11,12	0.74	0	15,15,17	0.80	0
7	MAN	Z	4	7	11,11,12	0.41	0	15,15,17	1.17	1 (6%)
7	MAN	Z	5	7	11,11,12	0.59	0	15,15,17	1.19	1 (6%)
7	MAN	Z	6	7	11,11,12	0.83	0	15,15,17	1.06	2 (13%)
7	MAN	Z	7	7	11,11,12	0.58	0	15,15,17	1.17	2 (13%)
7	MAN	Z	8	7	11,11,12	0.47	0	15,15,17	1.28	2 (13%)
7	MAN	Z	9	7	11,11,12	0.69	0	15,15,17	1.02	2 (13%)
10	NAG	a	1	4,10	14,14,15	0.36	0	17,19,21	0.67	1 (5%)
10	NAG	a	2	10	14,14,15	0.29	0	17,19,21	0.39	0
10	BMA	a	3	10	11,11,12	0.57	0	15,15,17	0.69	0
5	NAG	b	1	4,5	14,14,15	0.40	0	17,19,21	0.87	1 (5%)
5	NAG	b	2	5	14,14,15	0.22	0	17,19,21	0.55	0
5	BMA	b	3	5	11,11,12	0.89	0	15,15,17	0.99	2 (13%)
5	MAN	b	4	5	11,11,12	0.79	1 (9%)	15,15,17	1.25	2 (13%)
5	MAN	b	5	5	11,11,12	0.79	0	15,15,17	1.01	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
5	NAG	F	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	2	5	-	2/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	1/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	4,6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	M	1	4,6	-	0/6/23/26	0/1/1/1
6	NAG	M	2	6	-	2/6/23/26	0/1/1/1
7	NAG	N	1	7,4	-	2/6/23/26	0/1/1/1
7	MAN	N	10	7	-	0/2/19/22	0/1/1/1
7	NAG	N	2	7	-	2/6/23/26	0/1/1/1
7	BMA	N	3	7	-	0/2/19/22	0/1/1/1
7	MAN	N	4	7	-	0/2/19/22	0/1/1/1
7	MAN	N	5	7	-	2/2/19/22	0/1/1/1
7	MAN	N	6	7	-	0/2/19/22	0/1/1/1
7	MAN	N	7	7	-	0/2/19/22	0/1/1/1
7	MAN	N	8	7	-	2/2/19/22	0/1/1/1
7	MAN	N	9	7	-	2/2/19/22	0/1/1/1
8	NAG	O	1	4,8	-	0/6/23/26	0/1/1/1
8	NAG	O	2	8	-	1/6/23/26	0/1/1/1
8	BMA	O	3	8	-	0/2/19/22	0/1/1/1
8	MAN	O	4	8	-	1/2/19/22	0/1/1/1
8	MAN	O	5	8	-	0/2/19/22	0/1/1/1
8	MAN	O	6	8	-	0/2/19/22	0/1/1/1
6	NAG	P	1	6,1	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	2/6/23/26	0/1/1/1
6	NAG	Q	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	Q	2	6	-	2/6/23/26	0/1/1/1
9	NAG	R	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	R	2	9	-	1/6/23/26	0/1/1/1
9	BMA	R	3	9	-	0/2/19/22	0/1/1/1
9	MAN	R	4	9	-	1/2/19/22	0/1/1/1
7	NAG	S	1	7,4	-	2/6/23/26	0/1/1/1
7	MAN	S	10	7	-	0/2/19/22	0/1/1/1
7	NAG	S	2	7	-	0/6/23/26	0/1/1/1
7	BMA	S	3	7	-	0/2/19/22	0/1/1/1
7	MAN	S	4	7	-	0/2/19/22	0/1/1/1
7	MAN	S	5	7	-	2/2/19/22	0/1/1/1
7	MAN	S	6	7	-	0/2/19/22	0/1/1/1
7	MAN	S	7	7	-	0/2/19/22	0/1/1/1
7	MAN	S	8	7	-	2/2/19/22	0/1/1/1
7	MAN	S	9	7	-	0/2/19/22	0/1/1/1
10	NAG	T	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	T	2	10	-	2/6/23/26	0/1/1/1
10	BMA	T	3	10	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	U	1	4,8	-	2/6/23/26	0/1/1/1
8	NAG	U	2	8	-	2/6/23/26	0/1/1/1
8	BMA	U	3	8	-	0/2/19/22	0/1/1/1
8	MAN	U	4	8	-	1/2/19/22	0/1/1/1
8	MAN	U	5	8	-	0/2/19/22	0/1/1/1
8	MAN	U	6	8	-	0/2/19/22	0/1/1/1
6	NAG	V	1	2,6	-	0/6/23/26	0/1/1/1
6	NAG	V	2	6	-	2/6/23/26	0/1/1/1
9	NAG	W	1	2,9	-	0/6/23/26	0/1/1/1
9	NAG	W	2	9	-	1/6/23/26	0/1/1/1
9	BMA	W	3	9	-	1/2/19/22	0/1/1/1
9	MAN	W	4	9	-	2/2/19/22	0/1/1/1
7	NAG	Z	1	7,4	-	2/6/23/26	0/1/1/1
7	MAN	Z	10	7	-	0/2/19/22	0/1/1/1
7	NAG	Z	2	7	-	2/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	4	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	5	7	-	2/2/19/22	0/1/1/1
7	MAN	Z	6	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	7	7	-	0/2/19/22	0/1/1/1
7	MAN	Z	8	7	-	2/2/19/22	0/1/1/1
7	MAN	Z	9	7	-	2/2/19/22	0/1/1/1
10	NAG	a	1	4,10	-	2/6/23/26	0/1/1/1
10	NAG	a	2	10	-	2/6/23/26	0/1/1/1
10	BMA	a	3	10	-	0/2/19/22	0/1/1/1
5	NAG	b	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	b	2	5	-	2/6/23/26	0/1/1/1
5	BMA	b	3	5	-	0/2/19/22	0/1/1/1
5	MAN	b	4	5	-	2/2/19/22	0/1/1/1
5	MAN	b	5	5	-	0/2/19/22	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	S	1	NAG	O5-C1	-4.08	1.37	1.43
7	S	2	NAG	O5-C1	-3.08	1.38	1.43
9	W	1	NAG	O5-C1	-2.77	1.39	1.43
8	U	4	MAN	C1-C2	2.48	1.57	1.52
7	Z	2	NAG	O5-C1	-2.47	1.39	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	1	NAG	O5-C1	-2.45	1.39	1.43
7	N	2	NAG	O5-C1	-2.44	1.39	1.43
8	U	3	BMA	C4-C3	2.28	1.58	1.52
8	O	4	MAN	C1-C2	2.26	1.57	1.52
7	S	7	MAN	O5-C1	-2.23	1.40	1.43
6	I	1	NAG	O5-C1	-2.22	1.40	1.43
7	S	10	MAN	O5-C1	-2.16	1.40	1.43
10	T	1	NAG	C1-C2	2.10	1.55	1.52
5	F	3	BMA	C1-C2	2.09	1.57	1.52
5	b	4	MAN	C1-C2	2.08	1.56	1.52
6	V	1	NAG	O5-C1	-2.06	1.40	1.43
7	S	9	MAN	O5-C1	-2.01	1.40	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	4	MAN	C1-O5-C5	4.00	117.61	112.19
7	N	4	MAN	C1-O5-C5	3.81	117.35	112.19
7	Z	4	MAN	C1-O5-C5	3.79	117.33	112.19
5	b	4	MAN	C1-O5-C5	3.56	117.02	112.19
9	W	4	MAN	C1-O5-C5	3.46	116.88	112.19
8	O	4	MAN	C1-O5-C5	3.26	116.61	112.19
7	Z	7	MAN	C1-O5-C5	3.09	116.37	112.19
7	N	7	MAN	C1-O5-C5	3.07	116.35	112.19
8	U	6	MAN	C1-O5-C5	2.96	116.20	112.19
8	U	4	MAN	C1-O5-C5	2.84	116.03	112.19
5	F	5	MAN	C1-O5-C5	2.79	115.97	112.19
9	R	4	MAN	C1-O5-C5	2.61	115.72	112.19
7	N	5	MAN	C1-O5-C5	2.60	115.72	112.19
8	O	5	MAN	C1-O5-C5	2.59	115.71	112.19
7	Z	5	MAN	C1-O5-C5	2.59	115.70	112.19
7	S	4	MAN	C1-O5-C5	2.56	115.66	112.19
8	O	3	BMA	C1-C2-C3	2.54	112.78	109.67
5	b	5	MAN	C1-O5-C5	2.53	115.62	112.19
8	U	4	MAN	O2-C2-C3	-2.53	105.07	110.14
7	N	8	MAN	C1-O5-C5	2.52	115.61	112.19
8	O	6	MAN	C1-O5-C5	2.51	115.60	112.19
5	b	4	MAN	O2-C2-C3	-2.51	105.11	110.14
7	Z	8	MAN	C1-O5-C5	2.51	115.59	112.19
7	S	6	MAN	C1-O5-C5	2.50	115.58	112.19
7	Z	6	MAN	C1-O5-C5	2.46	115.53	112.19
9	W	1	NAG	C1-O5-C5	2.45	115.52	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	S	8	MAN	O2-C2-C3	-2.45	105.24	110.14
7	N	6	MAN	C1-O5-C5	2.44	115.50	112.19
7	N	9	MAN	O2-C2-C3	-2.42	105.29	110.14
7	Z	9	MAN	O2-C2-C3	-2.41	105.32	110.14
7	S	1	NAG	C1-O5-C5	-2.37	108.98	112.19
8	O	5	MAN	O2-C2-C3	-2.34	105.44	110.14
8	O	6	MAN	O2-C2-C3	-2.32	105.48	110.14
8	O	4	MAN	O2-C2-C3	-2.29	105.56	110.14
7	N	9	MAN	C1-O5-C5	2.28	115.28	112.19
8	U	1	NAG	C1-O5-C5	2.27	115.26	112.19
7	Z	9	MAN	C1-O5-C5	2.26	115.26	112.19
7	N	8	MAN	O2-C2-C3	-2.26	105.61	110.14
7	Z	8	MAN	O2-C2-C3	-2.26	105.61	110.14
10	a	1	NAG	C1-O5-C5	2.26	115.25	112.19
7	Z	6	MAN	O2-C2-C3	-2.25	105.63	110.14
7	N	6	MAN	O2-C2-C3	-2.24	105.66	110.14
7	S	10	MAN	O2-C2-C3	-2.23	105.67	110.14
8	U	6	MAN	O2-C2-C3	-2.23	105.67	110.14
7	S	5	MAN	O2-C2-C3	-2.23	105.67	110.14
7	Z	7	MAN	O2-C2-C3	-2.21	105.71	110.14
7	N	7	MAN	O2-C2-C3	-2.21	105.72	110.14
5	F	5	MAN	O2-C2-C3	-2.21	105.72	110.14
5	F	4	MAN	O2-C2-C3	-2.17	105.79	110.14
7	S	8	MAN	C1-O5-C5	2.16	115.12	112.19
8	U	5	MAN	O2-C2-C3	-2.15	105.83	110.14
7	S	4	MAN	O2-C2-C3	-2.14	105.85	110.14
7	S	1	NAG	C3-C4-C5	2.14	114.05	110.24
5	b	5	MAN	O2-C2-C3	-2.13	105.87	110.14
7	S	6	MAN	O2-C2-C3	-2.11	105.91	110.14
7	S	7	MAN	O2-C2-C3	-2.10	105.93	110.14
9	W	4	MAN	O2-C2-C3	-2.09	105.94	110.14
5	b	3	BMA	C1-O5-C5	2.07	115.00	112.19
7	N	10	MAN	O2-C2-C3	-2.06	106.01	110.14
5	b	3	BMA	C1-C2-C3	2.04	112.18	109.67
5	b	1	NAG	C3-C4-C5	2.04	113.88	110.24
7	Z	10	MAN	O2-C2-C3	-2.03	106.07	110.14
9	R	4	MAN	O2-C2-C3	-2.03	106.08	110.14

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	N	1	NAG	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6
7	N	8	MAN	O5-C5-C6-O6
7	Z	8	MAN	O5-C5-C6-O6
10	a	2	NAG	O5-C5-C6-O6
10	T	2	NAG	O5-C5-C6-O6
7	N	1	NAG	C4-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
7	N	8	MAN	C4-C5-C6-O6
7	Z	8	MAN	C4-C5-C6-O6
7	S	8	MAN	O5-C5-C6-O6
7	S	5	MAN	O5-C5-C6-O6
8	U	2	NAG	O5-C5-C6-O6
10	T	1	NAG	C4-C5-C6-O6
8	U	2	NAG	C4-C5-C6-O6
10	T	2	NAG	C4-C5-C6-O6
10	a	2	NAG	C4-C5-C6-O6
7	S	5	MAN	C4-C5-C6-O6
7	N	5	MAN	O5-C5-C6-O6
7	S	1	NAG	O5-C5-C6-O6
7	Z	5	MAN	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
7	N	9	MAN	O5-C5-C6-O6
7	Z	9	MAN	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
7	S	8	MAN	C4-C5-C6-O6
10	T	1	NAG	O5-C5-C6-O6
5	b	2	NAG	O5-C5-C6-O6
6	M	2	NAG	O5-C5-C6-O6
8	U	1	NAG	O5-C5-C6-O6
9	W	4	MAN	O5-C5-C6-O6
7	Z	5	MAN	C4-C5-C6-O6
7	N	5	MAN	C4-C5-C6-O6
6	P	2	NAG	O5-C5-C6-O6
6	V	2	NAG	O5-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
8	U	1	NAG	C4-C5-C6-O6
5	b	4	MAN	O5-C5-C6-O6
7	N	9	MAN	C4-C5-C6-O6
7	S	1	NAG	C4-C5-C6-O6
7	Z	9	MAN	C4-C5-C6-O6
8	O	4	MAN	O5-C5-C6-O6
9	R	4	MAN	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
8	O	2	NAG	O5-C5-C6-O6
6	I	2	NAG	C4-C5-C6-O6
10	a	1	NAG	C4-C5-C6-O6
8	U	4	MAN	O5-C5-C6-O6
7	N	2	NAG	C4-C5-C6-O6
7	Z	2	NAG	C4-C5-C6-O6
5	F	4	MAN	O5-C5-C6-O6
6	M	2	NAG	C4-C5-C6-O6
5	b	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6
9	W	2	NAG	O5-C5-C6-O6
6	P	2	NAG	C4-C5-C6-O6
10	a	1	NAG	O5-C5-C6-O6
6	V	2	NAG	C4-C5-C6-O6
7	N	2	NAG	O5-C5-C6-O6
7	Z	2	NAG	O5-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
6	Q	2	NAG	C4-C5-C6-O6
9	R	2	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
9	W	4	MAN	C4-C5-C6-O6
9	W	3	BMA	C4-C5-C6-O6
5	b	4	MAN	C4-C5-C6-O6

There are no ring outliers.

