Full wwPDB EM Validation Report

Mar 9, 2026 – 02:55 PM UTC

PDB ID	:	8DOW / pdb_00008dow
EMDB ID	:	EMD-27624
Title	:	Cryo-EM structure of HIV-1 Env(CH848 10.17 DS.SOSIP_DT) in complex with DH1030.1 Fab
Authors	:	Gobeil, S.; Acharya, P.
Deposited on	:	2022-07-14
Resolution	:	3.69 Å(reported)
Based on initial models	:	8DKF, 6UM6

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 (i) symbol.

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

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

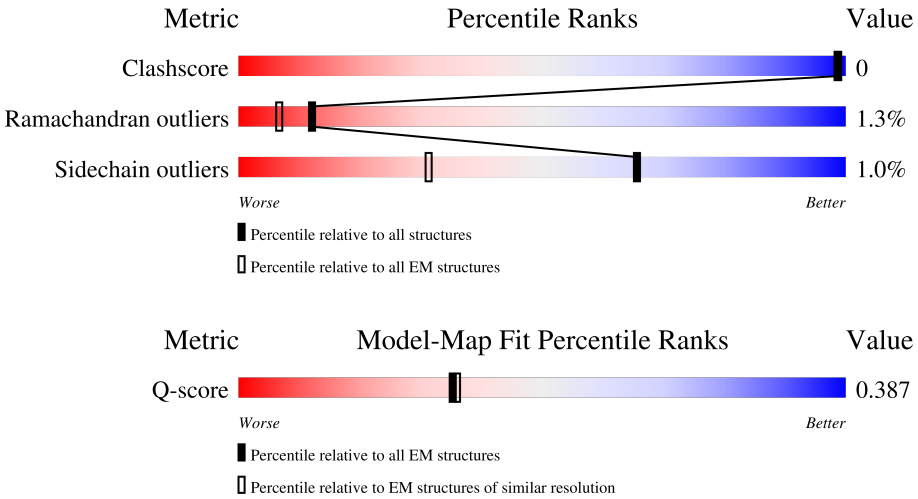
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.69 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11284 (3.19 - 4.18)

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	463	95%
1	E	463	5% 95% 5%
1	I	463	94% 5%
2	B	161	6% 80% 18%

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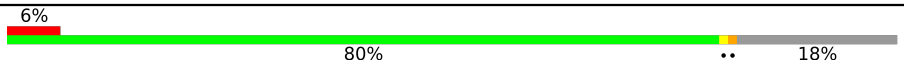
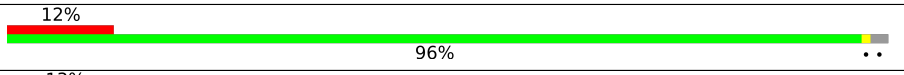
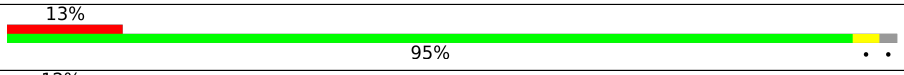
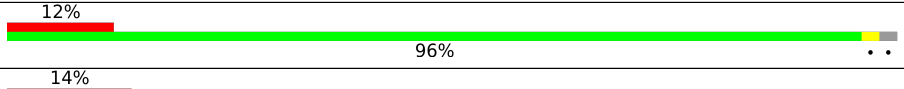
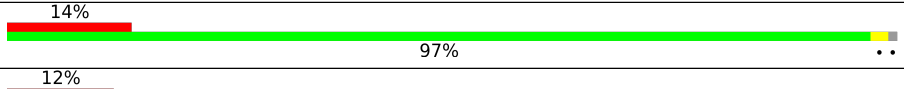
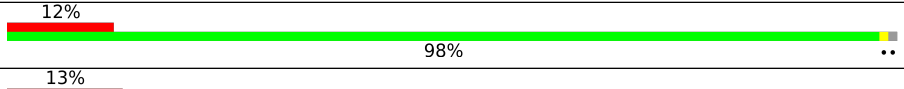
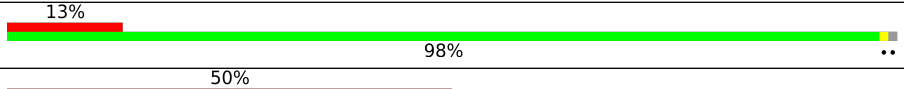
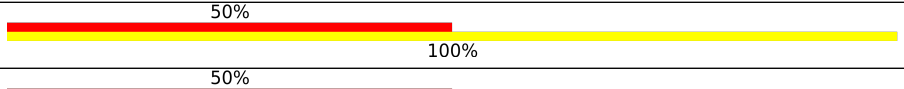
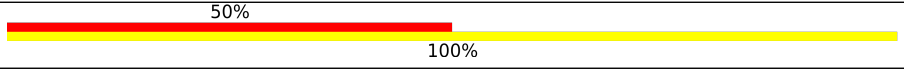
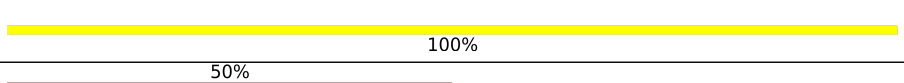
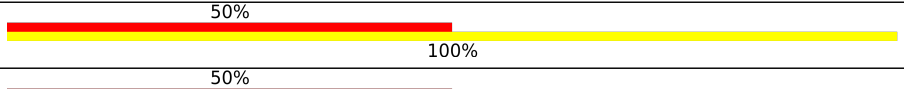
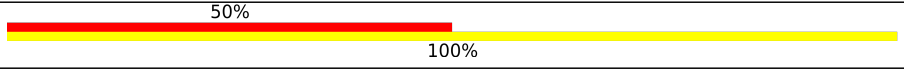
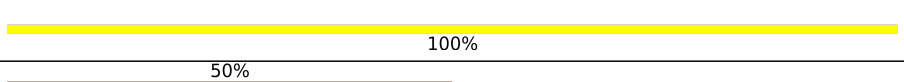
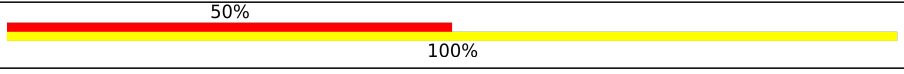
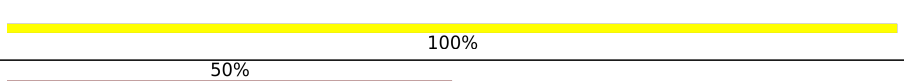
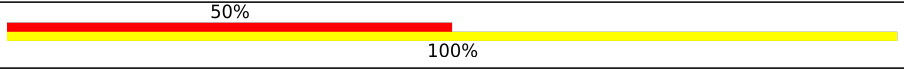
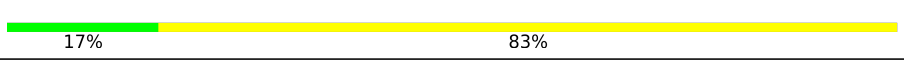
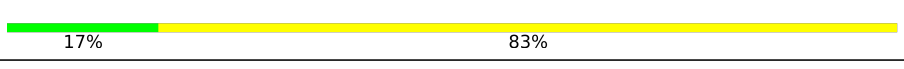
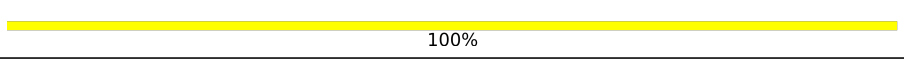
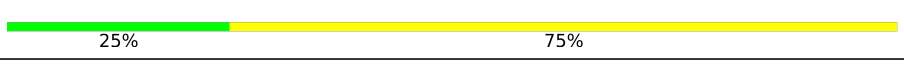
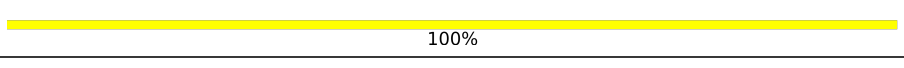
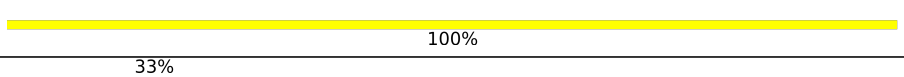
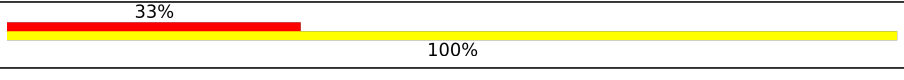
Mol	Chain	Length	Quality of chain
2	F	161	
2	J	161	
3	C	230	
3	G	230	
3	K	230	
4	D	219	
4	H	219	
4	L	219	
5	M	2	
5	P	2	
5	Q	2	
5	R	2	
5	T	2	
5	U	2	
5	X	2	
5	Y	2	
5	Z	2	
6	N	6	
6	S	6	
6	W	6	
7	O	4	
7	V	4	
7	a	4	
8	b	3	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 25053 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 Envelope glycoprotein gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	462	Total	C	N	O	S	0	0
			3613	2261	625	698	29		
1	E	462	Total	C	N	O	S	0	0
			3613	2261	625	698	29		
1	I	462	Total	C	N	O	S	0	0
			3613	2261	625	698	29		

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	expression tag	UNP A0A1W6IPB2
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	201	CYS	VAL	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	31	ALA	-	expression tag	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	201	CYS	VAL	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

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Chain	Residue	Modelled	Actual	Comment	Reference
I	31	ALA	-	expression tag	UNP A0A1W6IPB2
I	32	GLU	-	expression tag	UNP A0A1W6IPB2
I	33	ASN	-	expression tag	UNP A0A1W6IPB2
I	133	ASP	ASN	conflict	UNP A0A1W6IPB2
I	138	THR	ASN	conflict	UNP A0A1W6IPB2
I	201	CYS	VAL	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 gp41.

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

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	504	VAL	-	expression tag	UNP Q2N0S7
B	505	GLY	-	expression tag	UNP Q2N0S7
B	506	ARG	-	expression tag	UNP Q2N0S7
B	507	ARG	-	expression tag	UNP Q2N0S7
B	508	ARG	-	expression tag	UNP Q2N0S7
B	509	ARG	-	expression tag	UNP Q2N0S7
B	510	ARG	-	expression tag	UNP Q2N0S7
B	559	PRO	ILE	conflict	UNP Q2N0S7
B	605	CYS	THR	conflict	UNP Q2N0S7
F	504	VAL	-	expression tag	UNP Q2N0S7
F	505	GLY	-	expression tag	UNP Q2N0S7
F	506	ARG	-	expression tag	UNP Q2N0S7
F	507	ARG	-	expression tag	UNP Q2N0S7
F	508	ARG	-	expression tag	UNP Q2N0S7
F	509	ARG	-	expression tag	UNP Q2N0S7
F	510	ARG	-	expression tag	UNP Q2N0S7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	559	PRO	ILE	conflict	UNP Q2N0S7
F	605	CYS	THR	conflict	UNP Q2N0S7
J	504	VAL	-	expression tag	UNP Q2N0S7
J	505	GLY	-	expression tag	UNP Q2N0S7
J	506	ARG	-	expression tag	UNP Q2N0S7
J	507	ARG	-	expression tag	UNP Q2N0S7
J	508	ARG	-	expression tag	UNP Q2N0S7
J	509	ARG	-	expression tag	UNP Q2N0S7
J	510	ARG	-	expression tag	UNP Q2N0S7
J	559	PRO	ILE	conflict	UNP Q2N0S7
J	605	CYS	THR	conflict	UNP Q2N0S7

- Molecule 3 is a protein called DH1030.1 Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	225	Total	C	N	O	S	0	0
			1725	1083	300	336	6		
3	G	225	Total	C	N	O	S	0	0
			1725	1083	300	336	6		
3	K	225	Total	C	N	O	S	0	0
			1725	1083	300	336	6		

- Molecule 4 is a protein called DH1030.1 Fab Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	217	Total	C	N	O	S	0	0
			1676	1050	287	334	5		
4	H	217	Total	C	N	O	S	0	0
			1676	1050	287	334	5		
4	L	217	Total	C	N	O	S	0	0
			1676	1050	287	334	5		

- 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		

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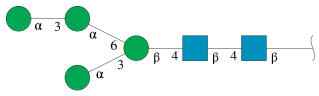
Mol	Chain	Residues	Atoms				AltConf	Trace
5	P	2	Total	C	N	O	0	0
			28	16	2	10		
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		
5	U	2	Total	C	N	O	0	0
			28	16	2	10		
5	X	2	Total	C	N	O	0	0
			28	16	2	10		
5	Y	2	Total	C	N	O	0	0
			28	16	2	10		
5	Z	2	Total	C	N	O	0	0
			28	16	2	10		

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

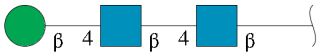


Mol	Chain	Residues	Atoms				AltConf	Trace
6	N	6	Total	C	N	O	0	0
			72	40	2	30		
6	S	6	Total	C	N	O	0	0
			72	40	2	30		
6	W	6	Total	C	N	O	0	0
			72	40	2	30		

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

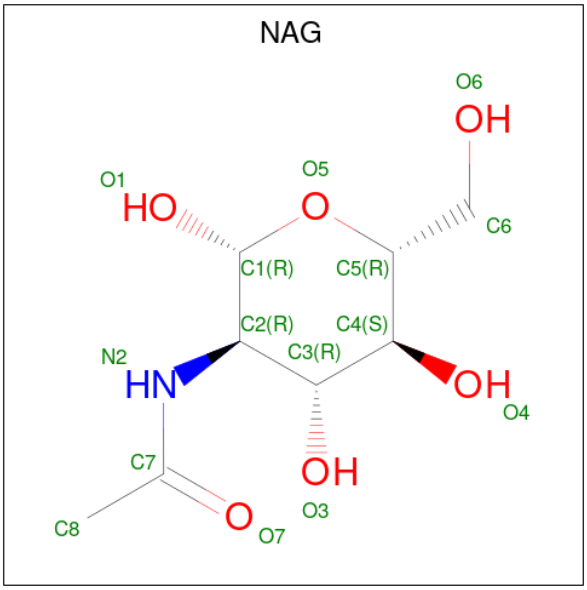
Mol	Chain	Residues	Atoms				AltConf	Trace
7	O	4	Total	C	N	O	0	0
			50	28	2	20		
7	V	4	Total	C	N	O	0	0
			50	28	2	20		
7	a	4	Total	C	N	O	0	0
			50	28	2	20		

- 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	b	3	Total	C	N	O	0	0
			39	22	2	15		

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



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	

Continued on next page...

Continued from previous page...

