Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 06:40 AM EST

PDB ID	:	6UM5
EMDB ID	:	EMD-20817
Title	:	Cryo-EM structure of HIV-1 neutralizing antibody DH270 UCA3 in complex with CH848 10.17DT Env
Authors	:	Acharya, P.; Henderson, R.C.; Saunders, K.O.; Haynes, B.F.
Deposited on	:	2019-10-09
Resolution	:	4.20 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

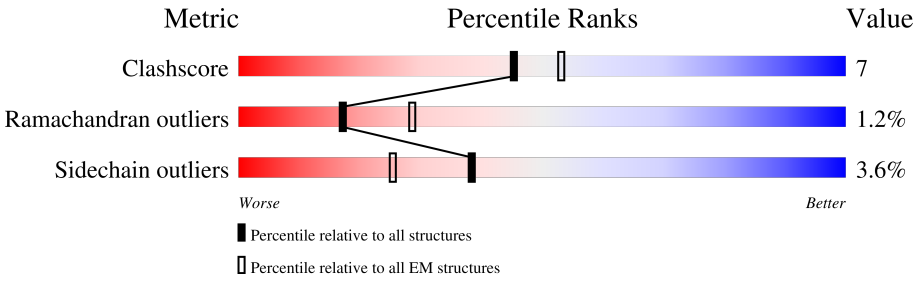
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	462	10% 81% 16% ·
1	E	462	10% 81% 16% ·
1	I	462	10% 82% 15% ·
2	B	153	14% 74% 10% · 14%
2	F	153	13% 75% 10% · 14%
2	J	153	13% 75% 10% · 14%
3	C	238	· 48% 5% 47%
3	G	238	· 48% · 47%

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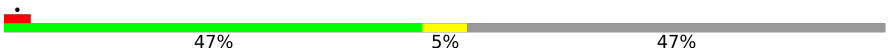
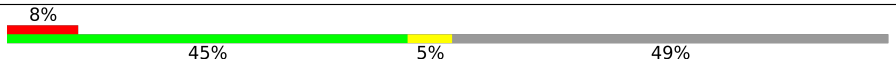
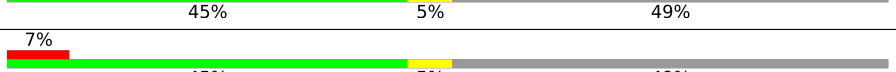
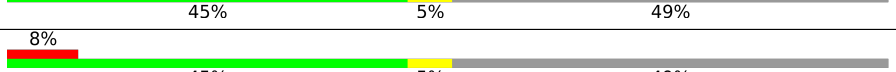
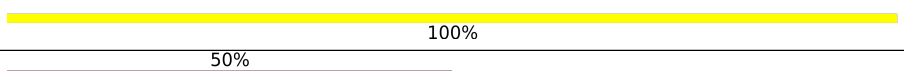
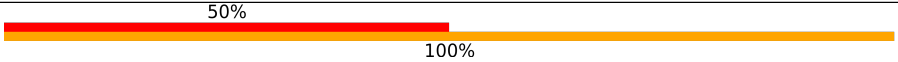
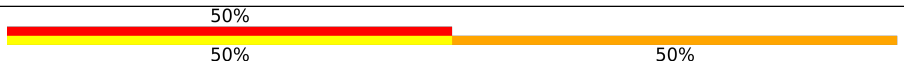
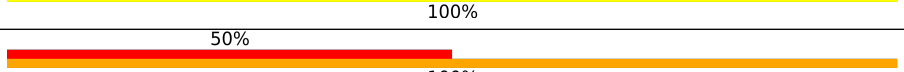
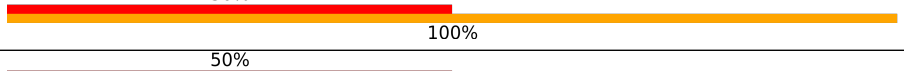
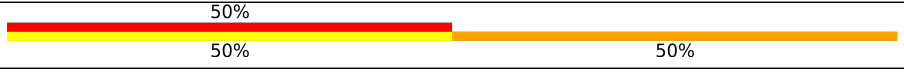
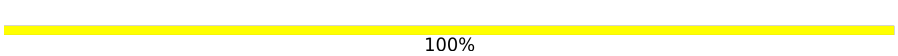
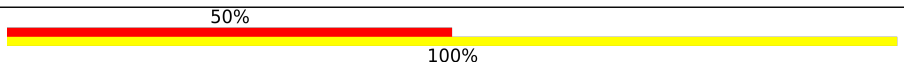
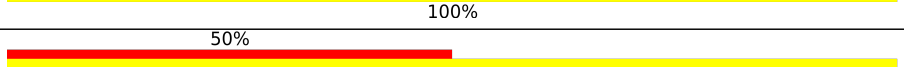
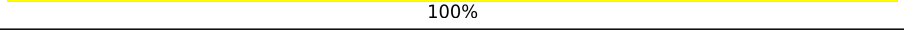
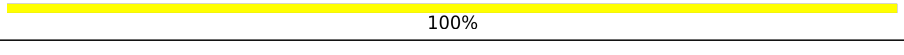
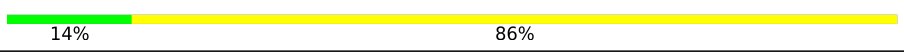
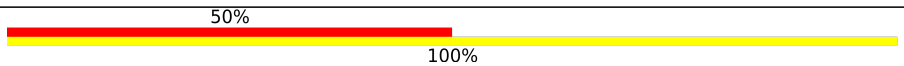
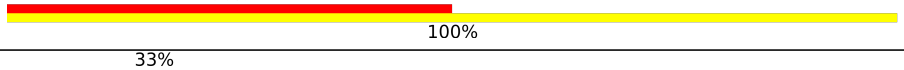
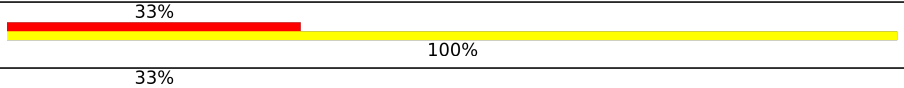
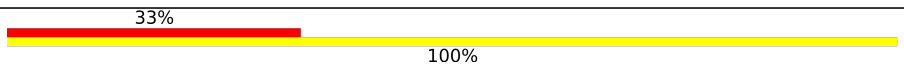
Mol	Chain	Length	Quality of chain
3	K	238	
4	D	216	
4	H	216	
4	L	216	
5	M	2	
5	Q	2	
5	S	2	
5	T	2	
5	X	2	
5	Z	2	
5	a	2	
5	e	2	
5	g	2	
6	N	7	
6	U	7	
6	b	7	
7	O	4	
7	V	4	
7	c	4	
8	P	3	
8	R	3	
8	W	3	
8	Y	3	
8	d	3	
8	f	3	

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
9	NAG	A	617	-	X	-	-
9	NAG	E	617	-	X	-	-
9	NAG	I	617	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 20562 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 CH848 10.17 DT gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	462	Total	C	N	O	S	0	0
			3615	2263	625	698	29		
1	E	462	Total	C	N	O	S	0	0
			3615	2263	625	698	29		
1	I	462	Total	C	N	O	S	0	0
			3615	2263	625	698	29		

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	expression tag	UNP A0A1W6IPB2
A	33	ASN	-	expression tag	UNP A0A1W6IPB2
A	133	ASP	ASN	conflict	UNP A0A1W6IPB2
A	138	THR	ASN	conflict	UNP A0A1W6IPB2
A	200	CYS	ALA	conflict	UNP A0A1W6IPB2
A	433	CYS	ALA	conflict	UNP A0A1W6IPB2
A	490	LYS	GLU	conflict	UNP A0A1W6IPB2
A	492	GLU	GLN	conflict	UNP A0A1W6IPB2
A	496	VAL	ILE	conflict	UNP A0A1W6IPB2
A	500	ARG	GLY	conflict	UNP A0A1W6IPB2
A	501	CYS	ALA	conflict	UNP A0A1W6IPB2
E	32	GLU	-	expression tag	UNP A0A1W6IPB2
E	33	ASN	-	expression tag	UNP A0A1W6IPB2
E	133	ASP	ASN	conflict	UNP A0A1W6IPB2
E	138	THR	ASN	conflict	UNP A0A1W6IPB2
E	200	CYS	ALA	conflict	UNP A0A1W6IPB2
E	433	CYS	ALA	conflict	UNP A0A1W6IPB2
E	490	LYS	GLU	conflict	UNP A0A1W6IPB2
E	492	GLU	GLN	conflict	UNP A0A1W6IPB2
E	496	VAL	ILE	conflict	UNP A0A1W6IPB2
E	500	ARG	GLY	conflict	UNP A0A1W6IPB2
E	501	CYS	ALA	conflict	UNP A0A1W6IPB2
I	32	GLU	-	expression tag	UNP A0A1W6IPB2
I	33	ASN	-	expression tag	UNP A0A1W6IPB2

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Chain	Residue	Modelled	Actual	Comment	Reference
I	133	ASP	ASN	conflict	UNP A0A1W6IPB2
I	138	THR	ASN	conflict	UNP A0A1W6IPB2
I	200	CYS	ALA	conflict	UNP A0A1W6IPB2
I	433	CYS	ALA	conflict	UNP A0A1W6IPB2
I	490	LYS	GLU	conflict	UNP A0A1W6IPB2
I	492	GLU	GLN	conflict	UNP A0A1W6IPB2
I	496	VAL	ILE	conflict	UNP A0A1W6IPB2
I	500	ARG	GLY	conflict	UNP A0A1W6IPB2
I	501	CYS	ALA	conflict	UNP A0A1W6IPB2

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	131	Total	C	N	O	S	0	0
			1030	652	177	195	6		
2	F	131	Total	C	N	O	S	0	0
			1030	652	177	195	6		
2	J	131	Total	C	N	O	S	0	0
			1030	652	177	195	6		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	605	CYS	THR	conflict	UNP Q2N0S7
F	605	CYS	THR	conflict	UNP Q2N0S7
J	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called DH270 UCA3 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			989	627	168	188	6		
3	G	126	Total	C	N	O	S	0	0
			989	627	168	188	6		
3	K	126	Total	C	N	O	S	0	0
			989	627	168	188	6		

- Molecule 4 is a protein called DH270 UCA3 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	110	Total	C	N	O	S	0	0
			796	492	133	167	4		

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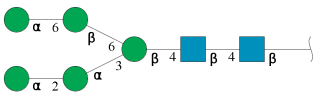
Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	110	Total	C	N	O	S	0	0
			796	492	133	167	4		
4	L	110	Total	C	N	O	S	0	0
			796	492	133	167	4		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	M	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		
5	a	2	Total	C	N	O	0	0
			28	16	2	10		
5	e	2	Total	C	N	O	0	0
			28	16	2	10		
5	g	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-beta-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.

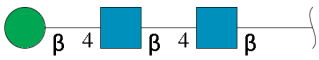


Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	7	Total 83	C 46	N 2	O 35	0	0
6	U	7	Total 83	C 46	N 2	O 35	0	0
6	b	7	Total 83	C 46	N 2	O 35	0	0

- Molecule 7 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

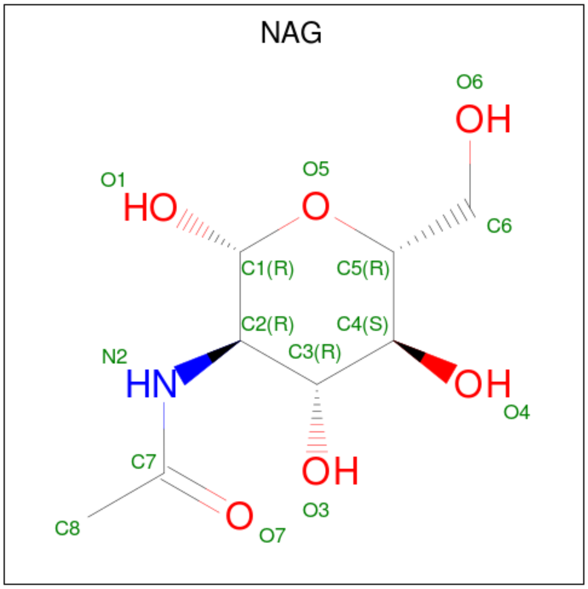
Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	4	Total 53	C 30	N 3	O 20	0	0
7	V	4	Total 53	C 30	N 3	O 20	0	0
7	c	4	Total 53	C 30	N 3	O 20	0	0

- Molecule 8 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				AltConf	Trace
8	P	3	Total 39	C 22	N 2	O 15	0	0
8	R	3	Total 39	C 22	N 2	O 15	0	0
8	W	3	Total 39	C 22	N 2	O 15	0	0
8	Y	3	Total 39	C 22	N 2	O 15	0	0
8	d	3	Total 39	C 22	N 2	O 15	0	0
8	f	3	Total 39	C 22	N 2	O 15	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total C N O 126 72 9 45	0
9	A	1	Total C N O 126 72 9 45	0
9	A	1	Total C N O 126 72 9 45	0
9	A	1	Total C N O 126 72 9 45	0
9	A	1	Total C N O 126 72 9 45	0
9	A	1	Total C N O 126 72 9 45	0
9	A	1	Total C N O 126 72 9 45	0
9	A	1	Total C N O 126 72 9 45	0
9	A	1	Total C N O 126 72 9 45	0
9	E	1	Total C N O 126 72 9 45	0
9	E	1	Total C N O 126 72 9 45	0
9	E	1	Total C N O 126 72 9 45	0

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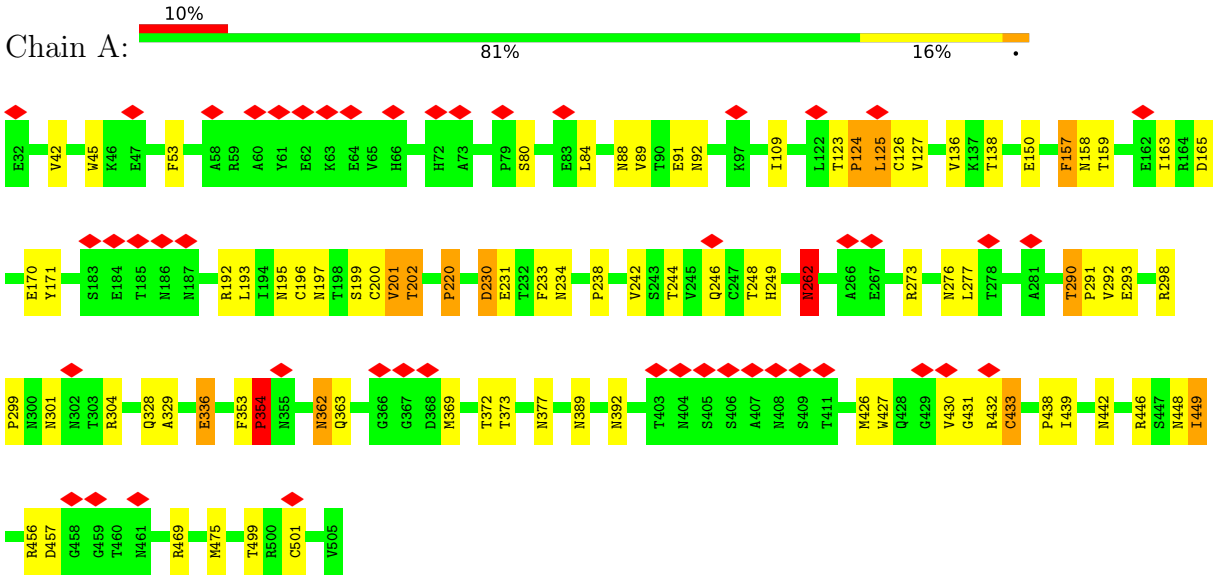
Mol	Chain	Residues	Atoms				AltConf
9	E	1	Total 126	C 72	N 9	O 45	0
9	E	1	Total 126	C 72	N 9	O 45	0
9	E	1	Total 126	C 72	N 9	O 45	0
9	E	1	Total 126	C 72	N 9	O 45	0
9	E	1	Total 126	C 72	N 9	O 45	0
9	E	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0
9	I	1	Total 126	C 72	N 9	O 45	0

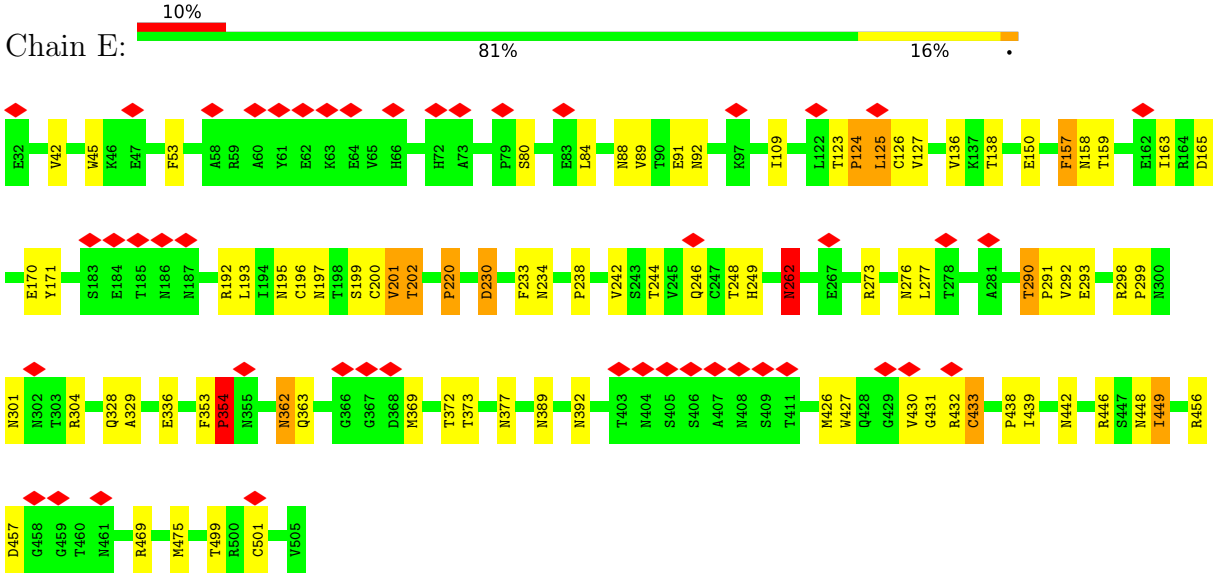
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

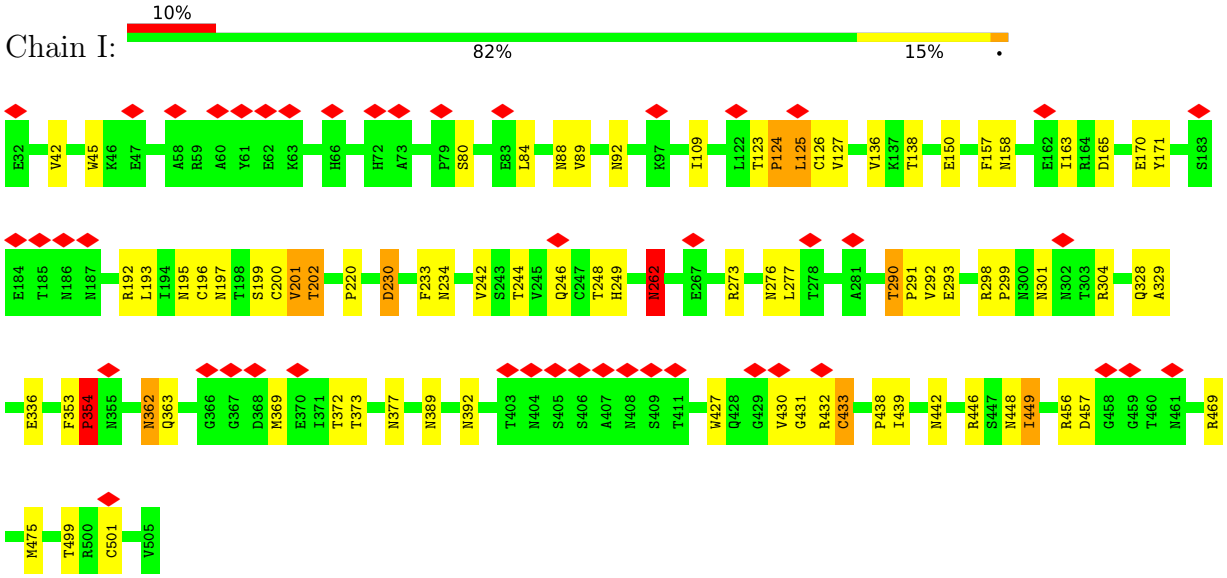
- Molecule 1: CH848 10.17 DT gp120



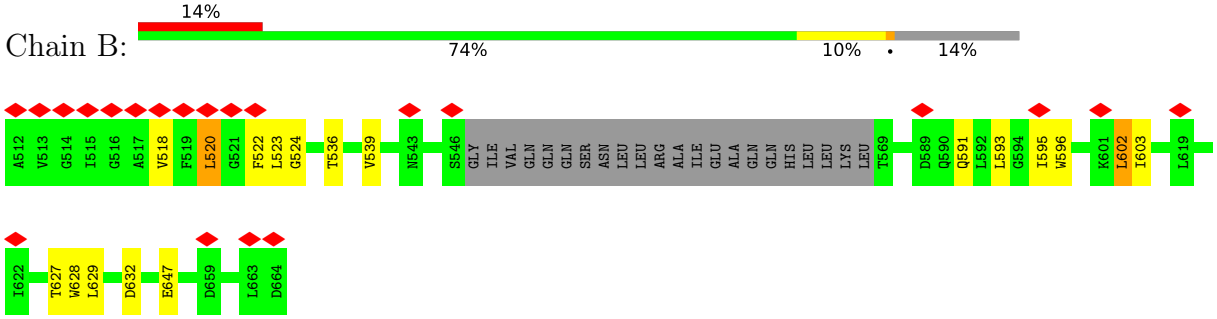
- Molecule 1: CH848 10.17 DT gp120



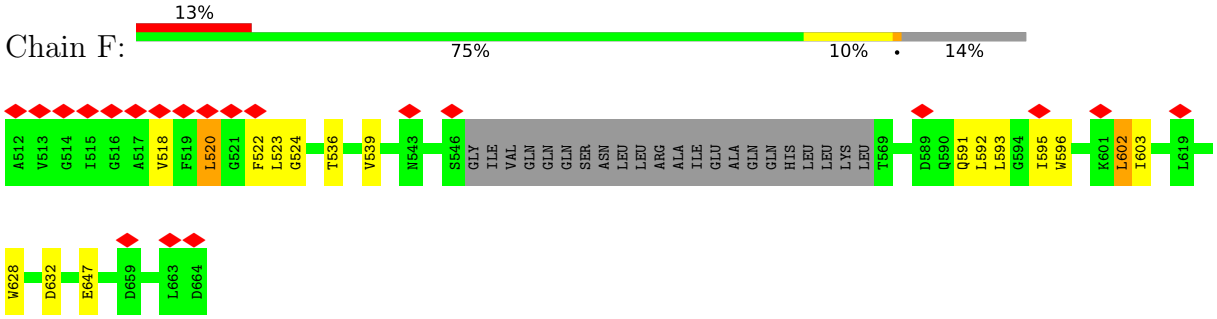
- Molecule 1: CH848 10.17 DT gp120



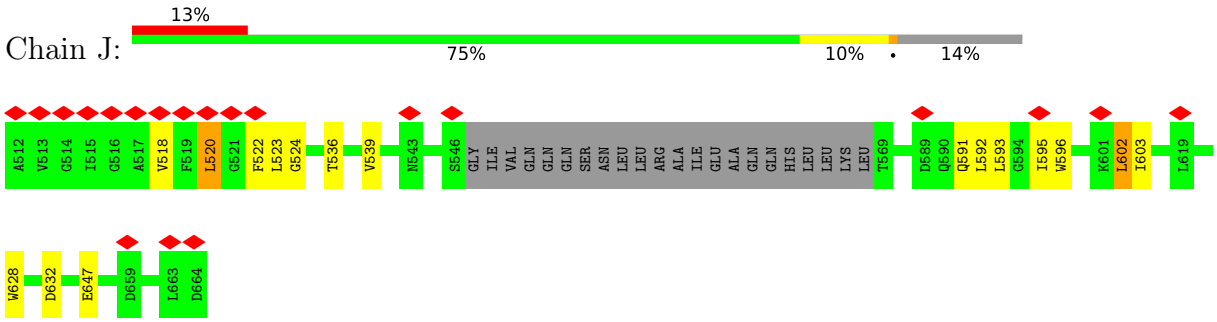
• Molecule 2: Envelope glycoprotein gp160



• Molecule 2: Envelope glycoprotein gp160

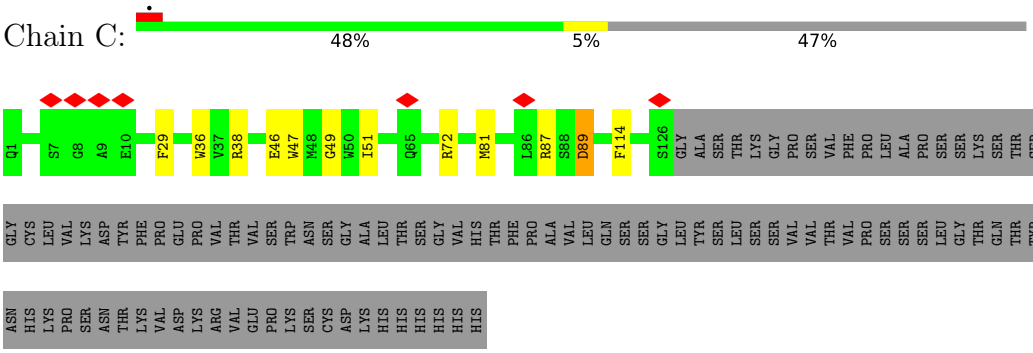


• Molecule 2: Envelope glycoprotein gp160



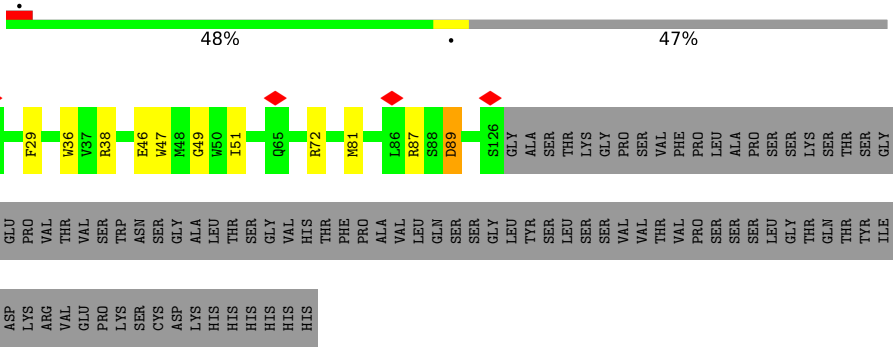
• Molecule 3: DH270 UCA3 Fab Heavy Chain

Chain C:



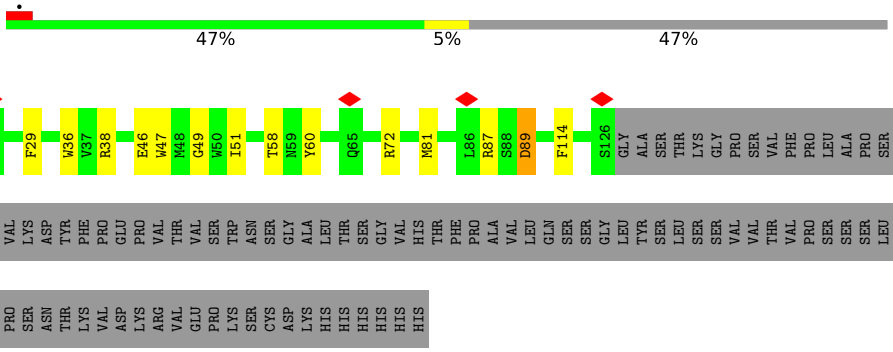
• Molecule 3: DH270 UCA3 Fab Heavy Chain

Chain G:



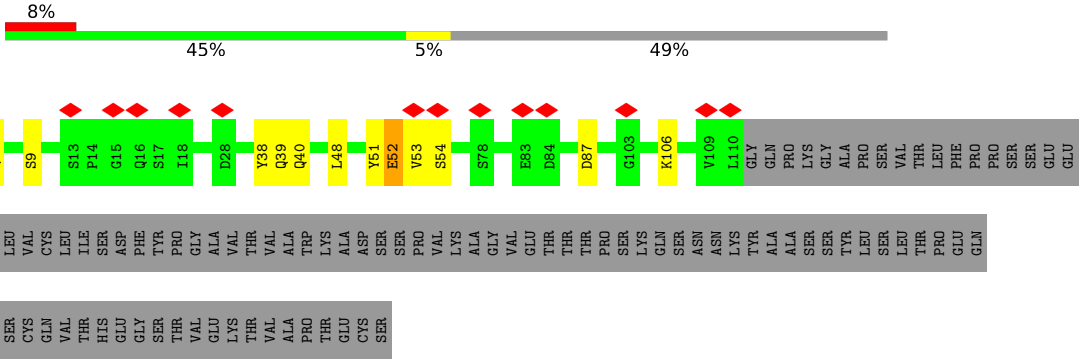
• Molecule 3: DH270 UCA3 Fab Heavy Chain

Chain K:



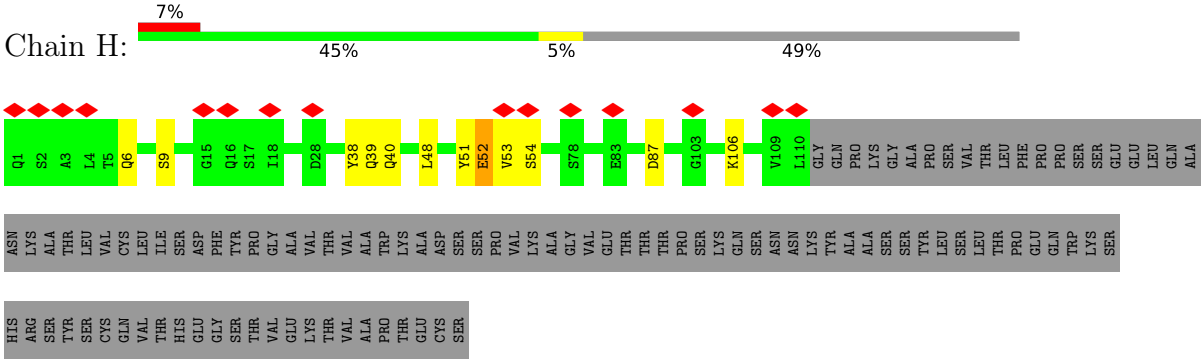
• Molecule 4: DH270 UCA3 Fab Light Chain

