Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 04:17 PM EDT

PDB ID	:	5T3X
Title	:	3.9 Angstrom Crystal Structure of a Fully and Natively Glycosylated BG505 SOSIP.664 HIV-1 Env Trimer in Complex with the Broadly Neutralizing Antibodies IOMA and 10-1074.
Authors	:	Gristick, H.B.; Bjorkman, P.J.
Deposited on	:	2016-08-26
Resolution	:	3.90 Å(reported)

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

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

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

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

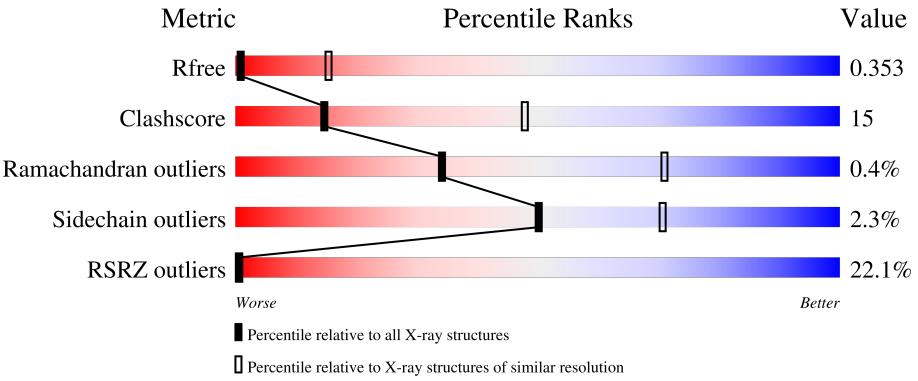
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.90 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	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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

Mol	Chain	Length	Quality of chain
1	B	153	10% 49% 32% · 18%
2	G	481	8% 58% 34% · 7%
3	H	238	29% 67% 29% · ·
4	L	214	20% 67% 29% · ·
5	D	232	29% 59% 37% · ·

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Mol	Chain	Length	Quality of chain
6	E	214	42% 67% 29%
7	A	2	100%
8	C	4	50% 50%
9	F	3	67% 33%
10	I	3	33% 33% 33%
11	J	13	38% 31% 31%
12	K	10	40% 40% 20%
13	M	9	22% 56% 22%
14	N	2	50% 50%
14	Q	2	100%
14	T	2	100%
15	O	7	14% 86%
16	P	16	19% 56% 25%
17	R	7	29% 29% 43%
18	S	10	20% 30% 50%
19	U	7	29% 71%
20	V	5	20% 40% 40%
21	W	6	33% 50% 17%
22	X	5	40% 20% 40%

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
12	GAL	K	6	-	-	-	X
13	SIA	M	7	-	-	-	X
13	NAG	M	9	-	-	-	X
15	MAN	O	5	-	-	-	X
15	MAN	O	6	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	MAN	O	7	-	-	-	X
16	SIA	P	12	-	-	-	X
16	NAG	P	13	-	-	-	X
16	GAL	P	14	-	-	-	X
16	NAG	P	15	-	-	-	X
16	FUC	P	16	-	-	-	X
17	NAG	R	1	-	-	-	X
17	NAG	R	2	-	-	-	X
17	NAG	R	5	-	-	-	X
18	MAN	S	9	-	-	-	X
19	NAG	U	1	-	-	-	X
19	NAG	U	2	-	-	-	X
20	MAN	V	4	-	-	-	X
21	MAN	W	5	-	-	-	X
22	NAG	X	1	-	-	-	X
22	MAN	X	4	-	-	-	X
22	MAN	X	5	-	-	-	X
7	FUC	A	2	-	-	-	X
9	FUC	F	3	-	-	-	X

2 Entry composition (i)

There are 23 unique types of molecules in this entry. The entry contains 12620 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	126	Total	C	N	O	S	0	0	0
			1001	633	172	190	6			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	449	Total	C	N	O	S	0	0	0
			3532	2217	623	665	27			

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called 10-1074 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	230	Total	C	N	O	S	0	0	0
			1753	1108	293	345	7			

- Molecule 4 is a protein called 10-1074 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	211	1607	1006	281	314	6	0	0	0

- Molecule 5 is a protein called IOMA Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	D	229	1742	1100	298	332	12	0	0	0

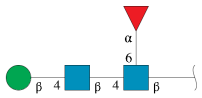
- Molecule 6 is a protein called IOMA Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	E	210	1558	976	261	317	4	0	0	0

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

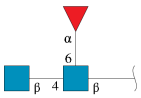
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
7	A	2	24	14	1	9	0	0	0

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



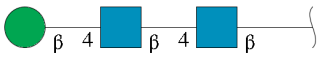
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	C	4	49	28	2	19	0	0	0

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



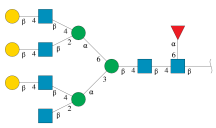
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	F	3	38	22	2	14	0	0	0

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



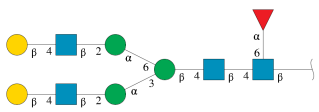
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
10	I	3	39	22	2	15	0	0	0

- Molecule 11 is an oligosaccharide called beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



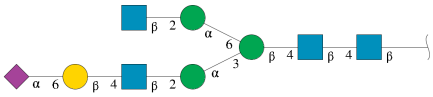
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
11	J	13	160	90	6	64	0	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
12	K	10	Total C N O 121 68 4 49	0	0	0

- Molecule 13 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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.

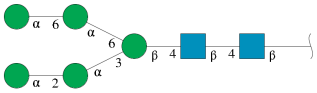


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
13	M	9	Total C N O 120 67 5 48	0	0	0

- Molecule 14 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

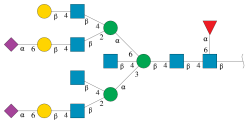
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
14	N	2	Total C N O 28 16 2 10	0	0	0
14	Q	2	Total C N O 28 16 2 10	0	0	0
14	T	2	Total C N O 28 16 2 10	0	0	0

- Molecule 15 is an oligosaccharide called 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.



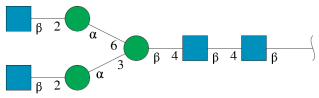
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	O	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 16 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



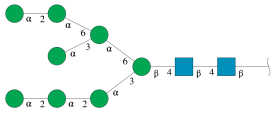
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
16	P	16	Total	C	N	O	0	0	0
			214	120	9	85			

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



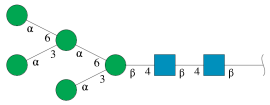
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	R	7	Total	C	N	O	0	0	0
			89	50	4	35			

- Molecule 18 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-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



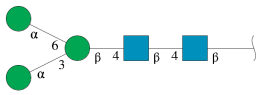
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	S	10	Total	C	N	O	0	0	0
			116	64	2	50			

- Molecule 19 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.



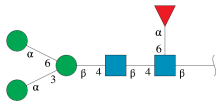
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	U	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 20 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
20	V	5	Total	C	N	O	0	0	0
			61	34	2	25			

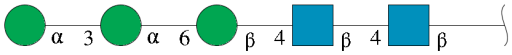
- Molecule 21 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	W	6	Total	C	N	O	0	0	0
			71	40	2	29			

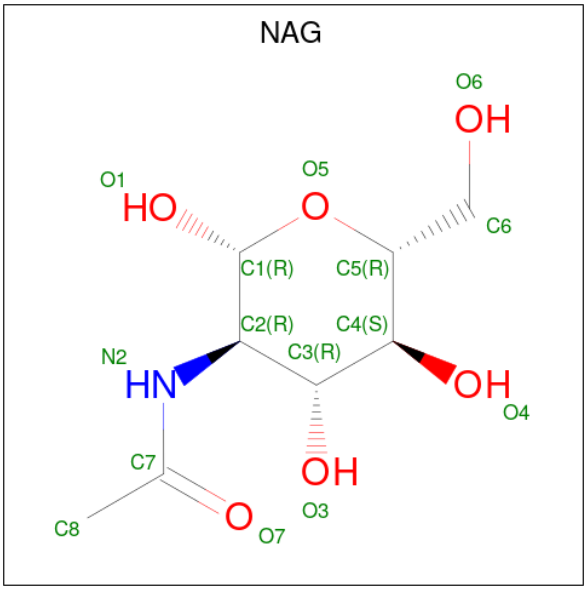
- Molecule 22 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-

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



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

- Molecule 23 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

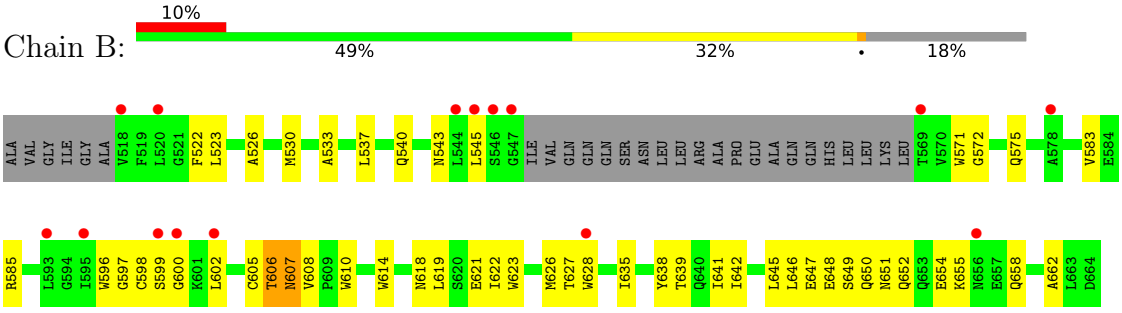


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	G	1	Total C N O 14 8 1 5	0	0

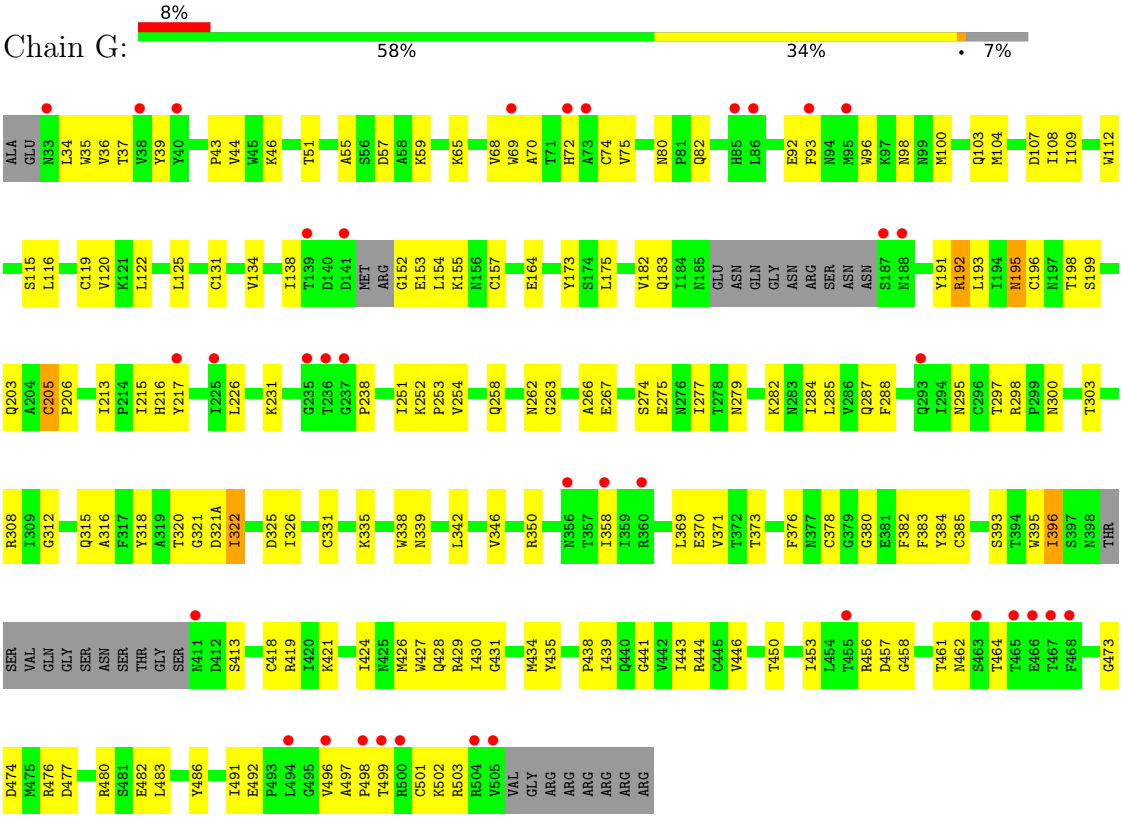
3 Residue-property plots (i)

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

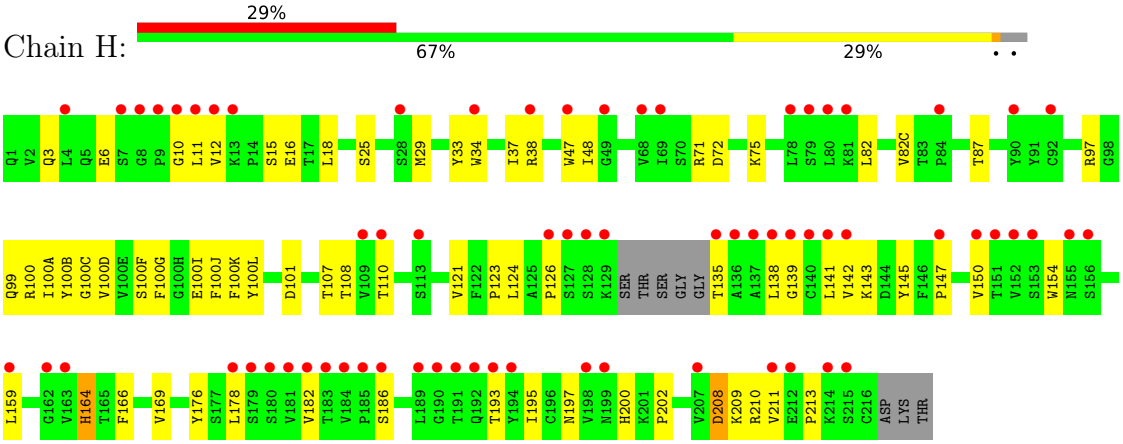
• Molecule 1: Envelope glycoprotein gp160



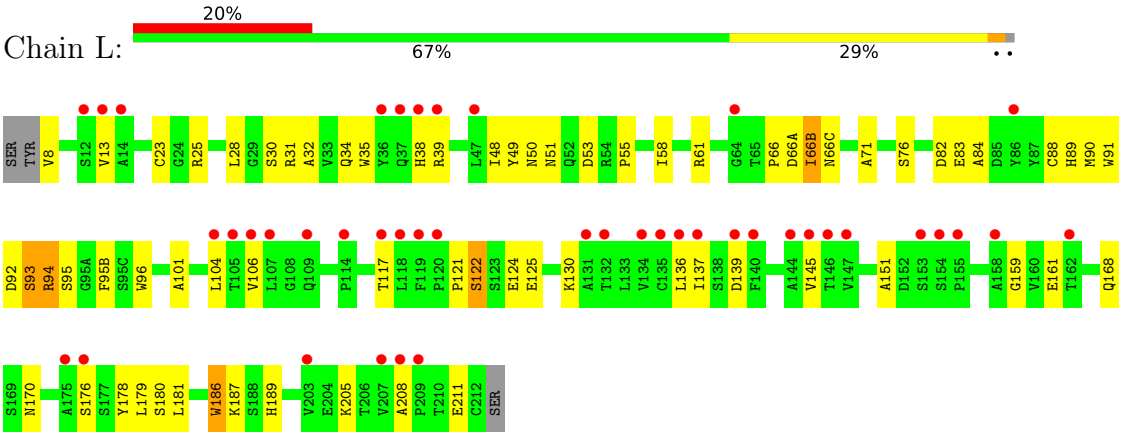
• Molecule 2: Envelope glycoprotein gp160



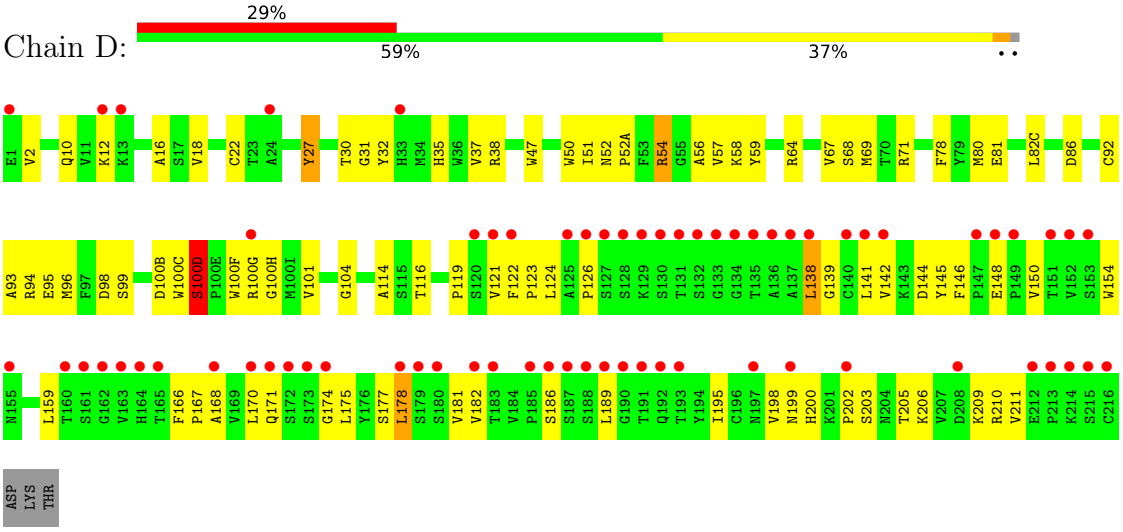
• Molecule 3: 10-1074 Heavy Chain



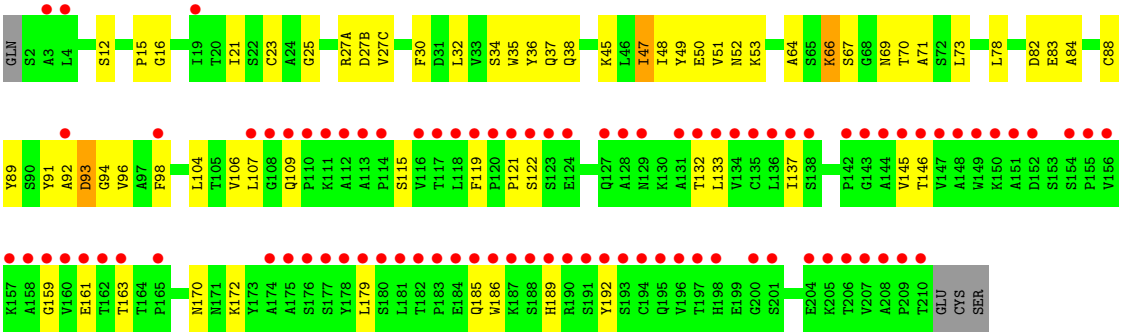
• Molecule 4: 10-1074 Light Chain



• Molecule 5: IOMA Heavy Chain

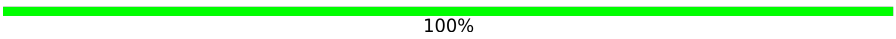


• Molecule 6: IOMA Light Chain



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

Chain A:



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

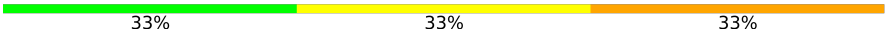
Chain C:

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

Chain F:

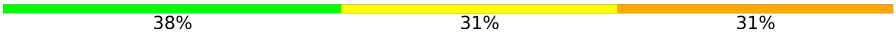
• Molecule 10: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

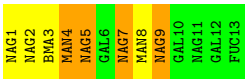
Chain I:



• Molecule 11: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)]alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

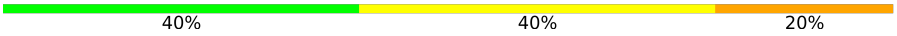
Chain J:

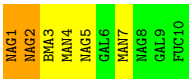




• Molecule 12: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyrano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

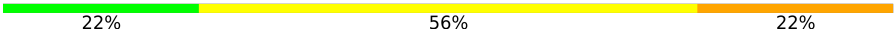
Chain K:

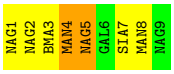




• Molecule 13: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:





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

Chain N:

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

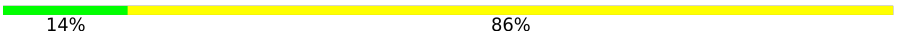
Chain Q:

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

Chain T:

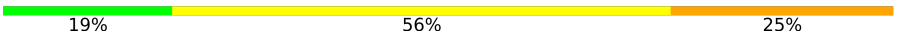
• Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

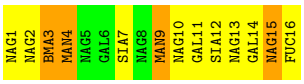
Chain O:



• Molecule 16: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-6)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

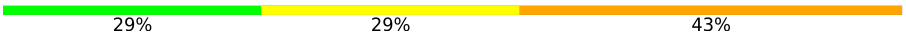
Chain P:





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

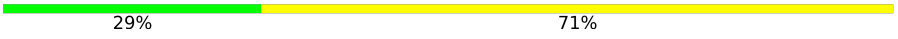


• Molecule 18: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

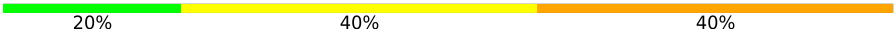
• Molecule 19: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



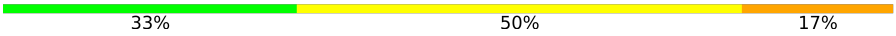
• Molecule 20: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



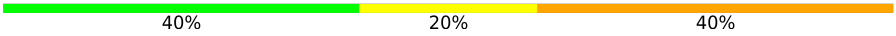
• Molecule 21: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