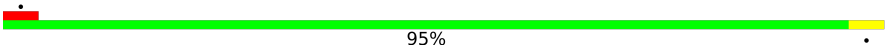
Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	A	1	Total	C	N	O	0
			14	8	1	5	
9	E	1	Total	C	N	O	0
			14	8	1	5	
9	E	1	Total	C	N	O	0
			14	8	1	5	
9	E	1	Total	C	N	O	0
			14	8	1	5	
9	E	1	Total	C	N	O	0
			14	8	1	5	
9	E	1	Total	C	N	O	0
			14	8	1	5	
9	E	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	
9	I	1	Total	C	N	O	0
			14	8	1	5	

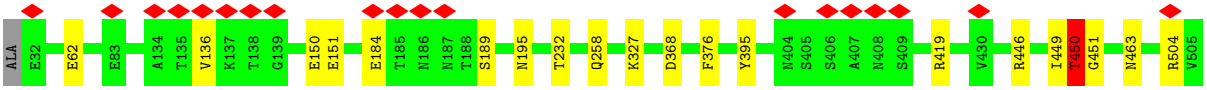
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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: Envelope glycoprotein gp120

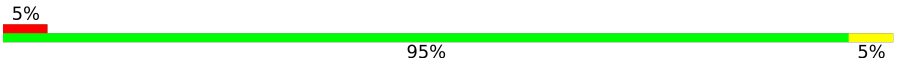
Chain A:

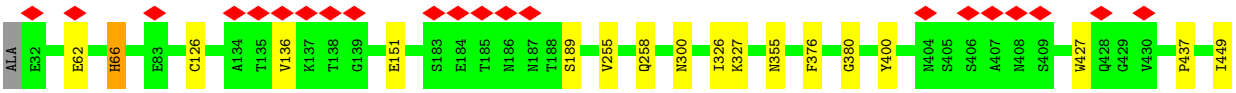


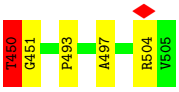


• Molecule 1: Envelope glycoprotein gp120

Chain E:

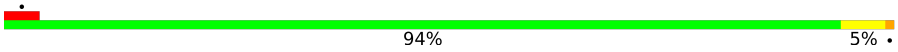


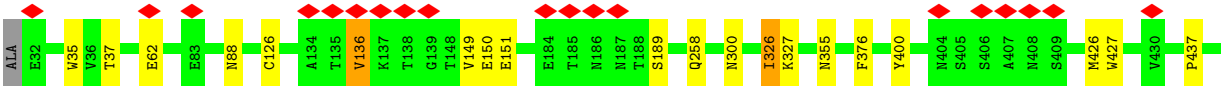


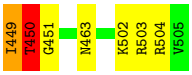


• Molecule 1: Envelope glycoprotein gp120

Chain I:

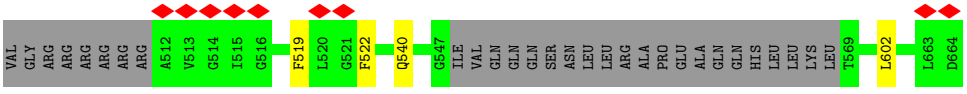






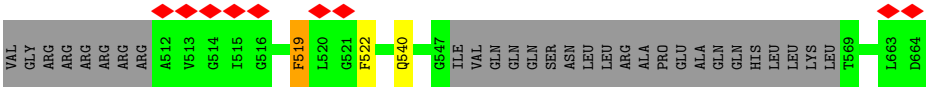
• Molecule 2: Envelope glycoprotein gp41

Chain B:



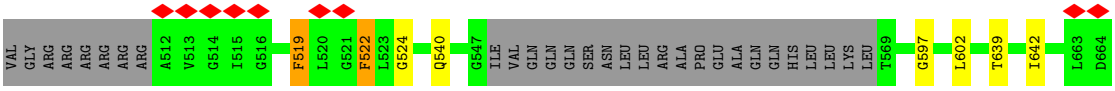
• Molecule 2: Envelope glycoprotein gp41

Chain F:



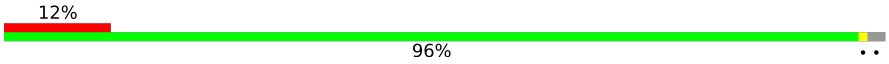
• Molecule 2: Envelope glycoprotein gp41

Chain J:



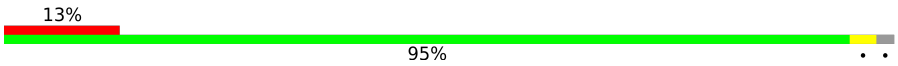
• Molecule 3: DH1030.1 Fab Heavy chain

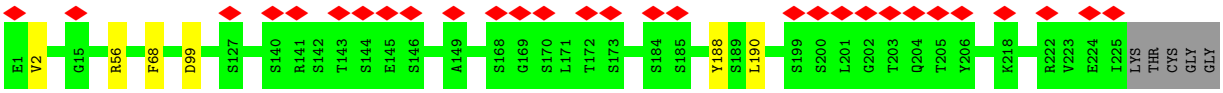
Chain C:



• Molecule 3: DH1030.1 Fab Heavy chain

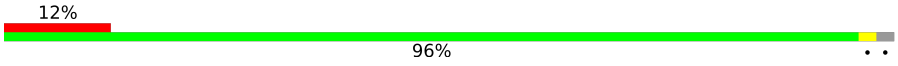
Chain G:





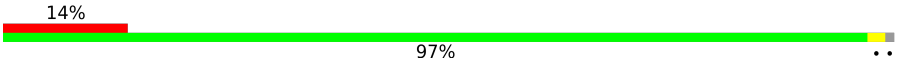
• Molecule 3: DH1030.1 Fab Heavy chain

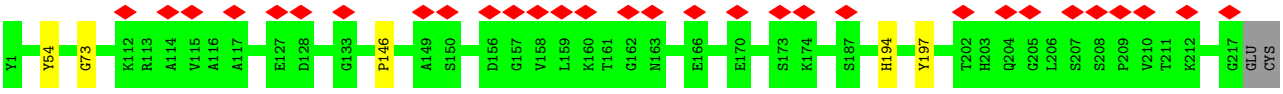
Chain K:



• Molecule 4: DH1030.1 Fab Light Chain

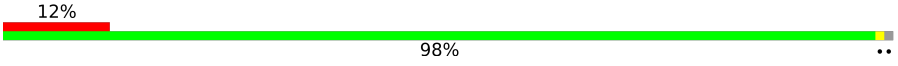
Chain D:

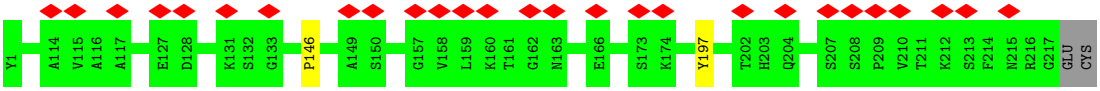




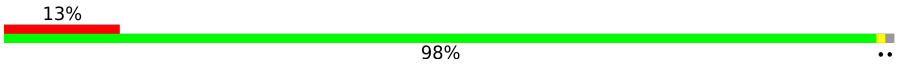
• Molecule 4: DH1030.1 Fab Light Chain

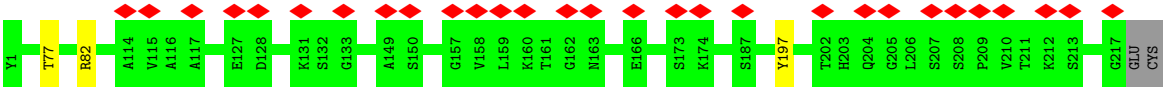
Chain H:





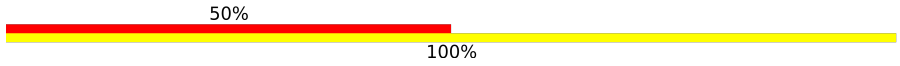
• Molecule 4: DH1030.1 Fab Light Chain



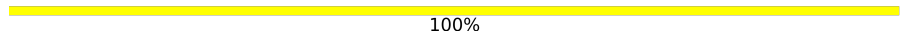


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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

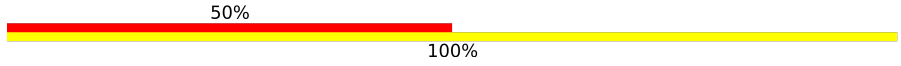


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



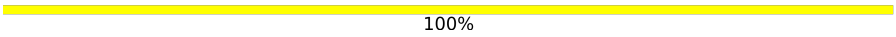
• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

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



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

Chain U:

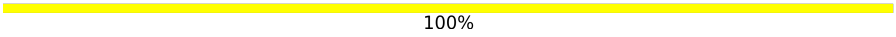


• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:

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

Chain Y:



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

Chain Z:

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

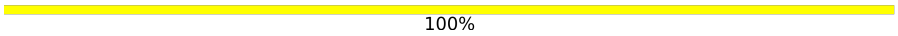
Chain N:

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

Chain S:

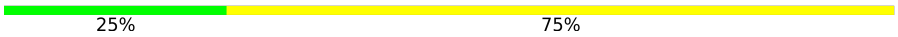
• Molecule 6: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:



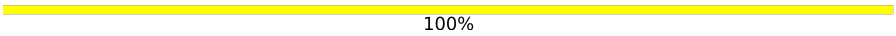
• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



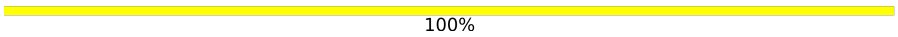
• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain V:



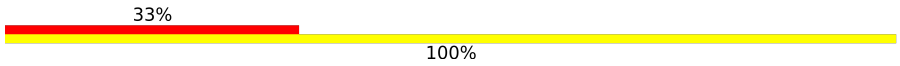
• Molecule 7: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a:



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

Chain b:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	296846	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 ($e^-/Å^2$)	54	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.663	Depositor
Minimum map value	-0.655	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.136	Depositor
Recommended contour level	0.9	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, BMA, MAN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.74	0/3690	1.31	7/5021 (0.1%)
1	E	0.74	0/3690	1.31	9/5021 (0.2%)
1	I	0.74	0/3690	1.31	10/5021 (0.2%)
2	B	0.70	0/1052	1.26	1/1427 (0.1%)
2	F	0.72	0/1052	1.28	1/1427 (0.1%)
2	J	0.71	0/1052	1.28	2/1427 (0.1%)
3	C	0.76	0/1769	1.27	1/2410 (0.0%)
3	G	0.76	0/1769	1.27	3/2410 (0.1%)
3	K	0.75	0/1769	1.27	1/2410 (0.0%)
4	D	0.75	0/1715	1.27	3/2334 (0.1%)
4	H	0.76	0/1715	1.30	2/2334 (0.1%)
4	L	0.76	0/1715	1.27	0/2334
All	All	0.74	0/24678	1.29	40/33576 (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
1	A	0	3
1	E	0	2
1	I	0	4
3	G	0	1
3	K	0	1
4	D	0	2
4	H	0	1
4	L	0	2
All	All	0	16

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	450	THR	N-CA-C	7.84	127.49	110.80
1	A	446	ARG	N-CA-C	7.81	122.22	109.72
2	F	519	PHE	CA-CB-CG	7.68	121.48	113.80
1	I	450	THR	N-CA-C	7.62	127.04	110.80
2	B	519	PHE	CA-CB-CG	7.52	121.32	113.80
1	A	376	PHE	CA-CB-CG	7.45	121.25	113.80
3	C	68	PHE	CA-CB-CG	7.27	121.07	113.80
3	K	68	PHE	CA-CB-CG	7.11	120.91	113.80
1	I	300	ASN	CA-CB-CG	7.08	119.68	112.60
1	A	450	THR	N-CA-C	7.06	125.83	110.80
2	J	519	PHE	CA-CB-CG	6.97	120.77	113.80
3	G	68	PHE	CA-CB-CG	6.22	120.02	113.80
1	I	376	PHE	CA-CB-CG	5.92	119.72	113.80
3	G	99	ASP	CA-C-N	5.79	129.12	120.83
3	G	99	ASP	C-N-CA	5.79	129.12	120.83
1	I	449	ILE	CA-C-N	5.79	132.59	121.54
1	I	449	ILE	C-N-CA	5.79	132.59	121.54
2	J	524	GLY	N-CA-C	5.76	120.79	114.40
1	A	449	ILE	CA-C-N	5.75	132.52	121.54
1	A	449	ILE	C-N-CA	5.75	132.52	121.54
1	I	449	ILE	N-CA-C	5.72	118.19	108.86
1	A	451	GLY	N-CA-C	-5.67	99.74	113.18
4	H	146	PRO	CA-C-N	5.61	127.80	120.28
4	H	146	PRO	C-N-CA	5.61	127.80	120.28
1	E	451	GLY	N-CA-C	-5.55	100.02	113.18
1	E	300	ASN	CA-CB-CG	5.39	117.99	112.60
4	D	146	PRO	CA-C-N	5.37	127.48	120.28
4	D	146	PRO	C-N-CA	5.37	127.48	120.28
1	E	376	PHE	CA-CB-CG	5.31	119.11	113.80
1	I	437	PRO	N-CA-CB	5.25	105.95	103.22
4	D	194	HIS	CB-CG-CD2	-5.16	124.49	131.20
1	E	497	ALA	N-CA-C	5.14	112.85	108.22
1	I	451	GLY	N-CA-C	-5.11	101.07	113.18
1	A	449	ILE	N-CA-C	5.10	117.17	108.86
1	I	450	THR	CA-C-N	5.10	131.40	121.41
1	I	450	THR	C-N-CA	5.10	131.40	121.41
1	E	449	ILE	CA-C-N	5.05	131.18	121.54
1	E	449	ILE	C-N-CA	5.05	131.18	121.54
1	E	437	PRO	N-CA-CB	5.03	105.83	103.22
1	E	66	HIS	CB-CG-CD2	-5.01	124.69	131.20

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	395	TYR	Sidechain
1	A	419	ARG	Sidechain
1	A	450	THR	Peptide
4	D	197	TYR	Sidechain
4	D	54	TYR	Sidechain
1	E	400	TYR	Sidechain
1	E	450	THR	Peptide
3	G	188	TYR	Sidechain
4	H	197	TYR	Sidechain
1	I	400	TYR	Sidechain
1	I	449	ILE	Peptide
1	I	450	THR	Peptide
1	I	503	ARG	Sidechain
3	K	65	ARG	Sidechain
4	L	197	TYR	Sidechain
4	L	82	ARG	Sidechain

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	3613	0	3522	0	0
1	E	3613	0	3522	1	0
1	I	3613	0	3521	2	0
2	B	1034	0	1014	0	0
2	F	1034	0	1014	2	0
2	J	1034	0	1014	1	0
3	C	1725	0	1668	0	0
3	G	1725	0	1668	1	0
3	K	1725	0	1668	0	0
4	D	1676	0	1628	0	0
4	H	1676	0	1628	0	0
4	L	1676	0	1628	0	0
5	M	28	0	25	0	0
5	P	28	0	25	0	0
5	Q	28	0	25	0	0
5	R	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	28	0	25	0	0
5	U	28	0	25	0	0
5	X	28	0	25	0	0
5	Y	28	0	25	0	0
5	Z	28	0	25	0	0
6	N	72	0	61	0	0
6	S	72	0	61	0	0
6	W	72	0	61	0	0
7	O	50	0	43	0	0
7	V	50	0	43	0	0
7	a	50	0	43	0	0
8	b	39	0	34	0	0
9	A	84	0	78	0	0
9	E	84	0	78	0	0
9	I	84	0	78	0	0
All	All	25053	0	24300	7	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 0.