Chain D:



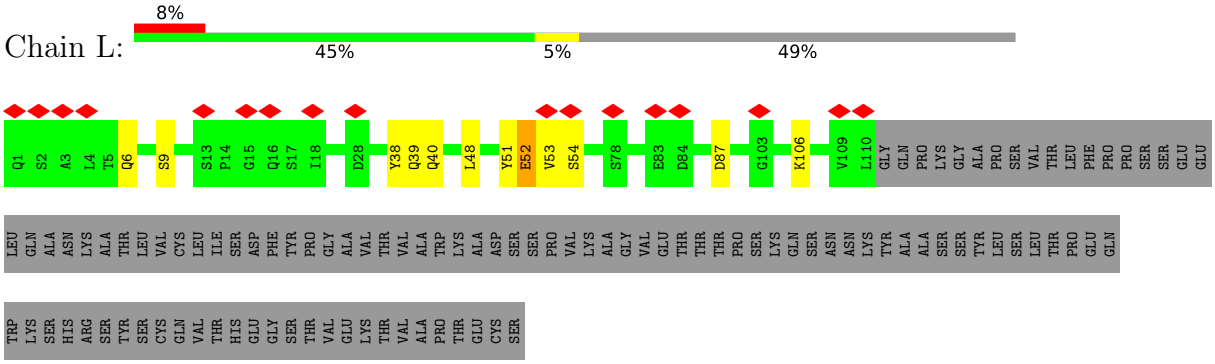
• Molecule 4: DH270 UCA3 Fab Light Chain

Chain H:



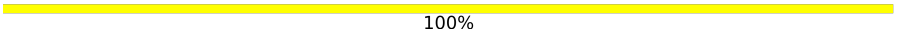
• Molecule 4: DH270 UCA3 Fab Light Chain

Chain L:



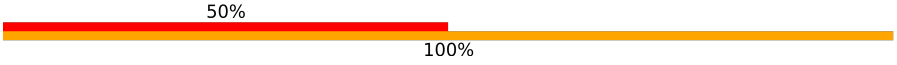
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:

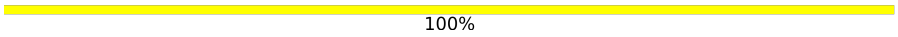


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain S:

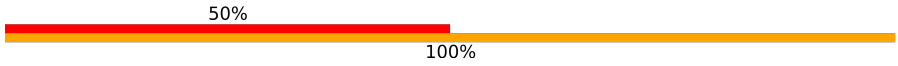
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

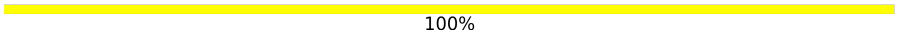


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:

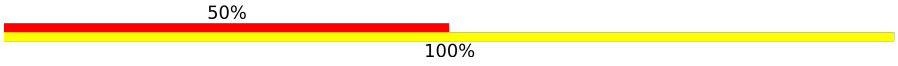


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain e:

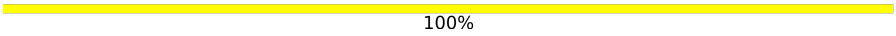
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:



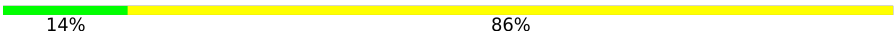
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:



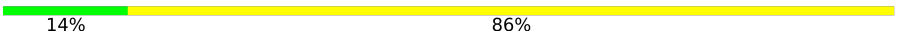
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:



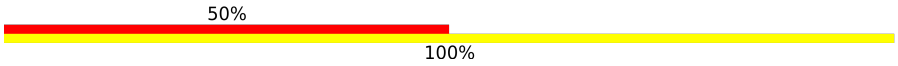
• Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain b:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

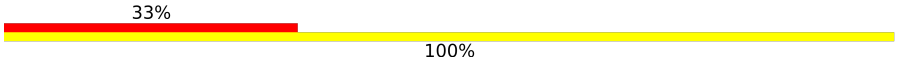
Chain V:

• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain c:

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

Chain P:

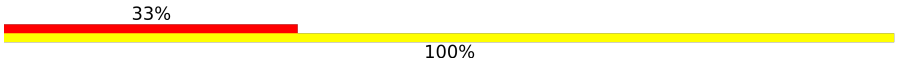


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:

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

Chain W:

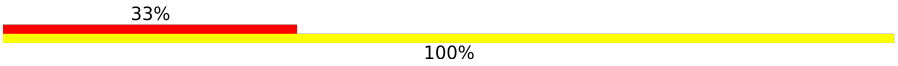


• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:

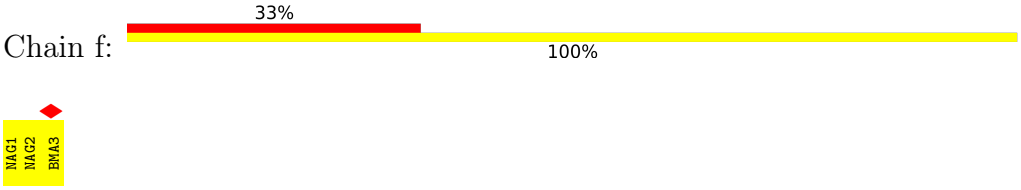
• Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d:



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

Chain f:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	22093	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.085	Depositor
Minimum map value	-0.945	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.091	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.57	3/3692 (0.1%)	0.75	9/5024 (0.2%)
1	E	0.57	3/3692 (0.1%)	0.75	9/5024 (0.2%)
1	I	0.57	3/3692 (0.1%)	0.75	9/5024 (0.2%)
2	B	0.41	0/1048	0.51	0/1422
2	F	0.41	0/1048	0.52	0/1422
2	J	0.41	0/1048	0.52	0/1422
3	C	0.42	0/1017	0.50	0/1381
3	G	0.42	0/1017	0.51	0/1381
3	K	0.42	0/1017	0.50	0/1381
4	D	0.36	0/811	0.50	0/1100
4	H	0.36	0/811	0.50	0/1100
4	L	0.36	0/811	0.50	0/1100
All	All	0.50	9/19704 (0.0%)	0.65	27/26781 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	1
4	H	0	1
4	L	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	354	PRO	N-CA	13.79	1.70	1.47
1	A	354	PRO	N-CA	13.78	1.70	1.47
1	E	354	PRO	N-CA	13.74	1.70	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	353	PHE	C-N	6.03	1.45	1.34
1	A	353	PHE	C-N	5.99	1.45	1.34
1	I	353	PHE	C-N	5.99	1.45	1.34
1	I	220	PRO	N-CD	-5.67	1.40	1.47
1	E	220	PRO	N-CD	-5.64	1.40	1.47
1	A	220	PRO	N-CD	-5.64	1.40	1.47

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	249	HIS	CB-CA-C	-11.28	87.84	110.40
1	E	249	HIS	CB-CA-C	-11.28	87.85	110.40
1	A	249	HIS	CB-CA-C	-11.27	87.86	110.40
1	E	197	ASN	CB-CA-C	-9.58	91.24	110.40
1	A	197	ASN	CB-CA-C	-9.57	91.26	110.40
1	I	197	ASN	CB-CA-C	-9.57	91.26	110.40
1	I	354	PRO	CA-N-CD	-7.75	100.64	111.50
1	A	354	PRO	CA-N-CD	-7.72	100.69	111.50
1	E	354	PRO	CA-N-CD	-7.71	100.70	111.50
1	I	353	PHE	CB-CA-C	5.90	122.19	110.40
1	A	353	PHE	CB-CA-C	5.89	122.18	110.40
1	E	353	PHE	CB-CA-C	5.88	122.17	110.40
1	E	248	THR	C-N-CA	5.84	136.31	121.70
1	I	248	THR	C-N-CA	5.84	136.31	121.70
1	A	248	THR	C-N-CA	5.84	136.30	121.70
1	E	448	ASN	C-N-CA	5.82	136.24	121.70
1	I	448	ASN	C-N-CA	5.82	136.24	121.70
1	A	448	ASN	C-N-CA	5.81	136.22	121.70
1	E	262	ASN	CB-CA-C	-5.72	98.95	110.40
1	A	262	ASN	CB-CA-C	-5.72	98.96	110.40
1	I	262	ASN	CB-CA-C	-5.72	98.96	110.40
1	A	362	ASN	CB-CA-C	-5.31	99.79	110.40
1	E	362	ASN	CB-CA-C	-5.30	99.80	110.40
1	I	362	ASN	CB-CA-C	-5.30	99.80	110.40
1	A	80	SER	C-N-CD	-5.06	109.48	120.60
1	I	80	SER	C-N-CD	-5.05	109.49	120.60
1	E	80	SER	C-N-CD	-5.05	109.49	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	52	GLU	Peptide
4	H	52	GLU	Peptide
4	L	52	GLU	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3615	0	3521	50	0
1	E	3615	0	3521	47	0
1	I	3615	0	3521	44	0
2	B	1030	0	1011	14	0
2	F	1030	0	1011	12	0
2	J	1030	0	1011	13	0
3	C	989	0	935	6	0
3	G	989	0	935	5	0
3	K	989	0	935	8	0
4	D	796	0	772	6	0
4	H	796	0	772	5	0
4	L	796	0	772	6	0
5	M	28	0	25	0	0
5	Q	28	0	25	3	0
5	S	28	0	25	2	0
5	T	28	0	25	0	0
5	X	28	0	25	3	0
5	Z	28	0	25	2	0
5	a	28	0	25	0	0
5	e	28	0	25	0	0
5	g	28	0	25	0	0
6	N	83	0	70	1	0
6	U	83	0	70	0	0
6	b	83	0	70	0	0
7	O	53	0	46	0	0
7	V	53	0	46	1	0
7	c	53	0	46	0	0
8	P	39	0	34	0	0
8	R	39	0	34	4	0
8	W	39	0	34	0	0
8	Y	39	0	34	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	d	39	0	34	0	0
8	f	39	0	34	0	0
9	A	126	0	117	15	0
9	E	126	0	117	16	0
9	I	126	0	117	14	0
All	All	20562	0	19845	262	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 7.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:354:PRO:N	1:I:354:PRO:CA	1.70	1.43
1:E:354:PRO:CA	1:E:354:PRO:N	1.70	1.42
1:A:354:PRO:N	1:A:354:PRO:CA	1.70	1.39
4:L:52:GLU:O	4:L:54:SER:N	2.09	0.86
4:H:52:GLU:O	4:H:54:SER:N	2.09	0.85
4:D:52:GLU:O	4:D:54:SER:N	2.09	0.85
1:I:201:VAL:HG12	1:I:201:VAL:O	1.84	0.78
9:A:630:NAG:O7	9:A:630:NAG:O3	2.02	0.78
1:E:201:VAL:HG12	1:E:201:VAL:O	1.84	0.77
9:E:630:NAG:O7	9:E:630:NAG:O3	2.02	0.77
9:I:630:NAG:O7	9:I:630:NAG:O3	2.02	0.76
1:A:201:VAL:HG12	1:A:201:VAL:O	1.84	0.76
9:E:626:NAG:HO4	9:E:626:NAG:HO6	1.22	0.74
9:E:631:NAG:O7	9:E:631:NAG:O3	2.06	0.72
9:A:631:NAG:O7	9:A:631:NAG:O3	2.06	0.72
9:E:631:NAG:O6	9:E:631:NAG:O4	2.04	0.72
9:I:631:NAG:O7	9:I:631:NAG:O3	2.07	0.71
1:I:233:PHE:O	1:I:273:ARG:NH2	2.25	0.70
1:E:233:PHE:O	1:E:273:ARG:NH2	2.25	0.70
2:F:602:LEU:HD12	2:F:603:ILE:H	1.55	0.70
2:J:602:LEU:HD12	2:J:603:ILE:H	1.55	0.70
2:B:602:LEU:HD12	2:B:603:ILE:H	1.55	0.69
1:A:233:PHE:O	1:A:273:ARG:NH2	2.25	0.69
1:A:277:LEU:O	1:A:456:ARG:NH2	2.27	0.68
1:I:277:LEU:O	1:I:456:ARG:NH2	2.27	0.68
1:E:277:LEU:O	1:E:456:ARG:NH2	2.27	0.68
9:I:617:NAG:O7	9:I:617:NAG:O3	2.12	0.67
9:I:626:NAG:O6	9:I:626:NAG:O4	2.03	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:617:NAG:O7	9:A:617:NAG:O3	2.12	0.67
9:A:626:NAG:O6	9:A:626:NAG:O4	2.03	0.67
9:A:631:NAG:O6	9:A:631:NAG:O4	2.04	0.67
9:I:622:NAG:O6	9:I:622:NAG:O4	2.12	0.67
9:E:619:NAG:C1	9:E:619:NAG:O7	2.44	0.66
9:I:631:NAG:O6	9:I:631:NAG:O4	2.04	0.66
9:I:627:NAG:O7	9:I:627:NAG:O3	2.16	0.64
8:Y:2:NAG:O7	8:Y:2:NAG:H3	1.99	0.63
7:V:2:NAG:O4	7:V:2:NAG:O6	2.15	0.63
9:A:619:NAG:C1	9:A:619:NAG:O7	2.44	0.62
9:I:619:NAG:C1	9:I:619:NAG:O7	2.44	0.62
8:R:2:NAG:H3	8:R:2:NAG:O7	1.98	0.62
9:E:627:NAG:O7	9:E:627:NAG:O3	2.16	0.62
5:S:2:NAG:O4	5:S:2:NAG:O6	2.11	0.62
9:A:627:NAG:O7	9:A:627:NAG:O3	2.16	0.62
9:E:619:NAG:O6	9:E:619:NAG:O4	2.09	0.61
9:E:617:NAG:O7	9:E:617:NAG:O3	2.12	0.60
5:X:1:NAG:H82	5:X:1:NAG:C1	2.32	0.60
5:Z:2:NAG:O6	5:Z:2:NAG:O4	2.11	0.59
8:Y:1:NAG:O3	8:Y:2:NAG:O5	2.12	0.59
5:Q:1:NAG:H82	5:Q:1:NAG:C1	2.32	0.59
1:I:200:CYS:O	1:I:202:THR:N	2.35	0.58
8:R:1:NAG:O7	8:R:1:NAG:O3	2.22	0.58
8:Y:1:NAG:O3	8:Y:1:NAG:O7	2.22	0.58
9:A:619:NAG:O6	9:A:619:NAG:O4	2.09	0.58
1:A:200:CYS:O	1:A:202:THR:N	2.35	0.58
9:E:622:NAG:O7	9:E:622:NAG:H3	2.01	0.58
1:E:200:CYS:O	1:E:202:THR:N	2.35	0.57
9:A:622:NAG:O6	9:A:622:NAG:O4	2.12	0.57
1:I:328:GLN:HA	1:I:329:ALA:HB3	1.88	0.56
2:F:536:THR:HG22	2:F:536:THR:O	2.06	0.55
1:A:328:GLN:HA	1:A:329:ALA:HB3	1.88	0.55
2:J:536:THR:O	2:J:536:THR:HG22	2.06	0.55
9:A:622:NAG:O7	9:A:622:NAG:H3	2.01	0.55
1:I:42:VAL:HG13	2:J:628:TRP:CG	2.42	0.55
2:B:536:THR:HG22	2:B:536:THR:O	2.06	0.55
1:E:328:GLN:HA	1:E:329:ALA:HB3	1.88	0.55
1:E:42:VAL:HG13	2:F:628:TRP:CG	2.42	0.54
1:E:45:TRP:HE1	2:F:523:LEU:CD2	2.20	0.54
9:E:632:NAG:O6	9:E:632:NAG:O4	2.18	0.54
3:K:114:PHE:HD2	4:L:38:TYR:HH	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:O	1:A:201:VAL:CG1	2.54	0.54
1:I:45:TRP:HE1	2:J:523:LEU:CD2	2.21	0.54
3:C:114:PHE:HD2	4:D:38:TYR:HH	1.56	0.54
1:I:290:THR:OG1	1:I:291:PRO:HA	2.08	0.54
1:A:42:VAL:HG13	2:B:628:TRP:CG	2.42	0.53
1:E:201:VAL:O	1:E:201:VAL:CG1	2.54	0.53
5:Z:2:NAG:HO4	5:Z:2:NAG:HO6	1.53	0.53
1:A:45:TRP:HE1	2:B:523:LEU:CD2	2.20	0.53
1:E:290:THR:OG1	1:E:291:PRO:HA	2.09	0.53
1:I:201:VAL:O	1:I:201:VAL:CG1	2.54	0.53
5:S:2:NAG:HO4	5:S:2:NAG:HO6	1.56	0.53
9:E:622:NAG:O6	9:E:622:NAG:O4	2.12	0.53
3:G:38:ARG:NH1	3:G:46:GLU:OE1	2.42	0.53
1:A:193:LEU:HD13	1:A:195:ASN:H	1.73	0.52
1:A:290:THR:OG1	1:A:291:PRO:HA	2.08	0.52
1:I:193:LEU:HD13	1:I:195:ASN:H	1.73	0.52
3:K:38:ARG:NH1	3:K:46:GLU:OE1	2.42	0.52
9:A:630:NAG:O6	9:A:630:NAG:O4	2.24	0.52
1:E:193:LEU:HD13	1:E:195:ASN:H	1.73	0.52
9:I:632:NAG:O6	9:I:632:NAG:O4	2.18	0.52
3:C:38:ARG:NH1	3:C:46:GLU:OE1	2.42	0.52
9:E:631:NAG:HO4	9:E:631:NAG:HO6	1.53	0.52
1:I:369:MET:O	1:I:373:THR:OG1	2.29	0.51
1:A:369:MET:O	1:A:373:THR:OG1	2.29	0.51
5:Q:2:NAG:C1	5:Q:2:NAG:O7	2.58	0.51
9:I:622:NAG:O7	9:I:622:NAG:H3	2.01	0.50
2:J:520:LEU:HD12	2:J:524:GLY:HA3	1.94	0.50
3:K:87:ARG:HB2	3:K:89:ASP:OD1	2.12	0.50
2:B:520:LEU:HD12	2:B:524:GLY:HA3	1.94	0.50
2:F:520:LEU:HD12	2:F:524:GLY:HA3	1.94	0.49
3:G:87:ARG:HB2	3:G:89:ASP:OD1	2.12	0.49
1:E:499:THR:HG23	1:E:501:CYS:H	1.78	0.49
1:I:363:GLN:O	1:I:469:ARG:NH1	2.46	0.49
1:A:363:GLN:O	1:A:469:ARG:NH1	2.46	0.49
3:K:89:ASP:OD1	3:K:89:ASP:N	2.34	0.49
1:E:363:GLN:O	1:E:469:ARG:NH1	2.46	0.49
1:A:499:THR:HG23	1:A:501:CYS:H	1.78	0.49
3:C:87:ARG:HB2	3:C:89:ASP:OD1	2.12	0.49
9:E:630:NAG:O6	9:E:630:NAG:O4	2.24	0.49
1:A:262:ASN:OD1	1:A:262:ASN:N	2.46	0.48
9:A:630:NAG:HO3	9:A:630:NAG:C7	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:9:SER:HA	4:D:106:LYS:O	2.13	0.48
1:I:499:THR:HG23	1:I:501:CYS:H	1.78	0.48
4:L:9:SER:HA	4:L:106:LYS:O	2.13	0.48
1:E:369:MET:O	1:E:373:THR:OG1	2.29	0.48
4:H:9:SER:HA	4:H:106:LYS:O	2.13	0.48
5:X:2:NAG:C1	5:X:2:NAG:O7	2.58	0.48
1:I:262:ASN:OD1	1:I:262:ASN:N	2.46	0.47
1:E:262:ASN:N	1:E:262:ASN:OD1	2.46	0.47
1:A:123:THR:HB	1:A:124:PRO:HD2	1.97	0.47
1:I:123:THR:HB	1:I:124:PRO:HD2	1.97	0.47
1:I:230:ASP:OD1	1:I:230:ASP:N	2.48	0.46
2:B:602:LEU:H	2:B:602:LEU:HG	1.43	0.46
1:A:304:ARG:HD2	1:A:438:PRO:O	2.16	0.46
1:A:124:PRO:O	1:A:125:LEU:HB2	2.16	0.46
4:D:38:TYR:OH	4:D:48:LEU:HD12	2.15	0.46
1:E:124:PRO:O	1:E:125:LEU:HB2	2.16	0.46
4:L:38:TYR:OH	4:L:48:LEU:HD12	2.15	0.46
1:A:246:GLN:N	1:A:246:GLN:OE1	2.48	0.46
1:E:304:ARG:HD2	1:E:438:PRO:O	2.16	0.46
1:A:123:THR:O	1:A:124:PRO:O	2.34	0.46
1:I:304:ARG:HD2	1:I:438:PRO:O	2.16	0.46
1:E:123:THR:O	1:E:124:PRO:O	2.34	0.46
1:I:123:THR:O	1:I:124:PRO:O	2.34	0.46
1:I:124:PRO:O	1:I:125:LEU:HB2	2.16	0.46
1:E:123:THR:HB	1:E:124:PRO:HD2	1.97	0.45
1:E:230:ASP:OD1	1:E:230:ASP:N	2.48	0.45
1:E:298:ARG:HB2	1:E:299:PRO:HD2	1.98	0.45
9:I:622:NAG:HO4	9:I:622:NAG:HO6	1.57	0.45
1:I:199:SER:O	1:I:433:CYS:SG	2.75	0.45
1:I:298:ARG:HB2	1:I:299:PRO:HD2	1.98	0.45
1:A:230:ASP:N	1:A:230:ASP:OD1	2.48	0.45
4:H:38:TYR:OH	4:H:48:LEU:HD12	2.15	0.45
4:H:39:GLN:HA	4:H:87:ASP:O	2.17	0.45
1:A:109:ILE:HG23	1:A:430:VAL:HG23	1.99	0.45
1:E:199:SER:O	1:E:433:CYS:SG	2.75	0.45
3:G:51:ILE:HG23	3:G:51:ILE:O	2.17	0.45
1:A:199:SER:O	1:A:433:CYS:SG	2.75	0.45
3:C:51:ILE:HG23	3:C:51:ILE:O	2.17	0.45
1:I:246:GLN:OE1	1:I:246:GLN:N	2.48	0.45
2:B:593:LEU:HD12	2:B:596:TRP:CH2	2.52	0.45
1:E:246:GLN:N	1:E:246:GLN:OE1	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:39:GLN:HA	4:L:87:ASP:O	2.17	0.45
4:D:39:GLN:HA	4:D:87:ASP:O	2.17	0.44
1:I:109:ILE:HG23	1:I:430:VAL:HG23	1.99	0.44
2:F:593:LEU:HD12	2:F:596:TRP:CH2	2.52	0.44
3:K:47:TRP:CZ2	3:K:49:GLY:HA2	2.52	0.44
1:E:109:ILE:HG23	1:E:430:VAL:HG23	1.99	0.44
3:G:47:TRP:CZ2	3:G:49:GLY:HA2	2.52	0.44
4:H:51:TYR:O	4:H:52:GLU:C	2.56	0.44
3:K:51:ILE:O	3:K:51:ILE:HG23	2.17	0.44
4:D:51:TYR:O	4:D:52:GLU:C	2.56	0.44
1:A:124:PRO:O	1:A:125:LEU:CB	2.66	0.44
1:A:298:ARG:HB2	1:A:299:PRO:HD2	1.98	0.44
1:I:389:ASN:OD1	1:I:389:ASN:N	2.51	0.44
3:K:36:TRP:CD2	3:K:81:MET:SD	3.11	0.44
3:C:36:TRP:CD2	3:C:81:MET:SD	3.11	0.44
1:E:126:CYS:O	1:I:163:ILE:HG23	2.17	0.44
3:G:36:TRP:CD2	3:G:81:MET:SD	3.11	0.44
2:J:593:LEU:HD12	2:J:596:TRP:CH2	2.52	0.44
1:A:126:CYS:O	1:E:163:ILE:HG23	2.18	0.44
9:A:627:NAG:HO3	9:A:627:NAG:C7	2.21	0.44
1:I:124:PRO:O	1:I:125:LEU:CB	2.66	0.44
5:Q:2:NAG:O7	5:Q:2:NAG:H3	2.18	0.44
3:C:47:TRP:CZ2	3:C:49:GLY:HA2	2.52	0.43
1:E:124:PRO:O	1:E:125:LEU:CB	2.66	0.43
1:E:127:VAL:HG12	1:I:165:ASP:OD1	2.18	0.43
1:E:426:MET:H	1:E:426:MET:HG2	1.67	0.43
9:I:630:NAG:O7	9:I:630:NAG:C3	2.65	0.43
8:Y:1:NAG:O4	8:Y:1:NAG:O6	2.27	0.43
2:F:518:VAL:O	2:F:539:VAL:HG11	2.18	0.43
2:F:647:GLU:OE1	2:J:539:VAL:CG2	2.66	0.43
2:J:518:VAL:O	2:J:539:VAL:HG11	2.18	0.43
1:A:127:VAL:HG12	1:E:165:ASP:OD1	2.19	0.43
1:A:163:ILE:HG23	1:I:126:CYS:O	2.18	0.43
1:E:293:GLU:OE1	1:E:446:ARG:NH2	2.44	0.43
9:E:630:NAG:O7	9:E:630:NAG:C3	2.65	0.43
1:A:389:ASN:OD1	1:A:389:ASN:N	2.51	0.43
1:I:292:VAL:O	1:I:449:ILE:HG22	2.19	0.43
1:A:84:LEU:HB3	1:A:244:THR:HG22	2.01	0.43
9:E:631:NAG:O7	9:E:631:NAG:C3	2.67	0.43
1:I:427:TRP:HE1	1:I:475:MET:CG	2.32	0.43
3:K:58:THR:HG1	3:K:60:TYR:HE2	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:51:TYR:O	4:L:52:GLU:C	2.56	0.43
1:A:292:VAL:O	1:A:449:ILE:HG22	2.19	0.43
2:B:539:VAL:CG2	2:J:647:GLU:OE1	2.67	0.43
2:B:602:LEU:CD1	2:B:603:ILE:H	2.28	0.43
1:E:136:VAL:HG13	1:E:138:THR:H	1.84	0.43
9:A:631:NAG:O7	9:A:631:NAG:C3	2.67	0.42
1:A:165:ASP:OD1	1:I:127:VAL:HG12	2.19	0.42
2:B:518:VAL:O	2:B:539:VAL:HG11	2.18	0.42
9:A:632:NAG:O6	9:A:632:NAG:O4	2.18	0.42
1:E:292:VAL:O	1:E:449:ILE:HG22	2.19	0.42
1:E:362:ASN:OD1	1:E:363:GLN:N	2.53	0.42
1:I:293:GLU:OE1	1:I:446:ARG:NH2	2.44	0.42
1:A:336:GLU:H	1:A:336:GLU:HG3	1.64	0.42
1:E:389:ASN:OD1	1:E:389:ASN:N	2.51	0.42
1:I:150:GLU:OE1	1:I:150:GLU:N	2.49	0.42
9:I:631:NAG:O7	9:I:631:NAG:C3	2.67	0.42
1:A:304:ARG:HD3	1:A:439:ILE:HA	2.02	0.42
1:I:362:ASN:OD1	1:I:363:GLN:N	2.52	0.42
1:A:427:TRP:HE1	1:A:475:MET:CG	2.32	0.42
2:B:647:GLU:OE1	2:F:539:VAL:CG2	2.67	0.42
1:I:84:LEU:HB3	1:I:244:THR:HG22	2.01	0.42
1:E:427:TRP:HE1	1:E:475:MET:CG	2.32	0.42
1:A:293:GLU:OE1	1:A:446:ARG:NH2	2.44	0.42
1:E:170:GLU:HG3	1:E:171:TYR:H	1.85	0.42
1:A:150:GLU:OE1	1:A:150:GLU:N	2.49	0.41
2:F:591:GLN:O	2:F:595:ILE:HG13	2.20	0.41
1:I:42:VAL:HG13	2:J:628:TRP:CD2	2.56	0.41
1:I:234:ASN:O	1:I:234:ASN:ND2	2.54	0.41
1:E:84:LEU:HB3	1:E:244:THR:HG22	2.01	0.41
1:I:170:GLU:HG3	1:I:171:TYR:H	1.85	0.41
8:Y:1:NAG:O7	8:Y:1:NAG:C3	2.68	0.41
1:A:136:VAL:HG13	1:A:138:THR:H	1.84	0.41
1:E:157:PHE:CE2	1:E:159:THR:HB	2.56	0.41
1:E:304:ARG:HD3	1:E:439:ILE:HA	2.02	0.41
1:I:432:ARG:O	1:I:432:ARG:HG3	2.20	0.41
8:R:1:NAG:O7	8:R:1:NAG:C3	2.68	0.41
1:A:42:VAL:HG13	2:B:628:TRP:CD2	2.56	0.41
1:A:157:PHE:CE2	1:A:159:THR:HB	2.56	0.41
1:A:170:GLU:HG3	1:A:171:TYR:H	1.85	0.41
1:A:234:ASN:ND2	1:A:234:ASN:O	2.53	0.41
1:I:304:ARG:HD3	1:I:439:ILE:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:GLY:O	1:A:433:CYS:N	2.54	0.41
1:E:150:GLU:OE1	1:E:150:GLU:N	2.49	0.41
1:I:431:GLY:O	1:I:433:CYS:N	2.54	0.41
1:A:53:PHE:CZ	1:A:220:PRO:HB3	2.56	0.41
1:E:234:ASN:O	1:E:234:ASN:ND2	2.54	0.41
1:E:431:GLY:O	1:E:433:CYS:N	2.54	0.41
1:E:432:ARG:O	1:E:432:ARG:HG3	2.20	0.41
9:E:619:NAG:HO4	9:E:619:NAG:HO6	1.56	0.41
2:F:592:LEU:O	2:F:596:TRP:NE1	2.54	0.41
1:I:136:VAL:HG13	1:I:138:THR:H	1.84	0.41
1:A:362:ASN:OD1	1:A:363:GLN:N	2.52	0.41
2:B:591:GLN:O	2:B:595:ILE:HG13	2.20	0.41
1:E:53:PHE:CZ	1:E:220:PRO:HB3	2.56	0.41
9:I:630:NAG:O6	9:I:630:NAG:O4	2.24	0.41
2:J:591:GLN:O	2:J:595:ILE:HG13	2.20	0.41
1:A:91:GLU:O	1:A:238:PRO:HA	2.22	0.40
1:A:426:MET:H	1:A:426:MET:HG2	1.67	0.40
1:E:42:VAL:HG13	2:F:628:TRP:CD2	2.56	0.40
1:E:91:GLU:O	1:E:238:PRO:HA	2.22	0.40
1:I:170:GLU:HG3	1:I:171:TYR:N	2.36	0.40
2:J:592:LEU:O	2:J:596:TRP:NE1	2.54	0.40
1:A:432:ARG:HG3	1:A:432:ARG:O	2.20	0.40
2:J:602:LEU:CD1	2:J:603:ILE:H	2.28	0.40
5:X:2:NAG:O7	5:X:2:NAG:H3	2.18	0.40
1:A:170:GLU:HG3	1:A:171:TYR:N	2.36	0.40
2:B:627:THR:HG23	2:B:629:LEU:H	1.87	0.40
8:R:1:NAG:O3	8:R:2:NAG:O5	2.12	0.40
1:A:231:GLU:H	1:A:231:GLU:CD	2.25	0.40
6:N:2:NAG:H83	6:N:2:NAG:H2	1.99	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	460/462 (100%)	414 (90%)	37 (8%)	9 (2%)	7 40
1	E	460/462 (100%)	414 (90%)	37 (8%)	9 (2%)	7 40
1	I	460/462 (100%)	414 (90%)	37 (8%)	9 (2%)	7 40
2	B	127/153 (83%)	120 (94%)	7 (6%)	0	100 100
2	F	127/153 (83%)	120 (94%)	7 (6%)	0	100 100
2	J	127/153 (83%)	120 (94%)	7 (6%)	0	100 100
3	C	124/238 (52%)	121 (98%)	3 (2%)	0	100 100
3	G	124/238 (52%)	121 (98%)	3 (2%)	0	100 100
3	K	124/238 (52%)	121 (98%)	3 (2%)	0	100 100
4	D	108/216 (50%)	105 (97%)	2 (2%)	1 (1%)	17 56
4	H	108/216 (50%)	105 (97%)	2 (2%)	1 (1%)	17 56
4	L	108/216 (50%)	105 (97%)	2 (2%)	1 (1%)	17 56
All	All	2457/3207 (77%)	2280 (93%)	147 (6%)	30 (1%)	17 50