30 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	Q	1	NAG	1	0
5	F	2	NAG	3	0
7	N	2	NAG	1	0
7	Z	6	MAN	5	0
5	F	1	NAG	1	0
7	N	1	NAG	2	0
7	Z	8	MAN	1	0
8	U	3	BMA	1	0
7	Z	5	MAN	1	0
8	U	2	NAG	2	0
6	M	1	NAG	1	0
8	U	1	NAG	2	0
7	N	9	MAN	3	0
7	S	9	MAN	4	0

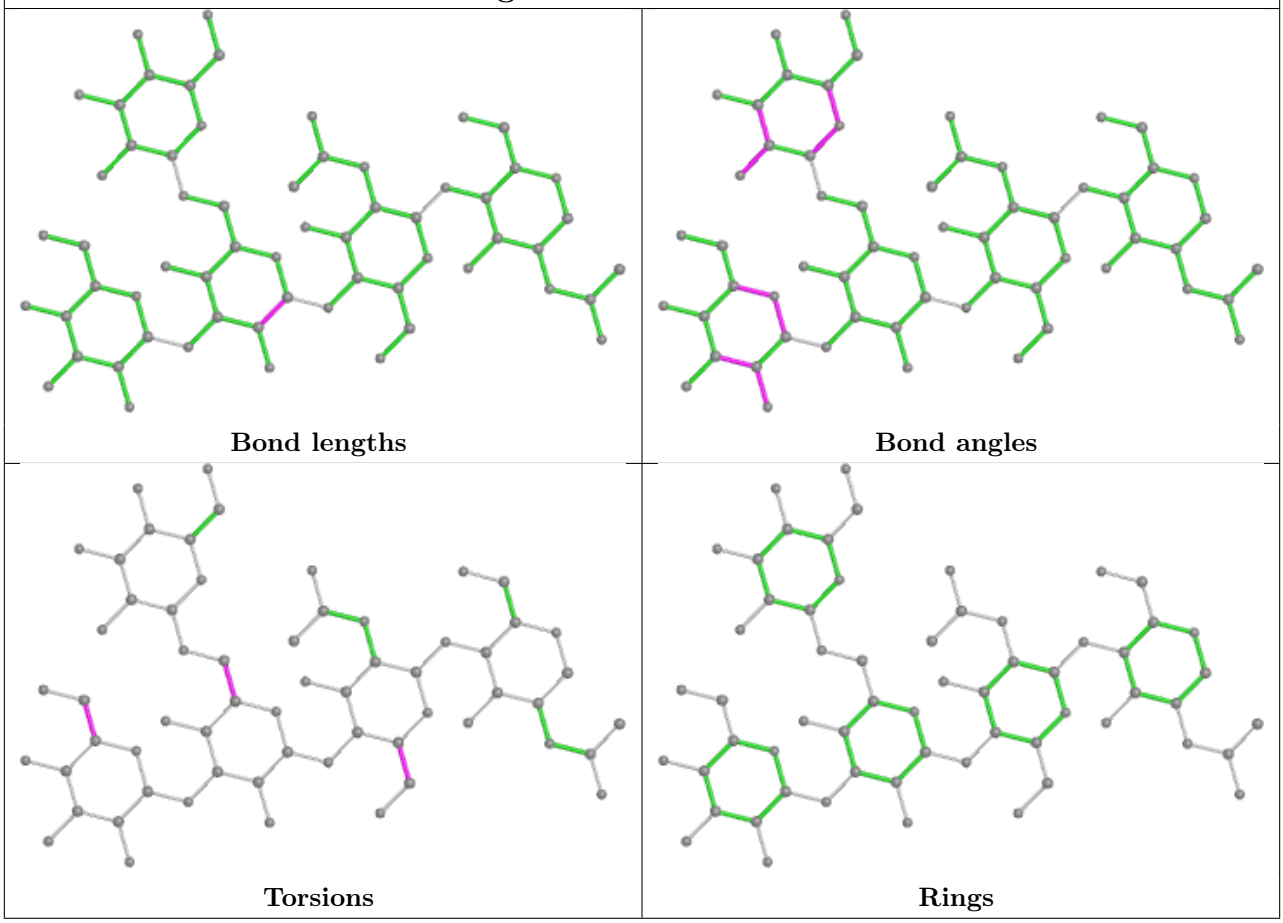
Continued on next page...

Continued from previous page...

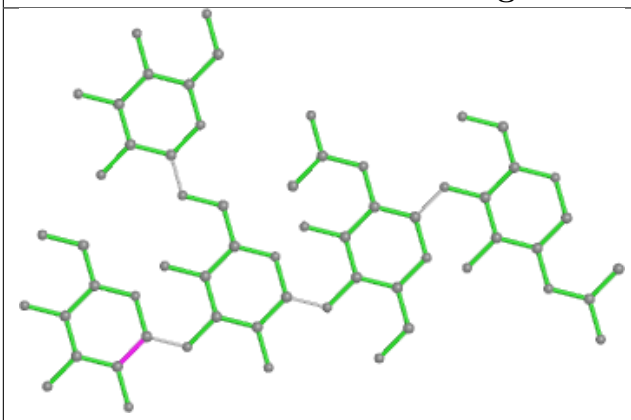
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	W	1	NAG	2	0
10	T	1	NAG	1	0
5	F	3	BMA	1	0
7	Z	9	MAN	6	0
7	S	2	NAG	1	0
9	W	2	NAG	3	0
7	S	1	NAG	1	0
7	N	6	MAN	1	0
9	R	2	NAG	1	0
8	O	2	NAG	2	0
8	O	1	NAG	7	0
8	U	5	MAN	1	0
9	R	1	NAG	1	0
6	M	2	NAG	1	0
7	S	3	BMA	1	0
6	Q	2	NAG	1	0