All (7) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:519:PHE:HA	2:F:522:PHE:HA	1.97	0.46
1:E:255:VAL:HG21	1:E:427:TRP:HE1	1.82	0.44
2:F:519:PHE:C	2:F:522:PHE:H	2.26	0.43
1:I:426:MET:HG3	1:I:427:TRP:CD2	2.54	0.43
2:J:519:PHE:HA	2:J:522:PHE:HA	2.03	0.41
3:G:190:LEU:HD12	3:G:190:LEU:C	2.46	0.40
1:I:35:TRP:CH2	1:I:502:LYS:HE3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	460/463 (99%)	415 (90%)	38 (8%)	7 (2%)	8 36
1	E	460/463 (99%)	416 (90%)	33 (7%)	11 (2%)	4 29
1	I	460/463 (99%)	414 (90%)	35 (8%)	11 (2%)	4 29
2	B	128/161 (80%)	114 (89%)	12 (9%)	2 (2%)	7 35
2	F	128/161 (80%)	114 (89%)	14 (11%)	0	100 100
2	J	128/161 (80%)	115 (90%)	10 (8%)	3 (2%)	5 30
3	C	223/230 (97%)	207 (93%)	14 (6%)	2 (1%)	14 45
3	G	223/230 (97%)	205 (92%)	16 (7%)	2 (1%)	14 45
3	K	223/230 (97%)	208 (93%)	13 (6%)	2 (1%)	14 45
4	D	215/219 (98%)	198 (92%)	16 (7%)	1 (0%)	24 56
4	H	215/219 (98%)	197 (92%)	18 (8%)	0	100 100
4	L	215/219 (98%)	199 (93%)	16 (7%)	0	100 100
All	All	3078/3219 (96%)	2802 (91%)	235 (8%)	41 (1%)	12 38

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	450	THR
1	A	189	SER
1	A	450	THR
1	E	327	LYS
1	I	62	GLU
1	I	327	LYS
1	I	355	ASN
1	A	62	GLU
1	A	327	LYS
2	B	522	PHE
1	E	62	GLU
1	E	189	SER
1	E	380	GLY
1	I	450	THR
1	I	463	ASN
2	J	602	LEU
3	K	173	SER
1	A	136	VAL
1	A	258	GLN

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Mol	Chain	Res	Type
1	A	463	ASN
4	D	73	GLY
1	E	136	VAL
1	E	355	ASN
3	G	2	VAL
1	I	88	ASN
1	I	136	VAL
1	I	189	SER
1	I	258	GLN
3	K	2	VAL
2	B	602	LEU
3	C	2	VAL
3	C	173	SER
1	E	126	CYS
1	E	258	GLN
1	E	493	PRO
3	G	56	ARG
1	I	126	CYS
2	J	522	PHE
1	E	326	ILE
2	J	597	GLY
1	I	326	ILE

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	411/411 (100%)	403 (98%)	8 (2%)	50	65
1	E	411/411 (100%)	407 (99%)	4 (1%)	68	74
1	I	411/411 (100%)	403 (98%)	8 (2%)	50	65
2	B	110/136 (81%)	109 (99%)	1 (1%)	70	75
2	F	110/136 (81%)	109 (99%)	1 (1%)	70	75
2	J	110/136 (81%)	107 (97%)	3 (3%)	39	59
3	C	192/195 (98%)	190 (99%)	2 (1%)	68	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	192/195 (98%)	192 (100%)	0	100	100
3	K	192/195 (98%)	192 (100%)	0	100	100
4	D	192/194 (99%)	192 (100%)	0	100	100
4	H	192/194 (99%)	192 (100%)	0	100	100
4	L	192/194 (99%)	191 (100%)	1 (0%)	81	80
All	All	2715/2808 (97%)	2687 (99%)	28 (1%)	65	74

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	150	GLU
1	A	151	GLU
1	A	184	GLU
1	A	195	ASN
1	A	232	THR
1	A	368	ASP
1	A	450	THR
1	A	504	ARG
2	B	540	GLN
3	C	2	VAL
3	C	119	VAL
1	E	66	HIS
1	E	151	GLU
1	E	450	THR
1	E	504	ARG
2	F	540	GLN
1	I	37	THR
1	I	136	VAL
1	I	149	VAL
1	I	150	GLU
1	I	151	GLU
1	I	326	ILE
1	I	450	THR
1	I	504	ARG
2	J	540	GLN
2	J	639	THR
2	J	642	ILE
4	L	77	THR

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	92	ASN
1	A	195	ASN
1	A	425	ASN
2	B	575	GLN
3	C	53	ASN
3	C	216	ASN
4	D	188	ASN
1	E	72	HIS
1	E	92	ASN
1	E	302	ASN
1	E	404	ASN
1	E	422	GLN
3	G	82	GLN
4	H	143	ASN
1	I	92	ASN
1	I	195	ASN
1	I	280	ASN
1	I	404	ASN
1	I	428	GLN
2	J	616	ASN
3	K	53	ASN
4	L	188	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

51 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	1,5	14,14,15	1.24	2 (14%)	17,19,21	0.95	0
5	NAG	M	2	5	14,14,15	1.33	3 (21%)	17,19,21	1.44	2 (11%)
6	NAG	N	1	1,6	14,14,15	0.83	0	17,19,21	1.02	0
6	NAG	N	2	6	14,14,15	1.15	2 (14%)	17,19,21	1.55	4 (23%)
6	BMA	N	3	6	11,11,12	1.23	1 (9%)	15,15,17	1.75	4 (26%)
6	MAN	N	4	6	11,11,12	1.13	0	15,15,17	1.70	2 (13%)
6	MAN	N	5	6	11,11,12	0.97	1 (9%)	15,15,17	1.49	2 (13%)
6	MAN	N	6	6	11,11,12	1.51	2 (18%)	15,15,17	1.39	2 (13%)
7	NAG	O	1	1,7	14,14,15	1.01	0	17,19,21	0.81	0
7	NAG	O	2	7	14,14,15	1.17	2 (14%)	17,19,21	1.17	2 (11%)
7	BMA	O	3	7	11,11,12	1.26	1 (9%)	15,15,17	1.42	3 (20%)
7	MAN	O	4	7	11,11,12	1.29	2 (18%)	15,15,17	1.08	2 (13%)
5	NAG	P	1	1,5	14,14,15	1.14	1 (7%)	17,19,21	0.77	0
5	NAG	P	2	5	14,14,15	1.31	2 (14%)	17,19,21	1.12	1 (5%)
5	NAG	Q	1	1,5	14,14,15	1.21	1 (7%)	17,19,21	0.78	0
5	NAG	Q	2	5	14,14,15	1.30	3 (21%)	17,19,21	1.18	2 (11%)
5	NAG	R	1	1,5	14,14,15	1.29	3 (21%)	17,19,21	0.80	0
5	NAG	R	2	5	14,14,15	1.35	2 (14%)	17,19,21	1.44	1 (5%)
6	NAG	S	1	1,6	14,14,15	0.85	0	17,19,21	1.04	0
6	NAG	S	2	6	14,14,15	1.07	1 (7%)	17,19,21	1.65	4 (23%)
6	BMA	S	3	6	11,11,12	1.19	1 (9%)	15,15,17	1.99	4 (26%)
6	MAN	S	4	6	11,11,12	1.42	3 (27%)	15,15,17	1.70	5 (33%)
6	MAN	S	5	6	11,11,12	1.01	1 (9%)	15,15,17	1.72	2 (13%)
6	MAN	S	6	6	11,11,12	1.53	2 (18%)	15,15,17	1.57	2 (13%)
5	NAG	T	1	1,5	14,14,15	1.15	2 (14%)	17,19,21	1.35	3 (17%)
5	NAG	T	2	5	14,14,15	1.20	2 (14%)	17,19,21	0.74	0
5	NAG	U	1	1,5	14,14,15	1.05	2 (14%)	17,19,21	0.70	0
5	NAG	U	2	5	14,14,15	1.15	1 (7%)	17,19,21	1.03	2 (11%)
7	NAG	V	1	1,7	14,14,15	1.08	1 (7%)	17,19,21	1.31	3 (17%)
7	NAG	V	2	7	14,14,15	1.23	2 (14%)	17,19,21	0.65	0
7	BMA	V	3	7	11,11,12	1.34	1 (9%)	15,15,17	1.75	3 (20%)
7	MAN	V	4	7	11,11,12	1.36	2 (18%)	15,15,17	1.17	1 (6%)
6	NAG	W	1	1,6	14,14,15	0.82	0	17,19,21	1.05	1 (5%)
6	NAG	W	2	6	14,14,15	1.15	2 (14%)	17,19,21	1.45	4 (23%)
6	BMA	W	3	6	11,11,12	1.28	1 (9%)	15,15,17	1.68	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	MAN	W	4	6	11,11,12	1.47	3 (27%)	15,15,17	1.71	5 (33%)
6	MAN	W	5	6	11,11,12	1.21	1 (9%)	15,15,17	1.67	3 (20%)
6	MAN	W	6	6	11,11,12	1.55	1 (9%)	15,15,17	1.43	4 (26%)
5	NAG	X	1	1,5	14,14,15	1.34	3 (21%)	17,19,21	0.82	0
5	NAG	X	2	5	14,14,15	1.30	2 (14%)	17,19,21	1.47	1 (5%)
5	NAG	Y	1	1,5	14,14,15	1.23	2 (14%)	17,19,21	0.72	0
5	NAG	Y	2	5	14,14,15	1.27	3 (21%)	17,19,21	0.97	1 (5%)
5	NAG	Z	1	1,5	14,14,15	1.37	3 (21%)	17,19,21	1.64	2 (11%)
5	NAG	Z	2	5	14,14,15	1.23	2 (14%)	17,19,21	1.18	3 (17%)
7	NAG	a	1	1,7	14,14,15	1.24	2 (14%)	17,19,21	1.34	2 (11%)
7	NAG	a	2	7	14,14,15	1.27	2 (14%)	17,19,21	1.15	2 (11%)
7	BMA	a	3	7	11,11,12	1.28	1 (9%)	15,15,17	0.76	0
7	MAN	a	4	7	11,11,12	1.35	2 (18%)	15,15,17	0.97	1 (6%)
8	NAG	b	1	1,8	14,14,15	1.22	1 (7%)	17,19,21	1.06	1 (5%)
8	NAG	b	2	8	14,14,15	1.34	2 (14%)	17,19,21	0.94	0
8	BMA	b	3	8	11,11,12	1.30	2 (18%)	15,15,17	0.78	0

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

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

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

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	6	MAN	O5-C5	3.29	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	2	NAG	O5-C5	3.16	1.49	1.43
5	M	2	NAG	O5-C5	3.11	1.49	1.43
7	a	2	NAG	O5-C5	3.05	1.49	1.43
5	Q	2	NAG	O5-C5	2.95	1.49	1.43
5	X	2	NAG	O5-C5	2.95	1.49	1.43
7	V	4	MAN	O5-C5	2.94	1.49	1.43
6	S	6	MAN	O5-C5	2.89	1.49	1.43
6	W	5	MAN	O5-C5	2.85	1.49	1.43
7	a	4	MAN	O5-C5	2.84	1.49	1.43
8	b	2	NAG	O5-C5	2.84	1.49	1.43
7	V	2	NAG	O5-C5	2.81	1.48	1.43
5	P	2	NAG	O5-C5	2.80	1.48	1.43
6	N	6	MAN	O5-C5	2.77	1.48	1.43
6	W	2	NAG	O5-C5	2.75	1.48	1.43
6	N	2	NAG	O5-C5	2.73	1.48	1.43
6	S	6	MAN	C2-C3	2.73	1.56	1.52
8	b	3	BMA	O5-C5	2.72	1.48	1.43
5	Y	2	NAG	O5-C5	2.70	1.48	1.43
7	a	3	BMA	O5-C5	2.66	1.48	1.43
7	V	3	BMA	O5-C5	2.62	1.48	1.43
5	Y	1	NAG	O5-C5	2.61	1.48	1.43
7	a	1	NAG	O5-C5	2.60	1.48	1.43
7	O	4	MAN	O5-C5	2.56	1.48	1.43
6	W	4	MAN	O5-C5	2.55	1.48	1.43
5	X	1	NAG	O5-C5	2.55	1.48	1.43
7	O	2	NAG	O5-C5	2.55	1.48	1.43
5	Z	2	NAG	O5-C5	2.52	1.48	1.43
6	N	5	MAN	O5-C5	2.51	1.48	1.43
5	T	1	NAG	O5-C5	2.44	1.48	1.43
7	O	3	BMA	O5-C5	2.43	1.48	1.43
6	N	6	MAN	C2-C3	2.39	1.56	1.52
6	W	3	BMA	O3-C3	2.39	1.48	1.43
5	M	1	NAG	O5-C5	2.38	1.48	1.43
5	P	1	NAG	O5-C5	2.38	1.48	1.43
5	X	1	NAG	C1-C2	2.37	1.55	1.52
5	Q	1	NAG	O5-C5	2.37	1.48	1.43
5	Z	1	NAG	C1-C2	2.36	1.55	1.52
8	b	1	NAG	O5-C5	2.36	1.48	1.43
6	S	2	NAG	O5-C5	2.35	1.48	1.43
6	S	5	MAN	O5-C5	2.35	1.48	1.43
5	R	1	NAG	C1-C2	2.35	1.55	1.52
6	N	3	BMA	O3-C3	2.34	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	4	MAN	O5-C1	2.33	1.47	1.43
5	Z	1	NAG	O5-C5	2.31	1.47	1.43
6	S	4	MAN	O5-C5	2.29	1.47	1.43
6	S	4	MAN	C2-C3	2.28	1.56	1.52
5	Y	1	NAG	O4-C4	2.28	1.48	1.43
5	U	2	NAG	O5-C5	2.28	1.47	1.43
5	P	2	NAG	O5-C1	2.27	1.47	1.43
6	W	4	MAN	C2-C3	2.27	1.56	1.52
7	V	2	NAG	O4-C4	2.27	1.48	1.43
5	Z	1	NAG	O4-C4	2.26	1.48	1.43
8	b	2	NAG	O4-C4	2.25	1.48	1.43
5	R	2	NAG	C1-C2	2.24	1.55	1.52
6	S	4	MAN	O3-C3	2.23	1.48	1.43
7	O	2	NAG	O4-C4	2.23	1.48	1.43
7	a	2	NAG	O4-C4	2.21	1.48	1.43
5	R	1	NAG	O5-C5	2.18	1.47	1.43
6	W	2	NAG	O5-C1	2.18	1.47	1.43
6	W	4	MAN	O3-C3	2.18	1.48	1.43
5	T	1	NAG	O4-C4	2.18	1.48	1.43
7	O	4	MAN	O5-C1	2.18	1.47	1.43
7	V	4	MAN	O5-C1	2.17	1.47	1.43
5	R	1	NAG	O4-C4	2.17	1.48	1.43
5	X	2	NAG	C1-C2	2.16	1.55	1.52
6	S	3	BMA	O3-C3	2.13	1.48	1.43
5	Q	2	NAG	C1-C2	2.13	1.55	1.52
5	Z	2	NAG	C1-C2	2.13	1.55	1.52
5	T	2	NAG	O5-C5	2.12	1.47	1.43
5	U	1	NAG	O5-C5	2.11	1.47	1.43
5	X	1	NAG	O4-C4	2.11	1.48	1.43
5	T	2	NAG	C1-C2	2.10	1.55	1.52
6	N	2	NAG	O5-C1	2.10	1.47	1.43
5	M	2	NAG	C1-C2	2.09	1.55	1.52
5	Y	2	NAG	C1-C2	2.09	1.55	1.52
7	a	1	NAG	C1-C2	2.08	1.55	1.52
5	Y	2	NAG	O5-C1	2.07	1.47	1.43
5	U	1	NAG	O4-C4	2.06	1.48	1.43
5	M	2	NAG	O5-C1	2.05	1.47	1.43
8	b	3	BMA	O5-C1	2.04	1.47	1.43
5	M	1	NAG	O4-C4	2.04	1.48	1.43
7	V	1	NAG	O5-C5	2.04	1.47	1.43
5	Q	2	NAG	O5-C1	2.03	1.47	1.43