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	VAL
1	A	124	PRO
1	A	201	VAL
1	A	449	ILE
4	D	53	VAL
1	E	89	VAL
1	E	124	PRO
1	E	201	VAL
1	E	449	ILE
4	H	53	VAL
1	I	89	VAL
1	I	124	PRO
1	I	201	VAL
1	I	449	ILE
4	L	53	VAL
1	A	354	PRO
1	E	354	PRO
1	I	354	PRO
1	A	125	LEU
1	A	202	THR
1	A	242	VAL
1	A	290	THR

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Mol	Chain	Res	Type
1	E	125	LEU
1	E	202	THR
1	E	242	VAL
1	E	290	THR
1	I	125	LEU
1	I	202	THR
1	I	242	VAL
1	I	290	THR

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	412/412 (100%)	395 (96%)	17 (4%)	30	56
1	E	412/412 (100%)	395 (96%)	17 (4%)	30	56
1	I	412/412 (100%)	395 (96%)	17 (4%)	30	56
2	B	110/129 (85%)	106 (96%)	4 (4%)	35	60
2	F	110/129 (85%)	106 (96%)	4 (4%)	35	60
2	J	110/129 (85%)	106 (96%)	4 (4%)	35	60
3	C	103/200 (52%)	100 (97%)	3 (3%)	42	64
3	G	103/200 (52%)	100 (97%)	3 (3%)	42	64
3	K	103/200 (52%)	100 (97%)	3 (3%)	42	64
4	D	90/181 (50%)	88 (98%)	2 (2%)	52	70
4	H	90/181 (50%)	88 (98%)	2 (2%)	52	70
4	L	90/181 (50%)	88 (98%)	2 (2%)	52	70
All	All	2145/2766 (78%)	2067 (96%)	78 (4%)	38	60

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	157	PHE
1	A	158	ASN
1	A	192	ARG
1	A	196	CYS
1	A	230	ASP
1	A	262	ASN
1	A	276	ASN
1	A	301	ASN
1	A	336	GLU
1	A	372	THR
1	A	377	ASN
1	A	392	ASN
1	A	433	CYS
1	A	442	ASN
1	A	457	ASP
2	B	520	LEU
2	B	522	PHE
2	B	602	LEU
2	B	632	ASP
3	C	29	PHE
3	C	72	ARG
3	C	89	ASP
4	D	6	GLN
4	D	40	GLN
1	E	88	ASN
1	E	92	ASN
1	E	157	PHE
1	E	158	ASN
1	E	192	ARG
1	E	196	CYS
1	E	230	ASP
1	E	262	ASN
1	E	276	ASN
1	E	301	ASN
1	E	336	GLU
1	E	372	THR
1	E	377	ASN
1	E	392	ASN
1	E	433	CYS
1	E	442	ASN
1	E	457	ASP
2	F	520	LEU

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Mol	Chain	Res	Type
2	F	522	PHE
2	F	602	LEU
2	F	632	ASP
3	G	29	PHE
3	G	72	ARG
3	G	89	ASP
4	H	6	GLN
4	H	40	GLN
1	I	88	ASN
1	I	92	ASN
1	I	157	PHE
1	I	158	ASN
1	I	192	ARG
1	I	196	CYS
1	I	230	ASP
1	I	262	ASN
1	I	276	ASN
1	I	301	ASN
1	I	336	GLU
1	I	372	THR
1	I	377	ASN
1	I	392	ASN
1	I	433	CYS
1	I	442	ASN
1	I	457	ASP
2	J	520	LEU
2	J	522	PHE
2	J	602	LEU
2	J	632	ASP
3	K	29	PHE
3	K	72	ARG
3	K	89	ASP
4	L	6	GLN
4	L	40	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	GLN
1	A	404	ASN
2	B	540	GLN
3	C	39	GLN

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Mol	Chain	Res	Type
3	C	65	GLN
4	D	1	GLN
4	D	40	GLN
1	E	203	GLN
1	E	404	ASN
2	F	540	GLN
3	G	39	GLN
3	G	65	GLN
4	H	1	GLN
4	H	40	GLN
1	I	203	GLN
1	I	404	ASN
2	J	540	GLN
2	J	591	GLN
3	K	39	GLN
3	K	65	GLN
4	L	1	GLN
4	L	40	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

69 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	M	1	5,1	14,14,15	0.74	1 (7%)	17,19,21	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	M	2	5	14,14,15	0.88	1 (7%)	17,19,21	0.49	0
6	NAG	N	1	6,1	14,14,15	0.75	1 (7%)	17,19,21	0.47	0
6	NAG	N	2	6	14,14,15	0.39	0	17,19,21	0.56	0
6	BMA	N	3	6	11,11,12	1.07	1 (9%)	15,15,17	0.84	1 (6%)
6	MAN	N	4	6	11,11,12	0.85	1 (9%)	15,15,17	1.19	3 (20%)
6	MAN	N	5	6	11,11,12	0.95	1 (9%)	15,15,17	1.20	1 (6%)
6	BMA	N	6	6	11,11,12	1.02	2 (18%)	15,15,17	1.15	1 (6%)
6	MAN	N	7	6	11,11,12	0.76	0	15,15,17	1.01	2 (13%)
7	NAG	O	1	7,1	14,14,15	2.04	6 (42%)	17,19,21	3.03	7 (41%)
7	NAG	O	2	7	14,14,15	0.88	0	17,19,21	2.81	7 (41%)
7	BMA	O	3	7	11,11,12	0.71	0	15,15,17	1.90	5 (33%)
7	NAG	O	4	7	14,14,15	0.54	0	17,19,21	1.82	6 (35%)
8	NAG	P	1	8,1	14,14,15	1.94	5 (35%)	17,19,21	3.09	9 (52%)
8	NAG	P	2	8	14,14,15	0.53	0	17,19,21	2.35	7 (41%)
8	BMA	P	3	8	11,11,12	0.70	0	15,15,17	2.18	6 (40%)
5	NAG	Q	1	5,1	14,14,15	1.96	4 (28%)	17,19,21	2.52	7 (41%)
5	NAG	Q	2	5	14,14,15	0.95	2 (14%)	17,19,21	1.92	5 (29%)
8	NAG	R	1	8,1	14,14,15	0.86	1 (7%)	17,19,21	1.93	4 (23%)
8	NAG	R	2	8	14,14,15	0.84	0	17,19,21	2.00	5 (29%)
8	BMA	R	3	8	11,11,12	0.49	0	15,15,17	1.51	3 (20%)
5	NAG	S	1	5,1	14,14,15	1.37	2 (14%)	17,19,21	1.73	5 (29%)
5	NAG	S	2	5	14,14,15	0.66	0	17,19,21	2.28	7 (41%)
5	NAG	T	1	5,1	14,14,15	0.73	1 (7%)	17,19,21	0.72	0
5	NAG	T	2	5	14,14,15	0.88	1 (7%)	17,19,21	0.49	0
6	NAG	U	1	6,1	14,14,15	0.75	1 (7%)	17,19,21	0.47	0
6	NAG	U	2	6	14,14,15	0.38	0	17,19,21	0.56	0
6	BMA	U	3	6	11,11,12	1.07	1 (9%)	15,15,17	0.85	1 (6%)
6	MAN	U	4	6	11,11,12	0.85	1 (9%)	15,15,17	1.19	3 (20%)
6	MAN	U	5	6	11,11,12	0.96	1 (9%)	15,15,17	1.20	1 (6%)
6	BMA	U	6	6	11,11,12	1.03	2 (18%)	15,15,17	1.15	1 (6%)
6	MAN	U	7	6	11,11,12	0.77	0	15,15,17	1.01	2 (13%)
7	NAG	V	1	7,1	14,14,15	2.04	6 (42%)	17,19,21	3.02	7 (41%)
7	NAG	V	2	7	14,14,15	0.88	0	17,19,21	2.81	7 (41%)
7	BMA	V	3	7	11,11,12	0.71	0	15,15,17	1.90	5 (33%)
7	NAG	V	4	7	14,14,15	0.54	0	17,19,21	1.82	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	W	1	8,1	14,14,15	1.95	5 (35%)	17,19,21	3.08	9 (52%)
8	NAG	W	2	8	14,14,15	0.53	0	17,19,21	2.35	7 (41%)
8	BMA	W	3	8	11,11,12	0.70	0	15,15,17	2.18	6 (40%)
5	NAG	X	1	5,1	14,14,15	1.96	4 (28%)	17,19,21	2.52	7 (41%)
5	NAG	X	2	5	14,14,15	0.95	2 (14%)	17,19,21	1.92	5 (29%)
8	NAG	Y	1	8,1	14,14,15	0.87	1 (7%)	17,19,21	1.93	4 (23%)
8	NAG	Y	2	8	14,14,15	0.84	0	17,19,21	2.00	5 (29%)
8	BMA	Y	3	8	11,11,12	0.51	0	15,15,17	1.51	3 (20%)
5	NAG	Z	1	5,1	14,14,15	1.37	2 (14%)	17,19,21	1.73	5 (29%)
5	NAG	Z	2	5	14,14,15	0.68	0	17,19,21	2.28	7 (41%)
5	NAG	a	1	5,1	14,14,15	0.75	1 (7%)	17,19,21	0.73	0
5	NAG	a	2	5	14,14,15	0.88	1 (7%)	17,19,21	0.49	0
6	NAG	b	1	6,1	14,14,15	0.75	1 (7%)	17,19,21	0.48	0
6	NAG	b	2	6	14,14,15	0.38	0	17,19,21	0.56	0
6	BMA	b	3	6	11,11,12	1.07	1 (9%)	15,15,17	0.85	1 (6%)
6	MAN	b	4	6	11,11,12	0.85	1 (9%)	15,15,17	1.19	3 (20%)
6	MAN	b	5	6	11,11,12	0.95	1 (9%)	15,15,17	1.20	1 (6%)
6	BMA	b	6	6	11,11,12	1.02	2 (18%)	15,15,17	1.16	1 (6%)
6	MAN	b	7	6	11,11,12	0.77	0	15,15,17	1.01	2 (13%)
7	NAG	c	1	7,1	14,14,15	2.05	5 (35%)	17,19,21	3.02	7 (41%)
7	NAG	c	2	7	14,14,15	0.87	0	17,19,21	2.82	7 (41%)
7	BMA	c	3	7	11,11,12	0.71	0	15,15,17	1.90	5 (33%)
7	NAG	c	4	7	14,14,15	0.54	0	17,19,21	1.82	6 (35%)
8	NAG	d	1	8,1	14,14,15	1.94	5 (35%)	17,19,21	3.09	9 (52%)
8	NAG	d	2	8	14,14,15	0.52	0	17,19,21	2.36	7 (41%)
8	BMA	d	3	8	11,11,12	0.70	0	15,15,17	2.18	6 (40%)
5	NAG	e	1	5,1	14,14,15	1.96	4 (28%)	17,19,21	2.52	7 (41%)
5	NAG	e	2	5	14,14,15	0.95	2 (14%)	17,19,21	1.92	5 (29%)
8	NAG	f	1	8,1	14,14,15	0.86	1 (7%)	17,19,21	1.93	4 (23%)
8	NAG	f	2	8	14,14,15	0.83	0	17,19,21	2.00	5 (29%)
8	BMA	f	3	8	11,11,12	0.51	0	15,15,17	1.51	3 (20%)
5	NAG	g	1	5,1	14,14,15	1.37	2 (14%)	17,19,21	1.73	5 (29%)
5	NAG	g	2	5	14,14,15	0.67	0	17,19,21	2.28	7 (41%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	BMA	V	3	7	-	0/2/19/22	0/1/1/1
7	NAG	V	4	7	-	1/6/23/26	0/1/1/1
8	NAG	W	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	W	2	8	-	0/6/23/26	0/1/1/1
8	BMA	W	3	8	-	1/2/19/22	0/1/1/1
5	NAG	X	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	X	2	5	-	3/6/23/26	0/1/1/1
8	NAG	Y	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	Y	2	8	-	2/6/23/26	0/1/1/1
8	BMA	Y	3	8	-	0/2/19/22	0/1/1/1
5	NAG	Z	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	Z	2	5	-	2/6/23/26	0/1/1/1
5	NAG	a	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	a	2	5	-	2/6/23/26	0/1/1/1
6	NAG	b	1	6,1	-	4/6/23/26	0/1/1/1
6	NAG	b	2	6	-	4/6/23/26	0/1/1/1
6	BMA	b	3	6	-	2/2/19/22	0/1/1/1
6	MAN	b	4	6	-	2/2/19/22	0/1/1/1
6	MAN	b	5	6	-	1/2/19/22	0/1/1/1
6	BMA	b	6	6	-	2/2/19/22	0/1/1/1
6	MAN	b	7	6	-	2/2/19/22	0/1/1/1
7	NAG	c	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	c	2	7	-	3/6/23/26	0/1/1/1
7	BMA	c	3	7	-	0/2/19/22	0/1/1/1
7	NAG	c	4	7	-	1/6/23/26	0/1/1/1
8	NAG	d	1	8,1	-	1/6/23/26	0/1/1/1
8	NAG	d	2	8	-	0/6/23/26	0/1/1/1
8	BMA	d	3	8	-	1/2/19/22	0/1/1/1
5	NAG	e	1	5,1	-	5/6/23/26	0/1/1/1
5	NAG	e	2	5	-	3/6/23/26	0/1/1/1
8	NAG	f	1	8,1	-	4/6/23/26	0/1/1/1
8	NAG	f	2	8	-	2/6/23/26	0/1/1/1
8	BMA	f	3	8	-	0/2/19/22	0/1/1/1
5	NAG	g	1	5,1	-	2/6/23/26	0/1/1/1
5	NAG	g	2	5	-	2/6/23/26	0/1/1/1

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	1	NAG	O5-C1	-5.66	1.34	1.43
5	Q	1	NAG	O5-C1	-5.66	1.34	1.43
5	X	1	NAG	O5-C1	-5.65	1.34	1.43
8	W	1	NAG	O5-C1	-4.11	1.37	1.43
8	d	1	NAG	O5-C1	-4.09	1.37	1.43
8	P	1	NAG	O5-C1	-4.08	1.37	1.43
7	c	1	NAG	C2-N2	-3.53	1.40	1.46
7	O	1	NAG	C2-N2	-3.50	1.40	1.46
7	V	1	NAG	C2-N2	-3.46	1.40	1.46
7	V	1	NAG	O5-C1	-3.30	1.38	1.43
7	O	1	NAG	O5-C1	-3.30	1.38	1.43
8	P	1	NAG	O5-C5	-3.28	1.36	1.43
8	W	1	NAG	O5-C5	-3.27	1.36	1.43
7	c	1	NAG	O5-C1	-3.27	1.38	1.43
8	d	1	NAG	O5-C5	-3.26	1.36	1.43
5	T	2	NAG	O5-C1	-2.98	1.38	1.43
5	a	2	NAG	O5-C1	-2.98	1.39	1.43
5	M	2	NAG	O5-C1	-2.97	1.39	1.43
7	c	1	NAG	C1-C2	-2.78	1.48	1.52
7	O	1	NAG	C1-C2	-2.78	1.48	1.52
7	V	1	NAG	C1-C2	-2.78	1.48	1.52
6	U	1	NAG	O5-C1	-2.76	1.39	1.43
6	U	3	BMA	O5-C1	-2.76	1.39	1.43
6	N	1	NAG	O5-C1	-2.76	1.39	1.43
6	b	1	NAG	O5-C1	-2.74	1.39	1.43
6	N	3	BMA	O5-C1	-2.74	1.39	1.43
5	X	1	NAG	C3-C2	-2.73	1.46	1.52
6	b	3	BMA	O5-C1	-2.73	1.39	1.43
5	e	1	NAG	C3-C2	-2.72	1.46	1.52
5	Q	1	NAG	C3-C2	-2.72	1.46	1.52
5	S	1	NAG	O5-C1	-2.60	1.39	1.43
5	g	1	NAG	O5-C1	-2.60	1.39	1.43
5	Z	1	NAG	O5-C1	-2.60	1.39	1.43
5	a	1	NAG	O5-C1	-2.57	1.39	1.43
5	Z	1	NAG	C1-C2	-2.54	1.48	1.52
5	M	1	NAG	O5-C1	-2.54	1.39	1.43
5	T	1	NAG	O5-C1	-2.53	1.39	1.43
5	S	1	NAG	C1-C2	-2.53	1.48	1.52
5	g	1	NAG	C1-C2	-2.51	1.48	1.52
7	c	1	NAG	C4-C5	-2.50	1.47	1.53
5	Q	1	NAG	O5-C5	-2.49	1.38	1.43
5	X	1	NAG	C1-C2	-2.48	1.48	1.52
5	e	1	NAG	C1-C2	-2.48	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	1	NAG	O5-C5	-2.47	1.38	1.43
5	Q	1	NAG	C1-C2	-2.47	1.48	1.52
7	O	1	NAG	C4-C5	-2.47	1.47	1.53
7	V	1	NAG	C4-C5	-2.46	1.47	1.53
5	e	1	NAG	O5-C5	-2.46	1.38	1.43
6	b	4	MAN	O5-C1	-2.41	1.39	1.43
6	N	4	MAN	O5-C1	-2.40	1.39	1.43
6	U	4	MAN	O5-C1	-2.40	1.39	1.43
7	c	1	NAG	C4-C3	-2.40	1.46	1.52
7	O	1	NAG	C4-C3	-2.39	1.46	1.52
7	V	1	NAG	C4-C3	-2.38	1.46	1.52
8	W	1	NAG	C4-C5	-2.32	1.48	1.53
8	P	1	NAG	C4-C5	-2.31	1.48	1.53
8	d	1	NAG	C4-C5	-2.31	1.48	1.53
8	P	1	NAG	C3-C2	-2.19	1.47	1.52
8	W	1	NAG	C3-C2	-2.19	1.47	1.52
8	d	1	NAG	C3-C2	-2.18	1.47	1.52
8	Y	1	NAG	O5-C1	-2.13	1.40	1.43
8	R	1	NAG	O5-C1	-2.12	1.40	1.43
8	f	1	NAG	O5-C1	-2.11	1.40	1.43
5	Q	2	NAG	C2-N2	-2.10	1.42	1.46
5	e	2	NAG	C2-N2	-2.09	1.42	1.46
8	W	1	NAG	C2-N2	-2.09	1.42	1.46
6	U	6	BMA	O5-C1	-2.09	1.40	1.43
6	U	5	MAN	O5-C1	-2.08	1.40	1.43
5	X	2	NAG	C2-N2	-2.08	1.42	1.46
5	X	2	NAG	C1-C2	-2.08	1.49	1.52
6	N	5	MAN	O5-C1	-2.07	1.40	1.43
6	N	6	BMA	O5-C1	-2.07	1.40	1.43
6	b	5	MAN	O5-C1	-2.07	1.40	1.43
6	b	6	BMA	O5-C1	-2.07	1.40	1.43
5	Q	2	NAG	C1-C2	-2.06	1.49	1.52
8	P	1	NAG	C2-N2	-2.05	1.42	1.46
8	d	1	NAG	C2-N2	-2.03	1.42	1.46
7	V	1	NAG	C3-C2	-2.03	1.48	1.52
7	O	1	NAG	C3-C2	-2.02	1.48	1.52
5	e	2	NAG	C1-C2	-2.02	1.49	1.52
6	U	6	BMA	C2-C3	2.02	1.55	1.52
6	b	6	BMA	C2-C3	2.01	1.55	1.52
6	N	6	BMA	C2-C3	2.00	1.55	1.52