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

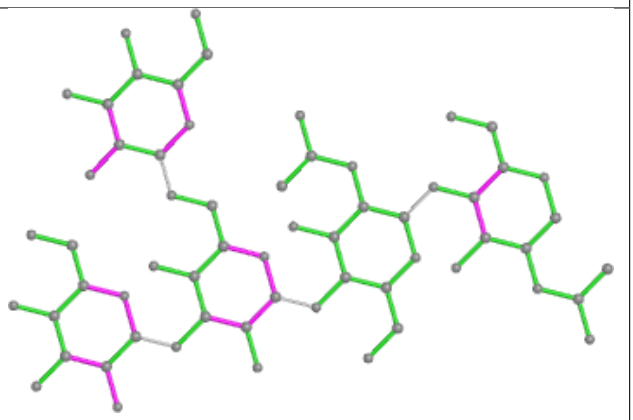
Oligosaccharide Chain F



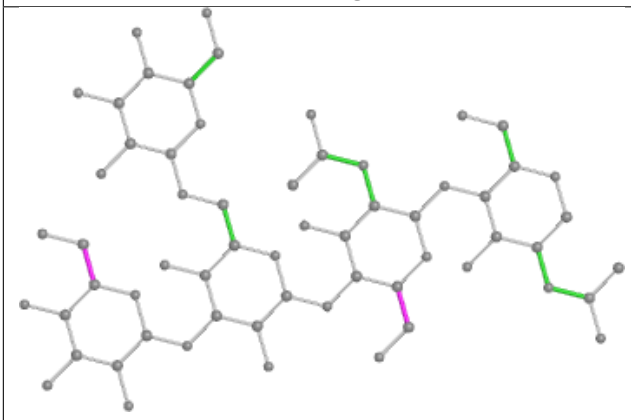
Oligosaccharide Chain b



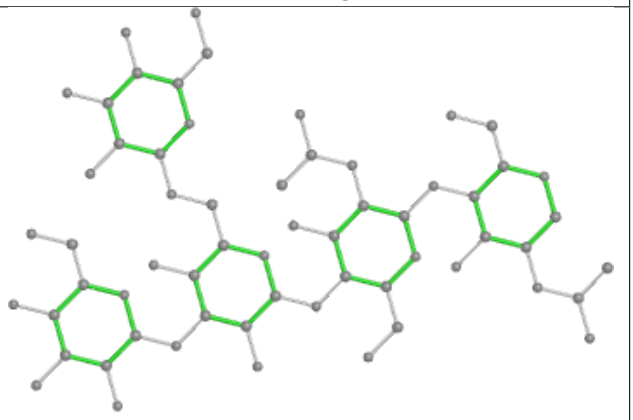
Bond lengths



Bond angles

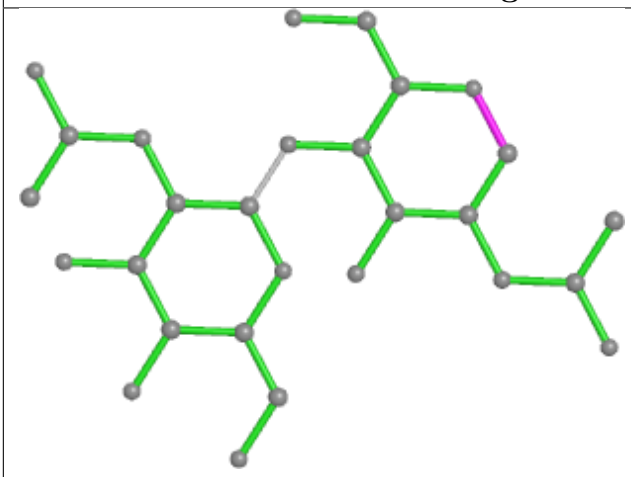


Torsions

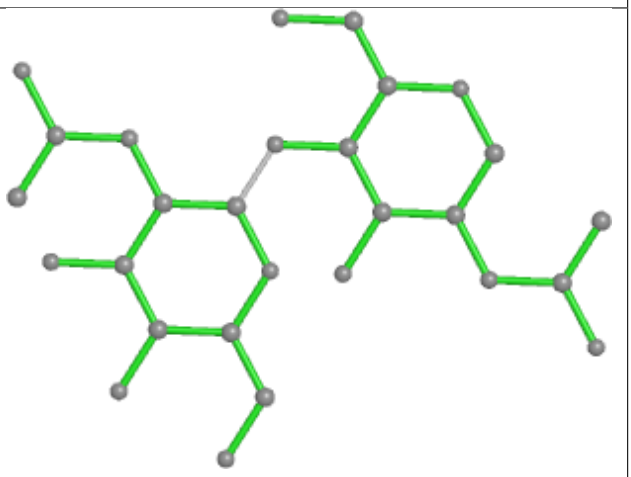


Rings

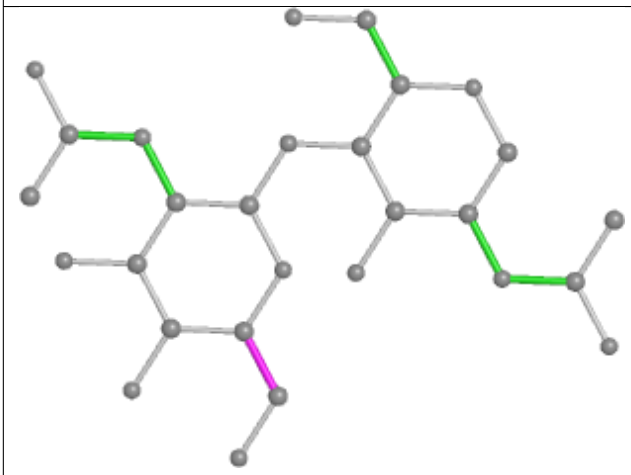
Oligosaccharide Chain I



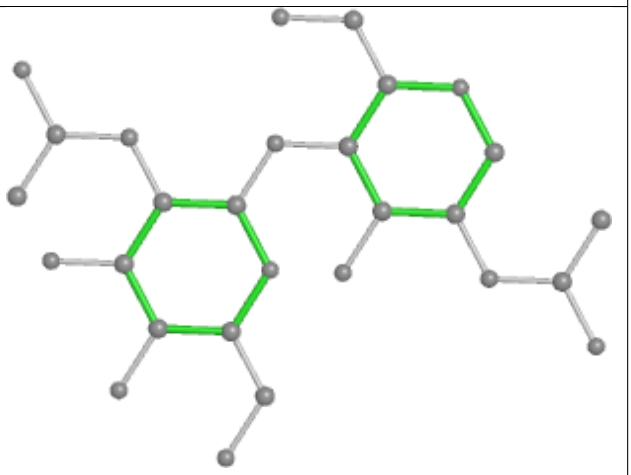
Bond lengths



Bond angles

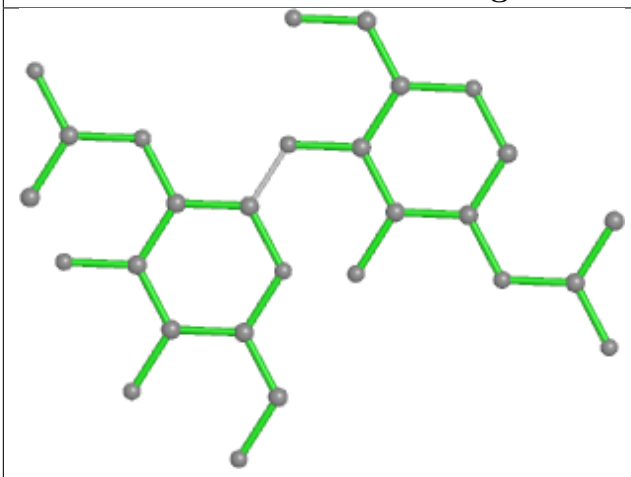


Torsions

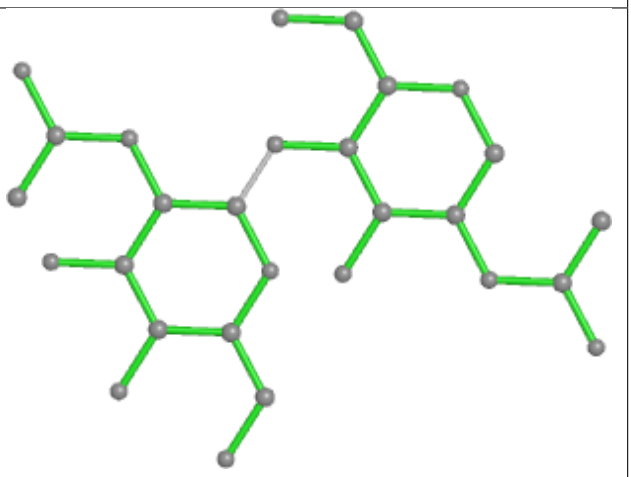


Rings

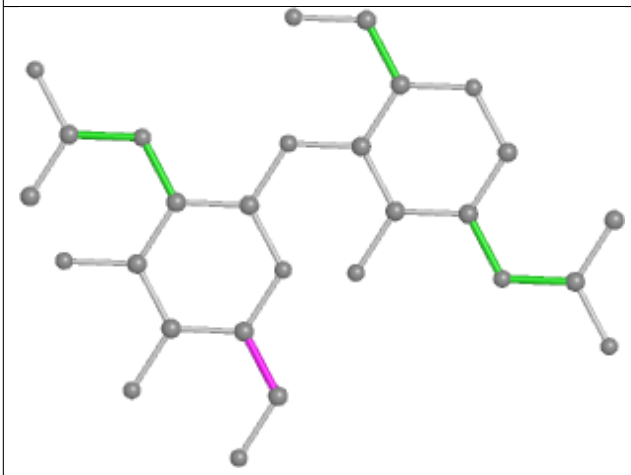
Oligosaccharide Chain M



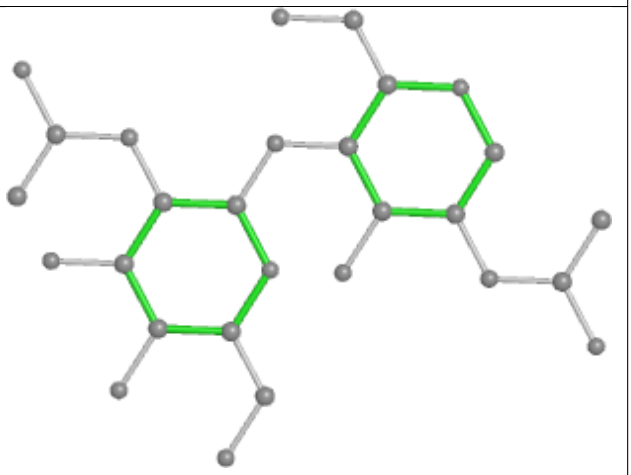
Bond lengths



Bond angles

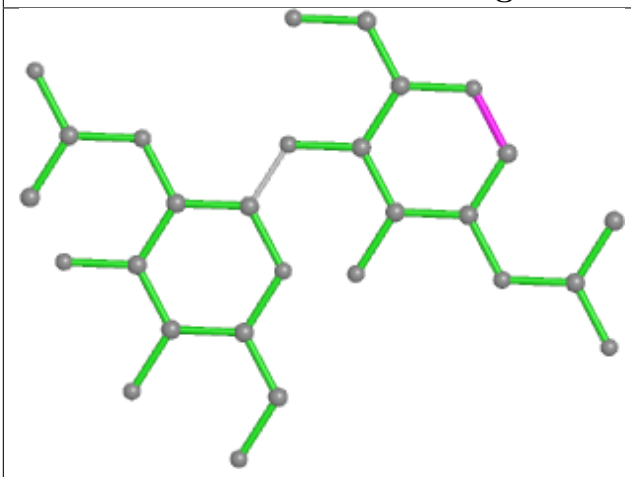


Torsions

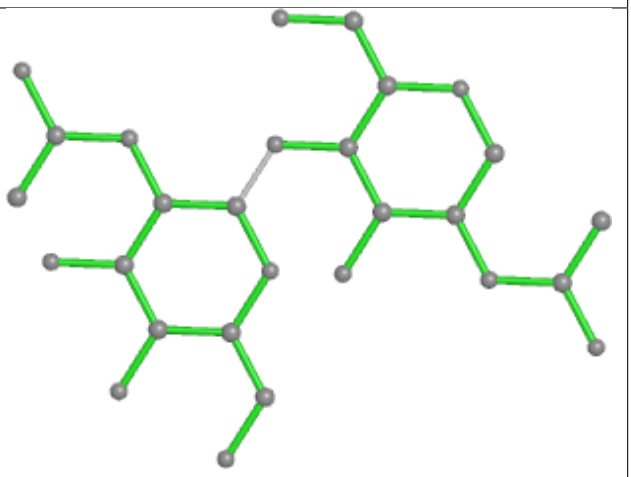


Rings

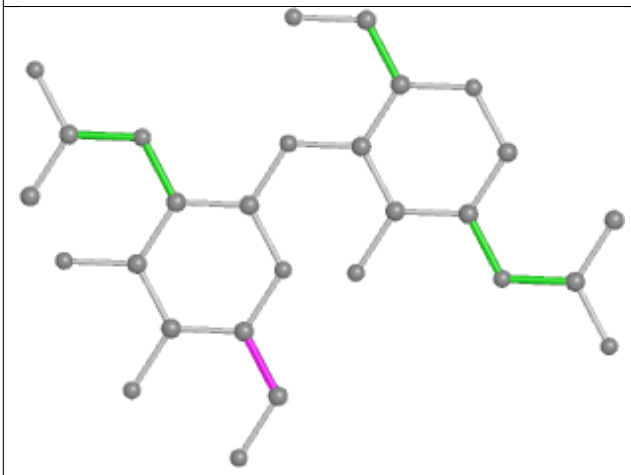
Oligosaccharide Chain P



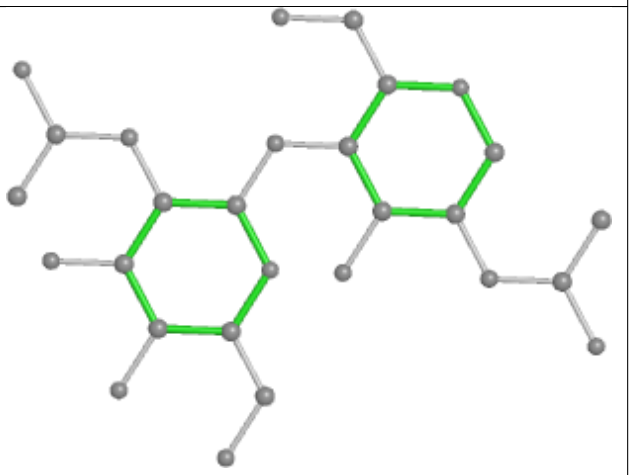
Bond lengths



Bond angles

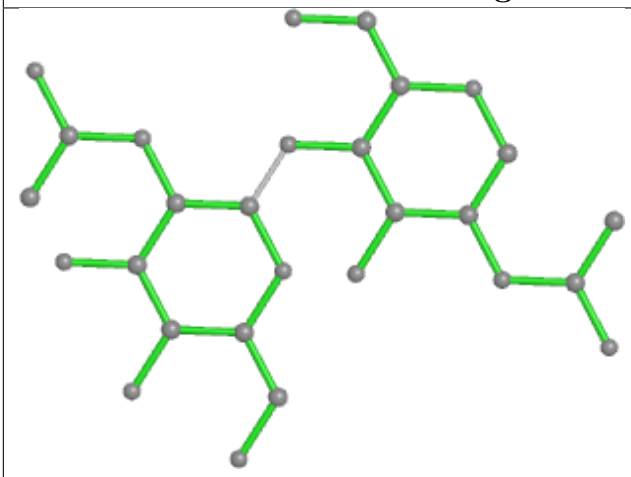


Torsions

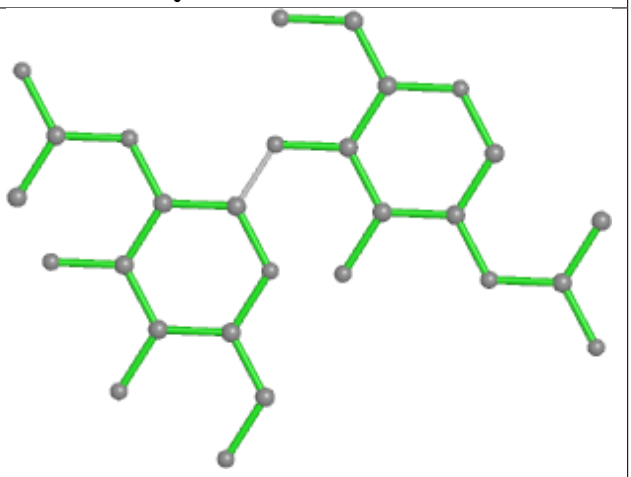


Rings

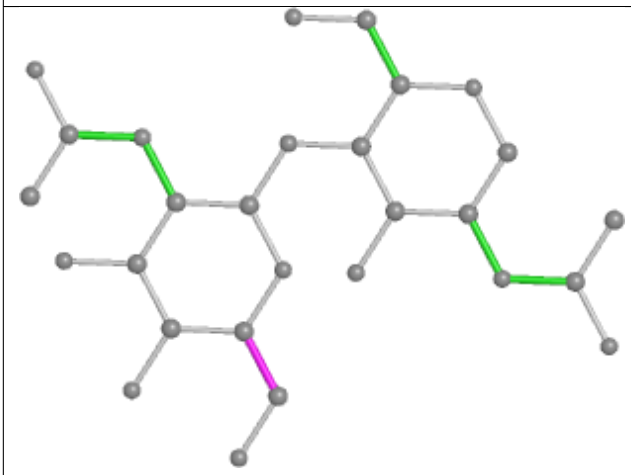
Oligosaccharide Chain Q



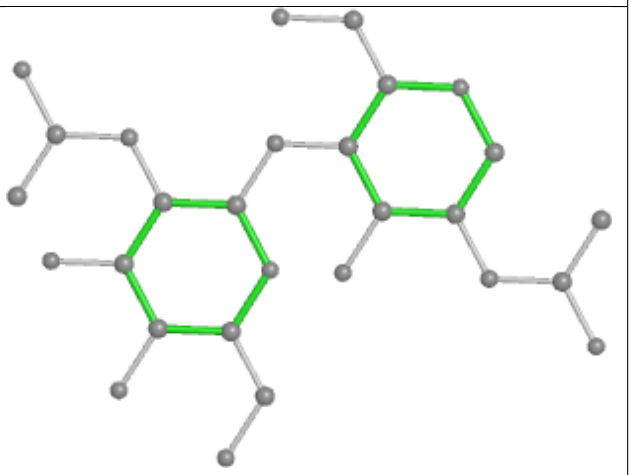
Bond lengths



Bond angles

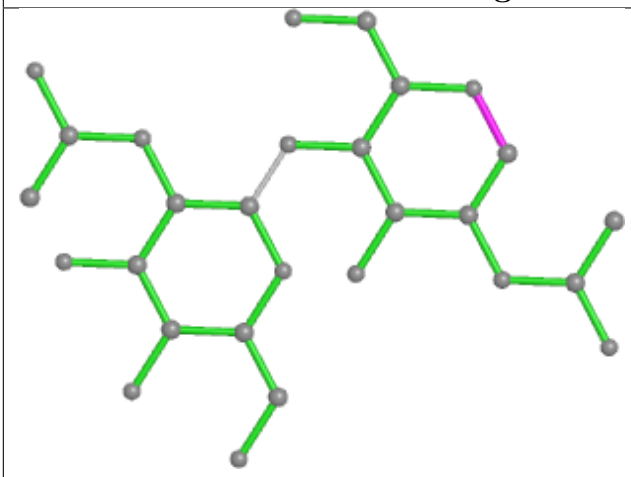


Torsions

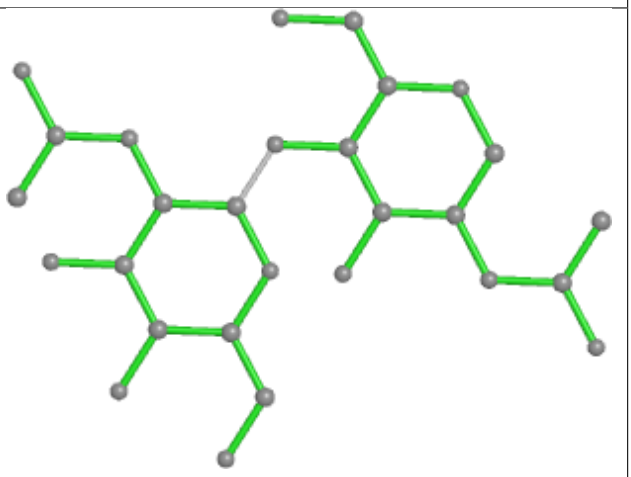


Rings

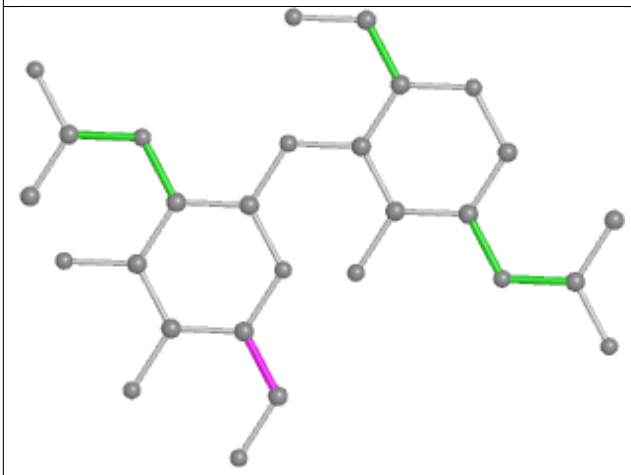
Oligosaccharide Chain V



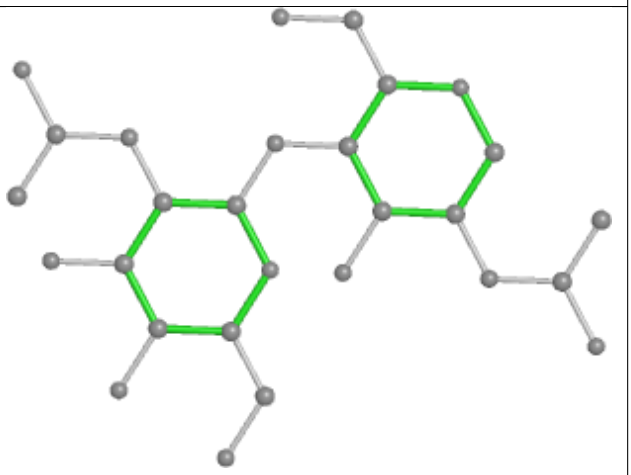
Bond lengths



Bond angles

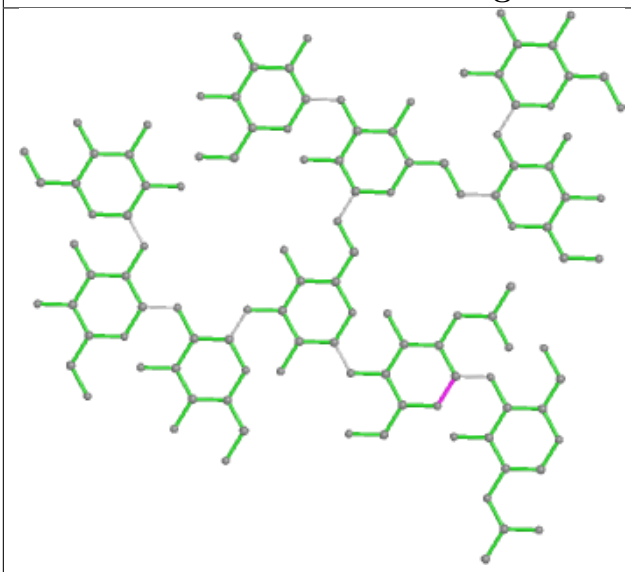


Torsions

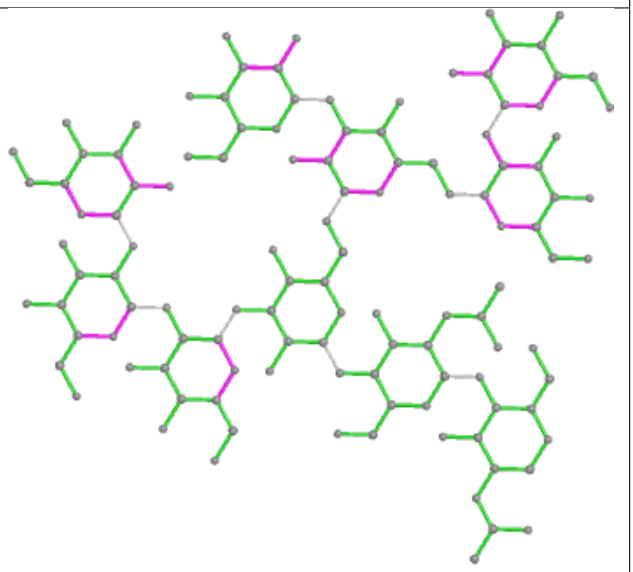


Rings

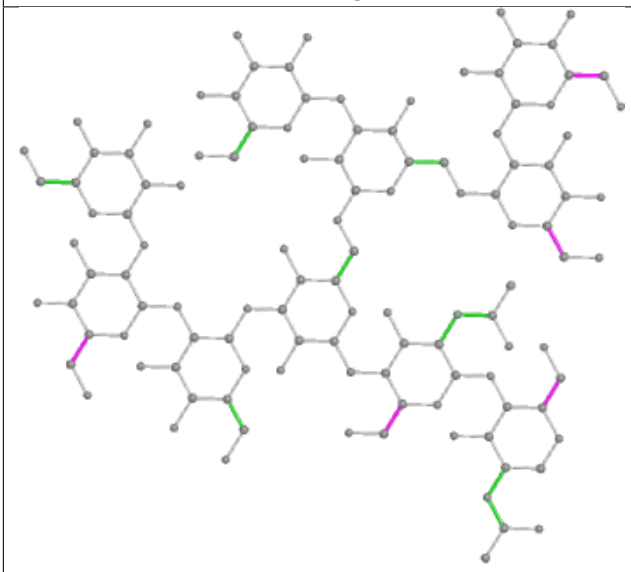
Oligosaccharide Chain N



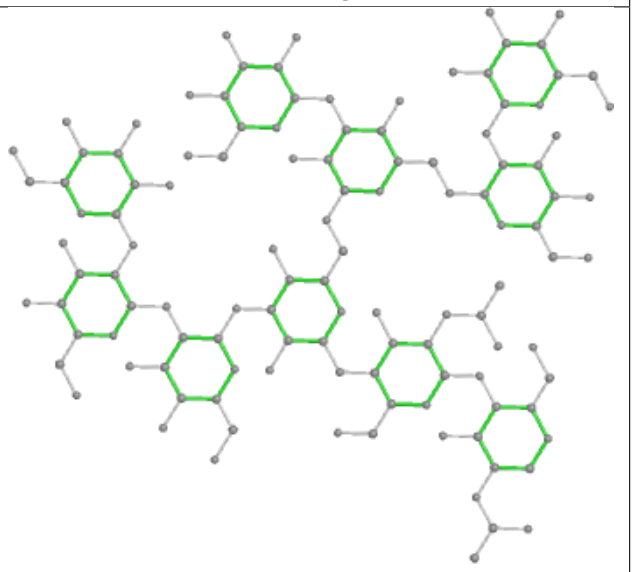
Bond lengths



Bond angles

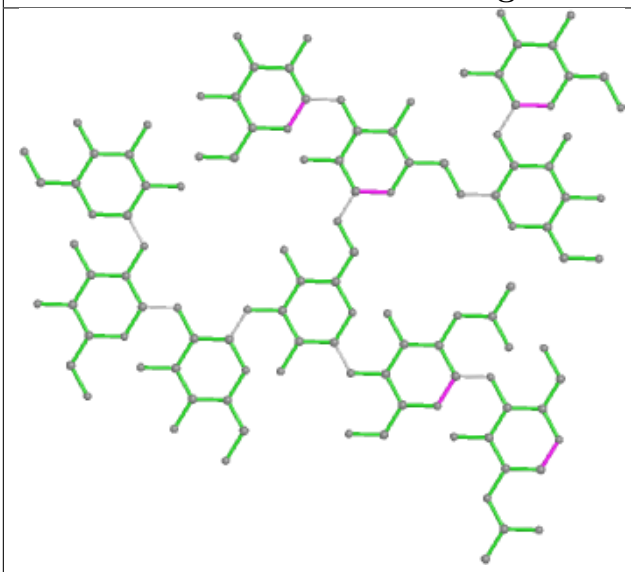


Torsions

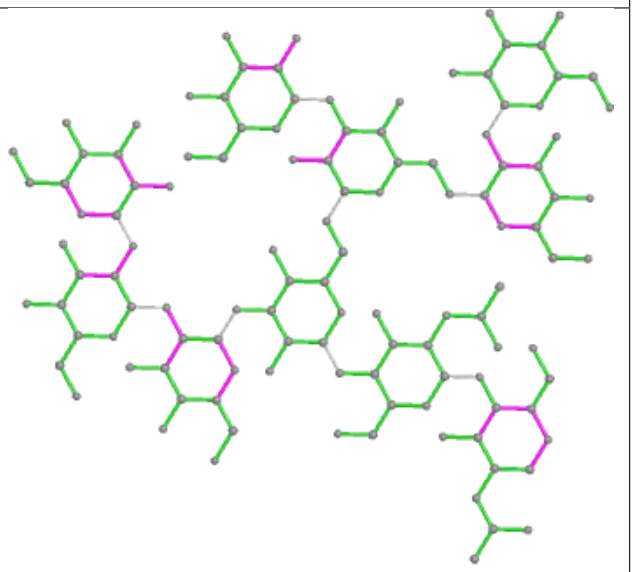


Rings

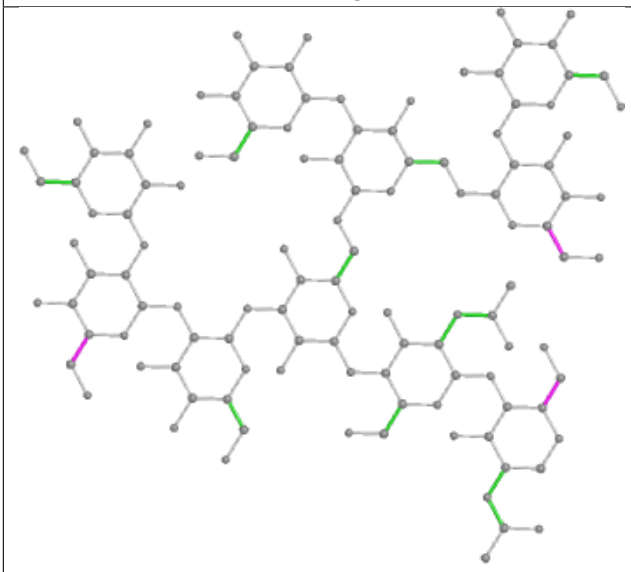
Oligosaccharide Chain S



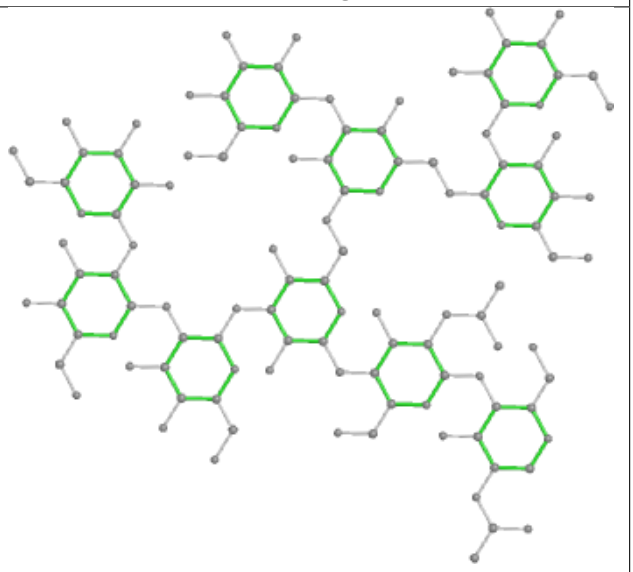
Bond lengths



Bond angles

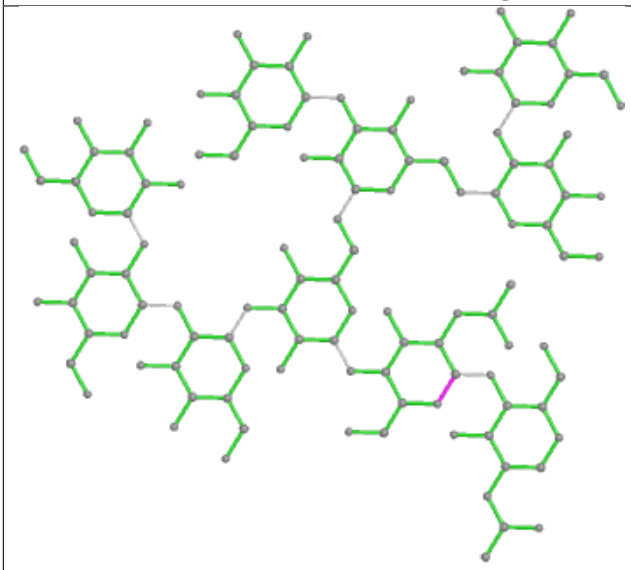


Torsions

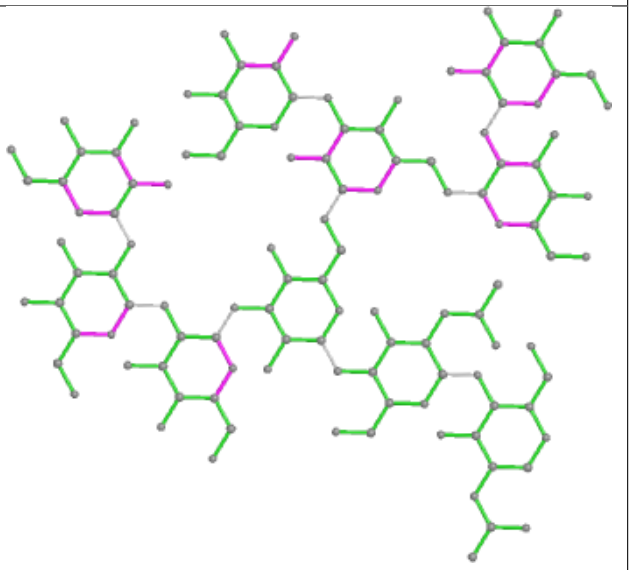


Rings

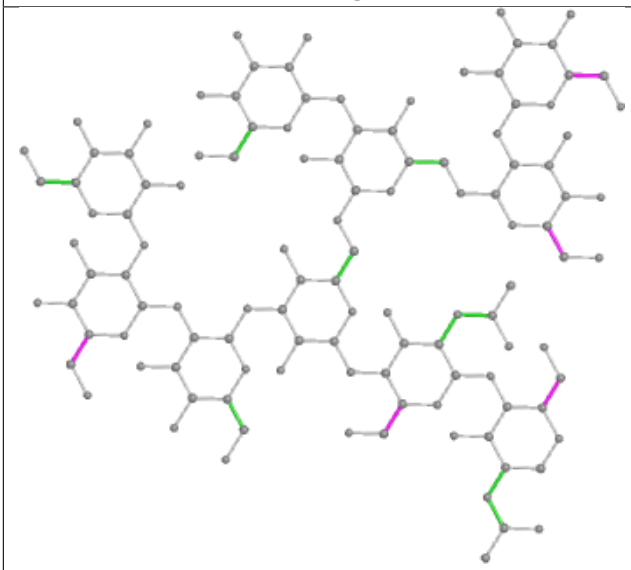
Oligosaccharide Chain Z



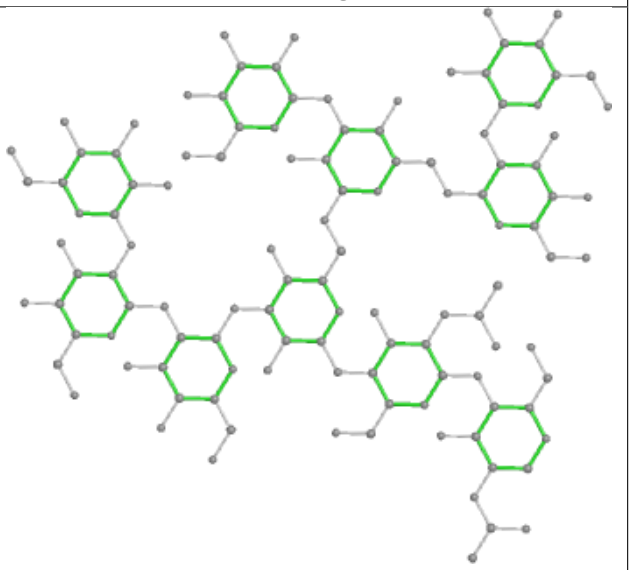
Bond lengths



Bond angles

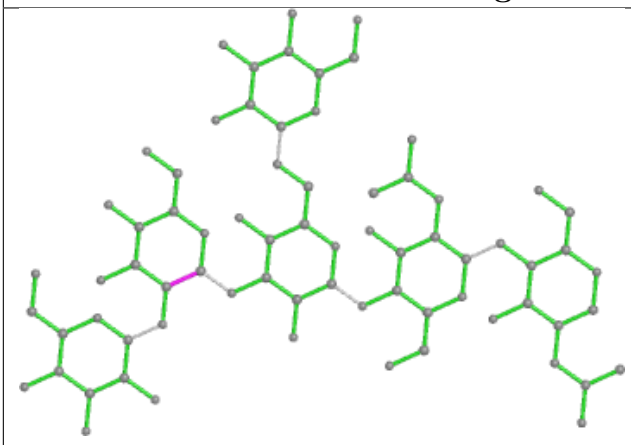


Torsions

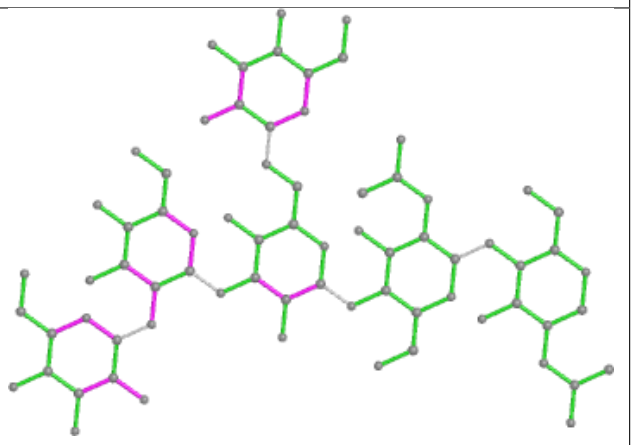


Rings

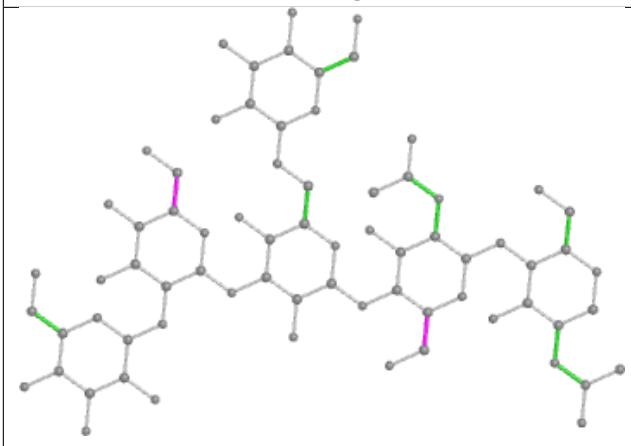