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Z	1	NAG	O5-C1-C2	5.65	120.03	111.29
5	X	2	NAG	O5-C1-C2	5.48	119.78	111.29
5	R	2	NAG	O5-C1-C2	5.35	119.58	111.29
6	S	3	BMA	C1-C2-C3	-5.04	102.30	109.64
5	M	2	NAG	O5-C1-C2	4.99	119.01	111.29
7	V	3	BMA	O5-C1-C2	4.75	122.13	110.79
6	S	5	MAN	C1-O5-C5	4.62	118.37	112.19
6	N	4	MAN	O3-C3-C2	-4.62	100.64	110.05
6	W	5	MAN	C1-O5-C5	4.48	118.19	112.19
7	V	4	MAN	C1-O5-C5	4.14	117.74	112.19
6	S	6	MAN	C1-O5-C5	3.87	117.37	112.19
6	N	3	BMA	O5-C1-C2	3.71	119.65	110.79
6	N	5	MAN	C1-O5-C5	3.71	117.16	112.19
6	N	2	NAG	C4-C3-C2	-3.66	105.65	111.02
6	W	3	BMA	C1-C2-C3	-3.57	104.45	109.64
6	S	2	NAG	C4-C3-C2	-3.55	105.81	111.02
7	a	1	NAG	C1-O5-C5	3.52	116.90	112.19
6	S	3	BMA	O5-C1-C2	3.46	119.05	110.79
6	W	2	NAG	C4-C3-C2	-3.38	106.07	111.02
6	N	6	MAN	C1-O5-C5	3.26	116.55	112.19
6	N	4	MAN	C1-C2-C3	3.25	114.37	109.64
6	W	4	MAN	C1-O5-C5	3.23	116.52	112.19
6	N	5	MAN	O5-C1-C2	3.19	118.39	110.79
5	T	1	NAG	C4-C3-C2	3.15	115.64	111.02
7	V	1	NAG	C1-C2-N2	3.12	115.34	110.43
6	W	4	MAN	O3-C3-C2	-3.11	103.70	110.05
6	W	6	MAN	C1-O5-C5	3.10	116.34	112.19
5	P	2	NAG	C1-O5-C5	3.10	116.34	112.19
6	S	4	MAN	C1-O5-C5	3.10	116.34	112.19
7	a	4	MAN	C1-O5-C5	3.08	116.31	112.19
6	S	4	MAN	C1-C2-C3	3.07	114.11	109.64
7	O	3	BMA	O5-C1-C2	2.97	117.88	110.79
7	a	2	NAG	O5-C1-C2	-2.95	106.73	111.29
6	N	2	NAG	C1-O5-C5	2.91	116.08	112.19
6	W	5	MAN	O5-C1-C2	2.82	117.51	110.79
6	S	2	NAG	C1-O5-C5	2.76	115.89	112.19
6	W	3	BMA	O5-C1-C2	2.74	117.33	110.79
6	S	2	NAG	O4-C4-C5	2.70	115.96	109.32
6	S	3	BMA	O3-C3-C4	2.67	116.67	110.38
6	W	4	MAN	C1-C2-C3	2.65	113.50	109.64
6	S	4	MAN	C3-C4-C5	2.65	115.03	110.23
6	S	6	MAN	O5-C1-C2	2.64	117.10	110.79
6	N	3	BMA	C1-C2-C3	-2.63	105.82	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	6	MAN	O5-C1-C2	2.62	117.03	110.79
6	N	3	BMA	C1-O5-C5	2.57	115.63	112.19
7	O	2	NAG	O5-C1-C2	-2.57	107.32	111.29
7	O	3	BMA	C1-O5-C5	2.56	115.61	112.19
7	V	3	BMA	O2-C2-C1	2.55	115.07	109.22
6	W	2	NAG	O4-C4-C5	2.55	115.61	109.32
6	S	5	MAN	O5-C1-C2	2.53	116.82	110.79
7	V	1	NAG	O5-C1-C2	-2.49	107.44	111.29
6	W	3	BMA	O3-C3-C4	2.47	116.19	110.38
7	O	2	NAG	C1-O5-C5	2.46	115.48	112.19
6	W	6	MAN	O5-C1-C2	2.45	116.64	110.79
5	Q	2	NAG	C1-O5-C5	2.45	115.47	112.19
6	W	2	NAG	O5-C5-C4	-2.44	104.89	110.83
7	O	4	MAN	C1-C2-C3	2.44	113.19	109.64
6	S	3	BMA	O2-C2-C1	2.42	114.77	109.22
6	W	4	MAN	O5-C1-C2	2.40	116.51	110.79
6	N	3	BMA	O2-C2-C1	2.39	114.70	109.22
5	Y	2	NAG	C1-O5-C5	2.36	115.35	112.19
5	Z	2	NAG	C1-O5-C5	2.35	115.33	112.19
8	b	1	NAG	O5-C1-C2	-2.34	107.67	111.29
5	U	2	NAG	C1-O5-C5	2.33	115.31	112.19
6	N	2	NAG	O4-C4-C5	2.32	115.05	109.32
7	a	1	NAG	C1-C2-N2	2.30	114.05	110.43
5	Z	1	NAG	O5-C5-C4	-2.28	105.27	110.83
6	W	1	NAG	O4-C4-C3	-2.26	105.06	110.38
5	T	1	NAG	C1-C2-N2	-2.25	106.88	110.43
6	S	2	NAG	O5-C5-C4	-2.24	105.37	110.83
5	Z	2	NAG	C1-C2-N2	2.21	113.92	110.43
6	W	2	NAG	C1-O5-C5	2.19	115.13	112.19
7	O	3	BMA	O2-C2-C1	2.19	114.23	109.22
6	S	4	MAN	O3-C3-C2	-2.18	105.61	110.05
6	W	4	MAN	C3-C4-C5	2.15	114.14	110.23
7	a	2	NAG	C1-O5-C5	2.13	115.04	112.19
7	V	3	BMA	C1-C2-C3	-2.13	106.55	109.64
6	W	6	MAN	O2-C2-C3	-2.10	105.80	110.15
5	Z	2	NAG	C2-N2-C7	2.10	125.71	122.90
5	M	2	NAG	O4-C4-C3	-2.09	105.46	110.38
5	T	1	NAG	O4-C4-C3	-2.06	105.51	110.38
6	W	5	MAN	O4-C4-C3	-2.06	105.52	110.38
6	N	2	NAG	O5-C5-C4	-2.05	105.83	110.83
6	S	4	MAN	O5-C1-C2	2.05	115.68	110.79
6	W	6	MAN	C1-C2-C3	2.05	112.63	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	V	1	NAG	C2-N2-C7	2.03	125.62	122.90
5	U	2	NAG	O5-C1-C2	-2.02	108.16	111.29
7	O	4	MAN	C1-O5-C5	2.01	114.88	112.19
5	Q	2	NAG	C1-C2-N2	2.00	113.59	110.43

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	2	NAG	C1-C2-N2-C7
7	V	1	NAG	C1-C2-N2-C7
7	a	3	BMA	O5-C5-C6-O6
6	S	4	MAN	O5-C5-C6-O6
6	S	4	MAN	C4-C5-C6-O6
5	Z	2	NAG	O5-C5-C6-O6
6	S	5	MAN	O5-C5-C6-O6
6	W	5	MAN	O5-C5-C6-O6
7	O	2	NAG	O5-C5-C6-O6
7	V	3	BMA	O5-C5-C6-O6
7	a	1	NAG	C4-C5-C6-O6
5	P	2	NAG	O5-C5-C6-O6
6	N	5	MAN	O5-C5-C6-O6
5	T	2	NAG	O5-C5-C6-O6
6	W	4	MAN	O5-C5-C6-O6
6	W	4	MAN	C4-C5-C6-O6
5	Q	2	NAG	C1-C2-N2-C7
5	U	2	NAG	C1-C2-N2-C7
5	Y	2	NAG	C1-C2-N2-C7
5	Z	1	NAG	C1-C2-N2-C7
7	a	1	NAG	C1-C2-N2-C7
7	a	2	NAG	C1-C2-N2-C7
5	P	2	NAG	C3-C2-N2-C7
5	Y	2	NAG	C3-C2-N2-C7
5	Z	1	NAG	C3-C2-N2-C7
8	b	2	NAG	C3-C2-N2-C7
7	a	1	NAG	O5-C5-C6-O6
5	M	2	NAG	C1-C2-N2-C7
5	P	2	NAG	C1-C2-N2-C7
5	R	2	NAG	C1-C2-N2-C7
5	X	2	NAG	C1-C2-N2-C7
8	b	1	NAG	C1-C2-N2-C7
8	b	2	NAG	C1-C2-N2-C7

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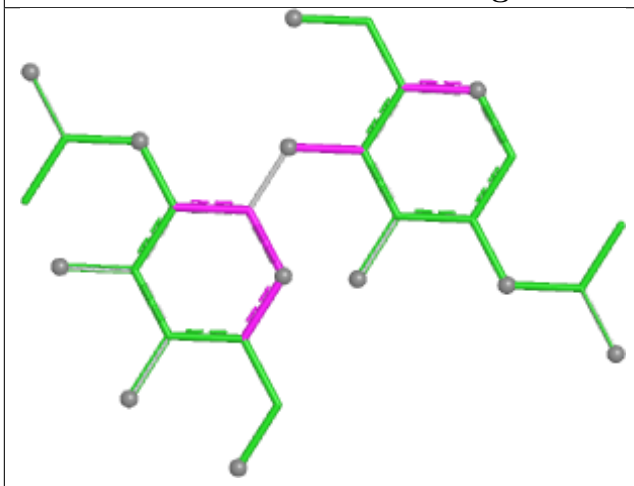
Mol	Chain	Res	Type	Atoms
5	Y	1	NAG	C4-C5-C6-O6
5	Q	2	NAG	C3-C2-N2-C7
5	U	2	NAG	C3-C2-N2-C7
7	V	1	NAG	C3-C2-N2-C7
7	a	1	NAG	C3-C2-N2-C7
7	a	2	NAG	C3-C2-N2-C7
8	b	1	NAG	C3-C2-N2-C7
7	a	3	BMA	C4-C5-C6-O6

There are no ring outliers.

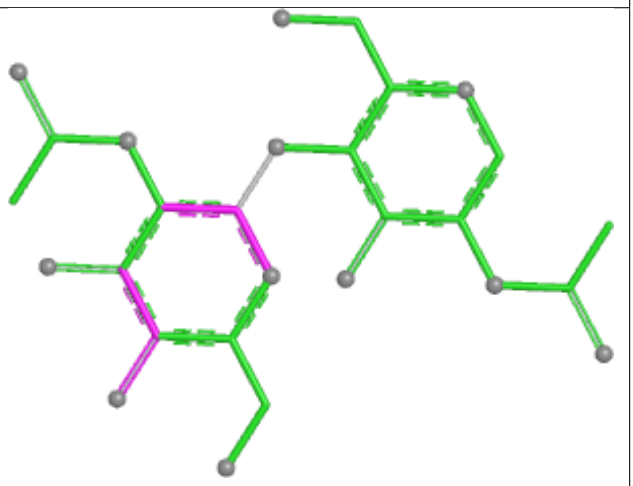
No monomer is involved in short contacts.