All (273) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	d	1	NAG	O5-C5-C6	-6.96	96.29	107.20
8	P	1	NAG	O5-C5-C6	-6.95	96.31	107.20
8	W	1	NAG	O5-C5-C6	-6.94	96.33	107.20
7	V	1	NAG	O5-C1-C2	-6.42	101.15	111.29
7	O	1	NAG	O5-C1-C2	-6.41	101.17	111.29
7	c	1	NAG	O5-C1-C2	-6.41	101.17	111.29
7	c	2	NAG	O5-C1-C2	-5.86	102.04	111.29
7	V	2	NAG	O5-C1-C2	-5.85	102.04	111.29
7	O	2	NAG	O5-C1-C2	-5.84	102.06	111.29
7	c	1	NAG	C2-N2-C7	-5.61	114.92	122.90
7	O	1	NAG	C2-N2-C7	-5.60	114.92	122.90
7	V	1	NAG	C2-N2-C7	-5.59	114.94	122.90
8	d	1	NAG	O4-C4-C3	-5.52	97.58	110.35
8	P	1	NAG	O4-C4-C3	-5.51	97.60	110.35
7	c	2	NAG	C3-C4-C5	-5.50	100.43	110.24
8	W	1	NAG	O4-C4-C3	-5.50	97.64	110.35
7	O	2	NAG	C3-C4-C5	-5.49	100.45	110.24
7	V	2	NAG	C3-C4-C5	-5.48	100.47	110.24
8	d	2	NAG	C1-C2-N2	5.35	119.63	110.49
8	W	2	NAG	C1-C2-N2	5.34	119.61	110.49
8	P	2	NAG	C1-C2-N2	5.34	119.61	110.49
7	O	1	NAG	C3-C4-C5	-4.94	101.42	110.24
7	V	1	NAG	C3-C4-C5	-4.93	101.44	110.24
5	Q	1	NAG	O3-C3-C2	-4.93	99.27	109.47
5	X	1	NAG	O3-C3-C2	-4.92	99.28	109.47
7	c	1	NAG	C3-C4-C5	-4.92	101.46	110.24
5	e	1	NAG	O3-C3-C2	-4.92	99.29	109.47
8	d	2	NAG	C4-C3-C2	-4.88	103.86	111.02
5	X	1	NAG	C1-C2-N2	4.87	118.81	110.49
5	e	1	NAG	C1-C2-N2	4.87	118.80	110.49
5	Q	1	NAG	C1-C2-N2	4.86	118.78	110.49
5	X	2	NAG	C2-N2-C7	-4.86	115.99	122.90
5	e	2	NAG	C2-N2-C7	-4.86	115.99	122.90
8	P	2	NAG	C4-C3-C2	-4.85	103.91	111.02
8	W	2	NAG	C4-C3-C2	-4.85	103.91	111.02
5	Q	2	NAG	C2-N2-C7	-4.84	116.01	122.90
8	f	1	NAG	O5-C5-C6	4.70	114.57	107.20
8	Y	1	NAG	O5-C5-C6	4.69	114.56	107.20
8	R	1	NAG	O5-C5-C6	4.69	114.56	107.20
7	O	1	NAG	O3-C3-C4	-4.42	100.12	110.35
7	V	1	NAG	O3-C3-C4	-4.42	100.14	110.35
7	c	1	NAG	O3-C3-C4	-4.41	100.15	110.35
8	P	3	BMA	C3-C4-C5	-4.18	102.79	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	d	1	NAG	C6-C5-C4	-4.18	103.22	113.00
8	P	1	NAG	C6-C5-C4	-4.17	103.24	113.00
8	d	3	BMA	C3-C4-C5	-4.16	102.81	110.24
8	W	3	BMA	C3-C4-C5	-4.16	102.82	110.24
8	W	1	NAG	C6-C5-C4	-4.16	103.26	113.00
8	d	1	NAG	O4-C4-C5	-4.10	99.11	109.30
8	P	1	NAG	O4-C4-C5	-4.10	99.12	109.30
8	W	1	NAG	O4-C4-C5	-4.09	99.13	109.30
5	S	2	NAG	C1-C2-N2	4.08	117.46	110.49
5	Z	2	NAG	C2-N2-C7	-4.08	117.09	122.90
5	Z	2	NAG	C1-C2-N2	4.08	117.45	110.49
5	g	2	NAG	C1-C2-N2	4.07	117.43	110.49
5	S	2	NAG	C2-N2-C7	-4.06	117.13	122.90
5	g	2	NAG	C2-N2-C7	-4.06	117.13	122.90
7	O	2	NAG	O5-C5-C6	4.05	113.55	107.20
7	c	2	NAG	O5-C5-C6	4.04	113.54	107.20
7	V	2	NAG	O5-C5-C6	4.04	113.54	107.20
5	Q	1	NAG	O4-C4-C3	-3.96	101.20	110.35
5	e	1	NAG	O4-C4-C3	-3.95	101.22	110.35
5	X	1	NAG	O4-C4-C3	-3.95	101.23	110.35
7	O	4	NAG	C1-O5-C5	3.93	117.51	112.19
8	f	3	BMA	O5-C5-C6	3.92	113.35	107.20
8	R	3	BMA	O5-C5-C6	3.91	113.34	107.20
8	Y	3	BMA	O5-C5-C6	3.91	113.34	107.20
7	c	4	NAG	C1-O5-C5	3.90	117.48	112.19
7	V	4	NAG	C1-O5-C5	3.90	117.48	112.19
7	V	1	NAG	O5-C5-C6	3.81	113.18	107.20
7	O	1	NAG	O5-C5-C6	3.80	113.16	107.20
7	c	1	NAG	O5-C5-C6	3.79	113.14	107.20
8	d	1	NAG	C4-C3-C2	-3.74	105.54	111.02
8	P	1	NAG	C4-C3-C2	-3.73	105.55	111.02
8	W	1	NAG	C4-C3-C2	-3.72	105.57	111.02
5	e	1	NAG	O5-C5-C6	-3.69	101.42	107.20
5	X	1	NAG	O5-C5-C6	-3.69	101.43	107.20
5	Q	1	NAG	O5-C5-C6	-3.68	101.43	107.20
5	g	2	NAG	O5-C5-C6	3.68	112.97	107.20
5	S	2	NAG	O5-C5-C6	3.68	112.97	107.20
8	f	2	NAG	O4-C4-C3	-3.65	101.91	110.35
8	Y	2	NAG	O4-C4-C3	-3.65	101.91	110.35
5	Z	2	NAG	O5-C5-C6	3.65	112.92	107.20
8	R	2	NAG	O4-C4-C3	-3.64	101.93	110.35
7	c	2	NAG	O3-C3-C2	3.64	116.99	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	2	NAG	O3-C3-C2	3.63	116.98	109.47
7	O	2	NAG	O3-C3-C2	3.63	116.98	109.47
7	V	4	NAG	O3-C3-C2	-3.62	101.97	109.47
7	O	4	NAG	O3-C3-C2	-3.61	101.99	109.47
7	O	2	NAG	O6-C6-C5	-3.61	98.92	111.29
7	c	2	NAG	O6-C6-C5	-3.60	98.92	111.29
7	c	4	NAG	O3-C3-C2	-3.60	102.01	109.47
7	V	2	NAG	O6-C6-C5	-3.60	98.93	111.29
8	R	2	NAG	C2-N2-C7	-3.59	117.80	122.90
8	f	2	NAG	C2-N2-C7	-3.58	117.80	122.90
8	Y	2	NAG	C2-N2-C7	-3.57	117.82	122.90
7	O	3	BMA	C6-C5-C4	-3.46	104.90	113.00
7	c	3	BMA	C6-C5-C4	-3.46	104.90	113.00
7	V	3	BMA	C6-C5-C4	-3.46	104.91	113.00
8	d	3	BMA	O3-C3-C4	3.37	118.14	110.35
8	W	3	BMA	O3-C3-C4	3.36	118.12	110.35
5	Q	2	NAG	O4-C4-C3	-3.36	102.59	110.35
8	d	3	BMA	O2-C2-C3	-3.35	103.42	110.14
8	P	3	BMA	O3-C3-C4	3.35	118.10	110.35
5	e	2	NAG	O4-C4-C3	-3.35	102.61	110.35
5	X	2	NAG	O4-C4-C3	-3.34	102.62	110.35
8	P	3	BMA	O2-C2-C3	-3.33	103.47	110.14
8	W	3	BMA	O2-C2-C3	-3.33	103.47	110.14
8	W	1	NAG	O3-C3-C4	-3.31	102.69	110.35
5	g	1	NAG	C3-C4-C5	-3.31	104.33	110.24
5	Z	1	NAG	C3-C4-C5	-3.31	104.34	110.24
5	S	1	NAG	C3-C4-C5	-3.30	104.35	110.24
8	P	1	NAG	O3-C3-C4	-3.29	102.73	110.35
8	f	2	NAG	C1-C2-N2	-3.29	104.87	110.49
8	Y	2	NAG	C1-C2-N2	-3.29	104.87	110.49
8	d	1	NAG	O3-C3-C4	-3.29	102.75	110.35
8	R	2	NAG	C1-C2-N2	-3.28	104.89	110.49
8	Y	1	NAG	O6-C6-C5	-3.14	100.53	111.29
8	f	1	NAG	O6-C6-C5	-3.13	100.54	111.29
8	R	1	NAG	O6-C6-C5	-3.13	100.55	111.29
8	f	1	NAG	O4-C4-C3	3.12	117.56	110.35
8	d	2	NAG	O5-C5-C6	-3.11	102.32	107.20
8	R	1	NAG	O4-C4-C3	3.11	117.55	110.35
8	Y	2	NAG	C1-O5-C5	3.11	116.41	112.19
8	R	2	NAG	C1-O5-C5	3.11	116.41	112.19
8	Y	1	NAG	O4-C4-C3	3.11	117.53	110.35
5	S	1	NAG	O7-C7-C8	3.11	127.83	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	2	NAG	C1-O5-C5	3.10	116.39	112.19
8	P	2	NAG	O5-C5-C6	-3.10	102.35	107.20
5	g	1	NAG	O7-C7-C8	3.10	127.81	122.06
8	W	2	NAG	O5-C5-C6	-3.09	102.35	107.20
5	Z	1	NAG	O7-C7-C8	3.09	127.80	122.06
5	g	2	NAG	C6-C5-C4	-3.07	105.81	113.00
5	S	2	NAG	C6-C5-C4	-3.07	105.82	113.00
5	Z	2	NAG	C6-C5-C4	-3.05	105.85	113.00
8	W	3	BMA	C1-C2-C3	-3.05	105.92	109.67
8	P	3	BMA	C1-C2-C3	-3.02	105.95	109.67
8	d	3	BMA	C1-C2-C3	-3.00	105.97	109.67
8	d	3	BMA	O4-C4-C5	-2.93	102.02	109.30
5	Q	1	NAG	C2-N2-C7	2.93	127.08	122.90
8	P	3	BMA	O4-C4-C5	-2.93	102.03	109.30
5	e	1	NAG	C2-N2-C7	2.92	127.07	122.90
7	O	2	NAG	C6-C5-C4	-2.92	106.16	113.00
8	W	3	BMA	O4-C4-C5	-2.92	102.05	109.30
7	V	2	NAG	C6-C5-C4	-2.92	106.17	113.00
5	X	1	NAG	C2-N2-C7	2.92	127.05	122.90
7	c	2	NAG	C6-C5-C4	-2.91	106.18	113.00
7	c	3	BMA	O3-C3-C2	2.90	115.55	109.99
7	V	3	BMA	O3-C3-C2	2.90	115.54	109.99
7	O	3	BMA	O3-C3-C2	2.89	115.52	109.99
5	g	2	NAG	O5-C1-C2	-2.83	106.81	111.29
5	Z	2	NAG	O5-C1-C2	-2.82	106.84	111.29
5	S	2	NAG	O5-C1-C2	-2.81	106.85	111.29
8	Y	1	NAG	C4-C3-C2	-2.78	106.94	111.02
8	f	1	NAG	C4-C3-C2	-2.78	106.94	111.02
8	R	1	NAG	C4-C3-C2	-2.78	106.95	111.02
8	W	1	NAG	C1-O5-C5	2.71	115.86	112.19
8	P	1	NAG	C1-O5-C5	2.70	115.85	112.19
6	U	5	MAN	O2-C2-C3	-2.69	104.75	110.14
6	b	5	MAN	O2-C2-C3	-2.69	104.75	110.14
8	d	1	NAG	C1-O5-C5	2.68	115.83	112.19
8	P	3	BMA	O5-C1-C2	-2.68	106.63	110.77
8	d	3	BMA	O5-C1-C2	-2.68	106.63	110.77
6	N	5	MAN	O2-C2-C3	-2.68	104.77	110.14
8	W	3	BMA	O5-C1-C2	-2.68	106.63	110.77
7	O	1	NAG	O4-C4-C3	2.66	116.49	110.35
7	c	1	NAG	O4-C4-C3	2.65	116.47	110.35
7	V	1	NAG	O4-C4-C3	2.65	116.47	110.35
7	V	3	BMA	O5-C1-C2	-2.58	106.79	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	3	BMA	O5-C1-C2	-2.58	106.79	110.77
7	c	3	BMA	O5-C1-C2	-2.58	106.80	110.77
8	f	2	NAG	O5-C5-C6	-2.54	103.22	107.20
8	R	2	NAG	O5-C5-C6	-2.53	103.23	107.20
8	Y	2	NAG	O5-C5-C6	-2.53	103.24	107.20
5	g	1	NAG	O3-C3-C2	-2.50	104.29	109.47
5	Z	1	NAG	O3-C3-C2	-2.50	104.29	109.47
5	S	1	NAG	O3-C3-C2	-2.50	104.30	109.47
5	e	1	NAG	C8-C7-N2	-2.48	111.90	116.10
5	Q	1	NAG	C8-C7-N2	-2.47	111.91	116.10
5	X	1	NAG	C8-C7-N2	-2.47	111.92	116.10
6	U	4	MAN	C1-O5-C5	2.44	115.50	112.19
8	d	2	NAG	O4-C4-C5	2.44	115.35	109.30
8	W	2	NAG	O4-C4-C5	2.43	115.34	109.30
8	P	2	NAG	O4-C4-C5	2.43	115.34	109.30
6	b	4	MAN	C1-O5-C5	2.43	115.48	112.19
6	N	4	MAN	C1-O5-C5	2.43	115.48	112.19
5	e	2	NAG	C1-C2-N2	-2.43	106.34	110.49
5	Q	2	NAG	C1-C2-N2	-2.43	106.34	110.49
5	X	2	NAG	C1-C2-N2	-2.42	106.35	110.49
6	U	3	BMA	O2-C2-C3	-2.41	105.31	110.14
6	N	3	BMA	O2-C2-C3	-2.40	105.32	110.14
6	b	3	BMA	O2-C2-C3	-2.40	105.32	110.14
8	W	1	NAG	C1-C2-N2	2.39	114.57	110.49
5	Z	2	NAG	O3-C3-C2	2.38	114.38	109.47
5	S	1	NAG	C8-C7-N2	-2.37	112.08	116.10
5	S	2	NAG	O3-C3-C2	2.37	114.38	109.47
5	g	2	NAG	O3-C3-C2	2.37	114.38	109.47
8	P	1	NAG	C1-C2-N2	2.36	114.52	110.49
7	V	4	NAG	C2-N2-C7	2.36	126.26	122.90
5	g	1	NAG	C8-C7-N2	-2.36	112.11	116.10
7	c	3	BMA	O4-C4-C3	-2.36	104.90	110.35
7	O	4	NAG	C2-N2-C7	2.36	126.26	122.90
7	O	3	BMA	O4-C4-C3	-2.36	104.90	110.35
5	Z	1	NAG	C8-C7-N2	-2.36	112.11	116.10
7	c	4	NAG	C2-N2-C7	2.36	126.26	122.90
7	V	3	BMA	O4-C4-C3	-2.35	104.91	110.35
8	d	1	NAG	C1-C2-N2	2.35	114.50	110.49
7	V	2	NAG	C4-C3-C2	-2.31	107.63	111.02
8	R	3	BMA	O3-C3-C2	-2.31	105.56	109.99
8	f	3	BMA	O3-C3-C2	-2.31	105.57	109.99
7	O	2	NAG	C4-C3-C2	-2.30	107.64	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	c	2	NAG	C4-C3-C2	-2.30	107.64	111.02
6	U	7	MAN	C1-O5-C5	2.30	115.31	112.19
8	Y	3	BMA	O3-C3-C2	-2.29	105.60	109.99
6	N	7	MAN	C1-O5-C5	2.28	115.28	112.19
6	b	7	MAN	C1-O5-C5	2.28	115.28	112.19
6	b	4	MAN	O2-C2-C3	-2.28	105.58	110.14
6	N	7	MAN	O2-C2-C3	-2.27	105.58	110.14
6	U	7	MAN	O2-C2-C3	-2.27	105.58	110.14
6	b	7	MAN	O2-C2-C3	-2.27	105.59	110.14
6	U	4	MAN	O2-C2-C3	-2.27	105.60	110.14
6	N	4	MAN	O2-C2-C3	-2.27	105.60	110.14
8	W	2	NAG	O5-C1-C2	-2.25	107.73	111.29
5	S	2	NAG	C4-C3-C2	-2.25	107.72	111.02
5	X	2	NAG	O5-C1-C2	2.25	114.84	111.29
5	g	2	NAG	C4-C3-C2	-2.25	107.72	111.02
5	e	2	NAG	O5-C1-C2	2.24	114.83	111.29
5	Q	2	NAG	O5-C1-C2	2.24	114.82	111.29
8	P	2	NAG	O5-C1-C2	-2.24	107.76	111.29
5	Z	2	NAG	C4-C3-C2	-2.24	107.74	111.02
8	d	1	NAG	O5-C1-C2	-2.23	107.76	111.29
8	P	1	NAG	O5-C1-C2	-2.22	107.78	111.29
8	d	2	NAG	O5-C1-C2	-2.22	107.78	111.29
8	d	2	NAG	O3-C3-C4	2.21	115.46	110.35
8	W	1	NAG	O5-C1-C2	-2.20	107.81	111.29
8	P	2	NAG	O3-C3-C4	2.20	115.43	110.35
8	W	2	NAG	O3-C3-C4	2.20	115.42	110.35
8	d	2	NAG	O3-C3-C2	2.15	113.91	109.47
5	g	1	NAG	C1-C2-N2	-2.15	106.82	110.49
8	W	2	NAG	O3-C3-C2	2.14	113.90	109.47
5	Z	1	NAG	C1-C2-N2	-2.14	106.83	110.49
5	S	1	NAG	C1-C2-N2	-2.14	106.83	110.49
8	P	2	NAG	O3-C3-C2	2.14	113.90	109.47
7	V	4	NAG	O5-C1-C2	-2.13	107.92	111.29
5	Q	1	NAG	C4-C3-C2	-2.13	107.90	111.02
5	e	1	NAG	C4-C3-C2	-2.12	107.91	111.02
5	X	1	NAG	C4-C3-C2	-2.12	107.92	111.02
6	b	4	MAN	O5-C1-C2	2.11	114.03	110.77
7	O	4	NAG	O5-C1-C2	-2.11	107.95	111.29
7	O	4	NAG	C1-C2-N2	2.11	114.10	110.49
7	c	4	NAG	C1-C2-N2	2.11	114.10	110.49
7	c	4	NAG	O5-C1-C2	-2.11	107.96	111.29
6	N	4	MAN	O5-C1-C2	2.10	114.02	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	4	NAG	C1-C2-N2	2.10	114.07	110.49
6	b	6	BMA	C3-C4-C5	-2.10	106.50	110.24
6	U	4	MAN	O5-C1-C2	2.09	114.00	110.77
6	N	6	BMA	C3-C4-C5	-2.08	106.53	110.24
6	U	6	BMA	C3-C4-C5	-2.08	106.53	110.24
8	R	3	BMA	C2-C3-C4	-2.06	107.33	110.89
7	V	4	NAG	O4-C4-C5	-2.06	104.19	109.30
8	Y	3	BMA	C2-C3-C4	-2.06	107.34	110.89
7	V	1	NAG	O6-C6-C5	-2.05	104.25	111.29
7	O	4	NAG	O4-C4-C5	-2.05	104.20	109.30
7	c	4	NAG	O4-C4-C5	-2.05	104.20	109.30
7	c	1	NAG	O6-C6-C5	-2.05	104.27	111.29
7	O	1	NAG	O6-C6-C5	-2.04	104.28	111.29
8	f	3	BMA	C2-C3-C4	-2.04	107.37	110.89
5	Q	2	NAG	C4-C3-C2	-2.03	108.04	111.02
5	e	2	NAG	C4-C3-C2	-2.02	108.05	111.02
7	V	3	BMA	O3-C3-C4	-2.02	105.68	110.35
7	O	3	BMA	O3-C3-C4	-2.02	105.69	110.35
5	X	2	NAG	C4-C3-C2	-2.01	108.07	111.02
7	c	3	BMA	O3-C3-C4	-2.01	105.71	110.35

There are no chirality outliers.

All (141) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Q	1	NAG	C8-C7-N2-C2
5	Q	1	NAG	O7-C7-N2-C2
5	X	1	NAG	C8-C7-N2-C2
5	X	1	NAG	O7-C7-N2-C2
5	e	1	NAG	C8-C7-N2-C2
5	e	1	NAG	O7-C7-N2-C2
8	R	1	NAG	C3-C2-N2-C7
8	R	1	NAG	C8-C7-N2-C2
8	R	1	NAG	O7-C7-N2-C2
8	Y	1	NAG	C3-C2-N2-C7
8	Y	1	NAG	C8-C7-N2-C2
8	Y	1	NAG	O7-C7-N2-C2
8	f	1	NAG	C3-C2-N2-C7
8	f	1	NAG	C8-C7-N2-C2
8	f	1	NAG	O7-C7-N2-C2
6	N	3	BMA	C4-C5-C6-O6
6	U	3	BMA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	b	3	BMA	C4-C5-C6-O6
5	S	1	NAG	C8-C7-N2-C2
5	S	1	NAG	O7-C7-N2-C2
5	Z	1	NAG	C8-C7-N2-C2
5	Z	1	NAG	O7-C7-N2-C2
5	g	1	NAG	C8-C7-N2-C2
5	g	1	NAG	O7-C7-N2-C2
6	N	3	BMA	O5-C5-C6-O6
6	U	3	BMA	O5-C5-C6-O6
6	b	3	BMA	O5-C5-C6-O6
6	N	7	MAN	C4-C5-C6-O6
6	U	7	MAN	C4-C5-C6-O6
6	b	7	MAN	C4-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
6	U	4	MAN	O5-C5-C6-O6
6	N	7	MAN	O5-C5-C6-O6
6	U	7	MAN	O5-C5-C6-O6
6	b	7	MAN	O5-C5-C6-O6
6	N	1	NAG	C4-C5-C6-O6
6	U	1	NAG	C4-C5-C6-O6
6	b	1	NAG	C4-C5-C6-O6
5	Q	2	NAG	C8-C7-N2-C2
5	X	2	NAG	C8-C7-N2-C2
5	e	2	NAG	C8-C7-N2-C2
6	b	4	MAN	O5-C5-C6-O6
5	Q	1	NAG	C1-C2-N2-C7
5	X	1	NAG	C1-C2-N2-C7
5	e	1	NAG	C1-C2-N2-C7
5	S	2	NAG	O5-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
5	g	2	NAG	O5-C5-C6-O6
6	N	6	BMA	C4-C5-C6-O6
6	U	6	BMA	C4-C5-C6-O6
6	b	6	BMA	C4-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	T	1	NAG	C4-C5-C6-O6
5	a	1	NAG	C4-C5-C6-O6
6	N	4	MAN	C4-C5-C6-O6
6	U	4	MAN	C4-C5-C6-O6
6	b	4	MAN	C4-C5-C6-O6
5	Q	2	NAG	O7-C7-N2-C2
5	X	2	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
5	e	2	NAG	O7-C7-N2-C2
6	N	2	NAG	C8-C7-N2-C2
6	N	2	NAG	O7-C7-N2-C2
6	U	2	NAG	C8-C7-N2-C2
6	U	2	NAG	O7-C7-N2-C2
6	b	2	NAG	C8-C7-N2-C2
6	b	2	NAG	O7-C7-N2-C2
5	M	2	NAG	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
5	a	2	NAG	O5-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	T	2	NAG	C4-C5-C6-O6
5	a	2	NAG	C4-C5-C6-O6
6	N	2	NAG	O5-C5-C6-O6
6	U	2	NAG	O5-C5-C6-O6
6	b	2	NAG	O5-C5-C6-O6
6	N	6	BMA	O5-C5-C6-O6
6	U	6	BMA	O5-C5-C6-O6
6	b	6	BMA	O5-C5-C6-O6
7	c	2	NAG	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	V	2	NAG	O5-C5-C6-O6
6	N	1	NAG	O5-C5-C6-O6
6	U	1	NAG	O5-C5-C6-O6
6	b	1	NAG	O5-C5-C6-O6
8	R	1	NAG	O5-C5-C6-O6
8	f	1	NAG	O5-C5-C6-O6
8	Y	1	NAG	O5-C5-C6-O6
5	T	1	NAG	O5-C5-C6-O6
5	a	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
7	O	1	NAG	C8-C7-N2-C2
7	V	1	NAG	C8-C7-N2-C2
7	c	1	NAG	C8-C7-N2-C2
7	O	2	NAG	C1-C2-N2-C7
7	V	2	NAG	C1-C2-N2-C7
7	c	2	NAG	C1-C2-N2-C7
8	P	3	BMA	O5-C5-C6-O6
8	W	3	BMA	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
6	U	5	MAN	O5-C5-C6-O6
6	b	5	MAN	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
8	d	3	BMA	O5-C5-C6-O6
5	Q	2	NAG	C3-C2-N2-C7
5	X	2	NAG	C3-C2-N2-C7
5	e	2	NAG	C3-C2-N2-C7
7	O	4	NAG	C3-C2-N2-C7
7	V	4	NAG	C3-C2-N2-C7
7	c	4	NAG	C3-C2-N2-C7
8	R	2	NAG	C1-C2-N2-C7
8	Y	2	NAG	C1-C2-N2-C7
8	f	2	NAG	C1-C2-N2-C7
6	N	2	NAG	C4-C5-C6-O6
6	U	2	NAG	C4-C5-C6-O6
6	b	2	NAG	C4-C5-C6-O6
5	e	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6
5	X	1	NAG	O5-C5-C6-O6
7	O	1	NAG	O7-C7-N2-C2
7	V	1	NAG	O7-C7-N2-C2
7	c	1	NAG	O7-C7-N2-C2
6	N	1	NAG	C1-C2-N2-C7
6	U	1	NAG	C1-C2-N2-C7
6	b	1	NAG	C1-C2-N2-C7
8	P	1	NAG	C1-C2-N2-C7
8	W	1	NAG	C1-C2-N2-C7
8	d	1	NAG	C1-C2-N2-C7
7	O	2	NAG	C3-C2-N2-C7
7	V	2	NAG	C3-C2-N2-C7
7	c	2	NAG	C3-C2-N2-C7
5	Q	1	NAG	C4-C5-C6-O6
5	X	1	NAG	C4-C5-C6-O6
5	e	1	NAG	C4-C5-C6-O6
5	g	2	NAG	C4-C5-C6-O6
5	S	2	NAG	C4-C5-C6-O6
5	Z	2	NAG	C4-C5-C6-O6
6	N	1	NAG	C3-C2-N2-C7
6	U	1	NAG	C3-C2-N2-C7
6	b	1	NAG	C3-C2-N2-C7
8	R	2	NAG	C3-C2-N2-C7
8	Y	2	NAG	C3-C2-N2-C7
8	f	2	NAG	C3-C2-N2-C7

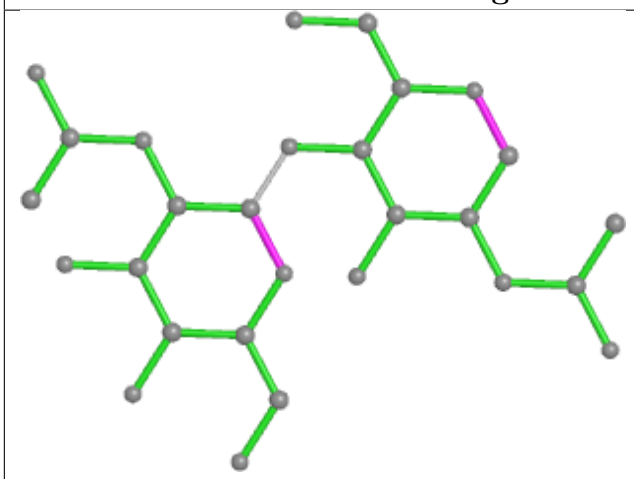
There are no ring outliers.

12 monomers are involved in 21 short contacts:

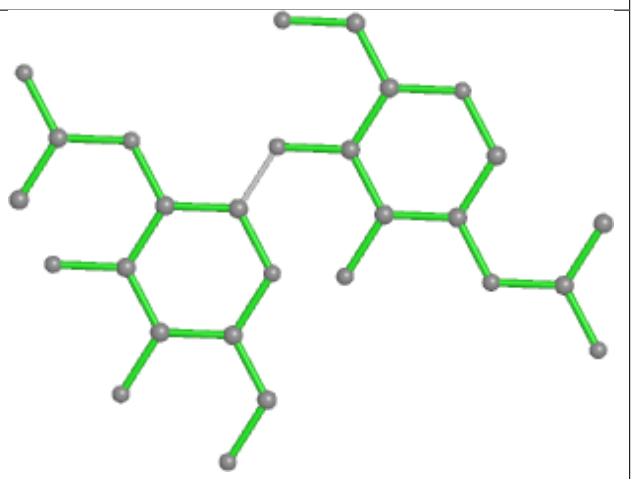
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	2	NAG	1	0
8	R	1	NAG	3	0
5	Z	2	NAG	2	0
8	R	2	NAG	2	0
5	X	1	NAG	1	0
8	Y	1	NAG	4	0
8	Y	2	NAG	2	0
5	S	2	NAG	2	0
5	Q	1	NAG	1	0
7	V	2	NAG	1	0
5	Q	2	NAG	2	0
5	X	2	NAG	2	0