Oligosaccharide Chain O



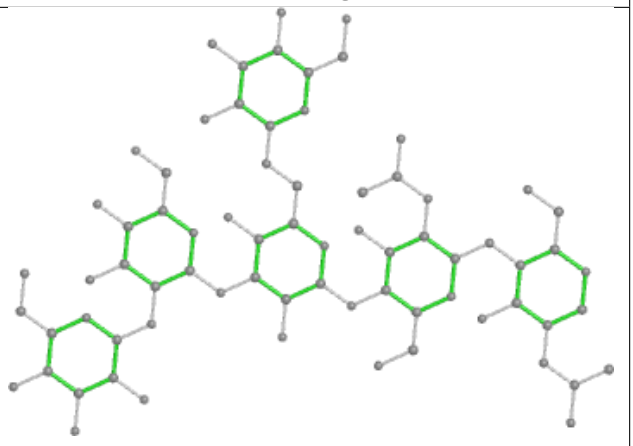
Bond lengths



Bond angles

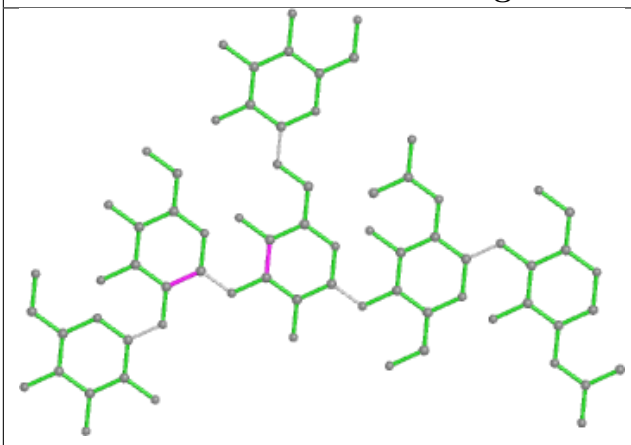


Torsions

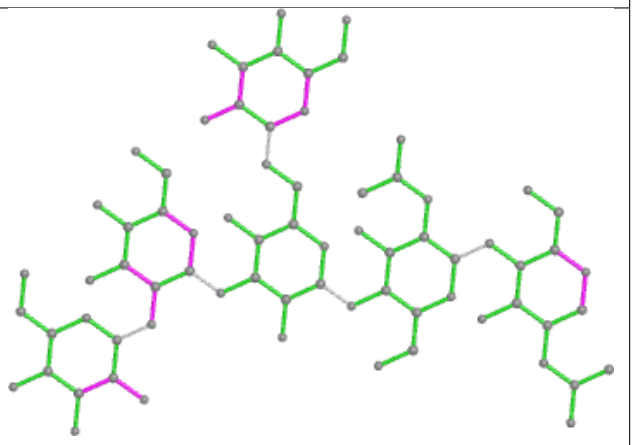


Rings

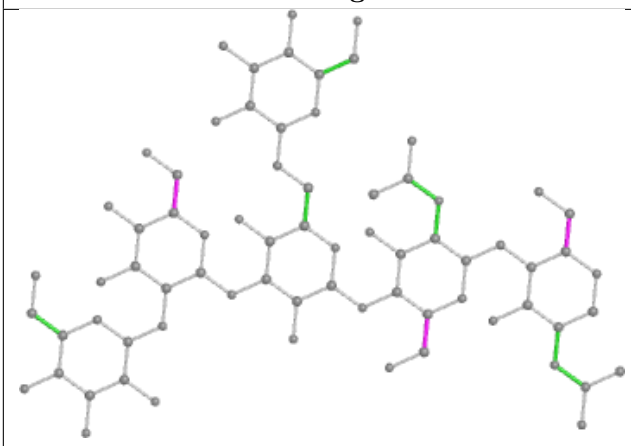
Oligosaccharide Chain U



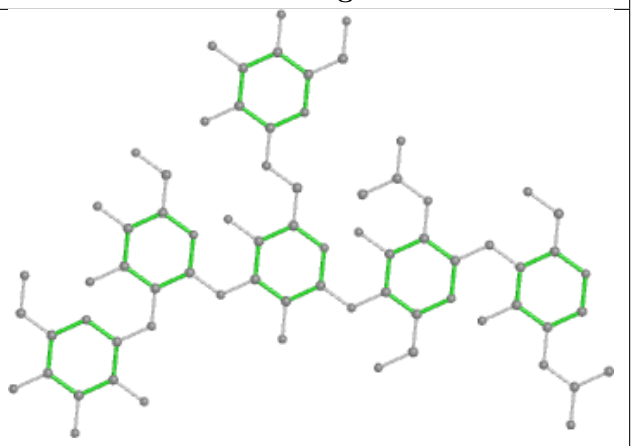
Bond lengths



Bond angles

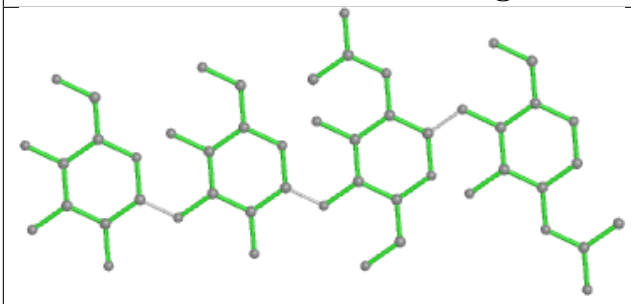


Torsions

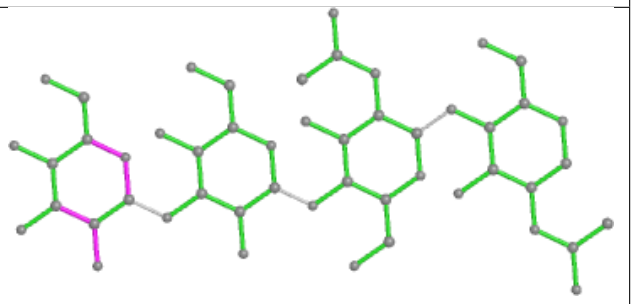


Rings

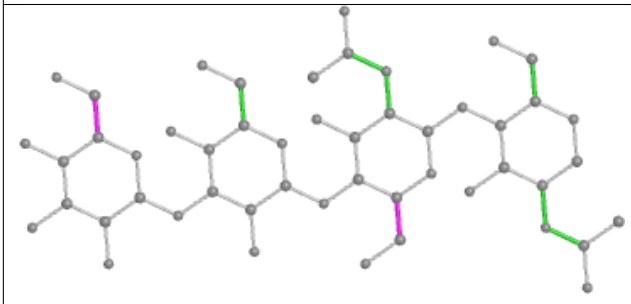
Oligosaccharide Chain R



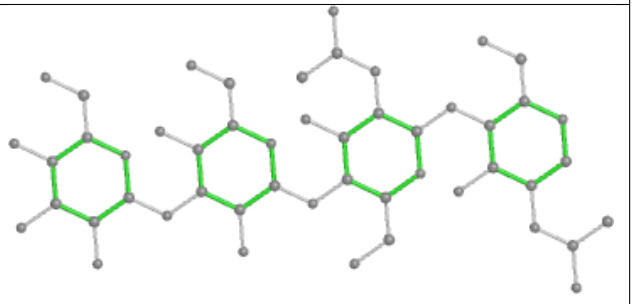
Bond lengths



Bond angles

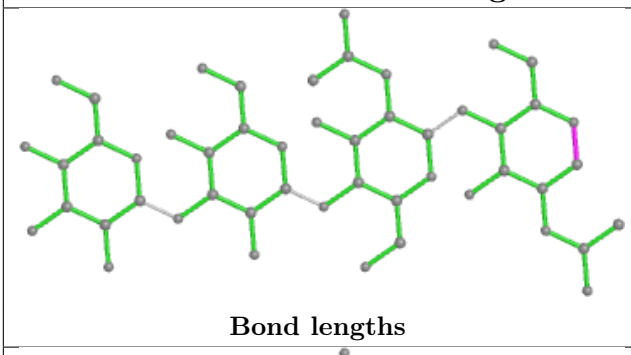


Torsions

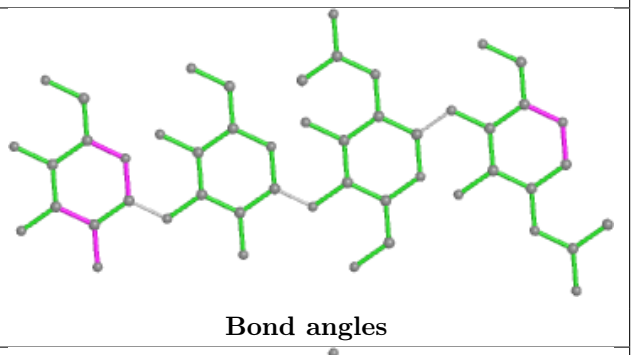


Rings

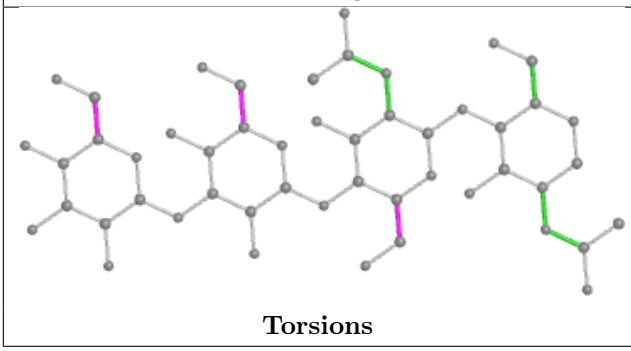
Oligosaccharide Chain W



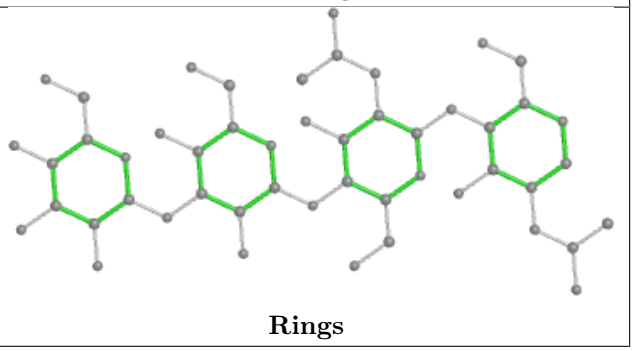
Bond lengths



Bond angles

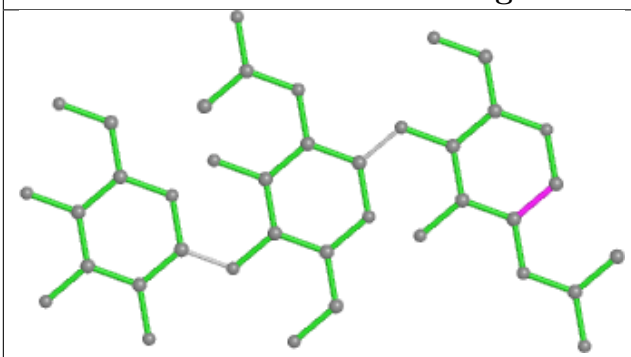


Torsions

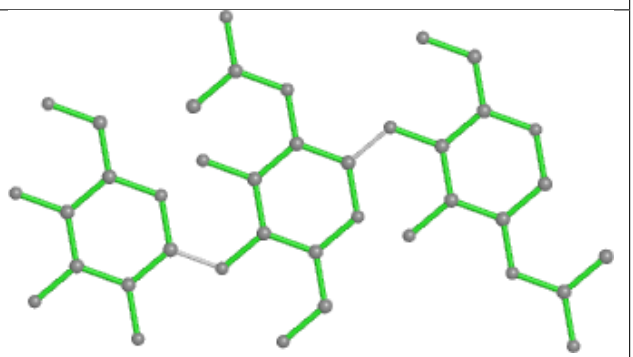


Rings

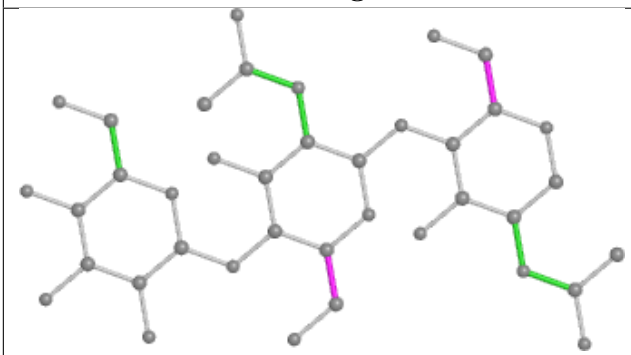
Oligosaccharide Chain T



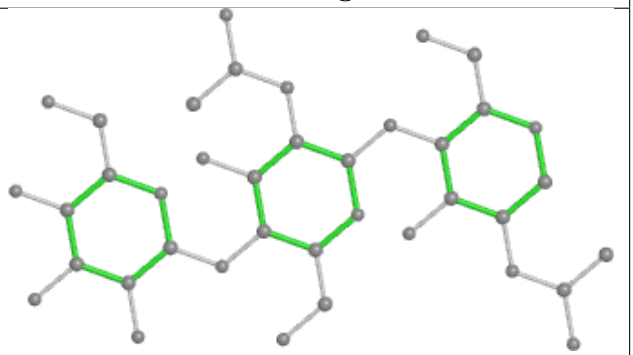
Bond lengths



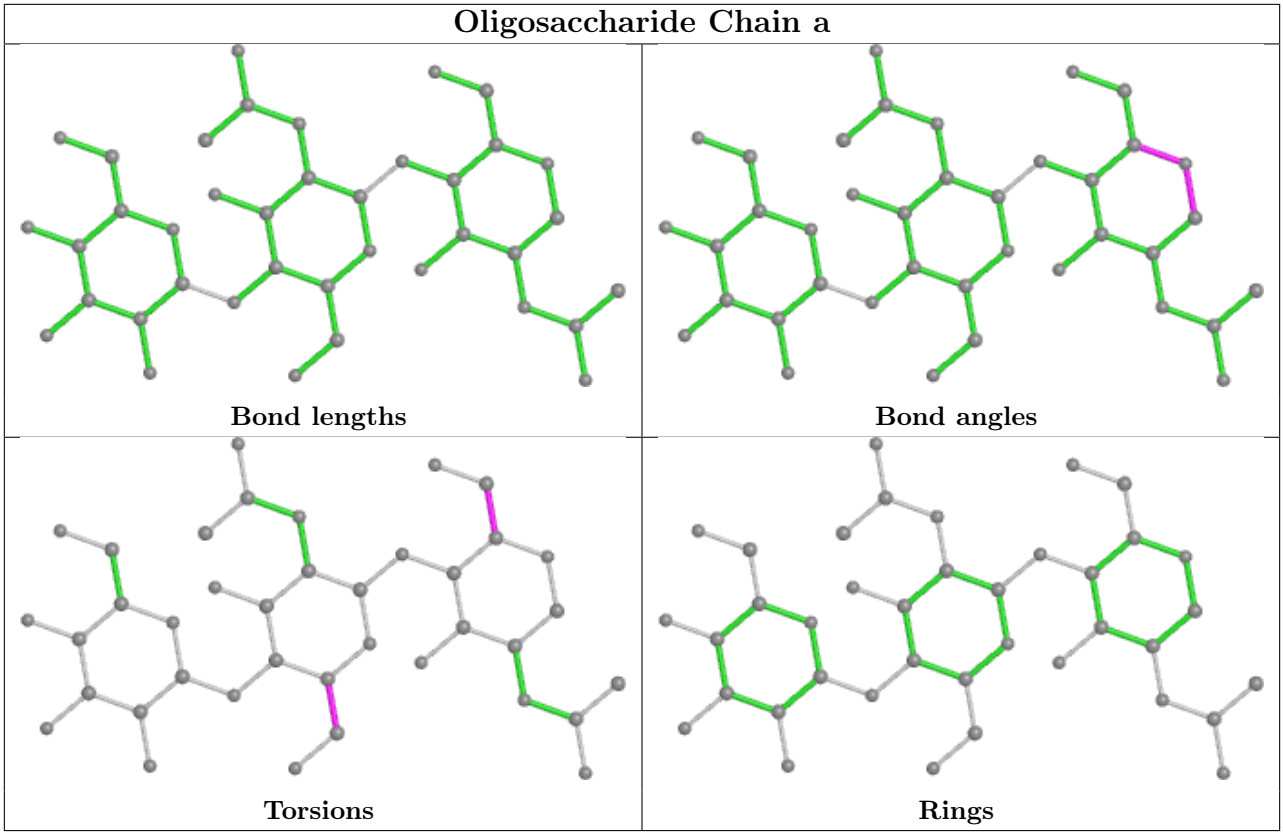
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	NAG	B	1040	2	14,14,15	0.29	0	17,19,21	0.54	0
11	NAG	A	1000	-	14,14,15	0.51	0	17,19,21	0.49	0
11	NAG	J	1042	2	14,14,15	0.59	0	17,19,21	0.73	1 (5%)
11	NAG	Y	1040	4	14,14,15	0.51	0	17,19,21	0.61	0
11	NAG	K	1040	4	14,14,15	0.58	0	17,19,21	0.47	0
11	NAG	Y	1041	4	14,14,15	0.95	1 (7%)	17,19,21	0.82	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	B	1040	2	-	2/6/23/26	0/1/1/1
11	NAG	A	1000	-	-	2/6/23/26	0/1/1/1
11	NAG	J	1042	2	-	2/6/23/26	0/1/1/1
11	NAG	Y	1040	4	-	0/6/23/26	0/1/1/1
11	NAG	K	1040	4	-	2/6/23/26	0/1/1/1
11	NAG	Y	1041	4	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Y	1041	NAG	C1-C2	2.93	1.56	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	Y	1041	NAG	C1-O5-C5	2.65	115.79	112.19
11	J	1042	NAG	C1-O5-C5	2.39	115.43	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	Y	1041	NAG	C1-C2-N2-C7
11	K	1040	NAG	C1-C2-N2-C7
11	B	1040	NAG	C1-C2-N2-C7
11	J	1042	NAG	C1-C2-N2-C7
11	A	1000	NAG	C1-C2-N2-C7
11	K	1040	NAG	C3-C2-N2-C7
11	A	1000	NAG	C4-C5-C6-O6
11	B	1040	NAG	C3-C2-N2-C7
11	J	1042	NAG	C3-C2-N2-C7
11	Y	1041	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Y	1041	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	A	224/244 (91%)	-0.53	0 100 100	94, 133, 173, 216	0
