Full wwPDB X-ray Structure Validation Report

Aug 22, 2020 – 04:35 PM BST

PDB ID	:	5I8H
Title	:	Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer in Complex with V3 Loop-targeting Antibody PGT122 Fab and Fusion Peptide-targeting Antibody VRC34.01 Fab
Authors	:	Xu, K.; Zhou, T.; Kwong, P.D.
Deposited on	:	2016-02-18
Resolution	:	4.30 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

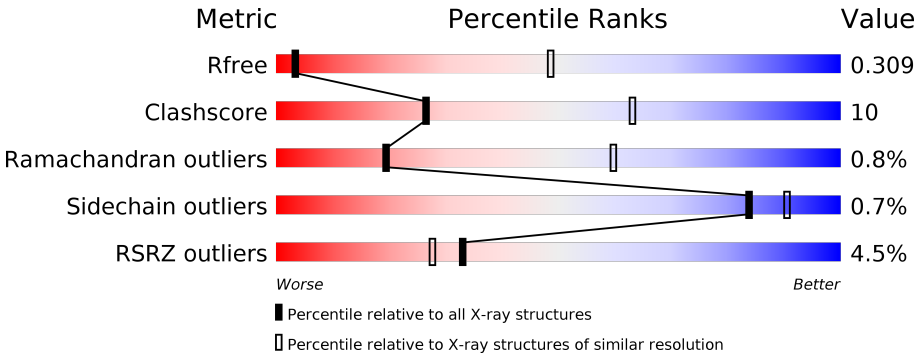
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.30 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	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	481	71% 22% • 5%
1	C	481	2% 68% 25% • 6%
2	B	153	58% 29% 14%
2	D	153	59% 26% • 14%
3	J	210	5% 70% 28% •
3	L	210	5% 69% 31%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	E	223	4% 91% 9%
4	G	223	3% 90% 10%
5	F	212	10% 97%
5	H	212	9% 96%
6	I	235	6% 65% 30%
6	K	235	9% 65% 30%
7	M	7	14% 57% 29%
7	Z	7	86% 14%
8	N	5	60% 40%
8	a	5	60% 40%
9	O	2	50% 50%
9	P	2	100%
9	Q	2	100%
9	T	2	100%
9	V	2	100%
9	W	2	100%
9	X	2	100%
9	b	2	50% 50%
9	c	2	100%
9	d	2	100%
9	f	2	100%
9	g	2	100%
9	i	2	100%
9	j	2	100%
10	R	6	50% 33% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	e	6	50% 50%
11	S	3	33% 67%
11	Y	3	67% 33%
11	k	3	67% 33%
11	l	3	100%
12	U	10	20% 60% 20%
12	h	10	20% 80%
13	m	4	75% 25%

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	BMA	S	3	-	-	-	X
11	NAG	k	2	-	-	-	X
11	BMA	k	3	-	-	-	X
11	NAG	l	2	-	-	-	X
11	BMA	l	3	-	-	-	X
12	MAN	h	10	-	-	-	X
14	NAG	A	942	-	-	-	X
14	NAG	B	902	-	-	-	X
14	NAG	B	903	-	-	-	X
14	NAG	C	909	-	-	-	X
14	NAG	I	305	-	-	-	X
14	NAG	K	301	-	-	-	X
7	MAN	Z	5	-	-	-	X
9	NAG	O	2	-	-	-	X
9	NAG	P	2	-	-	-	X
9	NAG	b	2	-	-	-	X
9	NAG	c	2	-	-	-	X
9	NAG	d	1	-	-	-	X
9	NAG	d	2	-	-	-	X
9	NAG	i	1	-	-	-	X
9	NAG	i	2	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 23938 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 BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3576	2243	632	673	28			
1	C	450	Total	C	N	O	S	0	0	0
			3542	2223	625	666	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	332	ASN	THR	conflict	UNP Q2N0S6
A	501	CYS	ALA	conflict	UNP Q2N0S6
A	509	ARG	GLU	conflict	UNP Q2N0S6
A	510	ARG	LYS	conflict	UNP Q2N0S6
A	512	ARG	-	expression tag	UNP Q2N0S6
A	513	ARG	-	expression tag	UNP Q2N0S6
C	332	ASN	THR	conflict	UNP Q2N0S6
C	501	CYS	ALA	conflict	UNP Q2N0S6
C	509	ARG	GLU	conflict	UNP Q2N0S6
C	510	ARG	LYS	conflict	UNP Q2N0S6
C	512	ARG	-	expression tag	UNP Q2N0S6
C	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 2 is a protein called BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1034	654	178	196	6			
2	D	132	Total	C	N	O	S	0	0	0
			1034	654	178	196	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S6
D	605	CYS	THR	conflict	UNP Q2N0S6

- Molecule 3 is a protein called PGT122 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			
3	J	210	Total	C	N	O	S	0	0	0
			1589	998	267	320	4			

- Molecule 4 is a protein called VRC34.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	223	Total	C	N	O	S	0	0	0
			1674	1054	285	329	6			
4	G	223	Total	C	N	O	S	0	0	0
			1674	1054	285	329	6			

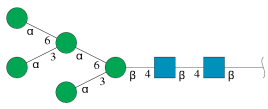
- Molecule 5 is a protein called VRC34.01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	212	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			
5	H	212	Total	C	N	O	S	0	0	0
			1628	1024	274	325	5			

- Molecule 6 is a protein called PGT122 Fab heavy chain.

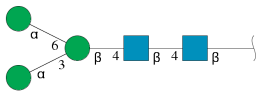
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	I	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			
6	K	228	Total	C	N	O	S	0	0	0
			1742	1109	295	333	5			

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



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

- Molecule 8 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-acetamido-2-deoxy-beta-D-glucopyranose.



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

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

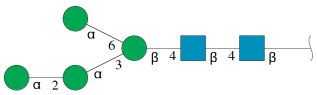
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	O	2	Total C N O 28 16 2 10	0	0	0
9	P	2	Total C N O 28 16 2 10	0	0	0
9	Q	2	Total C N O 28 16 2 10	0	0	0
9	T	2	Total C N O 28 16 2 10	0	0	0
9	V	2	Total C N O 28 16 2 10	0	0	0
9	W	2	Total C N O 28 16 2 10	0	0	0
9	X	2	Total C N O 28 16 2 10	0	0	0
9	b	2	Total C N O 28 16 2 10	0	0	0

Continued on next page...

Continued from previous page...

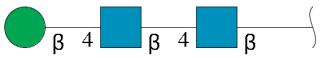
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	c	2	Total C N O 28 16 2 10	0	0	0
9	d	2	Total C N O 28 16 2 10	0	0	0
9	f	2	Total C N O 28 16 2 10	0	0	0
9	g	2	Total C N O 28 16 2 10	0	0	0
9	i	2	Total C N O 28 16 2 10	0	0	0
9	j	2	Total C N O 28 16 2 10	0	0	0

- Molecule 10 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
10	R	6	Total C N O 72 40 2 30	0	0	0
10	e	6	Total C N O 72 40 2 30	0	0	0

- Molecule 11 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



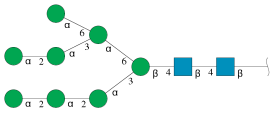
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
11	S	3	Total C N O 39 22 2 15	0	0	0
11	Y	3	Total C N O 39 22 2 15	0	0	0
11	k	3	Total C N O 39 22 2 15	0	0	0

Continued on next page...

Continued from previous page...

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

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

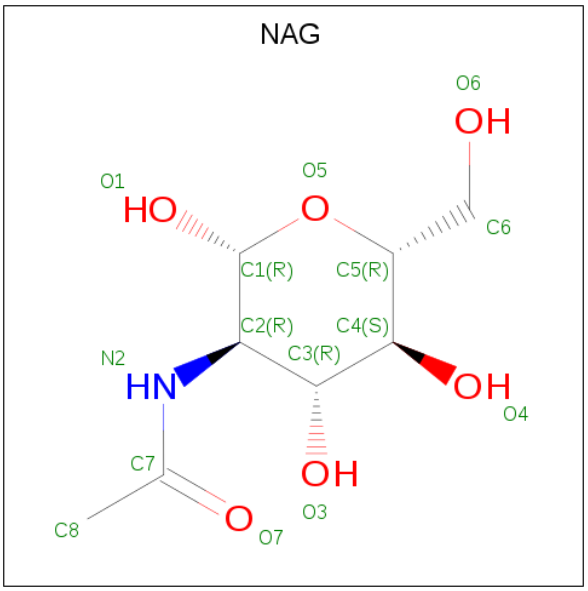


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	U	10	Total C N O 116 64 2 50	0	0	0
12	h	10	Total C N O 116 64 2 50	0	0	0

- Molecule 13 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
13	m	4	Total C N O 50 28 2 20	0	0	0

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

Continued from previous page...

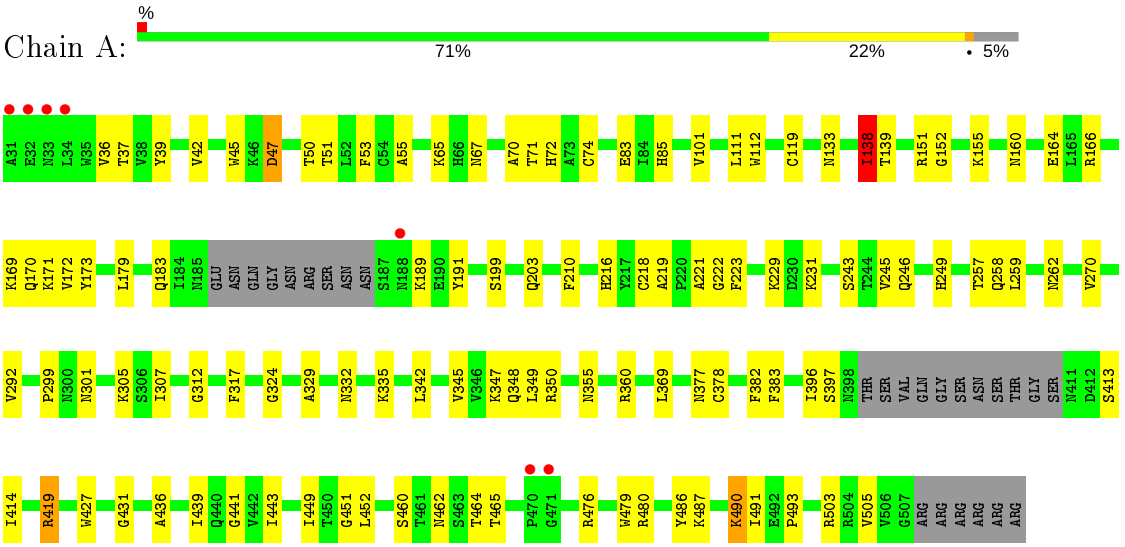
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	I	1	Total	C	N	O	0	0
			14	8	1	5		
14	K	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots (i)

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

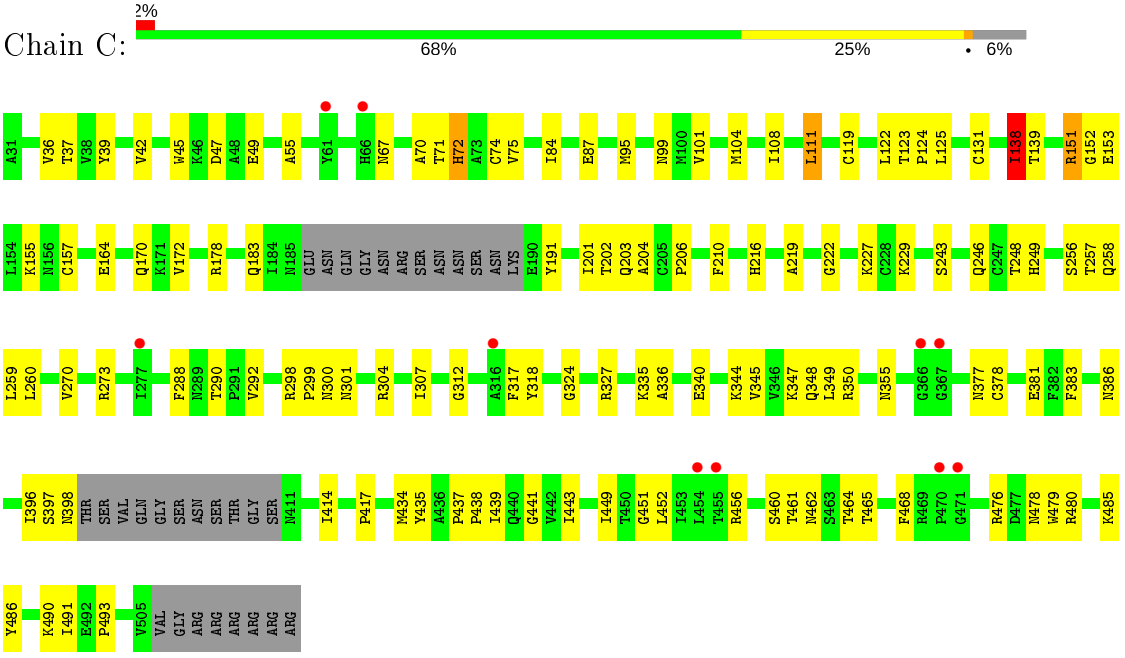
- Molecule 1: BG505 SOSIP.664 gp120

Chain A:



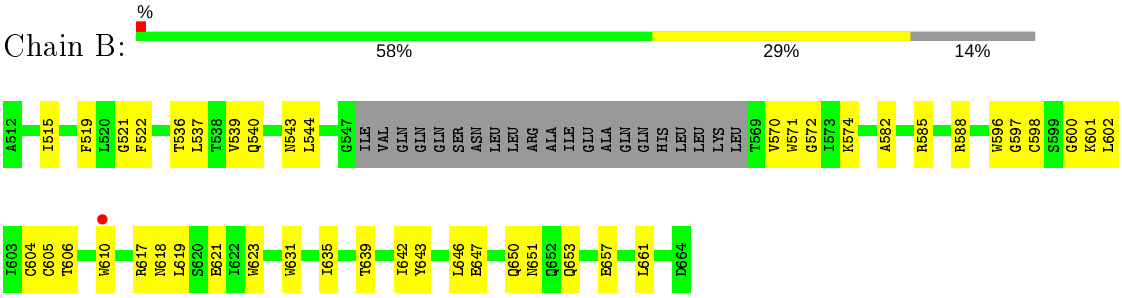
- Molecule 1: BG505 SOSIP.664 gp120

Chain C:



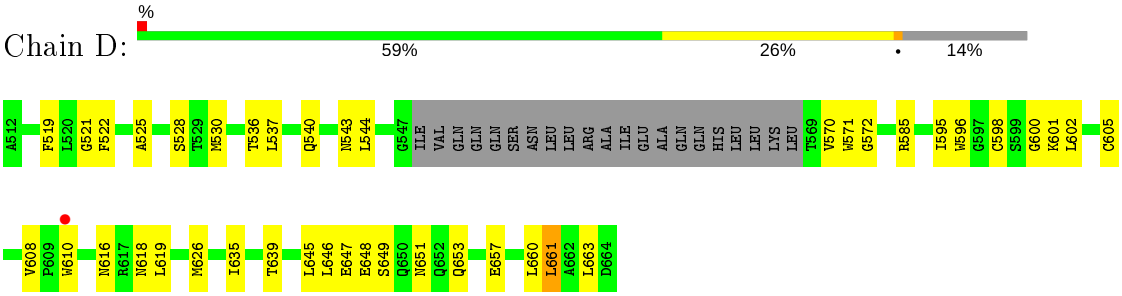
• Molecule 2: BG505 SOSIP.664 gp41

Chain B:



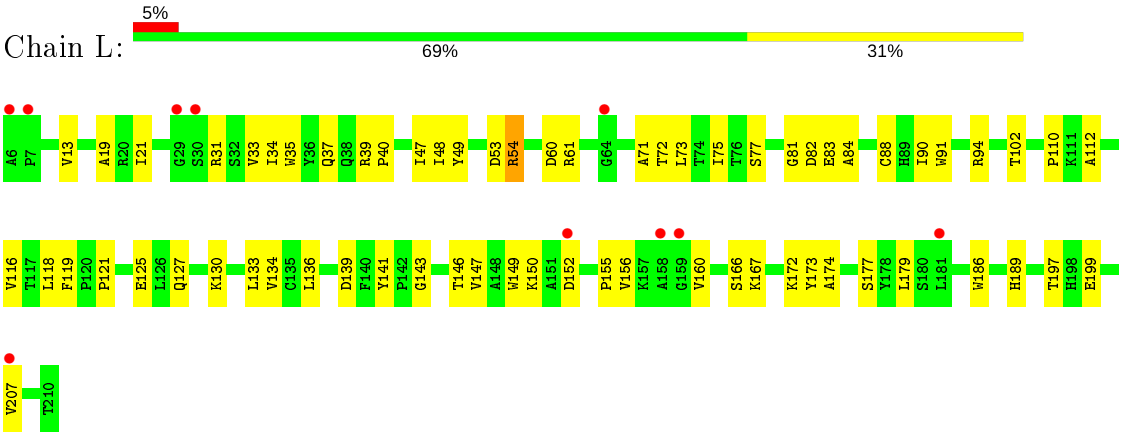
• Molecule 2: BG505 SOSIP.664 gp41

Chain D:



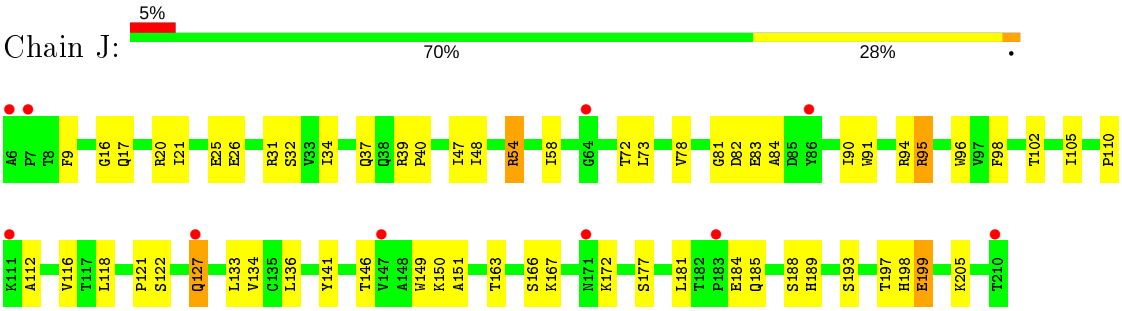
• Molecule 3: PGT122 Fab light chain

Chain L:



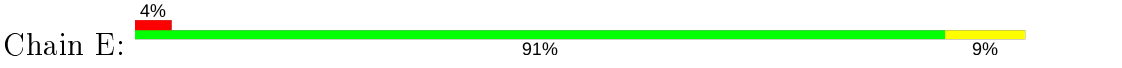
• Molecule 3: PGT122 Fab light chain

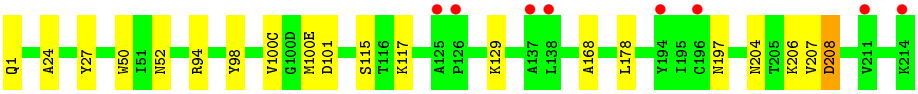
Chain J:



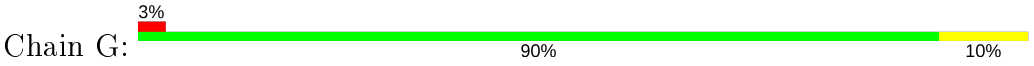
• Molecule 4: VRC34.01 Fab heavy chain

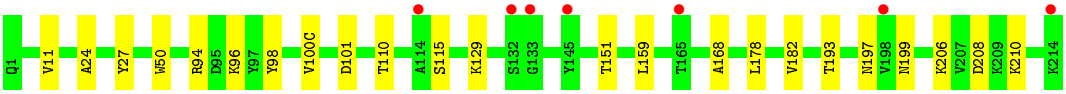
Chain E:



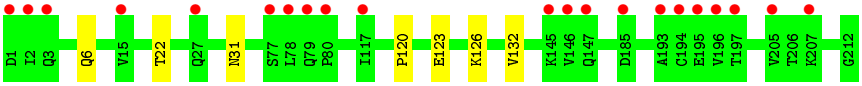


• Molecule 4: VRC34.01 Fab heavy chain

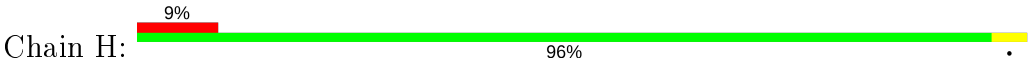




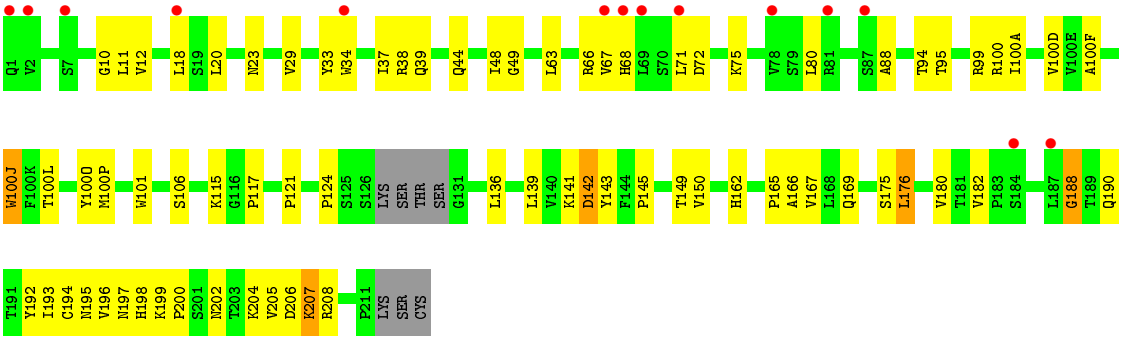
• Molecule 5: VRC34.01 Fab light chain



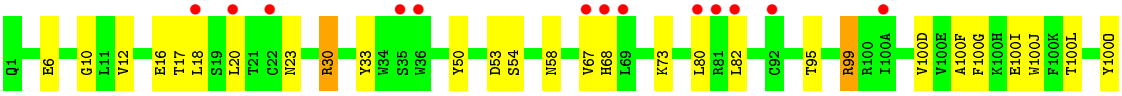
• Molecule 5: VRC34.01 Fab light chain

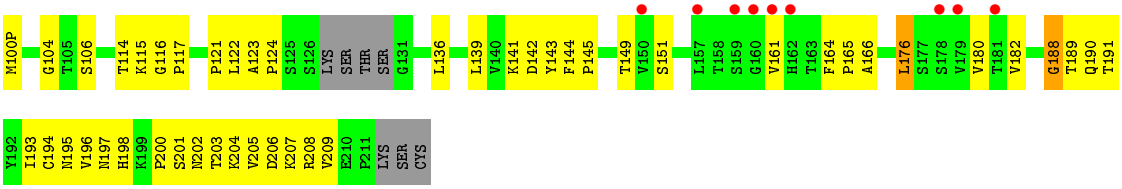


• Molecule 6: PGT122 Fab heavy chain



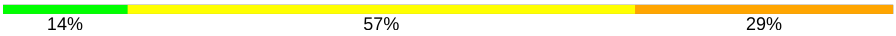
• Molecule 6: PGT122 Fab heavy chain





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

Chain M:



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

Chain Z:

• Molecule 8: 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 8: 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 a:

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

Chain O:

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

Chain P: 100%

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

Chain Q: 100%

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

Chain T: 100%

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

Chain V: 100%

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

Chain W: 100%

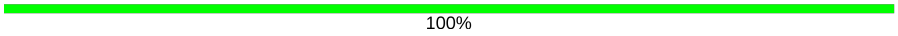
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 100%

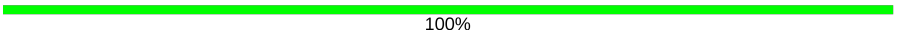
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b: 50% 50%

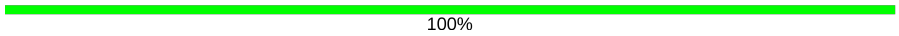
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c: 

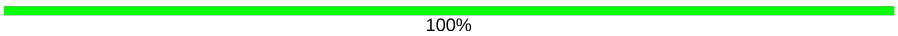
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 

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

Chain f: 

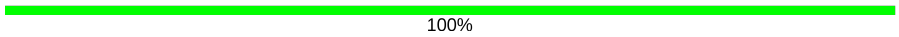
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 

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

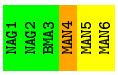
Chain i: 

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

Chain j: 

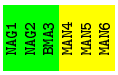
• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



• Molecule 10: 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 e:



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

Chain S:

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

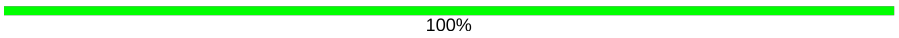
Chain Y:

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

Chain k:

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

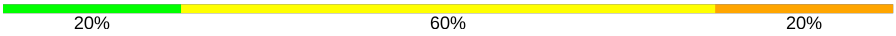
Chain l:



• Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranos

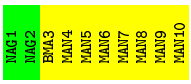
e-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



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

Chain h:



• Molecule 13: 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 m:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	252.30Å 252.30Å 561.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.34 – 4.30 48.34 – 4.30	Depositor EDS
% Data completeness (in resolution range)	54.9 (48.34-4.30) 55.1 (48.34-4.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.74 (at 4.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.281 , 0.309 0.281 , 0.309	Depositor DCC
R_{free} test set	1319 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	127.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 116.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	23938	wwPDB-VP
Average B, all atoms (Å^2)	215.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.8659e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.34	0/3650	0.66	3/4956 (0.1%)
1	C	0.34	0/3616	0.63	2/4911 (0.0%)
2	B	0.33	0/1052	0.59	0/1427
2	D	0.31	0/1052	0.61	1/1427 (0.1%)
3	J	0.36	0/1632	0.64	1/2236 (0.0%)
3	L	0.57	4/1632 (0.2%)	0.62	1/2236 (0.0%)
4	E	0.31	0/1715	0.56	0/2337
4	G	0.28	0/1715	0.50	0/2337
5	F	0.28	0/1665	0.52	0/2262
5	H	0.26	0/1665	0.50	0/2262
6	I	0.32	0/1789	0.65	3/2443 (0.1%)
6	K	0.33	0/1789	0.66	4/2443 (0.2%)
All	All	0.34	4/22972 (0.0%)	0.61	15/31277 (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	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	54	ARG	CZ-NH1	-11.18	1.18	1.33
3	L	54	ARG	NE-CZ	-9.07	1.21	1.33
3	L	54	ARG	CZ-NH2	-7.11	1.23	1.33
3	L	54	ARG	CD-NE	-7.05	1.34	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	176	LEU	CA-CB-CG	9.21	136.48	115.30
1	A	138	ILE	CG1-CB-CG2	-9.11	91.35	111.40
6	K	176	LEU	CA-CB-CG	8.41	134.65	115.30
1	C	138	ILE	CG1-CB-CG2	-8.06	93.68	111.40
1	A	490	LYS	CA-CB-CG	6.53	127.77	113.40
1	A	166	ARG	CA-CB-CG	6.03	126.66	113.40
6	K	23	ASN	N-CA-CB	-5.61	100.50	110.60
6	I	23	ASN	N-CA-CB	-5.50	100.70	110.60
6	K	99	ARG	CG-CD-NE	-5.47	100.32	111.80
6	I	23	ASN	CB-CA-C	5.37	121.15	110.40
2	D	661	LEU	CB-CG-CD2	5.25	119.93	111.00
6	K	30	ARG	NE-CZ-NH1	-5.25	117.67	120.30
3	J	127	GLN	N-CA-CB	-5.22	101.21	110.60
1	C	111	LEU	CB-CG-CD1	-5.18	102.20	111.00
3	L	54	ARG	CG-CD-NE	-5.05	101.19	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	208	ASP	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	3576	0	3509	88	0
1	C	3542	0	3471	90	0
2	B	1034	0	1011	42	0
2	D	1034	0	1012	31	0
3	J	1589	0	1530	55	0
3	L	1589	0	1529	54	0
4	E	1674	0	1638	25	0
4	G	1674	0	1638	20	0
5	F	1628	0	1588	12	0
5	H	1628	0	1588	8	0
6	I	1742	0	1713	59	0
6	K	1742	0	1715	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	M	83	0	69	3	0
7	Z	83	0	70	2	0
8	N	61	0	52	0	0
8	a	61	0	52	0	0
9	O	28	0	25	4	0
9	P	28	0	25	0	0
9	Q	28	0	25	0	0
9	T	28	0	25	0	0
9	V	28	0	25	0	0
9	W	28	0	25	0	0
9	X	28	0	25	0	0
9	b	28	0	25	0	0
9	c	28	0	25	0	0
9	d	28	0	25	0	0
9	f	28	0	25	0	0
9	g	28	0	25	0	0
9	i	28	0	25	0	0
9	j	28	0	25	0	0
10	R	72	0	61	2	0
10	e	72	0	61	0	0
11	S	39	0	34	0	0
11	Y	39	0	34	1	0
11	k	39	0	34	0	0
11	l	39	0	34	0	0
12	U	116	0	97	1	0
12	h	116	0	97	0	0
13	m	50	0	42	0	0
14	A	56	0	52	3	0
14	B	42	0	39	0	0
14	C	70	0	65	1	0
14	D	28	0	26	0	0
14	I	14	0	13	0	0
14	K	14	0	13	0	0
All	All	23938	0	23237	479	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 10.