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

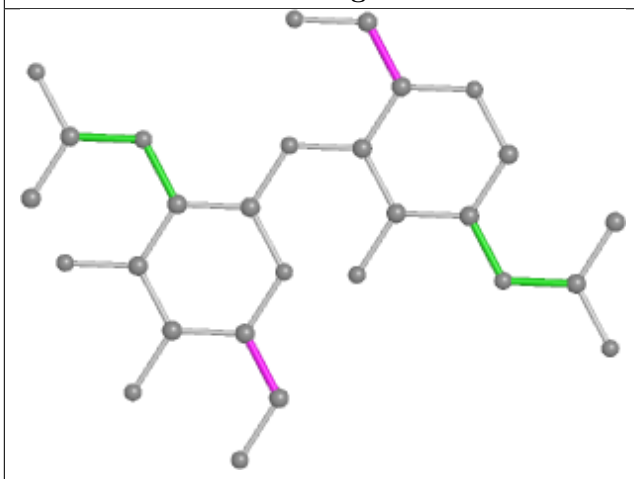
Oligosaccharide Chain M



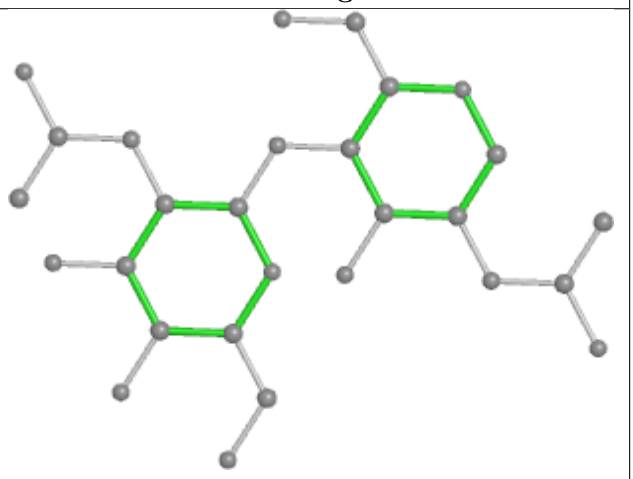
Bond lengths



Bond angles

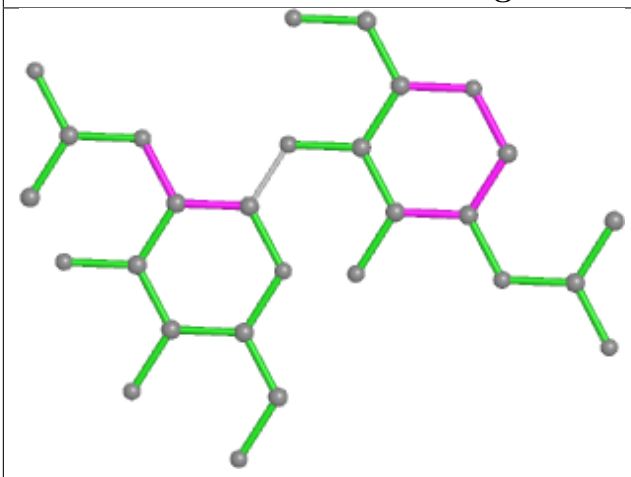


Torsions

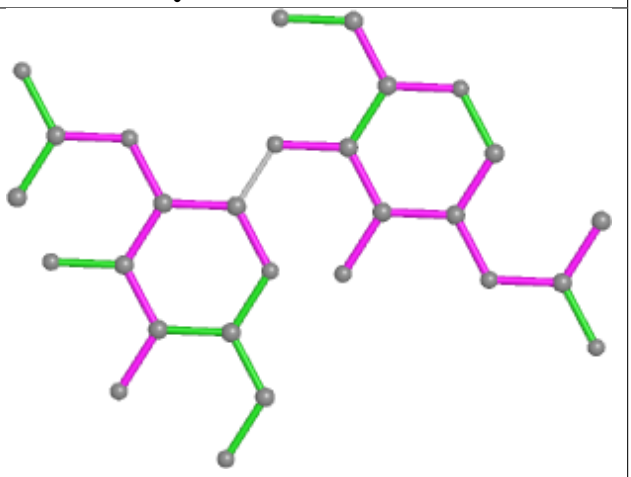


Rings

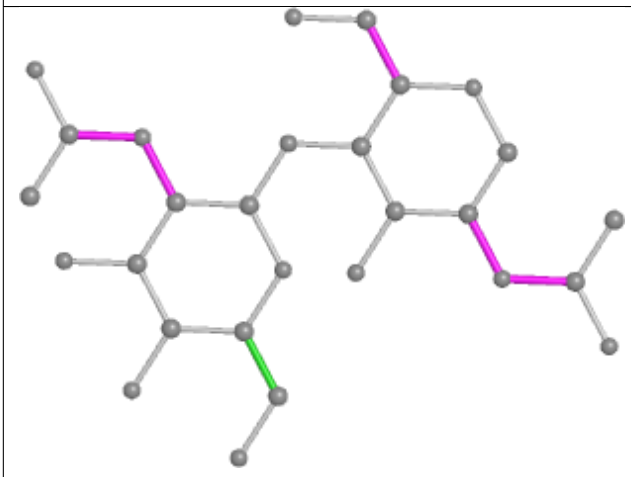
Oligosaccharide Chain Q



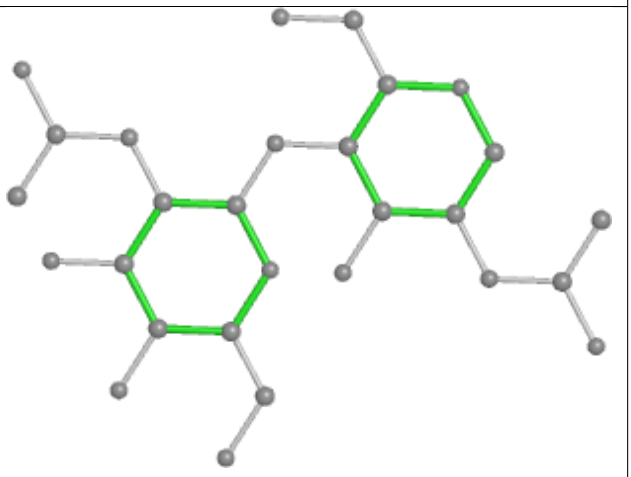
Bond lengths



Bond angles

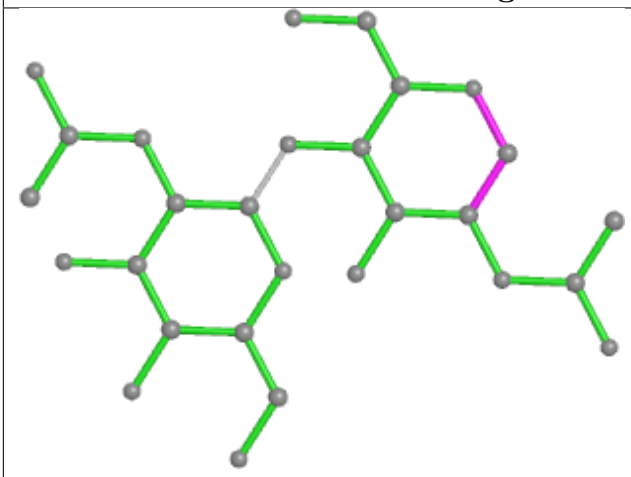


Torsions

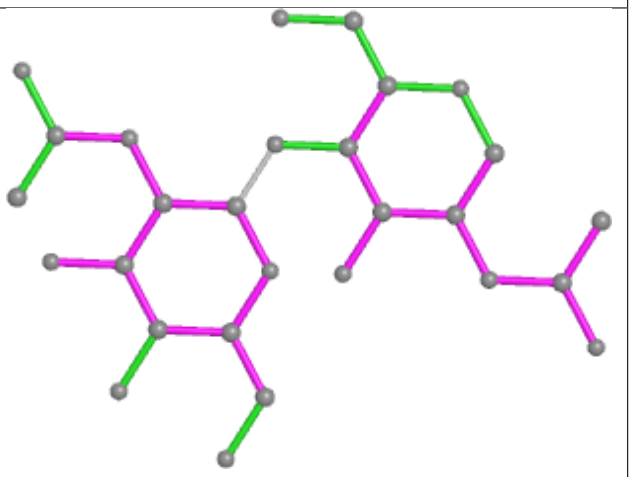


Rings

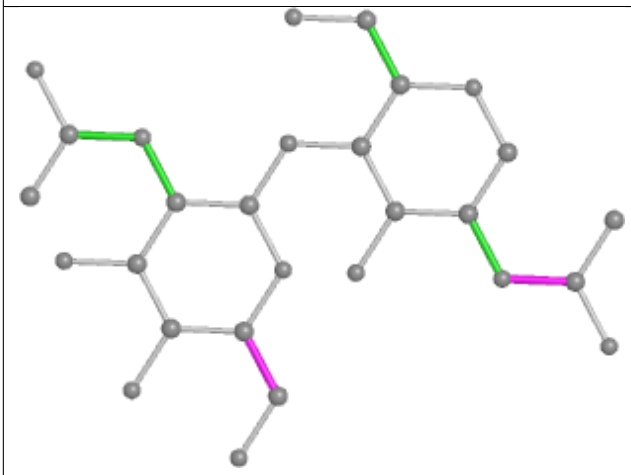
Oligosaccharide Chain S



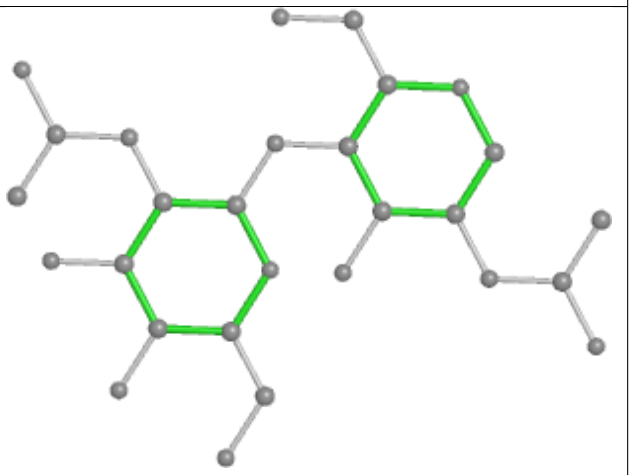
Bond lengths



Bond angles

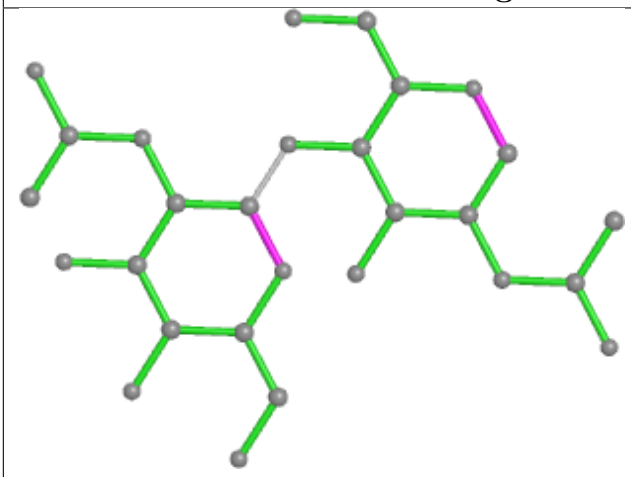


Torsions



Rings

Oligosaccharide Chain T



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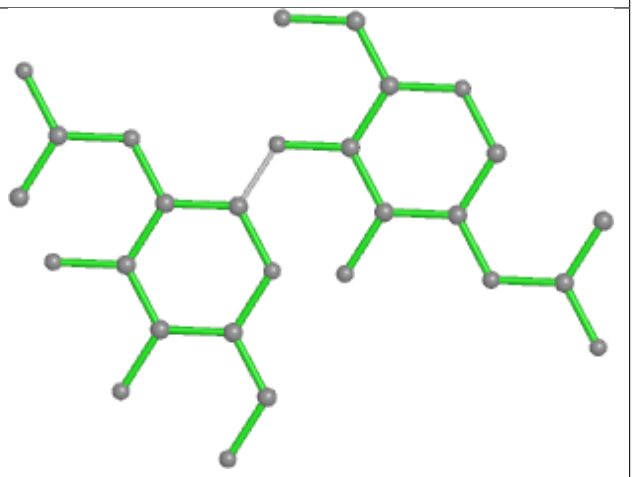

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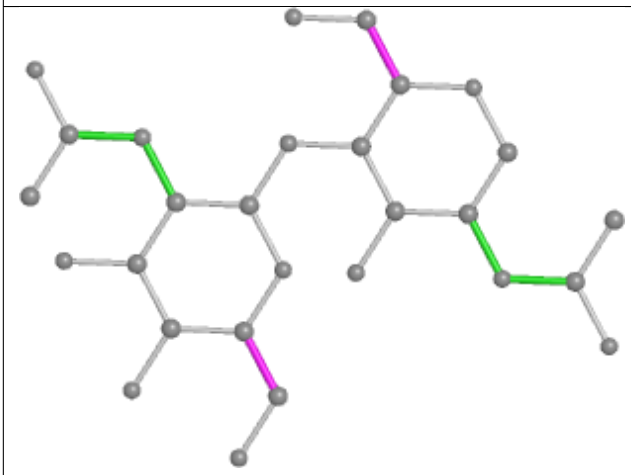

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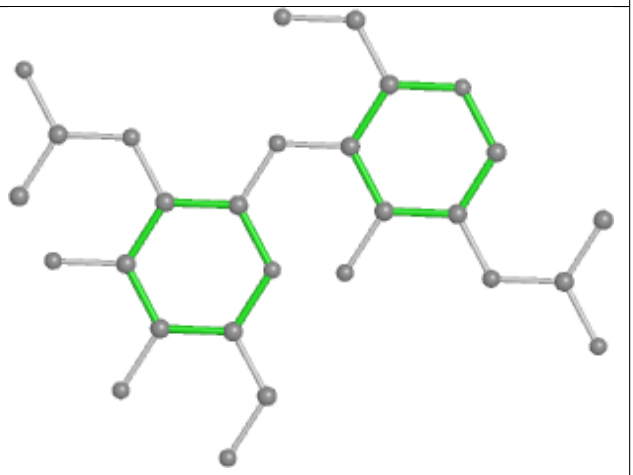
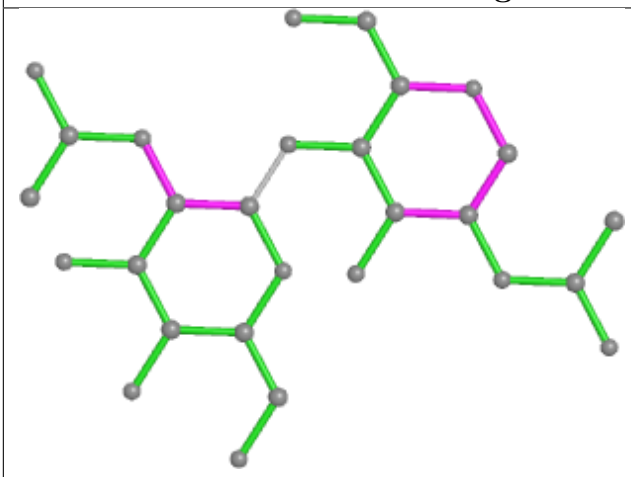


Rings

Oligosaccharide Chain X



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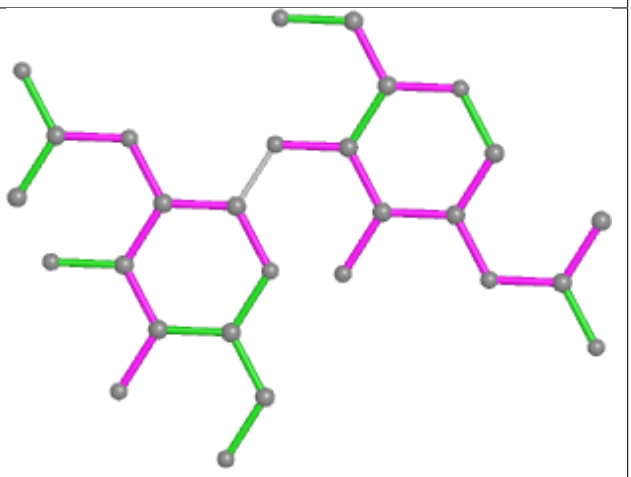

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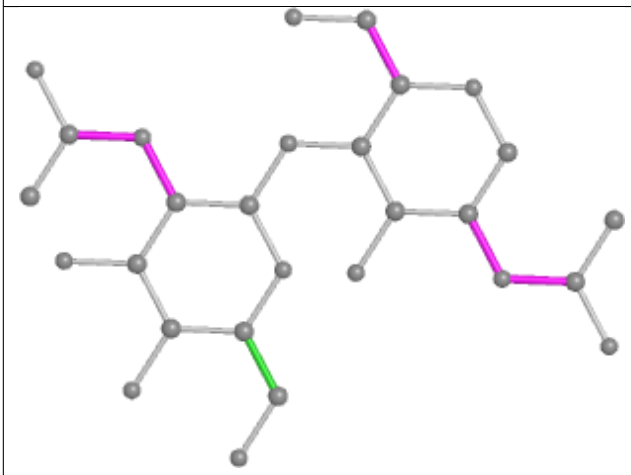
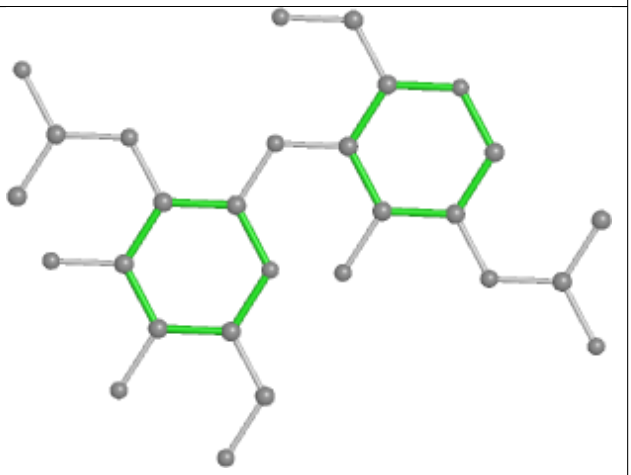
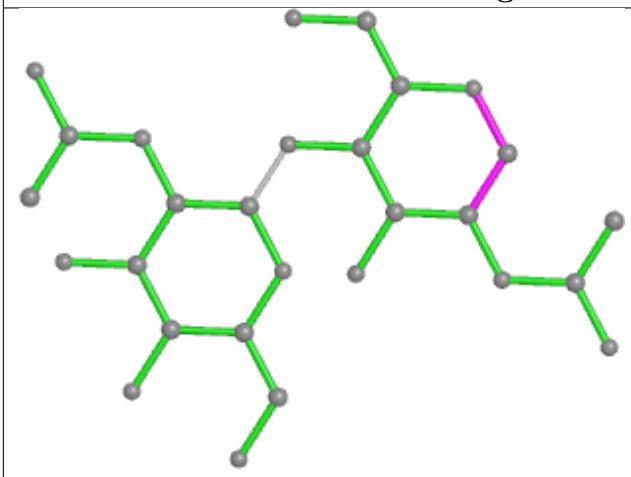


Torsions



Rings

Oligosaccharide Chain Z



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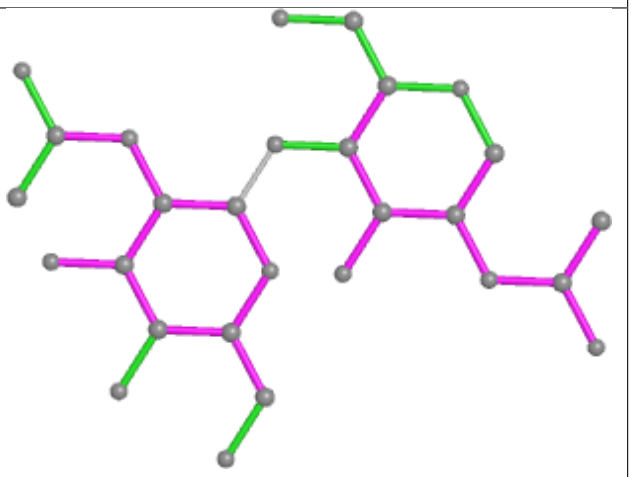
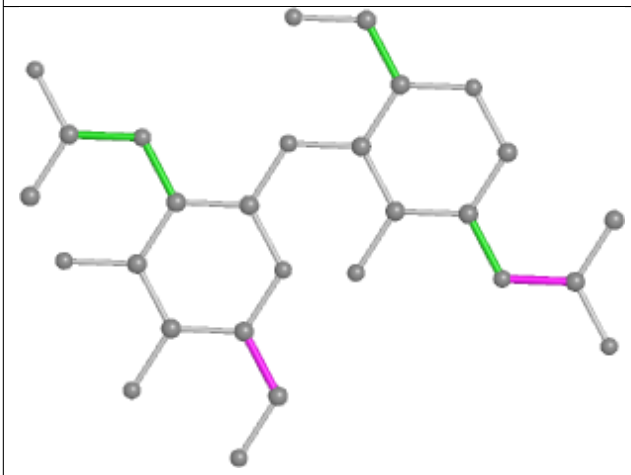
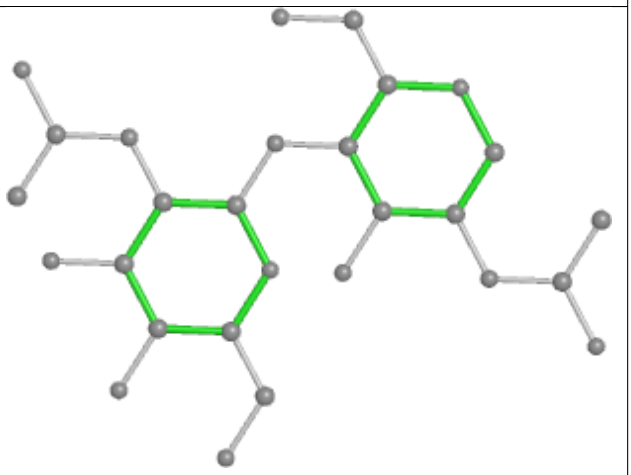


Bond angles

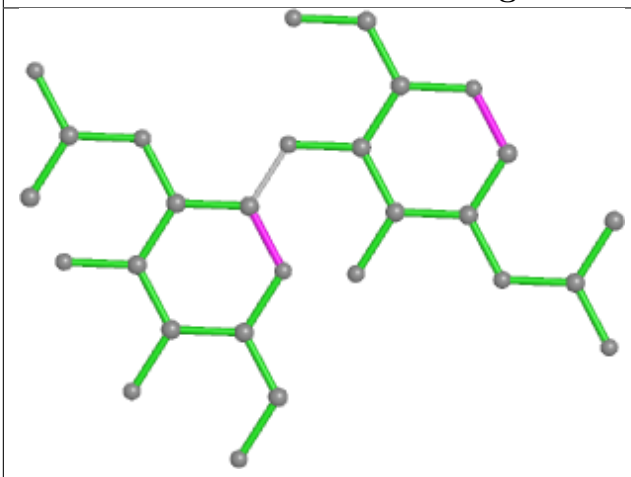


Torsions



Rings

Oligosaccharide Chain a



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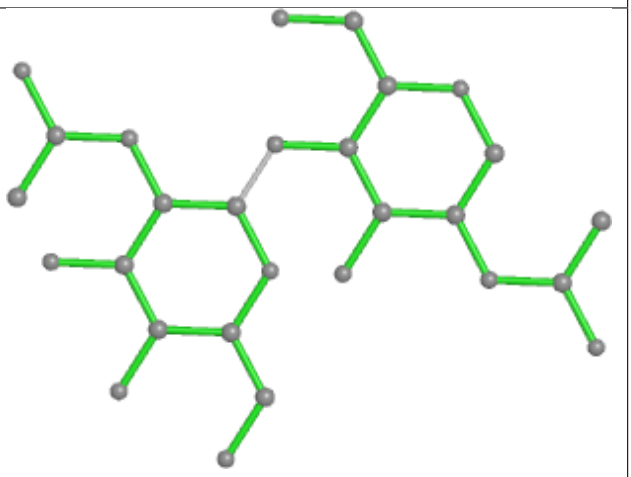

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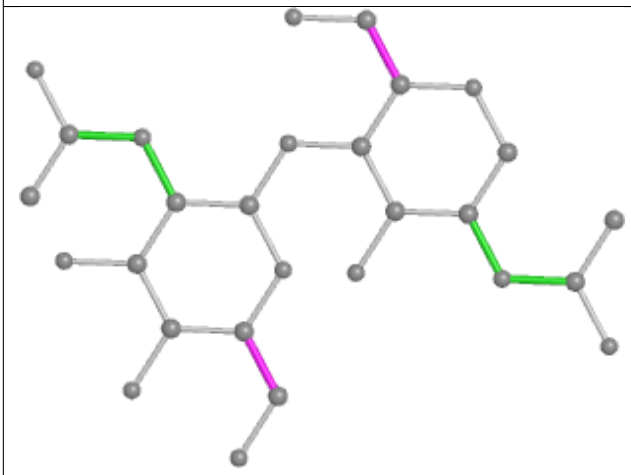

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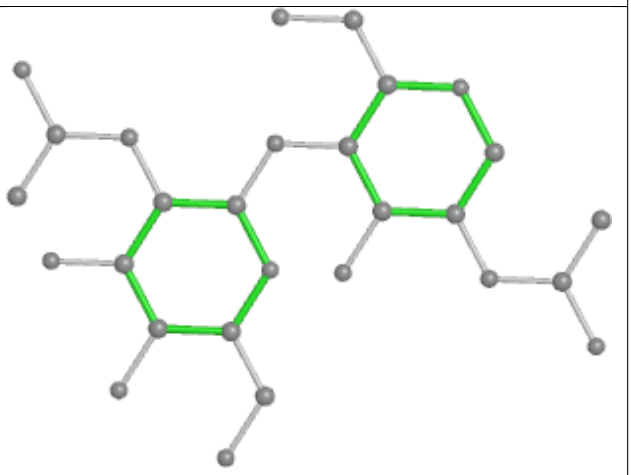
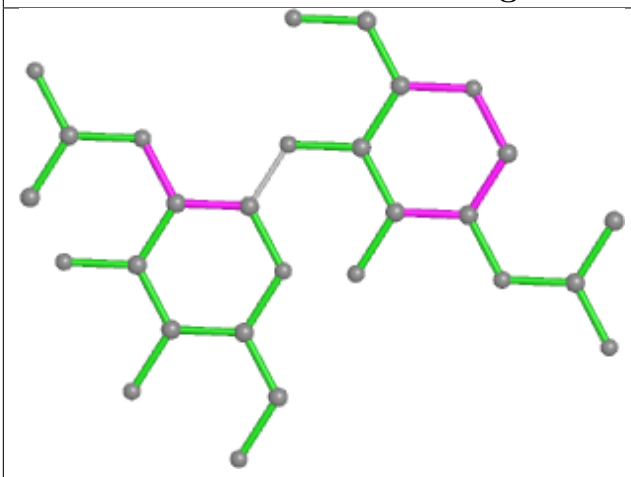


Rings

Oligosaccharide Chain e



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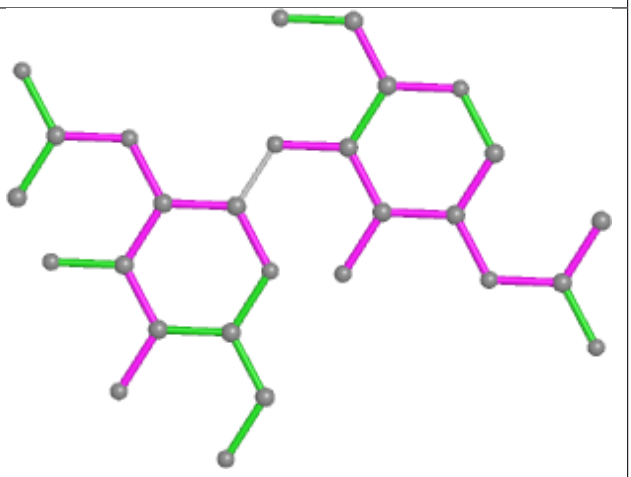

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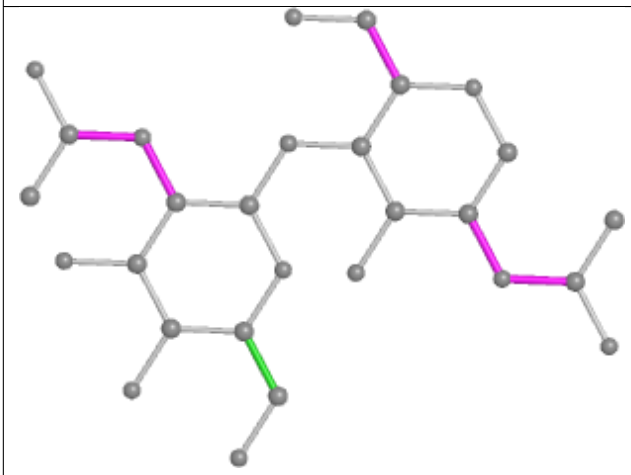

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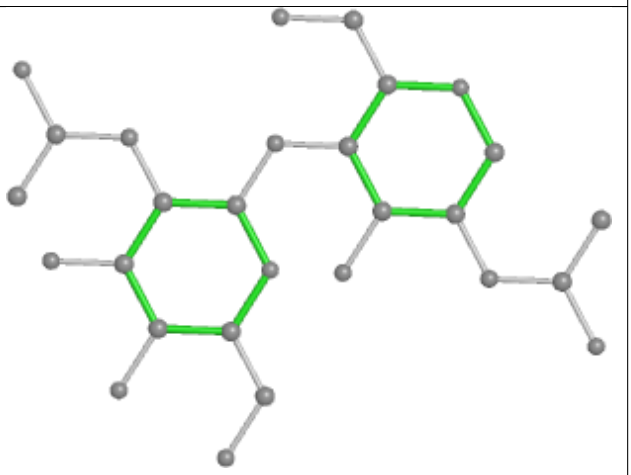
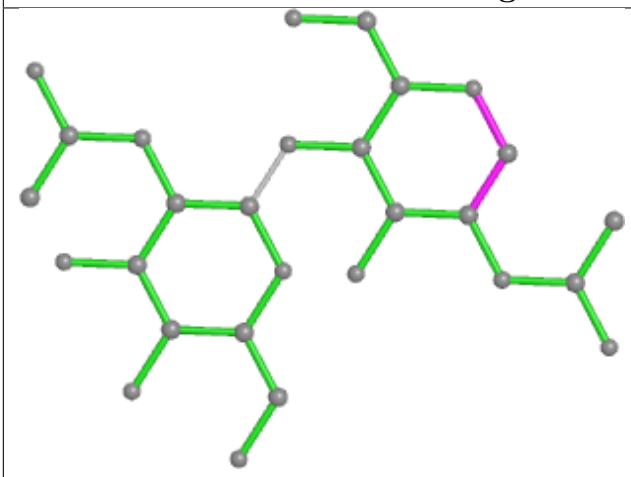


Rings

Oligosaccharide Chain g



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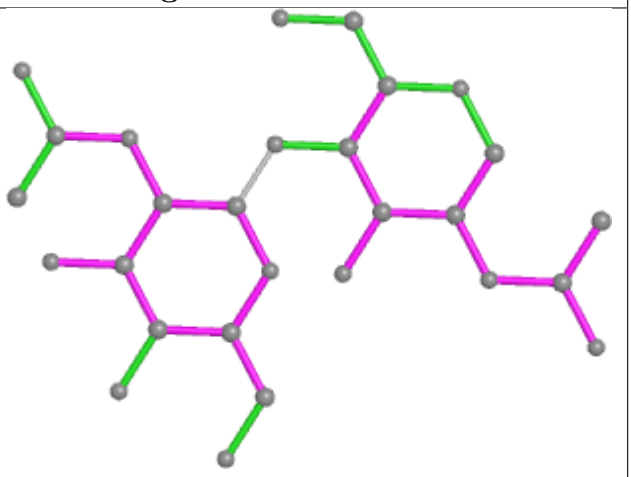
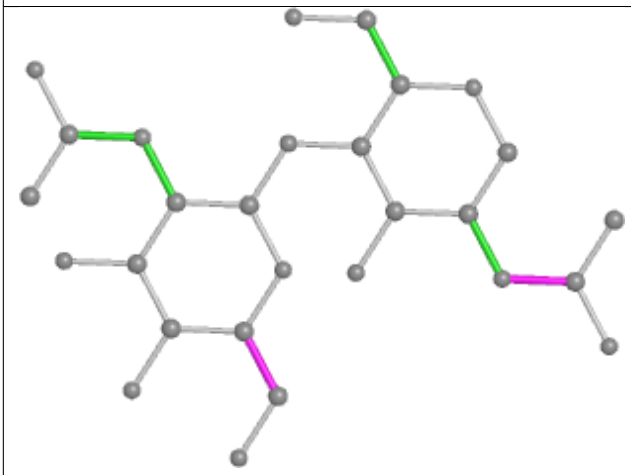


Bond angles



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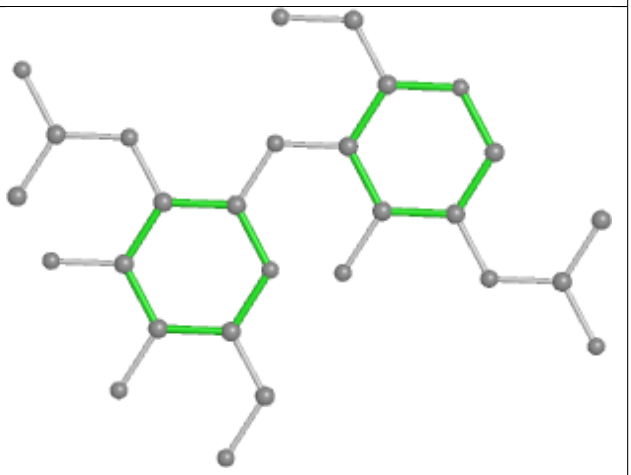
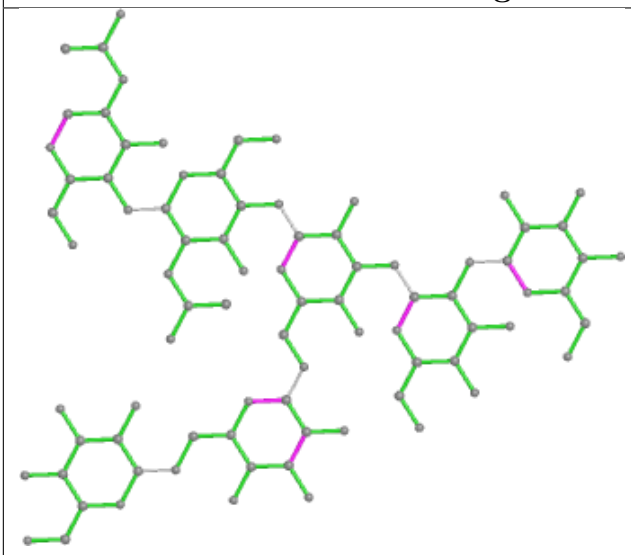


Rings

Oligosaccharide Chain N



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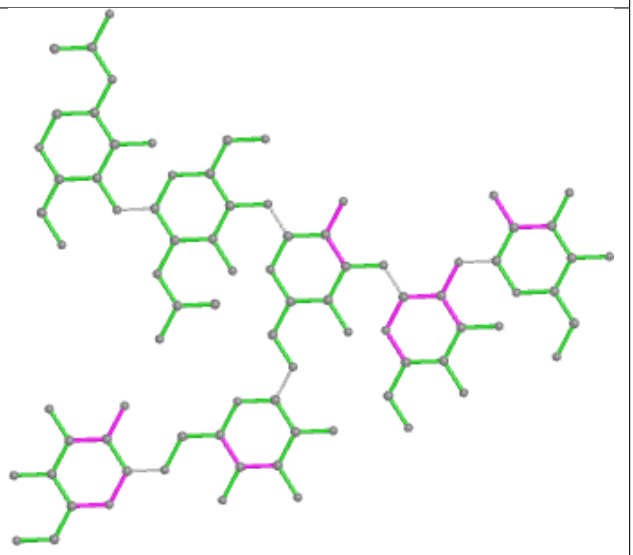

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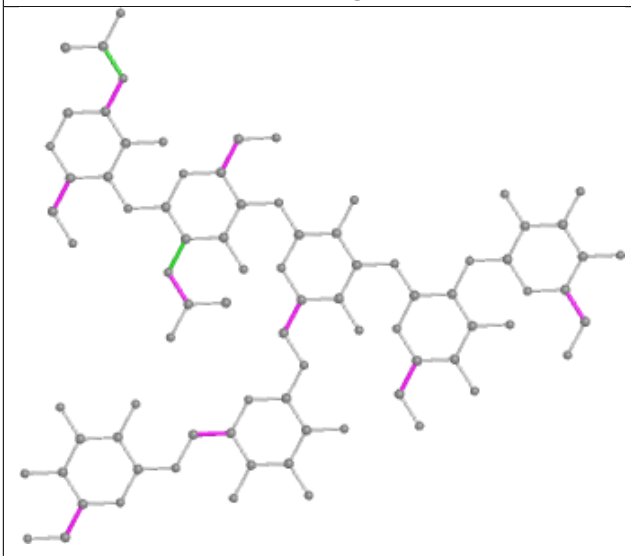