• Molecule 22: 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 X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	217.51Å 217.51Å 156.01Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	80.63 – 3.90 80.63 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (80.63-3.90) 95.7 (80.63-3.90)	Depositor EDS
R_{merge}	0.35	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 3.89Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.296 , 0.331 0.317 , 0.353	Depositor DCC
R_{free} test set	1276 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	134.0	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 326.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.075 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.160 for k,h,-l	Depositor
Outliers	0 of 25075 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12620	wwPDB-VP
Average B, all atoms (Å^2)	302.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	B	0.25	0/1019	0.45	0/1382
2	G	0.28	0/3605	0.53	2/4895 (0.0%)
3	H	0.25	0/1796	0.48	0/2450
4	L	0.26	0/1649	0.47	0/2250
5	D	0.27	0/1790	0.55	2/2437 (0.1%)
6	E	0.26	0/1596	0.50	0/2175
All	All	0.26	0/11455	0.51	4/15589 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	100(D)	SER	C-N-CD	-8.05	102.89	120.60
2	G	458	GLY	O-C-N	-8.00	109.61	123.20
5	D	100(D)	SER	C-N-CA	6.31	148.50	122.00
2	G	458	GLY	CA-C-N	5.83	127.86	116.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1001	0	976	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	3532	0	3462	132	0
3	H	1753	0	1719	52	0
4	L	1607	0	1550	52	0
5	D	1742	0	1698	72	0
6	E	1558	0	1511	52	0
7	A	24	0	22	0	0
8	C	49	0	43	0	0
9	F	38	0	34	0	0
10	I	39	0	34	1	0
11	J	160	0	136	2	0
12	K	121	0	103	1	0
13	M	120	0	101	1	0
14	N	28	0	25	0	0
14	Q	28	0	25	0	0
14	T	28	0	25	0	0
15	O	83	0	70	2	0
16	P	214	0	180	5	0
17	R	89	0	76	3	0
18	S	116	0	97	4	0
19	U	83	0	70	0	0
20	V	61	0	52	1	0
21	W	71	0	61	1	0
22	X	61	0	52	1	0
23	G	14	0	13	1	0
All	All	12620	0	12135	378	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 15.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:55:ALA:HB3	2:G:216:HIS:HB2	1.57	0.87
6:E:47:ILE:HG22	6:E:48:ILE:HG12	1.61	0.82
2:G:119:CYS:SG	2:G:205:CYS:N	2.50	0.81
5:D:199:ASN:OD1	5:D:206:LYS:NZ	2.13	0.80
2:G:297:THR:HG22	2:G:444:ARG:HG3	1.63	0.78
5:D:119:PRO:HB3	5:D:145:TYR:HB3	1.66	0.77
2:G:51:THR:HA	2:G:103:GLN:HE22	1.52	0.75
2:G:175:LEU:O	2:G:320:THR:OG1	2.06	0.73
5:D:119:PRO:HD2	5:D:205:THR:HB	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:ILE:HG21	2:G:496:VAL:HG11	1.72	0.72
3:H:100:ARG:NH2	4:L:66(A):ASP:OD2	2.22	0.72
1:B:606:THR:HG21	1:B:646:LEU:HD22	1.71	0.72
5:D:52(A):PRO:HG3	5:D:78:PHE:HZ	1.54	0.71
4:L:13:VAL:HG23	4:L:104:LEU:HD11	1.75	0.69
5:D:35:HIS:HD2	5:D:50:TRP:HB3	1.55	0.69
2:G:65:LYS:HB2	2:G:68:VAL:HG23	1.75	0.69
5:D:51:ILE:HG23	5:D:57:VAL:HG12	1.74	0.69
5:D:150:VAL:HG11	5:D:198:VAL:HG13	1.75	0.68
16:P:3:BMA:H2	16:P:4:MAN:H5	1.75	0.68
2:G:279:ASN:HD22	2:G:282:LYS:HG2	1.58	0.68
11:J:5:NAG:H81	11:J:9:NAG:H82	1.76	0.67
1:B:606:THR:OG1	2:G:36:VAL:O	2.11	0.67
2:G:69:TRP:HE1	2:G:253:PRO:HG2	1.60	0.67
4:L:39:ARG:NH1	4:L:83:GLU:O	2.27	0.67
2:G:303:THR:HB	2:G:321:GLY:HA3	1.75	0.67
2:G:131:CYS:HB3	2:G:155:LYS:HB3	1.77	0.66
2:G:92:GLU:HA	2:G:238:PRO:HA	1.77	0.66
4:L:25:ARG:HH21	4:L:90:MET:H	1.42	0.66
3:H:38:ARG:HG3	3:H:48:ILE:HD11	1.79	0.65
3:H:16:GLU:H	3:H:82(C):VAL:HG22	1.61	0.65
2:G:258:GLN:NE2	2:G:371:VAL:O	2.29	0.65
2:G:424:ILE:HG22	2:G:426:MET:H	1.63	0.64
6:E:48:ILE:HG21	6:E:64:ALA:HB3	1.78	0.64
3:H:195:ILE:HG12	3:H:210:ARG:HG2	1.79	0.64
3:H:11:LEU:HD13	3:H:147:PRO:HG3	1.80	0.64
5:D:37:VAL:HG22	5:D:47:TRP:HA	1.81	0.63
3:H:100(B):TYR:CE2	4:L:93:SER:HB2	2.34	0.63
4:L:159:GLY:O	4:L:180:SER:N	2.27	0.63
2:G:456:ARG:NH2	6:E:93:ASP:OD1	2.25	0.62
4:L:83:GLU:HG2	4:L:106:VAL:H	1.64	0.62
6:E:66:LYS:HA	6:E:71:ALA:HA	1.81	0.62
4:L:23:CYS:HB2	4:L:71:ALA:HB3	1.81	0.62
1:B:596:TRP:O	1:B:651:ASN:ND2	2.32	0.62
1:B:526:ALA:HA	2:G:43:PRO:HB2	1.82	0.62
4:L:61:ARG:NH1	4:L:76:SER:O	2.29	0.61
4:L:35:TRP:HB2	4:L:48:ILE:HB	1.81	0.61
3:H:3:GLN:HG3	3:H:25:SER:HB2	1.82	0.61
2:G:439:ILE:HB	2:G:443:ILE:HD11	1.81	0.61
1:B:654:GLU:OE1	2:G:503:ARG:NH1	2.32	0.61
5:D:123:PRO:HD3	5:D:209:LYS:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:251:ILE:HG23	2:G:482:GLU:HG3	1.83	0.60
5:D:27:TYR:HE2	5:D:32:TYR:HB2	1.65	0.60
2:G:266:ALA:N	2:G:288:PHE:O	2.31	0.60
6:E:23:CYS:HB3	6:E:71:ALA:HB3	1.81	0.60
2:G:477:ASP:OD1	2:G:480:ARG:NH1	2.34	0.60
1:B:540:GLN:HE22	2:G:43:PRO:HG3	1.66	0.60
1:B:537:LEU:HD13	1:B:602:LEU:O	2.02	0.60
4:L:137:ILE:HD13	4:L:145:VAL:HG11	1.83	0.60
3:H:47:TRP:HE3	4:L:96:TRP:HA	1.67	0.60
4:L:25:ARG:NH2	4:L:90:MET:H	2.00	0.59
5:D:95:GLU:HA	5:D:100(H):GLY:O	2.03	0.59
4:L:28:LEU:HB3	4:L:94:ARG:HB2	1.84	0.59
2:G:274:SER:HB3	2:G:277:ILE:HG12	1.85	0.59
1:B:533:ALA:HB1	2:G:43:PRO:HG2	1.85	0.58
5:D:35:HIS:CD2	5:D:50:TRP:HB3	2.37	0.58
5:D:142:VAL:HG11	5:D:150:VAL:HG21	1.85	0.58
20:V:1:NAG:O3	20:V:2:NAG:N2	2.35	0.58
6:E:34:SER:N	6:E:89:TYR:O	2.31	0.58
2:G:195:ASN:ND2	2:G:199:SER:O	2.34	0.58
5:D:2:VAL:HG11	5:D:94:ARG:HH12	1.67	0.58
5:D:141:LEU:HD12	5:D:178:LEU:O	2.03	0.58
1:B:598:CYS:C	1:B:600:GLY:H	2.08	0.58
1:B:638:TYR:HA	1:B:641:ILE:HD12	1.86	0.58
5:D:195:ILE:HG12	5:D:210:ARG:HG2	1.86	0.57
4:L:179:LEU:HG	4:L:181:LEU:HD13	1.86	0.57
5:D:150:VAL:HB	5:D:178:LEU:HD21	1.86	0.57
5:D:10:GLN:HB3	5:D:12:LYS:HE2	1.86	0.57
5:D:116:THR:HG23	5:D:203:SER:HA	1.86	0.57
5:D:145:TYR:HE1	5:D:148:GLU:HA	1.70	0.57
6:E:92:ALA:C	6:E:94:GLY:H	2.07	0.57
1:B:650:GLN:O	1:B:654:GLU:N	2.32	0.57
5:D:47:TRP:HZ2	5:D:50:TRP:HD1	1.52	0.57
1:B:647:GLU:HG3	1:B:648:GLU:HG3	1.87	0.57
3:H:100:ARG:NH1	3:H:100(A):ILE:O	2.37	0.57
6:E:109:GLN:HE22	6:E:172:LYS:HG2	1.68	0.57
2:G:370:GLU:OE1	2:G:428:GLN:NE2	2.38	0.56
22:X:1:NAG:O3	22:X:2:NAG:N2	2.38	0.56
2:G:182:VAL:HG13	2:G:192:ARG:HD3	1.87	0.56
1:B:606:THR:OG1	2:G:36:VAL:HG23	2.06	0.56
2:G:34:LEU:HB3	2:G:498:PRO:HB2	1.86	0.56
2:G:285:LEU:HD22	2:G:453:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:147:PRO:O	3:H:200:HIS:NE2	2.38	0.56
2:G:441:GLY:HA3	17:R:1:NAG:H82	1.88	0.56
5:D:68:SER:HB3	5:D:81:GLU:HB3	1.87	0.56
5:D:18:VAL:HG23	5:D:82(C):LEU:HD11	1.88	0.56
3:H:193:THR:HG21	3:H:210:ARG:CZ	2.36	0.56
2:G:155:LYS:O	2:G:175:LEU:HA	2.05	0.56
5:D:52(A):PRO:HG3	5:D:78:PHE:CZ	2.39	0.56
2:G:369:LEU:O	2:G:373:THR:OG1	2.23	0.55
5:D:159:LEU:HD21	5:D:182:VAL:HG21	1.88	0.55
4:L:32:ALA:N	4:L:91:TRP:O	2.32	0.55
2:G:385:CYS:HA	2:G:418:CYS:HA	1.87	0.55
6:E:21:ILE:HD12	6:E:73:LEU:HD23	1.88	0.55
2:G:380:GLY:HA3	2:G:439:ILE:HG13	1.89	0.54
4:L:117:THR:HA	4:L:205:LYS:HG3	1.89	0.54
4:L:186:TRP:CD1	4:L:187:LYS:HG3	2.42	0.54
5:D:142:VAL:O	5:D:177:SER:HA	2.06	0.54
6:E:15:PRO:HD3	6:E:106:VAL:HG13	1.88	0.54
2:G:193:LEU:HB2	2:G:196:CYS:SG	2.47	0.54
2:G:69:TRP:CG	2:G:70:ALA:N	2.75	0.54
2:G:325:ASP:OD1	4:L:30:SER:N	2.25	0.54
12:K:1:NAG:H62	12:K:2:NAG:H82	1.89	0.54
5:D:52:ASN:HB3	5:D:56:ALA:HB3	1.90	0.54
1:B:628:TRP:CD1	2:G:43:PRO:HD2	2.42	0.54
1:B:530:MET:HG2	1:B:628:TRP:CG	2.43	0.54
2:G:100:MET:HB2	2:G:483:LEU:HD13	1.90	0.54
5:D:69:MET:HG2	5:D:80:MET:HG2	1.90	0.54
2:G:119:CYS:HB3	2:G:203:GLN:O	2.08	0.53
1:B:545:LEU:HD11	1:B:583:VAL:HG12	1.89	0.53
6:E:92:ALA:O	6:E:94:GLY:N	2.34	0.53
4:L:50:ASN:O	18:S:5:MAN:O3	2.24	0.53
3:H:166:PHE:HB3	4:L:176:SER:HB3	1.90	0.53
2:G:98:ASN:ND2	2:G:486:TYR:O	2.42	0.53
6:E:50:GLU:OE1	6:E:53:LYS:NZ	2.29	0.53
2:G:320:THR:HG22	2:G:438:PRO:HG3	1.91	0.52
3:H:142:VAL:HB	3:H:178:LEU:HG	1.92	0.52
6:E:121:PRO:HD2	6:E:186:TRP:CZ2	2.44	0.52
2:G:252:LYS:HE3	2:G:262:ASN:HB3	1.91	0.52
5:D:22:CYS:O	5:D:78:PHE:N	2.40	0.52
2:G:183:GLN:HA	2:G:191:TYR:HA	1.92	0.52
2:G:430:ILE:HG22	2:G:431:GLY:H	1.75	0.52
3:H:123:PRO:HD2	4:L:124:GLU:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:166:PHE:CZ	4:L:136:LEU:HB3	2.44	0.52
2:G:499:THR:HG23	2:G:501:CYS:H	1.75	0.52
3:H:169:VAL:HG21	4:L:161:GLU:HB3	1.90	0.52
11:J:4:MAN:O3	11:J:7:NAG:O5	2.20	0.52
1:B:610:TRP:NE1	1:B:614:TRP:O	2.42	0.52
2:G:358:ILE:HG12	2:G:396:ILE:HG23	1.91	0.52
2:G:473:GLY:O	5:D:54:ARG:NH1	2.40	0.51
3:H:100(A):ILE:HG12	3:H:100(J):PHE:HB3	1.92	0.51
5:D:52:ASN:N	5:D:56:ALA:O	2.38	0.51
6:E:145:VAL:HG12	6:E:146:THR:N	2.25	0.51
1:B:523:LEU:HA	1:B:540:GLN:NE2	2.25	0.51
4:L:208:ALA:HB3	4:L:211:GLU:HG3	1.93	0.51
6:E:89:TYR:CE1	6:E:96:VAL:HG13	2.46	0.51
10:I:1:NAG:O6	10:I:2:NAG:N2	2.43	0.51
16:P:9:MAN:O5	16:P:15:NAG:H82	2.11	0.51
1:B:572:GLY:O	1:B:575:GLN:NE2	2.43	0.51
2:G:55:ALA:O	2:G:216:HIS:N	2.36	0.51
2:G:153:GLU:HG3	2:G:419:ARG:HH21	1.75	0.51
3:H:100(D):VAL:HA	18:S:2:NAG:H2	1.92	0.51
4:L:34:GLN:HE21	4:L:91:TRP:HD1	1.59	0.51
5:D:35:HIS:N	5:D:93:ALA:O	2.38	0.51
3:H:99:GLN:HG3	3:H:100(J):PHE:CD2	2.45	0.51
6:E:12:SER:HB2	6:E:107:LEU:HD13	1.91	0.51
4:L:31:ARG:NH2	4:L:66:PRO:O	2.43	0.51
1:B:523:LEU:HA	1:B:540:GLN:HE21	1.74	0.51
3:H:101:ASP:OD1	3:H:101:ASP:N	2.44	0.51
4:L:31:ARG:O	4:L:51:ASN:ND2	2.43	0.51
4:L:82:ASP:HB2	4:L:106:VAL:HG21	1.93	0.51
5:D:126:PRO:HA	6:E:119:PHE:CE1	2.46	0.51
2:G:263:GLY:O	2:G:450:THR:HG21	2.12	0.50
2:G:55:ALA:N	2:G:216:HIS:O	2.44	0.50
4:L:28:LEU:O	4:L:92:ASP:HB2	2.11	0.50
2:G:274:SER:HB2	2:G:284:ILE:HG23	1.94	0.50
1:B:610:TRP:CD2	2:G:498:PRO:HB3	2.47	0.50
2:G:266:ALA:HB2	2:G:287:GLN:HB3	1.92	0.50
3:H:6:GLU:N	3:H:6:GLU:OE1	2.44	0.50
3:H:126:PRO:HD2	3:H:213:PRO:HA	1.94	0.50
5:D:31:GLY:O	5:D:98:ASP:HB3	2.12	0.50
1:B:610:TRP:CE3	2:G:36:VAL:HG12	2.47	0.50
5:D:186:SER:HA	5:D:189:LEU:HG	1.92	0.50
2:G:335:LYS:H	2:G:413:SER:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:12:VAL:HG21	3:H:18:LEU:HD12	1.94	0.49
5:D:30:THR:HA	5:D:52(A):PRO:HB2	1.94	0.49
5:D:100(G):ARG:HA	6:E:89:TYR:CE2	2.47	0.49
2:G:164:GLU:HA	2:G:312:GLY:O	2.12	0.49
2:G:55:ALA:HA	2:G:75:VAL:O	2.13	0.49
5:D:144:ASP:HA	5:D:175:LEU:HB3	1.94	0.49
6:E:37:GLN:N	6:E:45:LYS:O	2.45	0.49
2:G:109:ILE:HG12	2:G:427:TRP:CD2	2.48	0.49
5:D:200:HIS:CE1	5:D:203:SER:HG	2.26	0.49
2:G:215:ILE:N	2:G:251:ILE:O	2.39	0.49
21:W:2:NAG:H4	21:W:3:BMA:O2	2.12	0.49
1:B:522:PHE:CD1	1:B:523:LEU:HG	2.47	0.48
3:H:29:MET:HA	3:H:34:TRP:HZ2	1.78	0.48
5:D:100(G):ARG:HE	6:E:49:TYR:HD2	1.61	0.48
1:B:522:PHE:CE2	1:B:540:GLN:HA	2.47	0.48
2:G:326:ILE:HG12	4:L:94:ARG:NE	2.28	0.48
5:D:100(C):TRP:O	5:D:100(D):SER:HB2	2.13	0.48
2:G:393:SER:HB3	2:G:395:TRP:HE1	1.77	0.48
4:L:35:TRP:CZ3	4:L:88:CYS:HB2	2.48	0.48
5:D:166:PHE:HE2	5:D:181:VAL:HG13	1.78	0.48
4:L:92:ASP:OD1	4:L:95:SER:OG	2.28	0.48
5:D:50:TRP:CE2	5:D:58:LYS:HB3	2.49	0.48
2:G:46:LYS:HG3	2:G:492:GLU:HG3	1.95	0.48
3:H:100(C):GLY:HA3	3:H:100(I):GLU:OE1	2.13	0.48
6:E:121:PRO:HD3	6:E:133:LEU:HD21	1.95	0.48
2:G:378:CYS:HB3	2:G:383:PHE:CE1	2.48	0.48
3:H:159:LEU:HG	3:H:182:VAL:HG21	1.96	0.48
5:D:167:PRO:HD2	6:E:163:THR:HB	1.95	0.48
5:D:59:TYR:O	5:D:64:ARG:NH2	2.47	0.48
6:E:36:TYR:HE1	6:E:89:TYR:HB3	1.79	0.48
2:G:279:ASN:HB2	16:P:16:FUC:H61	1.96	0.47
3:H:100(K):PHE:HE2	4:L:91:TRP:HB3	1.79	0.47
2:G:474:ASP:OD1	2:G:476:ARG:NH1	2.47	0.47
5:D:99:SER:OG	5:D:100(B):ASP:O	2.32	0.47
1:B:635:ILE:O	1:B:639:THR:HG23	2.14	0.47
3:H:121:VAL:HA	3:H:141:LEU:O	2.14	0.47
4:L:122:SER:OG	4:L:125:GLU:N	2.33	0.47
2:G:104:MET:HG2	2:G:217:TYR:CZ	2.50	0.47
17:R:2:NAG:O3	17:R:3:BMA:O2	2.19	0.47
4:L:55:PRO:HD2	4:L:58:ILE:HG13	1.97	0.47
1:B:605:CYS:HA	2:G:37:THR:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:ASN:OD1	1:B:607:ASN:N	2.47	0.47
2:G:107:ASP:OD2	2:G:217:TYR:OH	2.32	0.47
6:E:27(B):ASP:O	6:E:30:PHE:HB2	2.14	0.47
6:E:185:GLN:O	6:E:192:TYR:OH	2.33	0.47
1:B:522:PHE:CE2	1:B:543:ASN:HB2	2.50	0.47
5:D:67:VAL:HG11	5:D:69:MET:HE3	1.97	0.46
1:B:571:TRP:CH2	2:G:74:CYS:HB2	2.50	0.46
2:G:279:ASN:ND2	2:G:282:LYS:HG2	2.25	0.46
2:G:298:ARG:HB2	2:G:383:PHE:HZ	1.79	0.46
2:G:338:TRP:O	2:G:342:LEU:HG	2.15	0.46
2:G:175:LEU:HD22	2:G:321(A):ASP:HA	1.97	0.46
3:H:38:ARG:HH12	3:H:82:LEU:HD22	1.79	0.46
3:H:124:LEU:HD23	4:L:122:SER:HB3	1.97	0.46
2:G:37:THR:OG1	2:G:497:ALA:O	2.33	0.46
2:G:206:PRO:HD3	2:G:318:TYR:CE2	2.51	0.46
1:B:645:LEU:HD12	1:B:649:SER:HB3	1.98	0.46
4:L:151:ALA:HB1	4:L:189:HIS:CD2	2.51	0.46
5:D:51:ILE:HD11	5:D:69:MET:HB3	1.98	0.46
6:E:27(B):ASP:OD1	6:E:27(C):VAL:N	2.43	0.46
13:M:4:MAN:H4	13:M:5:NAG:H83	1.97	0.46
5:D:168:ALA:HA	5:D:178:LEU:HB3	1.98	0.46
6:E:145:VAL:HG12	6:E:146:THR:H	1.80	0.46
2:G:192:ARG:NH2	2:G:193:LEU:O	2.44	0.46
4:L:8:VAL:HG12	4:L:101:ALA:HB3	1.98	0.45
1:B:651:ASN:O	1:B:655:LYS:HB2	2.15	0.45
3:H:166:PHE:CG	4:L:136:LEU:HD22	2.51	0.45
4:L:34:GLN:HB2	4:L:89:HIS:HB3	1.98	0.45
6:E:48:ILE:HA	6:E:53:LYS:O	2.16	0.45
2:G:122:LEU:O	2:G:125:LEU:HB2	2.16	0.45
5:D:138:LEU:HB2	5:D:211:VAL:HG11	1.98	0.45
4:L:49:TYR:O	4:L:53:ASP:HB2	2.16	0.45
4:L:66(A):ASP:O	18:S:4:MAN:O3	2.29	0.45
3:H:135:THR:N	3:H:186:SER:HG	2.14	0.45
5:D:38:ARG:HH22	5:D:86:ASP:HA	1.81	0.45
2:G:384:TYR:CE1	2:G:421:LYS:HB3	2.51	0.45
1:B:658:GLN:O	1:B:662:ALA:N	2.50	0.45
2:G:44:VAL:HG12	2:G:492:GLU:HB2	1.98	0.45
5:D:96:MET:HG2	5:D:101:VAL:HG23	1.97	0.45
1:B:623:TRP:HH2	2:G:39:TYR:CE1	2.35	0.45
5:D:121:VAL:HG21	5:D:198:VAL:HG11	1.99	0.45
6:E:35:TRP:CZ3	6:E:88:CYS:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:80:ASN:O	2:G:82:GLN:N	2.49	0.44
3:H:142:VAL:HG11	3:H:150:VAL:HG11	1.99	0.44
1:B:571:TRP:HZ3	2:G:72:HIS:H	1.65	0.44
2:G:339:ASN:OD1	23:G:3390:NAG:N2	2.51	0.44
2:G:434:MET:HG2	2:G:435:TYR:N	2.33	0.44
2:G:35:TRP:O	2:G:498:PRO:HA	2.18	0.44
2:G:384:TYR:O	2:G:419:ARG:N	2.46	0.44
16:P:4:MAN:H2	16:P:15:NAG:H61	1.99	0.44
5:D:170:LEU:HD11	5:D:174:GLY:HA2	1.98	0.44
5:D:171:GLN:HG2	6:E:161:GLU:OE1	2.18	0.44
6:E:185:GLN:O	6:E:189:HIS:ND1	2.48	0.44
1:B:610:TRP:HE3	2:G:36:VAL:HG12	1.83	0.44
1:B:618:ASN:HB2	1:B:621:GLU:HG3	1.98	0.44
2:G:120:VAL:HG11	2:G:316:ALA:O	2.17	0.44
3:H:10:GLY:HA3	3:H:202:PRO:HG3	2.00	0.44
4:L:66(B):ILE:O	4:L:66(C):ASN:HB2	2.18	0.44
5:D:122:PHE:CE2	5:D:141:LEU:HD23	2.53	0.44
2:G:198:THR:OG1	2:G:199:SER:N	2.51	0.43
18:S:8:MAN:H2	18:S:9:MAN:H2	1.78	0.43
2:G:298:ARG:HB2	2:G:383:PHE:CZ	2.53	0.43
2:G:350:ARG:NH2	2:G:396:ILE:O	2.48	0.43
6:E:16:GLY:H	6:E:78:LEU:HB2	1.82	0.43
2:G:312:GLY:HA2	2:G:315:GLN:HB2	1.98	0.43
2:G:393:SER:HB3	2:G:395:TRP:NE1	2.32	0.43
3:H:139:GLY:HA2	3:H:154:TRP:CZ2	2.53	0.43
4:L:139:ASP:OD1	4:L:170:ASN:ND2	2.52	0.43
3:H:164:HIS:NE2	4:L:168:GLN:OE1	2.51	0.43
5:D:16:ALA:O	5:D:82(C):LEU:HG	2.18	0.43
5:D:92:CYS:O	5:D:104:GLY:N	2.48	0.43
5:D:124:LEU:HB3	6:E:119:PHE:CD2	2.53	0.43
2:G:69:TRP:CH2	2:G:108:ILE:HG23	2.54	0.43
5:D:122:PHE:HE2	5:D:141:LEU:HD23	1.83	0.43
6:E:170:ASN:OD1	6:E:170:ASN:N	2.39	0.43
2:G:112:TRP:O	2:G:115:SER:OG	2.31	0.43
2:G:279:ASN:OD1	5:D:100(F):TRP:NE1	2.48	0.43
2:G:321(A):ASP:OD1	2:G:322:ILE:N	2.51	0.43
3:H:87:THR:HG23	3:H:110:THR:HA	2.00	0.43
3:H:107:THR:OG1	3:H:108:THR:N	2.50	0.43
5:D:100(G):ARG:HA	6:E:89:TYR:HE2	1.83	0.43
3:H:209:LYS:HE2	3:H:209:LYS:HB2	1.78	0.43
6:E:30:PHE:HB3	6:E:32:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:50:GLU:HB2	6:E:53:LYS:HG2	1.99	0.43
6:E:83:GLU:HG3	6:E:104:LEU:O	2.19	0.43
17:R:2:NAG:H61	17:R:6:MAN:H3	2.01	0.43
2:G:96:TRP:CG	2:G:275:GLU:HB2	2.54	0.43
2:G:157:CYS:O	2:G:173:TYR:HA	2.18	0.43
2:G:231:LYS:HD2	2:G:267:GLU:HG3	2.01	0.43
2:G:380:GLY:HA3	2:G:439:ILE:CG1	2.48	0.43
2:G:462:ASN:OD1	6:E:27(A):ARG:NH1	2.52	0.43
6:E:89:TYR:HB2	6:E:98:PHE:CD1	2.53	0.43
2:G:93:PHE:HZ	2:G:226:LEU:HB2	1.84	0.42
2:G:252:LYS:O	2:G:254:VAL:N	2.52	0.42
2:G:300:ASN:HB3	2:G:322:ILE:HD13	2.01	0.42
5:D:141:LEU:HD11	5:D:177:SER:OG	2.19	0.42
3:H:100(G):PHE:HB2	3:H:100(I):GLU:HG3	2.01	0.42
5:D:145:TYR:HD1	5:D:200:HIS:NE2	2.17	0.42
5:D:200:HIS:CD2	5:D:202:PRO:HD2	2.54	0.42
6:E:25:GLY:O	6:E:69:ASN:HB3	2.19	0.42
1:B:610:TRP:CH2	2:G:498:PRO:HD3	2.53	0.42
1:B:614:TRP:CD1	1:B:638:TYR:CG	3.08	0.42
1:B:622:ILE:O	1:B:626:MET:HB2	2.20	0.42
6:E:32:LEU:HD12	6:E:91:TYR:HB3	2.02	0.42
1:B:607:ASN:HA	2:G:502:LYS:HG3	2.02	0.42
5:D:145:TYR:CE1	5:D:150:VAL:HG23	2.55	0.42
1:B:597:GLY:HA3	2:G:503:ARG:CZ	2.50	0.42
1:B:608:VAL:HB	2:G:36:VAL:CG2	2.50	0.42
2:G:226:LEU:O	2:G:486:TYR:HA	2.20	0.42
6:E:115:SER:O	6:E:137:ILE:HA	2.20	0.42
1:B:614:TRP:CZ3	1:B:642:ILE:HG12	2.55	0.42
2:G:427:TRP:O	2:G:429:ARG:N	2.53	0.42
4:L:32:ALA:HA	4:L:51:ASN:ND2	2.35	0.42
2:G:376:PHE:O	2:G:382:PHE:HA	2.19	0.42
3:H:138:LEU:HD13	3:H:211:VAL:HG11	2.02	0.42
4:L:38:HIS:O	4:L:84:ALA:HB1	2.19	0.42
4:L:161:GLU:HB2	4:L:178:TYR:HB2	2.01	0.42
5:D:100(G):ARG:HG3	5:D:100(H):GLY:N	2.35	0.42
5:D:139:GLY:HA2	5:D:154:TRP:CH2	2.55	0.42
1:B:596:TRP:CD1	1:B:646:LEU:HB2	2.54	0.41
2:G:116:LEU:HD22	2:G:434:MET:HG3	2.02	0.41
3:H:197:ASN:ND2	3:H:208:ASP:OD2	2.53	0.41
2:G:134:VAL:HB	2:G:154:LEU:O	2.20	0.41
3:H:15:SER:N	3:H:82(C):VAL:O	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:143:LYS:HZ3	4:L:130:LYS:HB3	1.85	0.41
5:D:145:TYR:CE1	5:D:148:GLU:HA	2.52	0.41
6:E:35:TRP:CD1	6:E:48:ILE:HB	2.56	0.41
1:B:523:LEU:HD11	2:G:491:ILE:HD11	2.02	0.41
1:B:540:GLN:HE22	2:G:43:PRO:CG	2.33	0.41
3:H:126:PRO:HB3	3:H:138:LEU:HB3	2.01	0.41
2:G:59:LYS:HA	2:G:59:LYS:HD2	1.84	0.41
3:H:72:ASP:HB3	3:H:75:LYS:HB2	2.02	0.41
3:H:150:VAL:HB	3:H:178:LEU:HD21	2.02	0.41
4:L:121:PRO:HD2	4:L:186:TRP:CE2	2.56	0.41
2:G:164:GLU:HG3	2:G:308:ARG:HB3	2.02	0.41
3:H:200:HIS:CD2	3:H:202:PRO:HD2	2.56	0.41
2:G:461:THR:HB	2:G:464:THR:HG21	2.02	0.41
3:H:33:TYR:HE2	3:H:97:ARG:HD3	1.86	0.41
3:H:100(D):VAL:HG13	3:H:100(G):PHE:HB2	2.01	0.41
1:B:646:LEU:O	1:B:650:GLN:HB2	2.19	0.41
2:G:346:VAL:O	2:G:350:ARG:HG3	2.20	0.41
6:E:23:CYS:O	6:E:71:ALA:N	2.32	0.41
1:B:585:ARG:NE	2:G:491:ILE:O	2.41	0.41
1:B:648:GLU:O	1:B:652:GLN:HB3	2.20	0.41
2:G:282:LYS:HA	2:G:282:LYS:HD3	1.84	0.41
2:G:295:ASN:O	2:G:331:CYS:HA	2.21	0.41
3:H:145:TYR:CZ	3:H:176:TYR:HB2	2.55	0.41
5:D:12:LYS:HG3	5:D:18:VAL:CG2	2.51	0.41
5:D:122:PHE:HB2	6:E:122:SER:OG	2.21	0.41
6:E:159:GLY:O	6:E:179:LEU:HA	2.21	0.41
16:P:15:NAG:HO3	16:P:15:NAG:C7	2.33	0.41
1:B:642:ILE:HD13	2:G:496:VAL:HG11	2.03	0.41
2:G:446:VAL:O	15:O:1:NAG:H5	2.21	0.41
3:H:29:MET:O	3:H:71:ARG:NH1	2.54	0.40
6:E:67:SER:N	6:E:70:THR:O	2.44	0.40
4:L:31:ARG:HA	4:L:92:ASP:HA	2.03	0.40
6:E:23:CYS:HB2	6:E:35:TRP:CH2	2.57	0.40
6:E:38:GLN:O	6:E:84:ALA:HB1	2.20	0.40
2:G:96:TRP:HH2	2:G:285:LEU:HG	1.86	0.40
6:E:82:ASP:O	6:E:104:LEU:HD23	2.22	0.40
15:O:4:MAN:H2	15:O:5:MAN:H2	1.65	0.40
2:G:213:ILE:O	2:G:215:ILE:HG13	2.22	0.40
5:D:114:ALA:HB3	5:D:146:PHE:CD1	2.57	0.40
2:G:152:GLY:C	2:G:154:LEU:H	2.25	0.40
6:E:132:THR:HA	6:E:179:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	122/153 (80%)	106 (87%)	15 (12%)	1 (1%)	19 57
2	G	441/481 (92%)	407 (92%)	32 (7%)	2 (0%)	29 67
3	H	226/238 (95%)	216 (96%)	10 (4%)	0	100 100
4	L	209/214 (98%)	199 (95%)	10 (5%)	0	100 100
5	D	227/232 (98%)	216 (95%)	10 (4%)	1 (0%)	34 71
6	E	208/214 (97%)	193 (93%)	13 (6%)	2 (1%)	15 52
All	All	1433/1532 (94%)	1337 (93%)	90 (6%)	6 (0%)	34 71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	599	SER
2	G	138	ILE
5	D	100(D)	SER
6	E	93	ASP
2	G	457	ASP
6	E	51	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	108/129 (84%)	104 (96%)	4 (4%)	34	60
2	G	401/428 (94%)	395 (98%)	6 (2%)	65	80
3	H	202/208 (97%)	197 (98%)	5 (2%)	47	69
4	L	175/178 (98%)	169 (97%)	6 (3%)	37	62
5	D	194/197 (98%)	189 (97%)	5 (3%)	46	68
6	E	173/177 (98%)	170 (98%)	3 (2%)	60	78
All	All	1253/1317 (95%)	1224 (98%)	29 (2%)	50	71