All (479) 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)
3:L:39:ARG:HD3	3:L:84:ALA:HB2	1.35	1.09
1:C:138:ILE:HG22	1:C:139:THR:HA	1.40	1.04
1:A:490:LYS:HG2	2:B:585:ARG:HH12	1.25	0.95
1:A:138:ILE:HG22	1:A:139:THR:HA	1.48	0.94
1:A:350:ARG:NH2	1:A:396:ILE:O	2.04	0.90
1:A:70:ALA:HB2	1:A:111:LEU:HD11	1.53	0.90
1:C:249:HIS:HD1	1:C:486:TYR:HH	1.21	0.87
3:L:34:ILE:HD13	6:K:100(O):TYR:HB3	1.56	0.87
1:A:249:HIS:HD1	1:A:486:TYR:HH	0.87	0.86
1:C:350:ARG:NH2	1:C:396:ILE:O	2.09	0.85
6:I:99:ARG:HG2	6:I:100(L):THR:HG22	1.59	0.84
6:K:121:PRO:HD3	6:K:207:LYS:HE3	1.59	0.84
3:L:39:ARG:HH12	3:L:82:ASP:C	1.81	0.84
1:A:292:VAL:HB	1:A:449:ILE:HB	1.60	0.83
3:L:127:GLN:NE2	4:E:117:LYS:HB2	1.93	0.83
3:J:39:ARG:HD3	3:J:84:ALA:HB2	1.60	0.82
5:F:126:LYS:NZ	6:K:115:LYS:HB2	1.95	0.81
4:G:210:LYS:HB3	6:I:202:ASN:HD22	1.47	0.79
6:K:30:ARG:HD3	6:K:73:LYS:HD2	1.64	0.79
3:J:54:ARG:NE	3:J:58:ILE:O	2.18	0.76
1:C:70:ALA:HB2	1:C:111:LEU:HD11	1.66	0.76
3:L:54:ARG:NH1	3:L:60:ASP:HA	1.99	0.76
1:A:219:ALA:O	1:A:246:GLN:NE2	2.19	0.76
2:D:570:VAL:HG12	2:D:571:TRP:H	1.50	0.75
2:B:570:VAL:HG12	2:B:571:TRP:H	1.50	0.75
1:A:490:LYS:CG	2:B:585:ARG:HH12	2.00	0.75
1:A:490:LYS:HG2	2:B:585:ARG:NH1	2.00	0.75
1:C:292:VAL:HB	1:C:449:ILE:HB	1.68	0.74
2:B:653:GLN:O	2:B:657:GLU:HG2	1.87	0.73
1:A:55:ALA:HB3	1:A:216:HIS:HB2	1.68	0.73
1:C:55:ALA:HB3	1:C:216:HIS:HB2	1.71	0.73
2:B:596:TRP:HE1	2:B:647:GLU:HG2	1.54	0.72
3:J:9:PHE:HD2	3:J:105:ILE:HD11	1.54	0.72
6:I:162:HIS:CE1	3:J:172:LYS:HZ2	2.07	0.71
2:B:536:THR:O	2:B:540:GLN:NE2	2.23	0.71
6:I:100:ARG:NH2	6:I:100(A):ILE:O	2.23	0.71
3:L:37:GLN:OE1	3:L:39:ARG:NH2	2.23	0.71
1:C:206:PRO:HG3	1:C:318:TYR:HE2	1.55	0.71
1:C:219:ALA:O	1:C:246:GLN:NE2	2.24	0.71
3:L:39:ARG:HG3	3:L:40:PRO:HD2	1.72	0.70
3:J:39:ARG:HG3	3:J:40:PRO:HD2	1.72	0.70
3:L:127:GLN:HE22	4:E:117:LYS:HB2	1.57	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:657:GLU:O	2:D:661:LEU:HG	1.91	0.70
3:J:83:GLU:HG2	3:J:167:LYS:HZ1	1.57	0.70
2:D:653:GLN:O	2:D:657:GLU:HG2	1.93	0.69
3:J:16:GLY:N	3:J:78:VAL:O	2.24	0.69
2:B:597:GLY:HA2	2:B:651:ASN:HD21	1.59	0.68
1:C:101:VAL:HG13	1:C:479:TRP:HB2	1.75	0.68
6:I:142:ASP:OD1	6:I:169:GLN:NE2	2.26	0.68
1:A:47:ASP:OD2	1:A:487:LYS:NZ	2.22	0.67
6:I:193:ILE:HG12	6:I:208:ARG:HB2	1.76	0.67
6:K:161:VAL:HG12	6:K:180:VAL:HG22	1.74	0.67
6:I:198:HIS:CD2	6:I:200:PRO:HD2	2.28	0.67
3:J:25:GLU:OE2	3:J:95:ARG:NH1	2.27	0.67
6:K:196:VAL:O	6:K:205:VAL:N	2.27	0.66
1:C:155:LYS:NZ	1:C:191:TYR:OH	2.19	0.66
3:J:198:HIS:CE1	3:J:199:GLU:HG2	2.31	0.66
3:L:39:ARG:CD	3:L:84:ALA:HB2	2.22	0.66
1:A:179:LEU:HD11	1:A:419:ARG:HG2	1.77	0.66
4:E:206:LYS:O	6:K:205:VAL:HA	1.95	0.65
1:C:123:THR:HG23	1:C:124:PRO:HD3	1.79	0.65
6:K:99:ARG:HG3	6:K:100(L):THR:HG22	1.76	0.65
3:L:39:ARG:NH1	3:L:82:ASP:C	2.49	0.65
3:L:150:LYS:HD3	3:L:155:PRO:HA	1.78	0.64
3:J:83:GLU:HG2	3:J:167:LYS:NZ	2.12	0.64
4:G:206:LYS:HD2	6:I:206:ASP:OD2	1.98	0.63
1:C:299:PRO:O	1:C:300:ASN:ND2	2.32	0.63
4:G:206:LYS:O	6:I:205:VAL:HA	1.99	0.63
1:C:87:GLU:HG2	7:Z:1:NAG:H82	1.80	0.63
1:A:101:VAL:HG13	1:A:479:TRP:HB2	1.81	0.62
2:D:660:LEU:HA	2:D:663:LEU:HD23	1.81	0.62
3:J:83:GLU:OE2	3:J:167:LYS:NZ	2.22	0.62
1:C:417:PRO:HG3	6:K:100(G):PHE:HZ	1.64	0.62
6:I:121:PRO:HD3	6:I:207:LYS:HZ3	1.65	0.62
4:G:98:TYR:HB2	4:G:100(C):VAL:HG21	1.81	0.62
1:A:464:THR:OG1	1:A:465:THR:N	2.33	0.62
4:G:210:LYS:HB3	6:I:202:ASN:ND2	2.15	0.61
6:K:198:HIS:N	6:K:203:THR:O	2.33	0.61
2:D:645:LEU:O	2:D:649:SER:OG	2.17	0.61
1:A:262:ASN:ND2	11:Y:1:NAG:O7	2.33	0.61
3:L:47:ILE:HG22	3:L:48:ILE:HG13	1.81	0.61
1:A:503:ARG:NH2	2:B:597:GLY:HA3	2.16	0.60
3:L:166:SER:OG	6:K:165:PRO:HG3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:139:ASP:H	3:L:172:LYS:HG3	1.65	0.60
5:F:126:LYS:HZ1	6:K:115:LYS:HB2	1.65	0.59
2:B:618:ASN:HB3	2:B:621:GLU:HB2	1.84	0.59
1:A:503:ARG:HH22	2:B:597:GLY:HA3	1.67	0.59
2:D:536:THR:O	2:D:540:GLN:NE2	2.35	0.59
3:L:167:LYS:HG3	3:L:173:TYR:CE2	2.38	0.59
2:B:606:THR:HG22	2:B:650:GLN:HE21	1.68	0.59
3:L:19:ALA:HB3	3:L:75:ILE:HB	1.85	0.59
6:K:188:GLY:HA3	6:K:190:GLN:N	2.17	0.59
1:C:229:LYS:HE3	1:C:243:SER:HB3	1.83	0.59
1:A:67:ASN:HD21	1:A:72:HIS:HB2	1.68	0.59
6:I:188:GLY:HA3	6:I:190:GLN:N	2.17	0.59
2:B:596:TRP:NE1	2:B:647:GLU:HG2	2.18	0.58
1:C:206:PRO:HG3	1:C:318:TYR:CE2	2.38	0.58
6:I:149:THR:OG1	6:I:197:ASN:HB3	2.03	0.58
1:A:39:TYR:HD2	2:B:537:LEU:HD11	1.68	0.58
6:K:139:LEU:HD21	6:K:141:LYS:HB2	1.85	0.58
6:K:53:ASP:OD2	6:K:73:LYS:HD3	2.03	0.58
6:K:6:GLU:OE2	6:K:104:GLY:N	2.36	0.58
1:A:138:ILE:HG22	1:A:139:THR:CA	2.29	0.58
3:L:167:LYS:HG3	3:L:173:TYR:CZ	2.38	0.58
3:L:31:ARG:NH1	3:L:90:ILE:HD12	2.19	0.58
1:C:299:PRO:C	1:C:300:ASN:HD22	2.07	0.57
4:E:206:LYS:HD2	6:K:206:ASP:OD2	2.04	0.57
3:L:54:ARG:HH11	3:L:60:ASP:HA	1.67	0.57
6:I:167:VAL:HB	3:J:163:THR:HG22	1.85	0.57
4:E:208:ASP:OD2	6:K:204:LYS:HB2	2.04	0.57
3:J:184:GLU:O	3:J:188:SER:OG	2.18	0.57
3:L:112:ALA:HB3	3:L:141:TYR:N	2.20	0.57
6:K:117:PRO:HB3	6:K:143:TYR:HB3	1.86	0.57
3:J:112:ALA:HB3	3:J:141:TYR:N	2.20	0.57
2:B:585:ARG:HG3	2:B:588:ARG:HH21	1.69	0.56
5:F:126:LYS:HZ2	6:K:115:LYS:HB2	1.68	0.56
1:C:476:ARG:O	1:C:480:ARG:HG3	2.04	0.56
1:A:138:ILE:CG2	1:A:139:THR:HA	2.29	0.56
1:C:491:ILE:O	2:D:585:ARG:NH2	2.39	0.56
3:J:25:GLU:CD	3:J:95:ARG:HH11	2.09	0.56
1:C:210:PHE:HD2	1:C:377:ASN:HD21	1.53	0.56
6:I:190:GLN:HG3	6:I:192:TYR:CE1	2.41	0.56
3:J:31:ARG:NH1	3:J:90:ILE:HD12	2.21	0.56
3:L:48:ILE:HG12	3:L:54:ARG:HG2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:ARG:O	1:C:153:GLU:N	2.39	0.55
1:C:300:ASN:ND2	1:C:327:ARG:O	2.35	0.55
3:J:47:ILE:HG22	3:J:48:ILE:HG13	1.89	0.55
1:C:227:LYS:HA	1:C:485:LYS:O	2.07	0.55
7:Z:2:NAG:H3	7:Z:2:NAG:H83	1.88	0.55
1:C:336:ALA:O	1:C:340:GLU:HG2	2.06	0.55
4:G:208:ASP:OD2	6:I:204:LYS:HB3	2.06	0.55
2:B:570:VAL:HG12	2:B:571:TRP:N	2.21	0.55
1:C:151:ARG:HH21	1:C:178:ARG:HD2	1.72	0.55
1:C:67:ASN:HD21	1:C:72:HIS:HB2	1.71	0.55
2:D:618:ASN:OD1	2:D:619:LEU:N	2.39	0.55
1:C:45:TRP:HB3	1:C:491:ILE:HD13	1.88	0.54
3:J:39:ARG:HH12	3:J:82:ASP:C	2.10	0.54
14:C:927:NAG:H83	14:C:927:NAG:H3	1.89	0.54
6:K:194:CYS:O	6:K:206:ASP:HA	2.07	0.54
1:A:36:VAL:HG12	2:B:610:TRP:HE3	1.71	0.54
4:E:168:ALA:HA	4:E:178:LEU:HB3	1.90	0.54
6:I:115:LYS:NZ	6:I:142:ASP:HB3	2.21	0.54
7:M:2:NAG:H83	7:M:2:NAG:H3	1.89	0.54
3:L:21:ILE:HB	3:L:73:LEU:HB3	1.90	0.54
3:J:118:LEU:HD12	3:J:134:VAL:O	2.07	0.54
1:C:70:ALA:CB	1:C:111:LEU:HD11	2.35	0.54
1:C:138:ILE:HG22	1:C:139:THR:CA	2.25	0.54
1:C:138:ILE:CG2	1:C:139:THR:HA	2.26	0.54
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.90	0.54
6:I:99:ARG:HD3	6:I:100(J):TRP:CZ3	2.43	0.54
3:J:146:THR:OG1	3:J:197:THR:HB	2.08	0.54
6:I:100(O):TYR:HB3	3:J:34:ILE:HD13	1.90	0.54
1:A:183:GLN:HA	1:A:191:TYR:HA	1.89	0.53
1:A:307:ILE:HD11	1:A:317:PHE:HD2	1.74	0.53
1:A:37:THR:HG22	2:B:605:CYS:HA	1.90	0.53
2:D:570:VAL:HG12	2:D:571:TRP:N	2.21	0.53
1:A:491:ILE:O	2:B:585:ARG:NH2	2.42	0.53
6:I:38:ARG:HB2	6:I:48:ILE:HD11	1.90	0.53
4:E:204:ASN:O	6:K:206:ASP:O	2.26	0.53
14:A:926:NAG:H3	14:A:926:NAG:H83	1.89	0.53
1:C:464:THR:OG1	1:C:465:THR:N	2.42	0.53
6:I:67:VAL:O	6:I:68:HIS:ND1	2.42	0.53
6:I:100(D):VAL:O	6:I:100(F):ALA:N	2.35	0.53
6:K:196:VAL:O	6:K:204:LYS:HA	2.09	0.53
1:A:378:CYS:HB3	1:A:383:PHE:CE1	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:21:ILE:HG23	3:J:102:THR:HB	1.90	0.53
1:A:270:VAL:HG23	1:A:348:GLN:HG3	1.90	0.53
6:K:20:LEU:HD12	6:K:80:LEU:HD22	1.90	0.53
3:J:112:ALA:HB3	3:J:141:TYR:H	1.74	0.53
2:B:515:ILE:HG23	4:E:52:ASN:HB2	1.91	0.52
1:C:36:VAL:HG21	2:D:646:LEU:HD21	1.91	0.52
6:I:121:PRO:HD3	6:I:207:LYS:NZ	2.25	0.52
2:D:530:MET:HG3	2:D:626:MET:O	2.09	0.52
6:I:34:TRP:CZ3	6:I:94:THR:HG22	2.44	0.52
9:O:2:NAG:H83	9:O:2:NAG:H3	1.89	0.52
2:B:618:ASN:OD1	2:B:619:LEU:N	2.43	0.52
6:K:100(D):VAL:O	6:K:100(F):ALA:N	2.36	0.52
3:L:118:LEU:HD12	3:L:134:VAL:O	2.10	0.52
3:L:47:ILE:HD12	3:L:47:ILE:N	2.25	0.52
1:A:347:LYS:HD2	1:A:350:ARG:HH12	1.74	0.51
1:A:67:ASN:ND2	1:A:72:HIS:HB2	2.25	0.51
2:D:596:TRP:CD1	2:D:647:GLU:HB3	2.45	0.51
3:L:143:GLY:HA3	3:L:173:TYR:CD2	2.46	0.51
9:O:1:NAG:H62	9:O:2:NAG:H82	1.91	0.51
1:A:85:HIS:HB3	4:E:27:TYR:HA	1.93	0.51
6:I:166:ALA:N	6:I:176:LEU:HD23	2.26	0.51
5:H:126:LYS:NZ	6:I:115:LYS:HB2	2.25	0.51
6:K:198:HIS:ND1	6:K:200:PRO:HD2	2.26	0.51
6:I:44:GLN:HG3	3:J:98:PHE:O	2.11	0.51
2:D:598:CYS:O	2:D:600:GLY:N	2.43	0.51
2:B:570:VAL:C	2:B:572:GLY:H	2.14	0.50
6:K:149:THR:OG1	6:K:197:ASN:HB3	2.11	0.50
1:A:210:PHE:HD2	1:A:377:ASN:HD21	1.57	0.50
1:C:396:ILE:HG22	1:C:398:ASN:H	1.76	0.50
1:C:386:ASN:HB3	1:C:417:PRO:HD2	1.93	0.50
1:C:201:ILE:HD11	1:C:435:TYR:HB2	1.94	0.50
1:A:332:ASN:HB3	1:A:413:SER:OG	2.11	0.50
1:A:45:TRP:HA	1:A:490:LYS:O	2.12	0.50
1:C:439:ILE:HB	1:C:443:ILE:HD11	1.93	0.50
1:A:179:LEU:CD1	1:A:419:ARG:HG2	2.40	0.50
2:D:608:VAL:HG21	2:D:646:LEU:HD23	1.93	0.50
6:I:180:VAL:HG12	6:I:182:VAL:HG13	1.93	0.50
6:I:199:LYS:HB2	6:I:200:PRO:HD3	1.93	0.50
3:J:83:GLU:CD	3:J:167:LYS:HZ2	2.11	0.50
6:K:194:CYS:SG	6:K:207:LYS:HB3	2.52	0.50
6:I:117:PRO:HB3	6:I:143:TYR:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:VAL:O	1:A:349:LEU:HG	2.12	0.49
2:B:598:CYS:O	2:B:600:GLY:N	2.44	0.49
1:A:171:LYS:NZ	9:O:1:NAG:HN2	2.10	0.49
1:C:298:ARG:NH2	1:C:439:ILE:O	2.45	0.49
1:C:476:ARG:HA	1:C:479:TRP:CD1	2.47	0.49
5:F:123:GLU:HG3	6:K:115:LYS:HA	1.93	0.49
6:K:10:GLY:HA2	6:K:106:SER:O	2.11	0.49
3:L:13:VAL:HG21	3:L:19:ALA:HA	1.94	0.49
1:C:350:ARG:HD3	1:C:355:ASN:O	2.11	0.49
1:C:183:GLN:HA	1:C:191:TYR:HA	1.95	0.49
1:C:67:ASN:ND2	1:C:72:HIS:HB2	2.27	0.49
3:L:61:ARG:HD2	3:L:77:SER:HB3	1.95	0.49
1:C:260:LEU:HD12	1:C:451:GLY:HA3	1.94	0.49
4:E:208:ASP:OD2	6:K:204:LYS:HD2	2.13	0.49
3:L:37:GLN:HB3	3:L:47:ILE:HD11	1.95	0.49
4:G:197:ASN:ND2	4:G:208:ASP:OD1	2.30	0.49
2:B:619:LEU:HD12	2:B:623:TRP:CD1	2.48	0.49
1:A:382:PHE:HE2	1:A:436:ALA:HB2	1.78	0.49
1:A:42:VAL:HG22	1:A:493:PRO:O	2.13	0.48
1:A:133:ASN:HD22	14:A:908:NAG:C7	2.25	0.48
1:A:36:VAL:HG12	2:B:610:TRP:CE3	2.47	0.48
1:C:460:SER:HA	1:C:461:THR:CG2	2.42	0.48
4:G:129:LYS:HD2	4:G:129:LYS:N	2.28	0.48
1:C:288:PHE:HE2	1:C:449:ILE:HG22	1.78	0.48
3:J:116:VAL:HG23	3:J:205:LYS:HE2	1.94	0.48
1:A:85:HIS:CB	4:E:27:TYR:HA	2.43	0.48
6:I:63:LEU:HD22	6:I:66:ARG:HH21	1.78	0.48
2:B:642:ILE:O	2:B:646:LEU:HG	2.12	0.48
1:C:324:GLY:O	3:L:94:ARG:HD2	2.13	0.48
1:C:39:TYR:HD2	2:D:537:LEU:HD11	1.79	0.48
1:C:460:SER:HB2	1:C:462:ASN:HB2	1.95	0.48
6:K:6:GLU:OE1	6:K:6:GLU:N	2.46	0.48
3:L:121:PRO:HD3	3:L:133:LEU:HD23	1.94	0.48
1:A:173:TYR:CZ	1:A:305:LYS:NZ	2.82	0.48
1:C:164:GLU:HG3	1:C:312:GLY:HA3	1.96	0.48
4:E:98:TYR:HB2	4:E:100(C):VAL:HG21	1.94	0.48
6:K:6:GLU:CD	6:K:104:GLY:H	2.16	0.48
1:C:490:LYS:HB2	2:D:585:ARG:HH12	1.79	0.48
6:I:162:HIS:CG	3:J:172:LYS:HZ2	2.31	0.48
1:C:122:LEU:HD13	1:C:125:LEU:HD11	1.96	0.48
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:31:ASN:HD21	7:M:4:MAN:H2	1.79	0.48
1:C:460:SER:HA	1:C:461:THR:HG22	1.96	0.48
3:L:21:ILE:O	3:L:72:THR:HA	2.14	0.48
1:C:122:LEU:HB3	1:C:125:LEU:CD1	2.44	0.47
1:C:204:ALA:HB2	1:C:434:MET:SD	2.53	0.47
3:L:156:VAL:HG11	3:L:179:LEU:HD11	1.96	0.47
1:A:65:LYS:HG3	10:R:4:MAN:O4	2.14	0.47
6:K:166:ALA:N	6:K:176:LEU:HD23	2.29	0.47
1:A:50:THR:HB	1:A:223:PHE:CE2	2.49	0.47
1:A:164:GLU:HG3	1:A:312:GLY:HA3	1.96	0.47
1:C:304:ARG:NH2	1:C:437:PRO:HB2	2.29	0.47
4:E:129:LYS:HA	4:E:129:LYS:HE3	1.96	0.47
4:E:1:GLN:N	4:E:1:GLN:CD	2.68	0.47
2:B:519:PHE:CE2	2:B:521:GLY:HA2	2.50	0.47
5:H:37:GLN:HB2	5:H:47:LEU:HD11	1.96	0.47
3:J:37:GLN:OE1	3:J:39:ARG:NH2	2.47	0.47
3:L:34:ILE:HG23	3:L:49:TYR:HA	1.96	0.47
1:A:439:ILE:HB	1:A:443:ILE:HD11	1.96	0.47
1:C:151:ARG:O	1:C:178:ARG:NH2	2.48	0.47
1:C:456:ARG:HD3	1:C:468:PHE:HE1	1.80	0.47
3:L:133:LEU:HD12	3:L:179:LEU:HD23	1.96	0.47
1:A:301:ASN:OD1	1:A:441:GLY:HA2	2.14	0.47
1:C:347:LYS:HD3	1:C:350:ARG:NH1	2.29	0.47
3:L:33:VAL:HG11	3:L:71:ALA:HB1	1.97	0.47
1:C:256:SER:O	1:C:478:ASN:ND2	2.46	0.46
6:I:11:LEU:HD12	6:I:145:PRO:HD3	1.97	0.46
4:G:115:SER:HB2	3:J:127:GLN:HG2	1.96	0.46
5:F:126:LYS:HZ1	6:K:115:LYS:CA	2.28	0.46
6:I:12:VAL:HG21	6:I:18:LEU:HD13	1.96	0.46
6:K:180:VAL:HG12	6:K:182:VAL:HG13	1.97	0.46
1:A:396:ILE:HG22	1:A:397:SER:H	1.80	0.46
1:C:36:VAL:HG12	2:D:610:TRP:HE3	1.81	0.46
6:I:196:VAL:O	6:I:205:VAL:N	2.40	0.46
3:J:21:ILE:O	3:J:72:THR:HA	2.14	0.46
1:A:257:THR:O	1:A:259:LEU:N	2.47	0.46
3:L:39:ARG:HH11	3:L:83:GLU:C	2.19	0.46
6:K:121:PRO:HD3	6:K:207:LYS:CE	2.39	0.46
1:A:222:GLY:HA2	2:B:544:LEU:HD12	1.97	0.46
6:I:72:ASP:OD2	6:I:75:LYS:HD2	2.16	0.46
6:I:139:LEU:HD21	6:I:141:LYS:HB2	1.98	0.46
6:I:196:VAL:O	6:I:204:LYS:HA	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HG2	1:A:172:VAL:HG13	1.97	0.45
5:F:123:GLU:OE2	6:K:116:GLY:N	2.46	0.45
4:G:24:ALA:HB1	4:G:27:TYR:CE1	2.51	0.45
1:A:490:LYS:HG2	2:B:585:ARG:HH22	1.82	0.45
1:A:189:LYS:HE3	14:A:908:NAG:H82	1.97	0.45
2:D:570:VAL:C	2:D:572:GLY:H	2.20	0.45
1:C:335:LYS:HA	1:C:414:ILE:HD11	1.98	0.45
2:D:519:PHE:CE2	2:D:521:GLY:HA2	2.51	0.45
2:D:522:PHE:CD1	2:D:543:ASN:HB2	2.52	0.45
6:K:196:VAL:N	6:K:205:VAL:O	2.37	0.45
1:A:299:PRO:HD2	1:A:329:ALA:HA	1.97	0.45
5:F:126:LYS:HZ1	6:K:115:LYS:CB	2.28	0.45
3:L:127:GLN:OE1	4:E:115:SER:O	2.35	0.45
4:E:197:ASN:ND2	4:E:208:ASP:OD1	2.35	0.45
6:K:144:PHE:HA	6:K:145:PRO:HA	1.77	0.45
2:B:635:ILE:O	2:B:639:THR:HG23	2.16	0.45
6:K:16:GLU:HG2	6:K:17:THR:H	1.82	0.45
6:I:33:TYR:HB2	6:I:95:THR:O	2.16	0.45
5:F:123:GLU:HA	5:F:126:LYS:HE2	1.98	0.45
1:A:179:LEU:HD22	1:A:369:LEU:HD22	1.99	0.45
1:C:95:MET:SD	1:C:273:ARG:HD3	2.57	0.45
5:H:126:LYS:HZ2	6:I:115:LYS:HB2	1.81	0.45
6:K:67:VAL:O	6:K:68:HIS:ND1	2.50	0.45
6:K:18:LEU:HB3	6:K:82:LEU:HB3	1.98	0.45
1:A:83:GLU:HG2	1:A:245:VAL:CG1	2.48	0.44
1:C:301:ASN:OD1	1:C:441:GLY:HA2	2.16	0.44
2:B:631:TRP:CE2	2:B:635:ILE:HG13	2.52	0.44
3:J:181:LEU:HD22	3:J:185:GLN:HG2	1.99	0.44
6:K:191:THR:HG22	6:K:193:ILE:HG13	1.98	0.44
1:C:257:THR:O	1:C:259:LEU:N	2.48	0.44
1:C:49:GLU:OE2	1:C:99:ASN:HB2	2.17	0.44
4:E:208:ASP:O	6:K:202:ASN:O	2.36	0.44
3:L:49:TYR:O	3:L:53:ASP:HB2	2.17	0.44
2:B:631:TRP:O	2:B:635:ILE:HG12	2.17	0.44
1:C:202:THR:O	1:C:434:MET:HA	2.18	0.44
1:C:37:THR:HG22	2:D:605:CYS:HA	1.99	0.44
3:J:116:VAL:HA	3:J:136:LEU:O	2.18	0.44
3:L:116:VAL:HA	3:L:136:LEU:O	2.18	0.44
2:B:522:PHE:CE1	2:B:543:ASN:HB2	2.53	0.44
1:C:378:CYS:HB3	1:C:383:PHE:CE1	2.52	0.44
5:F:31:ASN:ND2	7:M:4:MAN:H2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:151:THR:OG1	4:G:199:ASN:HB2	2.18	0.44
4:G:96:LYS:HE2	5:H:49:TYR:CE2	2.53	0.44
6:K:100(D):VAL:HG22	6:K:100(I):GLU:OE1	2.18	0.44
1:C:42:VAL:HG22	1:C:493:PRO:O	2.18	0.44
2:D:651:ASN:HD22	2:D:651:ASN:N	2.15	0.44
3:J:150:LYS:HB2	3:J:193:SER:OG	2.18	0.44
3:L:119:PHE:HB3	6:K:122:LEU:HD22	2.00	0.44
1:C:222:GLY:HA2	2:D:544:LEU:HD12	1.99	0.44
3:J:151:ALA:HB1	3:J:189:HIS:CD2	2.51	0.44
1:A:221:ALA:HB3	2:B:582:ALA:HB1	2.00	0.44
2:B:574:LYS:HD2	2:B:574:LYS:HA	1.83	0.44
2:B:619:LEU:HD12	2:B:623:TRP:HD1	1.82	0.44
5:H:123:GLU:HA	5:H:126:LYS:HE2	1.99	0.44
4:E:129:LYS:N	4:E:129:LYS:HD2	2.33	0.43
6:I:100(P):MET:SD	6:I:100(P):MET:N	2.91	0.43
3:J:20:ARG:HA	3:J:73:LEU:O	2.18	0.43
3:J:32:SER:HB3	3:J:91:TRP:HB2	2.00	0.43
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.85	0.43
2:B:536:THR:HG22	2:B:539:VAL:HB	2.01	0.43
4:E:24:ALA:HB1	4:E:27:TYR:CE1	2.54	0.43
6:I:49:GLY:HA2	3:J:96:TRP:CZ3	2.53	0.43
6:I:49:GLY:HA2	3:J:96:TRP:HZ3	1.82	0.43
6:K:136:LEU:HG	6:K:209:VAL:HG11	2.00	0.43
4:E:94:ARG:NH2	4:E:101:ASP:OD2	2.28	0.43
4:G:94:ARG:NH2	4:G:101:ASP:OD2	2.38	0.43
6:K:50:TYR:CE1	6:K:58:ASN:HB3	2.54	0.43
3:L:31:ARG:HA	3:L:91:TRP:O	2.17	0.43
1:C:270:VAL:HG23	1:C:348:GLN:HG3	2.00	0.43
4:G:168:ALA:HA	4:G:178:LEU:HB3	2.00	0.43
6:I:145:PRO:HD2	6:I:200:PRO:CB	2.48	0.43
6:I:20:LEU:HD12	6:I:80:LEU:HD22	2.01	0.43
4:E:204:ASN:HB3	6:K:208:ARG:H	1.83	0.43
6:I:165:PRO:HG3	3:J:166:SER:OG	2.18	0.43
6:I:194:CYS:O	6:I:206:ASP:HA	2.19	0.43
6:K:33:TYR:HB2	6:K:95:THR:O	2.17	0.43
1:A:324:GLY:O	3:J:94:ARG:HD2	2.19	0.43
3:L:149:TRP:CD1	3:L:160:VAL:HG12	2.53	0.43
1:A:65:LYS:HE3	10:R:4:MAN:O3	2.19	0.43
4:G:11:VAL:HG22	4:G:110:THR:HB	1.99	0.43
3:J:17:GLN:O	3:J:78:VAL:HG23	2.18	0.43
3:L:54:ARG:HH12	3:L:60:ASP:HA	1.80	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:GLY:O	1:A:452:LEU:HD23	2.18	0.43
3:L:119:PHE:CD1	6:K:122:LEU:HB3	2.54	0.43
6:K:188:GLY:HA3	6:K:189:THR:C	2.38	0.43
6:K:114:THR:HG22	6:K:201:SER:OG	2.18	0.43
1:C:119:CYS:HB3	1:C:203:GLN:O	2.19	0.43
3:J:105:ILE:HD12	3:J:105:ILE:N	2.33	0.43
3:L:174:ALA:HB1	6:K:164:PHE:CD2	2.54	0.43
1:A:50:THR:OG1	1:A:51:THR:N	2.52	0.43
1:C:170:GLN:HG2	1:C:172:VAL:HG13	2.00	0.43
5:F:120:PRO:HD3	5:F:132:VAL:HG22	2.01	0.43
6:K:151:SER:OG	6:K:195:ASN:HB2	2.19	0.43
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.54	0.43
1:A:169:LYS:HE2	1:A:169:LYS:HB2	1.82	0.42
3:J:121:PRO:HD3	3:J:133:LEU:CD2	2.49	0.42
3:J:54:ARG:CZ	3:J:58:ILE:O	2.66	0.42
2:D:635:ILE:O	2:D:639:THR:HG23	2.19	0.42
3:J:149:TRP:HE1	3:J:177:SER:HG	1.67	0.42
3:L:21:ILE:HG23	3:L:102:THR:HB	2.00	0.42
3:L:39:ARG:CZ	3:L:81:GLY:O	2.67	0.42
1:A:223:PHE:CD1	1:A:223:PHE:N	2.87	0.42
1:A:223:PHE:HD1	1:A:223:PHE:N	2.18	0.42
1:A:350:ARG:HD3	1:A:355:ASN:O	2.19	0.42
3:J:54:ARG:NH2	3:J:58:ILE:O	2.53	0.42
3:J:31:ARG:HA	3:J:91:TRP:O	2.19	0.42
2:D:525:ALA:HB1	2:D:528:SER:HB2	2.01	0.42
6:I:37:ILE:HD13	6:I:101:TRP:CZ3	2.54	0.42
3:L:147:VAL:HG11	3:L:177:SER:OG	2.19	0.42
1:A:476:ARG:O	1:A:480:ARG:HG3	2.19	0.42
1:C:437:PRO:HA	1:C:438:PRO:HD3	1.96	0.42
3:L:112:ALA:HB3	3:L:141:TYR:H	1.83	0.42
3:L:125:GLU:HG3	3:L:130:LYS:O	2.20	0.42
3:L:146:THR:OG1	3:L:197:THR:HB	2.19	0.42
3:L:186:TRP:HH2	3:L:207:VAL:HG22	1.84	0.42
1:A:169:LYS:HD3	1:A:169:LYS:H	1.85	0.42
2:B:522:PHE:CD1	2:B:543:ASN:HB2	2.55	0.42
1:A:229:LYS:O	4:E:1:GLN:HG2	2.20	0.42
6:I:162:HIS:CG	3:J:172:LYS:NZ	2.88	0.42
3:L:152:ASP:OD1	3:L:189:HIS:HB3	2.20	0.42
1:A:160:ASN:HD22	9:O:1:NAG:H83	1.85	0.42
1:A:229:LYS:HE3	1:A:243:SER:OG	2.18	0.42
1:C:67:ASN:OD1	1:C:72:HIS:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:47:LEU:HA	5:H:58:VAL:HG21	2.02	0.42
6:I:115:LYS:HZ2	6:I:142:ASP:HB3	1.84	0.42
1:A:347:LYS:HD2	1:A:350:ARG:NH1	2.35	0.41
1:C:349:LEU:HD13	1:C:468:PHE:CE2	2.55	0.41
2:D:522:PHE:CE1	2:D:543:ASN:HB2	2.55	0.41
6:K:198:HIS:O	6:K:202:ASN:N	2.53	0.41
4:E:207:VAL:HG13	6:K:203:THR:HG23	2.01	0.41
1:C:307:ILE:HD11	1:C:317:PHE:HD2	1.85	0.41
1:C:206:PRO:CG	1:C:318:TYR:HE2	2.30	0.41
6:K:12:VAL:HG21	6:K:18:LEU:HD13	2.02	0.41
4:G:159:LEU:HD21	4:G:182:VAL:HG21	2.01	0.41
1:A:335:LYS:HG2	1:A:414:ILE:CG1	2.50	0.41
1:C:216:HIS:ND1	1:C:248:THR:O	2.40	0.41
6:I:10:GLY:HA2	6:I:106:SER:O	2.20	0.41
3:J:39:ARG:CZ	3:J:81:GLY:O	2.69	0.41
1:C:104:MET:O	1:C:108:ILE:HG12	2.21	0.41
1:C:451:GLY:O	1:C:452:LEU:HD23	2.21	0.41
1:C:55:ALA:HA	1:C:75:VAL:O	2.20	0.41
6:K:100(P):MET:SD	6:K:100(P):MET:N	2.94	0.41
1:A:199:SER:HB2	1:A:431:GLY:HA2	2.03	0.41
1:A:53:PHE:CZ	1:A:218:CYS:HB2	2.56	0.41
1:C:131:CYS:HA	1:C:157:CYS:HA	2.02	0.41
4:G:96:LYS:HE2	5:H:49:TYR:CZ	2.55	0.41
6:K:197:ASN:OD1	6:K:198:HIS:N	2.53	0.41
1:A:53:PHE:CE2	1:A:218:CYS:HB2	2.56	0.41
1:A:222:GLY:C	1:A:223:PHE:HD1	2.24	0.41
1:C:345:VAL:O	1:C:349:LEU:HG	2.21	0.41
5:F:6:GLN:HA	5:F:22:THR:O	2.20	0.41
6:I:188:GLY:HA3	6:I:190:GLN:H	1.84	0.41
3:J:39:ARG:NH1	3:J:81:GLY:O	2.54	0.41
1:A:307:ILE:HD11	1:A:317:PHE:CD2	2.54	0.41
1:A:460:SER:HB3	1:A:462:ASN:CA	2.51	0.41
1:C:101:VAL:HG21	1:C:480:ARG:HG2	2.01	0.41
6:I:29:VAL:CG1	6:I:71:LEU:HD22	2.50	0.41
3:J:25:GLU:CG	3:J:26:GLU:N	2.84	0.41
1:A:382:PHE:CE2	1:A:436:ALA:HB2	2.56	0.41
1:C:298:ARG:NH1	1:C:381:GLU:OE2	2.49	0.41
2:D:595:ILE:HD12	2:D:647:GLU:OE2	2.21	0.41
4:G:115:SER:CB	3:J:127:GLN:HG2	2.51	0.41
6:I:39:GLN:C	6:I:88:ALA:HB1	2.40	0.41
12:U:8:MAN:H2	12:U:9:MAN:H2	1.81	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:CYS:HB2	2:D:571:TRP:CH2	2.55	0.41
2:B:657:GLU:O	2:B:661:LEU:HG	2.20	0.40
1:C:84:ILE:HD13	2:D:522:PHE:N	2.36	0.40
6:K:123:ALA:HA	6:K:124:PRO:HD3	1.97	0.40
1:A:112:TRP:CD2	1:A:427:TRP:HZ3	2.39	0.40
1:C:290:THR:OG1	1:C:344:LYS:NZ	2.54	0.40
1:C:490:LYS:HB2	2:D:585:ARG:NH1	2.36	0.40
4:E:208:ASP:O	6:K:203:THR:HA	2.22	0.40
6:I:115:LYS:HZ3	6:I:142:ASP:HB3	1.87	0.40
6:I:150:VAL:HA	6:I:195:ASN:O	2.21	0.40
4:G:115:SER:HB3	3:J:127:GLN:CD	2.42	0.40
2:B:643:TYR:O	2:B:647:GLU:HG3	2.21	0.40
4:G:193:THR:HG23	4:G:210:LYS:HE3	2.03	0.40
6:I:121:PRO:O	3:J:122:SER:HB3	2.21	0.40
6:I:124:PRO:HG3	6:I:136:LEU:HD12	2.04	0.40
6:I:162:HIS:ND1	3:J:172:LYS:NZ	2.70	0.40
6:K:151:SER:O	6:K:195:ASN:N	2.34	0.40
1:A:155:LYS:HD3	1:A:155:LYS:HA	1.88	0.40
1:A:119:CYS:HB3	1:A:203:GLN:O	2.22	0.40
1:A:112:TRP:CG	1:A:427:TRP:HZ3	2.39	0.40
1:A:74:CYS:HB2	2:B:571:TRP:CH2	2.56	0.40
2:B:536:THR:O	2:B:536:THR:HG22	2.21	0.40
2:D:616:ASN:OD1	2:D:616:ASN:N	2.54	0.40
4:E:94:ARG:O	4:E:100(E):MET:HA	2.21	0.40
5:H:115:VAL:HA	5:H:135:LEU:O	2.21	0.40
6:K:53:ASP:OD1	6:K:54:SER:N	2.44	0.40
1:C:396:ILE:CG2	1:C:397:SER:N	2.84	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	449/481 (93%)	405 (90%)	38 (8%)	6 (1%)	12	48
1	C	444/481 (92%)	402 (90%)	37 (8%)	5 (1%)	14	52
2	B	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	9	45
2	D	128/153 (84%)	113 (88%)	13 (10%)	2 (2%)	9	45
3	J	208/210 (99%)	194 (93%)	12 (6%)	2 (1%)	15	54
3	L	208/210 (99%)	194 (93%)	12 (6%)	2 (1%)	15	54
4	E	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
4	G	221/223 (99%)	218 (99%)	3 (1%)	0	100	100
5	F	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
5	H	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
6	I	224/235 (95%)	213 (95%)	9 (4%)	2 (1%)	17	56
6	K	224/235 (95%)	212 (95%)	10 (4%)	2 (1%)	17	56
All	All	2875/3028 (95%)	2691 (94%)	161 (6%)	23 (1%)	19	60