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

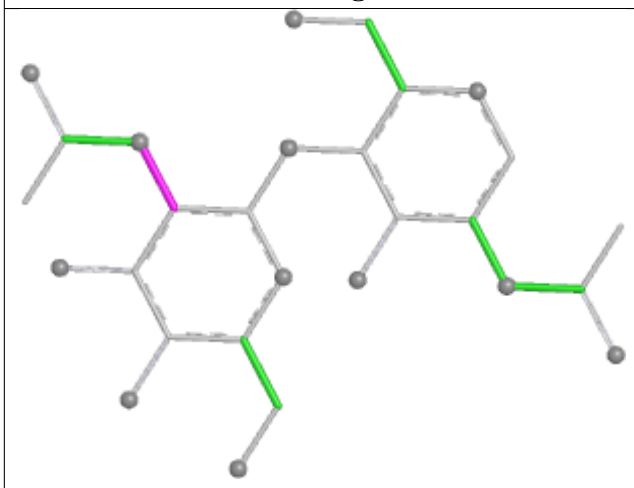
Oligosaccharide Chain M



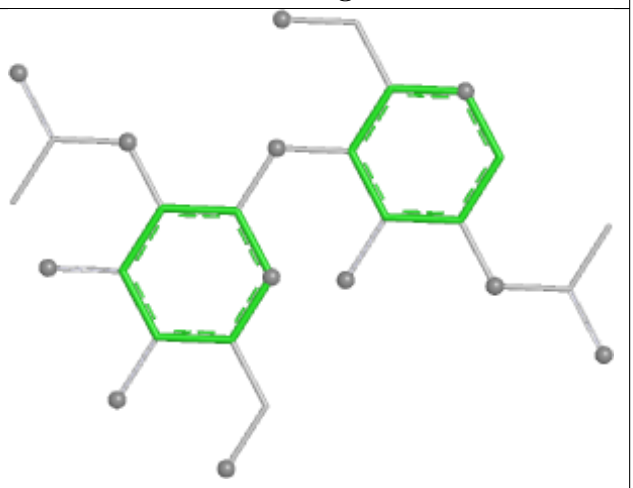
Bond lengths



Bond angles

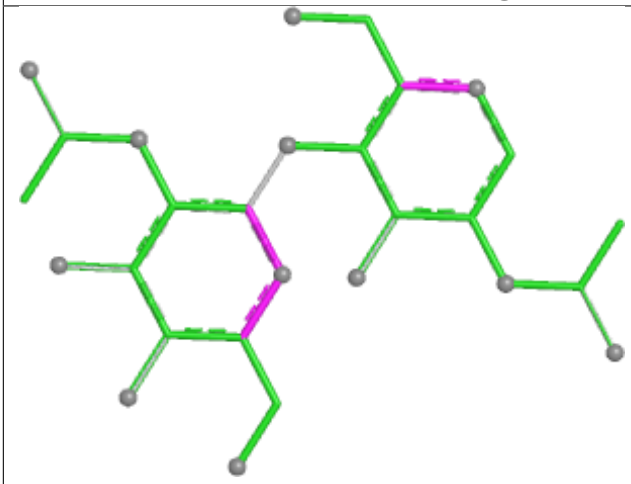


Torsions

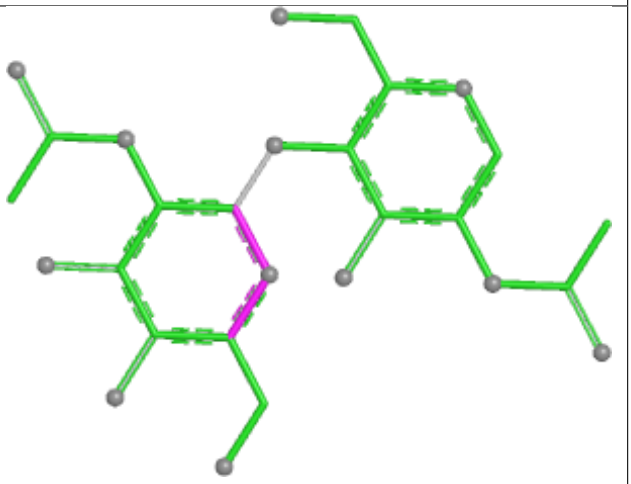


Rings

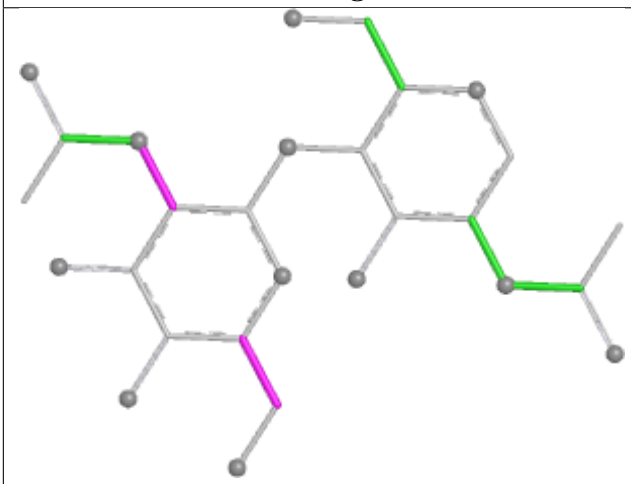
Oligosaccharide Chain P



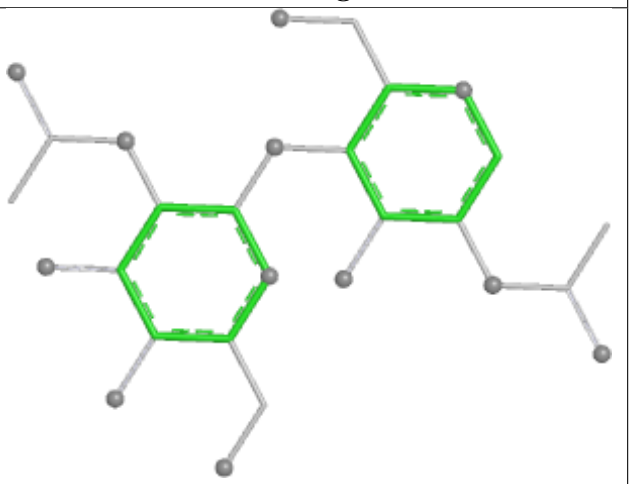
Bond lengths



Bond angles

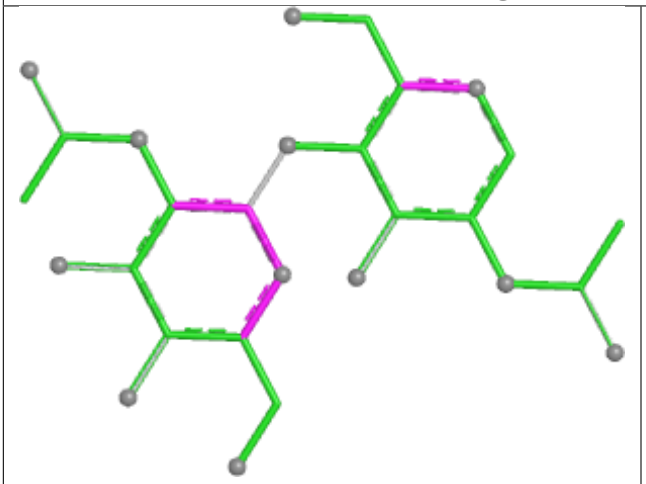


Torsions

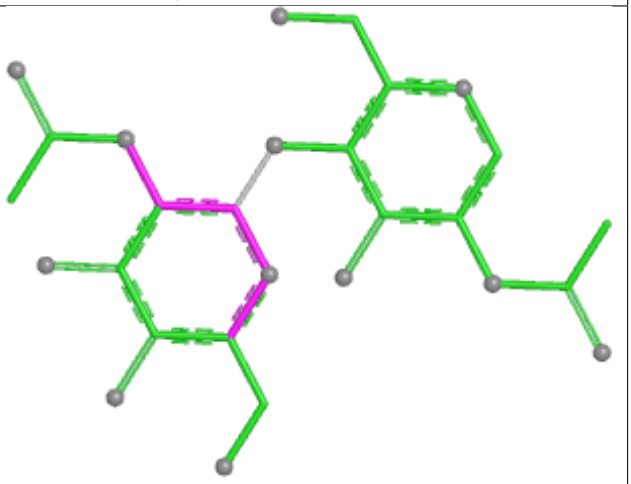


Rings

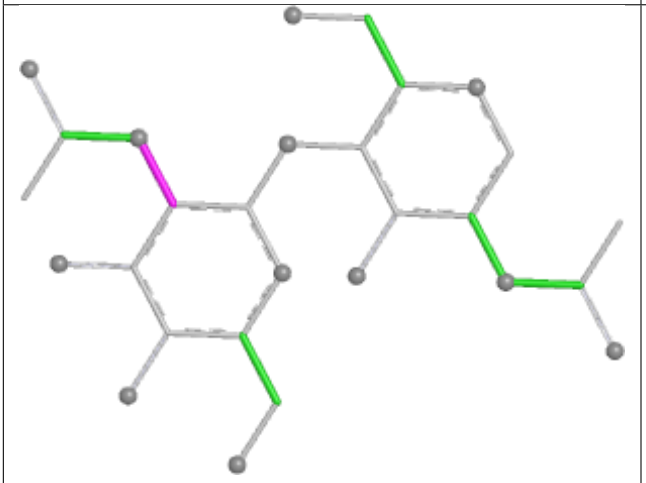
Oligosaccharide Chain Q



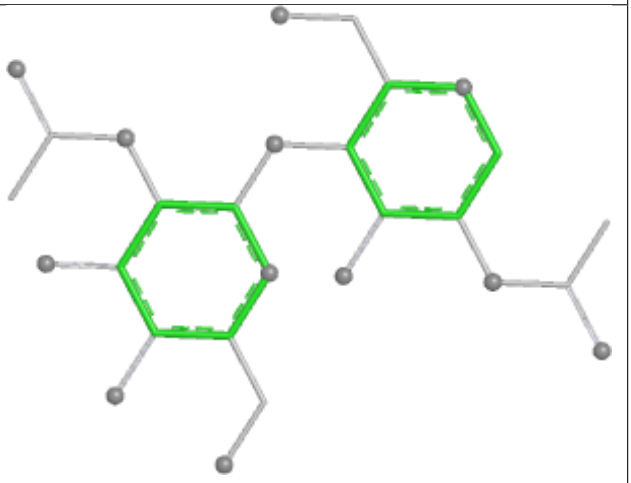
Bond lengths



Bond angles

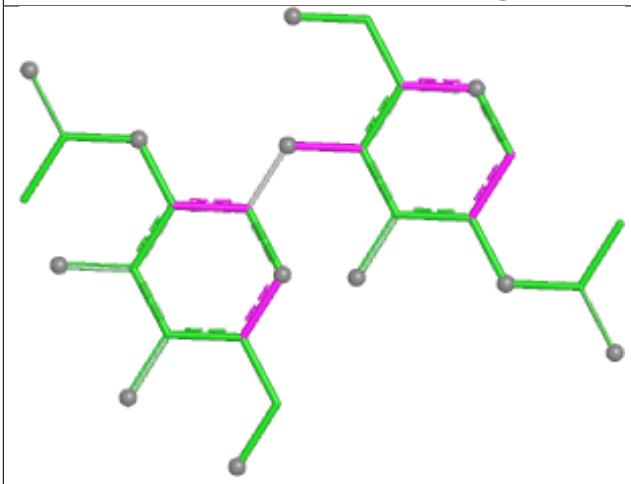


Torsions

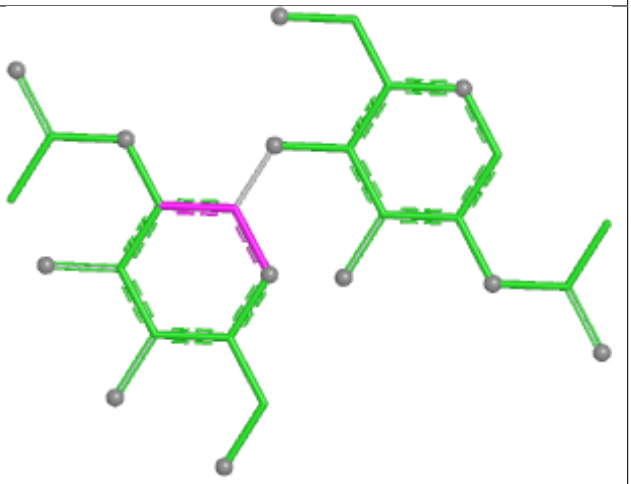


Rings

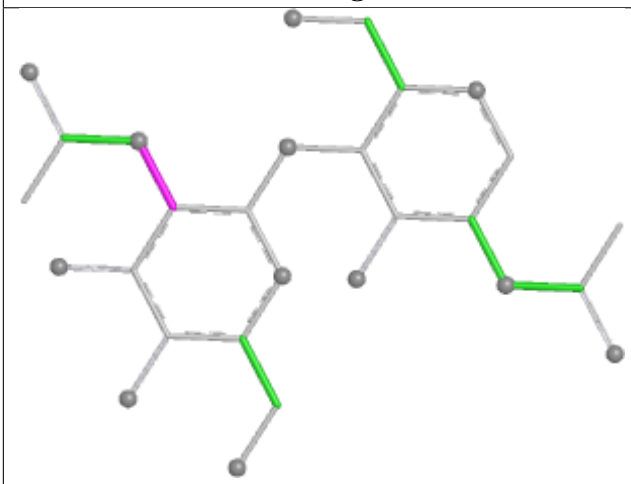
Oligosaccharide Chain R



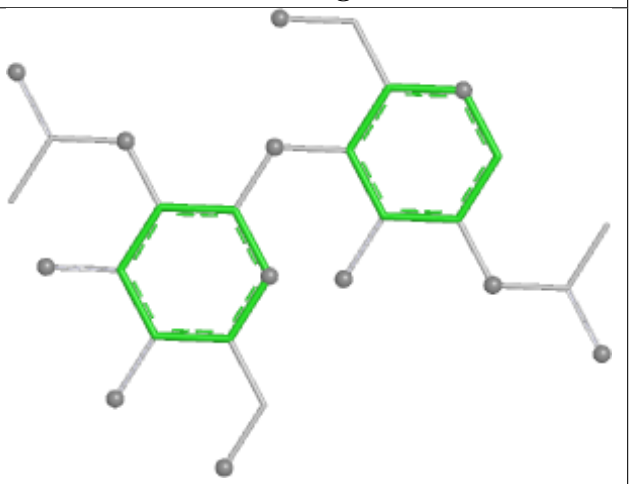
Bond lengths



Bond angles

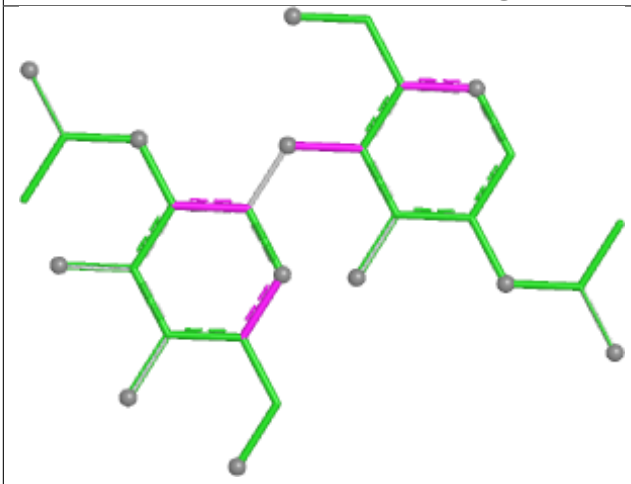


Torsions



Rings

Oligosaccharide Chain T



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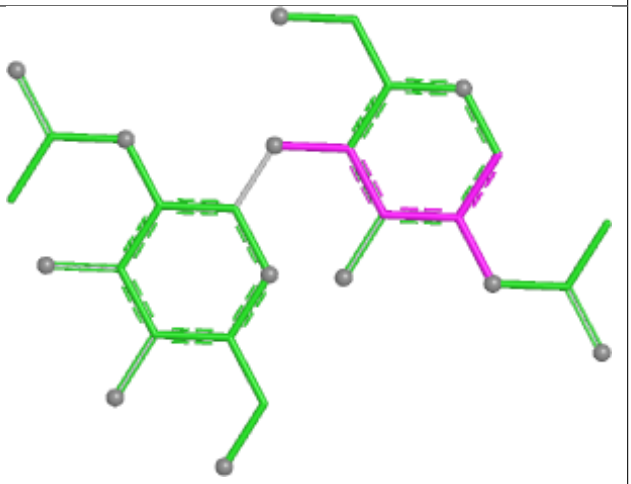

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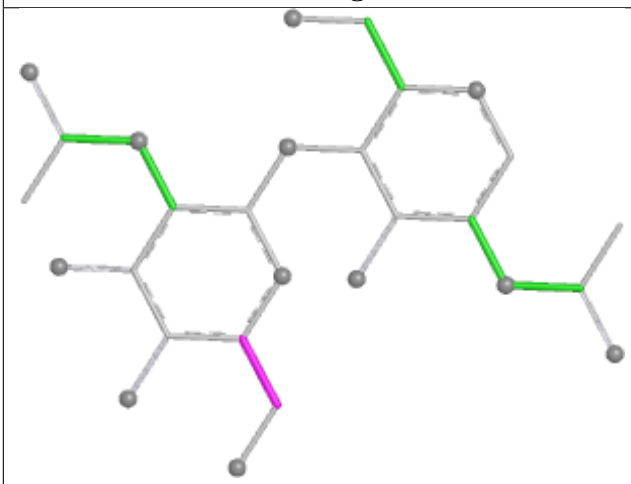

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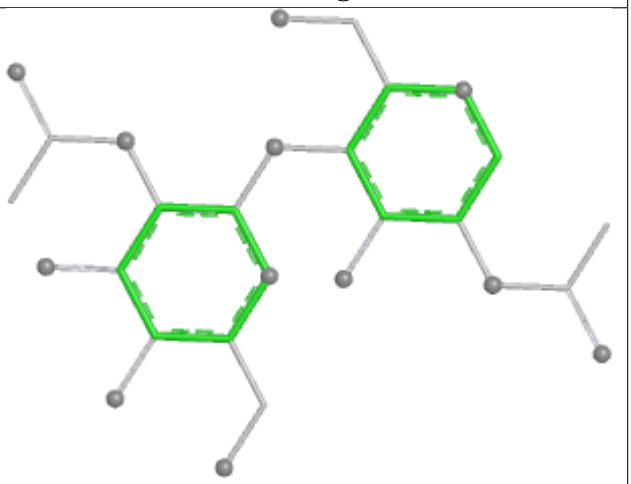
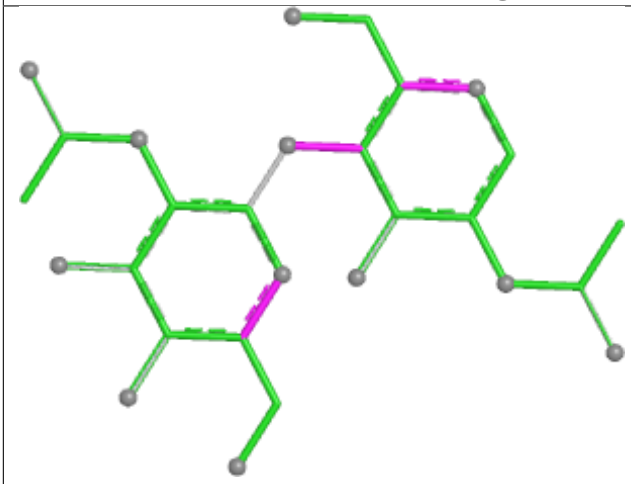