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	606	THR
1	B	607	ASN
1	B	619	LEU
1	B	627	THR
2	G	57	ASP
2	G	192	ARG
2	G	195	ASN
2	G	205	CYS
2	G	322	ILE
2	G	396	ILE
3	H	37	ILE
3	H	100(F)	SER
3	H	100(L)	TYR
3	H	164	HIS
3	H	208	ASP
4	L	66(B)	ILE
4	L	93	SER
4	L	94	ARG
4	L	95(B)	PHE
4	L	122	SER
4	L	186	TRP
5	D	27	TYR
5	D	54	ARG
5	D	71	ARG
5	D	138	LEU
5	D	178	LEU
6	E	47	ILE
6	E	52	ASN
6	E	66	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	540	GLN
2	G	428	GLN
3	H	60	ASN
3	H	171	GLN
4	L	52	GLN
5	D	35	HIS
5	D	155	ASN
6	E	109	GLN

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

113 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	A	1	7,1	14,14,15	0.28	0	17,19,21	0.81	0
7	FUC	A	2	7	10,10,11	0.75	0	14,14,16	0.89	0
8	NAG	C	1	8,1	14,14,15	0.34	0	17,19,21	1.51	2 (11%)
8	NAG	C	2	8	14,14,15	0.31	0	17,19,21	1.03	1 (5%)
8	BMA	C	3	8	11,11,12	0.26	0	15,15,17	0.74	0
8	FUC	C	4	8	10,10,11	0.68	0	14,14,16	0.84	0
9	NAG	F	1	9,2	14,14,15	0.31	0	17,19,21	0.95	1 (5%)
9	NAG	F	2	9	14,14,15	0.28	0	17,19,21	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	FUC	F	3	9	10,10,11	0.73	0	14,14,16	0.93	0
10	NAG	I	1	2,10	14,14,15	0.43	0	17,19,21	1.41	4 (23%)
10	NAG	I	2	10	14,14,15	0.32	0	17,19,21	0.94	0
10	BMA	I	3	10	11,11,12	0.25	0	15,15,17	0.84	0
11	NAG	J	1	2,11	14,14,15	0.38	0	17,19,21	0.85	1 (5%)
11	GAL	J	10	11	11,11,12	0.24	0	15,15,17	0.77	0
11	NAG	J	11	11	14,14,15	0.33	0	17,19,21	0.85	0
11	GAL	J	12	11	11,11,12	0.26	0	15,15,17	0.79	0
11	FUC	J	13	11	10,10,11	0.70	0	14,14,16	0.84	0
11	NAG	J	2	11	14,14,15	0.36	0	17,19,21	1.08	2 (11%)
11	BMA	J	3	11	11,11,12	0.46	0	15,15,17	1.38	3 (20%)
11	MAN	J	4	11	11,11,12	0.40	0	15,15,17	1.92	3 (20%)
11	NAG	J	5	11	14,14,15	0.47	0	17,19,21	1.30	1 (5%)
11	GAL	J	6	11	11,11,12	0.25	0	15,15,17	0.79	0
11	NAG	J	7	11	14,14,15	0.31	0	17,19,21	1.08	1 (5%)
11	MAN	J	8	11	11,11,12	0.50	0	15,15,17	1.89	2 (13%)
11	NAG	J	9	11	14,14,15	0.35	0	17,19,21	1.10	2 (11%)
12	NAG	K	1	2,12	14,14,15	0.47	0	17,19,21	1.35	2 (11%)
12	FUC	K	10	12	10,10,11	0.71	0	14,14,16	0.93	0
12	NAG	K	2	12	14,14,15	0.57	0	17,19,21	2.21	4 (23%)
12	BMA	K	3	12	11,11,12	0.36	0	15,15,17	1.64	3 (20%)
12	MAN	K	4	12	11,11,12	0.39	0	15,15,17	1.08	2 (13%)
12	NAG	K	5	12	14,14,15	0.34	0	17,19,21	1.01	1 (5%)
12	GAL	K	6	12	11,11,12	0.28	0	15,15,17	0.78	0
12	MAN	K	7	12	11,11,12	0.25	0	15,15,17	1.05	1 (6%)
12	NAG	K	8	12	14,14,15	0.25	0	17,19,21	0.63	0
12	GAL	K	9	12	11,11,12	0.25	0	15,15,17	0.79	0
13	NAG	M	1	2,13	14,14,15	0.56	0	17,19,21	2.53	7 (41%)
13	NAG	M	2	13	14,14,15	0.69	0	17,19,21	1.96	5 (29%)
13	BMA	M	3	13	11,11,12	0.54	0	15,15,17	1.54	3 (20%)
13	MAN	M	4	13	11,11,12	0.40	0	15,15,17	1.50	3 (20%)
13	NAG	M	5	13	14,14,15	0.33	0	17,19,21	0.84	1 (5%)
13	GAL	M	6	13	11,11,12	0.26	0	15,15,17	0.89	0
13	SIA	M	7	13	20,20,21	2.01	2 (10%)	24,28,31	1.60	4 (16%)
13	MAN	M	8	13	11,11,12	0.26	0	15,15,17	1.09	1 (6%)
13	NAG	M	9	13	14,14,15	0.26	0	17,19,21	0.69	0
14	NAG	N	1	2,14	14,14,15	0.33	0	17,19,21	1.38	2 (11%)
14	NAG	N	2	14	14,14,15	0.25	0	17,19,21	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
15	NAG	O	1	2,15	14,14,15	0.37	0	17,19,21	0.85	0
15	NAG	O	2	15	14,14,15	0.30	0	17,19,21	1.23	2 (11%)
15	BMA	O	3	15	11,11,12	0.32	0	15,15,17	0.87	0
15	MAN	O	4	15	11,11,12	0.25	0	15,15,17	0.91	0
15	MAN	O	5	15	11,11,12	0.29	0	15,15,17	0.84	0
15	MAN	O	6	15	11,11,12	0.28	0	15,15,17	0.85	1 (6%)
15	MAN	O	7	15	11,11,12	0.34	0	15,15,17	0.92	1 (6%)
16	NAG	P	1	2,16	14,14,15	0.48	0	17,19,21	1.23	2 (11%)
16	NAG	P	10	16	14,14,15	0.39	0	17,19,21	1.43	4 (23%)
16	GAL	P	11	16	11,11,12	0.29	0	15,15,17	1.12	1 (6%)
16	SIA	P	12	16	20,20,21	1.99	2 (10%)	24,28,31	1.65	4 (16%)
16	NAG	P	13	16	14,14,15	0.45	0	17,19,21	1.10	2 (11%)
16	GAL	P	14	16	11,11,12	0.25	0	15,15,17	0.93	1 (6%)
16	NAG	P	15	16	14,14,15	0.54	0	17,19,21	1.22	2 (11%)
16	FUC	P	16	16	10,10,11	0.62	0	14,14,16	0.92	0
16	NAG	P	2	16	14,14,15	0.30	0	17,19,21	1.08	3 (17%)
16	BMA	P	3	16	11,11,12	0.43	0	15,15,17	1.84	7 (46%)
16	MAN	P	4	16	11,11,12	0.36	0	15,15,17	1.66	5 (33%)
16	NAG	P	5	16	14,14,15	0.28	0	17,19,21	0.58	0
16	GAL	P	6	16	11,11,12	0.26	0	15,15,17	0.78	0
16	SIA	P	7	16	20,20,21	1.99	2 (10%)	24,28,31	1.61	4 (16%)
16	NAG	P	8	16	14,14,15	0.28	0	17,19,21	0.68	0
16	MAN	P	9	16	11,11,12	0.93	0	15,15,17	3.01	10 (66%)
14	NAG	Q	1	2,14	14,14,15	0.36	0	17,19,21	0.77	0
14	NAG	Q	2	14	14,14,15	0.29	0	17,19,21	0.71	0
17	NAG	R	1	2,17	14,14,15	0.48	0	17,19,21	1.80	5 (29%)
17	NAG	R	2	17	14,14,15	0.36	0	17,19,21	0.91	2 (11%)
17	BMA	R	3	17	11,11,12	0.30	0	15,15,17	1.03	1 (6%)
17	MAN	R	4	17	11,11,12	0.28	0	15,15,17	1.12	1 (6%)
17	NAG	R	5	17	14,14,15	0.30	0	17,19,21	0.45	0
17	MAN	R	6	17	11,11,12	0.26	0	15,15,17	0.89	0
17	NAG	R	7	17	14,14,15	0.27	0	17,19,21	0.70	0
18	NAG	S	1	18,2	14,14,15	0.30	0	17,19,21	0.75	0
18	MAN	S	10	18	11,11,12	0.27	0	15,15,17	0.80	0
18	NAG	S	2	18	14,14,15	0.25	0	17,19,21	1.33	2 (11%)
18	BMA	S	3	18	11,11,12	0.32	0	15,15,17	0.98	1 (6%)
18	MAN	S	4	18	11,11,12	0.35	0	15,15,17	1.49	2 (13%)
18	MAN	S	5	18	11,11,12	0.34	0	15,15,17	1.38	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
18	MAN	S	6	18	11,11,12	0.22	0	15,15,17	1.02	1 (6%)
18	MAN	S	7	18	11,11,12	0.25	0	15,15,17	1.28	2 (13%)
18	MAN	S	8	18	11,11,12	0.46	0	15,15,17	1.34	1 (6%)
18	MAN	S	9	18	11,11,12	0.23	0	15,15,17	0.88	1 (6%)
14	NAG	T	1	2,14	14,14,15	0.35	0	17,19,21	0.67	0
14	NAG	T	2	14	14,14,15	0.31	0	17,19,21	0.65	0
19	NAG	U	1	2,19	14,14,15	0.53	0	17,19,21	2.17	4 (23%)
19	NAG	U	2	19	14,14,15	0.45	0	17,19,21	1.83	3 (17%)
19	BMA	U	3	19	11,11,12	0.40	0	15,15,17	1.27	2 (13%)
19	MAN	U	4	19	11,11,12	0.39	0	15,15,17	0.99	1 (6%)
19	MAN	U	5	19	11,11,12	0.27	0	15,15,17	0.88	0
19	MAN	U	6	19	11,11,12	0.28	0	15,15,17	0.87	0
19	MAN	U	7	19	11,11,12	0.32	0	15,15,17	0.86	1 (6%)
20	NAG	V	1	20,2	14,14,15	0.32	0	17,19,21	1.27	3 (17%)
20	NAG	V	2	20	14,14,15	0.61	0	17,19,21	1.78	5 (29%)
20	BMA	V	3	20	11,11,12	0.35	0	15,15,17	1.17	2 (13%)
20	MAN	V	4	20	11,11,12	0.28	0	15,15,17	0.81	1 (6%)
20	MAN	V	5	20	11,11,12	0.28	0	15,15,17	0.77	0
21	NAG	W	1	2,21	14,14,15	0.36	0	17,19,21	1.00	0
21	NAG	W	2	21	14,14,15	0.28	0	17,19,21	0.82	0
21	BMA	W	3	21	11,11,12	0.46	0	15,15,17	1.59	2 (13%)
21	MAN	W	4	21	11,11,12	0.27	0	15,15,17	0.80	1 (6%)
21	MAN	W	5	21	11,11,12	0.27	0	15,15,17	0.84	0
21	FUC	W	6	21	10,10,11	0.90	0	14,14,16	1.07	1 (7%)
22	NAG	X	1	2,22	14,14,15	0.29	0	17,19,21	1.17	1 (5%)
22	NAG	X	2	22	14,14,15	0.58	0	17,19,21	2.14	6 (35%)
22	BMA	X	3	22	11,11,12	0.32	0	15,15,17	1.15	2 (13%)
22	MAN	X	4	22	11,11,12	0.25	0	15,15,17	0.73	0
22	MAN	X	5	22	11,11,12	0.25	0	15,15,17	0.77	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
7	NAG	A	1	7,1	-	0/6/23/26	0/1/1/1
7	FUC	A	2	7	-	-	0/1/1/1

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	GAL	M	6	13	-	2/2/19/22	0/1/1/1
13	SIA	M	7	13	-	3/18/34/38	0/1/1/1
13	MAN	M	8	13	-	0/2/19/22	0/1/1/1
13	NAG	M	9	13	-	2/6/23/26	0/1/1/1
14	NAG	N	1	2,14	-	0/6/23/26	0/1/1/1
14	NAG	N	2	14	-	2/6/23/26	0/1/1/1
15	NAG	O	1	2,15	-	2/6/23/26	0/1/1/1
15	NAG	O	2	15	-	1/6/23/26	0/1/1/1
15	BMA	O	3	15	-	1/2/19/22	0/1/1/1
15	MAN	O	4	15	-	0/2/19/22	0/1/1/1
15	MAN	O	5	15	-	1/2/19/22	0/1/1/1
15	MAN	O	6	15	-	2/2/19/22	0/1/1/1
15	MAN	O	7	15	-	2/2/19/22	0/1/1/1
16	NAG	P	1	2,16	-	2/6/23/26	0/1/1/1
16	NAG	P	10	16	-	4/6/23/26	0/1/1/1
16	GAL	P	11	16	-	0/2/19/22	0/1/1/1
16	SIA	P	12	16	-	1/18/34/38	0/1/1/1
16	NAG	P	13	16	-	2/6/23/26	0/1/1/1
16	GAL	P	14	16	-	0/2/19/22	0/1/1/1
16	NAG	P	15	16	-	1/6/23/26	0/1/1/1
16	FUC	P	16	16	-	-	0/1/1/1
16	NAG	P	2	16	-	1/6/23/26	0/1/1/1
16	BMA	P	3	16	-	2/2/19/22	0/1/1/1
16	MAN	P	4	16	-	2/2/19/22	0/1/1/1
16	NAG	P	5	16	-	2/6/23/26	0/1/1/1
16	GAL	P	6	16	-	2/2/19/22	0/1/1/1
16	SIA	P	7	16	-	4/18/34/38	0/1/1/1
16	NAG	P	8	16	-	0/6/23/26	0/1/1/1
16	MAN	P	9	16	-	0/2/19/22	0/1/1/1
14	NAG	Q	1	2,14	-	1/6/23/26	0/1/1/1
14	NAG	Q	2	14	-	0/6/23/26	0/1/1/1
17	NAG	R	1	2,17	-	0/6/23/26	0/1/1/1
17	NAG	R	2	17	-	2/6/23/26	0/1/1/1
17	BMA	R	3	17	-	0/2/19/22	0/1/1/1
17	MAN	R	4	17	-	0/2/19/22	0/1/1/1
17	NAG	R	5	17	-	2/6/23/26	0/1/1/1
17	MAN	R	6	17	-	2/2/19/22	0/1/1/1
17	NAG	R	7	17	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	NAG	S	1	18,2	-	0/6/23/26	0/1/1/1
18	MAN	S	10	18	-	0/2/19/22	0/1/1/1
18	NAG	S	2	18	-	1/6/23/26	0/1/1/1
18	BMA	S	3	18	-	0/2/19/22	0/1/1/1
18	MAN	S	4	18	-	0/2/19/22	0/1/1/1
18	MAN	S	5	18	-	1/2/19/22	0/1/1/1
18	MAN	S	6	18	-	0/2/19/22	0/1/1/1
18	MAN	S	7	18	-	0/2/19/22	0/1/1/1
18	MAN	S	8	18	-	2/2/19/22	0/1/1/1
18	MAN	S	9	18	-	0/2/19/22	0/1/1/1
14	NAG	T	1	2,14	-	0/6/23/26	0/1/1/1
14	NAG	T	2	14	-	2/6/23/26	0/1/1/1
19	NAG	U	1	2,19	-	0/6/23/26	0/1/1/1
19	NAG	U	2	19	-	2/6/23/26	0/1/1/1
19	BMA	U	3	19	-	0/2/19/22	0/1/1/1
19	MAN	U	4	19	-	1/2/19/22	0/1/1/1
19	MAN	U	5	19	-	1/2/19/22	0/1/1/1
19	MAN	U	6	19	-	0/2/19/22	0/1/1/1
19	MAN	U	7	19	-	1/2/19/22	0/1/1/1
20	NAG	V	1	20,2	-	2/6/23/26	0/1/1/1
20	NAG	V	2	20	-	1/6/23/26	0/1/1/1
20	BMA	V	3	20	-	0/2/19/22	0/1/1/1
20	MAN	V	4	20	-	0/2/19/22	0/1/1/1
20	MAN	V	5	20	-	0/2/19/22	0/1/1/1
21	NAG	W	1	2,21	-	0/6/23/26	0/1/1/1
21	NAG	W	2	21	-	1/6/23/26	0/1/1/1
21	BMA	W	3	21	-	0/2/19/22	0/1/1/1
21	MAN	W	4	21	-	0/2/19/22	0/1/1/1
21	MAN	W	5	21	-	0/2/19/22	0/1/1/1
21	FUC	W	6	21	-	-	0/1/1/1
22	NAG	X	1	2,22	-	2/6/23/26	0/1/1/1
22	NAG	X	2	22	-	2/6/23/26	0/1/1/1
22	BMA	X	3	22	-	0/2/19/22	0/1/1/1
22	MAN	X	4	22	-	2/2/19/22	0/1/1/1
22	MAN	X	5	22	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	M	7	SIA	C2-C1	7.60	1.59	1.52
16	P	12	SIA	C2-C1	7.53	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	P	7	SIA	C2-C1	7.51	1.59	1.52
13	M	7	SIA	O6-C2	2.76	1.47	1.43
16	P	7	SIA	O6-C2	2.72	1.47	1.43
16	P	12	SIA	O6-C2	2.61	1.47	1.43

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	K	2	NAG	C2-N2-C7	6.75	132.51	122.90
19	U	1	NAG	O4-C4-C5	6.20	124.69	109.30
13	M	1	NAG	O3-C3-C2	-5.98	97.10	109.47
22	X	2	NAG	O4-C4-C3	-5.64	97.31	110.35
11	J	8	MAN	O2-C2-C3	5.51	121.17	110.14
16	P	9	MAN	O4-C4-C5	5.22	122.26	109.30
11	J	4	MAN	C1-C2-C3	-5.21	103.26	109.67
16	P	9	MAN	O2-C2-C3	5.07	120.30	110.14
16	P	7	SIA	O1A-C1-C2	-4.38	112.22	122.57
22	X	2	NAG	O5-C1-C2	-4.35	104.42	111.29
16	P	12	SIA	O1A-C1-C2	-4.34	112.33	122.57
16	P	9	MAN	O5-C5-C6	-4.32	100.42	107.20
16	P	4	MAN	O5-C1-C2	-4.27	104.18	110.77
19	U	2	NAG	O4-C4-C5	4.22	119.77	109.30
13	M	7	SIA	O1A-C1-C2	-4.13	112.80	122.57
13	M	1	NAG	O4-C4-C3	-4.13	100.79	110.35
13	M	1	NAG	O4-C4-C5	-4.10	99.11	109.30
13	M	2	NAG	O4-C4-C3	-4.00	101.09	110.35
13	M	2	NAG	C4-C3-C2	3.99	116.87	111.02
18	S	8	MAN	C1-O5-C5	-3.92	106.89	112.19
17	R	1	NAG	O5-C5-C6	-3.89	101.10	107.20
8	C	1	NAG	O5-C5-C6	3.87	113.27	107.20
20	V	2	NAG	O5-C1-C2	-3.86	105.20	111.29
16	P	9	MAN	O2-C2-C1	3.81	116.95	109.15
12	K	1	NAG	C1-O5-C5	3.73	117.25	112.19
19	U	2	NAG	C1-O5-C5	3.69	117.19	112.19
19	U	1	NAG	C1-O5-C5	3.68	117.18	112.19
19	U	2	NAG	O4-C4-C3	3.67	118.84	110.35
14	N	1	NAG	O4-C4-C3	3.65	118.79	110.35
18	S	4	MAN	C1-C2-C3	3.64	114.14	109.67
13	M	7	SIA	C6-O6-C2	3.64	119.12	111.34
17	R	1	NAG	O4-C4-C3	-3.62	101.98	110.35
11	J	4	MAN	O4-C4-C5	3.50	118.00	109.30
13	M	2	NAG	O5-C1-C2	-3.45	105.84	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	9	MAN	O5-C1-C2	-3.44	105.46	110.77
11	J	8	MAN	O3-C3-C2	3.41	116.53	109.99
16	P	7	SIA	C6-O6-C2	3.41	118.63	111.34
21	W	3	BMA	O5-C1-C2	-3.33	105.62	110.77
17	R	1	NAG	O5-C1-C2	-3.31	106.06	111.29
13	M	1	NAG	O5-C1-C2	-3.31	106.07	111.29
20	V	2	NAG	O4-C4-C3	-3.30	102.72	110.35
16	P	1	NAG	O4-C4-C5	-3.26	101.21	109.30
16	P	10	NAG	C1-O5-C5	3.24	116.58	112.19
18	S	5	MAN	O5-C1-C2	-3.23	105.79	110.77
13	M	4	MAN	C1-C2-C3	-3.22	105.71	109.67
21	W	3	BMA	O2-C2-C3	-3.20	103.74	110.14
16	P	9	MAN	C1-C2-C3	3.19	113.58	109.67
16	P	12	SIA	C6-O6-C2	3.18	118.13	111.34
12	K	2	NAG	C8-C7-N2	3.17	121.46	116.10
18	S	4	MAN	O2-C2-C3	3.17	116.48	110.14
12	K	1	NAG	O5-C1-C2	-3.16	106.30	111.29
16	P	3	BMA	C1-C2-C3	3.14	113.53	109.67
13	M	2	NAG	O4-C4-C5	-3.14	101.50	109.30
12	K	3	BMA	O5-C5-C6	3.14	112.13	107.20
16	P	13	NAG	C1-O5-C5	3.13	116.44	112.19
13	M	3	BMA	O5-C1-C2	-3.11	105.97	110.77
11	J	5	NAG	C8-C7-N2	-3.06	110.91	116.10
12	K	2	NAG	O5-C1-C2	-3.04	106.49	111.29
13	M	1	NAG	C1-O5-C5	-3.01	108.11	112.19
12	K	3	BMA	C1-C2-C3	3.00	113.35	109.67
10	I	1	NAG	O5-C1-C2	-2.95	106.63	111.29
11	J	7	NAG	C1-O5-C5	2.94	116.18	112.19
22	X	1	NAG	O4-C4-C3	-2.93	103.56	110.35
20	V	2	NAG	O4-C4-C5	-2.92	102.03	109.30
20	V	3	BMA	C1-C2-C3	2.91	113.24	109.67
11	J	9	NAG	C1-O5-C5	2.88	116.10	112.19
19	U	3	BMA	C1-C2-C3	2.87	113.19	109.67
12	K	4	MAN	C1-O5-C5	-2.83	108.35	112.19
16	P	2	NAG	O4-C4-C5	-2.79	102.36	109.30
14	N	1	NAG	C4-C3-C2	-2.79	106.93	111.02
13	M	3	BMA	C1-O5-C5	-2.78	108.43	112.19
19	U	1	NAG	C4-C3-C2	-2.75	106.98	111.02
20	V	1	NAG	C3-C4-C5	-2.74	105.36	110.24
12	K	7	MAN	O5-C1-C2	-2.73	106.56	110.77
16	P	12	SIA	O6-C2-C3	-2.69	106.75	110.46
10	I	1	NAG	C2-N2-C7	-2.67	119.10	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	P	15	NAG	O5-C1-C2	-2.64	107.11	111.29
18	S	6	MAN	O5-C1-C2	-2.63	106.71	110.77
16	P	3	BMA	O5-C5-C6	2.62	111.32	107.20
12	K	2	NAG	C1-C2-N2	2.62	114.97	110.49
17	R	4	MAN	O5-C1-C2	-2.62	106.72	110.77
16	P	3	BMA	O3-C3-C2	-2.62	104.97	109.99
19	U	1	NAG	O5-C1-C2	-2.61	107.17	111.29
16	P	10	NAG	O5-C5-C6	-2.60	103.13	107.20
16	P	10	NAG	O4-C4-C5	2.60	115.75	109.30
22	X	3	BMA	O5-C1-C2	-2.59	106.77	110.77
19	U	3	BMA	O5-C1-C2	-2.57	106.80	110.77
22	X	3	BMA	C1-O5-C5	-2.57	108.71	112.19
11	J	3	BMA	C1-C2-C3	2.57	112.82	109.67
13	M	1	NAG	C4-C3-C2	2.56	114.77	111.02
18	S	7	MAN	C1-C2-C3	-2.55	106.53	109.67
16	P	9	MAN	O4-C4-C3	-2.53	104.49	110.35
22	X	2	NAG	C1-C2-N2	2.53	114.81	110.49
13	M	4	MAN	O5-C1-C2	-2.51	106.90	110.77
16	P	4	MAN	C1-O5-C5	2.50	115.57	112.19
10	I	1	NAG	O4-C4-C5	-2.49	103.10	109.30
16	P	7	SIA	O1B-C1-O1A	2.49	129.74	124.09
18	S	2	NAG	C1-C2-N2	2.46	114.69	110.49
21	W	6	FUC	O2-C2-C1	2.46	114.18	109.15
19	U	4	MAN	O5-C1-C2	-2.45	106.99	110.77
15	O	7	MAN	C1-O5-C5	-2.44	108.89	112.19
16	P	3	BMA	O4-C4-C3	2.43	115.96	110.35
18	S	3	BMA	O3-C3-C2	-2.43	105.34	109.99
16	P	3	BMA	C2-C3-C4	-2.42	106.70	110.89
16	P	12	SIA	O1B-C1-O1A	2.42	129.59	124.09
16	P	9	MAN	C3-C4-C5	-2.42	105.92	110.24
11	J	4	MAN	O5-C1-C2	-2.42	107.04	110.77
20	V	1	NAG	O5-C1-C2	-2.41	107.48	111.29
13	M	8	MAN	O5-C1-C2	-2.41	107.06	110.77
13	M	5	NAG	O5-C1-C2	-2.39	107.51	111.29
12	K	5	NAG	O5-C1-C2	-2.39	107.51	111.29
17	R	2	NAG	O5-C1-C2	-2.38	107.52	111.29
13	M	4	MAN	O2-C2-C3	-2.38	105.37	110.14
11	J	9	NAG	C2-N2-C7	-2.38	119.52	122.90
13	M	7	SIA	O1B-C1-O1A	2.36	129.45	124.09
19	U	7	MAN	O5-C1-C2	-2.34	107.15	110.77
13	M	3	BMA	O3-C3-C4	-2.34	104.94	110.35
11	J	3	BMA	O3-C3-C2	-2.34	105.52	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	O	2	NAG	O5-C1-C2	-2.33	107.61	111.29
22	X	2	NAG	C2-N2-C7	2.32	126.21	122.90
16	P	3	BMA	C3-C4-C5	-2.32	106.10	110.24
12	K	3	BMA	O3-C3-C4	-2.31	105.01	110.35
16	P	3	BMA	O3-C3-C4	2.28	115.63	110.35
16	P	15	NAG	O5-C5-C6	2.28	110.78	107.20
16	P	9	MAN	C1-O5-C5	2.27	115.26	112.19
11	J	2	NAG	O5-C1-C2	-2.26	107.71	111.29
15	O	2	NAG	O4-C4-C5	-2.24	103.72	109.30
11	J	1	NAG	O5-C1-C2	-2.23	107.77	111.29
17	R	1	NAG	C4-C3-C2	2.20	114.25	111.02
16	P	10	NAG	C6-C5-C4	-2.20	107.84	113.00
8	C	1	NAG	O4-C4-C5	-2.19	103.85	109.30
20	V	2	NAG	C1-C2-N2	2.19	114.22	110.49
18	S	9	MAN	O5-C1-C2	-2.18	107.40	110.77
16	P	11	GAL	O5-C1-C2	-2.18	107.41	110.77
16	P	7	SIA	C4-C3-C2	2.18	113.71	109.81
16	P	1	NAG	O3-C3-C2	-2.17	104.97	109.47
22	X	2	NAG	C4-C3-C2	2.16	114.19	111.02
13	M	7	SIA	O6-C2-C3	-2.16	107.48	110.46
15	O	6	MAN	O5-C1-C2	-2.15	107.44	110.77
16	P	13	NAG	O5-C5-C6	-2.15	103.83	107.20
13	M	2	NAG	C1-O5-C5	-2.15	109.28	112.19
16	P	14	GAL	O5-C1-C2	-2.14	107.47	110.77
16	P	4	MAN	O2-C2-C1	-2.12	104.81	109.15
18	S	2	NAG	O4-C4-C5	-2.12	104.04	109.30
12	K	4	MAN	O5-C5-C6	2.12	110.52	107.20
20	V	1	NAG	O5-C5-C6	2.11	110.52	107.20
13	M	1	NAG	O3-C3-C4	-2.07	105.56	110.35
9	F	1	NAG	O5-C1-C2	-2.07	108.02	111.29
20	V	3	BMA	O3-C3-C2	-2.07	106.04	109.99
8	C	2	NAG	C1-O5-C5	2.06	114.98	112.19
18	S	7	MAN	O3-C3-C4	2.06	115.11	110.35
16	P	9	MAN	C6-C5-C4	2.06	117.82	113.00
10	I	1	NAG	O4-C4-C3	-2.06	105.59	110.35
17	R	2	NAG	O4-C4-C3	-2.06	105.60	110.35
16	P	2	NAG	O4-C4-C3	-2.05	105.62	110.35
18	S	5	MAN	O2-C2-C1	-2.04	104.97	109.15
16	P	4	MAN	O4-C4-C5	-2.04	104.23	109.30
17	R	3	BMA	O5-C1-C2	-2.04	107.63	110.77
11	J	2	NAG	O5-C5-C6	2.03	110.39	107.20
11	J	3	BMA	C6-C5-C4	-2.03	108.24	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	R	1	NAG	C1-C2-N2	2.02	113.94	110.49
16	P	4	MAN	C3-C4-C5	-2.02	106.64	110.24
22	X	2	NAG	O4-C4-C5	-2.02	104.29	109.30
21	W	4	MAN	O5-C1-C2	-2.01	107.67	110.77
16	P	2	NAG	O5-C1-C2	-2.01	108.11	111.29
20	V	2	NAG	C2-N2-C7	2.00	125.75	122.90
20	V	4	MAN	O5-C1-C2	-2.00	107.68	110.77

There are no chirality outliers.