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	ILE
1	C	138	ILE
3	L	110	PRO
3	J	110	PRO
1	A	71	THR
1	C	71	THR
1	A	151	ARG
1	A	152	GLY
2	B	602	LEU
1	C	152	GLY
2	D	602	LEU
1	A	258	GLN
1	C	151	ARG
1	C	258	GLN
3	L	199	GLU
6	K	142	ASP
2	B	601	LYS
2	D	601	LYS
6	I	142	ASP
3	J	199	GLU
1	A	505	VAL
6	K	188	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	I	188	GLY

5.3.2 Protein sidechains

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	405/428 (95%)	401 (99%)	4 (1%)	76 86
1	C	401/428 (94%)	399 (100%)	2 (0%)	88 93
2	B	110/129 (85%)	108 (98%)	2 (2%)	59 77
2	D	110/129 (85%)	109 (99%)	1 (1%)	78 88
3	J	178/178 (100%)	176 (99%)	2 (1%)	73 85
3	L	178/178 (100%)	178 (100%)	0	100 100
4	E	187/187 (100%)	186 (100%)	1 (0%)	88 93
4	G	187/187 (100%)	186 (100%)	1 (0%)	88 93
5	F	185/185 (100%)	185 (100%)	0	100 100
5	H	185/185 (100%)	184 (100%)	1 (0%)	88 93
6	I	198/205 (97%)	195 (98%)	3 (2%)	65 80
6	K	198/205 (97%)	197 (100%)	1 (0%)	88 93
All	All	2522/2624 (96%)	2504 (99%)	18 (1%)	84 90

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ASP
1	A	231	LYS
1	A	360	ARG
1	A	419	ARG
2	B	604	CYS
2	B	617	ARG
1	C	47	ASP
1	C	72	HIS
4	E	50	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	G	50	TRP
2	D	648	GLU
5	H	33	LEU
6	I	100(J)	TRP
6	I	175	SER
6	I	207	LYS
3	J	54	ARG
3	J	95	ARG
6	K	100(J)	TRP

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

Mol	Chain	Res	Type
2	B	650	GLN
2	B	651	ASN
1	C	195	ASN
6	I	202	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