Rings

Oligosaccharide Chain U



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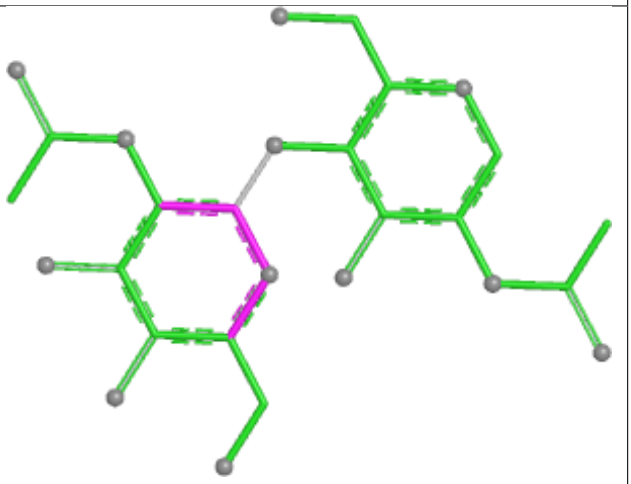
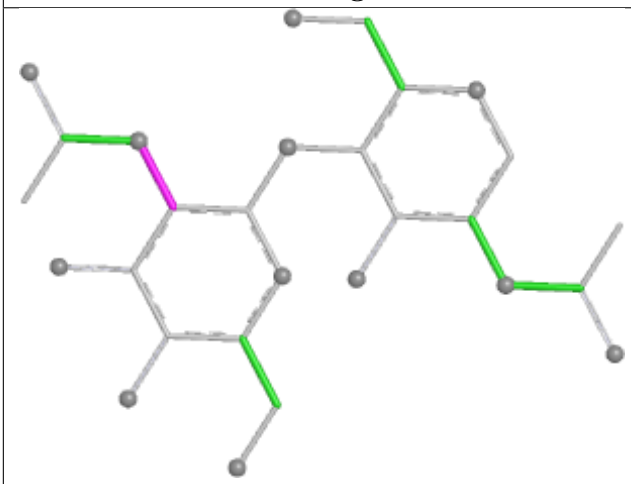
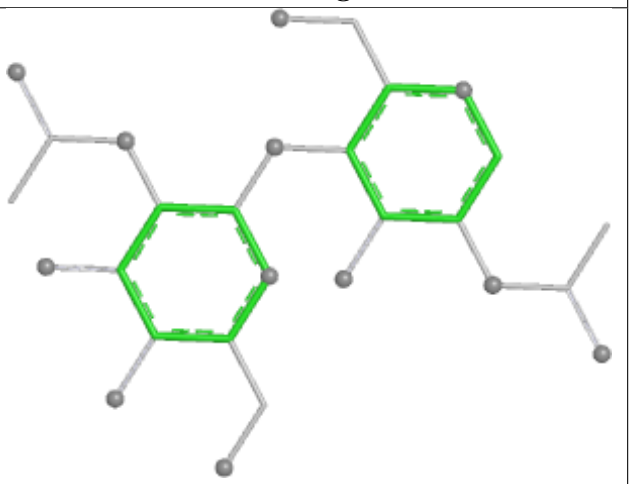