All (111) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	P	7	SIA	O1A-C1-C2-O6
16	P	3	BMA	O5-C5-C6-O6
13	M	3	BMA	O5-C5-C6-O6
13	M	4	MAN	O5-C5-C6-O6
16	P	6	GAL	O5-C5-C6-O6
12	K	3	BMA	O5-C5-C6-O6
14	N	2	NAG	O5-C5-C6-O6
11	J	11	NAG	O5-C5-C6-O6
18	S	8	MAN	O5-C5-C6-O6
13	M	3	BMA	C4-C5-C6-O6
16	P	1	NAG	O5-C5-C6-O6
16	P	10	NAG	O5-C5-C6-O6
16	P	6	GAL	C4-C5-C6-O6
12	K	7	MAN	O5-C5-C6-O6
13	M	2	NAG	O5-C5-C6-O6
17	R	7	NAG	O5-C5-C6-O6
16	P	3	BMA	C4-C5-C6-O6
17	R	6	MAN	C4-C5-C6-O6
12	K	3	BMA	C4-C5-C6-O6
17	R	6	MAN	O5-C5-C6-O6
13	M	4	MAN	C4-C5-C6-O6
17	R	7	NAG	C4-C5-C6-O6
14	N	2	NAG	C4-C5-C6-O6
16	P	1	NAG	C4-C5-C6-O6
16	P	4	MAN	O5-C5-C6-O6
11	J	11	NAG	C4-C5-C6-O6
17	R	5	NAG	O5-C5-C6-O6
12	K	7	MAN	C4-C5-C6-O6
12	K	1	NAG	C8-C7-N2-C2
12	K	1	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
12	K	2	NAG	C8-C7-N2-C2
12	K	2	NAG	O7-C7-N2-C2
12	K	8	NAG	C8-C7-N2-C2
12	K	8	NAG	O7-C7-N2-C2
13	M	5	NAG	C8-C7-N2-C2
13	M	5	NAG	O7-C7-N2-C2
13	M	9	NAG	C8-C7-N2-C2
13	M	9	NAG	O7-C7-N2-C2
16	P	5	NAG	C8-C7-N2-C2
16	P	5	NAG	O7-C7-N2-C2
16	P	10	NAG	C8-C7-N2-C2
16	P	10	NAG	O7-C7-N2-C2
17	R	7	NAG	C8-C7-N2-C2
17	R	7	NAG	O7-C7-N2-C2
13	M	2	NAG	C4-C5-C6-O6
16	P	10	NAG	C4-C5-C6-O6
18	S	8	MAN	C4-C5-C6-O6
15	O	6	MAN	O5-C5-C6-O6
9	F	1	NAG	O5-C5-C6-O6
15	O	7	MAN	O5-C5-C6-O6
22	X	4	MAN	O5-C5-C6-O6
13	M	6	GAL	C4-C5-C6-O6
17	R	5	NAG	C4-C5-C6-O6
15	O	7	MAN	C4-C5-C6-O6
19	U	2	NAG	O5-C5-C6-O6
22	X	4	MAN	C4-C5-C6-O6
15	O	6	MAN	C4-C5-C6-O6
11	J	3	BMA	C4-C5-C6-O6
22	X	1	NAG	C4-C5-C6-O6
16	P	4	MAN	C4-C5-C6-O6
20	V	1	NAG	C4-C5-C6-O6
9	F	2	NAG	O5-C5-C6-O6
10	I	2	NAG	C4-C5-C6-O6
9	F	2	NAG	C4-C5-C6-O6
13	M	1	NAG	C4-C5-C6-O6
22	X	1	NAG	O5-C5-C6-O6
13	M	6	GAL	O5-C5-C6-O6
15	O	1	NAG	C4-C5-C6-O6
10	I	1	NAG	O5-C5-C6-O6
17	R	2	NAG	O5-C5-C6-O6
18	S	5	MAN	O5-C5-C6-O6
19	U	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
15	O	1	NAG	O5-C5-C6-O6
9	F	1	NAG	C4-C5-C6-O6
12	K	2	NAG	O5-C5-C6-O6
11	J	2	NAG	O5-C5-C6-O6
13	M	7	SIA	C6-C7-C8-O8
16	P	15	NAG	O5-C5-C6-O6
11	J	9	NAG	O5-C5-C6-O6
13	M	1	NAG	O5-C5-C6-O6
15	O	5	MAN	O5-C5-C6-O6
16	P	12	SIA	O1A-C1-C2-O6
11	J	9	NAG	C4-C5-C6-O6
19	U	2	NAG	C4-C5-C6-O6
10	I	2	NAG	O5-C5-C6-O6
20	V	1	NAG	O5-C5-C6-O6
16	P	7	SIA	O1A-C1-C2-C3
16	P	7	SIA	O1B-C1-C2-C3
14	T	2	NAG	C4-C5-C6-O6
15	O	3	BMA	C4-C5-C6-O6
16	P	13	NAG	C1-C2-N2-C7
8	C	2	NAG	C3-C2-N2-C7
15	O	2	NAG	C3-C2-N2-C7
18	S	2	NAG	C3-C2-N2-C7
20	V	2	NAG	C3-C2-N2-C7
16	P	13	NAG	O5-C5-C6-O6
21	W	2	NAG	O5-C5-C6-O6
22	X	2	NAG	C1-C2-N2-C7
19	U	4	MAN	O5-C5-C6-O6
11	J	3	BMA	O5-C5-C6-O6
14	Q	1	NAG	O5-C5-C6-O6
14	T	2	NAG	O5-C5-C6-O6
13	M	2	NAG	C1-C2-N2-C7
13	M	7	SIA	O7-C7-C8-O8
16	P	7	SIA	O1B-C1-C2-O6
16	P	2	NAG	C4-C5-C6-O6
13	M	7	SIA	O1A-C1-C2-O6
12	K	2	NAG	C3-C2-N2-C7
22	X	2	NAG	C3-C2-N2-C7
19	U	7	MAN	C4-C5-C6-O6
17	R	2	NAG	C4-C5-C6-O6

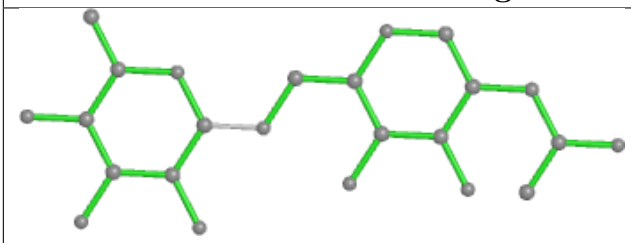
There are no ring outliers.

33 monomers are involved in 22 short contacts:

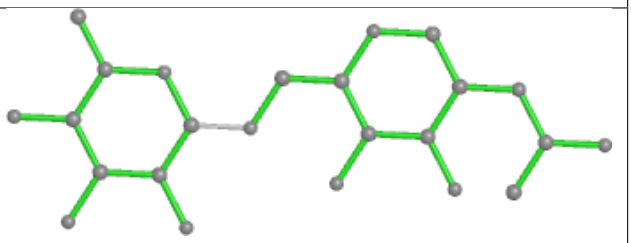
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	J	5	NAG	1	0
17	R	1	NAG	1	0
16	P	16	FUC	1	0
11	J	4	MAN	1	0
13	M	5	NAG	1	0
11	J	7	NAG	1	0
17	R	3	BMA	1	0
18	S	9	MAN	1	0
16	P	15	NAG	3	0
12	K	1	NAG	1	0
16	P	3	BMA	1	0
22	X	1	NAG	1	0
17	R	2	NAG	2	0
17	R	6	MAN	1	0
13	M	4	MAN	1	0
20	V	1	NAG	1	0
15	O	5	MAN	1	0
18	S	2	NAG	1	0
20	V	2	NAG	1	0
15	O	4	MAN	1	0
21	W	2	NAG	1	0
22	X	2	NAG	1	0
18	S	4	MAN	1	0
16	P	4	MAN	2	0
18	S	8	MAN	1	0
11	J	9	NAG	1	0
16	P	9	MAN	1	0
12	K	2	NAG	1	0
15	O	1	NAG	1	0
10	I	2	NAG	1	0
18	S	5	MAN	1	0
21	W	3	BMA	1	0
10	I	1	NAG	1	0

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

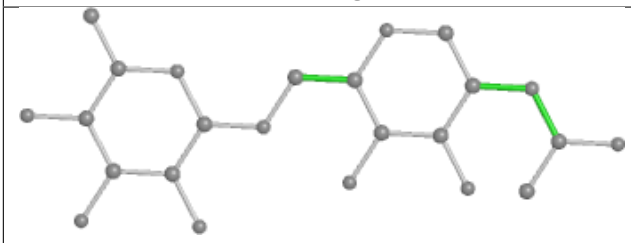
Oligosaccharide Chain A



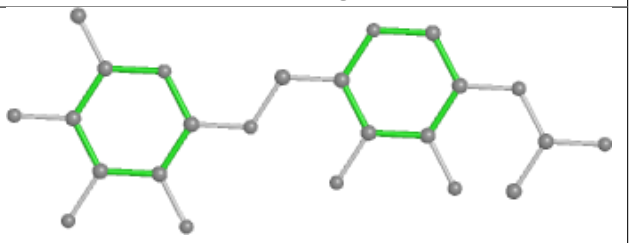
Bond lengths



Bond angles

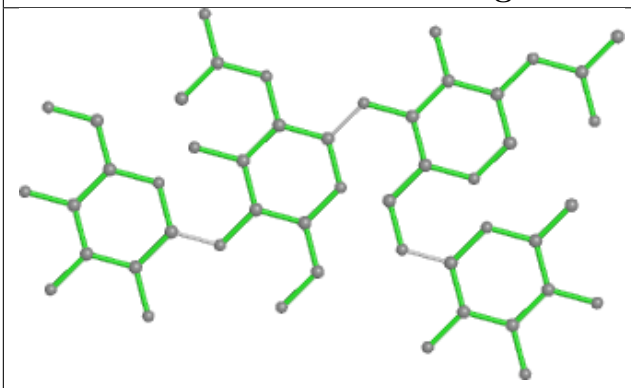


Torsions

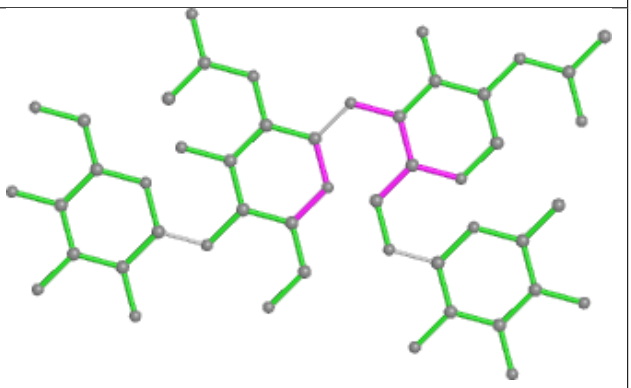


Rings

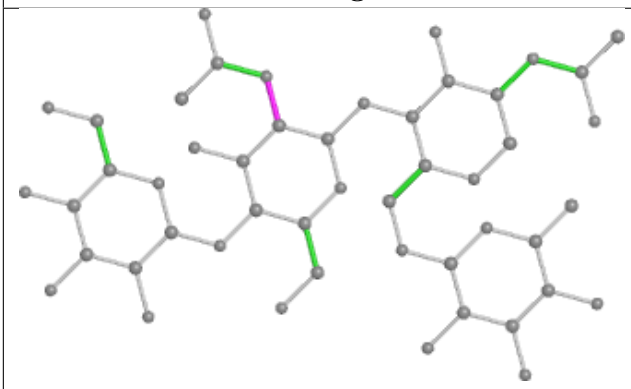
Oligosaccharide Chain C



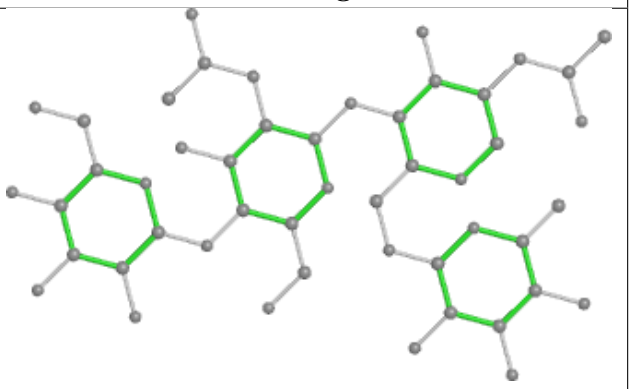
Bond lengths



Bond angles

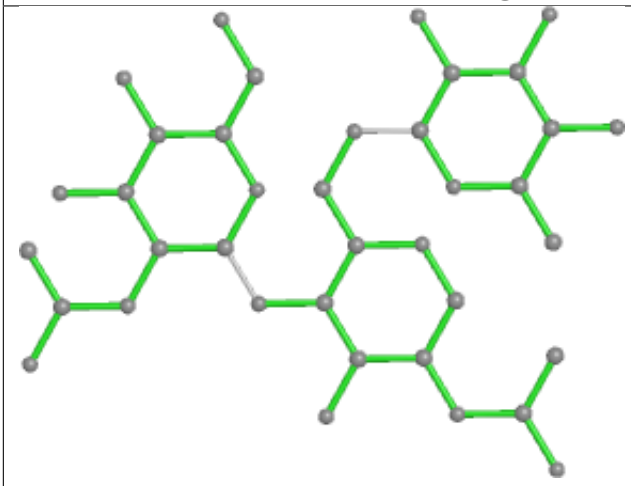


Torsions

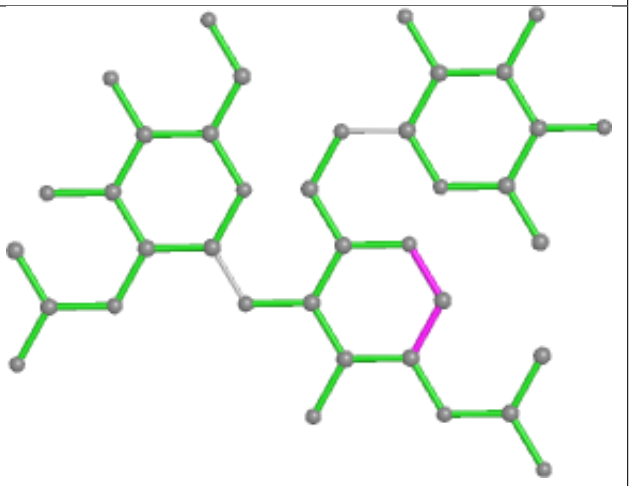


Rings

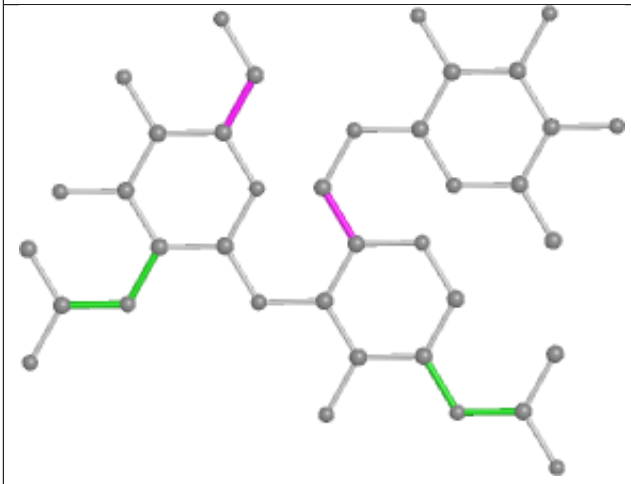
Oligosaccharide Chain F



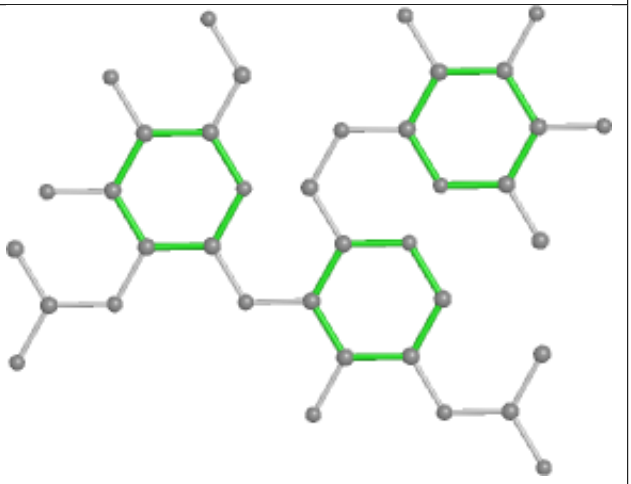
Bond lengths



Bond angles

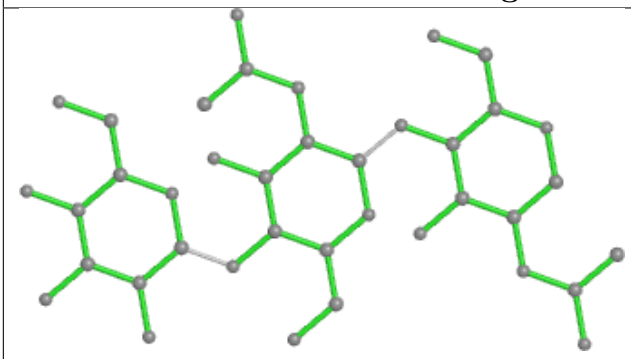


Torsions

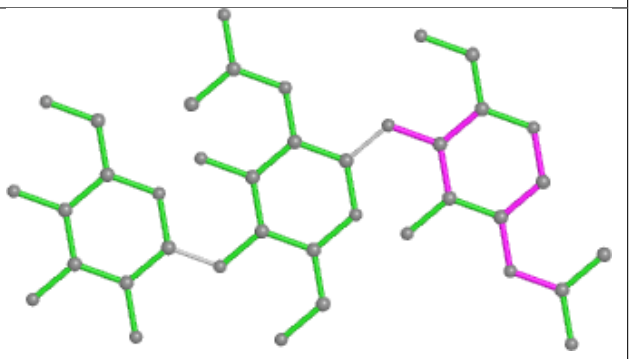


Rings

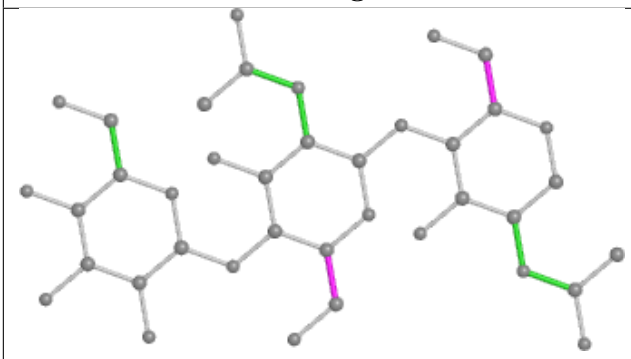
Oligosaccharide Chain I



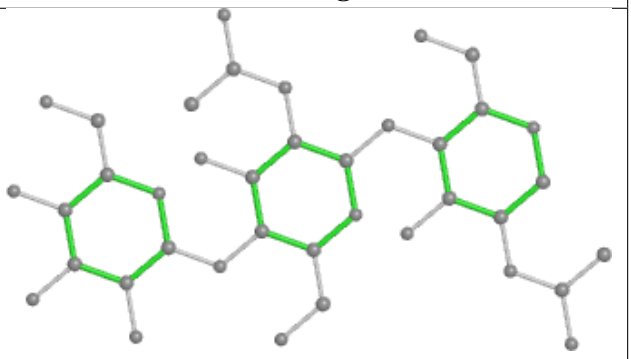
Bond lengths



Bond angles

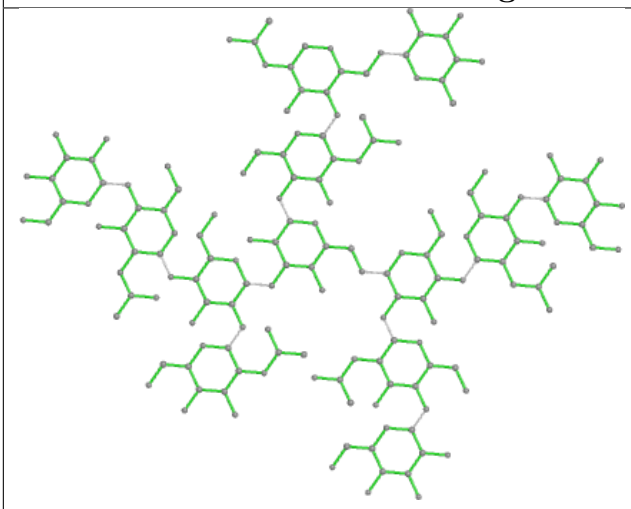


Torsions

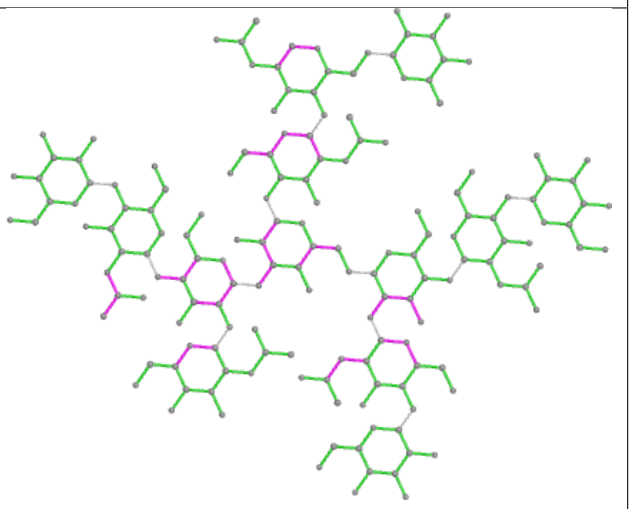


Rings

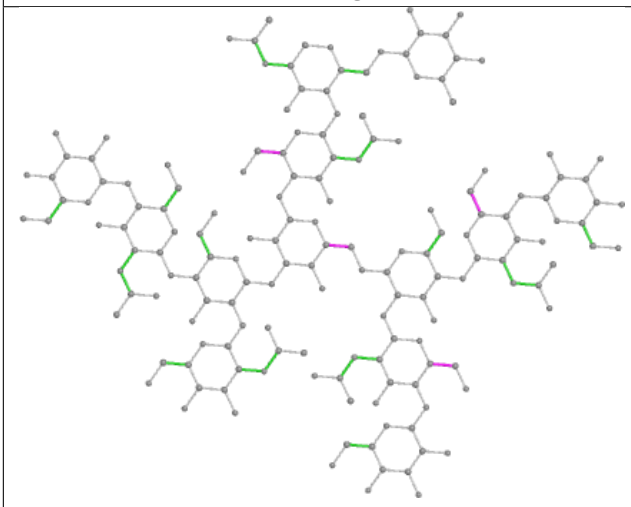
Oligosaccharide Chain J



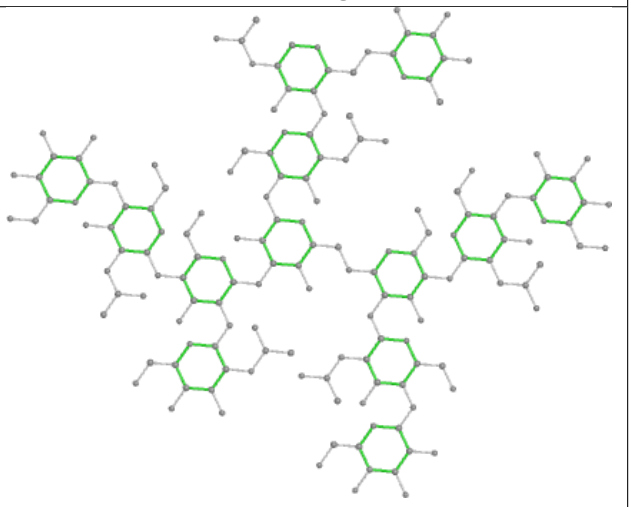
Bond lengths



Bond angles

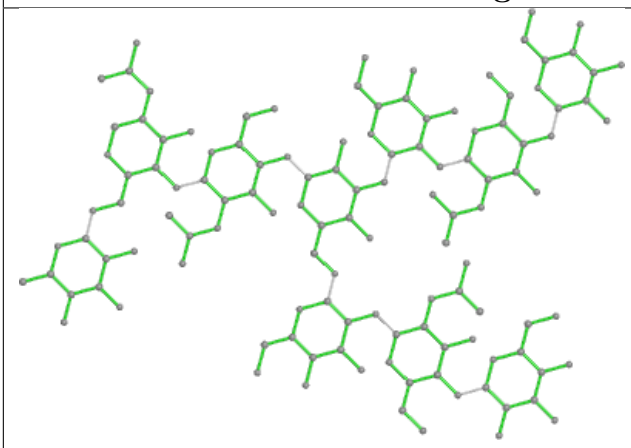


Torsions

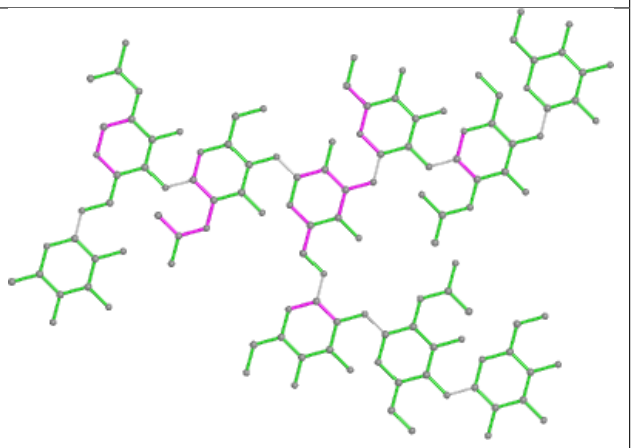


Rings

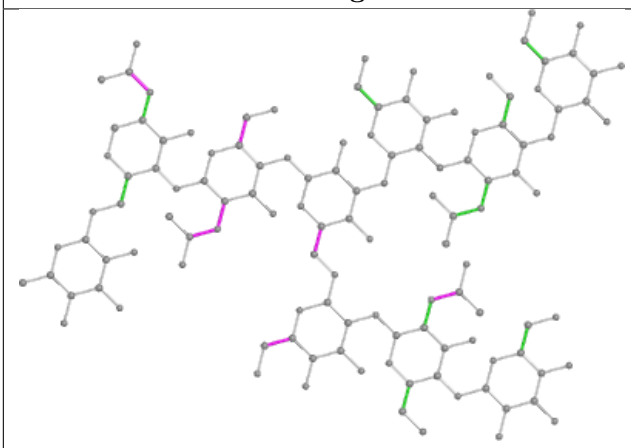
Oligosaccharide Chain K



Bond lengths



Bond angles



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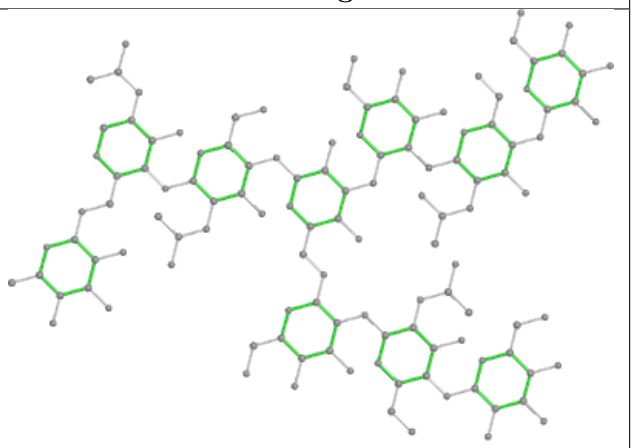
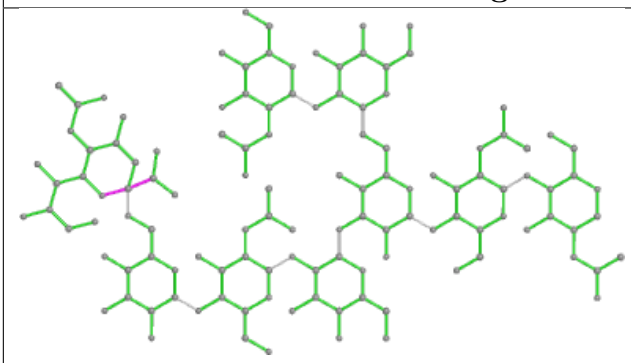
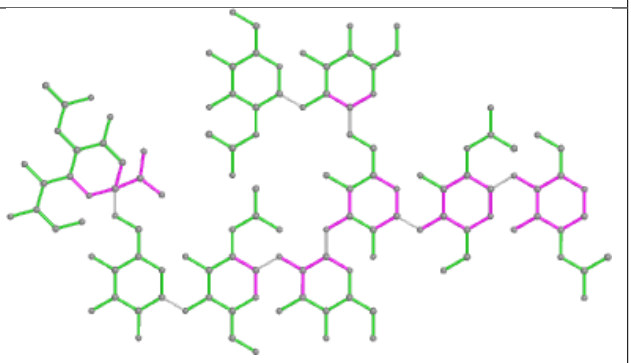