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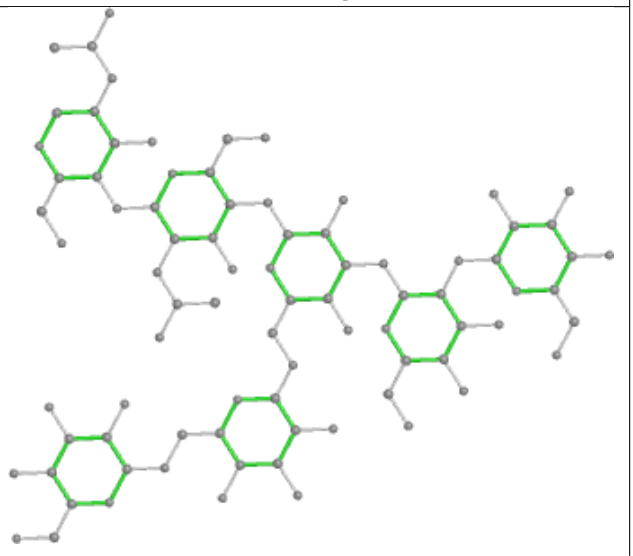
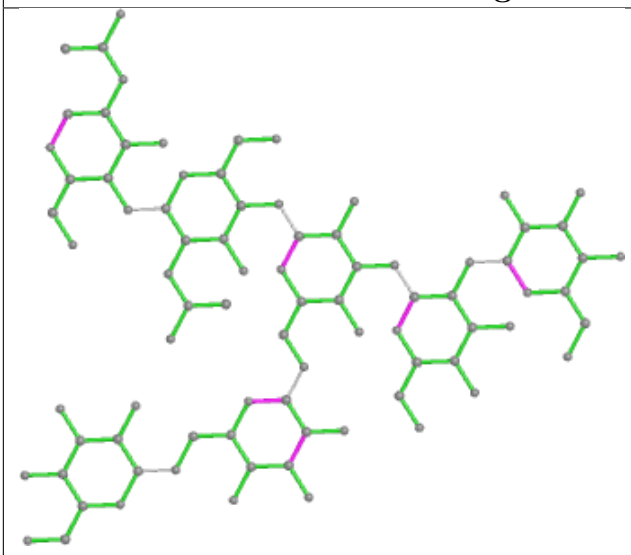


Rings

Oligosaccharide Chain U



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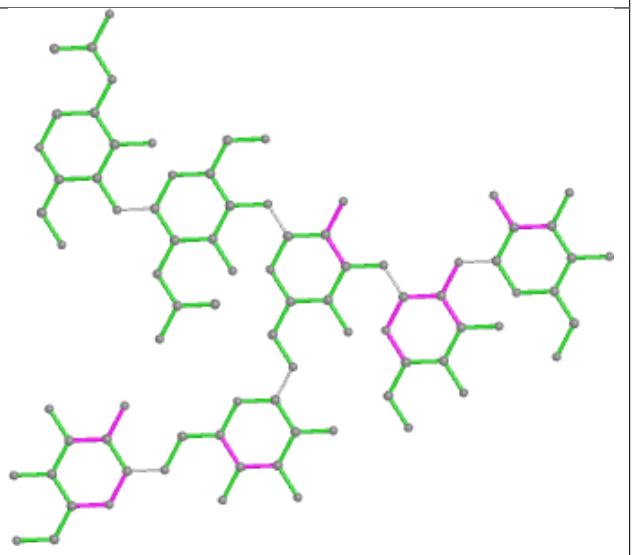
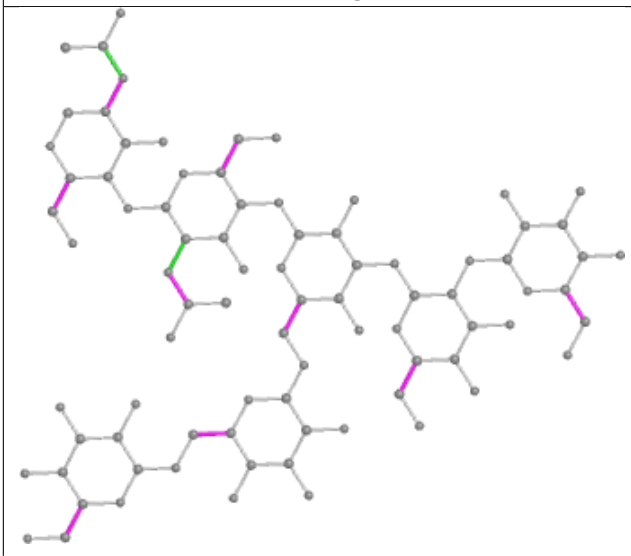


Bond angles



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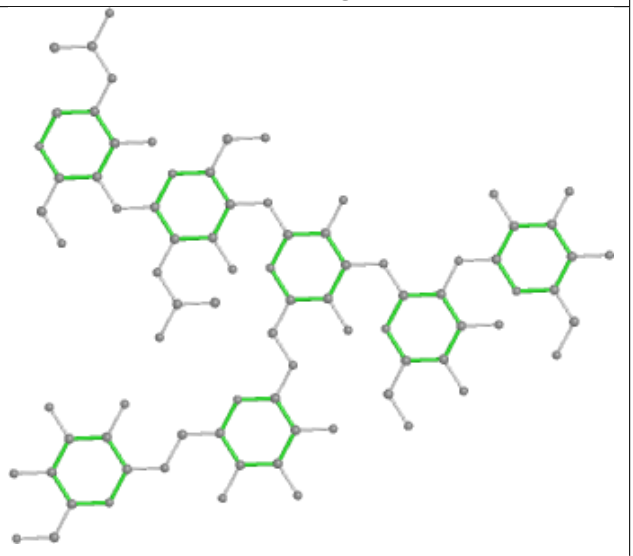
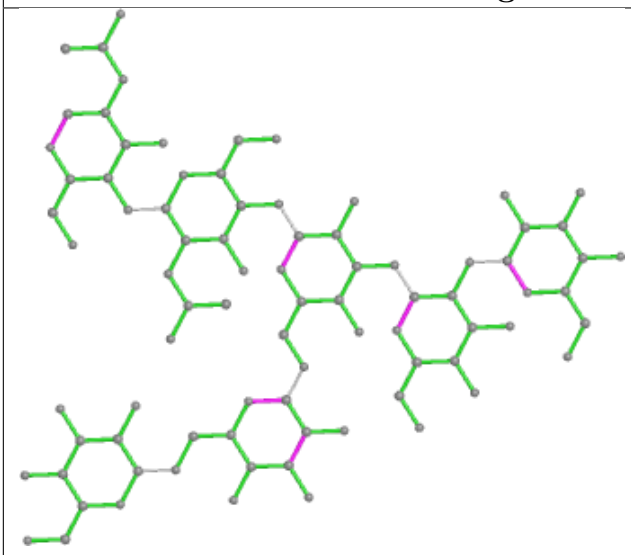


Rings

Oligosaccharide Chain b



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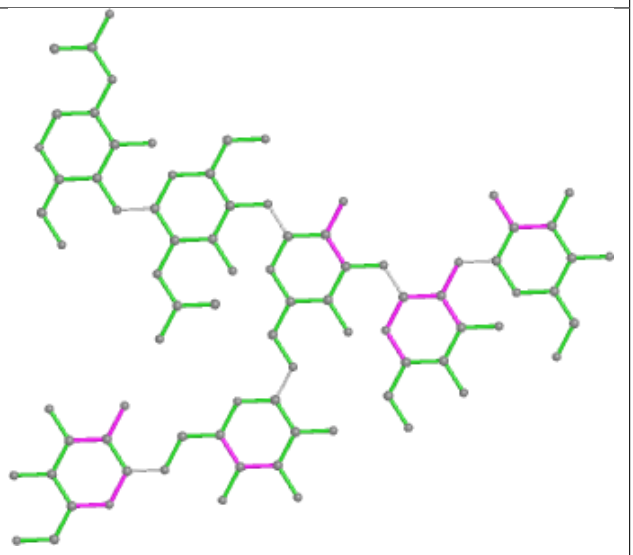
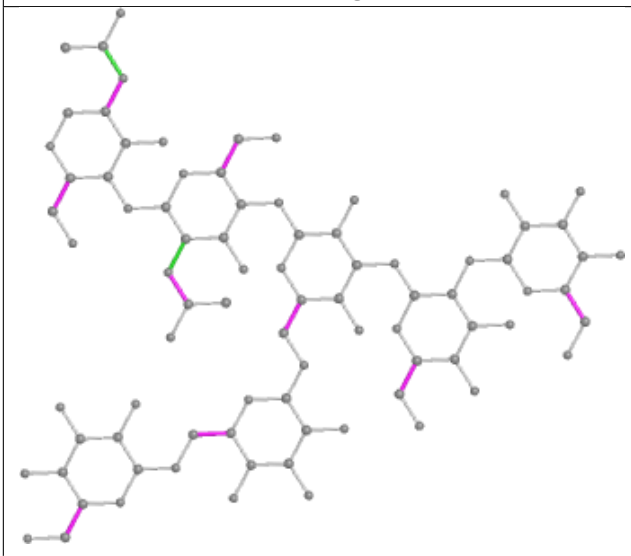


Bond angles



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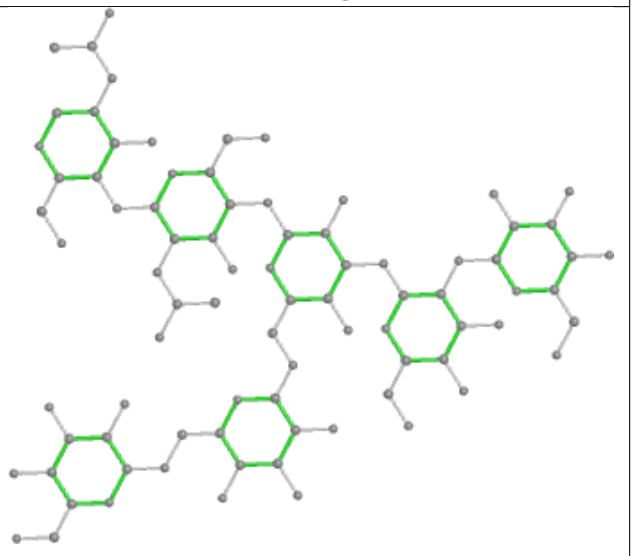
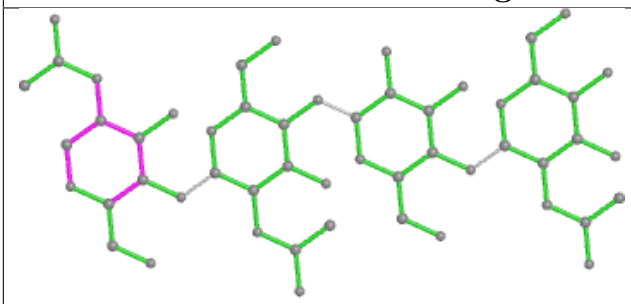
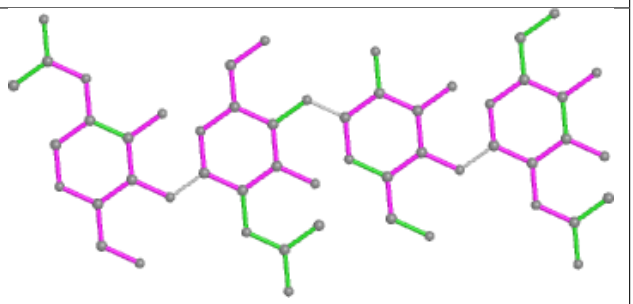
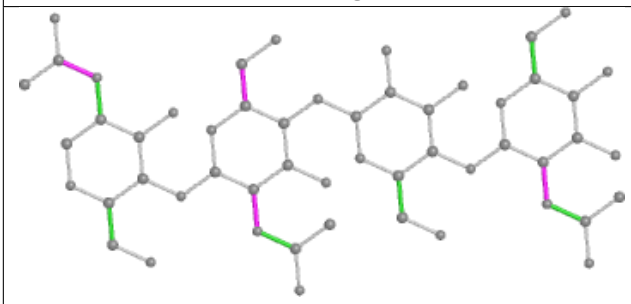
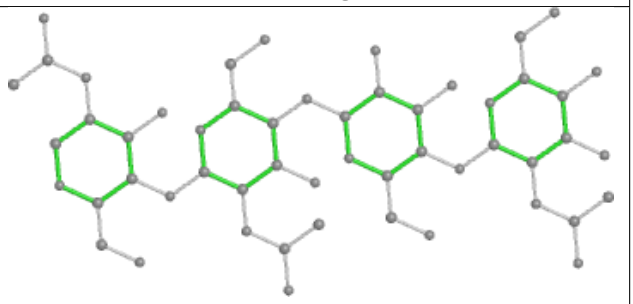
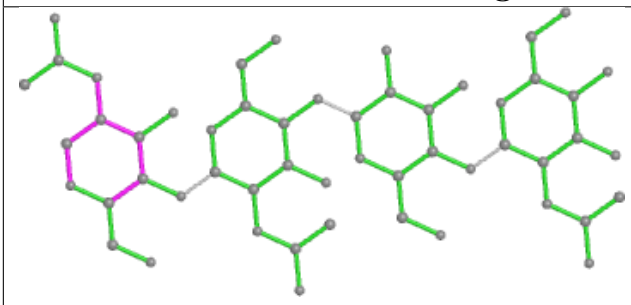
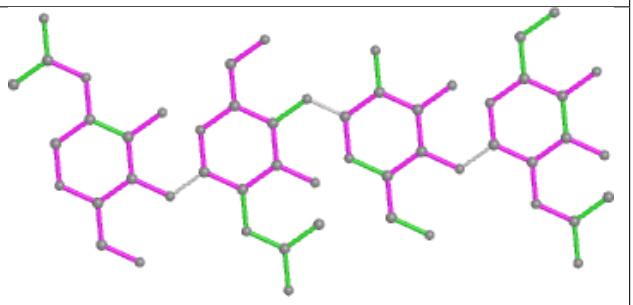
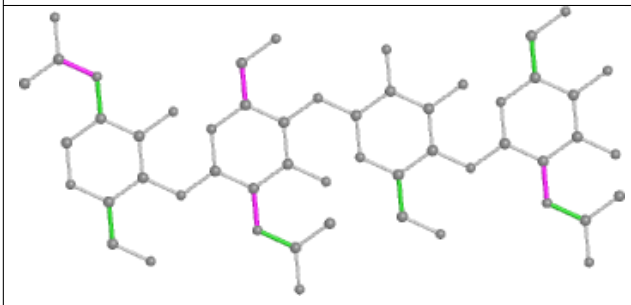
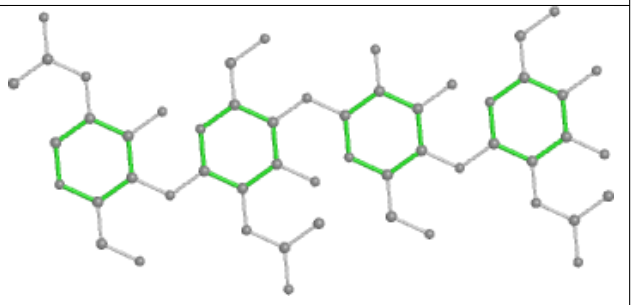
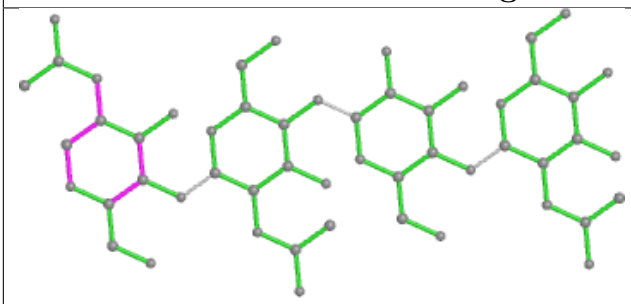


Rings

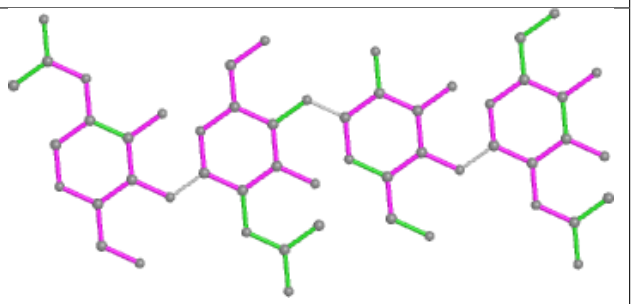
Oligosaccharide Chain O	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain V	
 Bond lengths	 Bond angles
 Torsions	 Rings

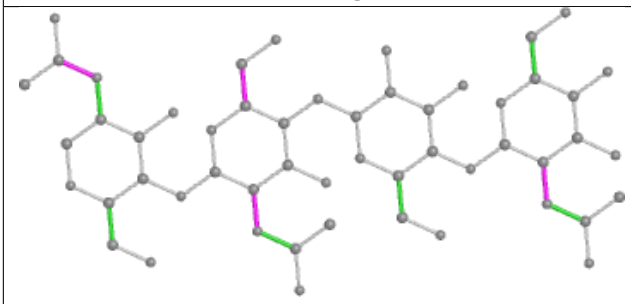
Oligosaccharide Chain c



Bond lengths



Bond angles



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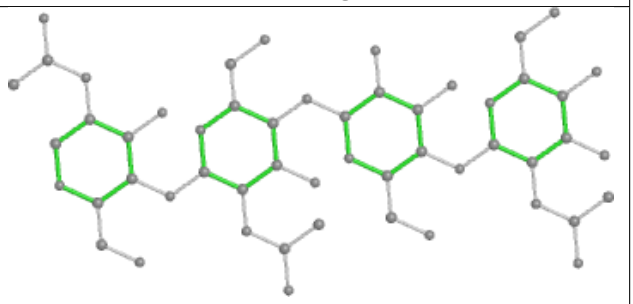
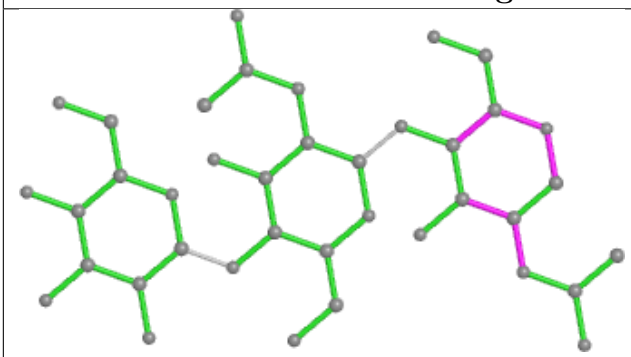
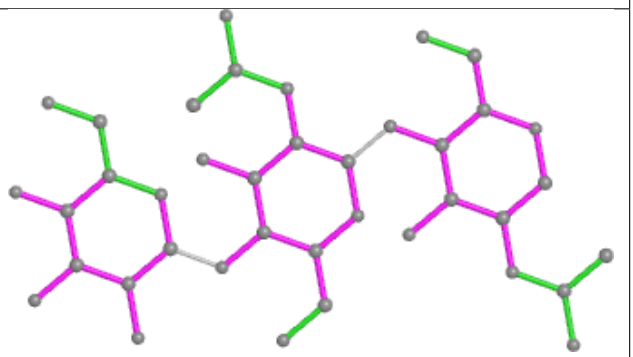