1	D	224/244 (91%)	-0.39	1 (0%) 92 86	102, 155, 201, 272	0
1	H	227/244 (93%)	-0.59	0 100 100	71, 121, 164, 195	0
2	B	124/153 (81%)	-0.59	1 (0%) 86 73	76, 115, 180, 236	0
2	J	124/153 (81%)	-0.63	0 100 100	67, 113, 178, 255	0
2	X	121/153 (79%)	-0.56	1 (0%) 86 73	74, 119, 177, 325	0
3	C	214/215 (99%)	-0.39	3 (1%) 75 59	91, 144, 203, 230	0
3	E	214/215 (99%)	-0.36	0 100 100	99, 167, 215, 277	0
3	L	214/215 (99%)	-0.61	1 (0%) 91 82	80, 122, 209, 246	0
4	G	398/479 (83%)	-0.40	2 (0%) 91 82	71, 167, 231, 277	0
4	K	405/479 (84%)	-0.40	1 (0%) 95 91	63, 167, 248, 316	0
4	Y	397/479 (82%)	-0.34	7 (1%) 68 51	66, 176, 239, 315	0
All	All	2886/3273 (88%)	-0.45	17 (0%) 89 80	63, 147, 222, 325	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	104	GLY	4.8
3	C	12	SER	3.3
2	X	649	SER	3.0
4	Y	153	GLU	2.9
4	Y	132	THR	2.8
3	C	197	THR	2.7
4	Y	70	ALA	2.6
2	B	519	PHE	2.5
4	G	473	GLY	2.4
4	Y	155	LYS	2.3
4	Y	457	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	K	70	ALA	2.2
3	C	204	PRO	2.1
4	G	295	ASN	2.1
4	Y	131	CYS	2.1
4	Y	154	LEU	2.0
3	L	154	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
8	MAN	U	5	11/12	0.49	0.37	172,209,213,214	0
6	NAG	Q	2	14/15	0.59	0.60	133,170,179,180	14
6	NAG	P	2	14/15	0.64	0.76	165,177,184,185	14
7	MAN	Z	10	11/12	0.65	0.58	121,125,133,138	11
10	NAG	a	2	14/15	0.65	0.39	145,169,180,182	14
5	MAN	F	5	11/12	0.66	0.52	126,135,143,153	11
9	MAN	W	4	11/12	0.67	0.41	205,211,221,222	0
8	BMA	U	3	11/12	0.67	0.30	152,163,172,186	0
8	MAN	U	4	11/12	0.68	0.34	175,177,194,206	0
10	BMA	a	3	11/12	0.69	0.27	184,194,202,210	0
5	MAN	b	5	11/12	0.71	0.20	168,173,179,183	0
10	NAG	a	1	14/15	0.74	0.38	104,118,150,154	14
7	MAN	N	10	11/12	0.75	0.30	157,162,178,181	0
9	BMA	W	3	11/12	0.75	0.29	147,166,181,198	0
6	NAG	Q	1	14/15	0.76	0.23	155,164,174,179	0
5	MAN	F	4	11/12	0.76	0.55	119,131,141,143	11
9	MAN	R	4	11/12	0.78	0.22	184,196,201,202	0
5	BMA	F	3	11/12	0.78	0.25	135,148,156,157	11
9	BMA	R	3	11/12	0.78	0.28	139,150,171,186	11
8	MAN	U	6	11/12	0.79	0.32	168,174,187,187	0
8	MAN	O	6	11/12	0.80	0.23	164,169,181,185	0
6	NAG	P	1	14/15	0.83	0.34	96,125,147,148	14

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MAN	S	10	11/12	0.83	0.21	148,156,162,166	0
10	BMA	T	3	11/12	0.83	0.25	147,151,156,158	11
8	NAG	U	2	14/15	0.84	0.27	134,146,162,176	14
8	NAG	U	1	14/15	0.85	0.20	115,132,139,142	14
5	MAN	b	4	11/12	0.85	0.20	170,174,183,187	0