Bond angles

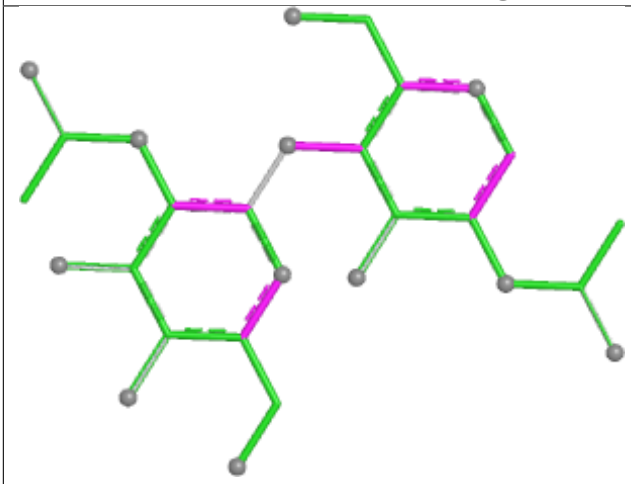


Torsions

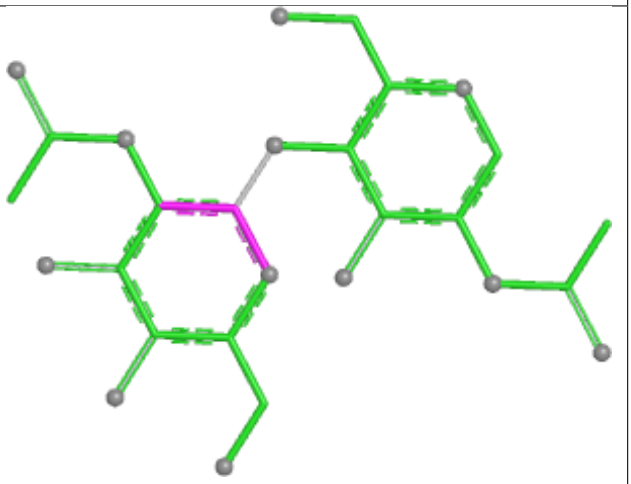


Rings

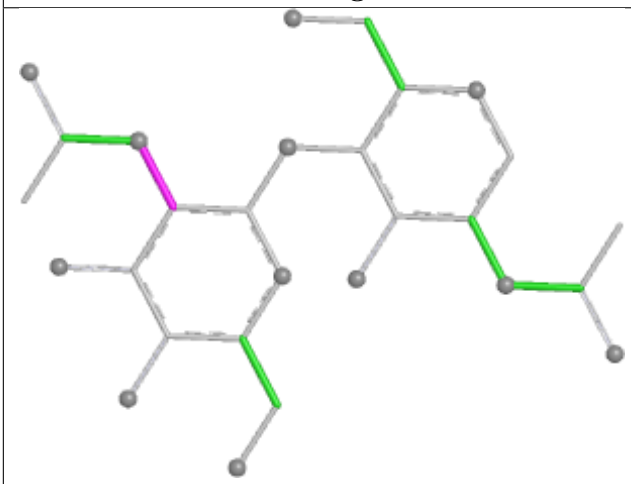
Oligosaccharide Chain X



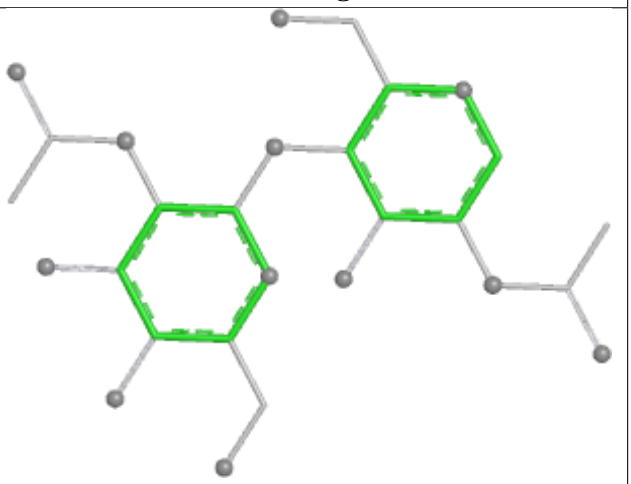
Bond lengths



Bond angles

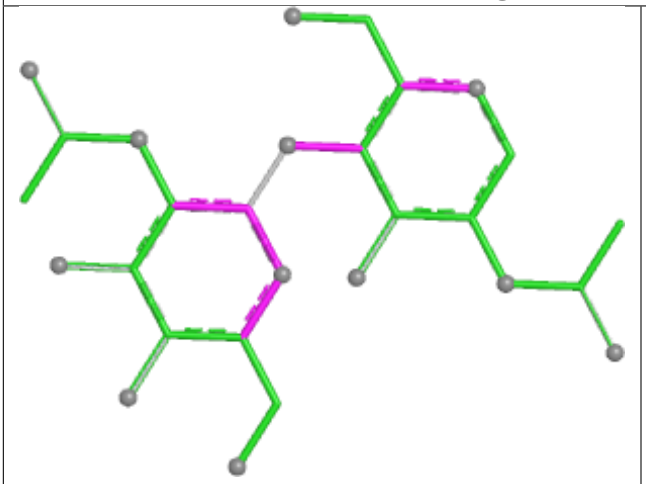


Torsions

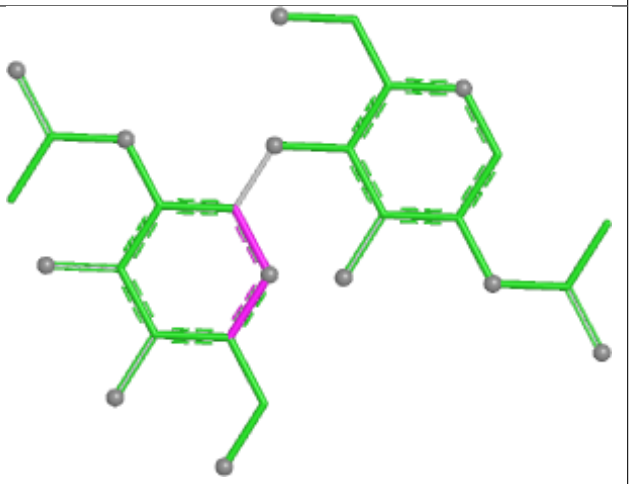


Rings

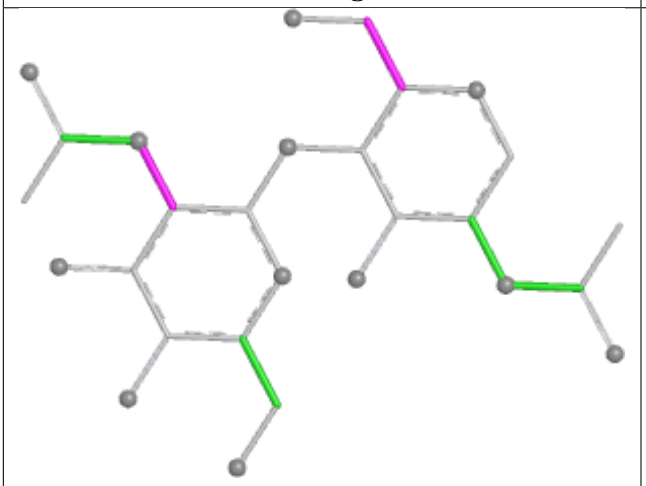
Oligosaccharide Chain Y



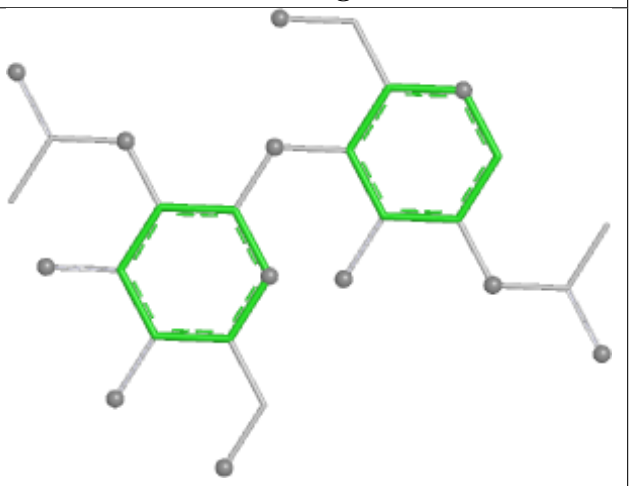
Bond lengths



Bond angles

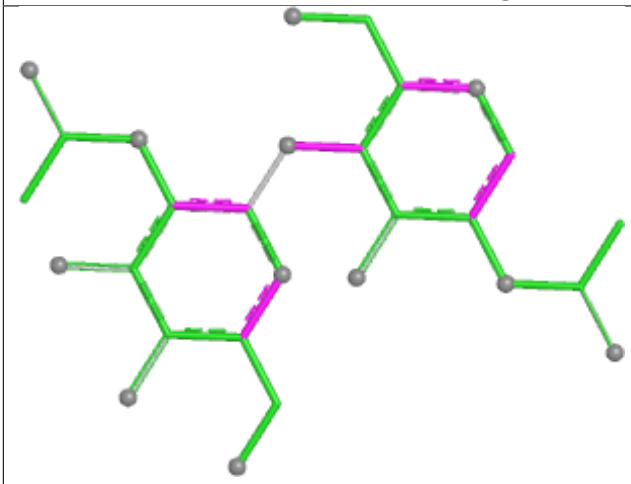


Torsions

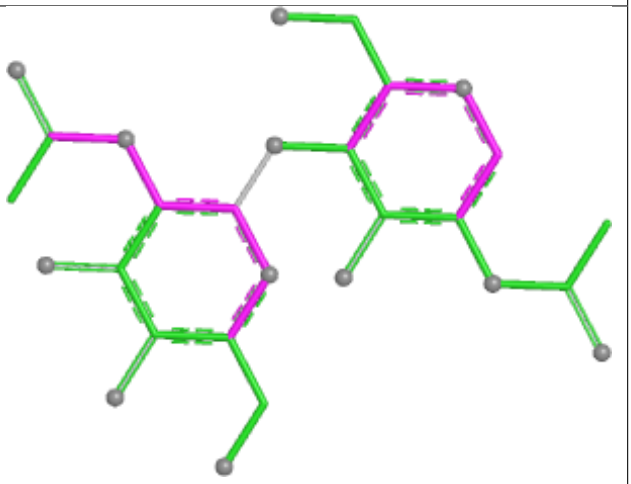


Rings

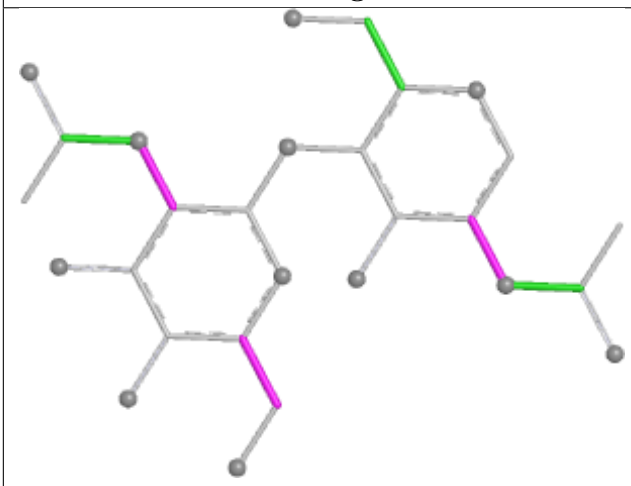
Oligosaccharide Chain Z



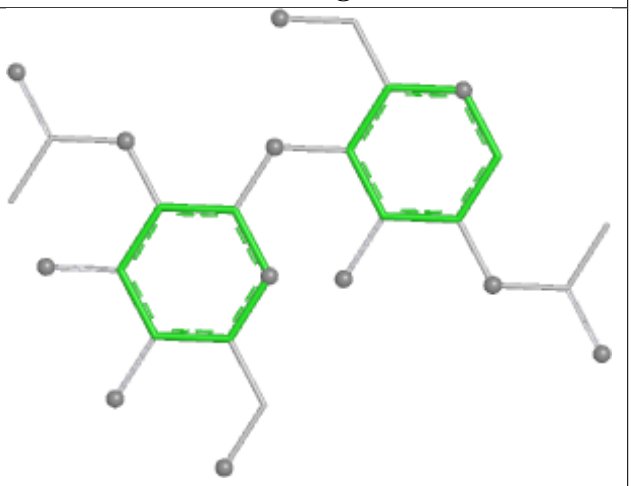
Bond lengths



Bond angles

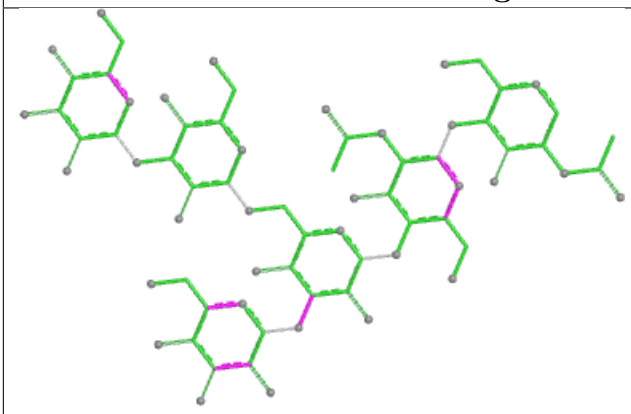


Torsions

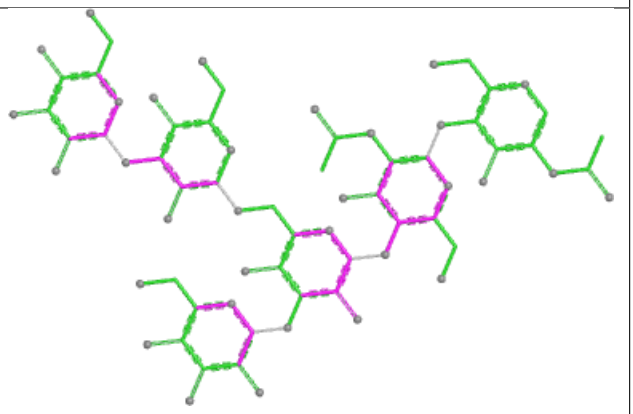


Rings

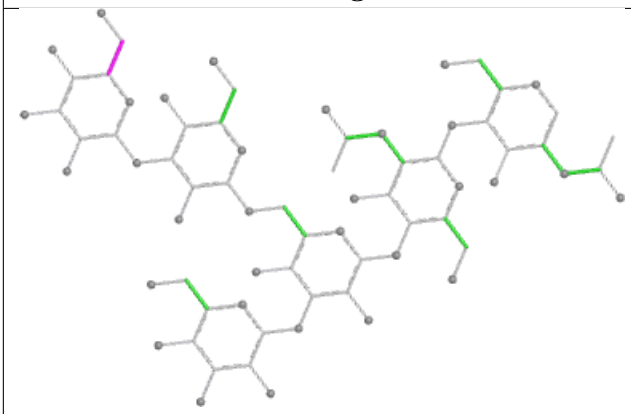
Oligosaccharide Chain N



Bond lengths



Bond angles



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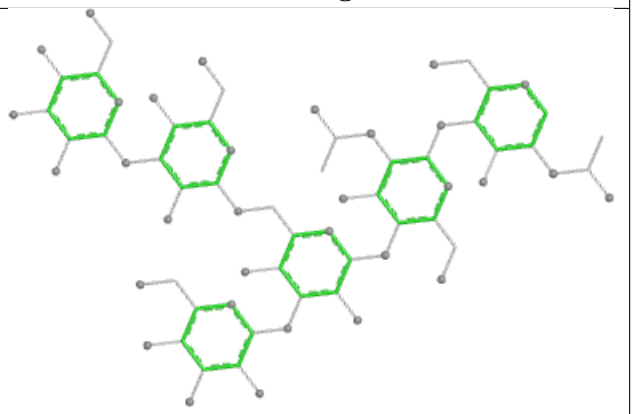
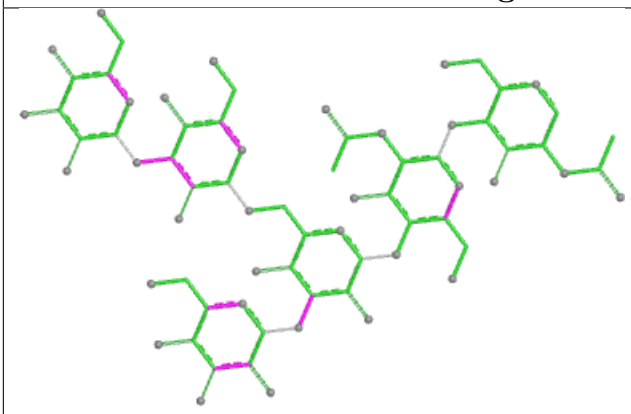


Rings

Oligosaccharide Chain S



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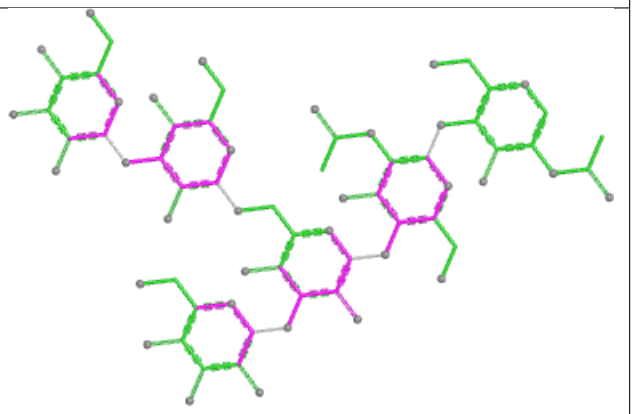

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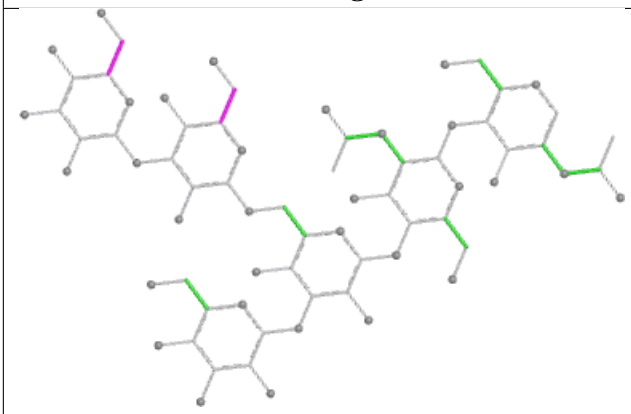
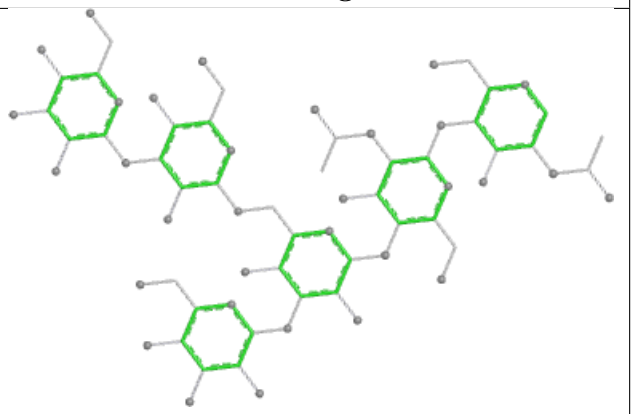
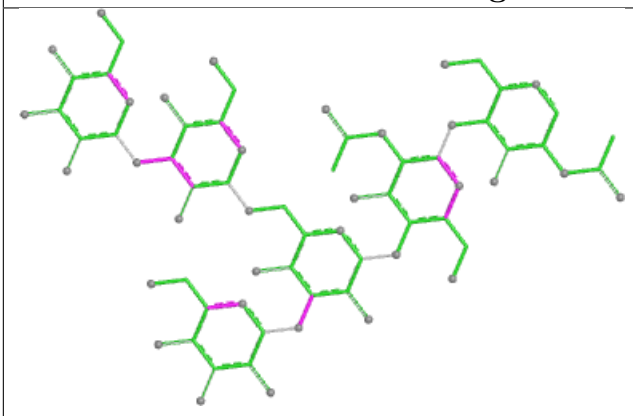


Torsions



Rings

Oligosaccharide Chain W



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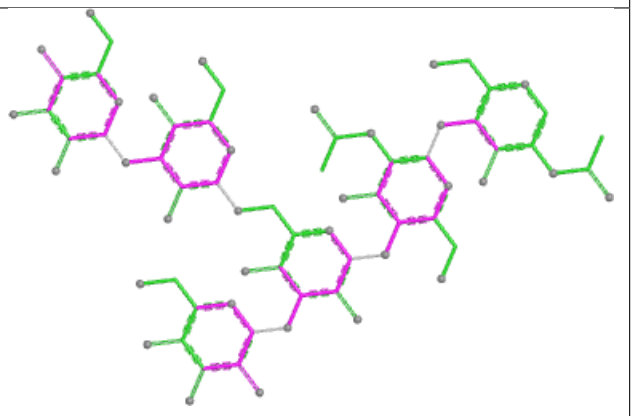
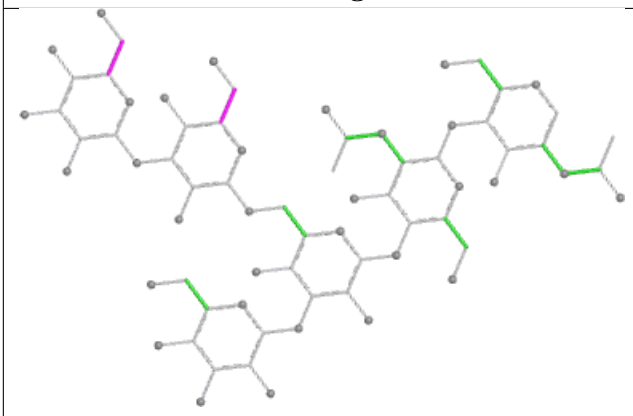


Bond angles



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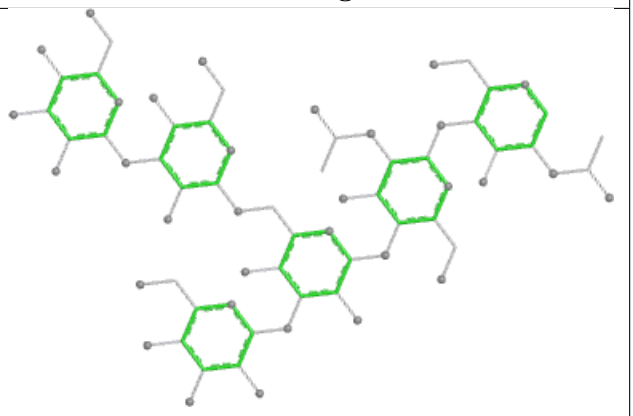
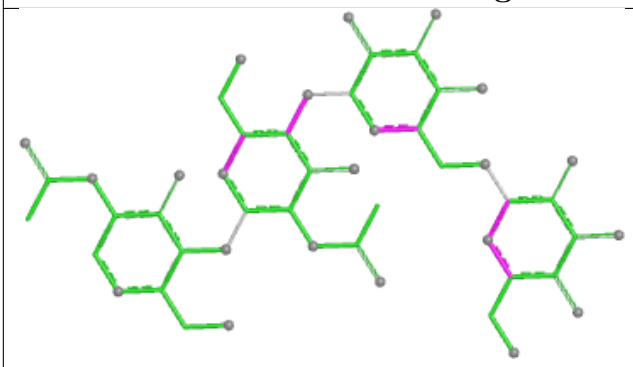
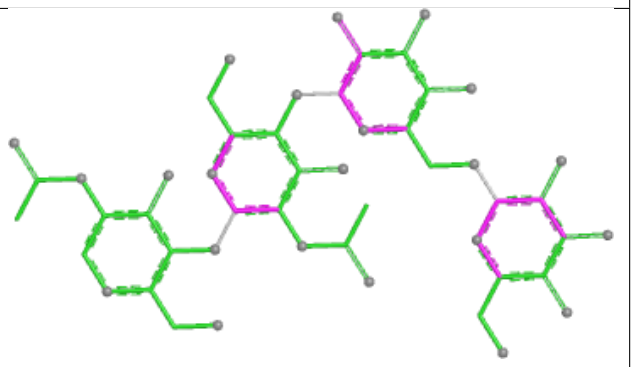


Rings

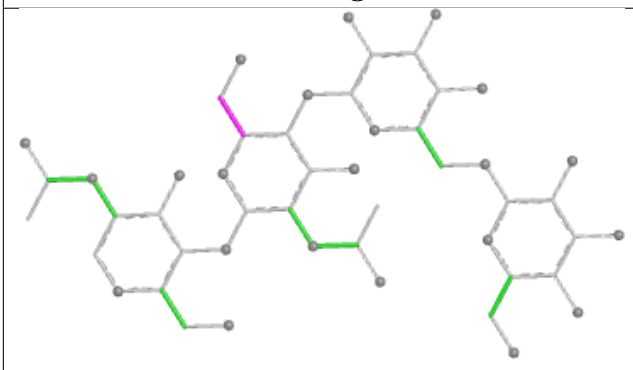
Oligosaccharide Chain O



Bond lengths



Bond angles



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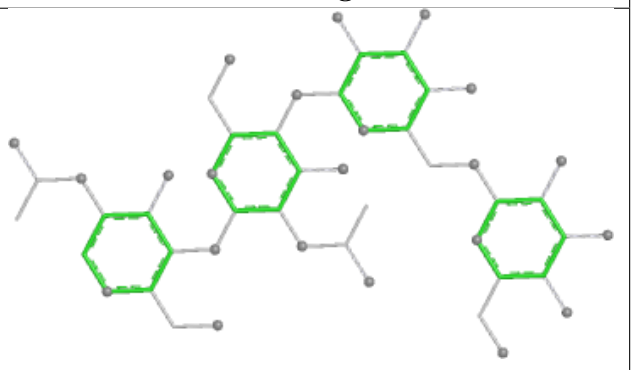
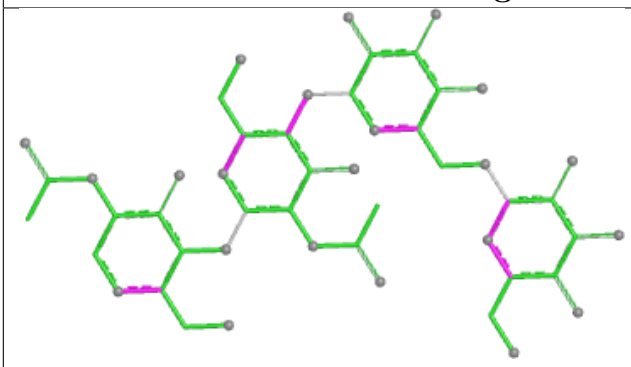
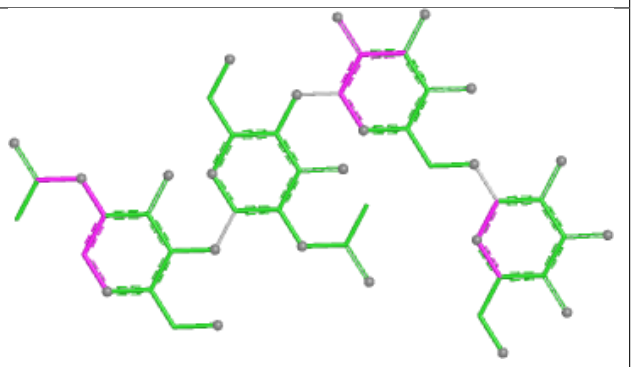