Rings

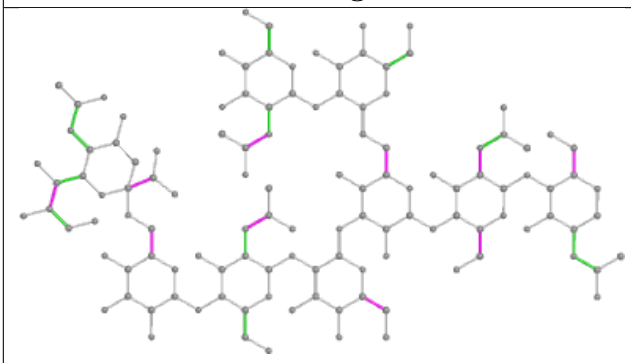
Oligosaccharide Chain M



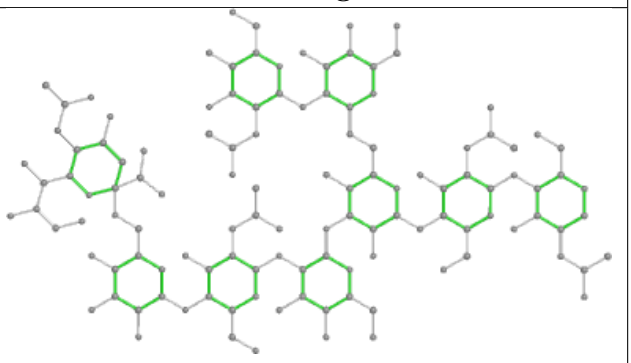
Bond lengths



Bond angles

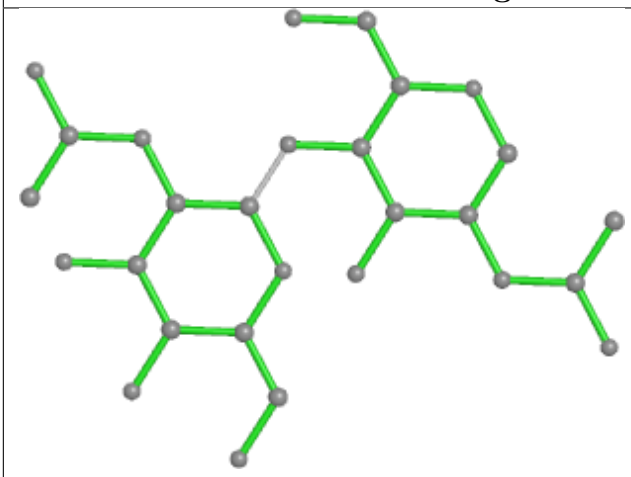


Torsions



Rings

Oligosaccharide Chain N



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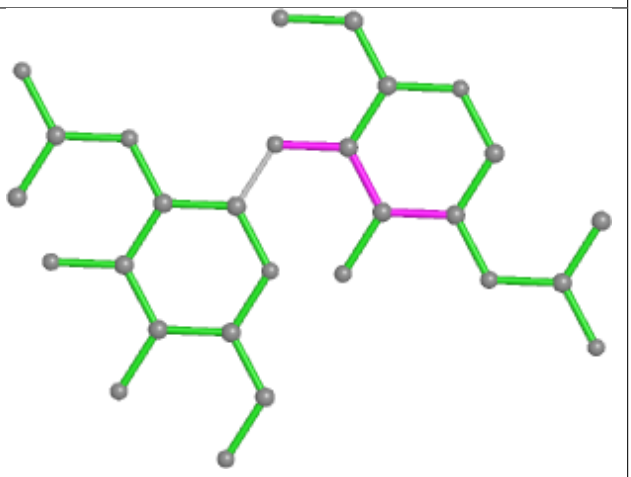
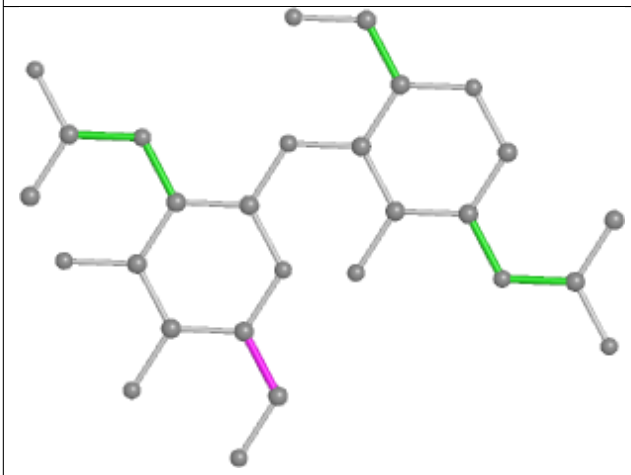


Bond angles



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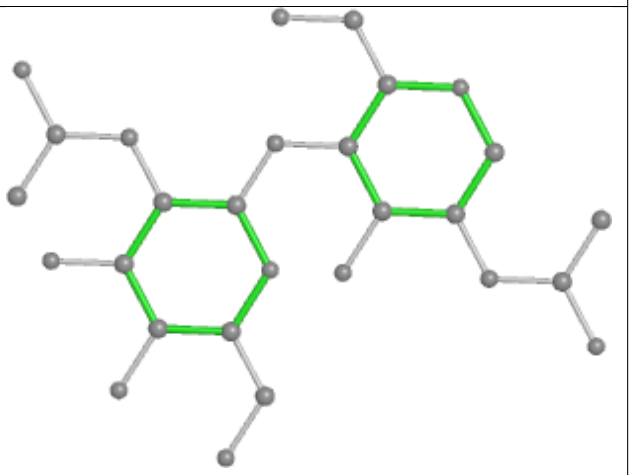
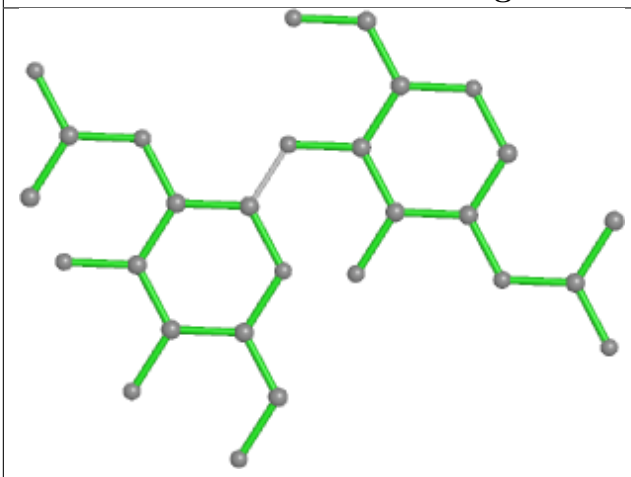
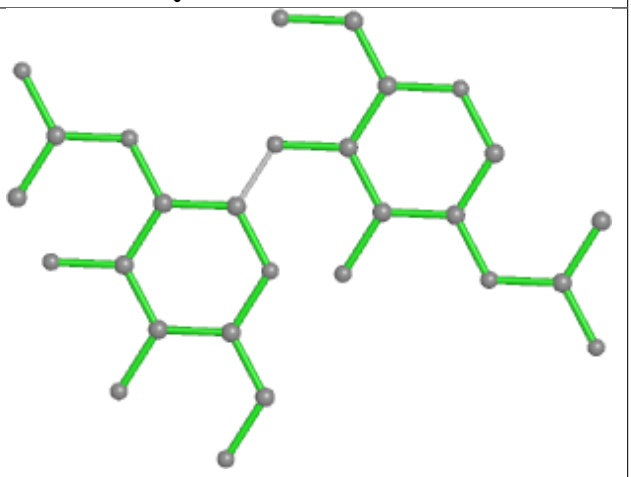


Rings

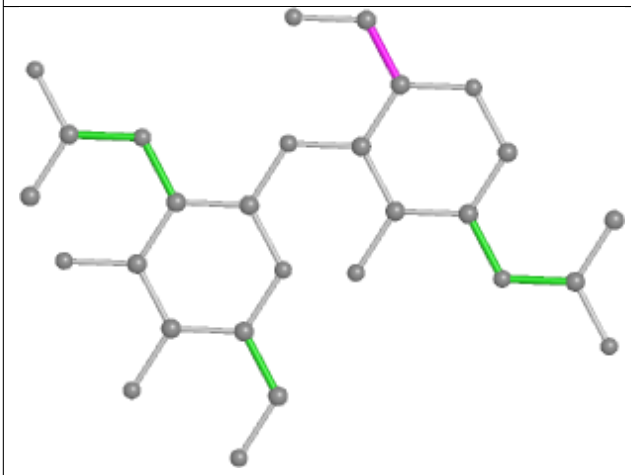
Oligosaccharide Chain Q



Bond lengths



Bond angles



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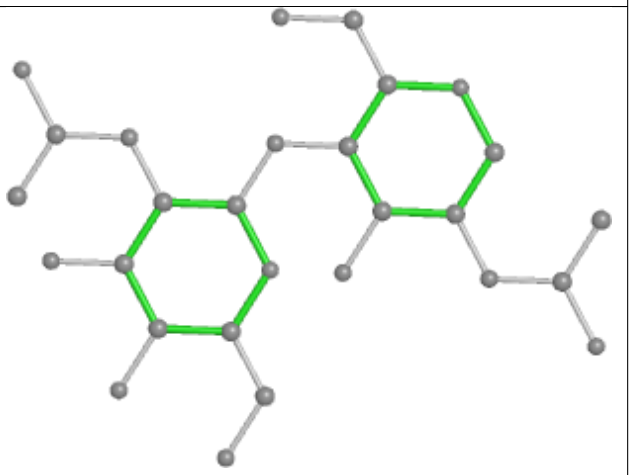
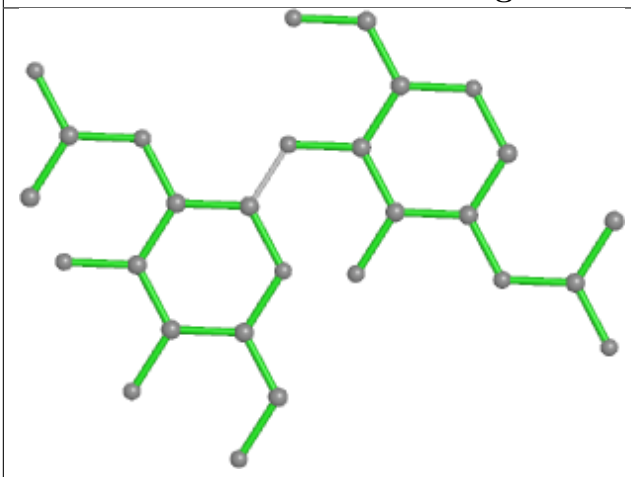


Rings

Oligosaccharide Chain T



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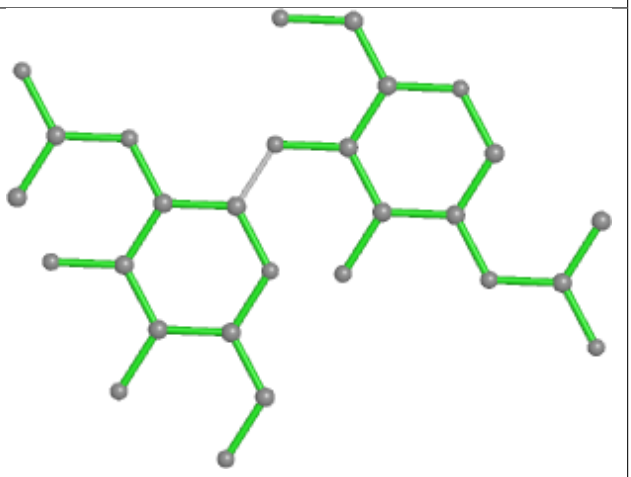
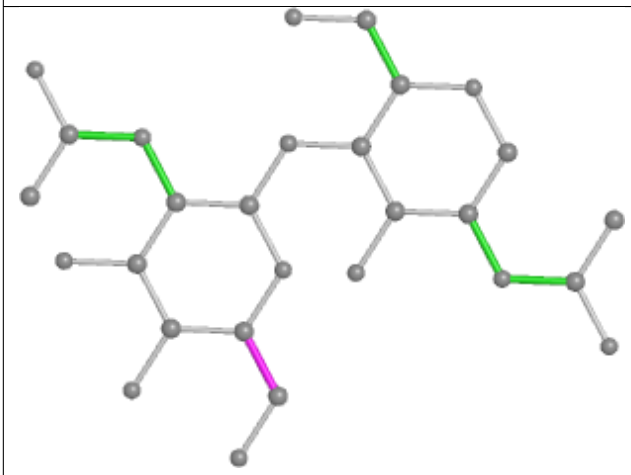


Bond angles



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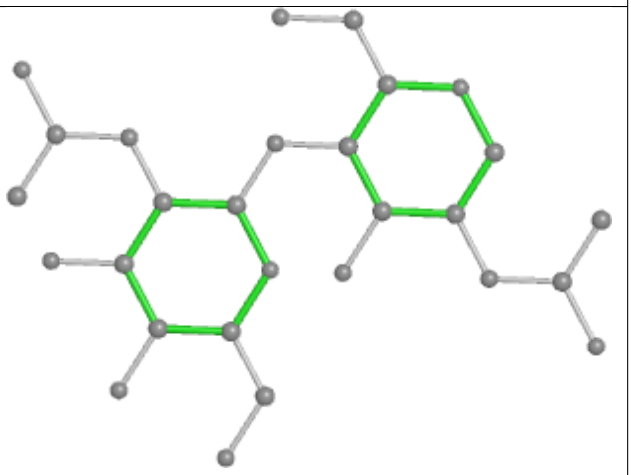
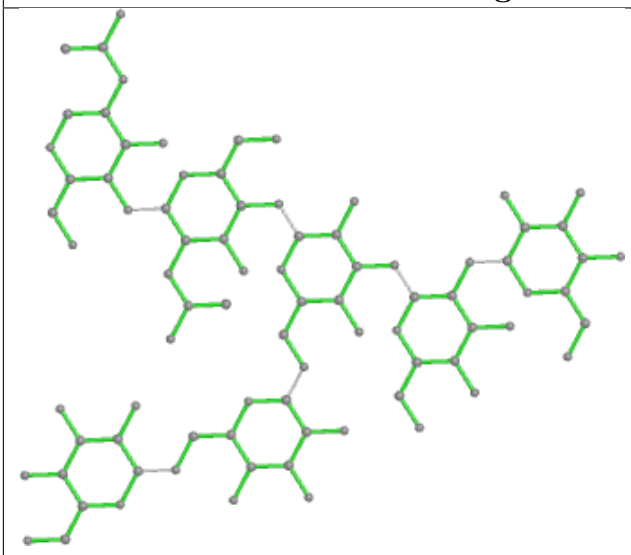
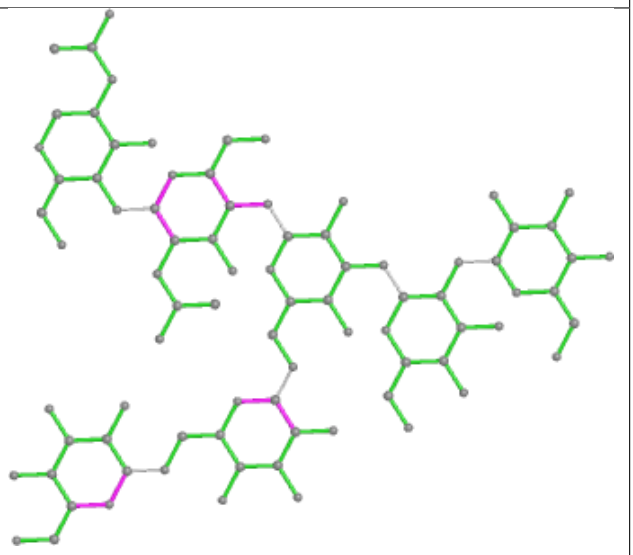


Rings

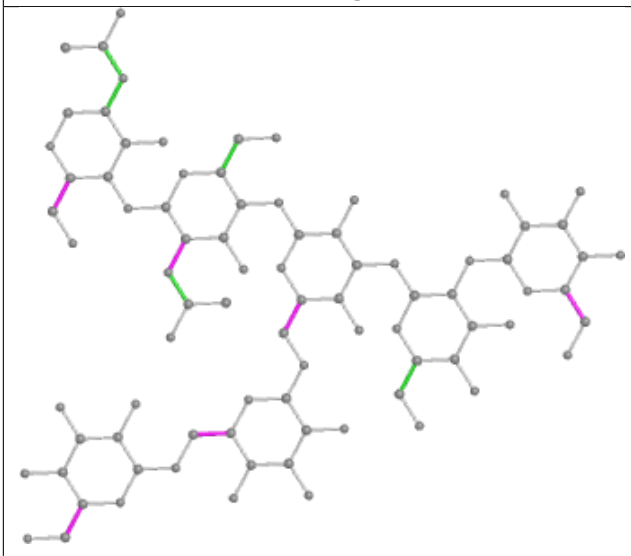
Oligosaccharide Chain O



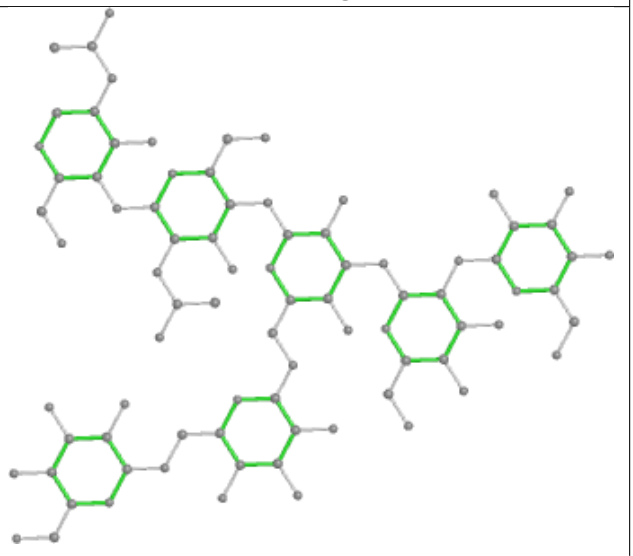
Bond lengths



Bond angles

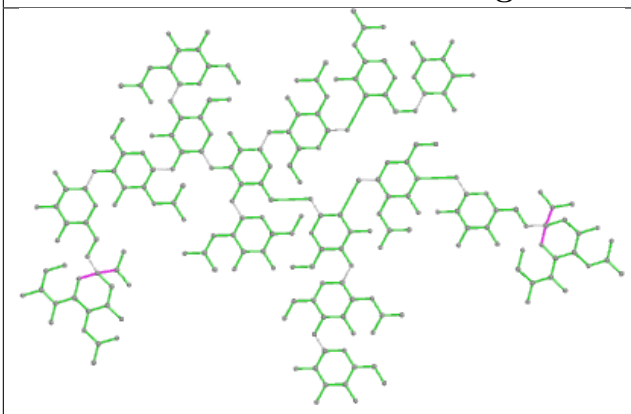


Torsions



Rings

Oligosaccharide Chain P



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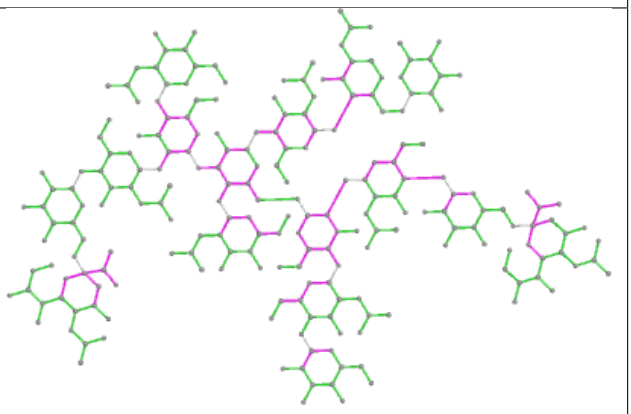
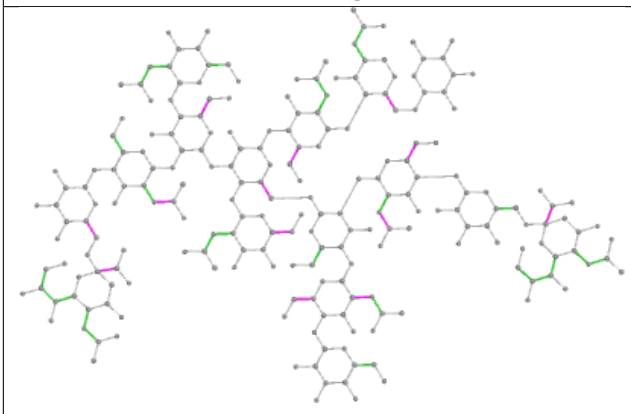


Bond angles



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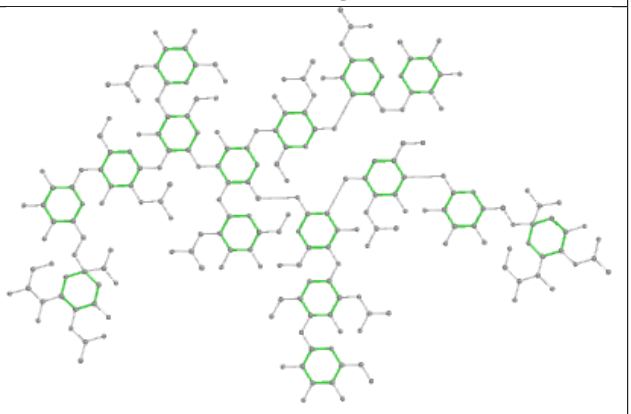
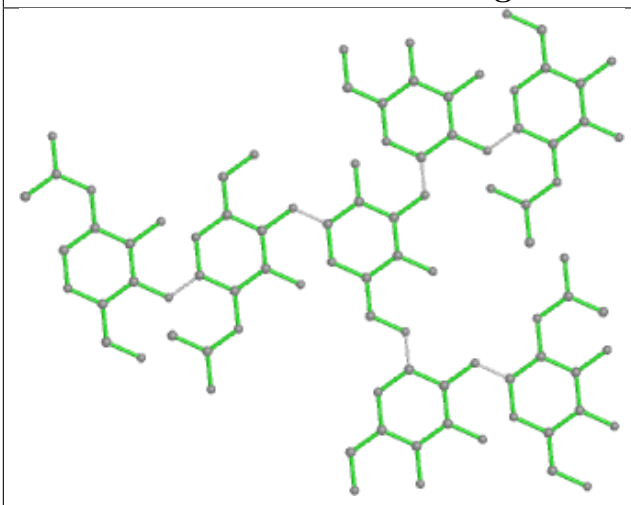
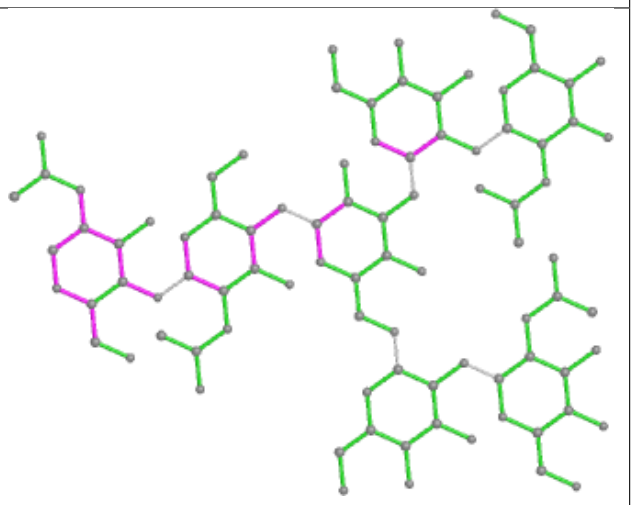