100 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	M	1	1,7	14,14,15	0.33	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	NAG	M	2	7	14,14,15	0.50	0	17,19,21	1.35	2 (11%)
7	BMA	M	3	7	11,11,12	0.66	0	15,15,17	0.91	1 (6%)
7	MAN	M	4	7	11,11,12	0.85	0	15,15,17	1.44	2 (13%)
7	MAN	M	5	7	11,11,12	1.27	1 (9%)	15,15,17	1.15	2 (13%)
7	MAN	M	6	7	11,11,12	4.19	9 (81%)	15,15,17	2.90	6 (40%)
7	MAN	M	7	7	11,11,12	0.67	0	15,15,17	1.19	3 (20%)
8	NAG	N	1	1,8	14,14,15	0.20	0	17,19,21	0.43	0
8	NAG	N	2	8	14,14,15	0.24	0	17,19,21	0.40	0
8	BMA	N	3	8	11,11,12	0.70	0	15,15,17	0.77	0
8	MAN	N	4	8	11,11,12	0.71	0	15,15,17	1.03	2 (13%)
8	MAN	N	5	8	11,11,12	0.70	0	15,15,17	1.08	2 (13%)
9	NAG	O	1	1,9	14,14,15	0.24	0	17,19,21	0.47	0
9	NAG	O	2	9	14,14,15	0.46	0	17,19,21	1.26	1 (5%)
9	NAG	P	1	1,9	14,14,15	0.20	0	17,19,21	0.42	0
9	NAG	P	2	9	14,14,15	0.31	0	17,19,21	0.41	0
9	NAG	Q	1	1,9	14,14,15	0.22	0	17,19,21	0.42	0
9	NAG	Q	2	9	14,14,15	0.28	0	17,19,21	0.38	0
10	NAG	R	1	10	14,14,15	0.20	0	17,19,21	0.54	0
10	NAG	R	2	10	14,14,15	0.28	0	17,19,21	0.52	0
10	BMA	R	3	10	11,11,12	0.58	0	15,15,17	0.69	0
10	MAN	R	4	10	11,11,12	0.53	0	15,15,17	1.05	2 (13%)
10	MAN	R	5	10	11,11,12	0.85	0	15,15,17	1.21	2 (13%)
10	MAN	R	6	10	11,11,12	0.69	0	15,15,17	1.06	1 (6%)
11	NAG	S	1	1,11	14,14,15	0.43	0	17,19,21	0.54	0
11	NAG	S	2	11	14,14,15	0.43	0	17,19,21	0.65	1 (5%)
11	BMA	S	3	11	11,11,12	1.24	1 (9%)	15,15,17	1.13	2 (13%)
9	NAG	T	1	1,9	14,14,15	0.25	0	17,19,21	0.38	0
9	NAG	T	2	9	14,14,15	0.29	0	17,19,21	0.43	0
12	NAG	U	1	1,12	14,14,15	0.18	0	17,19,21	0.44	0
12	MAN	U	10	12	11,11,12	0.71	0	15,15,17	0.98	2 (13%)
12	NAG	U	2	12	14,14,15	0.22	0	17,19,21	0.53	0
12	BMA	U	3	12	11,11,12	0.81	0	15,15,17	1.31	3 (20%)
12	MAN	U	4	12	11,11,12	0.63	0	15,15,17	1.07	1 (6%)
12	MAN	U	5	12	11,11,12	0.78	0	15,15,17	0.98	1 (6%)
12	MAN	U	6	12	11,11,12	0.79	1 (9%)	15,15,17	1.37	1 (6%)
12	MAN	U	7	12	11,11,12	0.59	0	15,15,17	0.95	1 (6%)
12	MAN	U	8	12	11,11,12	0.75	1 (9%)	15,15,17	1.00	2 (13%)
12	MAN	U	9	12	11,11,12	0.89	1 (9%)	15,15,17	1.15	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	V	1	9	14,14,15	0.30	0	17,19,21	0.37	0
9	NAG	V	2	9	14,14,15	0.23	0	17,19,21	0.41	0
9	NAG	W	1	1,9	14,14,15	0.26	0	17,19,21	0.63	0
9	NAG	W	2	9	14,14,15	0.28	0	17,19,21	0.43	0
9	NAG	X	1	1,9	14,14,15	0.21	0	17,19,21	0.44	0
9	NAG	X	2	9	14,14,15	0.25	0	17,19,21	0.44	0
11	NAG	Y	1	1,11	14,14,15	0.75	1 (7%)	17,19,21	0.56	0
11	NAG	Y	2	11	14,14,15	0.26	0	17,19,21	0.42	0
11	BMA	Y	3	11	11,11,12	0.62	0	15,15,17	0.78	0
7	NAG	Z	1	1,7	14,14,15	0.39	0	17,19,21	0.56	0
7	NAG	Z	2	7	14,14,15	0.61	0	17,19,21	1.57	3 (17%)
7	BMA	Z	3	7	11,11,12	1.53	1 (9%)	15,15,17	1.59	2 (13%)
7	MAN	Z	4	7	11,11,12	1.69	2 (18%)	15,15,17	1.27	1 (6%)
7	MAN	Z	5	7	11,11,12	2.51	4 (36%)	15,15,17	2.80	9 (60%)
7	MAN	Z	6	7	11,11,12	1.77	1 (9%)	15,15,17	1.25	1 (6%)
7	MAN	Z	7	7	11,11,12	1.18	2 (18%)	15,15,17	1.36	3 (20%)
8	NAG	a	1	1,8	14,14,15	0.32	0	17,19,21	0.39	0
8	NAG	a	2	8	14,14,15	0.23	0	17,19,21	0.39	0
8	BMA	a	3	8	11,11,12	0.79	0	15,15,17	0.76	0
8	MAN	a	4	8	11,11,12	0.68	0	15,15,17	1.01	1 (6%)
8	MAN	a	5	8	11,11,12	0.75	1 (9%)	15,15,17	1.08	2 (13%)
9	NAG	b	1	1,9	14,14,15	0.26	0	17,19,21	0.45	0
9	NAG	b	2	9	14,14,15	0.54	0	17,19,21	1.28	2 (11%)
9	NAG	c	1	1,9	14,14,15	0.21	0	17,19,21	0.43	0
9	NAG	c	2	9	14,14,15	0.30	0	17,19,21	0.42	0
9	NAG	d	1	1,9	14,14,15	0.26	0	17,19,21	0.40	0
9	NAG	d	2	9	14,14,15	0.30	0	17,19,21	0.39	0
10	NAG	e	1	1,10	14,14,15	0.44	0	17,19,21	0.56	0
10	NAG	e	2	10	14,14,15	0.25	0	17,19,21	0.46	0
10	BMA	e	3	10	11,11,12	0.69	0	15,15,17	0.78	0
10	MAN	e	4	10	11,11,12	0.72	0	15,15,17	1.07	2 (13%)
10	MAN	e	5	10	11,11,12	0.81	0	15,15,17	1.18	2 (13%)
10	MAN	e	6	10	11,11,12	0.60	0	15,15,17	1.07	2 (13%)
9	NAG	f	1	1,9	14,14,15	0.51	0	17,19,21	0.52	0
9	NAG	f	2	9	14,14,15	0.32	0	17,19,21	0.38	0
9	NAG	g	1	1,9	14,14,15	0.23	0	17,19,21	0.37	0
9	NAG	g	2	9	14,14,15	0.29	0	17,19,21	0.44	0
12	NAG	h	1	1,12	14,14,15	0.20	0	17,19,21	0.46	0
12	MAN	h	10	12	11,11,12	0.73	0	15,15,17	1.03	2 (13%)
12	NAG	h	2	12	14,14,15	0.22	0	17,19,21	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	BMA	h	3	12	11,11,12	0.68	0	15,15,17	1.27	2 (13%)
12	MAN	h	4	12	11,11,12	0.80	0	15,15,17	1.08	2 (13%)
12	MAN	h	5	12	11,11,12	0.86	0	15,15,17	1.04	1 (6%)
12	MAN	h	6	12	11,11,12	0.89	1 (9%)	15,15,17	1.36	1 (6%)
12	MAN	h	7	12	11,11,12	0.67	0	15,15,17	0.94	2 (13%)
12	MAN	h	8	12	11,11,12	0.71	0	15,15,17	0.97	1 (6%)
12	MAN	h	9	12	11,11,12	0.86	0	15,15,17	1.25	2 (13%)
9	NAG	i	1	1,9	14,14,15	0.38	0	17,19,21	0.52	0
9	NAG	i	2	9	14,14,15	0.26	0	17,19,21	0.46	0
9	NAG	j	1	1,9	14,14,15	0.41	0	17,19,21	0.66	0
9	NAG	j	2	9	14,14,15	0.33	0	17,19,21	0.43	0
11	NAG	k	1	1,11	14,14,15	0.42	0	17,19,21	0.57	0
11	NAG	k	2	11	14,14,15	0.37	0	17,19,21	0.74	0
11	BMA	k	3	11	11,11,12	0.74	0	15,15,17	0.88	1 (6%)
11	NAG	l	1	1,11	14,14,15	0.34	0	17,19,21	0.61	0
11	NAG	l	2	11	14,14,15	0.29	0	17,19,21	0.35	0
11	BMA	l	3	11	11,11,12	0.57	0	15,15,17	0.81	0
13	NAG	m	1	1,13	14,14,15	0.45	0	17,19,21	0.54	0
13	NAG	m	2	13	14,14,15	0.37	0	17,19,21	0.37	0
13	BMA	m	3	13	11,11,12	0.59	0	15,15,17	0.76	0
13	MAN	m	4	13,6	11,11,12	0.96	1 (9%)	15,15,17	1.22	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	M	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	M	2	7	-	3/6/23/26	0/1/1/1
7	BMA	M	3	7	-	2/2/19/22	0/1/1/1
7	MAN	M	4	7	-	0/2/19/22	1/1/1/1
7	MAN	M	5	7	-	0/2/19/22	0/1/1/1
7	MAN	M	6	7	-	0/2/19/22	1/1/1/1
7	MAN	M	7	7	-	0/2/19/22	0/1/1/1
8	NAG	N	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	N	2	8	-	2/6/23/26	0/1/1/1
8	BMA	N	3	8	-	2/2/19/22	0/1/1/1
8	MAN	N	4	8	-	1/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MAN	N	5	8	-	0/2/19/22	0/1/1/1
9	NAG	O	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	O	2	9	-	4/6/23/26	0/1/1/1
9	NAG	P	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	P	2	9	-	2/6/23/26	0/1/1/1
9	NAG	Q	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	Q	2	9	-	1/6/23/26	0/1/1/1
10	NAG	R	1	10	-	0/6/23/26	0/1/1/1
10	NAG	R	2	10	-	0/6/23/26	0/1/1/1
10	BMA	R	3	10	-	0/2/19/22	0/1/1/1
10	MAN	R	4	10	-	2/2/19/22	0/1/1/1
10	MAN	R	5	10	-	0/2/19/22	1/1/1/1
10	MAN	R	6	10	-	0/2/19/22	0/1/1/1
11	NAG	S	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	S	2	11	-	1/6/23/26	0/1/1/1
11	BMA	S	3	11	-	2/2/19/22	0/1/1/1
9	NAG	T	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	T	2	9	-	2/6/23/26	0/1/1/1
12	NAG	U	1	1,12	-	2/6/23/26	0/1/1/1
12	MAN	U	10	12	-	0/2/19/22	0/1/1/1
12	NAG	U	2	12	-	3/6/23/26	0/1/1/1
12	BMA	U	3	12	-	0/2/19/22	0/1/1/1
12	MAN	U	4	12	-	0/2/19/22	0/1/1/1
12	MAN	U	5	12	-	0/2/19/22	0/1/1/1
12	MAN	U	6	12	-	1/2/19/22	0/1/1/1
12	MAN	U	7	12	-	2/2/19/22	0/1/1/1
12	MAN	U	8	12	-	0/2/19/22	0/1/1/1
12	MAN	U	9	12	-	0/2/19/22	1/1/1/1
9	NAG	V	1	9	-	0/6/23/26	0/1/1/1
9	NAG	V	2	9	-	2/6/23/26	0/1/1/1
9	NAG	W	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	W	2	9	-	0/6/23/26	0/1/1/1
9	NAG	X	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	X	2	9	-	2/6/23/26	0/1/1/1
11	NAG	Y	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	Y	2	11	-	2/6/23/26	0/1/1/1
11	BMA	Y	3	11	-	1/2/19/22	0/1/1/1
7	NAG	Z	1	1,7	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	Z	2	7	-	3/6/23/26	0/1/1/1
7	BMA	Z	3	7	-	2/2/19/22	0/1/1/1
7	MAN	Z	4	7	-	0/2/19/22	1/1/1/1
7	MAN	Z	5	7	-	1/2/19/22	1/1/1/1
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
8	NAG	a	1	1,8	-	2/6/23/26	0/1/1/1
8	NAG	a	2	8	-	2/6/23/26	0/1/1/1
8	BMA	a	3	8	-	2/2/19/22	0/1/1/1
8	MAN	a	4	8	-	1/2/19/22	0/1/1/1
8	MAN	a	5	8	-	0/2/19/22	0/1/1/1
9	NAG	b	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	b	2	9	-	5/6/23/26	0/1/1/1
9	NAG	c	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	c	2	9	-	2/6/23/26	0/1/1/1
9	NAG	d	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	d	2	9	-	1/6/23/26	0/1/1/1
10	NAG	e	1	1,10	-	0/6/23/26	0/1/1/1
10	NAG	e	2	10	-	0/6/23/26	0/1/1/1
10	BMA	e	3	10	-	0/2/19/22	0/1/1/1
10	MAN	e	4	10	-	2/2/19/22	0/1/1/1
10	MAN	e	5	10	-	0/2/19/22	1/1/1/1
10	MAN	e	6	10	-	0/2/19/22	0/1/1/1
9	NAG	f	1	1,9	-	2/6/23/26	0/1/1/1
9	NAG	f	2	9	-	1/6/23/26	0/1/1/1
9	NAG	g	1	1,9	-	0/6/23/26	0/1/1/1
9	NAG	g	2	9	-	2/6/23/26	0/1/1/1
12	NAG	h	1	1,12	-	1/6/23/26	0/1/1/1
12	MAN	h	10	12	-	0/2/19/22	0/1/1/1
12	NAG	h	2	12	-	3/6/23/26	0/1/1/1
12	BMA	h	3	12	-	0/2/19/22	0/1/1/1
12	MAN	h	4	12	-	0/2/19/22	0/1/1/1
12	MAN	h	5	12	-	0/2/19/22	0/1/1/1
12	MAN	h	6	12	-	1/2/19/22	0/1/1/1
12	MAN	h	7	12	-	2/2/19/22	0/1/1/1
12	MAN	h	8	12	-	0/2/19/22	0/1/1/1
12	MAN	h	9	12	-	0/2/19/22	1/1/1/1
9	NAG	i	1	1,9	-	1/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	i	2	9	-	2/6/23/26	0/1/1/1
9	NAG	j	1	1,9	-	4/6/23/26	0/1/1/1
9	NAG	j	2	9	-	0/6/23/26	0/1/1/1
11	NAG	k	1	1,11	-	0/6/23/26	0/1/1/1
11	NAG	k	2	11	-	1/6/23/26	0/1/1/1
11	BMA	k	3	11	-	0/2/19/22	0/1/1/1
11	NAG	l	1	1,11	-	2/6/23/26	0/1/1/1
11	NAG	l	2	11	-	0/6/23/26	0/1/1/1
11	BMA	l	3	11	-	2/2/19/22	0/1/1/1
13	NAG	m	1	1,13	-	2/6/23/26	0/1/1/1
13	NAG	m	2	13	-	1/6/23/26	0/1/1/1
13	BMA	m	3	13	-	0/2/19/22	0/1/1/1
13	MAN	m	4	13,6	-	1/2/19/22	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	6	MAN	O5-C5	7.14	1.57	1.43
7	M	6	MAN	O2-C2	5.55	1.55	1.43
7	M	6	MAN	C4-C5	5.43	1.64	1.53
7	M	6	MAN	C2-C3	5.39	1.60	1.52
7	Z	5	MAN	C1-C2	4.77	1.63	1.52
7	Z	6	MAN	C1-C2	4.73	1.63	1.52
7	Z	4	MAN	C1-C2	4.49	1.62	1.52
7	Z	3	BMA	O5-C1	-4.36	1.36	1.43
7	M	6	MAN	O4-C4	-3.74	1.34	1.43
7	Z	5	MAN	O5-C5	3.71	1.51	1.43
7	Z	5	MAN	C4-C5	3.68	1.60	1.53
7	M	6	MAN	C4-C3	3.64	1.61	1.52
7	M	6	MAN	O3-C3	3.64	1.51	1.43
7	Z	5	MAN	C2-C3	3.56	1.57	1.52
7	M	5	MAN	O5-C1	-3.43	1.38	1.43
7	M	6	MAN	O5-C1	-2.78	1.39	1.43
7	Z	7	MAN	O5-C1	-2.67	1.39	1.43
13	m	4	MAN	C1-C2	2.49	1.57	1.52
11	Y	1	NAG	O5-C1	2.41	1.47	1.43
12	h	6	MAN	C1-C2	2.39	1.57	1.52
7	Z	7	MAN	O5-C5	2.29	1.48	1.43
12	U	6	MAN	C1-C2	2.16	1.57	1.52
7	Z	4	MAN	C4-C5	2.12	1.57	1.53
11	S	3	BMA	O5-C5	2.11	1.47	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	U	9	MAN	C1-C2	2.10	1.57	1.52
7	M	6	MAN	C1-C2	2.07	1.56	1.52
12	U	8	MAN	C1-C2	2.05	1.56	1.52
8	a	5	MAN	C1-C2	2.01	1.56	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	6	MAN	O3-C3-C2	6.44	122.33	109.99
7	Z	5	MAN	C1-C2-C3	6.02	117.07	109.67
7	Z	5	MAN	O5-C5-C6	5.55	115.90	107.20
7	M	6	MAN	C3-C4-C5	-5.15	101.05	110.24
7	M	6	MAN	O5-C5-C6	4.67	114.53	107.20
7	Z	2	NAG	C2-N2-C7	4.54	129.37	122.90
9	O	2	NAG	C2-N2-C7	4.44	129.22	122.90
7	M	2	NAG	C2-N2-C7	4.42	129.20	122.90
9	b	2	NAG	C2-N2-C7	4.42	129.20	122.90
7	Z	3	BMA	O6-C6-C5	-4.39	96.22	111.29
12	h	6	MAN	C1-O5-C5	4.22	117.92	112.19
12	U	6	MAN	C1-O5-C5	4.11	117.76	112.19
7	M	4	MAN	C1-O5-C5	3.90	117.47	112.19
7	Z	6	MAN	C1-O5-C5	3.84	117.39	112.19
12	h	9	MAN	C1-O5-C5	3.73	117.25	112.19
7	Z	5	MAN	O5-C5-C4	3.59	119.56	110.83
10	R	5	MAN	C1-O5-C5	3.50	116.93	112.19
10	e	5	MAN	C1-O5-C5	3.48	116.90	112.19
7	Z	2	NAG	O4-C4-C5	-3.38	100.89	109.30
12	U	9	MAN	C1-O5-C5	3.38	116.77	112.19
7	M	6	MAN	O2-C2-C1	3.33	115.97	109.15
7	Z	4	MAN	O5-C5-C6	-3.21	102.17	107.20
12	h	5	MAN	C1-O5-C5	3.13	116.44	112.19
12	U	4	MAN	C1-O5-C5	3.06	116.33	112.19
12	h	4	MAN	C1-O5-C5	2.94	116.17	112.19
12	U	5	MAN	C1-O5-C5	2.93	116.17	112.19
7	Z	7	MAN	O2-C2-C3	-2.83	104.47	110.14
12	U	3	BMA	C1-O5-C5	2.78	115.96	112.19
10	e	4	MAN	C1-O5-C5	2.77	115.94	112.19
7	M	6	MAN	C6-C5-C4	2.75	119.46	113.00
12	h	3	BMA	C1-O5-C5	2.73	115.89	112.19
10	R	4	MAN	C1-O5-C5	2.70	115.85	112.19
12	h	8	MAN	C1-O5-C5	2.68	115.82	112.19
10	R	6	MAN	C1-O5-C5	2.67	115.81	112.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Z	5	MAN	C6-C5-C4	2.61	119.12	113.00
12	U	8	MAN	C1-O5-C5	2.61	115.72	112.19
7	M	7	MAN	C1-O5-C5	2.60	115.72	112.19
7	Z	7	MAN	O5-C1-C2	2.60	114.79	110.77
7	M	5	MAN	O2-C2-C3	-2.54	105.04	110.14
8	a	4	MAN	C1-O5-C5	2.54	115.63	112.19
10	e	6	MAN	C1-O5-C5	2.54	115.63	112.19
10	R	4	MAN	O2-C2-C3	-2.50	105.12	110.14
7	Z	3	BMA	O2-C2-C3	-2.48	105.16	110.14
8	a	5	MAN	C1-O5-C5	2.44	115.50	112.19
8	N	4	MAN	C1-O5-C5	2.43	115.49	112.19
7	Z	7	MAN	C1-O5-C5	2.41	115.46	112.19
7	Z	5	MAN	C1-O5-C5	2.39	115.43	112.19
7	Z	5	MAN	O3-C3-C2	2.35	114.50	109.99
8	N	5	MAN	C1-O5-C5	2.34	115.36	112.19
12	h	10	MAN	C1-O5-C5	2.33	115.35	112.19
13	m	4	MAN	C1-O5-C5	2.31	115.32	112.19
7	M	5	MAN	O5-C1-C2	2.30	114.33	110.77
12	h	10	MAN	O2-C2-C3	-2.28	105.58	110.14
7	M	4	MAN	O2-C2-C3	-2.25	105.62	110.14
10	e	4	MAN	O2-C2-C3	-2.24	105.65	110.14
12	U	10	MAN	C1-O5-C5	2.24	115.22	112.19
8	N	5	MAN	O2-C2-C3	-2.23	105.66	110.14
7	Z	5	MAN	O2-C2-C1	2.23	113.71	109.15
12	U	3	BMA	O5-C1-C2	2.23	114.21	110.77
7	Z	2	NAG	C1-C2-N2	2.18	114.22	110.49
7	Z	5	MAN	O2-C2-C3	-2.18	105.77	110.14
7	Z	5	MAN	C3-C4-C5	-2.17	106.37	110.24
7	M	2	NAG	C1-C2-N2	2.16	114.18	110.49
11	S	3	BMA	C1-C2-C3	-2.16	107.02	109.67
11	S	3	BMA	O2-C2-C3	-2.15	105.83	110.14
10	R	5	MAN	O2-C2-C3	-2.15	105.84	110.14
10	e	5	MAN	O2-C2-C3	-2.14	105.86	110.14
12	h	9	MAN	O2-C2-C3	-2.12	105.89	110.14
7	M	6	MAN	C1-C2-C3	2.12	112.27	109.67
7	M	7	MAN	O2-C2-C3	-2.12	105.90	110.14
12	U	10	MAN	O2-C2-C3	-2.10	105.92	110.14
12	h	7	MAN	O2-C2-C3	-2.09	105.96	110.14
12	U	8	MAN	O2-C2-C3	-2.09	105.96	110.14
7	M	3	BMA	O6-C6-C5	-2.08	104.15	111.29
8	N	4	MAN	O2-C2-C3	-2.08	105.97	110.14
8	a	5	MAN	O2-C2-C3	-2.08	105.98	110.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	e	6	MAN	O2-C2-C3	-2.07	105.99	110.14
7	M	7	MAN	O5-C1-C2	2.06	113.96	110.77
9	b	2	NAG	C1-C2-N2	2.06	114.01	110.49
12	U	9	MAN	O2-C2-C3	-2.05	106.03	110.14
11	S	2	NAG	O4-C4-C5	-2.04	104.23	109.30
11	k	3	BMA	C1-O5-C5	2.03	114.94	112.19
12	U	3	BMA	C1-C2-C3	2.02	112.15	109.67
12	h	4	MAN	O2-C2-C1	2.02	113.29	109.15
12	h	3	BMA	C1-C2-C3	2.02	112.14	109.67
12	U	7	MAN	C1-O5-C5	2.01	114.92	112.19
12	h	7	MAN	C1-O5-C5	2.00	114.90	112.19

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	N	3	BMA	C4-C5-C6-O6
8	a	3	BMA	C4-C5-C6-O6
12	U	2	NAG	O5-C5-C6-O6
7	Z	3	BMA	C4-C5-C6-O6
9	T	2	NAG	O5-C5-C6-O6
12	h	2	NAG	O5-C5-C6-O6
7	M	3	BMA	O5-C5-C6-O6
11	S	1	NAG	O5-C5-C6-O6
9	i	2	NAG	O5-C5-C6-O6
9	g	2	NAG	O5-C5-C6-O6
10	e	4	MAN	O5-C5-C6-O6
10	R	4	MAN	O5-C5-C6-O6
9	i	2	NAG	C4-C5-C6-O6
8	N	3	BMA	O5-C5-C6-O6
8	a	3	BMA	O5-C5-C6-O6
8	a	2	NAG	C4-C5-C6-O6
9	f	1	NAG	O5-C5-C6-O6
11	l	3	BMA	O5-C5-C6-O6
8	N	2	NAG	C4-C5-C6-O6
9	g	2	NAG	C4-C5-C6-O6
13	m	1	NAG	O5-C5-C6-O6
8	a	2	NAG	O5-C5-C6-O6
12	U	2	NAG	C4-C5-C6-O6
7	M	3	BMA	C4-C5-C6-O6
11	S	1	NAG	C4-C5-C6-O6
9	V	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	b	1	NAG	C4-C5-C6-O6
9	d	1	NAG	C4-C5-C6-O6
8	N	1	NAG	C4-C5-C6-O6
9	O	1	NAG	C4-C5-C6-O6
9	T	2	NAG	C4-C5-C6-O6
7	Z	3	BMA	O5-C5-C6-O6
10	e	4	MAN	C4-C5-C6-O6
10	R	4	MAN	C4-C5-C6-O6
13	m	1	NAG	C4-C5-C6-O6
12	h	2	NAG	C4-C5-C6-O6
9	O	2	NAG	C8-C7-N2-C2
9	O	2	NAG	O7-C7-N2-C2
11	l	1	NAG	C8-C7-N2-C2
11	l	1	NAG	O7-C7-N2-C2
11	Y	1	NAG	C8-C7-N2-C2
11	Y	1	NAG	O7-C7-N2-C2
9	P	1	NAG	C8-C7-N2-C2
9	P	1	NAG	O7-C7-N2-C2
9	O	1	NAG	C8-C7-N2-C2
9	O	1	NAG	O7-C7-N2-C2
7	M	2	NAG	C8-C7-N2-C2
7	M	2	NAG	O7-C7-N2-C2
9	b	2	NAG	C8-C7-N2-C2
9	b	2	NAG	O7-C7-N2-C2
9	b	1	NAG	C8-C7-N2-C2
9	b	1	NAG	O7-C7-N2-C2
9	c	1	NAG	C8-C7-N2-C2
9	c	1	NAG	O7-C7-N2-C2
7	Z	2	NAG	C8-C7-N2-C2
7	Z	2	NAG	O7-C7-N2-C2
8	N	2	NAG	O5-C5-C6-O6
9	X	2	NAG	O5-C5-C6-O6
9	c	2	NAG	O5-C5-C6-O6
9	V	2	NAG	O5-C5-C6-O6
9	b	1	NAG	O5-C5-C6-O6
9	j	1	NAG	O5-C5-C6-O6
8	a	1	NAG	C4-C5-C6-O6
9	f	1	NAG	C4-C5-C6-O6
9	Q	1	NAG	C4-C5-C6-O6
9	W	1	NAG	O5-C5-C6-O6
9	P	2	NAG	O5-C5-C6-O6
7	Z	1	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
9	d	1	NAG	O5-C5-C6-O6
9	O	1	NAG	O5-C5-C6-O6
11	Y	3	BMA	O5-C5-C6-O6
11	S	3	BMA	C4-C5-C6-O6
9	j	1	NAG	C4-C5-C6-O6
8	N	1	NAG	O5-C5-C6-O6
12	h	7	MAN	O5-C5-C6-O6
12	U	7	MAN	O5-C5-C6-O6
7	M	1	NAG	O5-C5-C6-O6
9	W	1	NAG	C4-C5-C6-O6
7	Z	1	NAG	C4-C5-C6-O6
9	b	2	NAG	O5-C5-C6-O6
9	X	2	NAG	C4-C5-C6-O6
7	M	1	NAG	C4-C5-C6-O6
9	Q	1	NAG	O5-C5-C6-O6
12	h	7	MAN	C4-C5-C6-O6
12	U	7	MAN	C4-C5-C6-O6
12	U	6	MAN	O5-C5-C6-O6
11	Y	2	NAG	O5-C5-C6-O6
12	h	6	MAN	O5-C5-C6-O6
7	Z	5	MAN	O5-C5-C6-O6
8	a	1	NAG	O5-C5-C6-O6
8	a	4	MAN	O5-C5-C6-O6
8	N	4	MAN	O5-C5-C6-O6
13	m	4	MAN	O5-C5-C6-O6
11	l	3	BMA	C4-C5-C6-O6
13	m	2	NAG	O5-C5-C6-O6
9	c	2	NAG	C4-C5-C6-O6
11	S	3	BMA	O5-C5-C6-O6
9	P	2	NAG	C4-C5-C6-O6
9	i	1	NAG	C4-C5-C6-O6
9	O	2	NAG	O5-C5-C6-O6
12	U	1	NAG	C4-C5-C6-O6
11	k	2	NAG	O5-C5-C6-O6
9	j	1	NAG	C3-C2-N2-C7
12	h	2	NAG	C3-C2-N2-C7
12	U	1	NAG	O5-C5-C6-O6
9	b	2	NAG	C4-C5-C6-O6
9	d	2	NAG	O5-C5-C6-O6
11	S	2	NAG	C4-C5-C6-O6
9	j	1	NAG	C1-C2-N2-C7
9	f	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	h	1	NAG	C4-C5-C6-O6
9	W	1	NAG	C1-C2-N2-C7
9	Q	2	NAG	O5-C5-C6-O6
11	Y	2	NAG	C4-C5-C6-O6
9	O	2	NAG	C3-C2-N2-C7
12	U	2	NAG	C3-C2-N2-C7
9	W	1	NAG	C3-C2-N2-C7
7	M	2	NAG	C3-C2-N2-C7
9	b	2	NAG	C3-C2-N2-C7
7	Z	2	NAG	C3-C2-N2-C7

All (8) ring outliers are listed below:

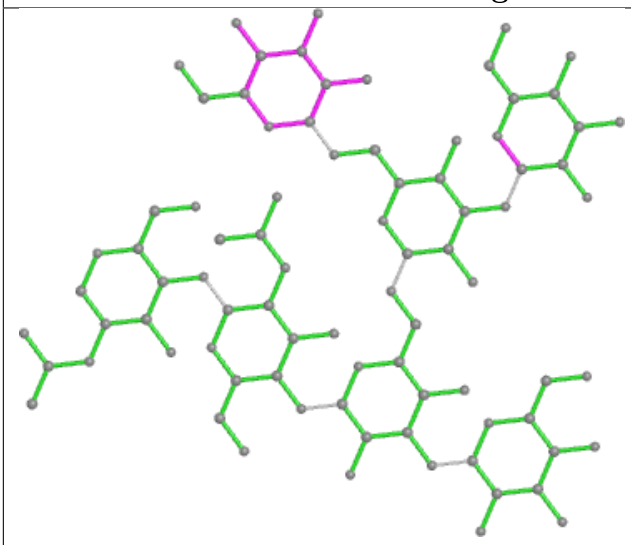
Mol	Chain	Res	Type	Atoms
7	M	4	MAN	C1-C2-C3-C4-C5-O5
7	Z	5	MAN	C1-C2-C3-C4-C5-O5
7	Z	4	MAN	C1-C2-C3-C4-C5-O5
12	U	9	MAN	C1-C2-C3-C4-C5-O5
12	h	9	MAN	C1-C2-C3-C4-C5-O5
10	R	5	MAN	C1-C2-C3-C4-C5-O5
7	M	6	MAN	C1-C2-C3-C4-C5-O5
10	e	5	MAN	C1-C2-C3-C4-C5-O5

10 monomers are involved in 13 short contacts:

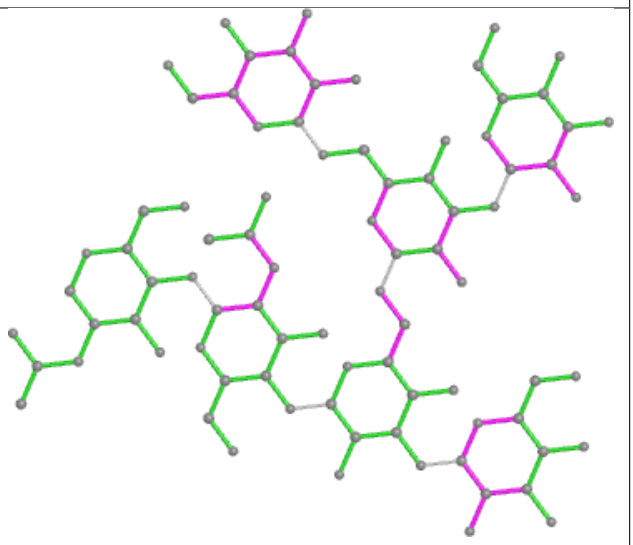
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	O	2	NAG	2	0
11	Y	1	NAG	1	0
12	U	9	MAN	1	0
9	O	1	NAG	3	0
7	M	2	NAG	1	0
7	Z	1	NAG	1	0
7	M	4	MAN	2	0
7	Z	2	NAG	1	0
12	U	8	MAN	1	0
10	R	4	MAN	2	0