8	NAG	O	1	14/15	0.86	0.22	117,135,150,161	14
6	NAG	M	2	14/15	0.86	0.19	155,163,180,181	0
6	NAG	I	2	14/15	0.86	0.31	157,164,178,178	14
10	NAG	T	2	14/15	0.86	0.22	114,128,145,149	14
8	MAN	O	5	11/12	0.87	0.14	182,193,197,198	0
7	NAG	Z	2	14/15	0.87	0.33	73,88,99,102	14
6	NAG	M	1	14/15	0.87	0.21	132,145,171,173	0
5	NAG	b	1	14/15	0.87	0.14	153,171,178,184	0
10	NAG	T	1	14/15	0.87	0.23	113,135,148,161	0
7	MAN	Z	8	11/12	0.88	0.33	110,123,137,141	11
6	NAG	I	1	14/15	0.89	0.35	125,137,150,154	14
7	MAN	Z	4	11/12	0.89	0.20	117,120,124,131	11
7	MAN	Z	7	11/12	0.89	0.34	109,115,125,126	11
5	BMA	b	3	11/12	0.89	0.28	152,158,170,178	0
5	NAG	F	2	14/15	0.90	0.21	106,124,138,153	0
6	NAG	V	2	14/15	0.90	0.26	158,170,180,183	0
7	MAN	Z	5	11/12	0.90	0.18	117,125,141,149	11
7	MAN	Z	6	11/12	0.90	0.24	115,121,131,133	11
9	NAG	R	2	14/15	0.90	0.32	93,103,111,125	14
8	MAN	O	4	11/12	0.91	0.23	171,189,201,208	0
7	MAN	N	8	11/12	0.91	0.17	114,133,145,153	0
5	NAG	b	2	14/15	0.91	0.19	155,168,187,195	0
7	MAN	N	6	11/12	0.91	0.18	126,127,144,162	0
7	NAG	Z	1	14/15	0.91	0.23	94,113,131,135	14
7	BMA	Z	3	11/12	0.92	0.18	95,106,115,125	11
7	MAN	S	8	11/12	0.92	0.16	123,128,153,162	0
9	NAG	W	1	14/15	0.92	0.26	70,86,110,126	14
9	NAG	W	2	14/15	0.92	0.24	80,98,116,132	14
9	NAG	R	1	14/15	0.92	0.24	56,77,98,109	14
6	NAG	V	1	14/15	0.92	0.15	124,140,154,155	0
8	BMA	O	3	11/12	0.93	0.17	132,136,155,163	0
7	MAN	Z	9	11/12	0.93	0.11	122,126,136,150	0
8	NAG	O	2	14/15	0.93	0.22	118,136,148,155	0
7	BMA	S	3	11/12	0.94	0.14	93,110,127,142	0
7	MAN	S	6	11/12	0.94	0.24	80,85,98,107	11
7	MAN	N	4	11/12	0.94	0.16	124,128,138,144	0
7	MAN	N	7	11/12	0.94	0.15	115,129,156,157	0

Continued on next page...

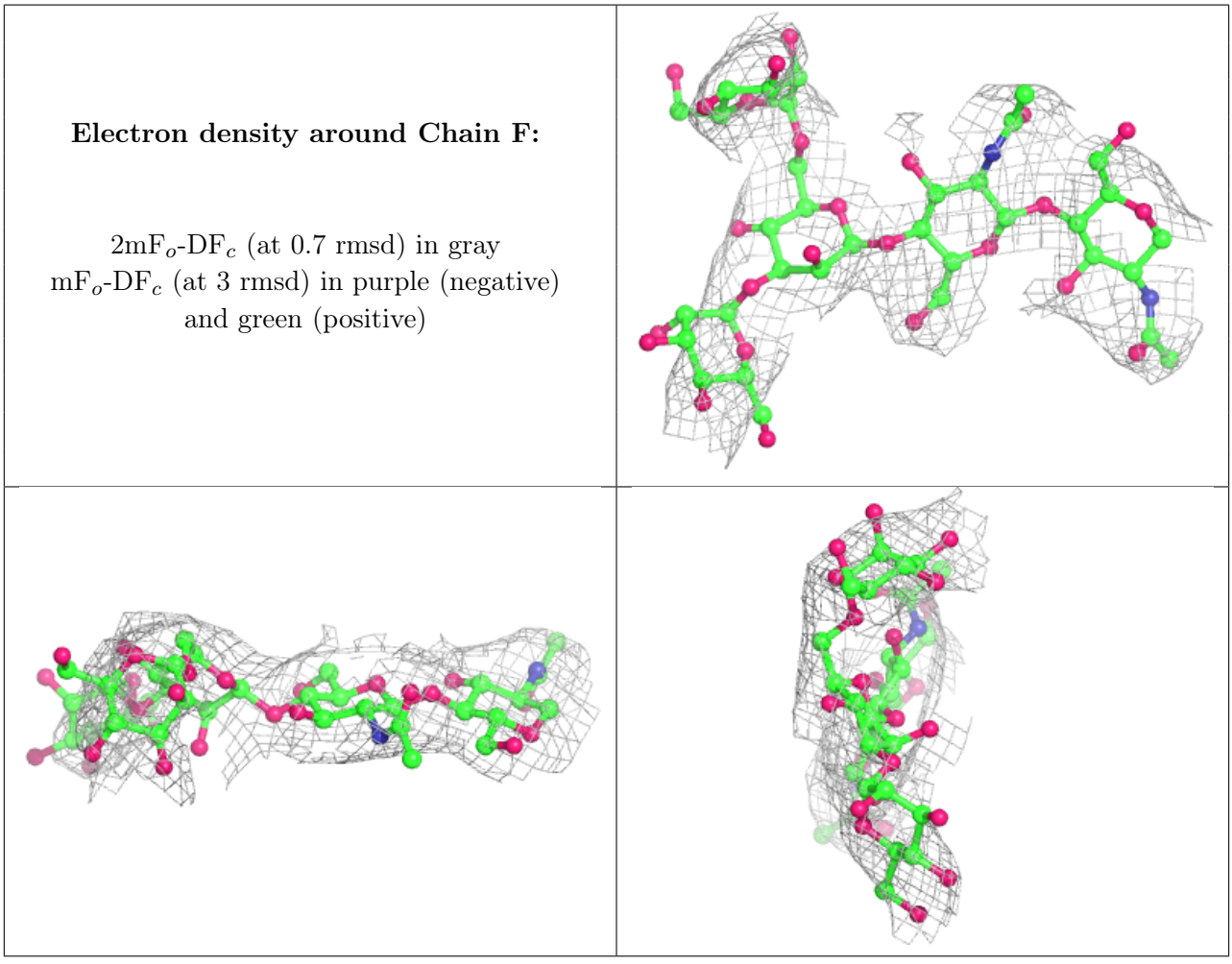
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	S	2	14/15	0.94	0.22	58,63,79,90	14
7	NAG	N	2	14/15	0.95	0.14	82,95,126,133	0
7	BMA	N	3	11/12	0.95	0.11	103,116,128,142	0
7	MAN	S	9	11/12	0.95	0.15	103,124,132,145	0
7	NAG	N	1	14/15	0.95	0.17	49,72,100,112	14
7	MAN	S	7	11/12	0.96	0.11	117,130,153,157	0
7	MAN	N	9	11/12	0.96	0.17	104,106,118,121	11
7	MAN	N	5	11/12	0.96	0.16	116,122,139,143	0
7	NAG	S	1	14/15	0.96	0.17	46,63,97,107	14
7	MAN	S	5	11/12	0.97	0.20	75,91,95,104	11
5	NAG	F	1	14/15	0.97	0.14	69,88,120,138	0
7	MAN	S	4	11/12	0.97	0.16	101,105,114,129	11

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.