Rings

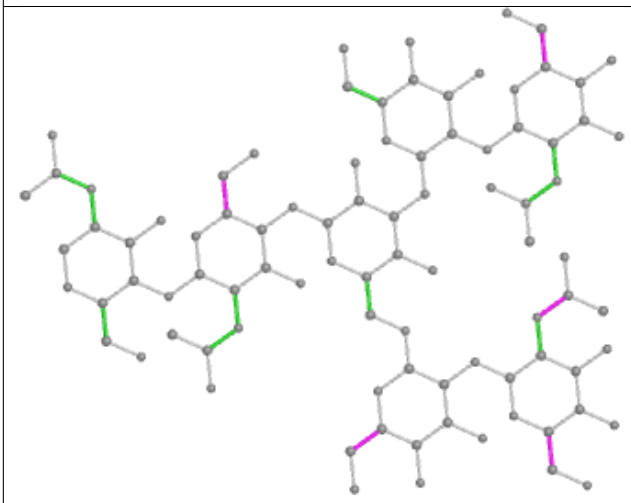
Oligosaccharide Chain R



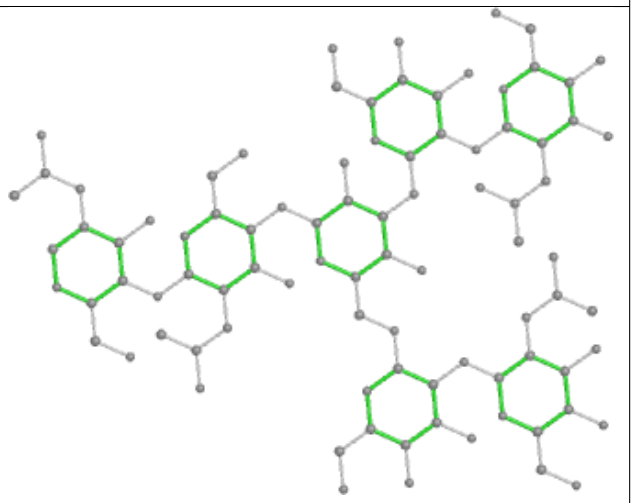
Bond lengths



Bond angles

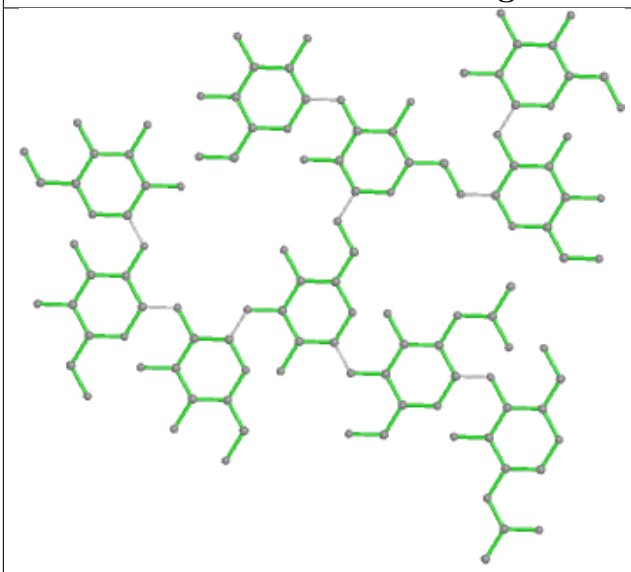


Torsions



Rings

Oligosaccharide Chain S



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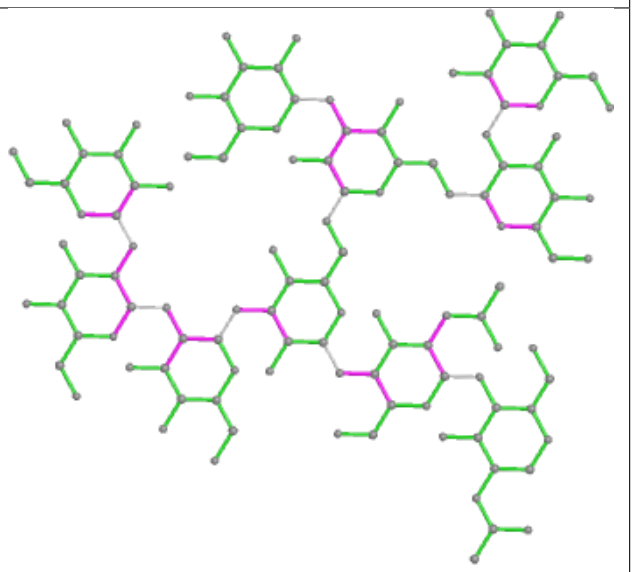
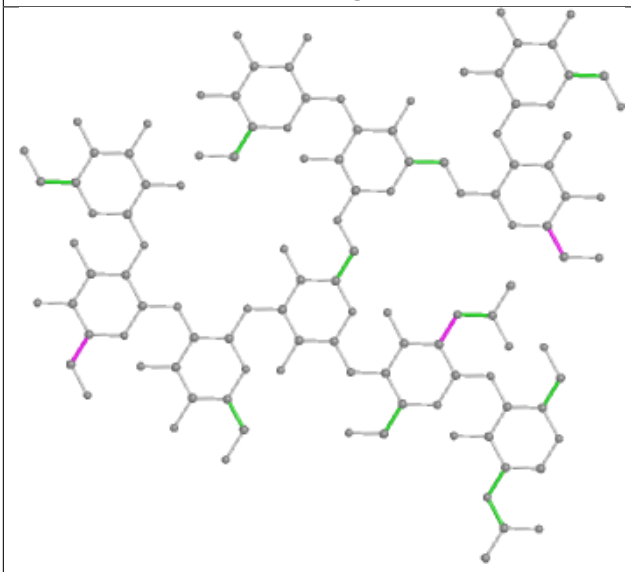


Bond angles



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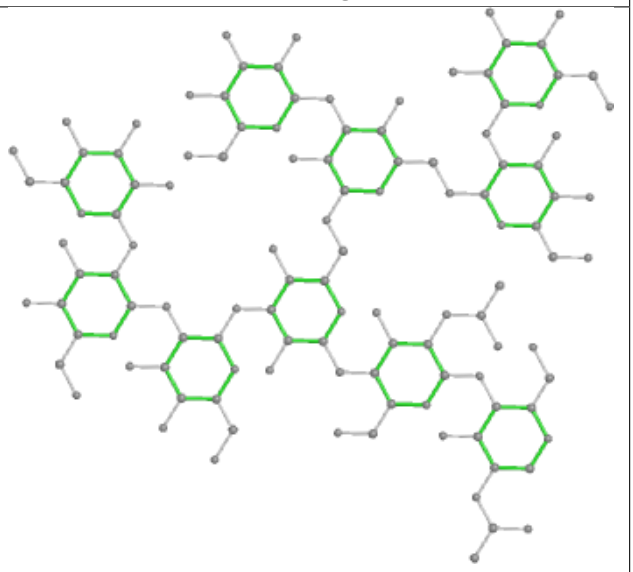
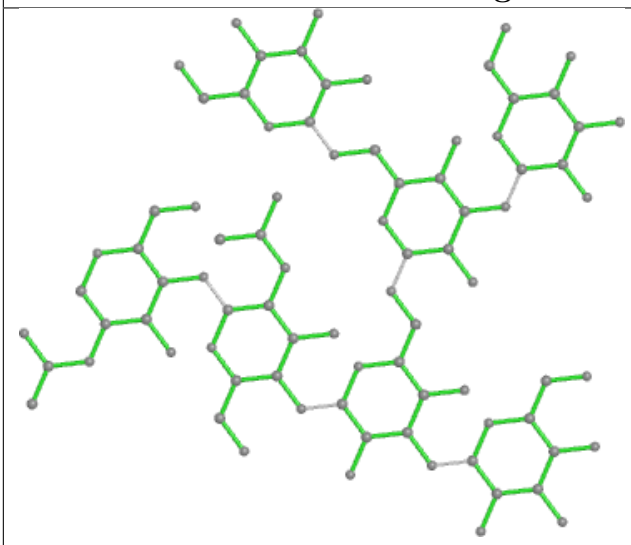


Rings

Oligosaccharide Chain U



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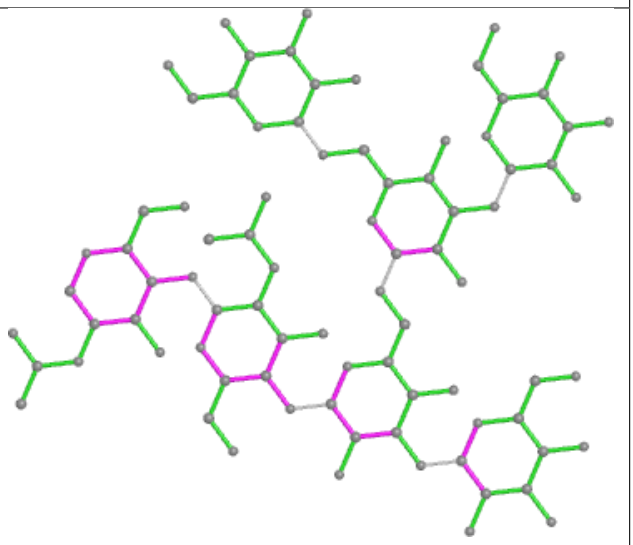
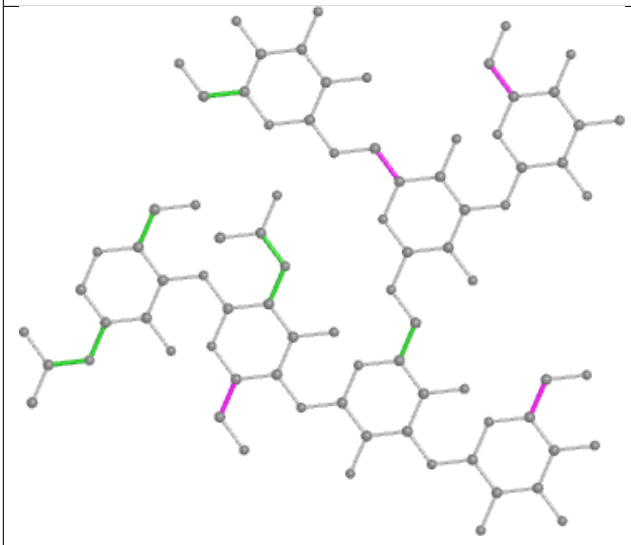


Bond angles



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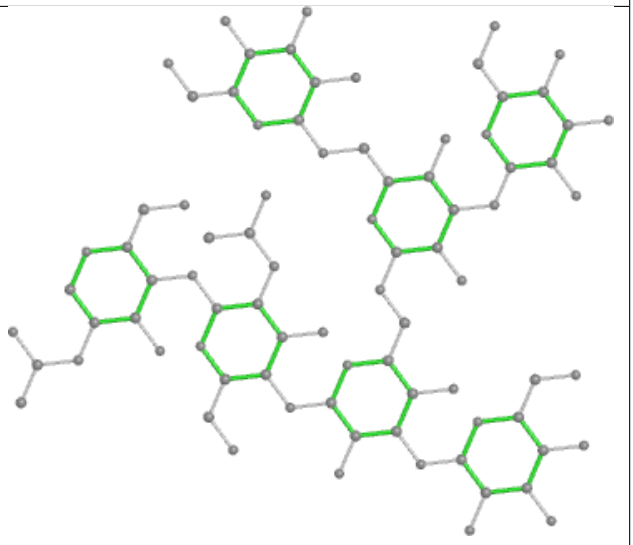
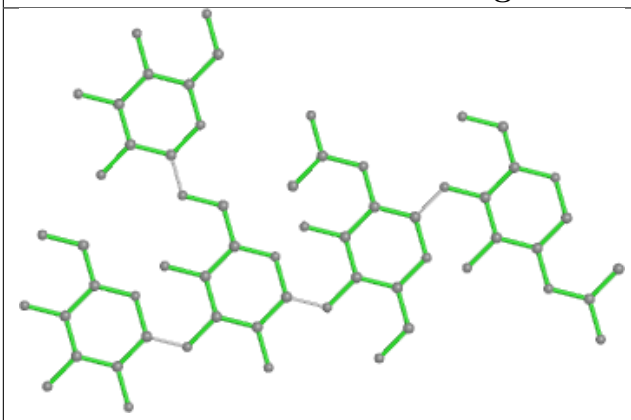
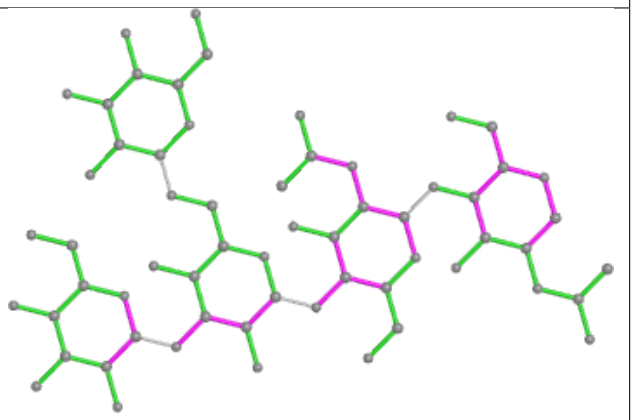


Rings

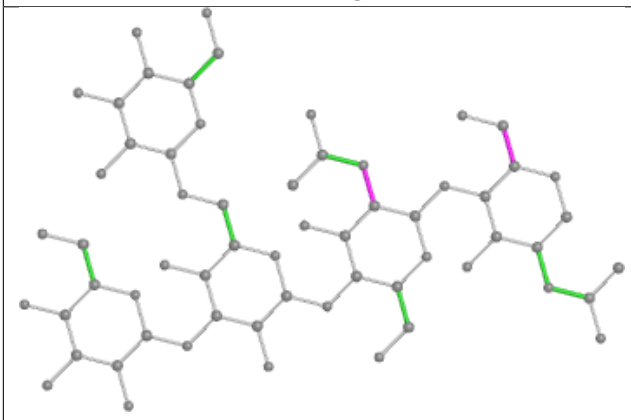
Oligosaccharide Chain V



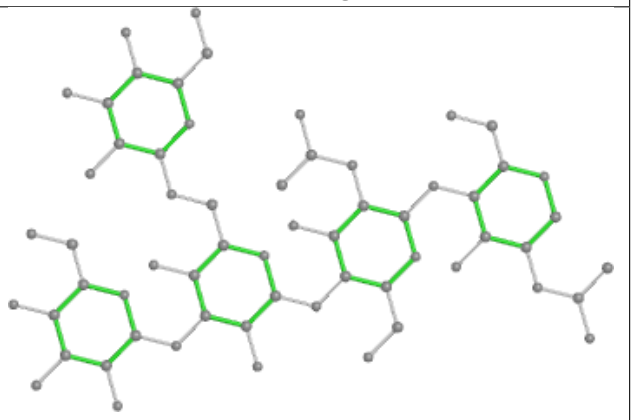
Bond lengths



Bond angles

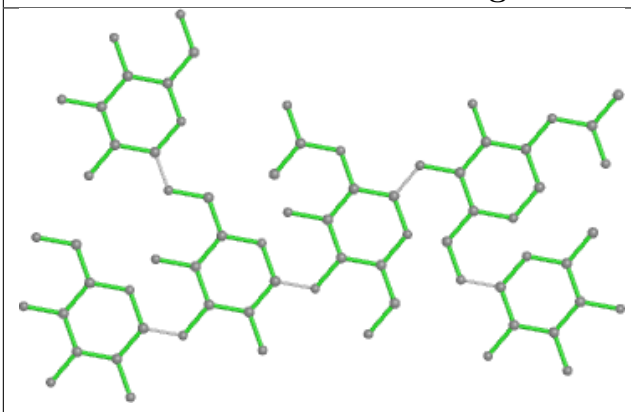


Torsions

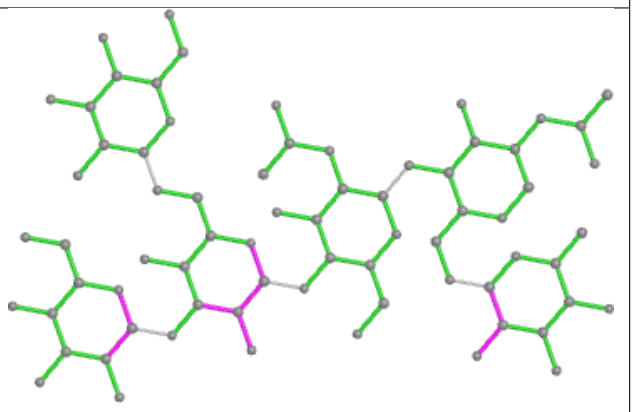


Rings

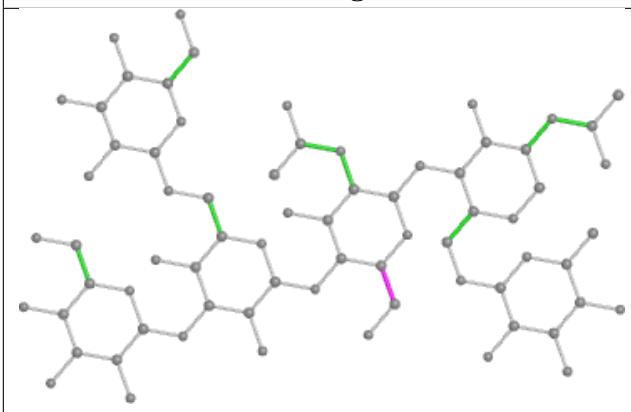
Oligosaccharide Chain W



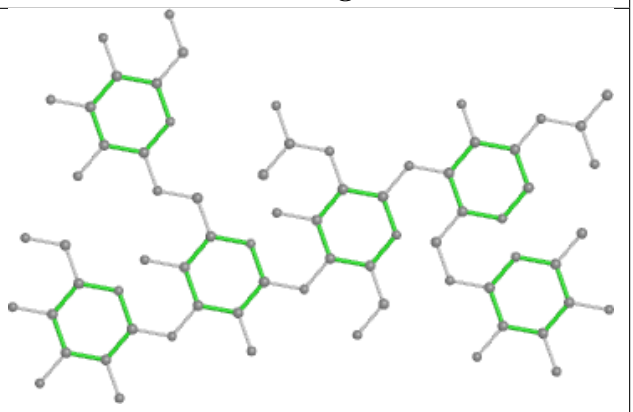
Bond lengths



Bond angles

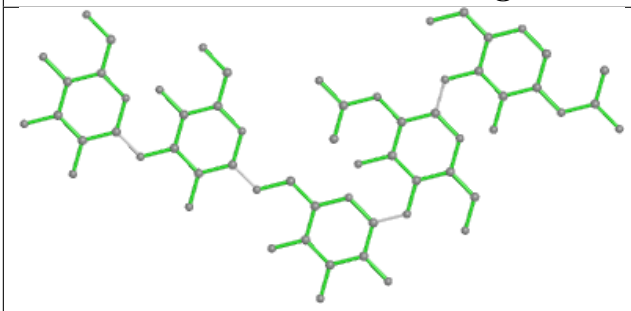


Torsions

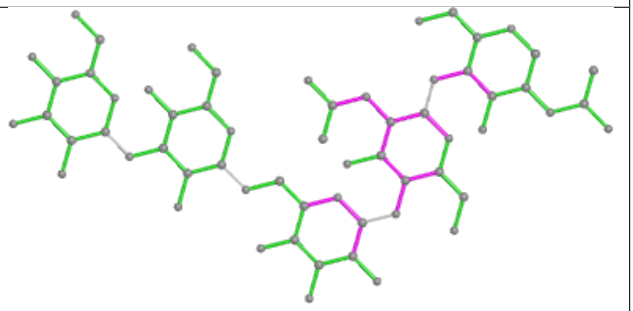


Rings

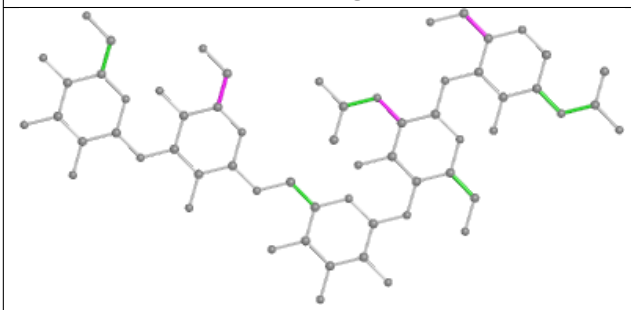
Oligosaccharide Chain X



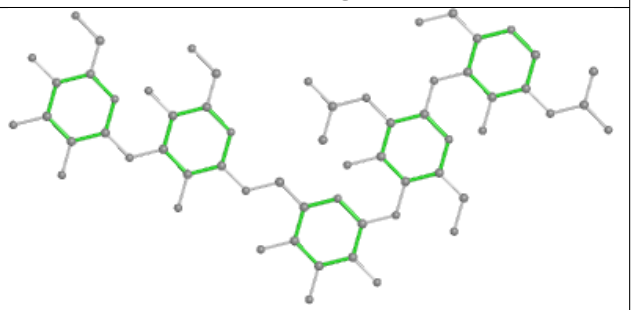
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
23	NAG	G	3390	2	14,14,15	0.32	0	17,19,21	0.64	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
23	NAG	G	3390	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	G	3390	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	B	126/153 (82%)	0.66	15 (11%)	4	4	163, 268, 331, 391	0
2	G	449/481 (93%)	0.59	37 (8%)	11	9	45, 199, 352, 455	0
3	H	230/238 (96%)	1.69	69 (30%)	0	0	154, 314, 444, 501	0
4	L	211/214 (98%)	0.98	43 (20%)	1	1	147, 347, 430, 482	0
5	D	229/232 (98%)	1.91	68 (29%)	0	0	109, 244, 640, 874	0
6	E	210/214 (98%)	3.39	89 (42%)	0	0	23, 310, 886, 970	0
All	All	1455/1532 (94%)	1.44	321 (22%)	0	0	23, 266, 631, 970	0

All (321) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	D	133	GLY	24.0
6	E	206	THR	21.3
6	E	155	PRO	21.3
6	E	148	ALA	20.8
5	D	216	CYS	20.1
6	E	146	THR	19.6
5	D	126	PRO	19.5
6	E	143	GLY	16.9
6	E	149	TRP	15.6
5	D	127	SER	15.5
6	E	190	ARG	15.3
6	E	188	SER	15.0
6	E	144	ALA	15.0
6	E	108	GLY	14.6
5	D	128	SER	14.4
5	D	134	GLY	14.4
5	D	135	THR	14.3
6	E	147	VAL	13.4
6	E	145	VAL	13.4

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Mol	Chain	Res	Type	RSRZ
6	E	210	THR	13.3
6	E	151	ALA	13.2
6	E	191	SER	12.9
5	D	161	SER	12.8
6	E	175	ALA	12.8
4	L	145	VAL	12.7
6	E	156	VAL	12.4
3	H	181	VAL	12.1
6	E	189	HIS	12.0
3	H	180	SER	11.9
3	H	152	VAL	11.8
3	H	135	THR	11.6
6	E	205	LYS	11.6
6	E	135	CYS	11.4
5	D	173	SER	11.2
5	D	160	THR	11.0
6	E	133	LEU	11.0
3	H	138	LEU	11.0
3	H	179	SER	10.9
6	E	117	THR	10.3
5	D	132	SER	10.3
5	D	162	GLY	10.2
6	E	193	SER	10.2
6	E	136	LEU	10.2
6	E	128	ALA	10.1
6	E	194	CYS	9.9
6	E	207	VAL	9.5
6	E	158	ALA	9.3
2	G	187	SER	9.3
6	E	157	LYS	9.1
6	E	118	LEU	9.0
3	H	10	GLY	8.8
3	H	212	GLU	8.8
6	E	107	LEU	8.7
3	H	184	VAL	8.5
6	E	195	GLN	8.5
5	D	192	GLN	8.3
6	E	111	LYS	8.2
3	H	11	LEU	8.1
4	L	144	ALA	8.1
3	H	151	THR	7.9
3	H	215	SER	7.9

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Mol	Chain	Res	Type	RSRZ
6	E	152	ASP	7.7
6	E	208	ALA	7.7
1	B	547	GLY	7.7
4	L	154	SER	7.6
6	E	176	SER	7.6
6	E	129	ASN	7.4
5	D	125	ALA	7.4
3	H	194	TYR	7.4
5	D	129	LYS	7.4
6	E	181	LEU	7.0
6	E	137	ILE	6.9
3	H	192	GLN	6.9
4	L	118	LEU	6.8
3	H	127	SER	6.8
3	H	186	SER	6.5
3	H	150	VAL	6.5
6	E	196	VAL	6.4
6	E	150	LYS	6.3
6	E	187	LYS	6.3
5	D	172	SER	6.2
3	H	136	ALA	6.1
2	G	188	ASN	6.1
6	E	209	PRO	6.1
6	E	204	GLU	6.1
5	D	208	ASP	6.1
5	D	151	THR	6.0
6	E	127	GLN	5.9
6	E	183	PRO	5.9
3	H	141	LEU	5.9
5	D	185	PRO	5.8
1	B	602	LEU	5.8
6	E	180	SER	5.8
5	D	165	THR	5.8
3	H	198	VAL	5.8
3	H	182	VAL	5.7
6	E	179	LEU	5.7
6	E	142	PRO	5.6
1	B	545	LEU	5.5
6	E	162	THR	5.5
6	E	124	GLU	5.4
3	H	9	PRO	5.4
6	E	120	PRO	5.4

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Mol	Chain	Res	Type	RSRZ
3	H	183	THR	5.4
6	E	134	VAL	5.3
2	G	465	THR	5.3
6	E	116	VAL	5.2
4	L	117	THR	5.2
6	E	192	TYR	5.1
1	B	520	LEU	5.1
5	D	140	CYS	5.1
5	D	152	VAL	5.1
6	E	3	ALA	5.1
3	H	190	GLY	5.0
5	D	174	GLY	5.0
4	L	104	LEU	4.9
6	E	182	THR	4.8
5	D	214	LYS	4.8
3	H	90	TYR	4.8
5	D	189	LEU	4.7
4	L	86	TYR	4.7
5	D	191	THR	4.7
5	D	137	ALA	4.6
6	E	201	SER	4.6
4	L	209	PRO	4.6
5	D	186	SER	4.6
2	G	236	THR	4.6
3	H	153	SER	4.5
6	E	112	ALA	4.5
5	D	136	ALA	4.5
6	E	197	THR	4.5
5	D	180	SER	4.5
3	H	81	LYS	4.4
4	L	132	THR	4.4
4	L	114	PRO	4.4
6	E	109	GLN	4.4
5	D	141	LEU	4.4
5	D	12	LYS	4.4
6	E	174	ALA	4.4
3	H	155	ASN	4.3
3	H	207	VAL	4.3
4	L	37	GLN	4.2
1	B	599	SER	4.2
3	H	178	LEU	4.2
6	E	122	SER	4.2