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

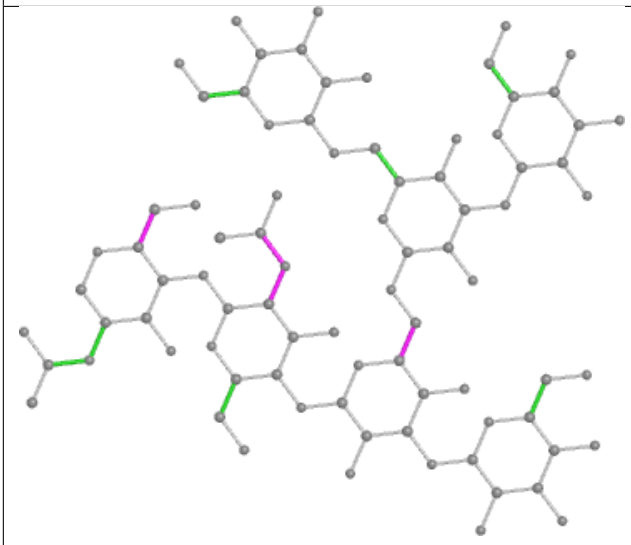
Oligosaccharide Chain M



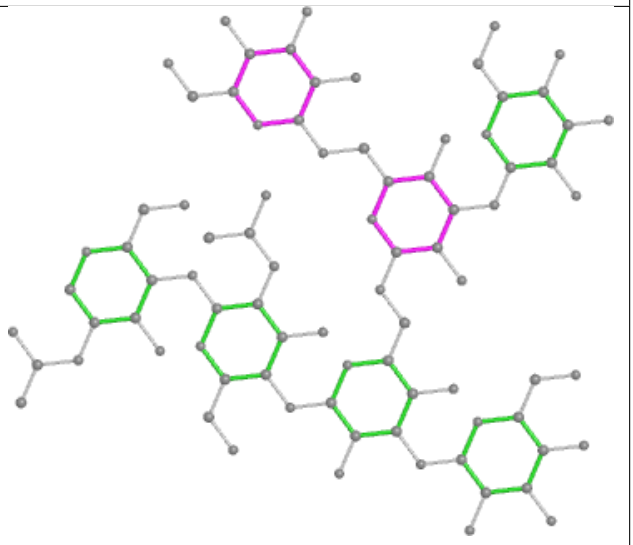
Bond lengths



Bond angles

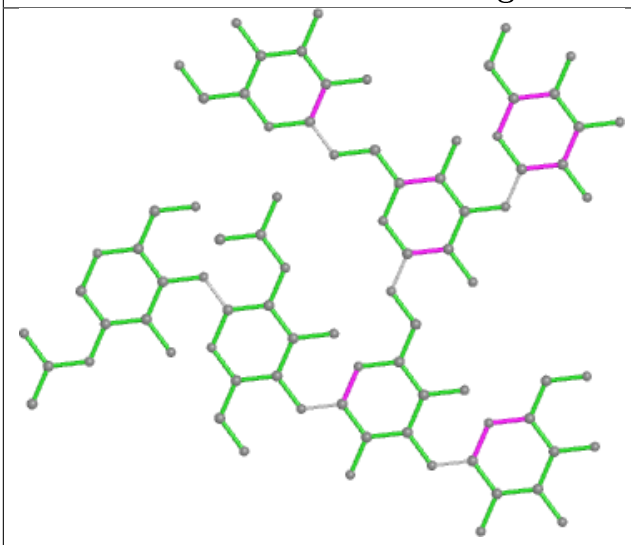


Torsions

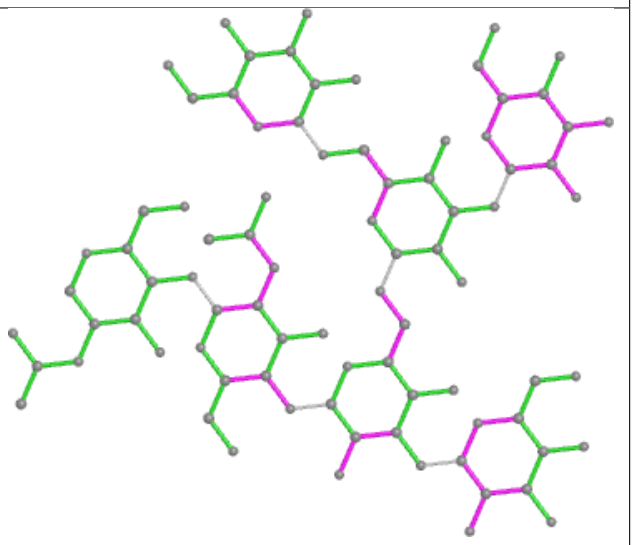


Rings

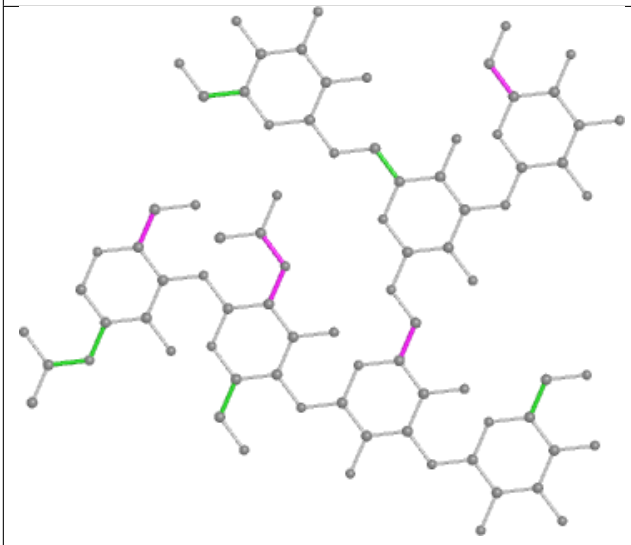
Oligosaccharide Chain Z



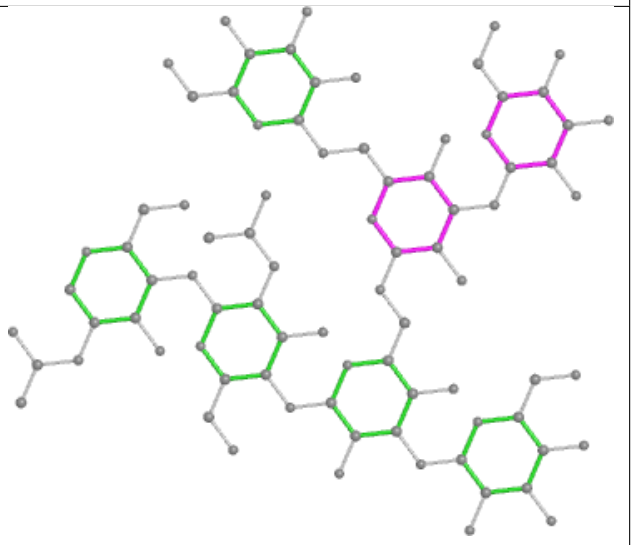
Bond lengths



Bond angles

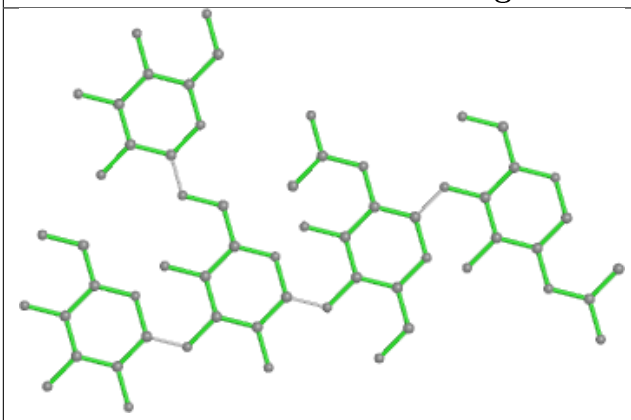


Torsions

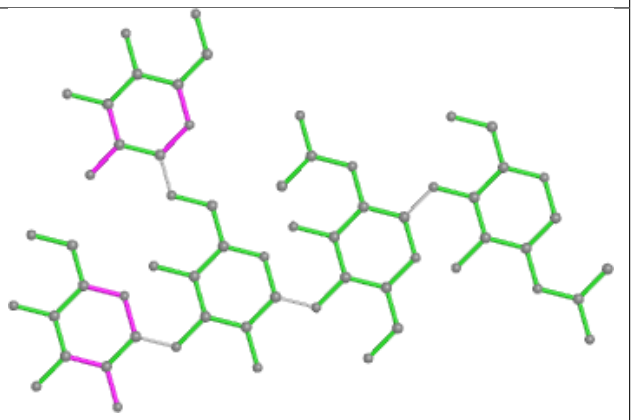


Rings

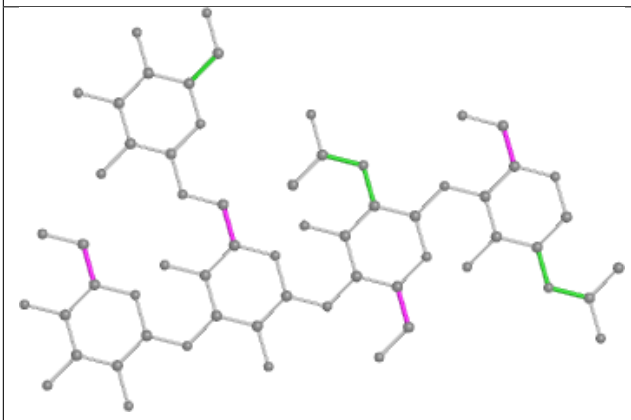
Oligosaccharide Chain N



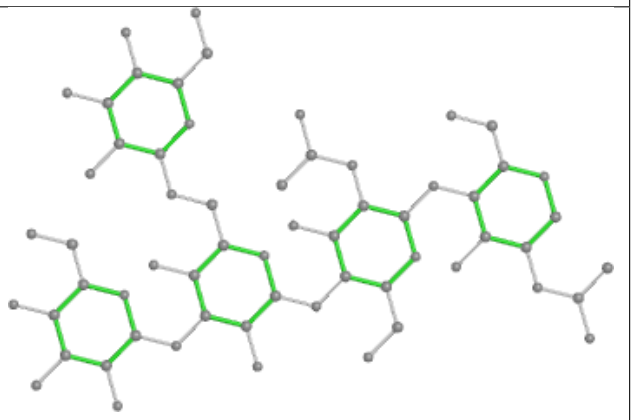
Bond lengths



Bond angles

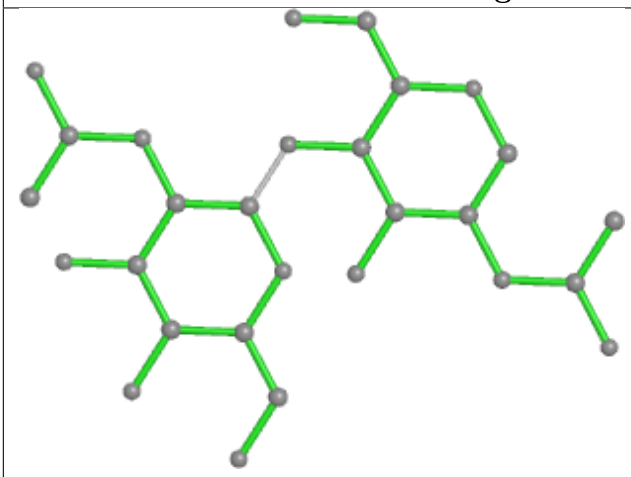


Torsions

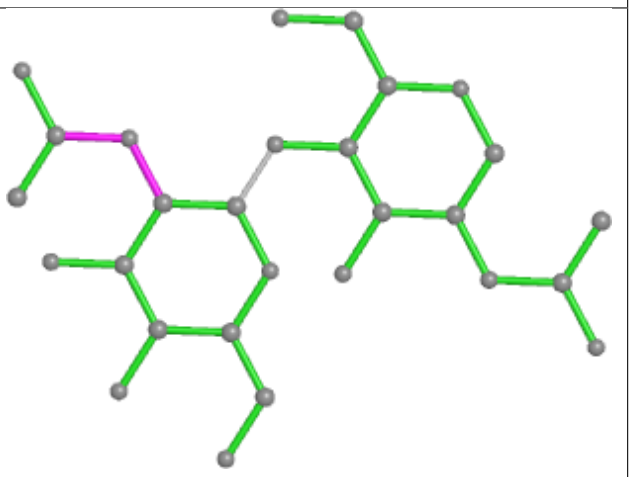


Rings

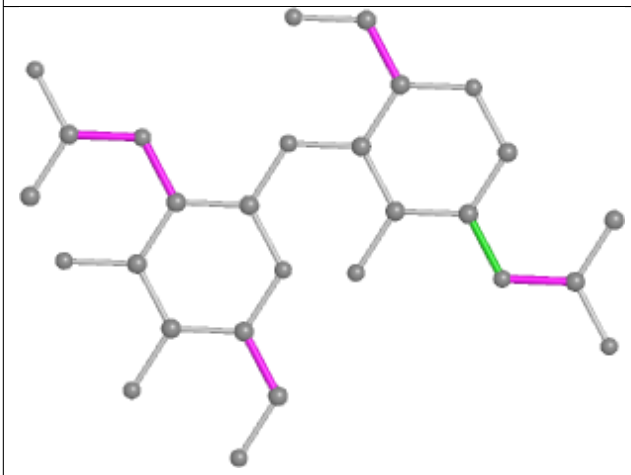
Oligosaccharide Chain O



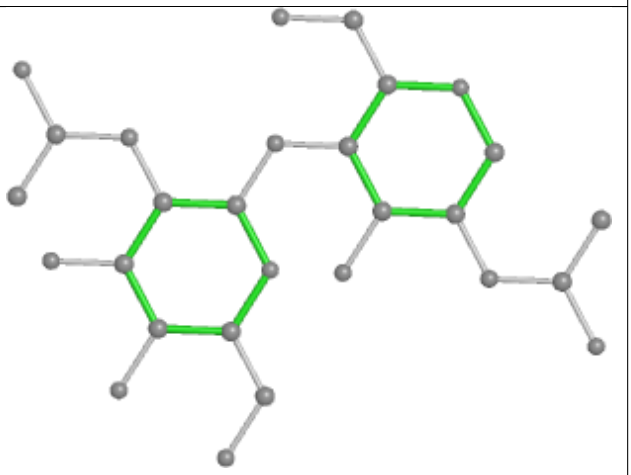
Bond lengths



Bond angles

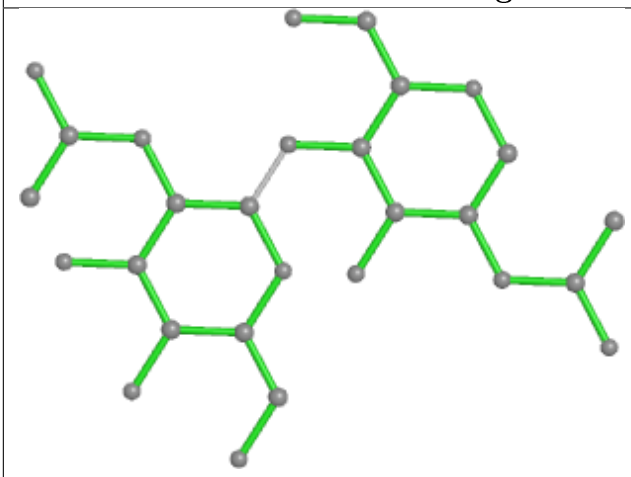


Torsions

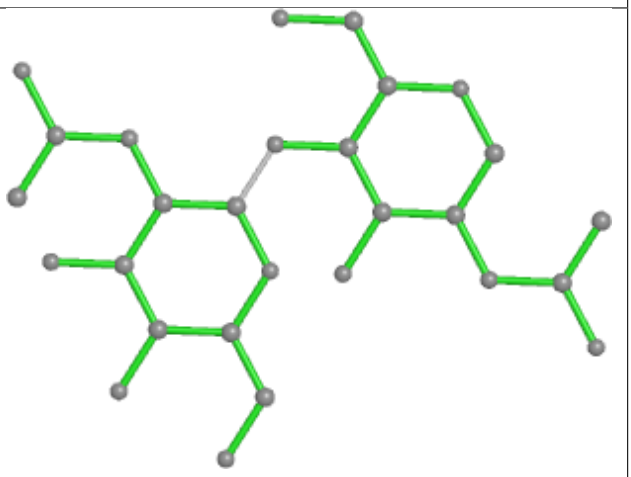


Rings

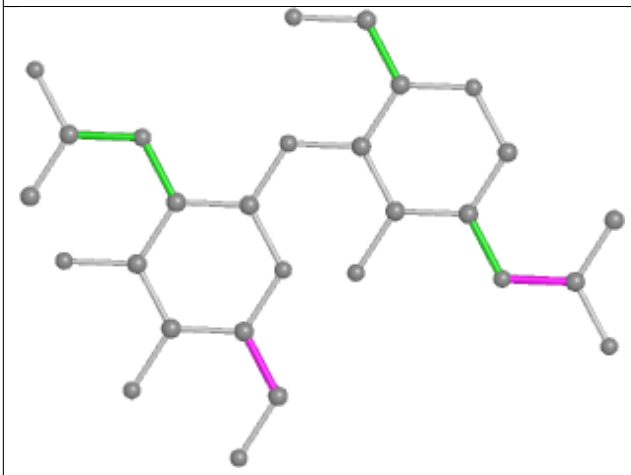
Oligosaccharide Chain P



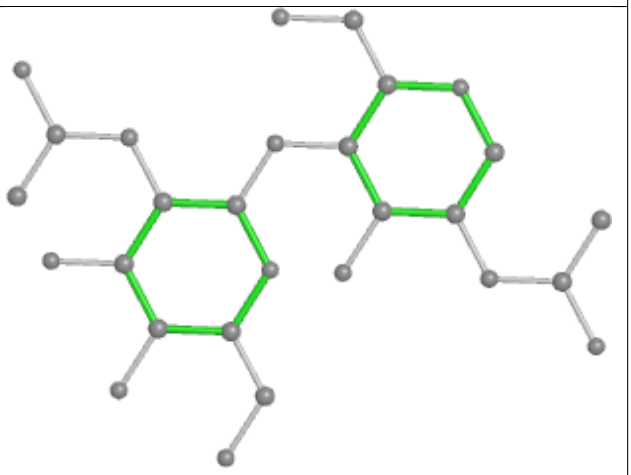
Bond lengths



Bond angles

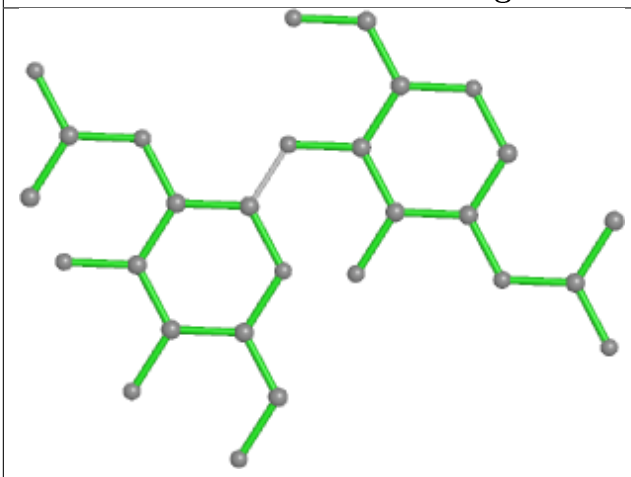


Torsions

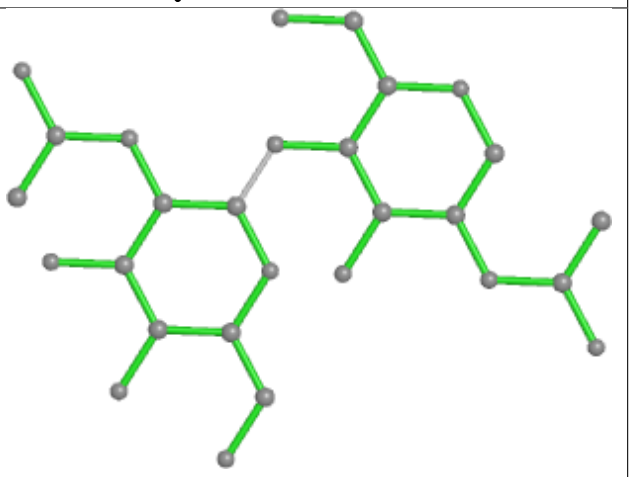


Rings

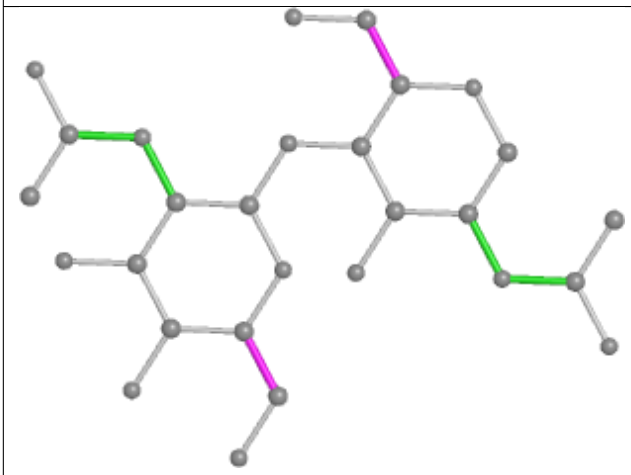
Oligosaccharide Chain Q



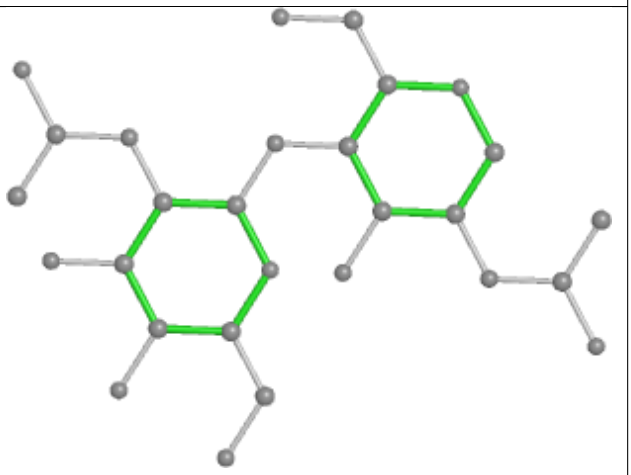
Bond lengths



Bond angles

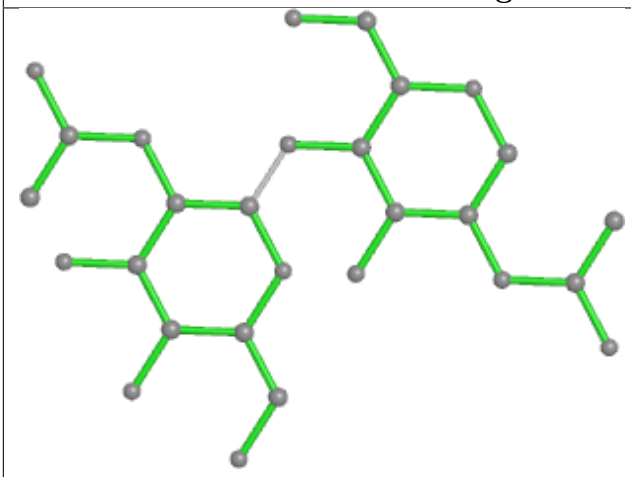


Torsions

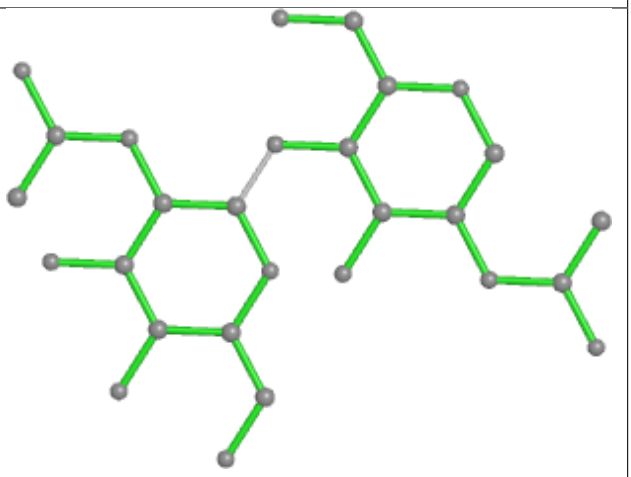


Rings

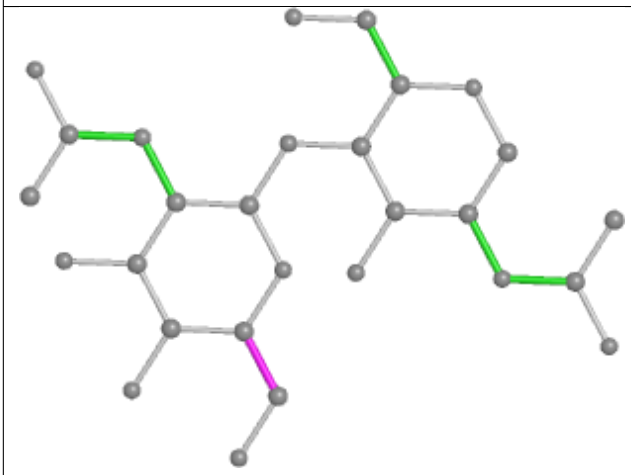
Oligosaccharide Chain T



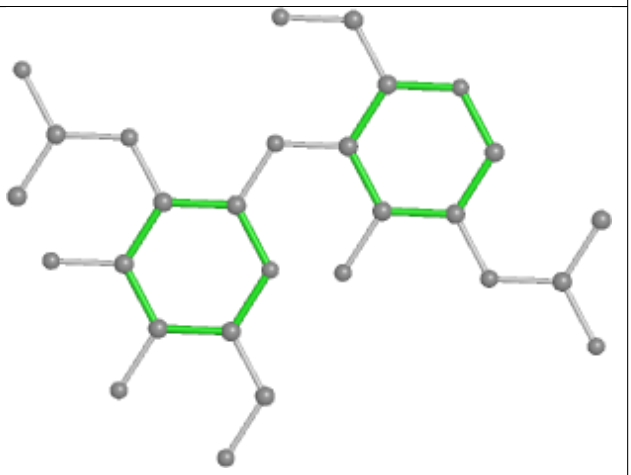
Bond lengths



Bond angles

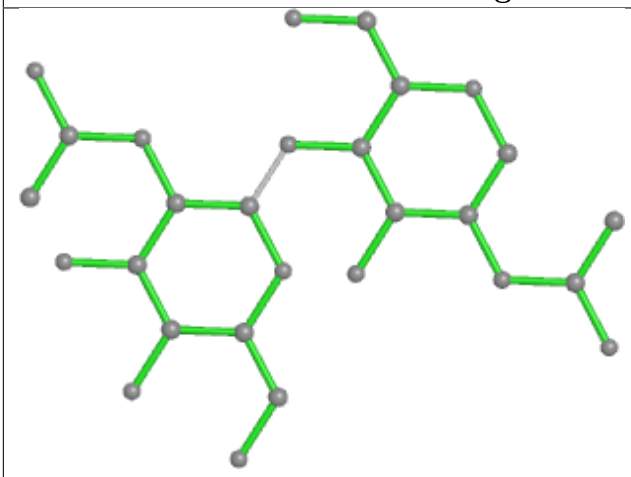