Rings

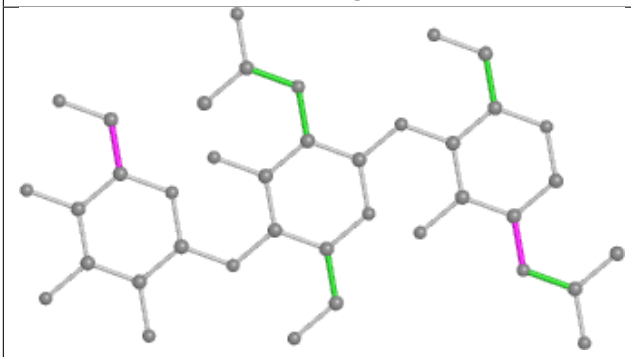
Oligosaccharide Chain P



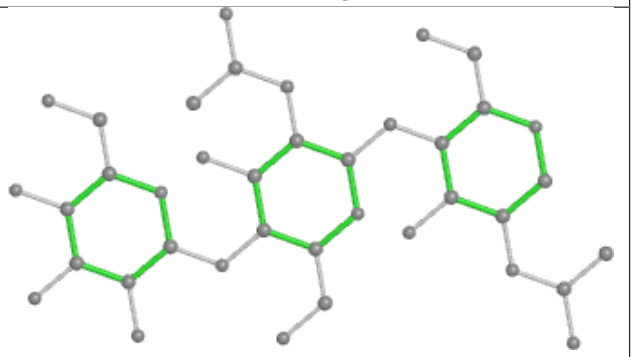
Bond lengths



Bond angles

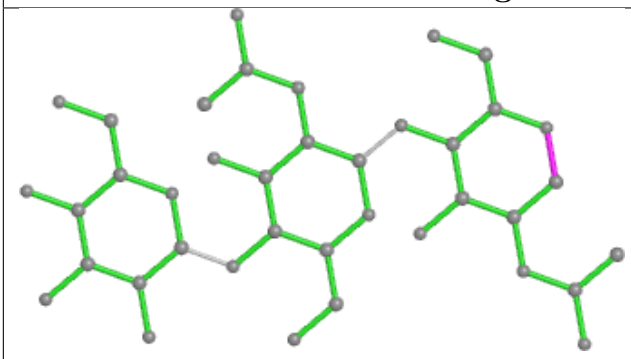


Torsions

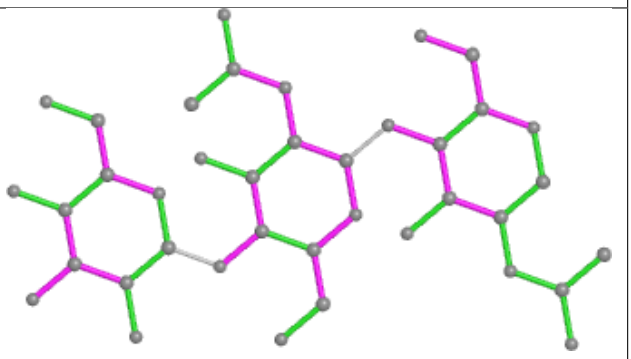


Rings

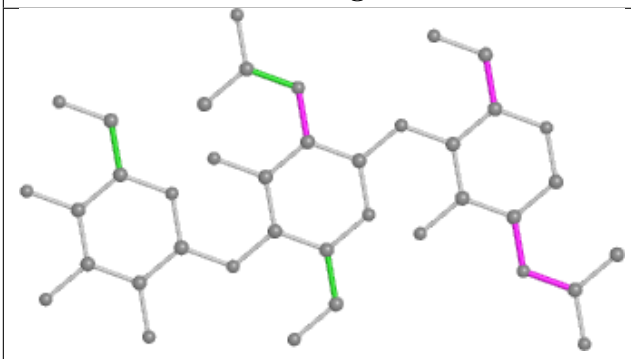
Oligosaccharide Chain R



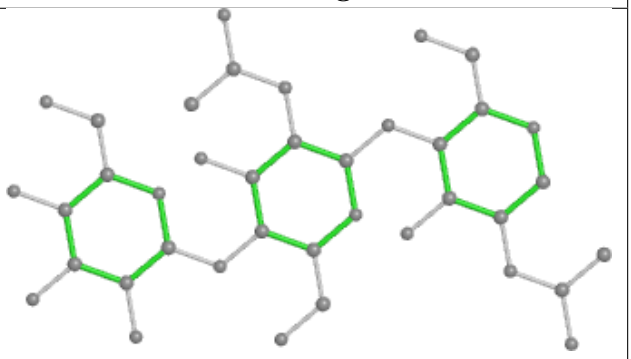
Bond lengths



Bond angles

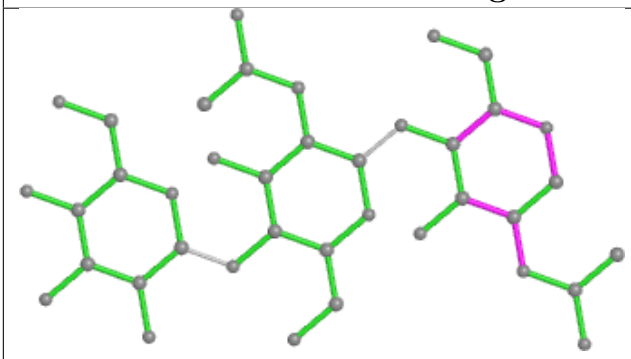


Torsions

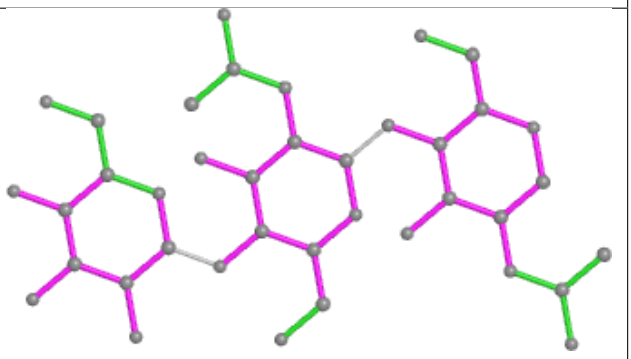


Rings

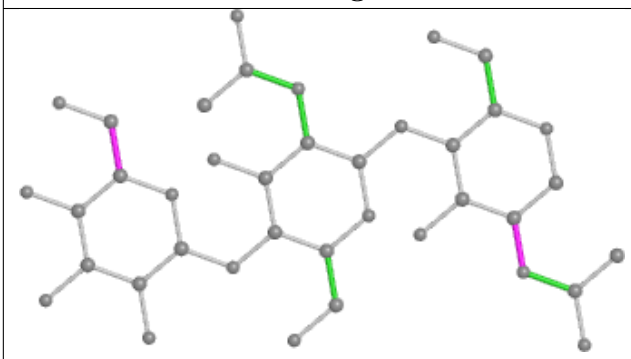
Oligosaccharide Chain W



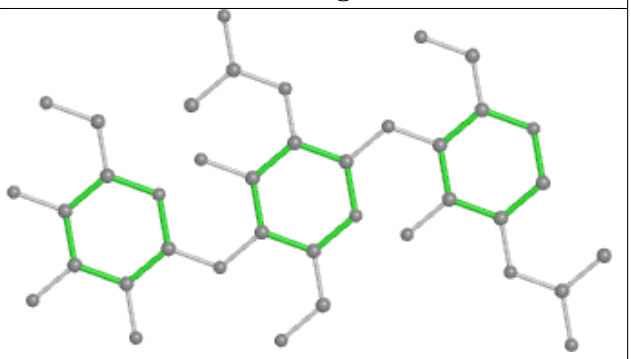
Bond lengths



Bond angles

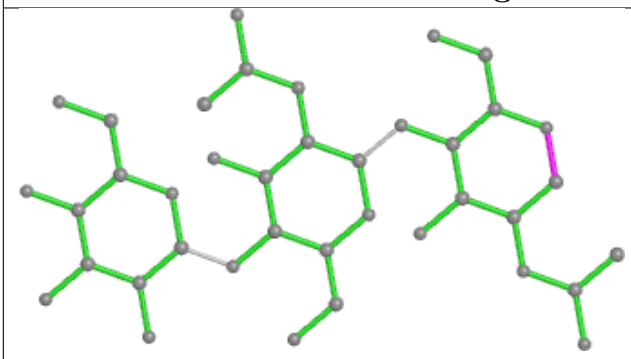


Torsions

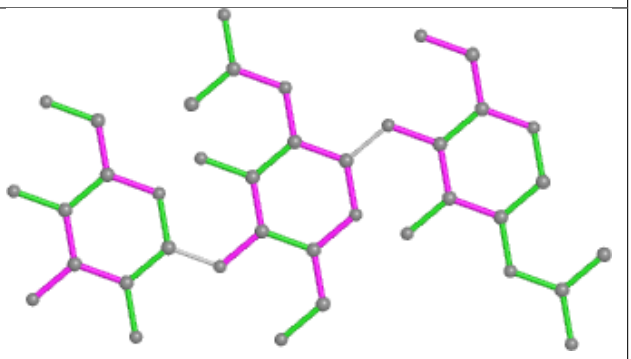


Rings

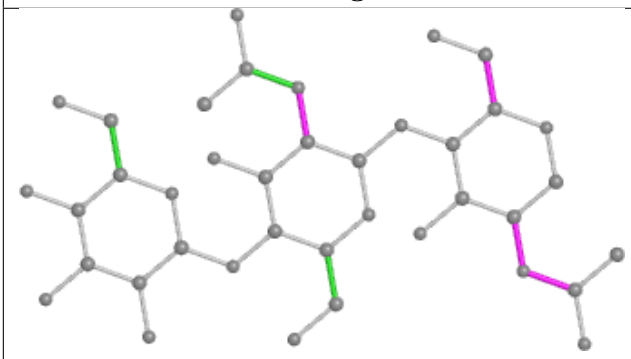
Oligosaccharide Chain Y



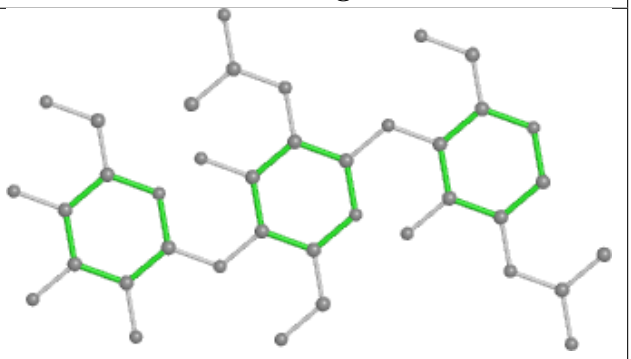
Bond lengths



Bond angles

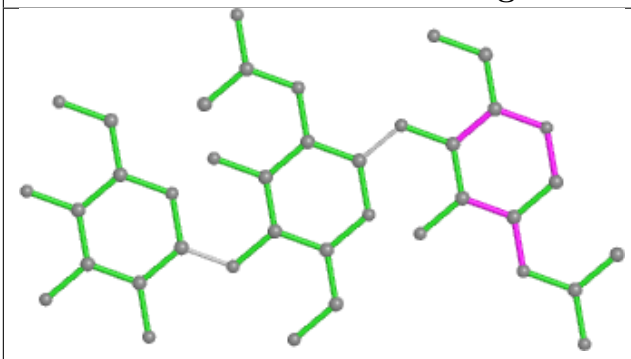


Torsions

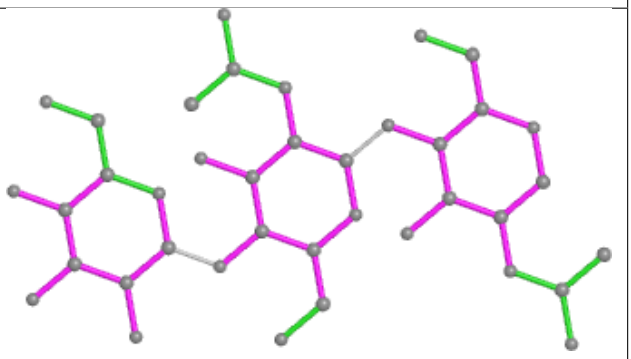


Rings

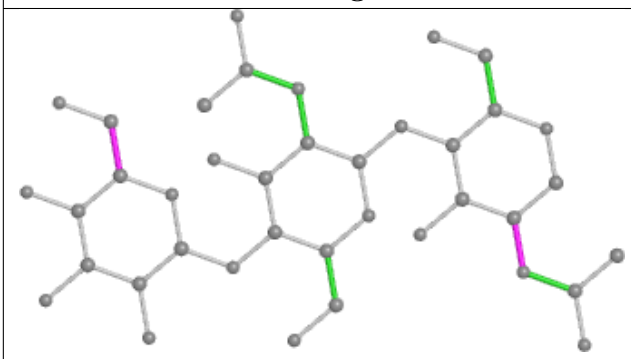
Oligosaccharide Chain d



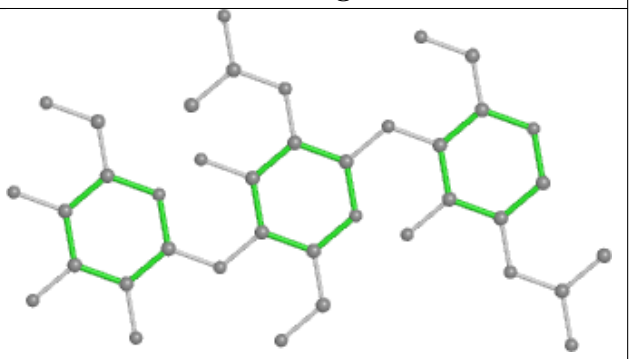
Bond lengths



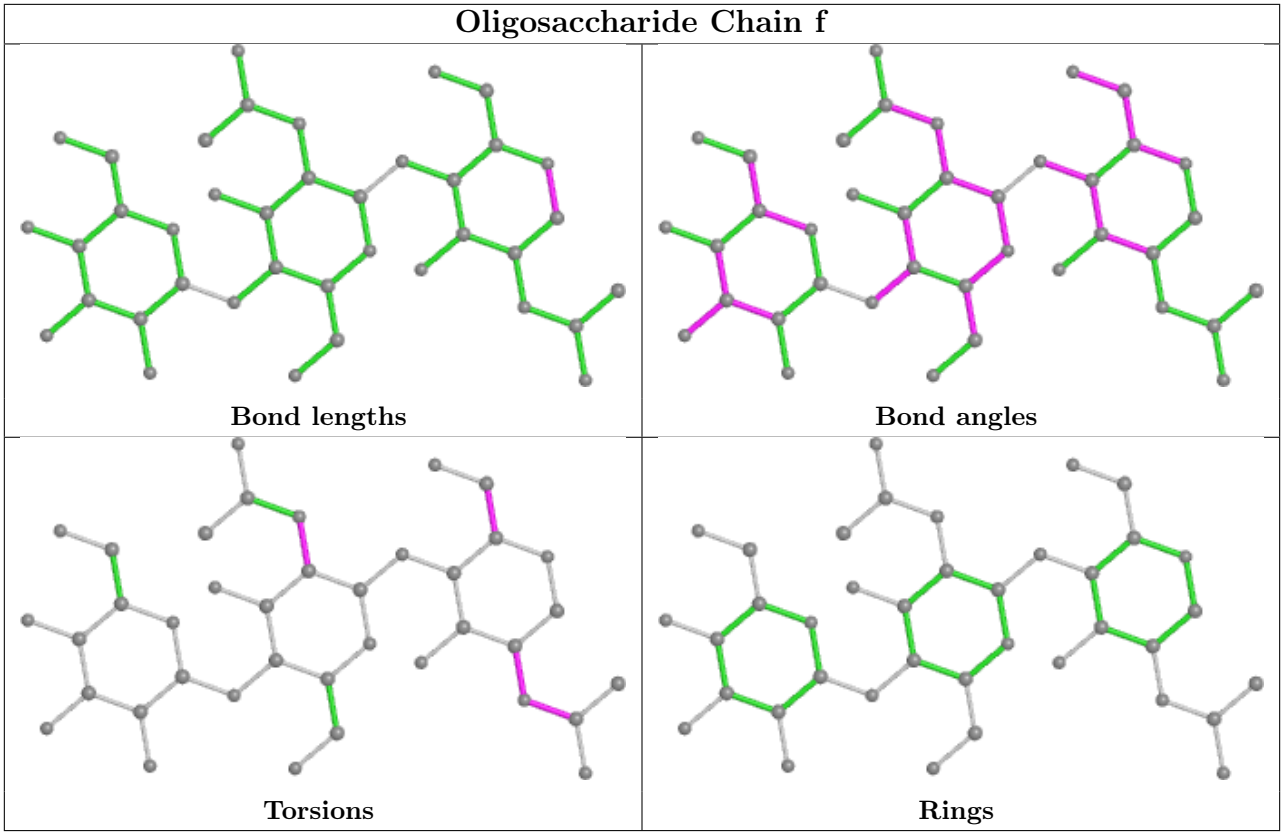
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	E	622	1	14,14,15	1.40	4 (28%)	17,19,21	2.36	7 (41%)
9	NAG	I	632	1	14,14,15	1.09	1 (7%)	17,19,21	2.75	6 (35%)
9	NAG	I	631	1	14,14,15	1.14	1 (7%)	17,19,21	1.78	6 (35%)
9	NAG	E	619	1	14,14,15	1.35	2 (14%)	17,19,21	1.98	6 (35%)
9	NAG	A	630	1	14,14,15	0.89	1 (7%)	17,19,21	2.23	7 (41%)
9	NAG	E	617	1	14,14,15	2.79	9 (64%)	17,19,21	3.09	9 (52%)
9	NAG	A	619	1	14,14,15	1.35	2 (14%)	17,19,21	1.99	6 (35%)
9	NAG	I	626	1	14,14,15	0.83	0	17,19,21	2.48	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	E	631	1	14,14,15	1.13	1 (7%)	17,19,21	1.78	6 (35%)
9	NAG	I	627	1	14,14,15	1.21	2 (14%)	17,19,21	1.78	4 (23%)
9	NAG	I	622	1	14,14,15	1.40	3 (21%)	17,19,21	2.37	7 (41%)
9	NAG	E	632	1	14,14,15	1.08	1 (7%)	17,19,21	2.76	6 (35%)
9	NAG	I	630	1	14,14,15	0.89	1 (7%)	17,19,21	2.23	7 (41%)
9	NAG	A	631	1	14,14,15	1.14	1 (7%)	17,19,21	1.78	6 (35%)
9	NAG	I	618	1	14,14,15	1.57	3 (21%)	17,19,21	2.54	6 (35%)
9	NAG	A	618	1	14,14,15	1.57	3 (21%)	17,19,21	2.54	6 (35%)
9	NAG	E	627	1	14,14,15	1.20	2 (14%)	17,19,21	1.79	5 (29%)
9	NAG	A	627	1	14,14,15	1.20	2 (14%)	17,19,21	1.78	4 (23%)
9	NAG	A	632	1	14,14,15	1.09	1 (7%)	17,19,21	2.75	6 (35%)
9	NAG	E	626	1	14,14,15	0.84	0	17,19,21	2.48	7 (41%)
9	NAG	I	617	1	14,14,15	2.80	9 (64%)	17,19,21	3.08	9 (52%)
9	NAG	A	626	1	14,14,15	0.84	0	17,19,21	2.48	7 (41%)
9	NAG	A	622	1	14,14,15	1.40	3 (21%)	17,19,21	2.37	7 (41%)
9	NAG	I	619	1	14,14,15	1.35	2 (14%)	17,19,21	1.99	6 (35%)
9	NAG	E	630	1	14,14,15	0.89	1 (7%)	17,19,21	2.23	7 (41%)
9	NAG	E	618	1	14,14,15	1.56	3 (21%)	17,19,21	2.54	6 (35%)
9	NAG	A	617	1	14,14,15	2.80	9 (64%)	17,19,21	3.08	9 (52%)

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
9	NAG	E	622	1	-	4/6/23/26	0/1/1/1
9	NAG	I	632	1	-	1/6/23/26	0/1/1/1
9	NAG	I	631	1	-	5/6/23/26	0/1/1/1
9	NAG	E	619	1	-	5/6/23/26	0/1/1/1
9	NAG	A	630	1	-	4/6/23/26	0/1/1/1
9	NAG	E	617	1	-	5/6/23/26	0/1/1/1
9	NAG	A	619	1	-	5/6/23/26	0/1/1/1
9	NAG	I	626	1	-	4/6/23/26	0/1/1/1
9	NAG	E	631	1	-	5/6/23/26	0/1/1/1
9	NAG	I	627	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	I	622	1	-	4/6/23/26	0/1/1/1
9	NAG	E	632	1	-	1/6/23/26	0/1/1/1
9	NAG	I	630	1	-	4/6/23/26	0/1/1/1
9	NAG	A	631	1	-	5/6/23/26	0/1/1/1
9	NAG	I	618	1	-	3/6/23/26	0/1/1/1
9	NAG	A	618	1	-	3/6/23/26	0/1/1/1
9	NAG	E	627	1	-	3/6/23/26	0/1/1/1
9	NAG	A	627	1	-	3/6/23/26	0/1/1/1
9	NAG	A	632	1	-	1/6/23/26	0/1/1/1
9	NAG	E	626	1	-	4/6/23/26	0/1/1/1
9	NAG	I	617	1	-	5/6/23/26	0/1/1/1
9	NAG	A	626	1	-	4/6/23/26	0/1/1/1
9	NAG	A	622	1	-	4/6/23/26	0/1/1/1
9	NAG	I	619	1	-	5/6/23/26	0/1/1/1
9	NAG	E	630	1	-	4/6/23/26	0/1/1/1
9	NAG	E	618	1	-	3/6/23/26	0/1/1/1
9	NAG	A	617	1	-	5/6/23/26	0/1/1/1

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	617	NAG	O5-C1	-4.66	1.36	1.43
9	I	617	NAG	O5-C1	-4.66	1.36	1.43
9	A	617	NAG	O5-C1	-4.65	1.36	1.43
9	A	617	NAG	O5-C5	-3.82	1.35	1.43
9	E	617	NAG	O5-C5	-3.81	1.35	1.43
9	I	617	NAG	O5-C5	-3.81	1.35	1.43
9	E	617	NAG	C3-C2	-3.75	1.44	1.52
9	I	617	NAG	C3-C2	-3.74	1.44	1.52
9	A	617	NAG	C3-C2	-3.71	1.44	1.52
9	I	617	NAG	C1-C2	-3.65	1.46	1.52
9	A	617	NAG	C1-C2	-3.65	1.46	1.52
9	E	617	NAG	C1-C2	-3.64	1.46	1.52
9	E	617	NAG	C4-C5	-3.22	1.46	1.53
9	A	617	NAG	C4-C5	-3.22	1.46	1.53
9	I	617	NAG	C4-C5	-3.22	1.46	1.53
9	A	618	NAG	O5-C1	-2.97	1.39	1.43
9	I	618	NAG	O5-C1	-2.94	1.39	1.43
9	E	618	NAG	O5-C1	-2.94	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	617	NAG	C2-N2	-2.93	1.41	1.46
9	I	617	NAG	C2-N2	-2.93	1.41	1.46
9	E	617	NAG	C2-N2	-2.88	1.41	1.46
9	I	632	NAG	C2-N2	-2.76	1.41	1.46
9	A	632	NAG	C2-N2	-2.74	1.41	1.46
9	E	632	NAG	C2-N2	-2.73	1.41	1.46
9	I	618	NAG	C4-C5	-2.64	1.47	1.53
9	A	618	NAG	C4-C5	-2.64	1.47	1.53
9	E	618	NAG	C4-C5	-2.63	1.47	1.53
9	A	617	NAG	C4-C3	-2.55	1.45	1.52
9	I	617	NAG	C4-C3	-2.53	1.45	1.52
9	I	618	NAG	O5-C5	-2.53	1.38	1.43
9	E	617	NAG	C4-C3	-2.52	1.45	1.52
9	A	627	NAG	O5-C1	-2.51	1.39	1.43
9	E	627	NAG	O5-C1	-2.49	1.39	1.43
9	I	627	NAG	O5-C1	-2.49	1.39	1.43
9	A	618	NAG	O5-C5	-2.49	1.38	1.43
9	E	618	NAG	O5-C5	-2.49	1.38	1.43
9	A	622	NAG	O5-C1	-2.48	1.39	1.43
9	I	622	NAG	O5-C1	-2.48	1.39	1.43
9	E	622	NAG	O5-C1	-2.47	1.39	1.43
9	I	622	NAG	C1-C2	-2.41	1.48	1.52
9	A	617	NAG	O4-C4	-2.41	1.37	1.43
9	E	617	NAG	O4-C4	-2.41	1.37	1.43
9	A	622	NAG	C1-C2	-2.41	1.48	1.52
9	E	622	NAG	C1-C2	-2.41	1.48	1.52
9	I	617	NAG	O4-C4	-2.41	1.37	1.43
9	I	617	NAG	O7-C7	-2.34	1.17	1.23
9	E	617	NAG	O7-C7	-2.33	1.18	1.23
9	A	617	NAG	O7-C7	-2.33	1.18	1.23
9	A	619	NAG	O5-C1	-2.17	1.40	1.43
9	E	619	NAG	O5-C1	-2.16	1.40	1.43
9	I	619	NAG	O5-C1	-2.16	1.40	1.43
9	E	630	NAG	C2-N2	-2.15	1.42	1.46
9	A	630	NAG	C2-N2	-2.15	1.42	1.46
9	I	630	NAG	C2-N2	-2.15	1.42	1.46
9	E	631	NAG	C4-C5	-2.14	1.48	1.53
9	I	631	NAG	C4-C5	-2.13	1.48	1.53
9	A	631	NAG	C4-C5	-2.13	1.48	1.53
9	I	627	NAG	C4-C5	-2.11	1.48	1.53
9	I	622	NAG	C4-C5	-2.07	1.48	1.53
9	A	627	NAG	C4-C5	-2.06	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	622	NAG	C4-C5	-2.06	1.48	1.53
9	E	627	NAG	C4-C5	-2.05	1.48	1.53
9	E	622	NAG	C4-C5	-2.04	1.48	1.53
9	I	619	NAG	C4-C5	-2.04	1.48	1.53
9	E	619	NAG	C4-C5	-2.04	1.48	1.53
9	A	619	NAG	C4-C5	-2.04	1.48	1.53
9	E	622	NAG	O5-C5	-2.01	1.39	1.43

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	632	NAG	O5-C5-C6	6.18	116.89	107.20
9	A	632	NAG	O5-C5-C6	6.16	116.87	107.20
9	I	632	NAG	O5-C1-C2	-6.16	101.57	111.29
9	A	632	NAG	O5-C1-C2	-6.15	101.58	111.29
9	E	632	NAG	O5-C1-C2	-6.15	101.58	111.29
9	I	632	NAG	O5-C5-C6	6.15	116.84	107.20
9	I	617	NAG	O4-C4-C5	-5.60	95.38	109.30
9	E	617	NAG	O4-C4-C5	-5.60	95.39	109.30
9	A	617	NAG	O4-C4-C5	-5.60	95.39	109.30
9	E	630	NAG	C2-N2-C7	-5.50	115.08	122.90
9	A	630	NAG	C2-N2-C7	-5.49	115.08	122.90
9	I	630	NAG	C2-N2-C7	-5.49	115.09	122.90
9	E	617	NAG	C3-C4-C5	-5.42	100.57	110.24
9	A	617	NAG	C3-C4-C5	-5.42	100.57	110.24
9	I	617	NAG	C3-C4-C5	-5.41	100.58	110.24
9	E	626	NAG	O5-C5-C6	5.37	115.63	107.20
9	I	626	NAG	O5-C5-C6	5.37	115.63	107.20
9	A	626	NAG	O5-C5-C6	5.37	115.63	107.20
9	A	622	NAG	O5-C5-C6	5.10	115.19	107.20
9	I	622	NAG	O5-C5-C6	5.10	115.19	107.20
9	E	622	NAG	O5-C5-C6	5.09	115.18	107.20
9	I	626	NAG	C1-C2-N2	4.94	118.93	110.49
9	A	626	NAG	C1-C2-N2	4.93	118.91	110.49
9	E	626	NAG	C1-C2-N2	4.91	118.88	110.49
9	E	617	NAG	C1-C2-N2	-4.85	102.20	110.49
9	I	617	NAG	C1-C2-N2	-4.85	102.20	110.49
9	A	617	NAG	C1-C2-N2	-4.84	102.22	110.49
9	E	618	NAG	C1-O5-C5	4.71	118.57	112.19
9	A	618	NAG	C1-O5-C5	4.69	118.55	112.19
9	I	618	NAG	C1-O5-C5	4.68	118.53	112.19
9	E	618	NAG	O5-C1-C2	-4.66	103.94	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	618	NAG	O5-C1-C2	-4.65	103.94	111.29
9	I	618	NAG	O5-C1-C2	-4.65	103.95	111.29
9	I	617	NAG	O5-C5-C6	4.47	114.21	107.20
9	A	617	NAG	O5-C5-C6	4.46	114.20	107.20
9	E	617	NAG	O5-C5-C6	4.46	114.20	107.20
9	I	622	NAG	C2-N2-C7	-4.31	116.77	122.90
9	A	622	NAG	C2-N2-C7	-4.29	116.80	122.90
9	E	618	NAG	O5-C5-C6	-4.28	100.49	107.20
9	E	622	NAG	C2-N2-C7	-4.28	116.80	122.90
9	I	618	NAG	O5-C5-C6	-4.27	100.50	107.20
9	A	618	NAG	O5-C5-C6	-4.27	100.51	107.20
9	A	617	NAG	O4-C4-C3	-4.17	100.71	110.35
9	E	617	NAG	O4-C4-C3	-4.16	100.72	110.35
9	I	617	NAG	O4-C4-C3	-4.16	100.73	110.35
9	I	618	NAG	C6-C5-C4	-4.01	103.62	113.00
9	A	618	NAG	C6-C5-C4	-4.00	103.63	113.00
9	E	618	NAG	C6-C5-C4	-3.99	103.65	113.00
9	E	626	NAG	O5-C1-C2	-3.85	105.21	111.29
9	A	626	NAG	O5-C1-C2	-3.83	105.24	111.29
9	I	626	NAG	O5-C1-C2	-3.83	105.24	111.29
9	E	618	NAG	O4-C4-C5	-3.79	99.88	109.30
9	A	618	NAG	O4-C4-C5	-3.79	99.88	109.30
9	I	618	NAG	O4-C4-C5	-3.79	99.90	109.30
9	I	619	NAG	O5-C5-C6	3.76	113.10	107.20
9	A	619	NAG	O5-C5-C6	3.75	113.08	107.20
9	E	619	NAG	O5-C5-C6	3.75	113.08	107.20
9	A	627	NAG	O3-C3-C4	-3.65	101.91	110.35
9	E	627	NAG	O3-C3-C4	-3.65	101.91	110.35
9	I	627	NAG	O3-C3-C4	-3.64	101.93	110.35
9	I	622	NAG	C1-C2-N2	-3.55	104.43	110.49
9	A	622	NAG	C1-C2-N2	-3.54	104.44	110.49
9	E	622	NAG	C1-C2-N2	-3.51	104.49	110.49
9	E	632	NAG	C2-N2-C7	-3.48	117.94	122.90
9	A	632	NAG	C2-N2-C7	-3.48	117.95	122.90
9	I	632	NAG	C2-N2-C7	-3.46	117.98	122.90
9	A	631	NAG	O5-C5-C6	3.37	112.48	107.20
9	E	631	NAG	O5-C5-C6	3.36	112.48	107.20
9	E	627	NAG	C6-C5-C4	-3.36	105.13	113.00
9	A	627	NAG	C6-C5-C4	-3.36	105.14	113.00
9	I	631	NAG	O5-C5-C6	3.36	112.47	107.20
9	A	626	NAG	C6-C5-C4	-3.36	105.14	113.00
9	I	626	NAG	C6-C5-C4	-3.36	105.14	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	E	626	NAG	C6-C5-C4	-3.36	105.14	113.00
9	I	627	NAG	C6-C5-C4	-3.35	105.16	113.00
9	E	626	NAG	C4-C3-C2	-3.26	106.24	111.02
9	A	626	NAG	C4-C3-C2	-3.25	106.25	111.02
9	E	619	NAG	O3-C3-C2	-3.25	102.74	109.47
9	I	619	NAG	O3-C3-C2	-3.25	102.74	109.47
9	A	619	NAG	O3-C3-C2	-3.24	102.76	109.47
9	I	626	NAG	C4-C3-C2	-3.24	106.27	111.02
9	I	619	NAG	C6-C5-C4	-3.23	105.44	113.00
9	E	619	NAG	C6-C5-C4	-3.23	105.44	113.00
9	A	619	NAG	C6-C5-C4	-3.23	105.44	113.00
9	I	617	NAG	O7-C7-N2	-3.22	116.03	121.95
9	E	617	NAG	O7-C7-N2	-3.21	116.05	121.95
9	A	617	NAG	O7-C7-N2	-3.21	116.05	121.95
9	E	632	NAG	C6-C5-C4	-3.20	105.52	113.00
9	A	632	NAG	C6-C5-C4	-3.18	105.55	113.00
9	I	632	NAG	C6-C5-C4	-3.18	105.56	113.00
9	A	630	NAG	C4-C3-C2	-3.11	106.45	111.02
9	I	630	NAG	C4-C3-C2	-3.11	106.47	111.02
9	I	632	NAG	C1-O5-C5	3.10	116.39	112.19
9	E	630	NAG	C4-C3-C2	-3.09	106.49	111.02
9	E	632	NAG	C1-O5-C5	3.09	116.38	112.19
9	I	630	NAG	O3-C3-C4	-3.08	103.22	110.35
9	A	630	NAG	O3-C3-C4	-3.08	103.23	110.35
9	A	632	NAG	C1-O5-C5	3.08	116.36	112.19
9	E	630	NAG	O3-C3-C4	-3.08	103.24	110.35
9	A	630	NAG	O3-C3-C2	3.05	115.78	109.47
9	E	630	NAG	O3-C3-C2	3.05	115.78	109.47
9	I	630	NAG	O3-C3-C2	3.04	115.77	109.47
9	I	632	NAG	C3-C4-C5	-3.03	104.84	110.24
9	A	632	NAG	C3-C4-C5	-3.01	104.87	110.24
9	E	632	NAG	C3-C4-C5	-3.01	104.87	110.24
9	I	617	NAG	C8-C7-N2	2.94	121.07	116.10
9	A	617	NAG	C8-C7-N2	2.92	121.05	116.10
9	E	617	NAG	C8-C7-N2	2.91	121.03	116.10
9	E	630	NAG	O5-C5-C6	2.83	111.64	107.20
9	I	630	NAG	O5-C5-C6	2.83	111.64	107.20
9	A	630	NAG	O5-C5-C6	2.82	111.63	107.20
9	E	619	NAG	O4-C4-C5	-2.75	102.47	109.30
9	I	619	NAG	O4-C4-C5	-2.75	102.47	109.30
9	A	619	NAG	O4-C4-C5	-2.75	102.48	109.30
9	E	617	NAG	O3-C3-C4	-2.74	104.00	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	617	NAG	O3-C3-C4	-2.73	104.04	110.35
9	I	617	NAG	O3-C3-C4	-2.73	104.05	110.35
9	A	631	NAG	C6-C5-C4	-2.72	106.62	113.00
9	E	631	NAG	C6-C5-C4	-2.71	106.65	113.00
9	I	631	NAG	C6-C5-C4	-2.71	106.67	113.00
9	E	630	NAG	C6-C5-C4	-2.67	106.76	113.00
9	I	630	NAG	C6-C5-C4	-2.67	106.76	113.00
9	A	630	NAG	C6-C5-C4	-2.66	106.76	113.00
9	A	627	NAG	C1-O5-C5	2.64	115.77	112.19
9	E	622	NAG	O3-C3-C4	2.63	116.44	110.35
9	A	622	NAG	O3-C3-C4	2.63	116.43	110.35
9	I	622	NAG	O3-C3-C4	2.62	116.42	110.35
9	I	627	NAG	C1-O5-C5	2.62	115.74	112.19
9	E	627	NAG	C1-O5-C5	2.62	115.74	112.19
9	A	631	NAG	C2-N2-C7	2.59	126.58	122.90
9	E	631	NAG	C2-N2-C7	2.58	126.58	122.90
9	I	631	NAG	C2-N2-C7	2.55	126.53	122.90
9	E	631	NAG	O4-C4-C3	2.53	116.20	110.35
9	A	631	NAG	O4-C4-C3	2.53	116.20	110.35
9	I	631	NAG	O4-C4-C3	2.53	116.19	110.35
9	A	622	NAG	C3-C4-C5	-2.49	105.80	110.24
9	I	631	NAG	C1-C2-N2	-2.48	106.25	110.49
9	E	622	NAG	C3-C4-C5	-2.48	105.81	110.24
9	I	622	NAG	C3-C4-C5	-2.48	105.81	110.24
9	E	631	NAG	C1-C2-N2	-2.48	106.26	110.49
9	A	631	NAG	C1-C2-N2	-2.46	106.28	110.49
9	I	626	NAG	C2-N2-C7	-2.42	119.46	122.90
9	A	626	NAG	C2-N2-C7	-2.41	119.47	122.90
9	E	626	NAG	C2-N2-C7	-2.40	119.49	122.90
9	E	617	NAG	C1-O5-C5	-2.37	108.98	112.19
9	A	617	NAG	C1-O5-C5	-2.37	108.98	112.19
9	I	617	NAG	C1-O5-C5	-2.37	108.98	112.19
9	E	622	NAG	O6-C6-C5	-2.36	103.21	111.29
9	A	622	NAG	O6-C6-C5	-2.35	103.23	111.29
9	I	622	NAG	O6-C6-C5	-2.35	103.24	111.29
9	I	631	NAG	C1-O5-C5	2.32	115.33	112.19
9	E	631	NAG	C1-O5-C5	2.31	115.32	112.19
9	A	631	NAG	C1-O5-C5	2.30	115.31	112.19
9	A	618	NAG	C1-C2-N2	2.26	114.36	110.49
9	I	618	NAG	C1-C2-N2	2.26	114.35	110.49
9	E	618	NAG	C1-C2-N2	2.25	114.34	110.49
9	I	619	NAG	C2-N2-C7	-2.21	119.75	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	619	NAG	O3-C3-C4	-2.21	105.25	110.35
9	A	619	NAG	O3-C3-C4	-2.20	105.26	110.35
9	A	619	NAG	C2-N2-C7	-2.20	119.77	122.90
9	E	619	NAG	C2-N2-C7	-2.20	119.77	122.90
9	E	619	NAG	O3-C3-C4	-2.19	105.29	110.35
9	A	630	NAG	O5-C1-C2	-2.14	107.91	111.29
9	E	630	NAG	O5-C1-C2	-2.14	107.91	111.29
9	I	630	NAG	O5-C1-C2	-2.14	107.91	111.29
9	E	627	NAG	O4-C4-C3	-2.05	105.62	110.35
9	A	627	NAG	O4-C4-C3	-2.04	105.64	110.35
9	I	627	NAG	O4-C4-C3	-2.03	105.66	110.35
9	I	626	NAG	C3-C4-C5	-2.03	106.62	110.24
9	E	626	NAG	C3-C4-C5	-2.02	106.63	110.24
9	A	626	NAG	C3-C4-C5	-2.02	106.64	110.24
9	I	622	NAG	O4-C4-C5	-2.02	104.29	109.30
9	E	622	NAG	O4-C4-C5	-2.01	104.30	109.30
9	E	627	NAG	C4-C3-C2	-2.01	108.08	111.02
9	A	622	NAG	O4-C4-C5	-2.00	104.33	109.30

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	617	NAG	O7-C7-N2-C2
9	A	622	NAG	C3-C2-N2-C7
9	A	622	NAG	C8-C7-N2-C2
9	A	622	NAG	O7-C7-N2-C2
9	A	626	NAG	C3-C2-N2-C7
9	A	630	NAG	C3-C2-N2-C7
9	E	617	NAG	O7-C7-N2-C2
9	E	622	NAG	C3-C2-N2-C7
9	E	622	NAG	C8-C7-N2-C2
9	E	622	NAG	O7-C7-N2-C2
9	E	626	NAG	C3-C2-N2-C7
9	E	630	NAG	C3-C2-N2-C7
9	I	617	NAG	O7-C7-N2-C2
9	I	622	NAG	C3-C2-N2-C7
9	I	622	NAG	C8-C7-N2-C2
9	I	622	NAG	O7-C7-N2-C2
9	I	626	NAG	C3-C2-N2-C7
9	I	630	NAG	C3-C2-N2-C7
9	A	617	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
9	E	617	NAG	C8-C7-N2-C2
9	I	617	NAG	C8-C7-N2-C2
9	A	618	NAG	C8-C7-N2-C2
9	A	619	NAG	C8-C7-N2-C2
9	A	626	NAG	C8-C7-N2-C2
9	A	630	NAG	C8-C7-N2-C2
9	A	631	NAG	C8-C7-N2-C2
9	E	618	NAG	C8-C7-N2-C2
9	E	619	NAG	C8-C7-N2-C2
9	E	626	NAG	C8-C7-N2-C2
9	E	630	NAG	C8-C7-N2-C2
9	E	631	NAG	C8-C7-N2-C2
9	I	618	NAG	C8-C7-N2-C2
9	I	619	NAG	C8-C7-N2-C2
9	I	626	NAG	C8-C7-N2-C2
9	I	630	NAG	C8-C7-N2-C2
9	I	631	NAG	C8-C7-N2-C2
9	A	617	NAG	O5-C5-C6-O6
9	E	617	NAG	O5-C5-C6-O6
9	I	617	NAG	O5-C5-C6-O6
9	A	617	NAG	C4-C5-C6-O6
9	E	617	NAG	C4-C5-C6-O6
9	I	617	NAG	C4-C5-C6-O6
9	A	618	NAG	O7-C7-N2-C2
9	A	630	NAG	O7-C7-N2-C2
9	E	618	NAG	O7-C7-N2-C2
9	I	618	NAG	O7-C7-N2-C2
9	I	630	NAG	O7-C7-N2-C2
9	A	619	NAG	O7-C7-N2-C2
9	A	626	NAG	O7-C7-N2-C2
9	A	631	NAG	O7-C7-N2-C2
9	E	619	NAG	O7-C7-N2-C2
9	E	626	NAG	O7-C7-N2-C2
9	E	630	NAG	O7-C7-N2-C2
9	E	631	NAG	O7-C7-N2-C2
9	I	619	NAG	O7-C7-N2-C2
9	I	626	NAG	O7-C7-N2-C2
9	I	631	NAG	O7-C7-N2-C2
9	A	618	NAG	C1-C2-N2-C7
9	A	619	NAG	C1-C2-N2-C7
9	E	618	NAG	C1-C2-N2-C7
9	E	619	NAG	C1-C2-N2-C7

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Mol	Chain	Res	Type	Atoms
9	I	618	NAG	C1-C2-N2-C7
9	I	619	NAG	C1-C2-N2-C7
9	A	631	NAG	O5-C5-C6-O6
9	E	631	NAG	O5-C5-C6-O6
9	I	631	NAG	O5-C5-C6-O6
9	A	626	NAG	O5-C5-C6-O6
9	E	626	NAG	O5-C5-C6-O6
9	I	626	NAG	O5-C5-C6-O6
9	A	627	NAG	C1-C2-N2-C7
9	E	627	NAG	C1-C2-N2-C7
9	I	627	NAG	C1-C2-N2-C7
9	A	630	NAG	O5-C5-C6-O6
9	E	630	NAG	O5-C5-C6-O6
9	I	630	NAG	O5-C5-C6-O6
9	A	622	NAG	O5-C5-C6-O6
9	E	622	NAG	O5-C5-C6-O6
9	I	622	NAG	O5-C5-C6-O6
9	A	619	NAG	O5-C5-C6-O6
9	E	619	NAG	O5-C5-C6-O6
9	I	619	NAG	O5-C5-C6-O6
9	A	631	NAG	C1-C2-N2-C7
9	E	631	NAG	C1-C2-N2-C7
9	I	631	NAG	C1-C2-N2-C7
9	A	632	NAG	O5-C5-C6-O6
9	E	632	NAG	O5-C5-C6-O6
9	I	632	NAG	O5-C5-C6-O6
9	A	627	NAG	C3-C2-N2-C7
9	A	631	NAG	C3-C2-N2-C7
9	E	627	NAG	C3-C2-N2-C7
9	E	631	NAG	C3-C2-N2-C7
9	I	627	NAG	C3-C2-N2-C7
9	I	631	NAG	C3-C2-N2-C7
9	A	617	NAG	C1-C2-N2-C7
9	E	617	NAG	C1-C2-N2-C7
9	I	617	NAG	C1-C2-N2-C7
9	A	627	NAG	C8-C7-N2-C2
9	E	627	NAG	C8-C7-N2-C2
9	I	627	NAG	C8-C7-N2-C2
9	A	619	NAG	C3-C2-N2-C7
9	E	619	NAG	C3-C2-N2-C7
9	I	619	NAG	C3-C2-N2-C7

There are no ring outliers.