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Mol	Chain	Res	Type	RSRZ
4	L	119	PHE	4.2
3	H	142	VAL	4.2
2	G	496	VAL	4.1
6	E	132	THR	4.1
6	E	154	SER	4.1
3	H	140	CYS	4.1
5	D	149	PRO	4.0
5	D	138	LEU	4.0
3	H	185	PRO	4.0
2	G	33	ASN	4.0
3	H	38	ARG	3.9
5	D	179	SER	3.9
5	D	130	SER	3.9
6	E	4	LEU	3.9
3	H	191	THR	3.8
3	H	193	THR	3.8
5	D	199	ASN	3.8
3	H	189	LEU	3.8
3	H	137	ALA	3.8
4	L	39	ARG	3.8
3	H	4	LEU	3.7
3	H	163	VAL	3.7
6	E	131	ALA	3.7
3	H	80	LEU	3.6
5	D	193	THR	3.6
6	E	159	GLY	3.6
6	E	113	ALA	3.5
4	L	139	ASP	3.5
4	L	176	SER	3.5
5	D	122	PHE	3.5
1	B	544	LEU	3.4
5	D	188	SER	3.5
3	H	69	ILE	3.4
4	L	38	HIS	3.4
4	L	203	VAL	3.4
4	L	208	ALA	3.4
3	H	214	LYS	3.3
5	D	120	SER	3.3
2	G	505	VAL	3.3
3	H	7	SER	3.3
5	D	131	THR	3.3
4	L	109	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
3	H	47	TRP	3.2
2	G	500	ARG	3.2
2	G	411	ASN	3.2
4	L	162	THR	3.2
3	H	12	VAL	3.2
6	E	184	GLU	3.2
1	B	578	ALA	3.2
2	G	93	PHE	3.2
4	L	135	CYS	3.2
3	H	113	SER	3.2
2	G	504	ARG	3.2
4	L	136	LEU	3.2
1	B	656	ASN	3.1
2	G	499	THR	3.1
2	G	494	LEU	3.1
4	L	155	PRO	3.1
3	H	49	GLY	3.1
5	D	202	PRO	3.1
6	E	185	GLN	3.0
4	L	207	VAL	3.0
6	E	200	GLY	3.0
1	B	546	SER	3.0
2	G	466	GLU	3.0
1	B	518	VAL	3.0
6	E	161	GLU	3.0
6	E	114	PRO	3.0
6	E	92	ALA	3.0
2	G	95	MET	3.0
2	G	498	PRO	3.0
4	L	140	PHE	3.0
5	D	100(G)	ARG	3.0
2	G	468	PHE	2.9
5	D	215	SER	2.9
3	H	129	LYS	2.9
3	H	110	THR	2.9
4	L	175	ALA	2.9
2	G	40	TYR	2.9
5	D	187	SER	2.9
6	E	198	HIS	2.9
1	B	569	THR	2.9
5	D	170	LEU	2.9
5	D	197	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
5	D	148	GLU	2.8
4	L	153	SER	2.8
6	E	123	SER	2.8
4	L	131	ALA	2.8
5	D	13	LYS	2.8
1	B	593	LEU	2.8
4	L	147	VAL	2.8
5	D	155	ASN	2.8
4	L	47	LEU	2.8
3	H	68	VAL	2.7
5	D	24	ALA	2.7
2	G	237	GLY	2.7
2	G	358	ILE	2.7
1	B	600	GLY	2.7
3	H	139	GLY	2.7
2	G	38	VAL	2.7
1	B	595	ILE	2.7
3	H	199	ASN	2.7
6	E	121	PRO	2.6
5	D	142	VAL	2.6
2	G	293	GLN	2.6
6	E	98	PHE	2.6
2	G	141	ASP	2.6
2	G	356	ASN	2.6
4	L	105	THR	2.6
4	L	13	VAL	2.6
2	G	467	THR	2.6
3	H	92	CYS	2.6
4	L	107	LEU	2.6
5	D	212	GLU	2.6
5	D	171	GLN	2.5
5	D	1	GLU	2.5
5	D	213	PRO	2.5
5	D	147	PRO	2.5
2	G	235	GLY	2.5
5	D	190	GLY	2.5
3	H	109	VAL	2.5
3	H	126	PRO	2.5
6	E	186	TRP	2.5
2	G	86	LEU	2.4
3	H	159	LEU	2.4
2	G	73	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
6	E	165	PRO	2.4
3	H	13	LYS	2.4
3	H	156	SER	2.4
5	D	153	SER	2.4
4	L	120	PRO	2.4
6	E	177	SER	2.3
3	H	8	GLY	2.3
5	D	183	THR	2.3
4	L	134	VAL	2.3
4	L	36	TYR	2.3
3	H	147	PRO	2.3
3	H	128	SER	2.3
3	H	211	VAL	2.3
2	G	72	HIS	2.3
6	E	160	VAL	2.3
3	H	84	PRO	2.3
4	L	158	ALA	2.2
3	H	162	GLY	2.2
3	H	34	TRP	2.2
4	L	106	VAL	2.2
5	D	163	VAL	2.2
5	D	33	HIS	2.2
3	H	28	SER	2.2
4	L	146	THR	2.2
6	E	163	THR	2.2
6	E	119	PHE	2.1
5	D	164	HIS	2.1
5	D	182	VAL	2.1
3	H	79	SER	2.1
4	L	137	ILE	2.1
6	E	178	TYR	2.1
4	L	64	GLY	2.1
2	G	463	SER	2.1
2	G	360	ARG	2.1
5	D	168	ALA	2.1
6	E	138	SER	2.1
3	H	78	LEU	2.1
2	G	85	HIS	2.1
4	L	12	SER	2.1
5	D	121	VAL	2.1
4	L	14	ALA	2.1
2	G	139	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	G	217	TYR	2.0
1	B	628	TRP	2.0
2	G	455	THR	2.0
2	G	69	TRP	2.0
6	E	110	PRO	2.0
2	G	225	ILE	2.0
6	E	19	ILE	2.0
5	D	178	LEU	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
16	MAN	P	9	11/12	0.42	0.34	390,390,390,390	0
16	NAG	P	13	14/15	0.43	0.44	394,394,394,394	0
16	NAG	P	10	14/15	0.44	0.39	404,417,422,424	0
16	NAG	P	2	14/15	0.46	0.29	297,317,320,320	0
16	FUC	P	16	10/11	0.48	0.59	309,309,309,309	0
17	BMA	R	3	11/12	0.48	0.20	350,357,361,366	0
12	NAG	K	5	14/15	0.49	0.25	363,363,363,363	0
15	MAN	O	6	11/12	0.49	0.50	318,335,341,351	0
19	BMA	U	3	11/12	0.49	0.36	397,414,429,431	0
16	GAL	P	11	11/12	0.56	0.20	435,435,435,435	0
11	MAN	J	8	11/12	0.57	0.19	330,330,330,330	0
18	MAN	S	9	11/12	0.58	0.46	280,280,280,280	0
7	FUC	A	2	10/11	0.58	0.55	312,312,312,312	0
20	MAN	V	4	11/12	0.58	0.42	313,318,336,356	0
15	BMA	O	3	11/12	0.59	0.38	287,304,319,321	0
15	MAN	O	7	11/12	0.59	0.51	399,413,420,421	0
13	NAG	M	5	14/15	0.60	0.35	355,368,372,374	0
19	MAN	U	5	11/12	0.61	0.32	342,342,342,342	0
11	MAN	J	4	11/12	0.62	0.18	340,340,340,340	0
22	MAN	X	5	11/12	0.62	0.71	408,410,419,425	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	NAG	J	9	14/15	0.65	0.20	315,315,315,315	0
16	GAL	P	14	11/12	0.65	0.50	367,367,367,367	0
15	MAN	O	5	11/12	0.65	0.43	311,311,311,311	0
12	MAN	K	4	11/12	0.66	0.25	338,338,338,338	0
17	NAG	R	2	14/15	0.66	0.43	338,352,362,366	0
16	SIA	P	12	20/21	0.66	0.48	456,456,456,456	0
21	MAN	W	4	11/12	0.66	0.38	294,294,294,294	0
16	NAG	P	15	14/15	0.66	0.47	376,376,376,376	0
16	NAG	P	1	14/15	0.67	0.32	289,299,317,320	0
21	MAN	W	5	11/12	0.67	0.58	400,400,400,400	0
9	FUC	F	3	10/11	0.67	0.50	318,324,334,342	0
12	GAL	K	6	11/12	0.68	0.42	411,411,411,411	0
12	NAG	K	2	14/15	0.69	0.23	277,290,302,308	0
11	NAG	J	11	14/15	0.69	0.35	383,383,383,383	0
12	MAN	K	7	11/12	0.69	0.23	350,350,350,350	0
16	NAG	P	8	14/15	0.70	0.24	371,371,371,371	0
9	NAG	F	2	14/15	0.70	0.33	336,357,359,360	0
20	BMA	V	3	11/12	0.71	0.24	318,336,351,352	0
13	NAG	M	9	14/15	0.71	0.45	307,320,324,326	0
20	MAN	V	5	11/12	0.71	0.38	314,331,337,347	0
19	NAG	U	2	14/15	0.71	0.74	431,431,431,431	0
13	GAL	M	6	11/12	0.71	0.22	358,363,372,375	0
22	MAN	X	4	11/12	0.71	0.42	380,397,403,413	0
17	NAG	R	7	14/15	0.71	0.35	332,345,349,351	0
14	NAG	T	1	14/15	0.72	0.18	385,385,385,385	0
21	NAG	W	2	14/15	0.72	0.22	300,321,323,323	0
16	BMA	P	3	11/12	0.72	0.24	355,362,366,371	0
19	MAN	U	7	11/12	0.72	0.38	370,375,393,413	0
13	SIA	M	7	20/21	0.72	0.42	371,371,371,371	0
11	NAG	J	7	14/15	0.72	0.27	340,340,340,340	0
9	NAG	F	1	14/15	0.73	0.27	331,341,358,361	0
17	MAN	R	4	11/12	0.74	0.28	317,323,334,335	0
17	NAG	R	5	14/15	0.74	0.52	347,356,371,376	0
19	MAN	U	6	11/12	0.74	0.36	355,370,377,378	0
15	MAN	O	4	11/12	0.74	0.35	281,286,304,324	0
14	NAG	T	2	14/15	0.74	0.22	369,369,369,369	0
11	GAL	J	6	11/12	0.74	0.27	350,350,350,350	0
12	BMA	K	3	11/12	0.75	0.10	330,330,330,330	0
11	NAG	J	5	14/15	0.76	0.18	346,346,346,346	0
7	NAG	A	1	14/15	0.76	0.22	285,298,351,352	0
17	NAG	R	1	14/15	0.77	0.45	258,258,258,258	0
13	MAN	M	8	11/12	0.77	0.26	283,291,296,297	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
22	NAG	X	1	14/15	0.77	0.42	215,226,243,248	0
10	NAG	I	2	14/15	0.77	0.22	271,271,271,271	0
16	NAG	P	5	14/15	0.77	0.15	352,366,370,372	0
16	SIA	P	7	20/21	0.78	0.21	397,397,397,397	0
14	NAG	N	2	14/15	0.78	0.37	270,272,275,276	0
19	NAG	U	1	14/15	0.78	0.43	290,299,323,342	0
11	BMA	J	3	11/12	0.78	0.15	313,313,313,313	0
21	BMA	W	3	11/12	0.78	0.19	314,321,325,329	0
13	NAG	M	2	14/15	0.79	0.34	221,241,244,244	0
11	FUC	J	13	10/11	0.79	0.35	294,294,294,294	0
21	FUC	W	6	10/11	0.79	0.39	308,313,323,331	0
8	FUC	C	4	10/11	0.80	0.26	351,351,351,351	0
11	GAL	J	10	11/12	0.80	0.22	336,336,336,336	0
12	NAG	K	8	14/15	0.80	0.19	339,352,356,358	0
12	GAL	K	9	11/12	0.80	0.19	350,355,364,366	0
11	GAL	J	12	11/12	0.81	0.39	401,401,401,401	0
18	MAN	S	7	11/12	0.81	0.27	208,225,231,240	0
18	MAN	S	8	11/12	0.81	0.26	261,274,297,307	0
19	MAN	U	4	11/12	0.82	0.21	350,368,374,383	0
11	NAG	J	2	14/15	0.82	0.27	254,274,287,287	0
8	BMA	C	3	11/12	0.82	0.38	311,311,311,311	0
10	BMA	I	3	11/12	0.83	0.23	274,274,274,274	0
14	NAG	Q	1	14/15	0.83	0.31	204,220,246,255	0
22	BMA	X	3	11/12	0.83	0.33	307,324,340,341	0
18	MAN	S	6	11/12	0.83	0.33	203,208,213,213	0
16	MAN	P	4	11/12	0.83	0.44	393,393,393,393	0
10	NAG	I	1	14/15	0.84	0.37	251,251,251,251	0
13	MAN	M	4	11/12	0.84	0.22	337,337,337,337	0
20	NAG	V	1	14/15	0.85	0.37	245,256,273,279	0
14	NAG	Q	2	14/15	0.85	0.35	283,298,308,317	0
21	NAG	W	1	14/15	0.85	0.25	296,306,324,327	0
16	GAL	P	6	11/12	0.86	0.12	351,351,351,351	0
22	NAG	X	2	14/15	0.86	0.42	241,258,278,284	0
12	FUC	K	10	10/11	0.86	0.57	329,329,329,329	0
18	MAN	S	5	11/12	0.86	0.16	180,183,196,204	0
13	NAG	M	1	14/15	0.86	0.39	198,208,226,229	0
20	NAG	V	2	14/15	0.87	0.34	326,343,363,369	0
14	NAG	N	1	14/15	0.87	0.29	232,246,263,271	0
12	NAG	K	1	14/15	0.87	0.34	236,260,269,281	0
18	MAN	S	10	11/12	0.88	0.35	250,252,261,267	0
18	MAN	S	4	11/12	0.88	0.19	195,200,218,238	0
15	NAG	O	2	14/15	0.88	0.33	203,219,240,245	0

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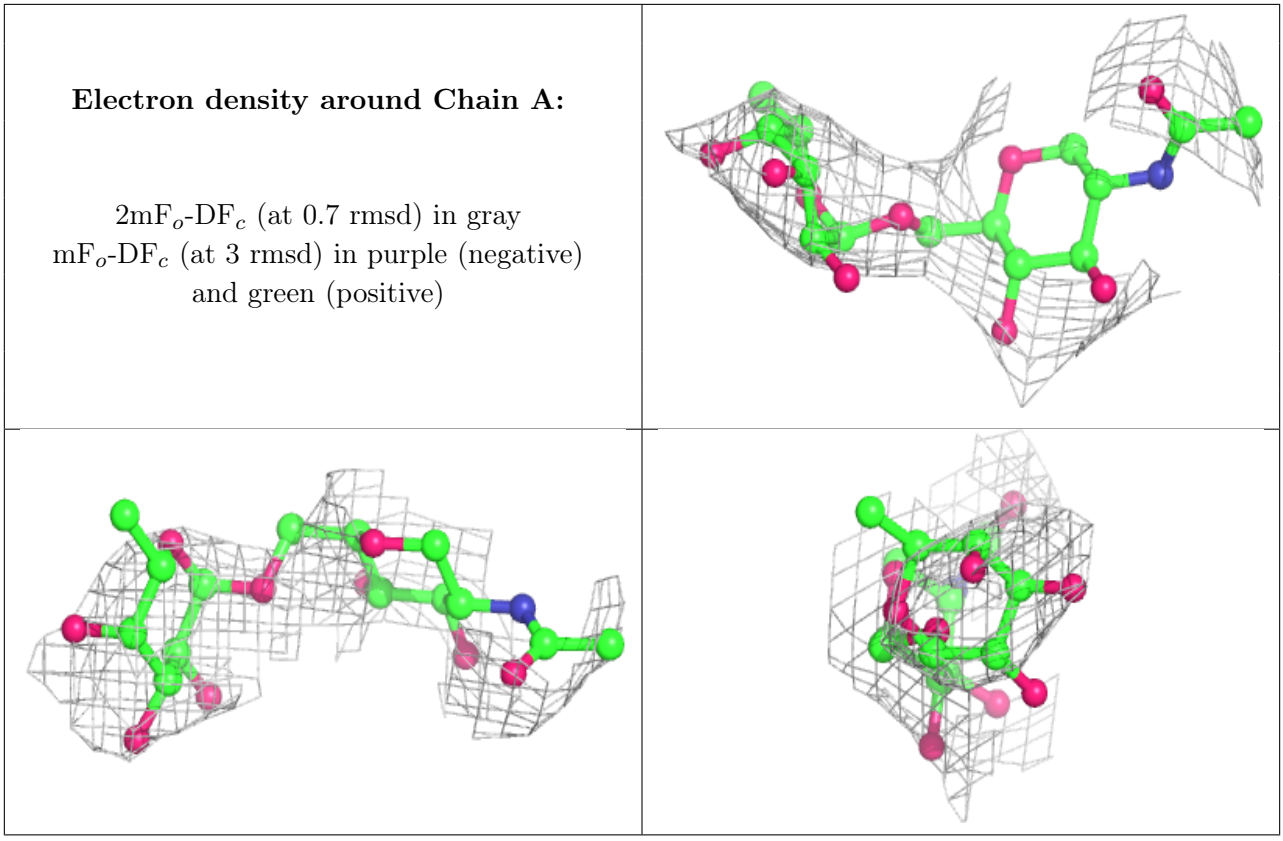
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
13	BMA	M	3	11/12	0.89	0.23	254,261,265,270	0
18	NAG	S	1	14/15	0.89	0.31	200,211,228,234	0
8	NAG	C	1	14/15	0.89	0.16	333,351,364,365	0
17	MAN	R	6	11/12	0.89	0.20	360,369,374,374	0
18	BMA	S	3	11/12	0.92	0.22	136,153,169,170	0
15	NAG	O	1	14/15	0.93	0.32	169,179,197,202	0
11	NAG	J	1	14/15	0.93	0.24	211,224,277,278	0
18	NAG	S	2	14/15	0.94	0.27	162,179,199,205	0
8	NAG	C	2	14/15	0.95	0.18	318,318,318,318	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.

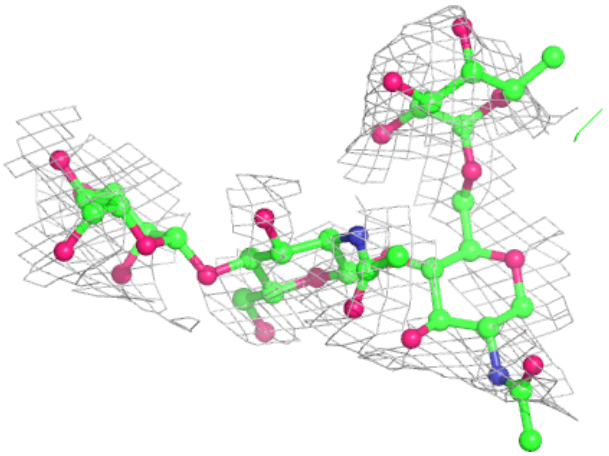
Electron density around Chain A:

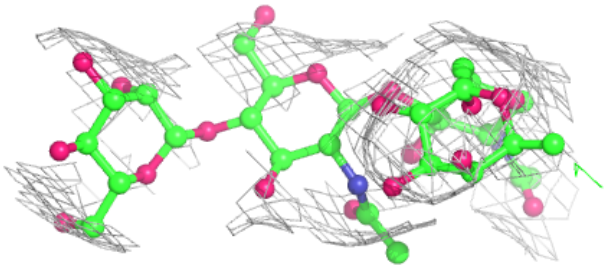
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

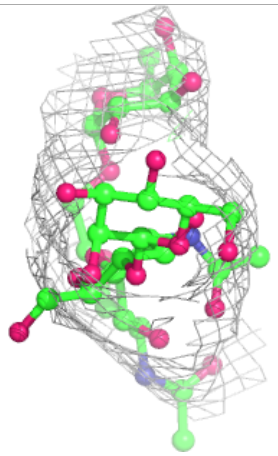


Electron density around Chain C:

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

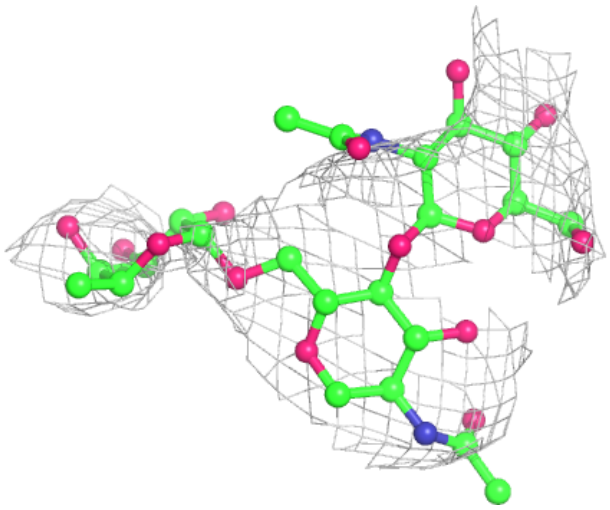


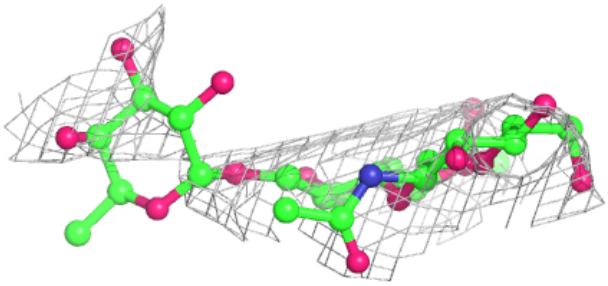


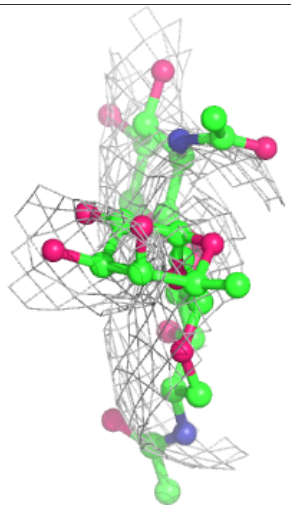


Electron density around Chain F:

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

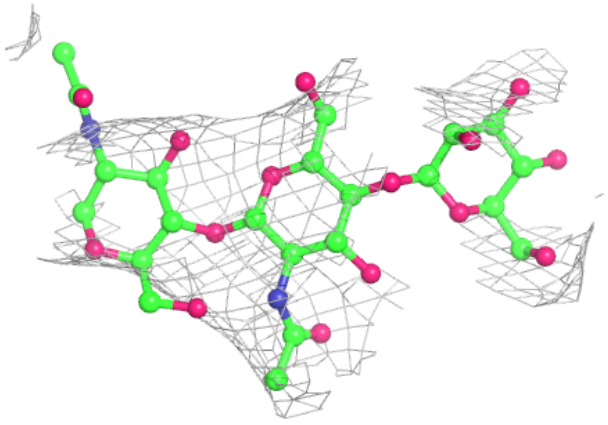


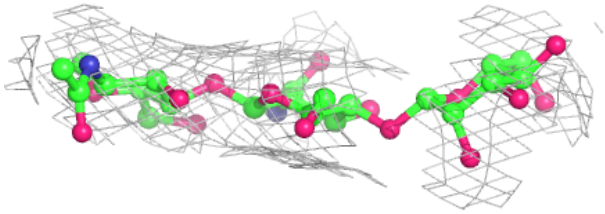


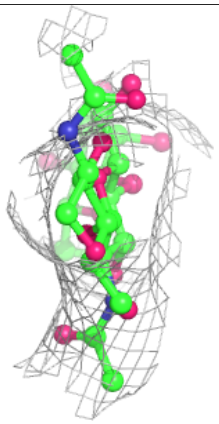


Electron density around Chain I:

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

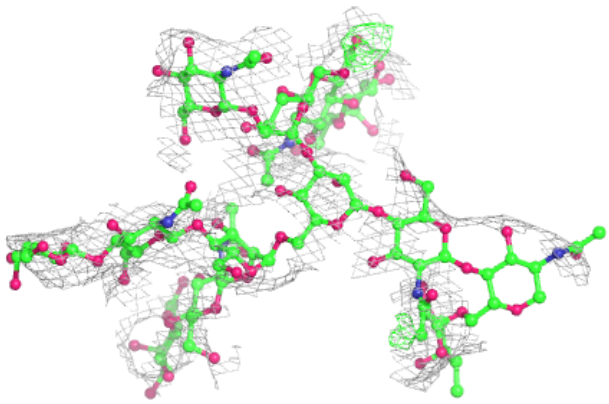


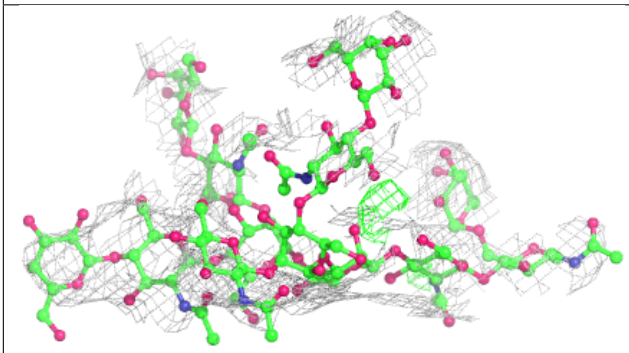


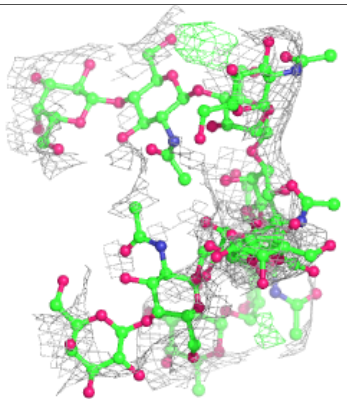


Electron density around Chain J:

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

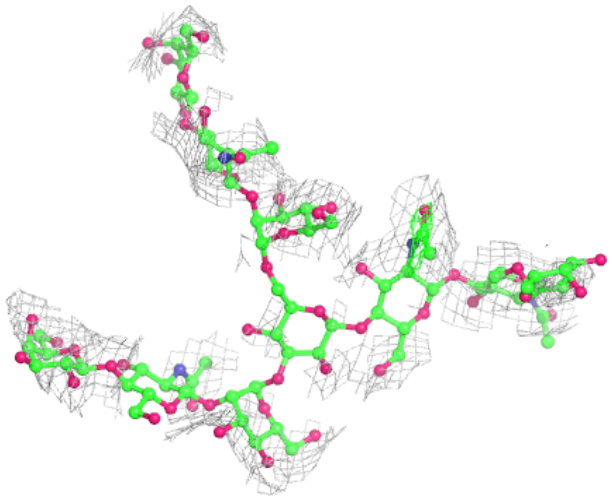


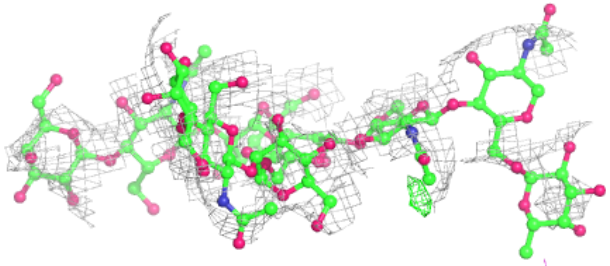


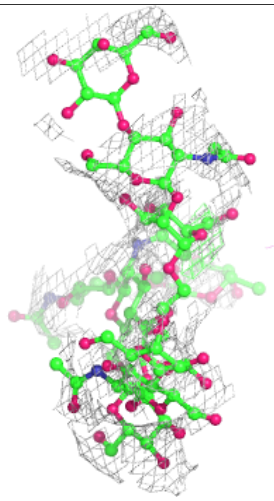


Electron density around Chain K:

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

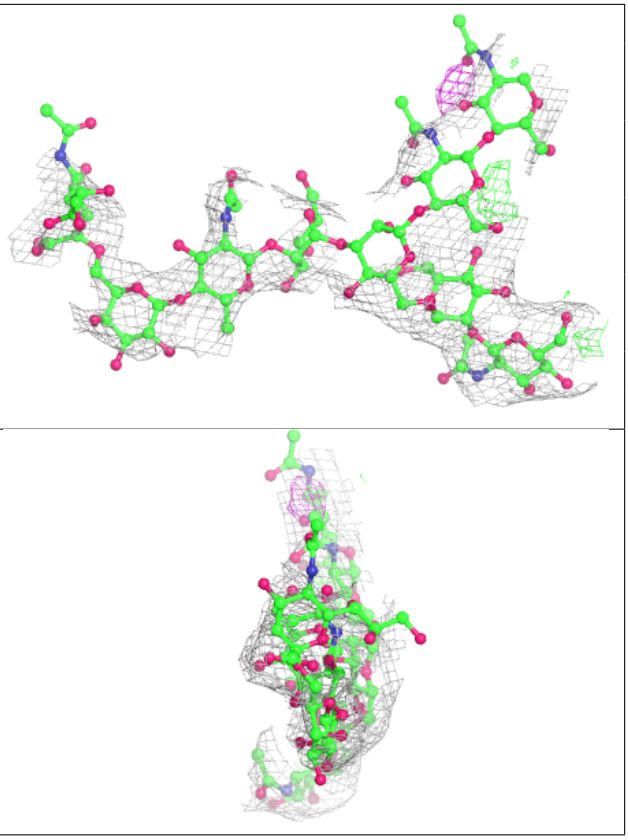


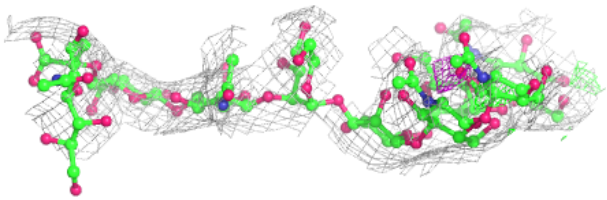




Electron density around Chain M:

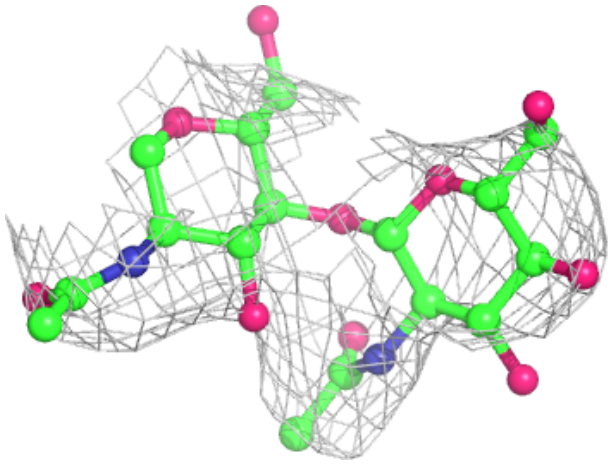
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

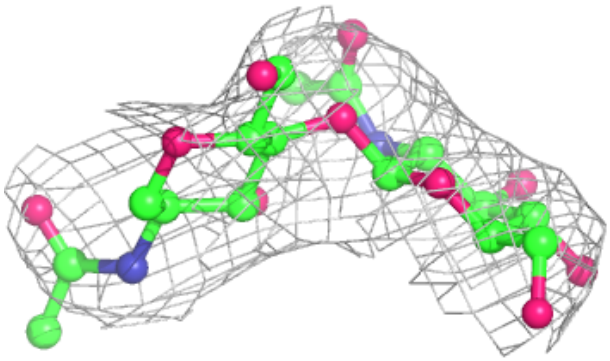


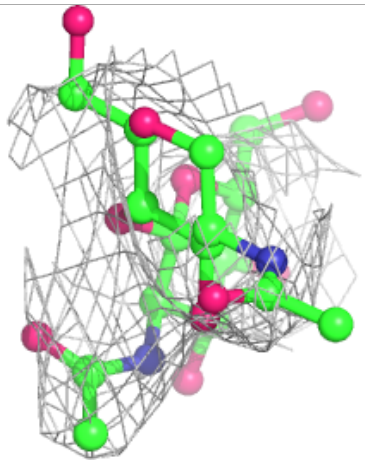


Electron density around Chain N:

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

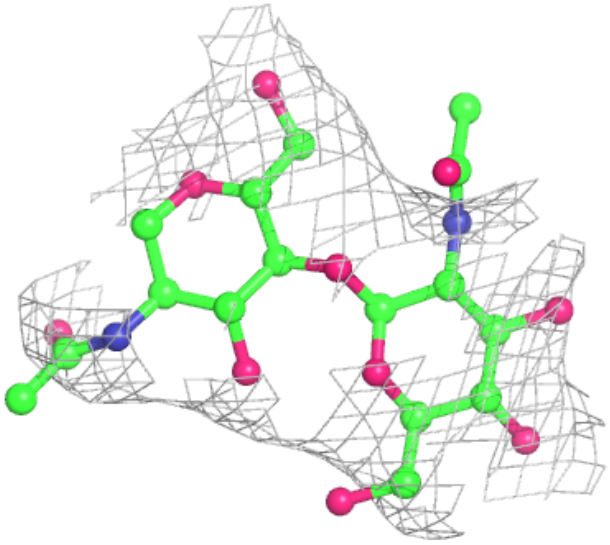


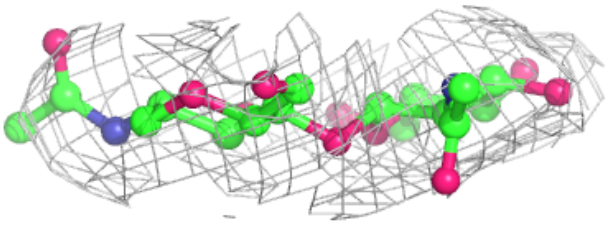


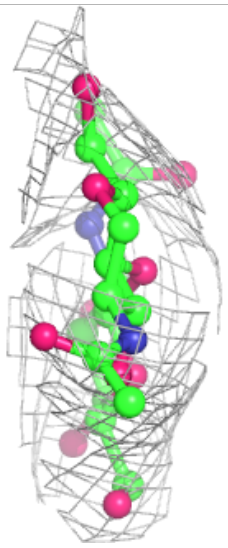


Electron density around Chain Q:

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

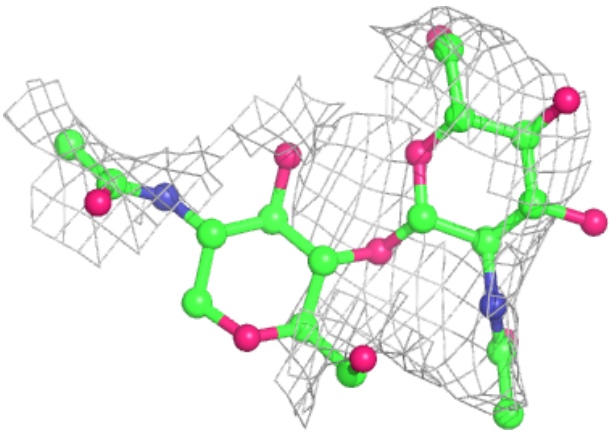


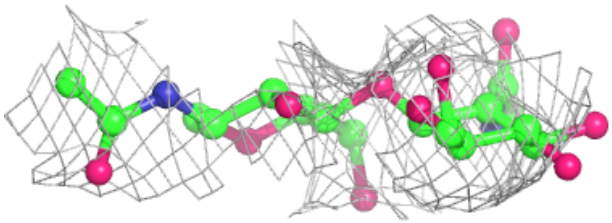


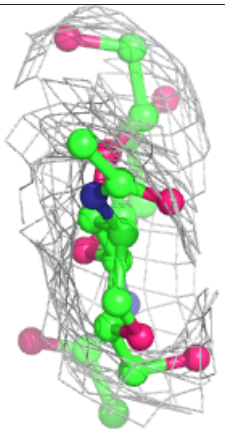


Electron density around Chain T:

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

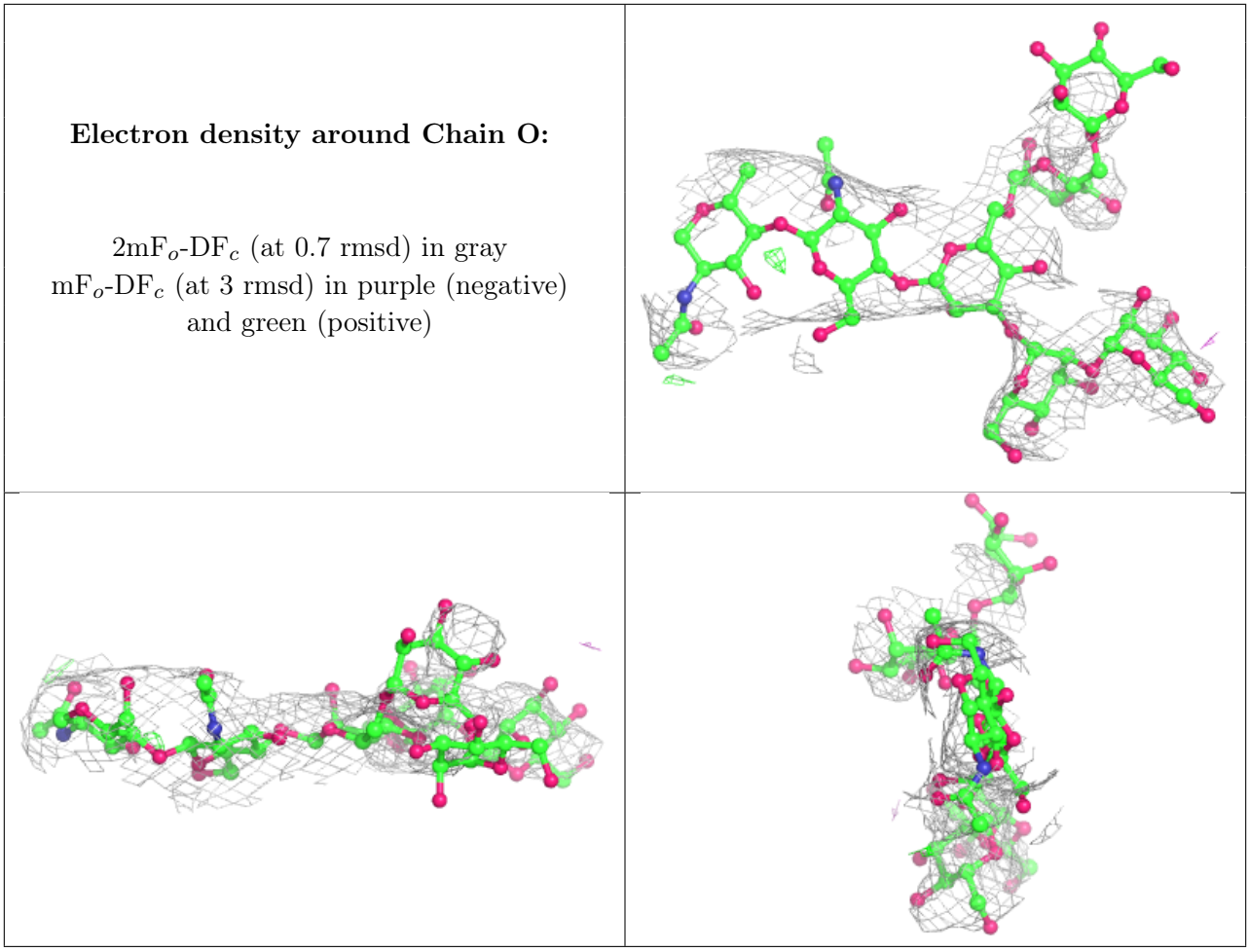






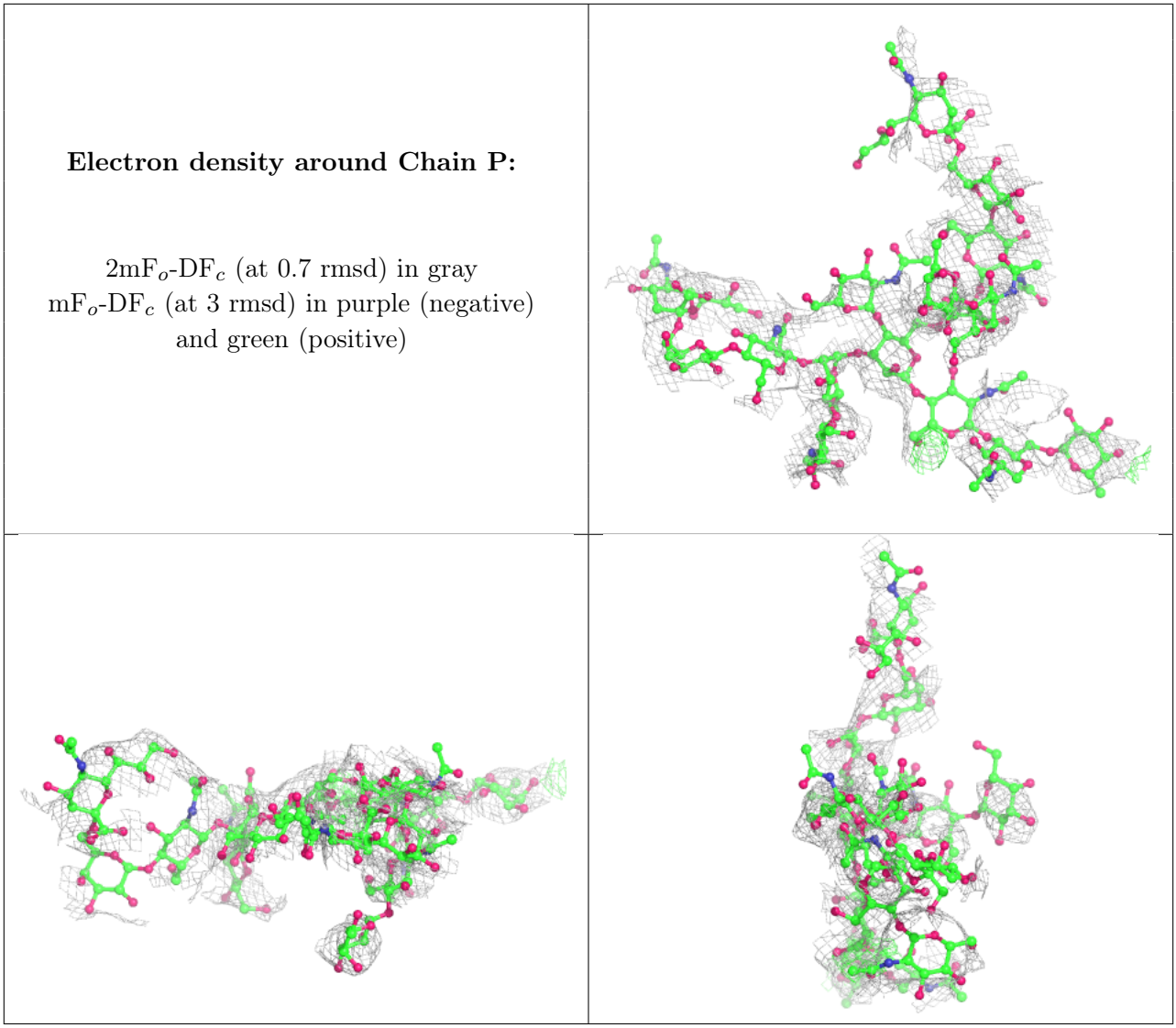
Electron density around Chain O:

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



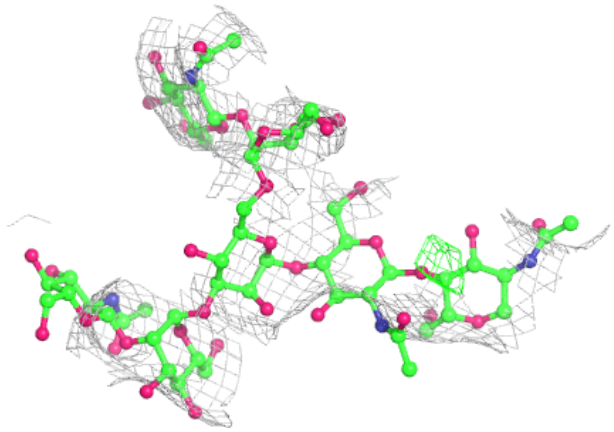
Electron density around Chain P:

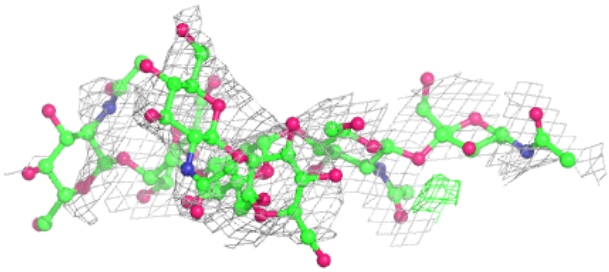
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

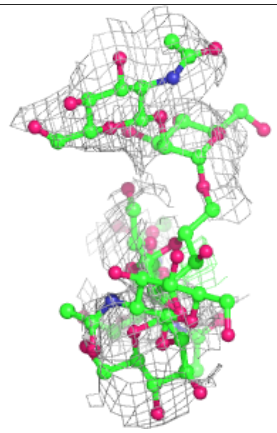


Electron density around Chain R:

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

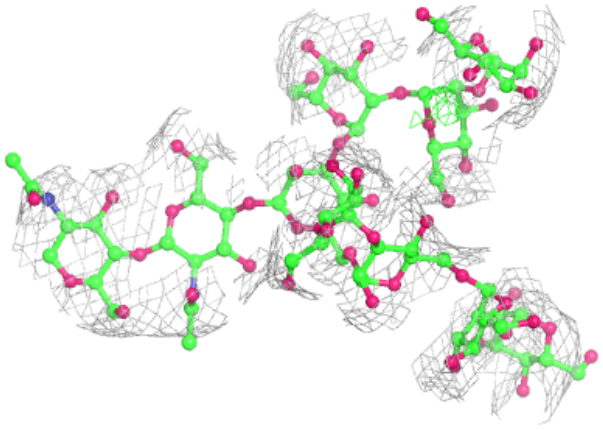


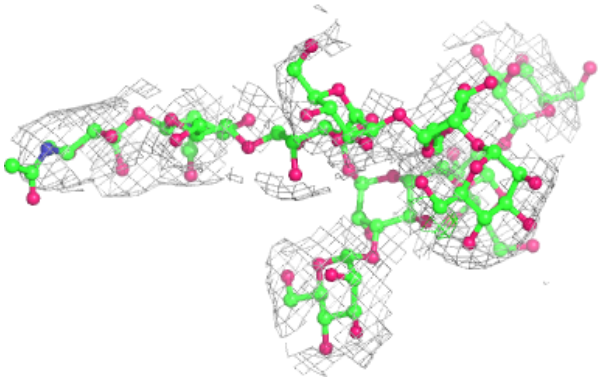


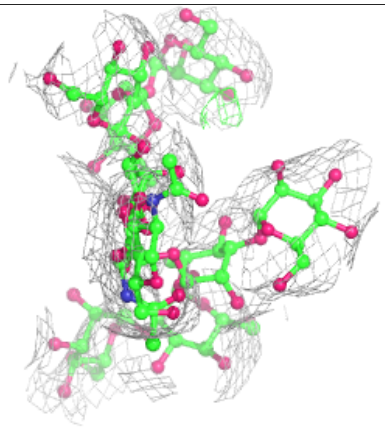


Electron density around Chain S:

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

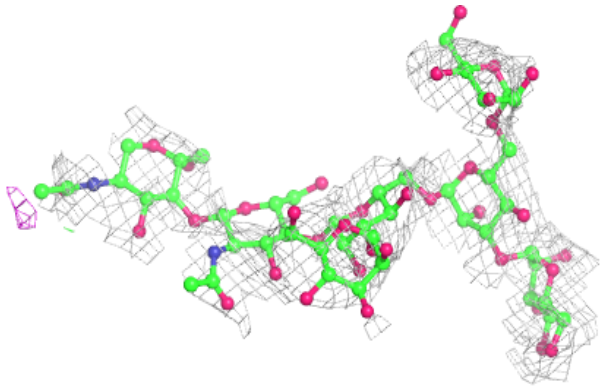


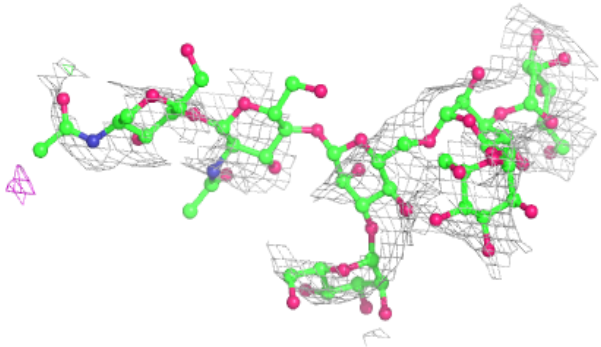


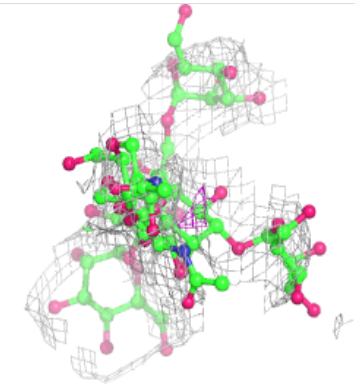


Electron density around Chain U:

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

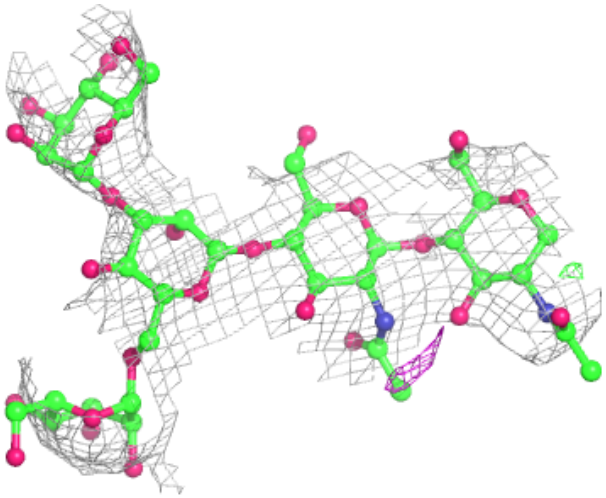


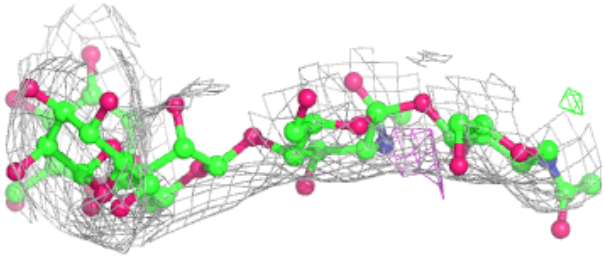


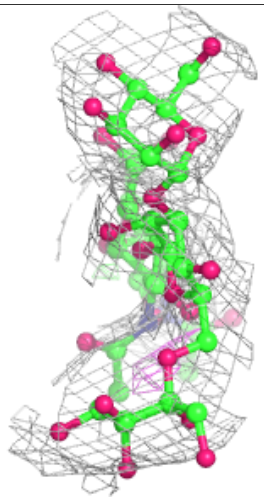


Electron density around Chain V:

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

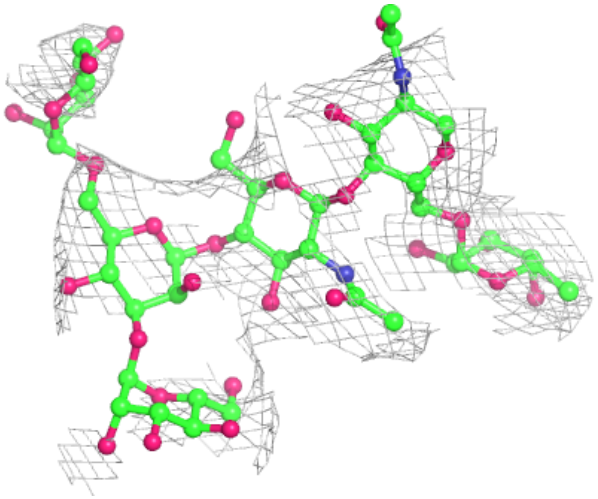


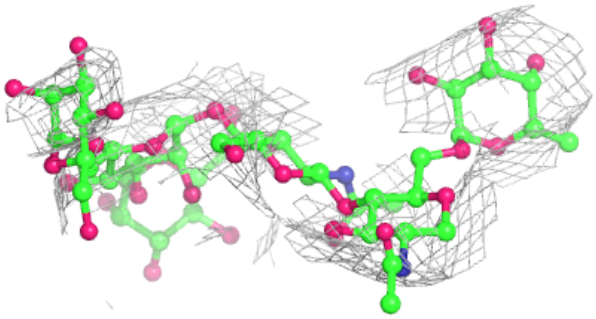


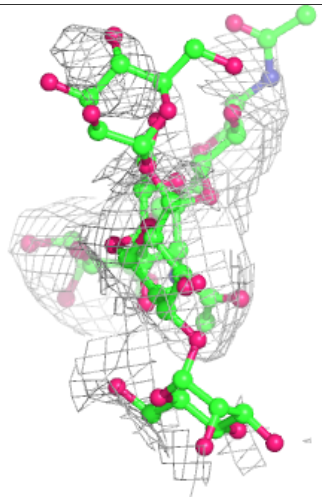


Electron density around Chain W:

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

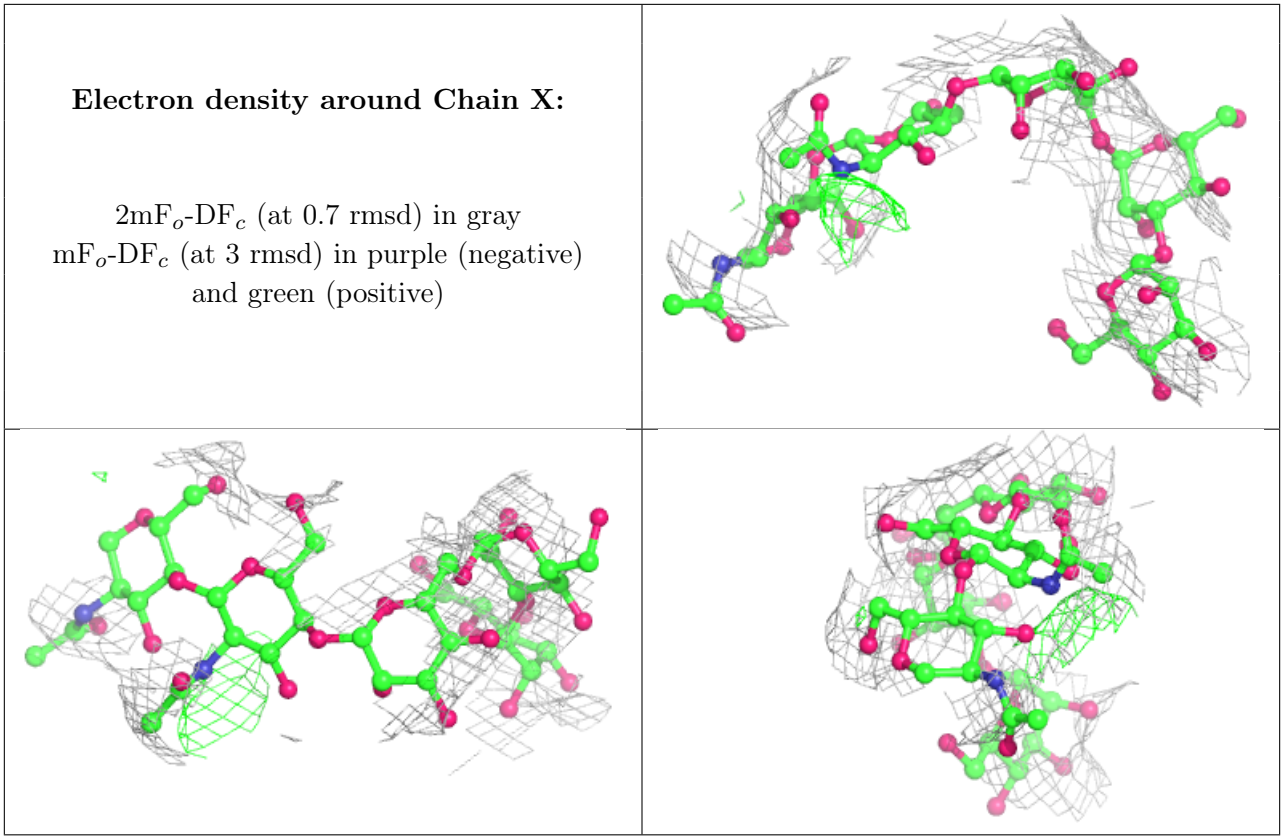






Electron density around Chain X:

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



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
23	NAG	G	3390	14/15	0.61	0.36	288,306,313,318	0

6.5 Other polymers

There are no such residues in this entry.