Torsions

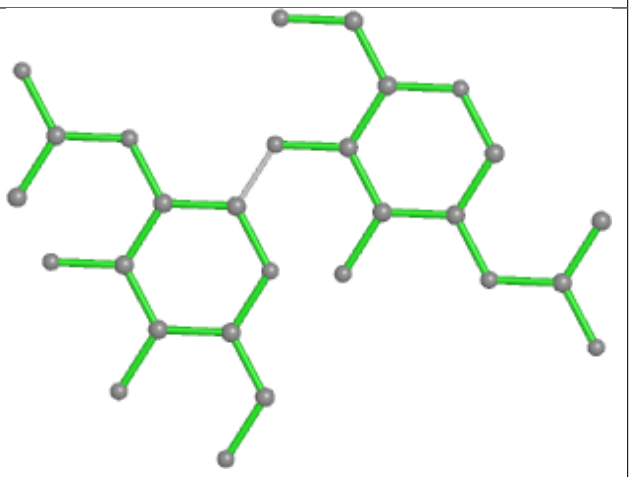


Rings

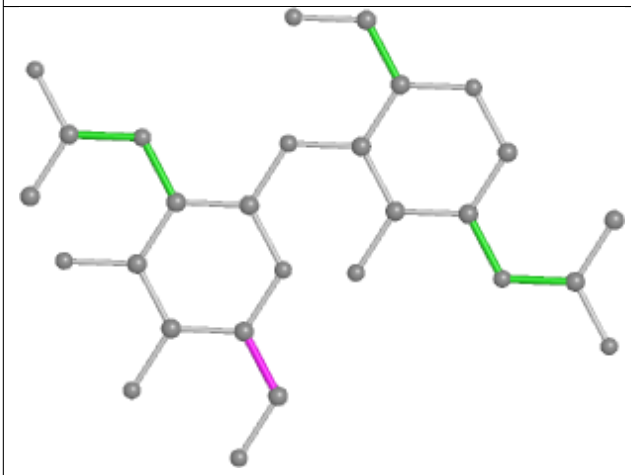
Oligosaccharide Chain V



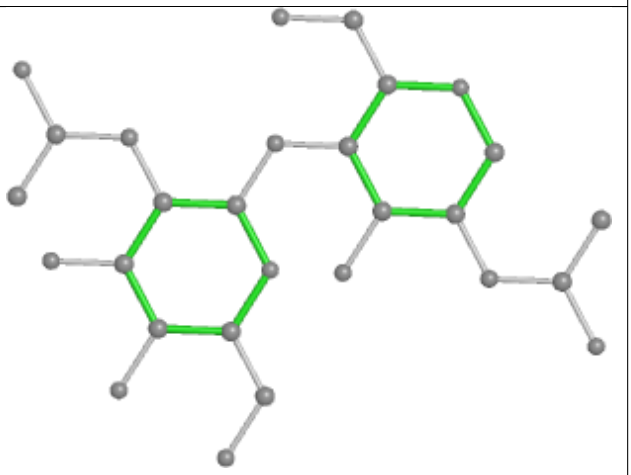
Bond lengths



Bond angles

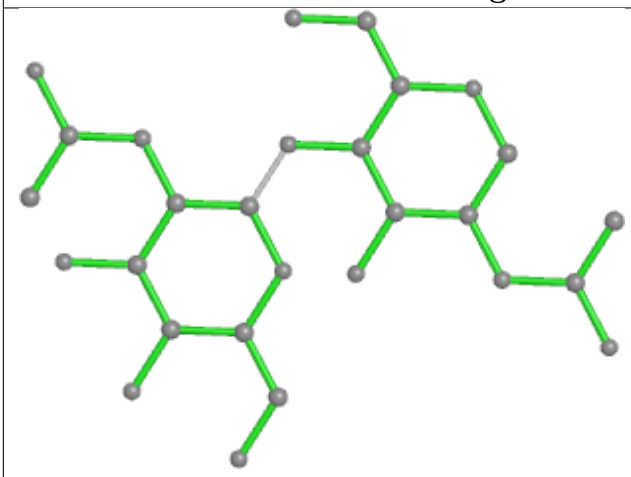


Torsions

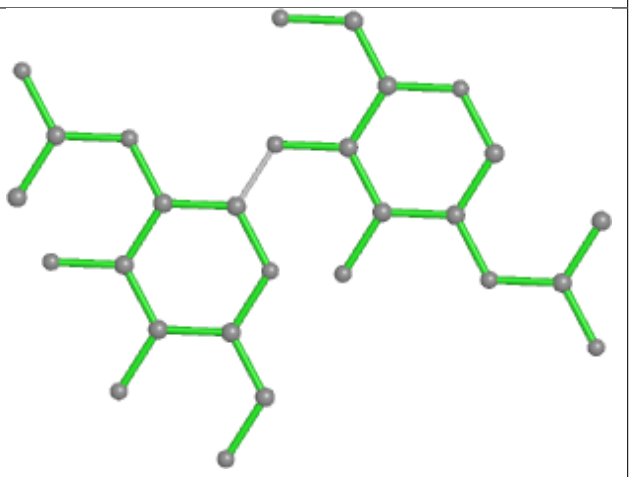


Rings

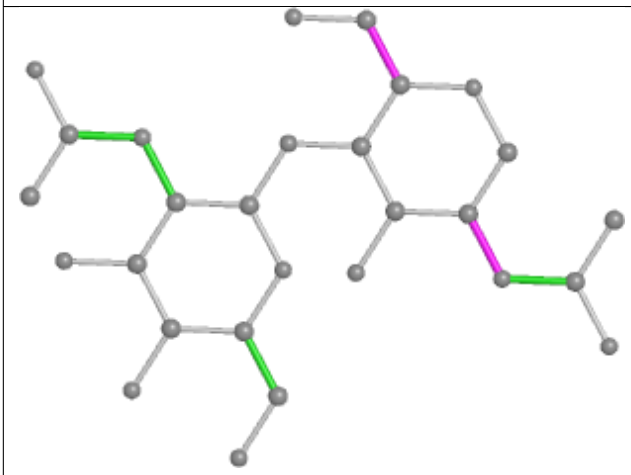
Oligosaccharide Chain W



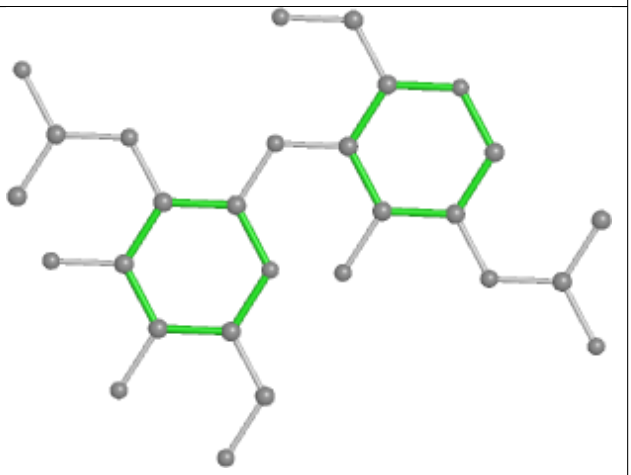
Bond lengths



Bond angles

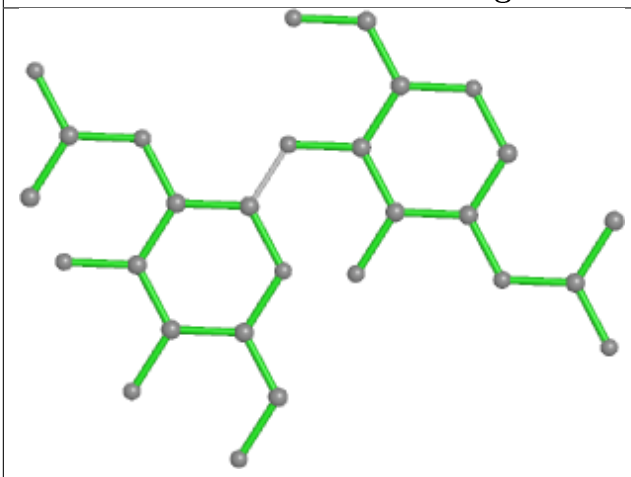


Torsions

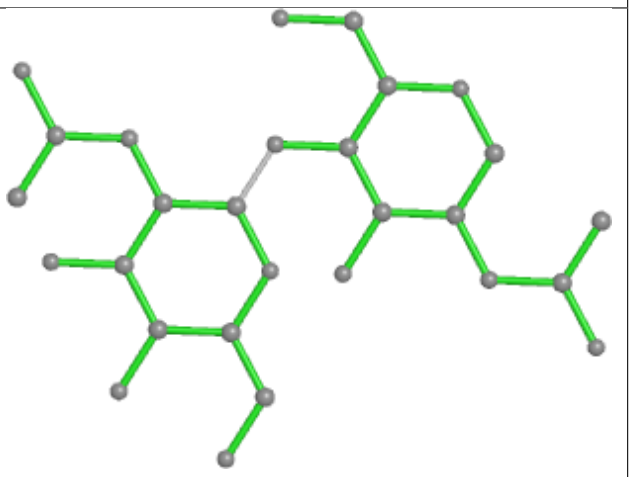


Rings

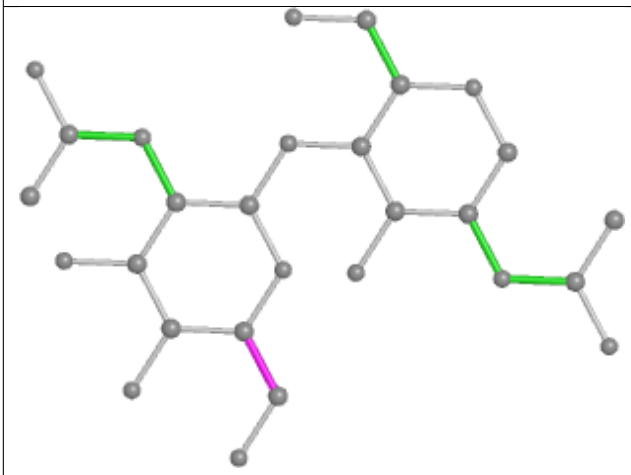
Oligosaccharide Chain X



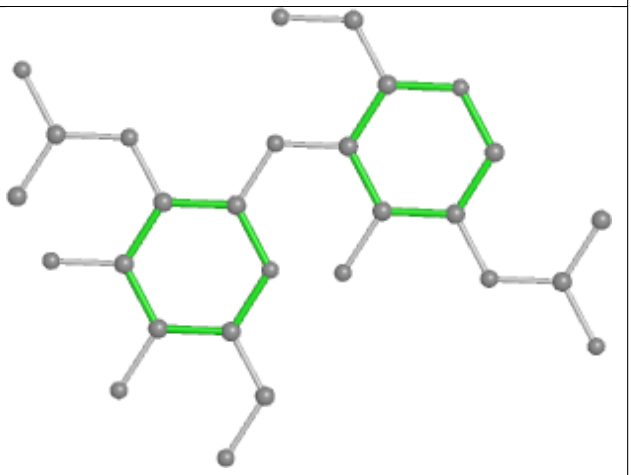
Bond lengths



Bond angles

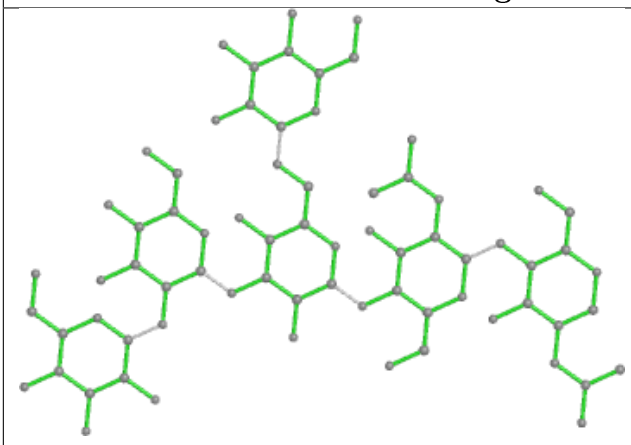


Torsions

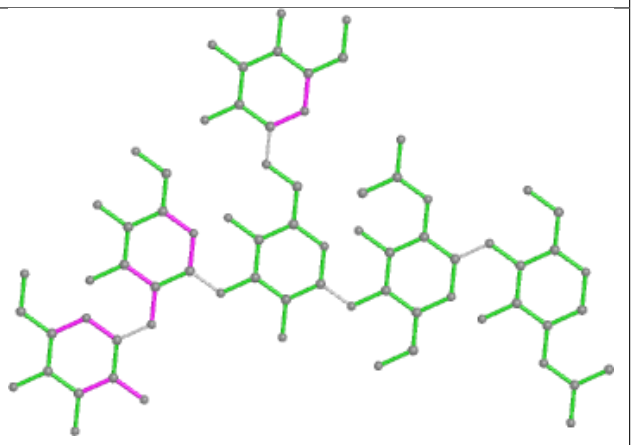


Rings

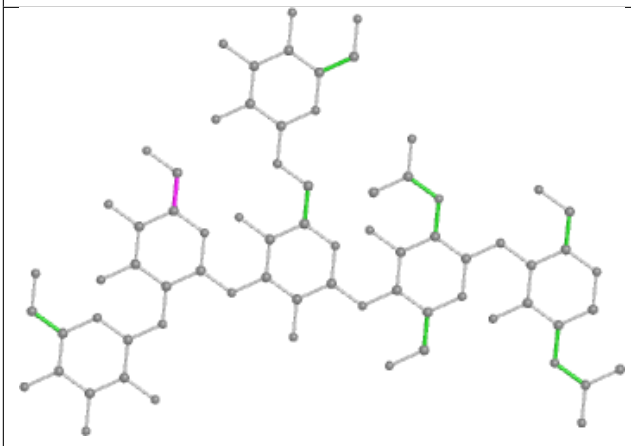
Oligosaccharide Chain R



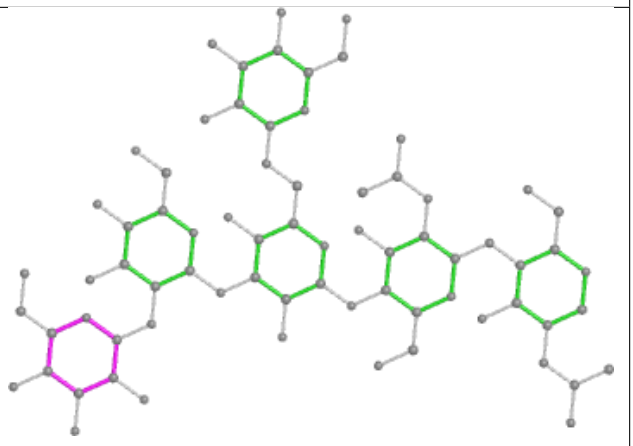
Bond lengths



Bond angles

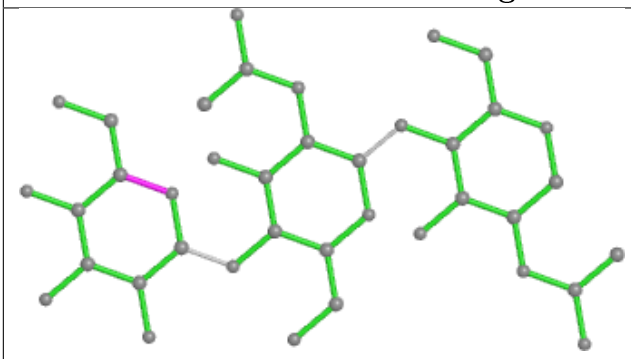


Torsions

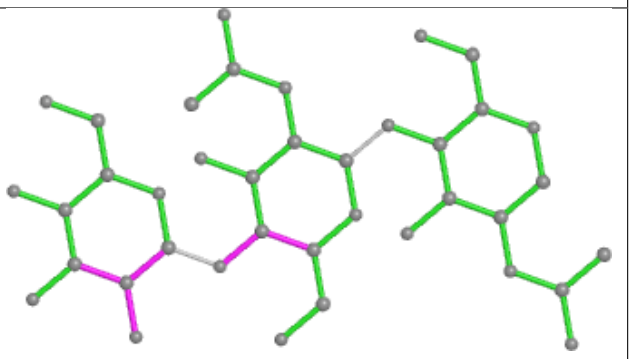


Rings

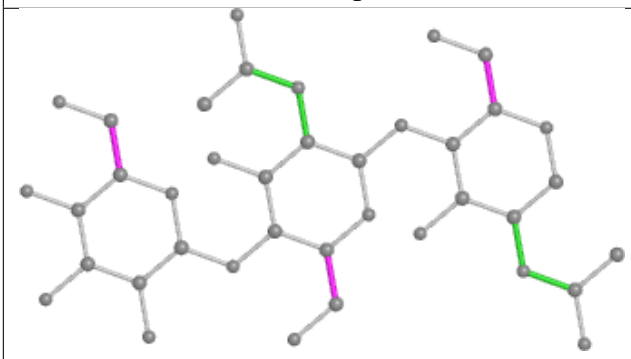
Oligosaccharide Chain S



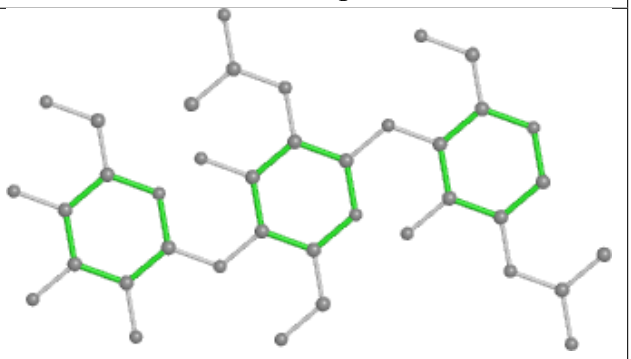
Bond lengths



Bond angles

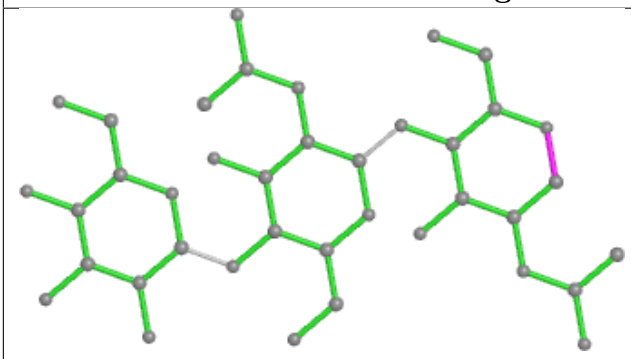


Torsions

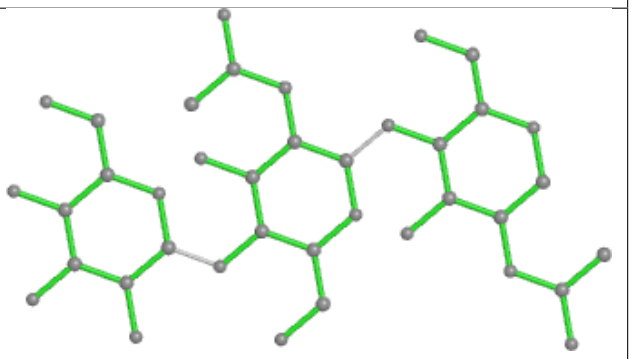


Rings

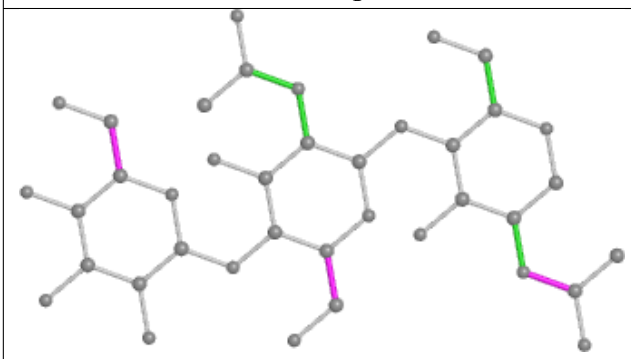
Oligosaccharide Chain Y



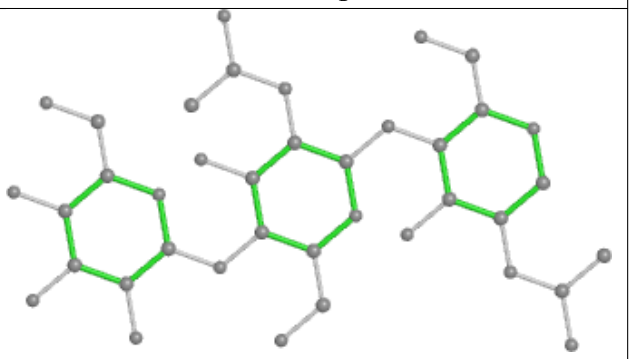
Bond lengths



Bond angles

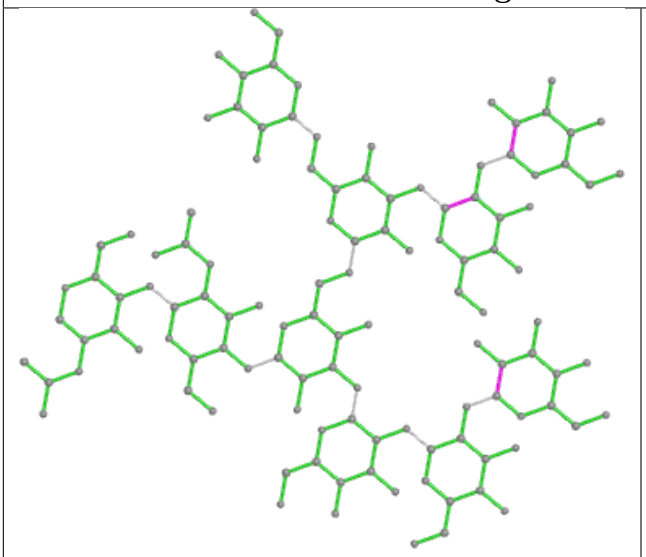


Torsions

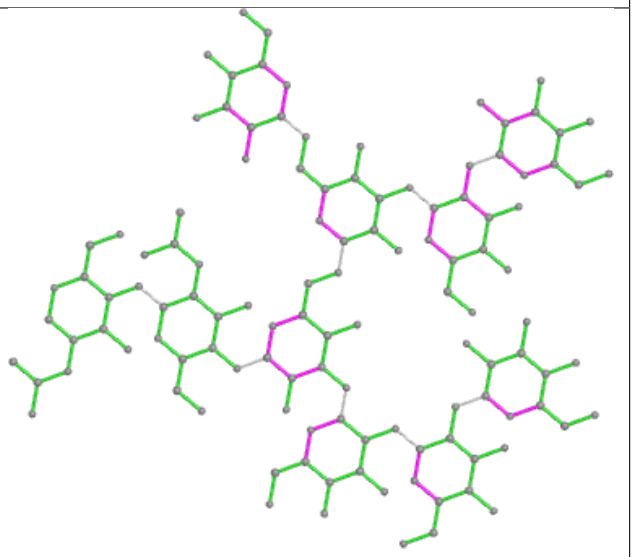


Rings

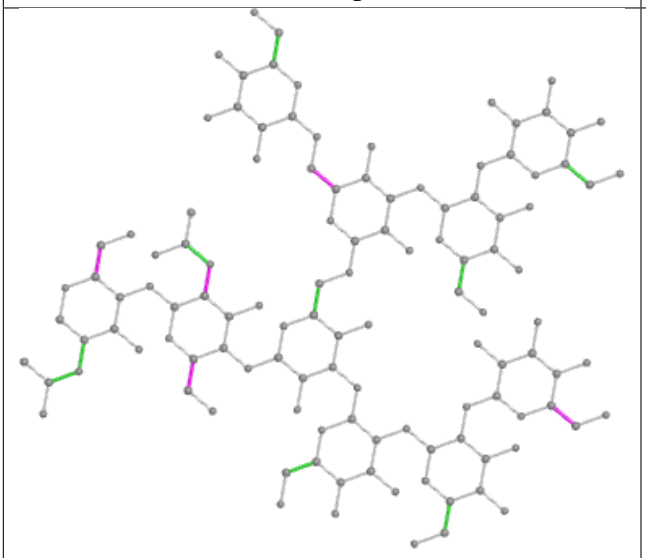
Oligosaccharide Chain U



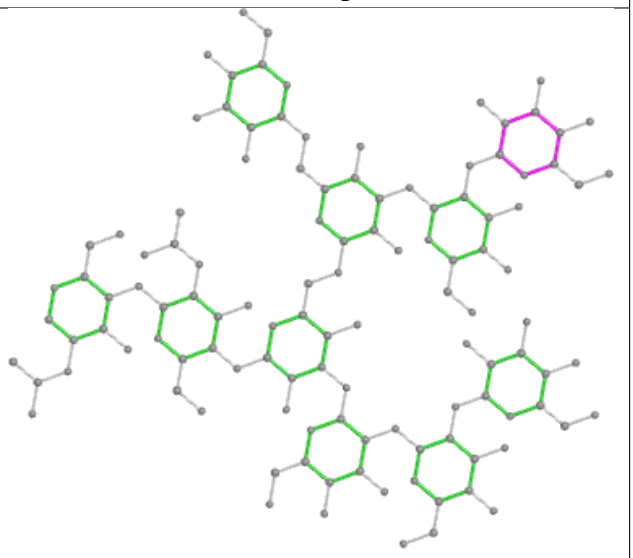
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry

16 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	$\#\|Z\|>2$
14	NAG	I	305	6	14,14,15	2.13	2 (14%)	17,19,21	0.89	0
14	NAG	D	901	2	14,14,15	0.39	0	17,19,21	0.59	0
14	NAG	K	301	6	14,14,15	2.05	2 (14%)	17,19,21	0.91	0
14	NAG	A	908	1	14,14,15	0.20	0	17,19,21	0.44	0
14	NAG	C	942	1	14,14,15	0.29	0	17,19,21	0.76	0
14	NAG	C	927	1	14,14,15	0.45	0	17,19,21	1.26	1 (5%)
14	NAG	C	908	1	14,14,15	0.28	0	17,19,21	0.41	0
14	NAG	B	902	2	14,14,15	0.16	0	17,19,21	0.47	0
14	NAG	C	953	1	14,14,15	0.28	0	17,19,21	0.43	0
14	NAG	D	902	2	14,14,15	0.36	0	17,19,21	0.38	0
14	NAG	A	926	1	14,14,15	0.44	0	17,19,21	1.26	1 (5%)
14	NAG	B	903	2	14,14,15	0.35	0	17,19,21	0.39	0
14	NAG	A	952	1	14,14,15	0.70	1 (7%)	17,19,21	0.47	0
14	NAG	A	942	1	14,14,15	0.19	0	17,19,21	0.35	0
14	NAG	C	909	1	14,14,15	0.35	0	17,19,21	0.50	0
14	NAG	B	901	2	14,14,15	0.31	0	17,19,21	0.57	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	NAG	I	305	6	-	1/6/23/26	0/1/1/1
14	NAG	D	901	2	-	2/6/23/26	0/1/1/1
14	NAG	K	301	6	-	2/6/23/26	0/1/1/1
14	NAG	A	908	1	-	1/6/23/26	0/1/1/1
14	NAG	C	942	1	-	4/6/23/26	0/1/1/1
14	NAG	C	927	1	-	5/6/23/26	0/1/1/1
14	NAG	C	908	1	-	1/6/23/26	0/1/1/1
14	NAG	B	902	2	-	2/6/23/26	0/1/1/1
14	NAG	C	953	1	-	2/6/23/26	0/1/1/1
14	NAG	D	902	2	-	2/6/23/26	0/1/1/1
14	NAG	A	926	1	-	5/6/23/26	0/1/1/1
14	NAG	B	903	2	-	2/6/23/26	0/1/1/1
14	NAG	A	952	1	-	0/6/23/26	0/1/1/1
14	NAG	A	942	1	-	2/6/23/26	0/1/1/1
14	NAG	C	909	1	-	2/6/23/26	0/1/1/1
14	NAG	B	901	2	-	1/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	I	305	NAG	O5-C1	7.41	1.55	1.43
14	K	301	NAG	O5-C1	7.14	1.55	1.43
14	I	305	NAG	C1-C2	-2.52	1.48	1.52
14	A	952	NAG	O5-C1	-2.45	1.39	1.43
14	K	301	NAG	C1-C2	-2.29	1.48	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	A	926	NAG	C2-N2-C7	4.33	129.07	122.90
14	C	927	NAG	C2-N2-C7	4.33	129.06	122.90

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	926	NAG	O5-C5-C6-O6
14	C	942	NAG	O5-C5-C6-O6
14	C	927	NAG	O5-C5-C6-O6
14	B	902	NAG	O5-C5-C6-O6
14	C	909	NAG	O5-C5-C6-O6
14	C	927	NAG	C4-C5-C6-O6
14	B	902	NAG	C4-C5-C6-O6
14	A	926	NAG	C4-C5-C6-O6
14	B	903	NAG	O5-C5-C6-O6
14	C	942	NAG	C4-C5-C6-O6
14	B	903	NAG	C4-C5-C6-O6
14	C	909	NAG	C4-C5-C6-O6
14	D	902	NAG	O5-C5-C6-O6
14	C	942	NAG	C8-C7-N2-C2
14	C	942	NAG	O7-C7-N2-C2
14	C	927	NAG	C8-C7-N2-C2
14	C	927	NAG	O7-C7-N2-C2
14	A	926	NAG	C8-C7-N2-C2
14	A	926	NAG	O7-C7-N2-C2
14	A	942	NAG	C8-C7-N2-C2
14	A	942	NAG	O7-C7-N2-C2
14	C	953	NAG	O5-C5-C6-O6
14	D	902	NAG	C4-C5-C6-O6
14	D	901	NAG	C4-C5-C6-O6
14	K	301	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
14	A	908	NAG	O5-C5-C6-O6
14	C	908	NAG	O5-C5-C6-O6
14	D	901	NAG	O5-C5-C6-O6
14	I	305	NAG	O5-C5-C6-O6
14	C	953	NAG	C4-C5-C6-O6
14	B	901	NAG	C4-C5-C6-O6
14	K	301	NAG	C4-C5-C6-O6
14	C	927	NAG	C3-C2-N2-C7
14	A	926	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	908	NAG	2	0
14	C	927	NAG	1	0
14	A	926	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	455/481 (94%)	-0.06	7 (1%) 73 64	118, 169, 241, 272	0
1	C	450/481 (93%)	-0.02	10 (2%) 62 52	125, 167, 239, 284	0
2	B	132/153 (86%)	-0.22	1 (0%) 86 79	115, 171, 238, 256	0
2	D	132/153 (86%)	-0.13	1 (0%) 86 79	122, 177, 233, 246	0
3	J	210/210 (100%)	0.14	10 (4%) 30 26	190, 267, 327, 375	0
3	L	210/210 (100%)	0.13	10 (4%) 30 26	188, 278, 318, 331	0
4	E	223/223 (100%)	0.08	8 (3%) 42 34	136, 205, 293, 332	0
4	G	223/223 (100%)	0.08	7 (3%) 49 39	141, 192, 284, 320	0
5	F	212/212 (100%)	0.30	21 (9%) 7 7	171, 266, 317, 340	0
5	H	212/212 (100%)	0.47	20 (9%) 8 8	157, 244, 296, 314	0
6	I	228/235 (97%)	0.18	14 (6%) 21 17	187, 251, 285, 313	0
6	K	228/235 (97%)	0.33	22 (9%) 8 7	188, 249, 281, 302	0
All	All	2915/3028 (96%)	0.10	131 (4%) 33 28	115, 214, 301, 375	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	126	PRO	7.3
5	F	194	CYS	6.3
5	H	113	PRO	5.7
3	J	6	ALA	5.3
5	F	78	LEU	5.2
6	K	67	VAL	5.0
1	A	32	GLU	4.7
3	J	64	GLY	4.7
6	K	159	SER	4.6
6	K	162	HIS	4.5
5	F	196	VAL	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	6	ALA	4.5
1	C	470	PRO	4.4
1	A	31	ALA	4.2
1	C	471	GLY	3.9
6	K	81	ARG	3.8
6	K	160	GLY	3.8
6	K	18	LEU	3.7
5	F	2	ILE	3.7
6	K	68	HIS	3.7
1	C	455	THR	3.6
5	H	194	CYS	3.6
6	K	80	LEU	3.5
4	E	137	ALA	3.5
6	K	69	LEU	3.5
4	G	133	GLY	3.4
6	I	81	ARG	3.4
5	H	201	LEU	3.4
5	F	146	VAL	3.3
1	C	66	HIS	3.3
6	I	71	LEU	3.3
6	K	82	LEU	3.1
6	K	20	LEU	3.1
5	F	77	SER	3.1
4	E	194	TYR	3.1
5	H	196	VAL	3.1
3	J	171	ASN	3.0
5	F	193	ALA	3.0
5	F	3	GLN	2.9
6	I	1	GLN	2.9
3	L	158	ALA	2.9
6	K	92	CYS	2.9
4	E	211	VAL	2.8
5	H	185	ASP	2.8
5	F	185	ASP	2.8
5	H	145	LYS	2.8
5	F	207	LYS	2.8
5	F	145	LYS	2.8
1	C	454	LEU	2.8
1	C	61	TYR	2.7
5	F	15	VAL	2.7
5	H	146	VAL	2.7
5	H	139	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	610	TRP	2.7
5	H	78	LEU	2.7
6	I	187	LEU	2.7
3	L	29	GLY	2.6
4	G	114	ALA	2.6
1	C	366	GLY	2.6
3	L	159	GLY	2.6
3	L	30	SER	2.6
4	E	214	LYS	2.6
1	C	277	ILE	2.6
5	H	199	GLN	2.6
3	J	7	PRO	2.6
5	H	112	ALA	2.5
5	H	152	ASN	2.5
5	F	147	GLN	2.5
6	K	181	THR	2.5
5	H	200	GLY	2.5
1	C	316	ALA	2.5
5	F	117	ILE	2.5
6	I	67	VAL	2.5
6	I	34	TRP	2.5
3	L	64	GLY	2.5
1	A	33	ASN	2.4
5	F	205	VAL	2.4
6	K	22	CYS	2.4
5	H	205	VAL	2.4
6	I	18	LEU	2.4
4	G	132	SER	2.3
1	A	471	GLY	2.3
4	E	138	LEU	2.3
6	K	179	VAL	2.3
3	J	183	PRO	2.3
3	L	207	VAL	2.3
1	C	367	GLY	2.3
4	G	214	LYS	2.3
6	K	36	TRP	2.3
3	J	86	TYR	2.3
6	I	2	VAL	2.3
5	F	1	ASP	2.2
5	H	104	VAL	2.2
5	H	166	GLN	2.2
6	I	87	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	34	LEU	2.2
6	I	78	VAL	2.2
5	H	117	ILE	2.2
3	L	181	LEU	2.2
3	L	152	ASP	2.2
6	I	68	HIS	2.2
3	L	7	PRO	2.2
4	E	125	ALA	2.2
4	E	196	CYS	2.2
6	K	161	VAL	2.2
6	K	100(A)	ILE	2.2
6	K	35	SER	2.2
1	A	470	PRO	2.2
5	H	75	VAL	2.1
6	I	7	SER	2.1
6	I	69	LEU	2.1
6	K	150	VAL	2.1
2	D	610	TRP	2.1
1	A	188	ASN	2.1
3	J	210	THR	2.1
4	G	165	THR	2.1
5	F	195	GLU	2.1
3	J	147	VAL	2.1
5	F	197	THR	2.1
5	H	86	TYR	2.1
5	F	80	PRO	2.1
6	K	178	SER	2.1
4	G	198	VAL	2.1
3	J	111	LYS	2.1
4	G	145	TYR	2.1
5	F	79	GLN	2.0
5	F	27	GLN	2.0
5	H	148	TRP	2.0
3	J	127	GLN	2.0
6	K	157	LEU	2.0
6	I	184	SER	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
11	BMA	k	3	11/12	0.55	0.64	273,279,285,287	0
8	MAN	N	5	11/12	0.62	0.24	288,291,294,297	0
9	NAG	b	2	14/15	0.62	0.64	224,237,247,255	0
13	BMA	m	3	11/12	0.62	0.25	259,268,274,282	0
11	NAG	k	2	14/15	0.62	0.42	241,271,282,284	0
9	NAG	c	2	14/15	0.64	1.06	224,242,261,263	0
8	BMA	N	3	11/12	0.64	0.26	256,265,276,285	0
11	BMA	l	3	11/12	0.65	0.68	268,300,328,382	0
9	NAG	P	2	14/15	0.65	0.67	235,250,266,269	0
11	NAG	l	2	14/15	0.65	0.45	226,247,272,300	0
9	NAG	i	2	14/15	0.67	1.01	276,295,304,306	0
8	MAN	a	5	11/12	0.72	0.20	291,294,295,297	0
11	BMA	S	3	11/12	0.72	0.43	238,239,241,241	0
12	MAN	h	10	11/12	0.73	0.45	207,223,229,232	0
7	MAN	Z	5	11/12	0.73	0.47	193,214,225,236	0
9	NAG	W	2	14/15	0.74	0.32	226,244,249,249	0
11	NAG	k	1	14/15	0.74	0.27	233,245,258,269	0
9	NAG	d	2	14/15	0.74	0.68	262,273,276,279	0
7	MAN	M	4	11/12	0.75	0.23	221,227,234,235	0
7	MAN	Z	6	11/12	0.76	0.38	220,225,239,240	0
12	MAN	U	9	11/12	0.76	0.40	237,244,248,248	0
11	BMA	Y	3	11/12	0.76	0.23	209,244,274,327	0
7	MAN	M	5	11/12	0.77	0.34	189,208,218,228	0
9	NAG	O	2	14/15	0.77	0.70	224,236,248,255	0
11	NAG	Y	2	14/15	0.77	0.28	199,221,246,273	0
9	NAG	d	1	14/15	0.79	0.61	216,233,245,258	0
13	NAG	m	1	14/15	0.79	0.27	213,241,264,267	0
9	NAG	i	1	14/15	0.79	0.79	229,247,272,295	0
11	NAG	S	2	14/15	0.80	0.29	212,223,235,244	0
7	MAN	M	6	11/12	0.81	0.39	219,226,240,243	0
9	NAG	P	1	14/15	0.81	0.36	167,198,218,233	0
9	NAG	f	1	14/15	0.81	0.23	175,193,219,228	0
12	MAN	h	5	11/12	0.81	0.21	214,223,238,241	0
9	NAG	b	1	14/15	0.81	0.25	174,198,206,219	0
11	NAG	Y	1	14/15	0.82	0.26	189,207,219,223	0
7	MAN	Z	4	11/12	0.82	0.25	199,208,215,215	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	NAG	V	2	14/15	0.82	0.51	252,267,276,276	0
7	NAG	M	1	14/15	0.82	0.40	163,173,183,185	0
13	MAN	m	4	11/12	0.82	0.34	245,269,280,281	0
11	NAG	l	1	14/15	0.83	0.25	196,212,229,234	0
8	MAN	N	4	11/12	0.84	0.25	241,253,257,259	0
9	NAG	V	1	14/15	0.84	0.34	219,234,259,280	0
8	BMA	a	3	11/12	0.84	0.14	245,253,263,273	0
9	NAG	X	2	14/15	0.84	0.30	243,268,273,274	0
9	NAG	T	2	14/15	0.84	0.43	222,235,246,253	0
7	BMA	M	3	11/12	0.84	0.37	192,202,224,227	0
8	MAN	a	4	11/12	0.85	0.20	229,240,246,246	0
10	MAN	e	4	11/12	0.85	0.37	248,257,269,274	0
13	NAG	m	2	14/15	0.85	0.20	242,251,265,266	0
9	NAG	Q	2	14/15	0.85	0.72	241,246,251,252	0
9	NAG	O	1	14/15	0.86	0.23	180,203,213,224	0
12	MAN	U	10	11/12	0.86	0.27	200,214,222,222	0
11	NAG	S	1	14/15	0.86	0.20	177,194,220,229	0
9	NAG	W	1	14/15	0.86	0.26	184,222,240,252	0
9	NAG	c	1	14/15	0.86	0.29	160,193,213,228	0
9	NAG	g	2	14/15	0.86	0.28	219,230,241,248	0
8	NAG	N	1	14/15	0.86	0.26	154,199,216,219	0
9	NAG	g	1	14/15	0.87	0.36	182,197,215,223	0
9	NAG	j	2	14/15	0.87	0.21	224,246,254,254	0
10	MAN	R	4	11/12	0.87	0.46	235,244,255,261	0
9	NAG	T	1	14/15	0.88	0.54	179,194,209,223	0
9	NAG	f	2	14/15	0.88	0.22	204,213,227,236	0
10	BMA	R	3	11/12	0.88	0.13	225,231,246,253	0
8	NAG	a	1	14/15	0.88	0.33	152,193,211,215	0
7	MAN	Z	7	11/12	0.89	0.45	196,199,218,231	0
10	MAN	e	5	11/12	0.89	0.26	254,262,264,266	0
10	MAN	e	6	11/12	0.89	0.20	246,266,272,274	0
10	BMA	e	3	11/12	0.89	0.12	238,243,259,266	0
8	NAG	N	2	14/15	0.89	0.47	219,233,244,254	0
9	NAG	j	1	14/15	0.90	0.24	178,218,237,249	0
12	NAG	U	1	14/15	0.90	0.24	171,178,197,199	0
10	MAN	R	6	11/12	0.90	0.12	232,250,257,258	0
12	MAN	h	6	11/12	0.90	0.21	229,236,242,244	0
7	BMA	Z	3	11/12	0.91	0.27	192,205,231,233	0
8	NAG	a	2	14/15	0.91	0.27	206,220,230,238	0
12	MAN	U	5	11/12	0.91	0.31	220,225,240,246	0
7	NAG	M	2	14/15	0.91	0.36	171,183,199,203	0
12	NAG	h	2	14/15	0.92	0.26	182,200,232,234	0

Continued on next page...

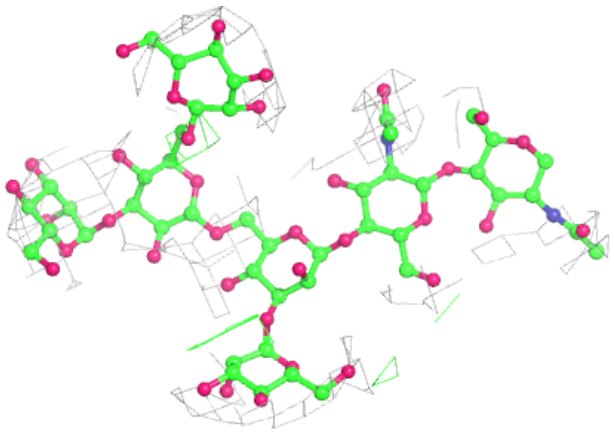
Continued from previous page...

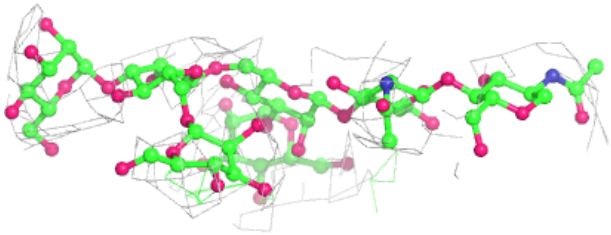
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	NAG	Z	1	14/15	0.92	0.30	177,185,200,200	0
12	MAN	h	4	11/12	0.92	0.14	194,198,219,238	0
9	NAG	X	1	14/15	0.92	0.24	231,245,265,272	0
12	MAN	h	7	11/12	0.92	0.15	201,219,226,237	0
12	MAN	h	9	11/12	0.92	0.21	227,237,242,243	0
7	NAG	Z	2	14/15	0.93	0.28	173,188,199,202	0
12	MAN	U	6	11/12	0.93	0.19	233,240,243,244	0
12	BMA	h	3	11/12	0.93	0.11	178,200,214,222	0
12	NAG	h	1	14/15	0.93	0.16	173,180,196,200	0
10	NAG	R	2	14/15	0.93	0.14	182,197,208,218	0
7	MAN	M	7	11/12	0.93	0.75	207,216,231,247	0
12	NAG	U	2	14/15	0.93	0.31	173,191,216,220	0
9	NAG	Q	1	14/15	0.93	0.48	193,211,222,236	0
10	NAG	e	2	14/15	0.93	0.19	197,210,221,229	0
12	MAN	U	4	11/12	0.94	0.18	193,197,218,238	0
12	MAN	U	8	11/12	0.94	0.28	235,238,245,250	0
12	MAN	h	8	11/12	0.95	0.12	236,237,242,246	0
10	MAN	R	5	11/12	0.95	0.31	226,232,234,235	0
10	NAG	R	1	14/15	0.96	0.25	134,153,170,180	0
10	NAG	e	1	14/15	0.96	0.27	150,168,186,195	0
12	MAN	U	7	11/12	0.96	0.19	189,208,215,222	0
12	BMA	U	3	11/12	0.96	0.21	178,197,213,217	0

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

Electron density around Chain M:

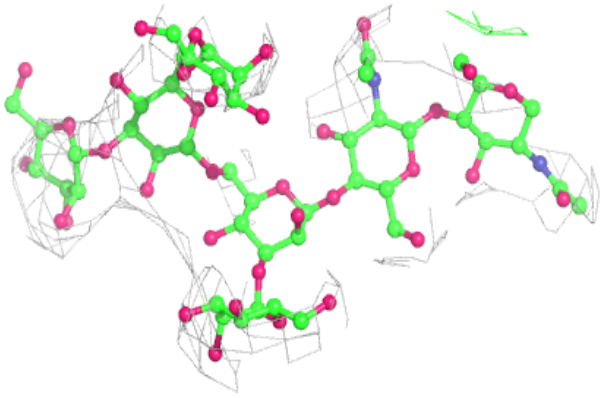
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

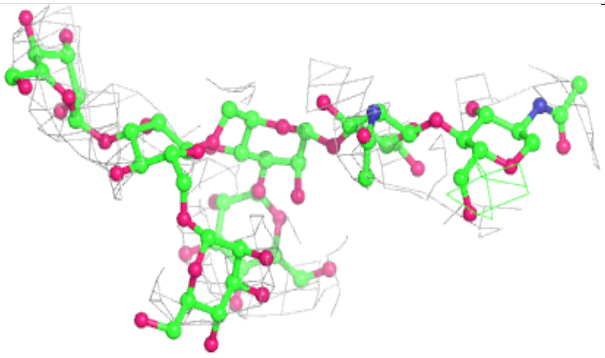


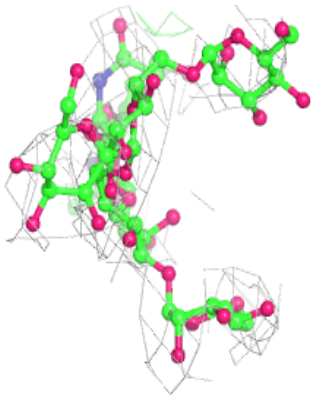


Electron density around Chain Z:

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

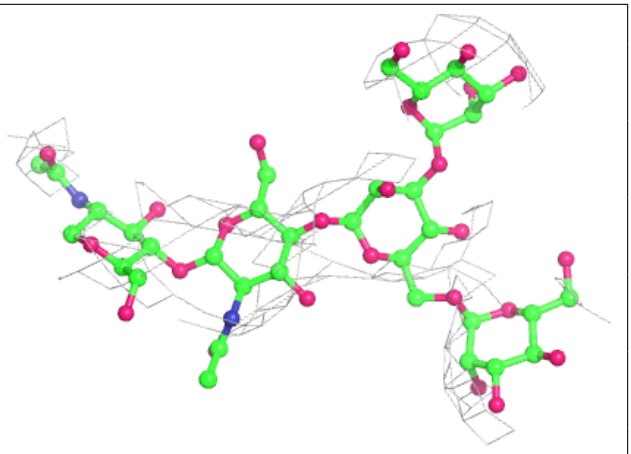


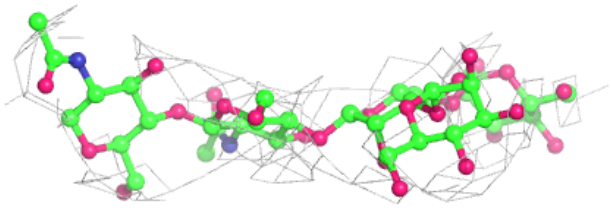


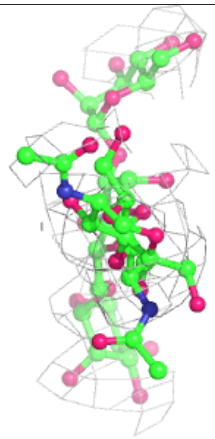


Electron density around Chain N:

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

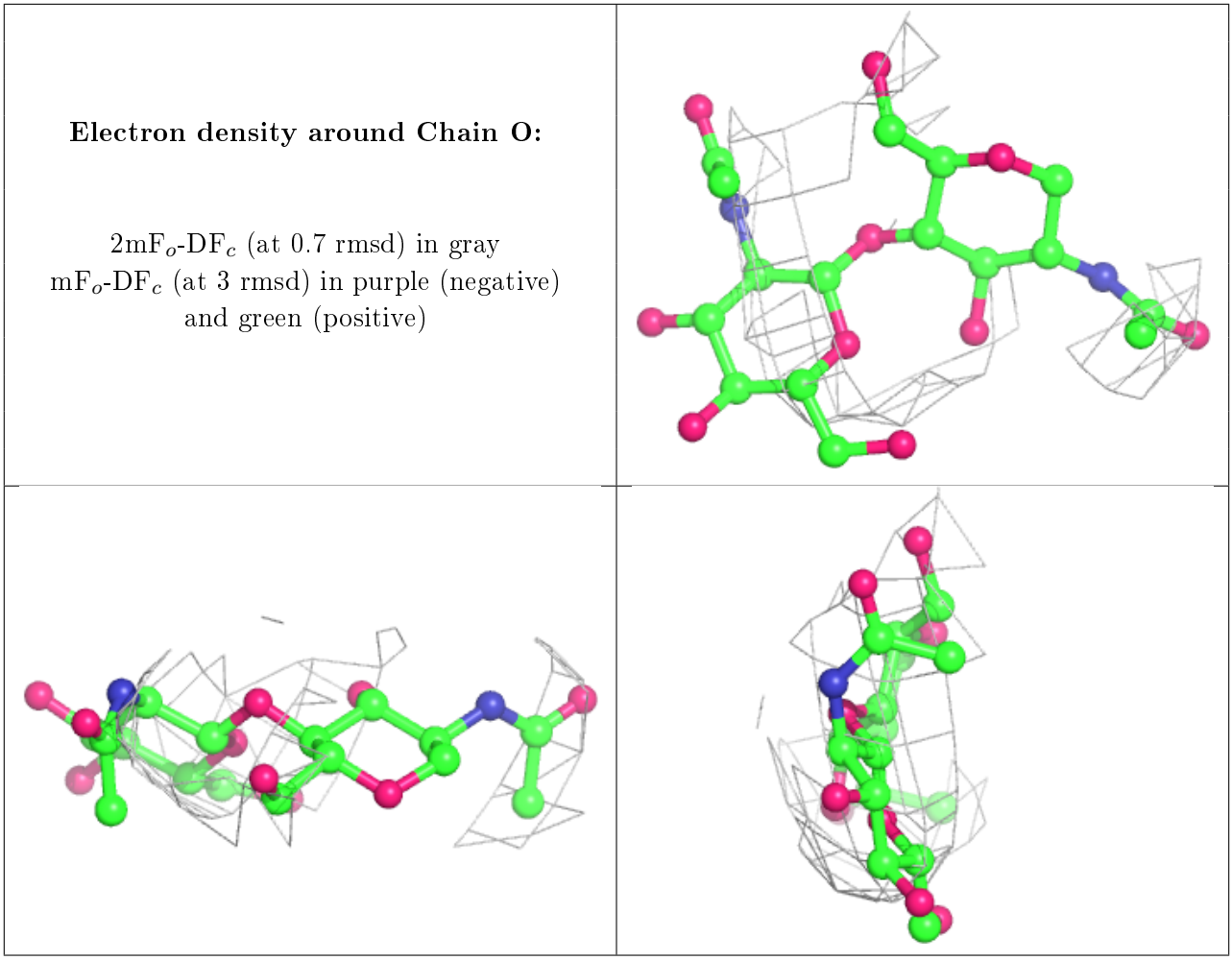






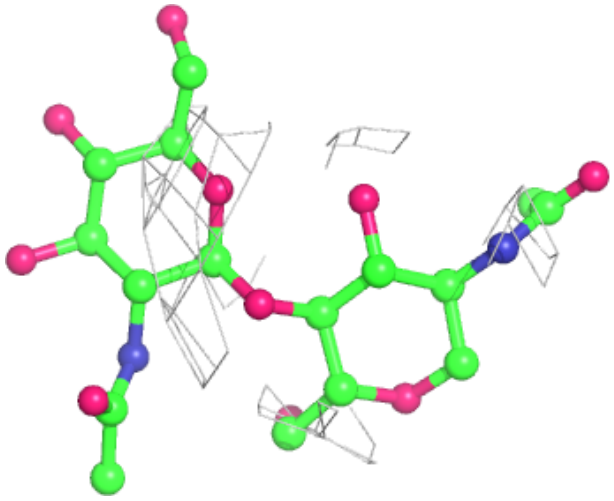
Electron density around Chain O:

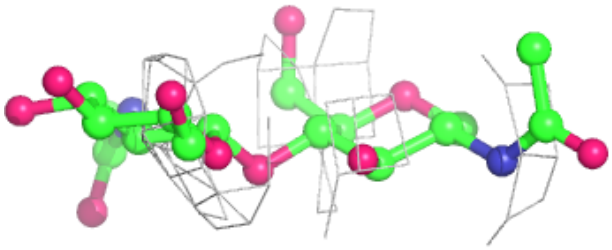
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

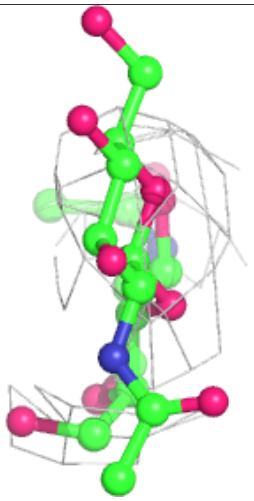


Electron density around Chain P:

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

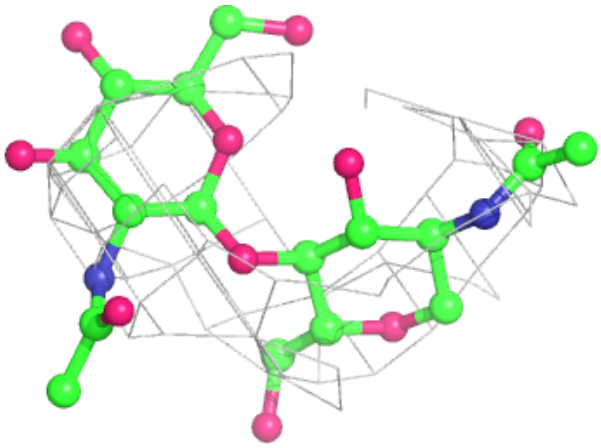


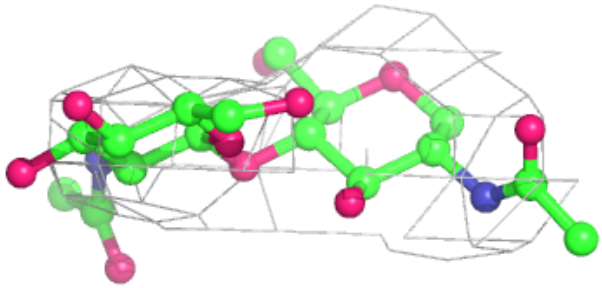


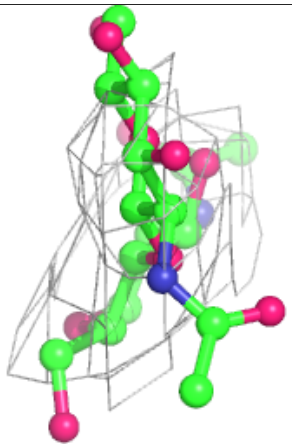


Electron density around Chain Q:

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

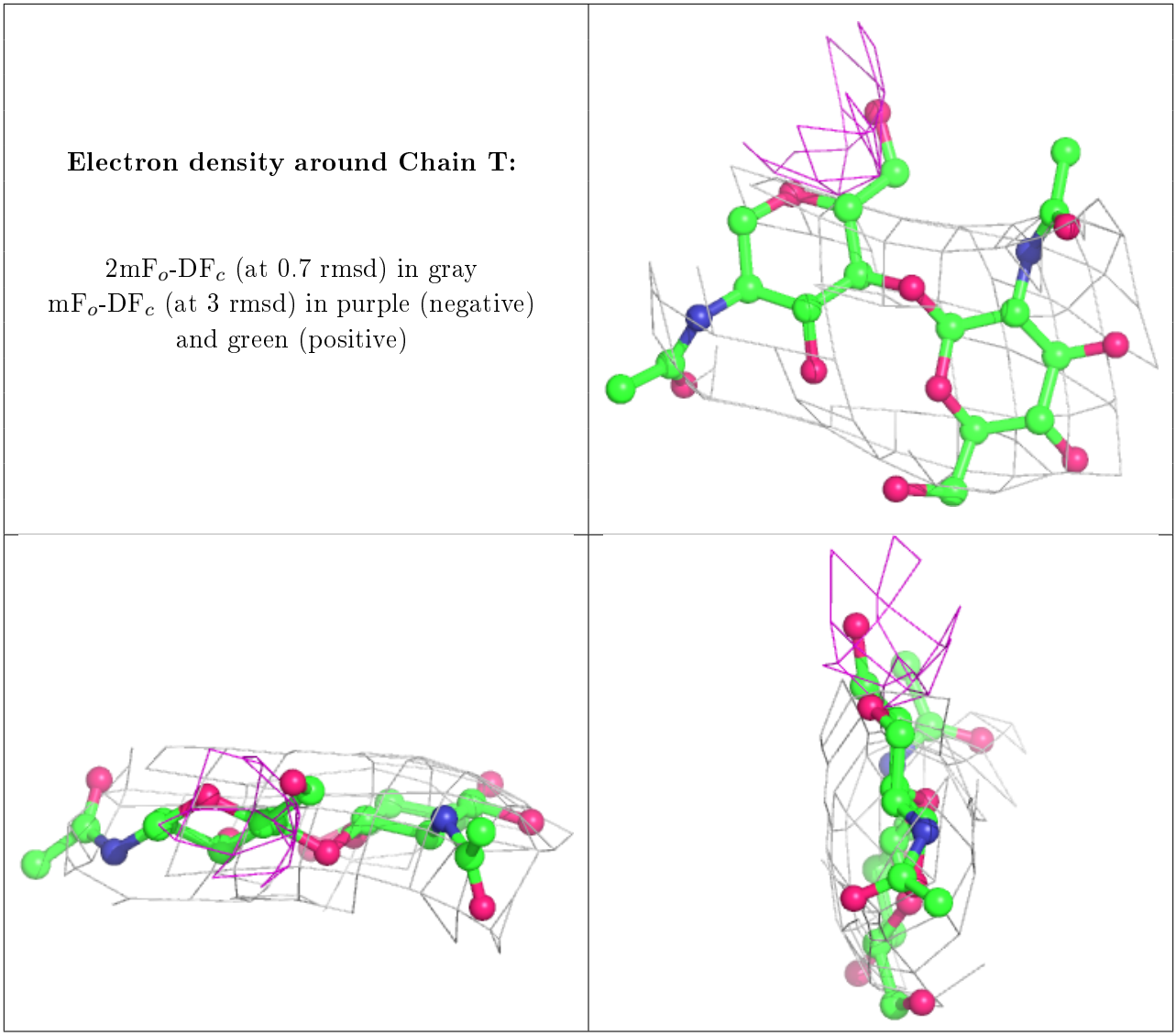






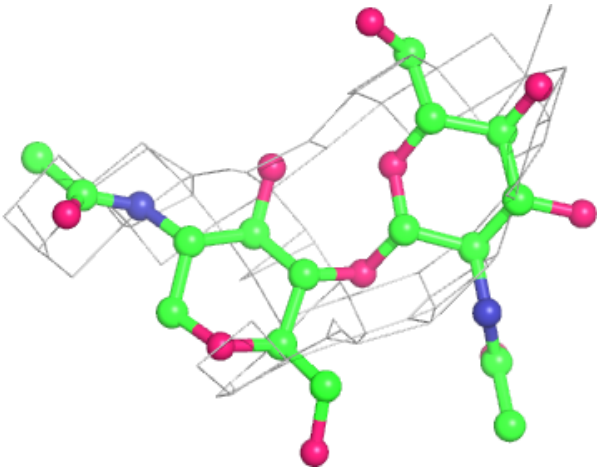
Electron density around Chain T:

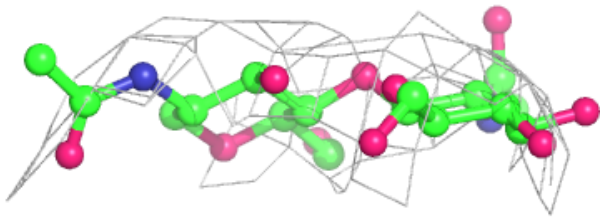
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

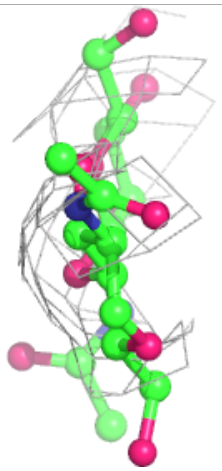


Electron density around Chain V:

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

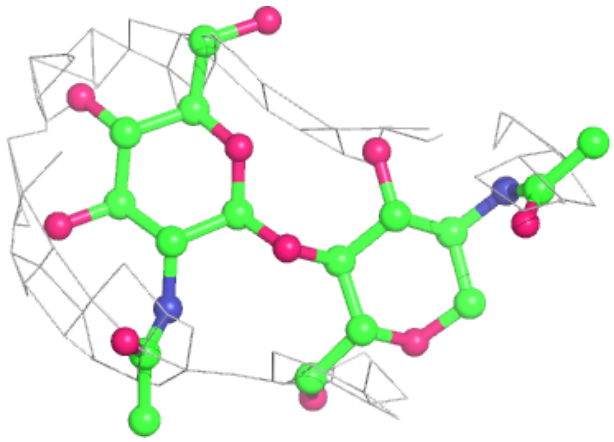


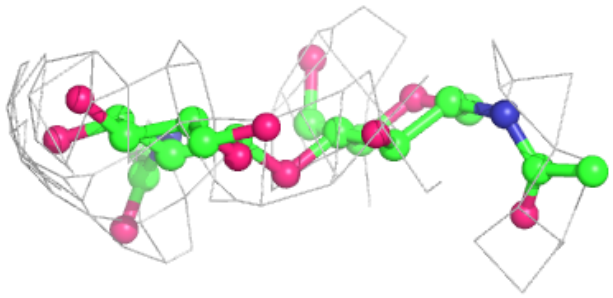


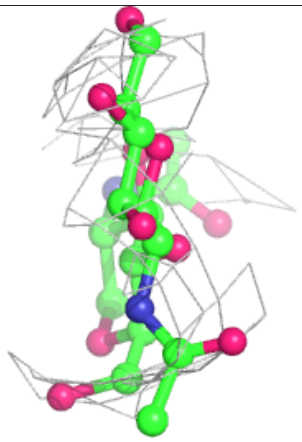


Electron density around Chain W:

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

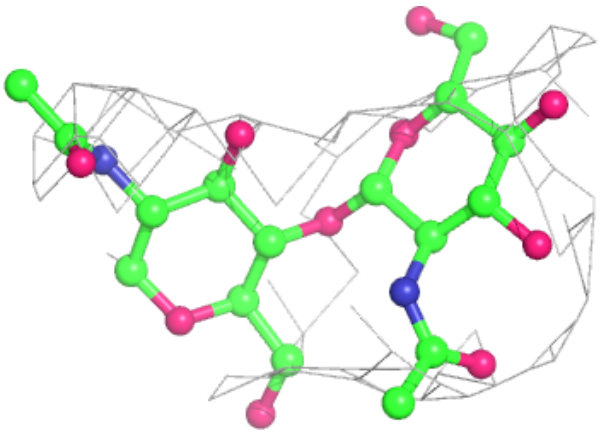


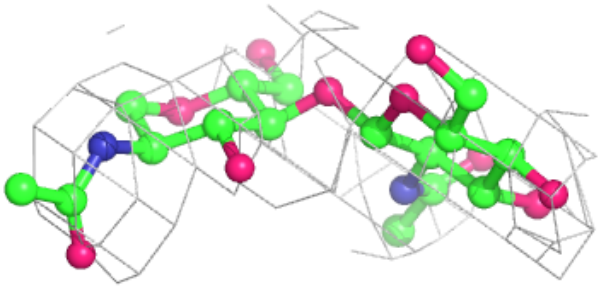


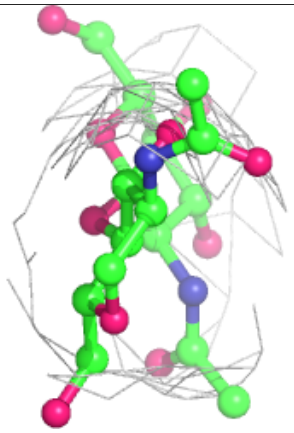


Electron density around Chain X:

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

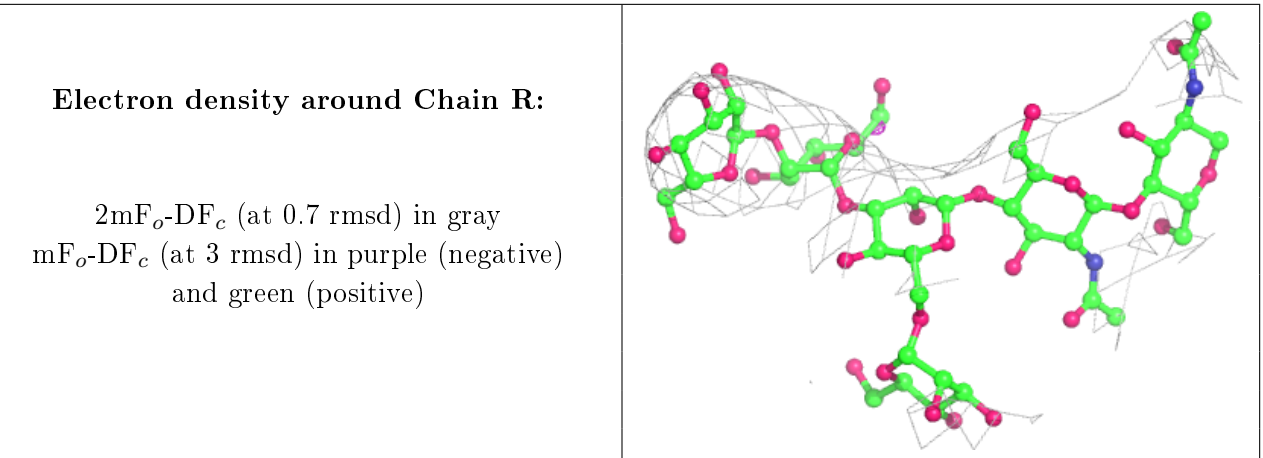


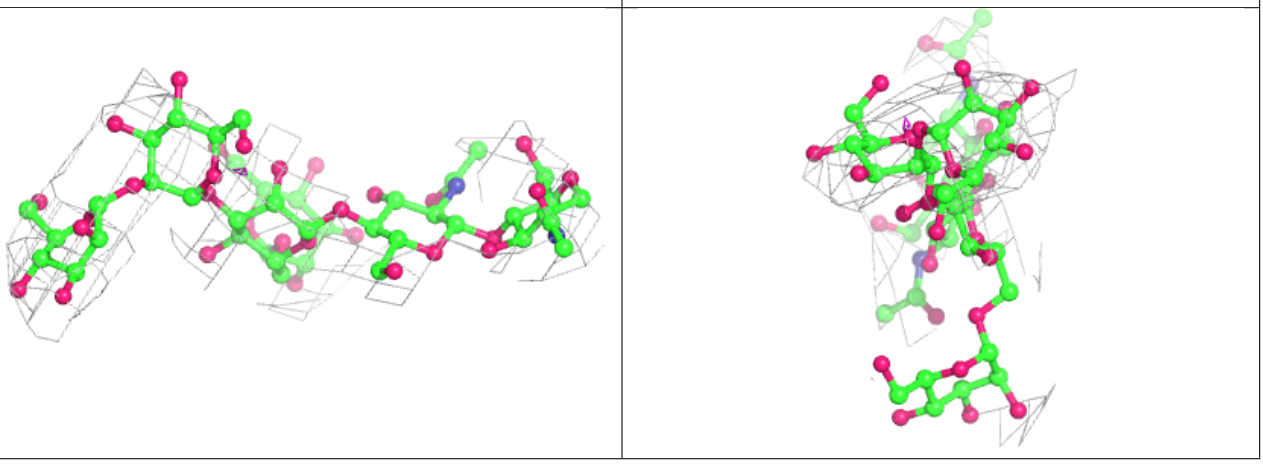




Electron density around Chain R:

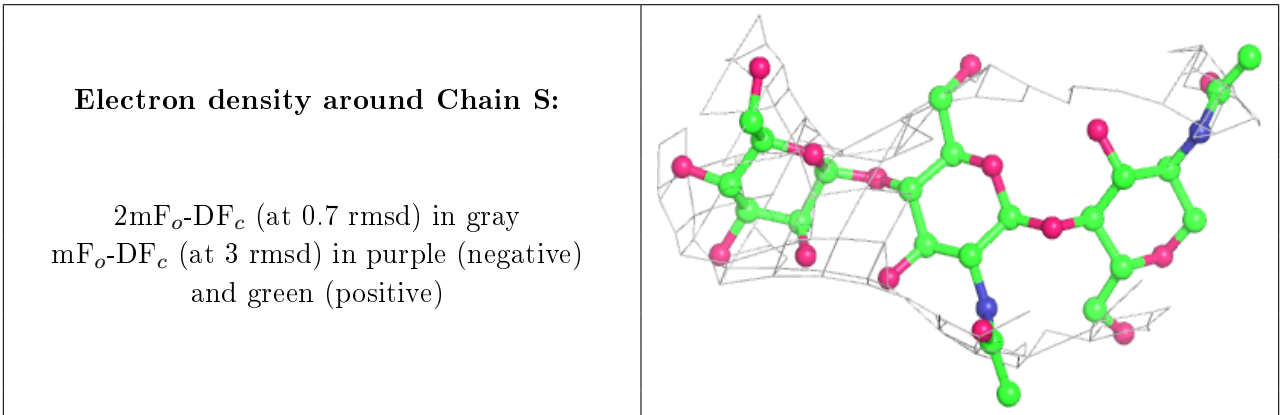
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

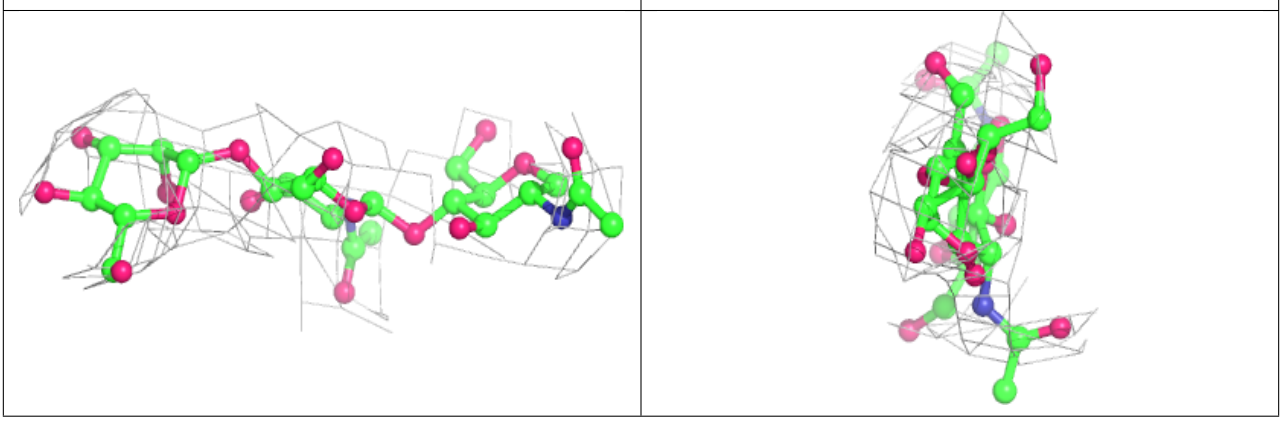




Electron density around Chain S:

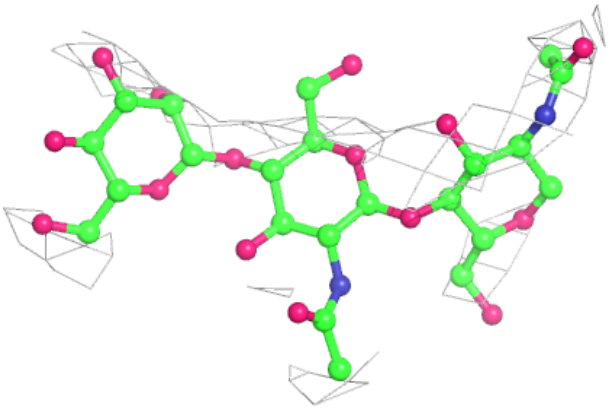
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

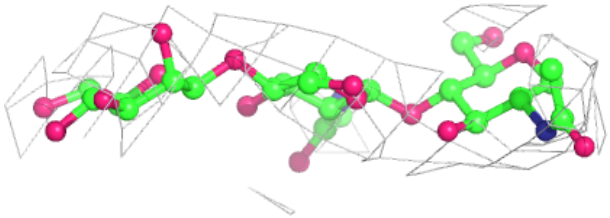


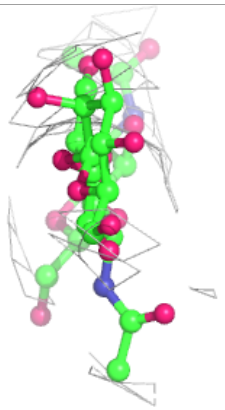


Electron density around Chain Y:

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

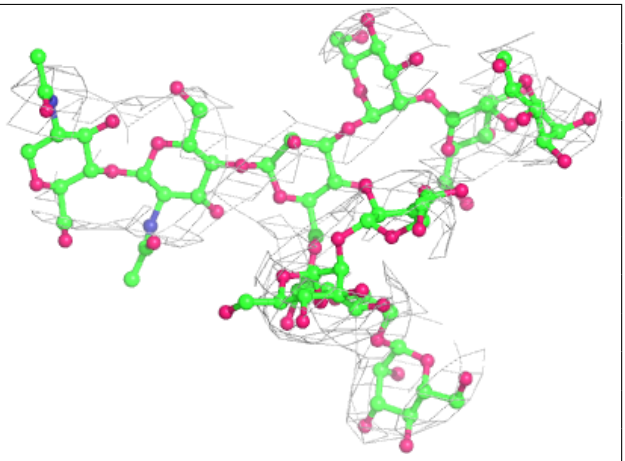


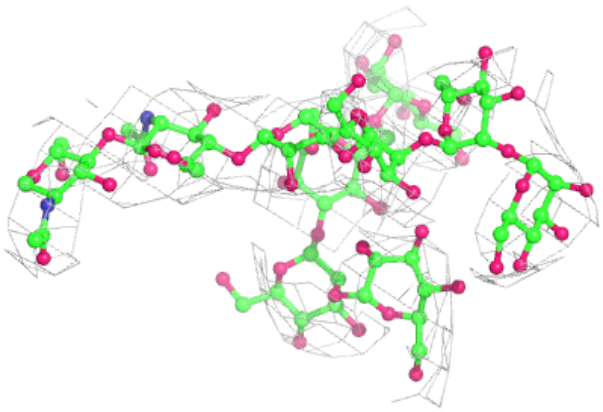


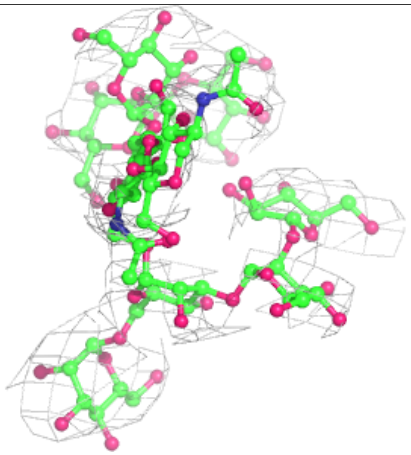


Electron density around Chain U:

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







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
14	NAG	I	305	14/15	0.05	1.66	262,282,291,294	0
14	NAG	K	301	14/15	0.43	0.87	255,274,293,293	0
14	NAG	B	902	14/15	0.52	1.27	260,274,299,300	0
14	NAG	C	909	14/15	0.57	0.43	197,225,250,254	0
14	NAG	D	902	14/15	0.60	0.24	225,248,271,272	0
14	NAG	A	942	14/15	0.64	0.52	246,259,268,272	0
14	NAG	D	901	14/15	0.77	0.37	265,277,303,319	0
14	NAG	B	903	14/15	0.79	0.43	230,262,292,295	0
14	NAG	C	908	14/15	0.80	0.28	232,249,265,272	0
14	NAG	A	908	14/15	0.82	0.26	217,234,248,253	0
14	NAG	C	953	14/15	0.82	0.16	212,234,244,246	0
14	NAG	C	942	14/15	0.83	0.32	230,246,255,260	0
14	NAG	A	926	14/15	0.85	0.30	210,217,221,223	0
14	NAG	C	927	14/15	0.87	0.67	218,225,232,234	0
14	NAG	B	901	14/15	0.88	0.34	239,260,288,303	0
14	NAG	A	952	14/15	0.89	0.16	233,255,262,265	0

6.5 Other polymers

There are no such residues in this entry.