24 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	622	NAG	2	0
9	I	632	NAG	1	0
9	I	631	NAG	3	0
9	E	619	NAG	3	0
9	A	630	NAG	3	0
9	E	617	NAG	1	0
9	A	619	NAG	2	0
9	I	626	NAG	1	0
9	E	631	NAG	4	0
9	I	627	NAG	1	0
9	I	622	NAG	3	0
9	E	632	NAG	1	0
9	I	630	NAG	3	0
9	A	631	NAG	3	0
9	E	627	NAG	1	0
9	A	627	NAG	2	0
9	A	632	NAG	1	0
9	E	626	NAG	1	0
9	I	617	NAG	1	0
9	A	626	NAG	1	0
9	A	622	NAG	2	0
9	I	619	NAG	1	0
9	E	630	NAG	3	0
9	A	617	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

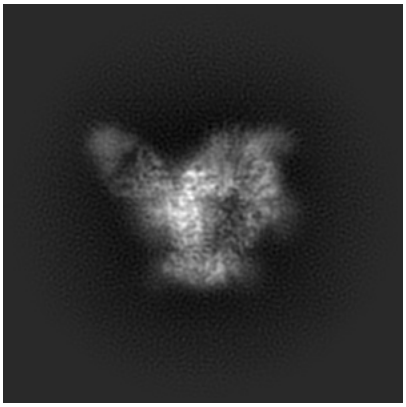
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20817. These allow visual inspection of the internal detail of the map and identification of artifacts.

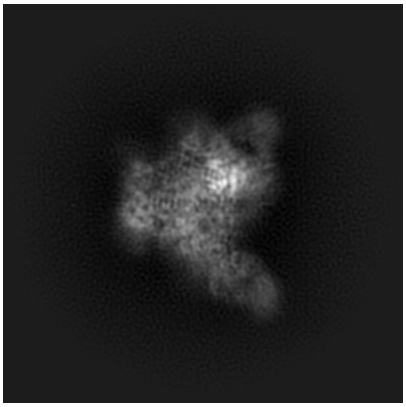
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

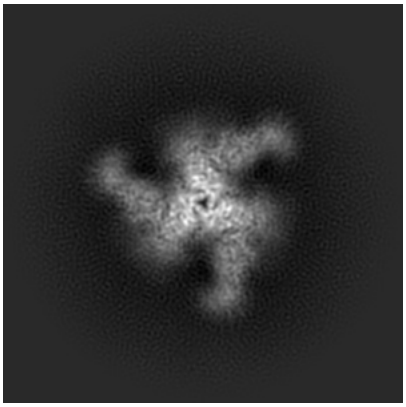
6.1.1 Primary map



X



Y

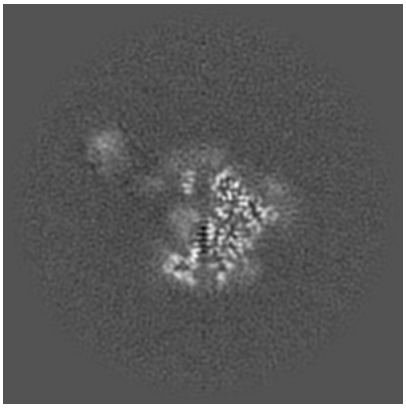


Z

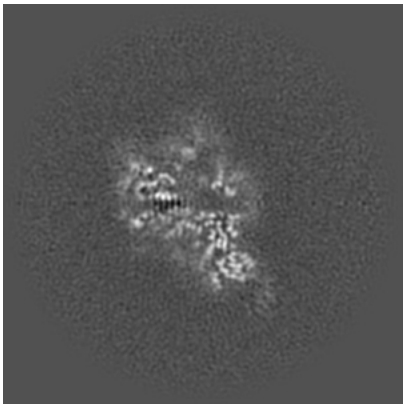
The images above show the map projected in three orthogonal directions.

6.2 Central slices

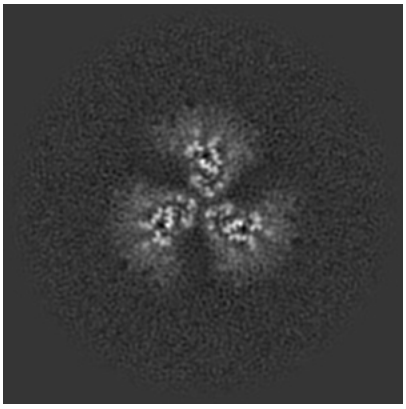
6.2.1 Primary map



X Index: 160



Y Index: 160

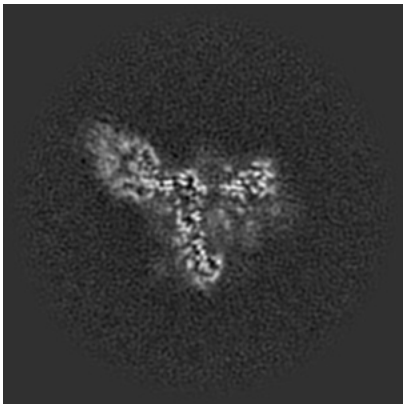


Z Index: 160

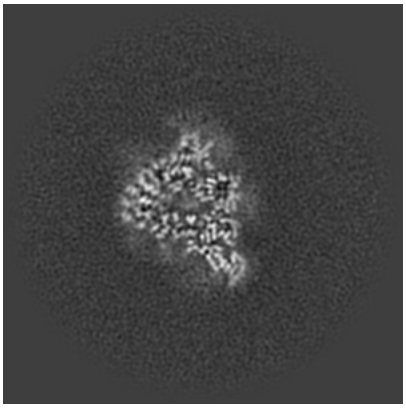
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

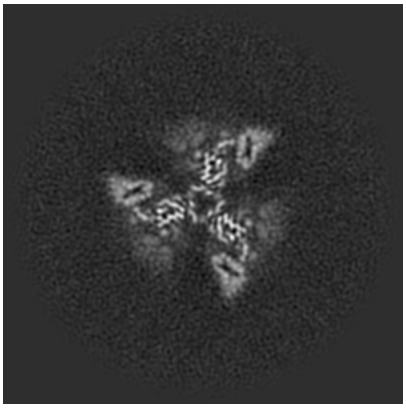
6.3.1 Primary map



X Index: 176



Y Index: 150

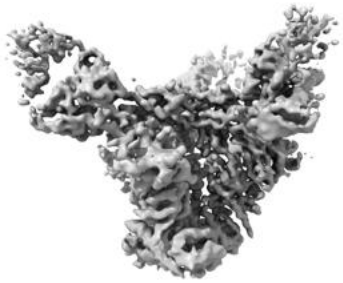


Z Index: 168

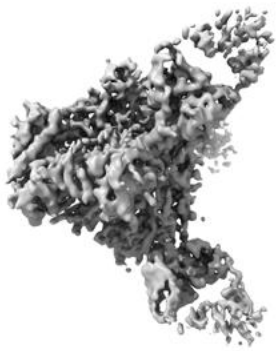
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

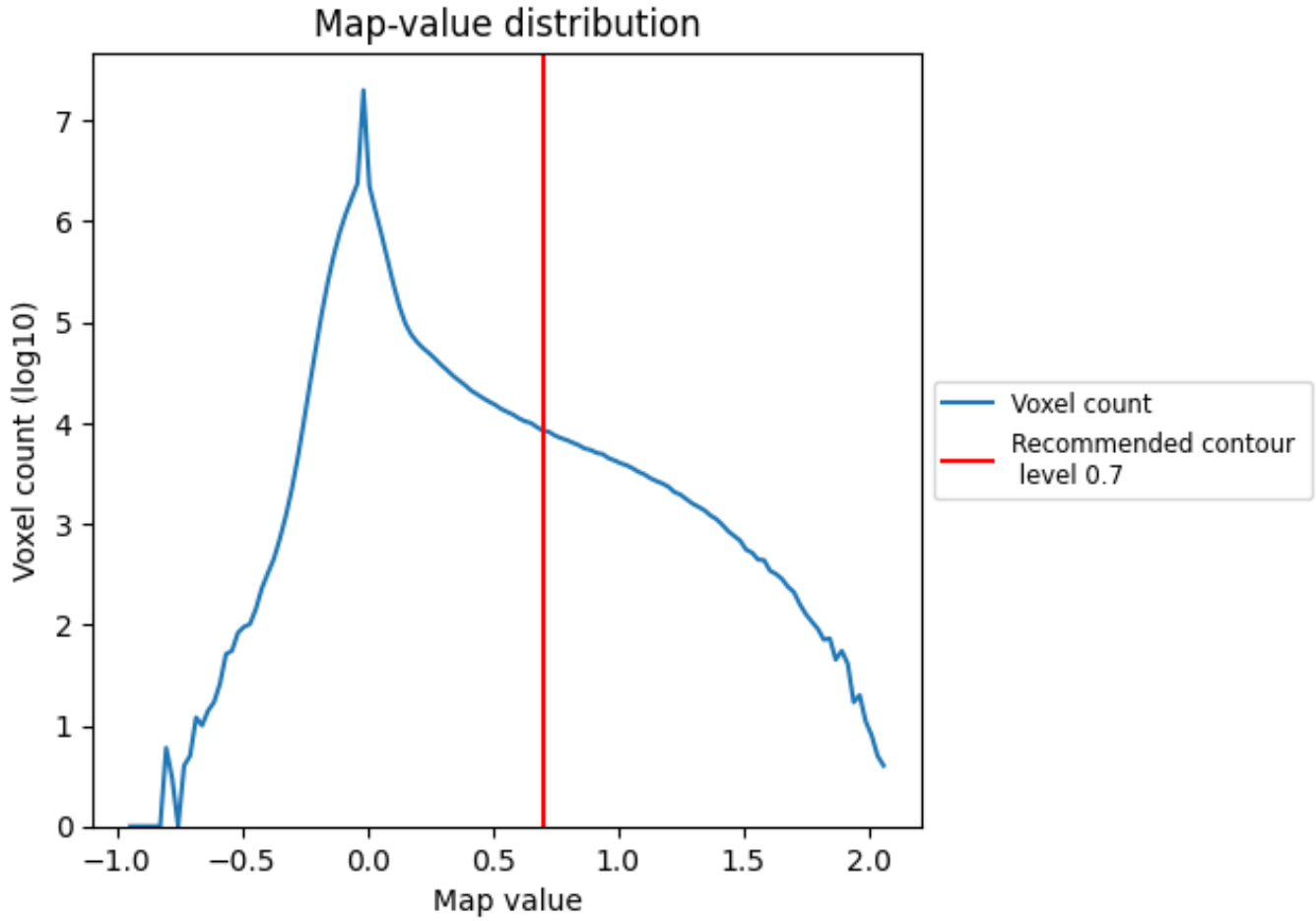
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

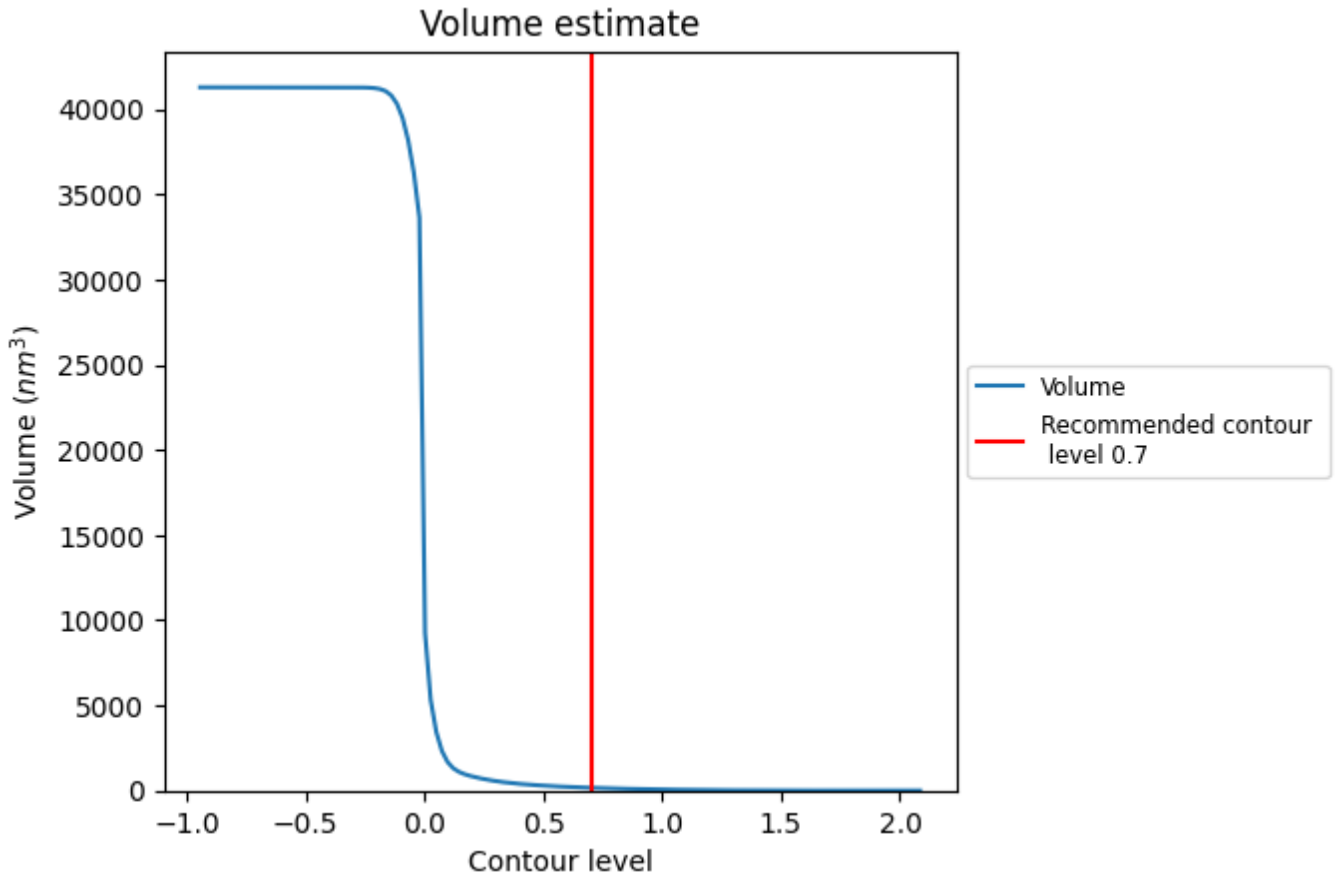
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

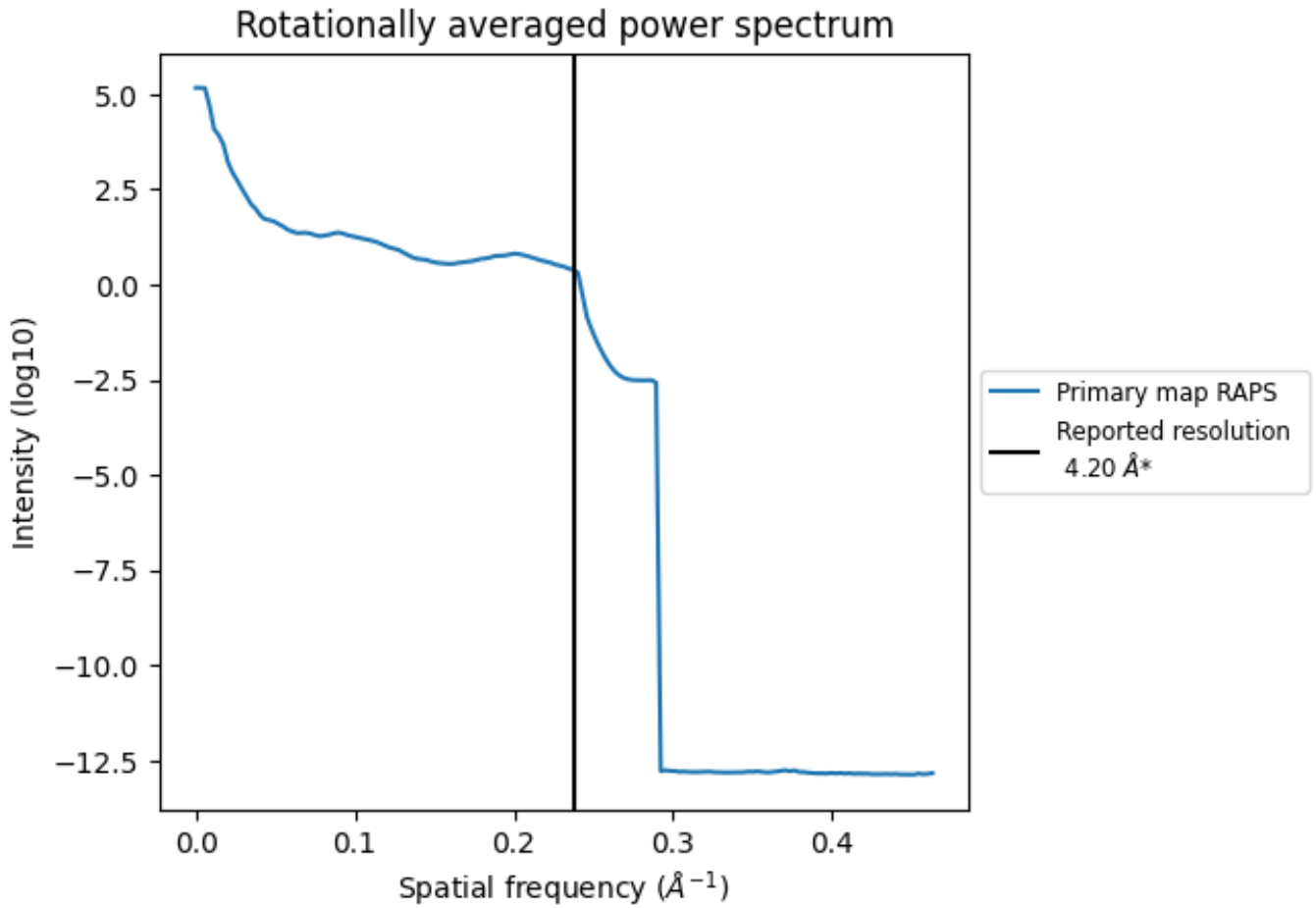
7.2 Volume estimate



The volume at the recommended contour level is 162 nm^3; this corresponds to an approximate mass of 146 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.238 $Å^{-1}$

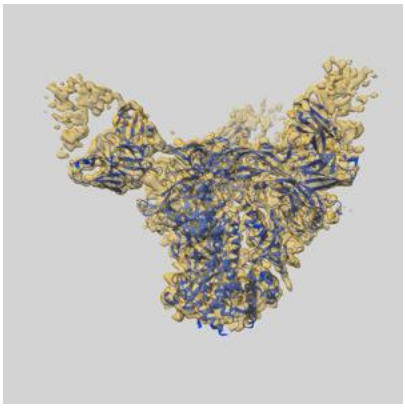
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

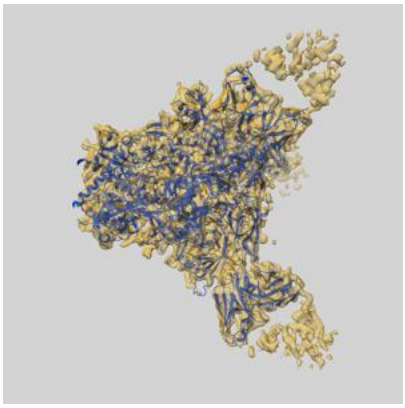
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-20817 and PDB model 6UM5. Per-residue inclusion information can be found in section 3 on page 11.

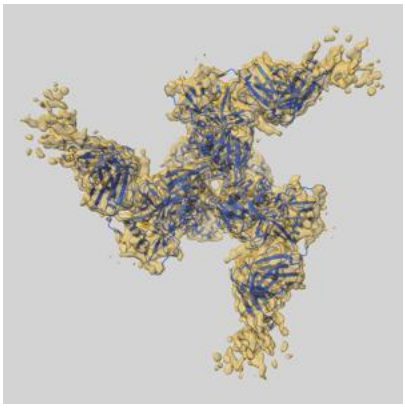
9.1 Map-model overlay



X



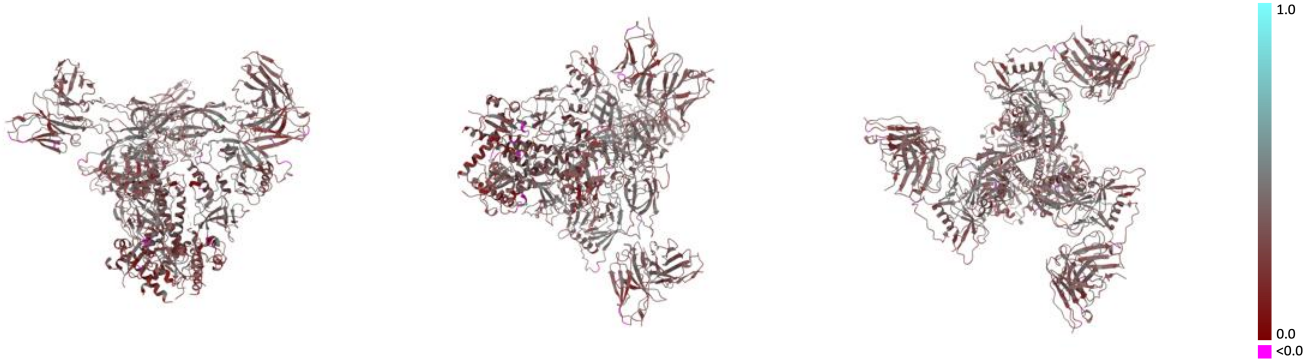
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



X Y Z

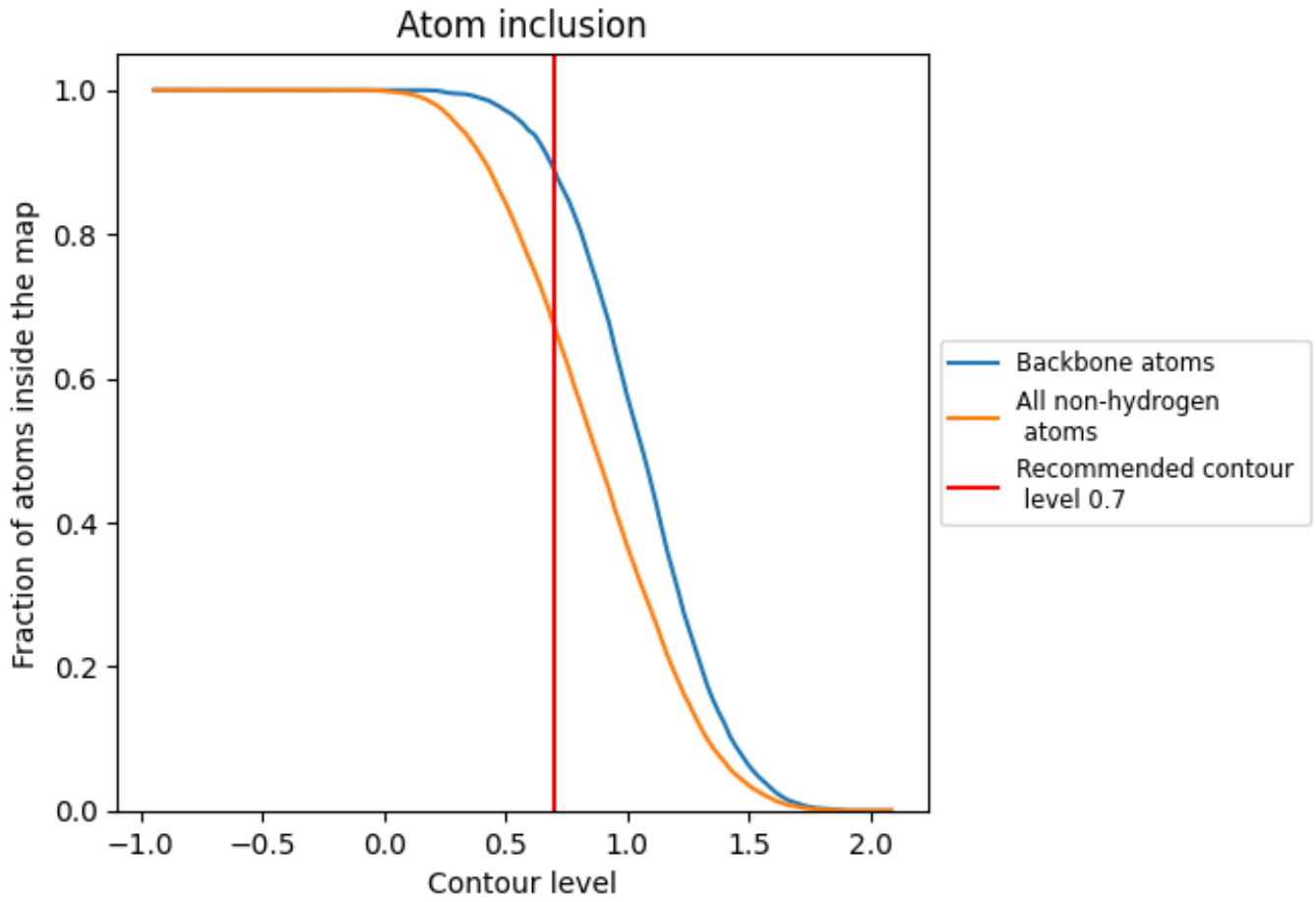
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.7).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6716	0.3470
A	0.6865	0.3620
B	0.6376	0.2830
C	0.7305	0.3540
D	0.6153	0.3100
E	0.6876	0.3630
F	0.6337	0.2800
G	0.7305	0.3550
H	0.6140	0.3120
I	0.6868	0.3630
J	0.6347	0.2830
K	0.7305	0.3550
L	0.6153	0.3160
M	0.6429	0.4250
N	0.7711	0.4500
O	0.4906	0.4570
P	0.4359	0.3860
Q	0.4643	0.4140
R	0.5641	0.4500
S	0.2857	0.4390
T	0.6429	0.4360
U	0.7711	0.4410
V	0.4906	0.4670
W	0.4359	0.3920
X	0.4643	0.4000
Y	0.5641	0.4430
Z	0.2857	0.4290
a	0.6429	0.4330
b	0.7831	0.4530
c	0.4906	0.4560
d	0.4615	0.3860
e	0.4643	0.4170
f	0.5385	0.4400
g	0.2857	0.4480