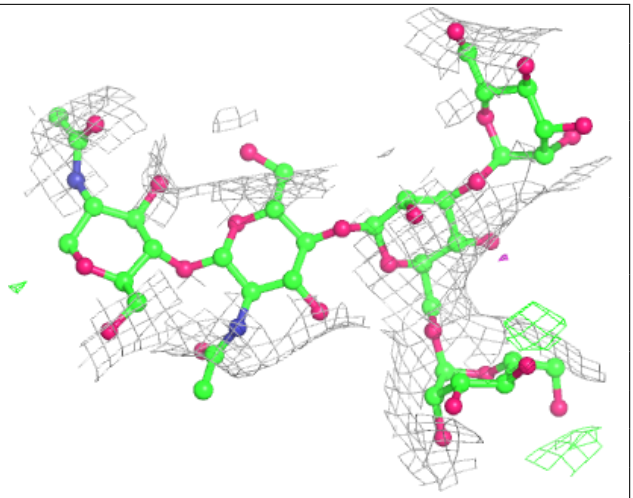
Electron density around Chain F:

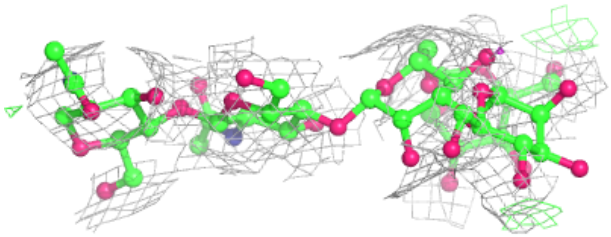
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

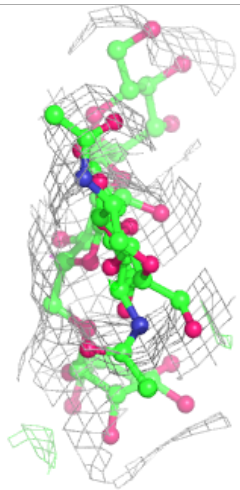


Electron density around Chain b:

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

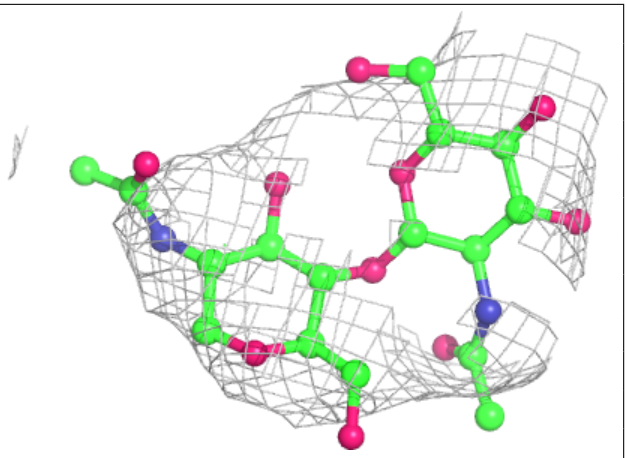


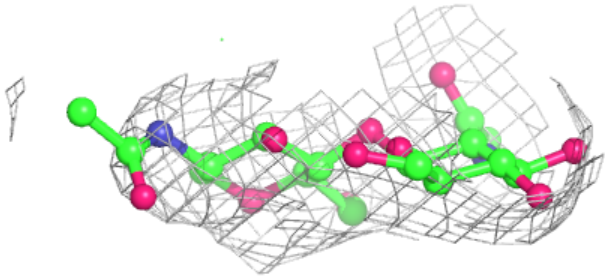


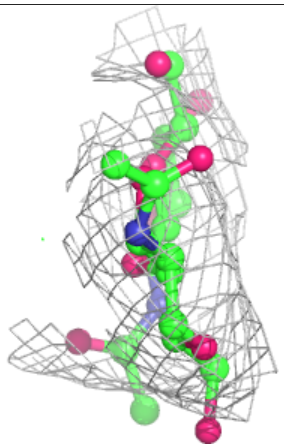


Electron density around Chain I:

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

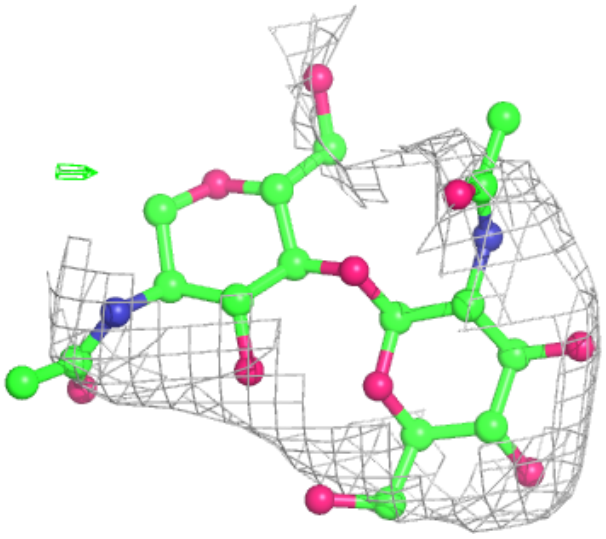


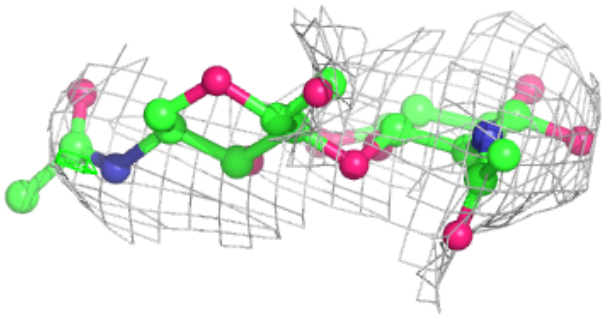


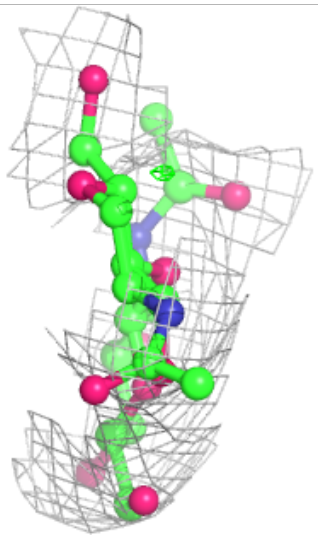


Electron density around Chain M:

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

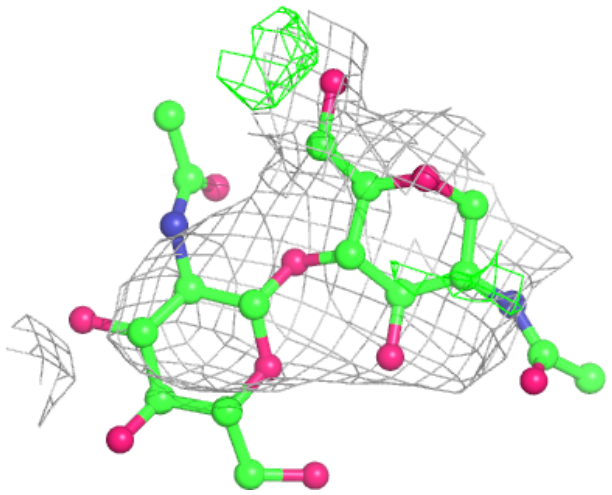


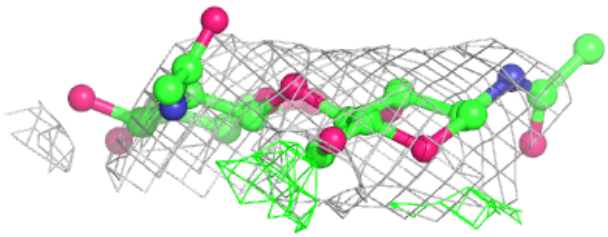


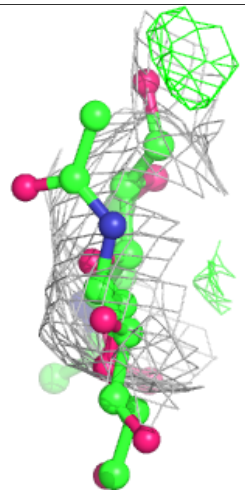


Electron density around Chain P:

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

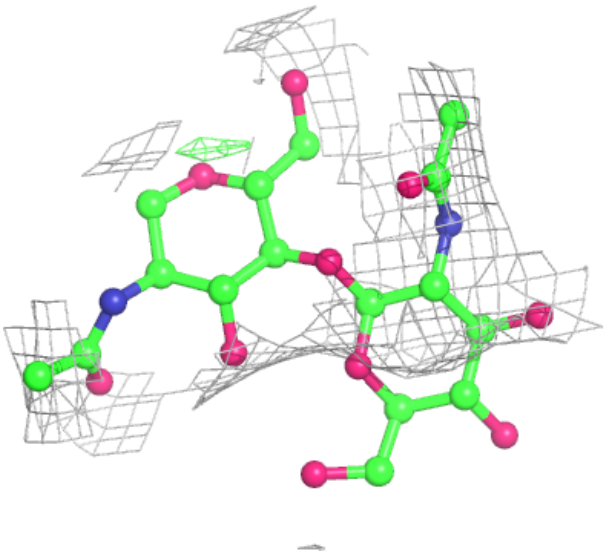


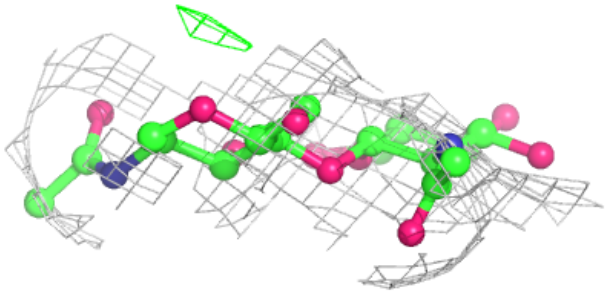


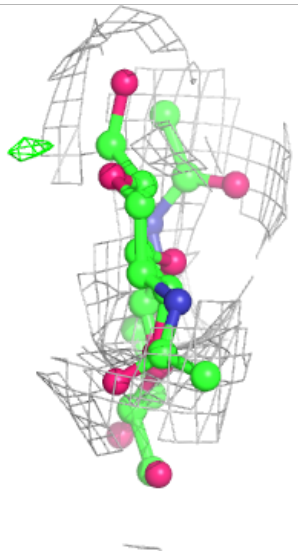


Electron density around Chain Q:

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

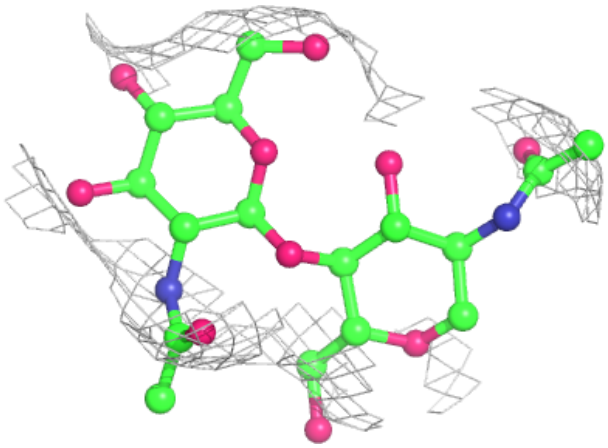


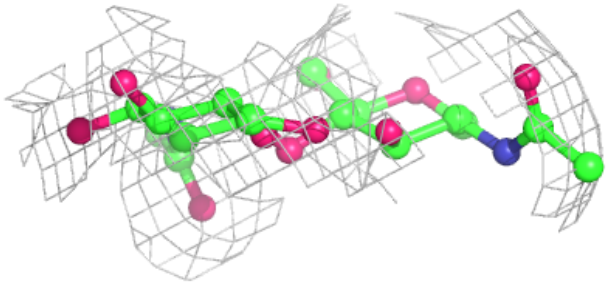


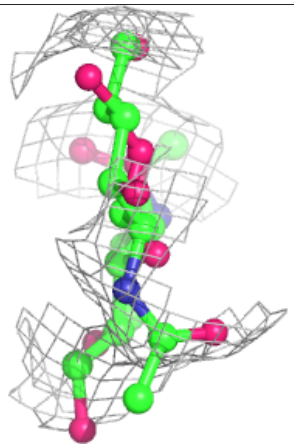


Electron density around Chain V:

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

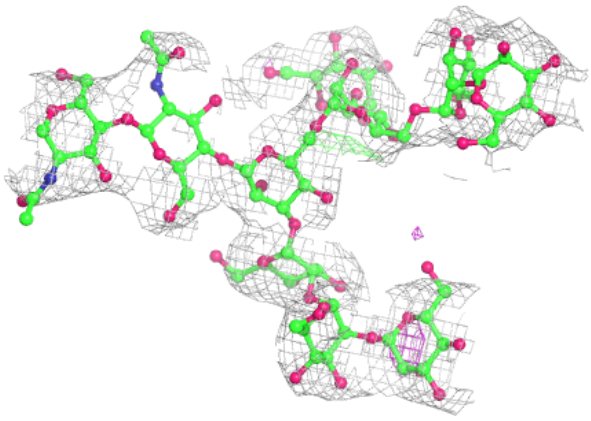


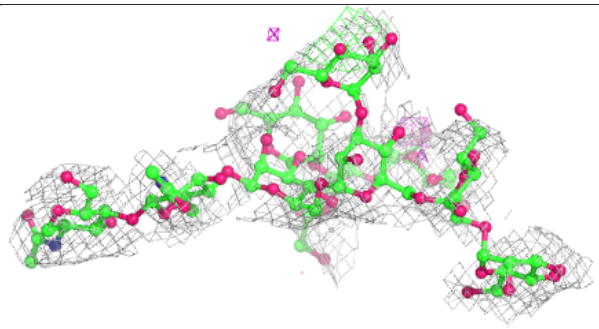


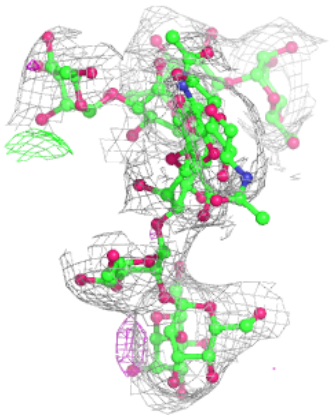


Electron density around Chain N:

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

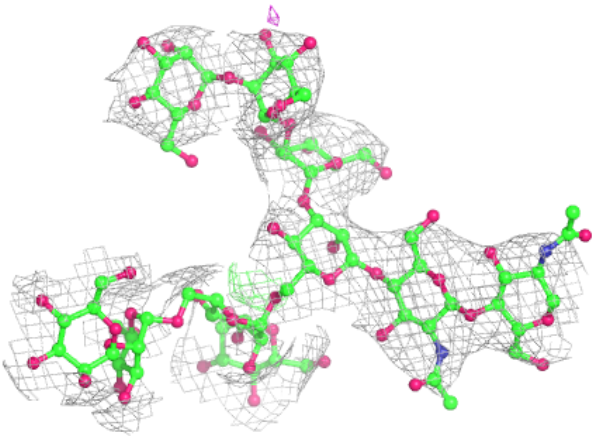


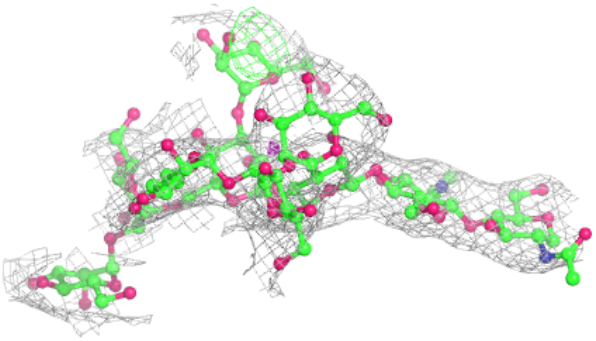


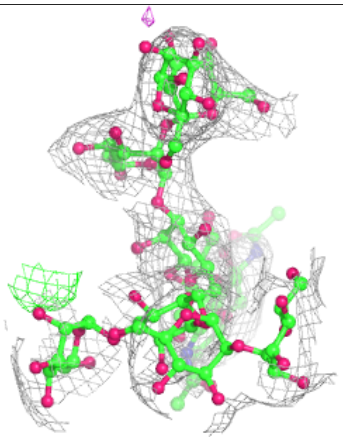


Electron density around Chain S:

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

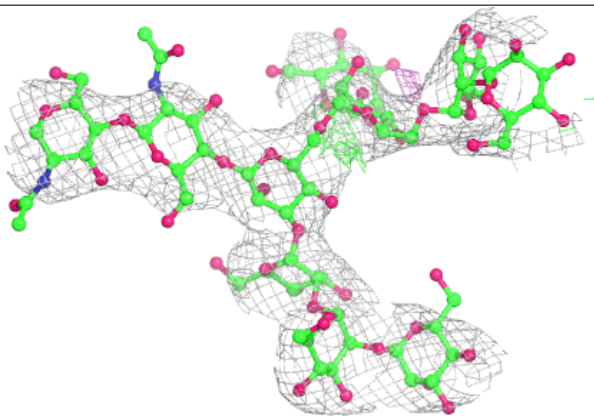


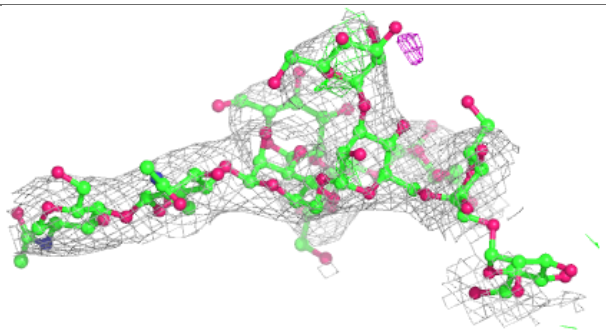


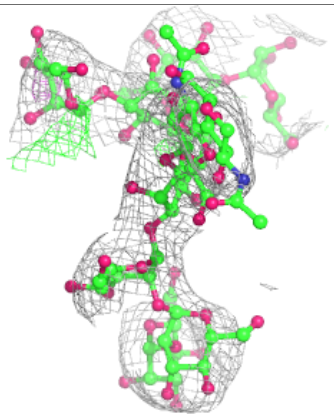


Electron density around Chain Z:

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

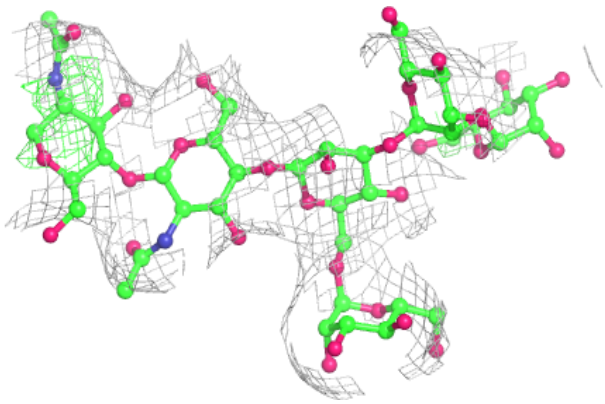


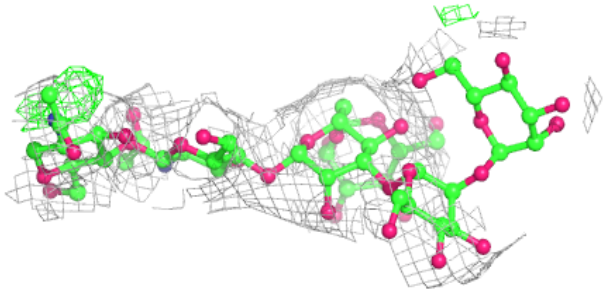


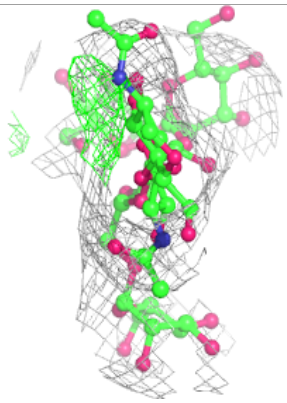


Electron density around Chain O:

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

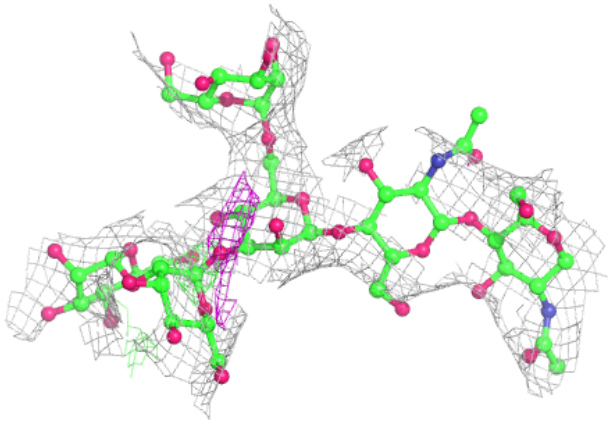


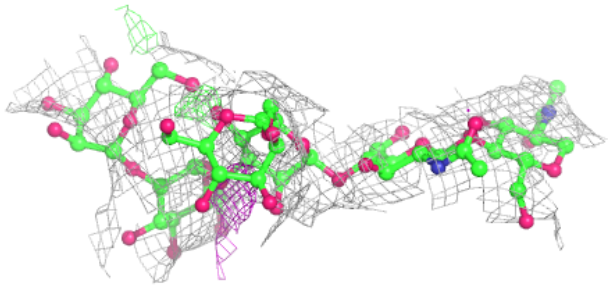


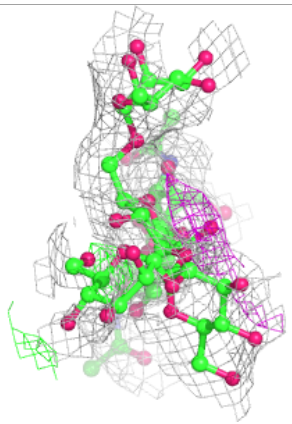


Electron density around Chain U:

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

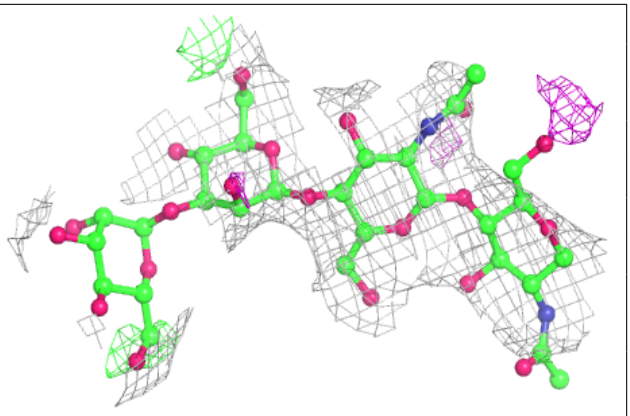


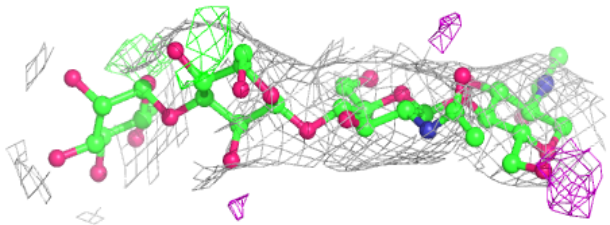


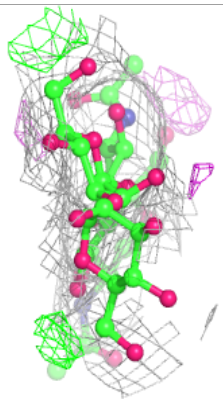


Electron density around Chain R:

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

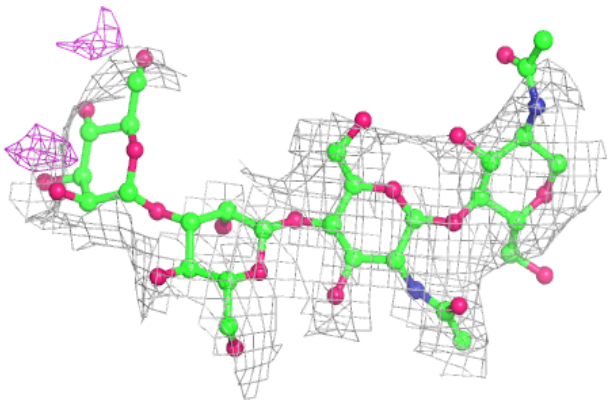


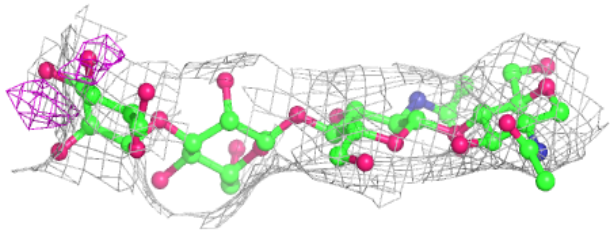


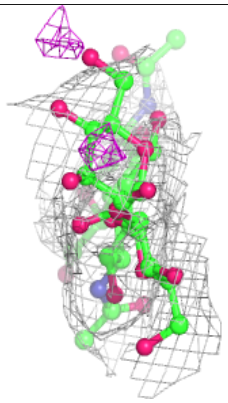


Electron density around Chain W:

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

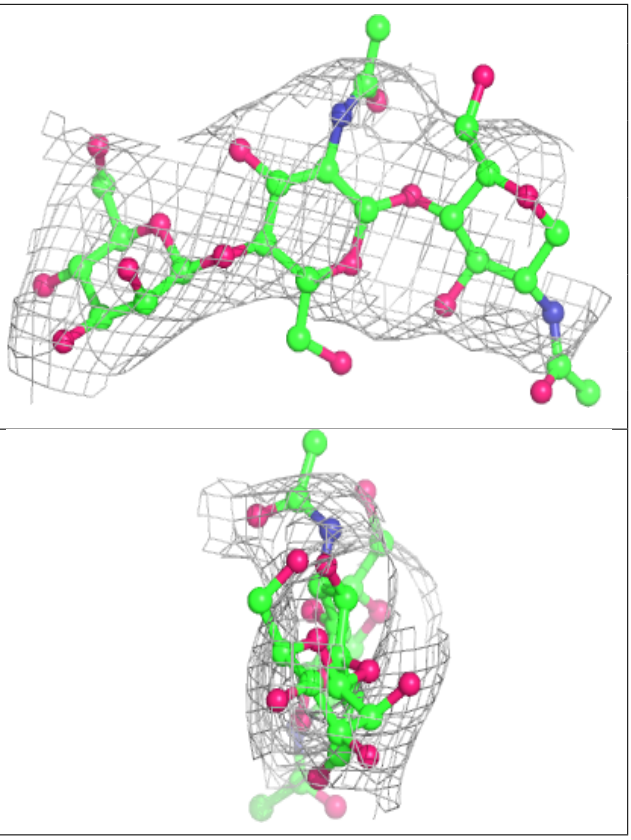






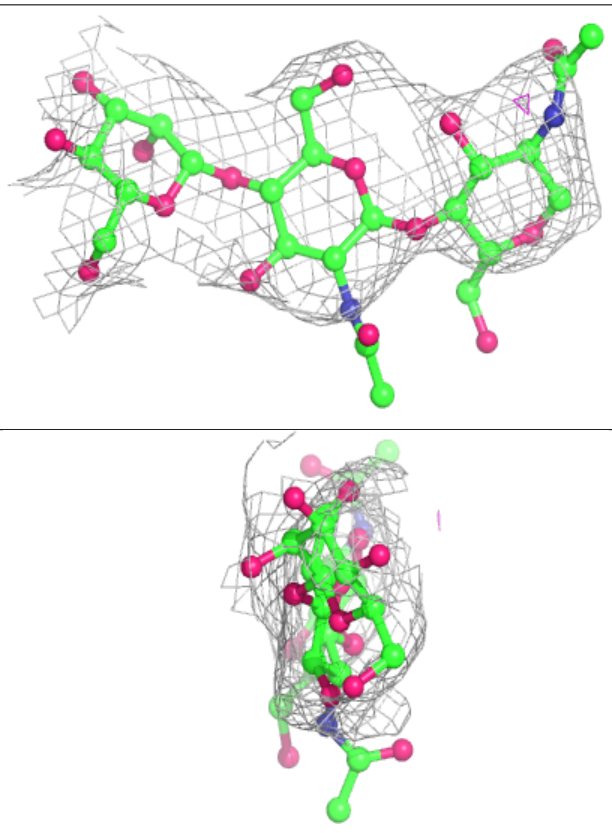
Electron density around Chain T:

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



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)



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
11	NAG	A	1000	14/15	0.48	0.44	157,166,174,175	14
11	NAG	K	1040	14/15	0.72	0.61	135,156,179,185	14
11	NAG	Y	1041	14/15	0.76	0.26	106,127,145,151	14
11	NAG	Y	1040	14/15	0.77	0.31	167,180,199,208	0
11	NAG	J	1042	14/15	0.81	0.33	115,125,139,145	14
11	NAG	B	1040	14/15	0.88	0.24	112,132,141,143	0

6.5 Other polymers

There are no such residues in this entry.