Rings

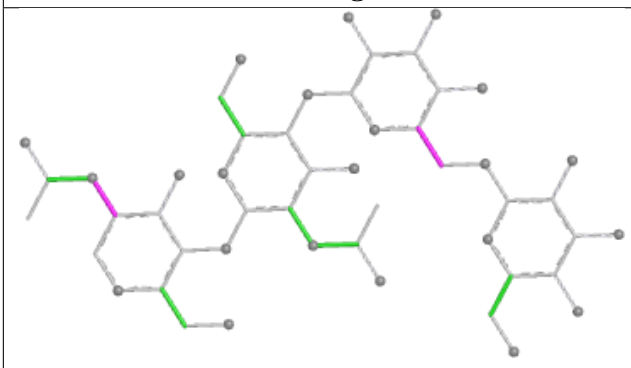
Oligosaccharide Chain V



Bond lengths



Bond angles



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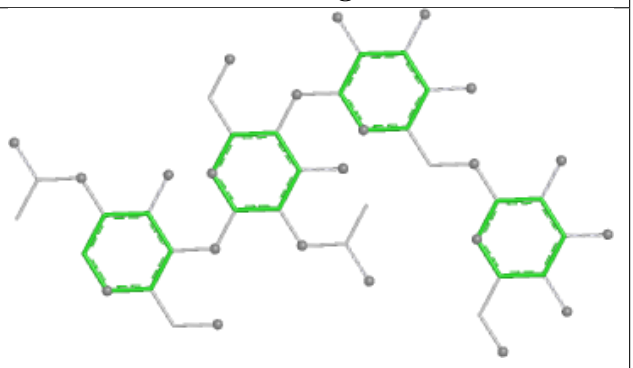
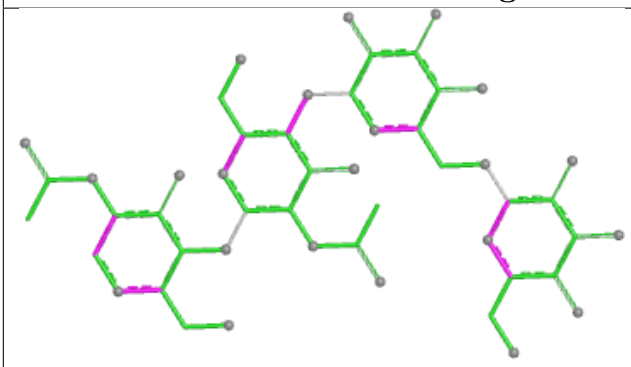
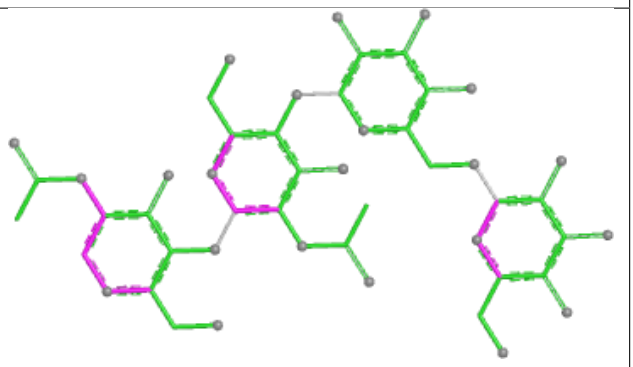


Rings

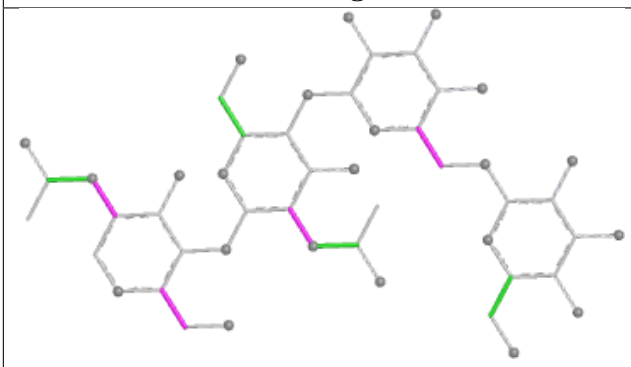
Oligosaccharide Chain a



Bond lengths



Bond angles



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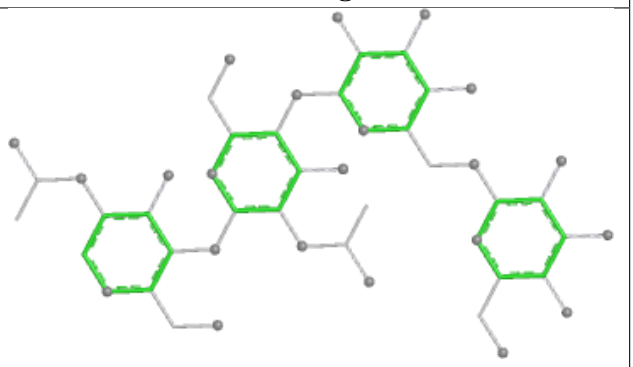
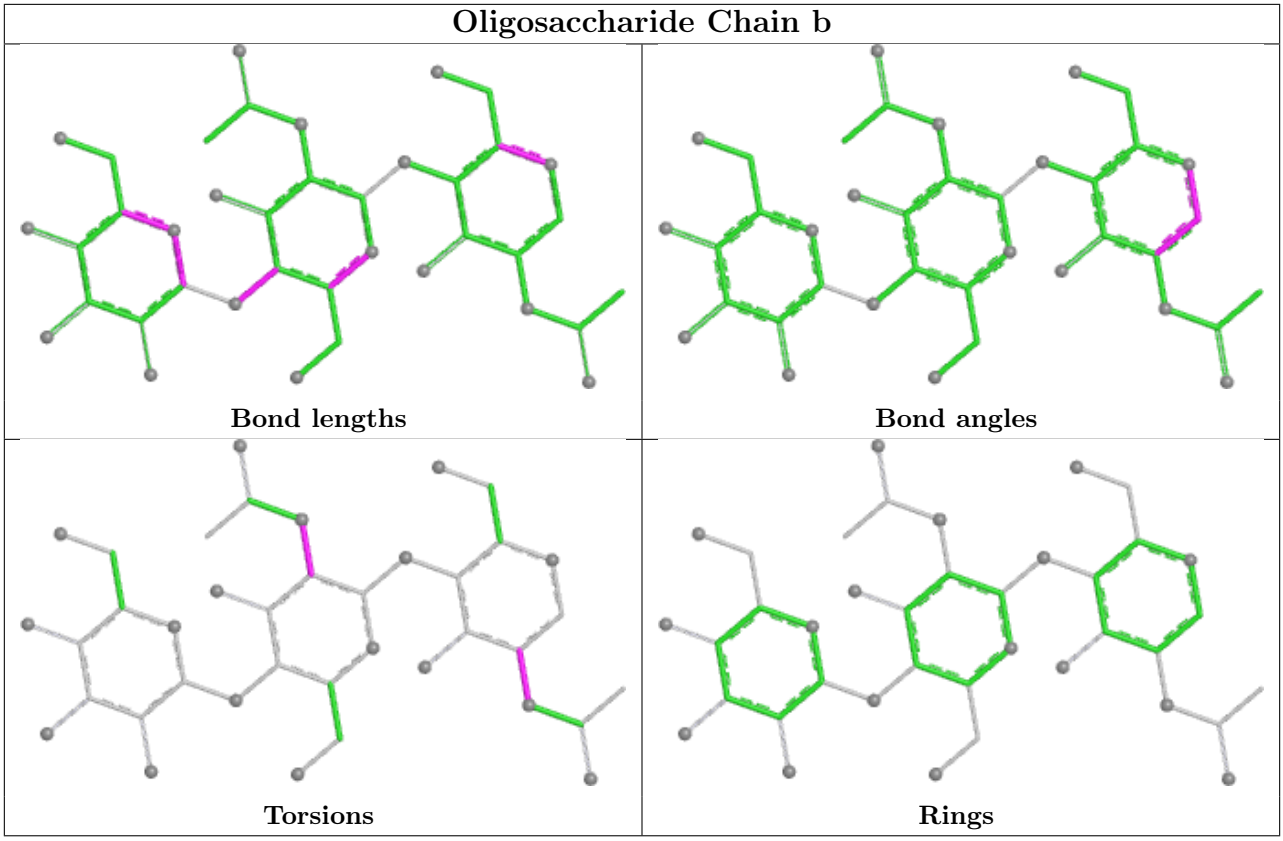


Rings



5.6 Ligand geometry (i)

18 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	A	601	1	14,14,15	1.08	1 (7%)	17,19,21	0.72	0
9	NAG	A	606	1	14,14,15	1.19	2 (14%)	17,19,21	0.87	1 (5%)
9	NAG	E	603	1	14,14,15	1.34	2 (14%)	17,19,21	0.77	1 (5%)
9	NAG	E	604	1	14,14,15	1.15	1 (7%)	17,19,21	0.69	0
9	NAG	I	602	1	14,14,15	1.03	1 (7%)	17,19,21	0.76	0
9	NAG	I	601	1	14,14,15	1.30	3 (21%)	17,19,21	0.89	1 (5%)
9	NAG	A	603	1	14,14,15	1.17	1 (7%)	17,19,21	1.18	1 (5%)
9	NAG	I	603	1	14,14,15	1.17	1 (7%)	17,19,21	0.78	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	NAG	I	605	1	14,14,15	1.25	2 (14%)	17,19,21	1.42	1 (5%)
9	NAG	A	602	1	14,14,15	1.17	2 (14%)	17,19,21	0.84	0
9	NAG	A	604	1	14,14,15	1.22	2 (14%)	17,19,21	0.69	0
9	NAG	A	605	1	14,14,15	1.22	1 (7%)	17,19,21	0.85	1 (5%)
9	NAG	I	604	1	14,14,15	1.16	1 (7%)	17,19,21	0.55	0
9	NAG	E	601	1	14,14,15	1.11	1 (7%)	17,19,21	0.75	1 (5%)
9	NAG	I	606	1	14,14,15	1.08	1 (7%)	17,19,21	0.90	1 (5%)
9	NAG	E	606	1	14,14,15	1.16	2 (14%)	17,19,21	0.75	0
9	NAG	E	605	1	14,14,15	1.10	1 (7%)	17,19,21	0.79	0
9	NAG	E	602	1	14,14,15	1.24	2 (14%)	17,19,21	1.17	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NAG	A	601	1	-	1/6/23/26	0/1/1/1
9	NAG	A	606	1	-	0/6/23/26	0/1/1/1
9	NAG	E	603	1	-	2/6/23/26	0/1/1/1
9	NAG	E	604	1	-	1/6/23/26	0/1/1/1
9	NAG	I	602	1	-	1/6/23/26	0/1/1/1
9	NAG	I	601	1	-	0/6/23/26	0/1/1/1
9	NAG	A	603	1	-	1/6/23/26	0/1/1/1
9	NAG	I	603	1	-	1/6/23/26	0/1/1/1
9	NAG	I	605	1	-	1/6/23/26	0/1/1/1
9	NAG	A	602	1	-	0/6/23/26	0/1/1/1
9	NAG	A	604	1	-	0/6/23/26	0/1/1/1
9	NAG	A	605	1	-	2/6/23/26	0/1/1/1
9	NAG	I	604	1	-	0/6/23/26	0/1/1/1
9	NAG	E	601	1	-	0/6/23/26	0/1/1/1
9	NAG	I	606	1	-	0/6/23/26	0/1/1/1
9	NAG	E	606	1	-	0/6/23/26	0/1/1/1
9	NAG	E	605	1	-	1/6/23/26	0/1/1/1
9	NAG	E	602	1	-	1/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	605	NAG	O5-C5	2.92	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	603	NAG	O5-C5	2.91	1.49	1.43
9	I	601	NAG	O5-C5	2.82	1.48	1.43
9	A	605	NAG	O5-C5	2.76	1.48	1.43
9	E	604	NAG	O5-C5	2.71	1.48	1.43
9	E	602	NAG	O5-C5	2.67	1.48	1.43
9	A	602	NAG	O5-C5	2.61	1.48	1.43
9	I	603	NAG	O5-C5	2.58	1.48	1.43
9	A	603	NAG	O5-C5	2.57	1.48	1.43
9	I	606	NAG	O5-C5	2.50	1.48	1.43
9	E	601	NAG	O5-C5	2.50	1.48	1.43
9	I	604	NAG	O5-C5	2.48	1.48	1.43
9	A	604	NAG	O5-C5	2.46	1.48	1.43
9	E	606	NAG	O5-C5	2.45	1.48	1.43
9	A	606	NAG	O5-C5	2.30	1.47	1.43
9	E	603	NAG	C1-C2	2.27	1.55	1.52
9	A	604	NAG	C1-C2	2.23	1.55	1.52
9	A	602	NAG	C1-C2	2.22	1.55	1.52
9	A	606	NAG	C1-C2	2.19	1.55	1.52
9	E	605	NAG	O5-C5	2.19	1.47	1.43
9	I	601	NAG	C1-C2	2.18	1.55	1.52
9	A	601	NAG	O5-C5	2.15	1.47	1.43
9	I	601	NAG	O5-C1	2.13	1.47	1.43
9	E	602	NAG	C1-C2	2.07	1.55	1.52
9	E	606	NAG	C1-C2	2.05	1.55	1.52
9	I	605	NAG	O5-C1	2.01	1.47	1.43
9	I	602	NAG	O5-C5	2.00	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	605	NAG	C1-O5-C5	4.73	118.52	112.19
9	E	602	NAG	C1-O5-C5	3.97	117.50	112.19
9	A	603	NAG	C1-O5-C5	3.67	117.10	112.19
9	A	605	NAG	C1-O5-C5	2.73	115.85	112.19
9	I	601	NAG	C1-O5-C5	2.70	115.81	112.19
9	A	606	NAG	C1-O5-C5	2.69	115.79	112.19
9	E	603	NAG	C1-O5-C5	2.27	115.23	112.19
9	I	603	NAG	C1-O5-C5	2.24	115.19	112.19
9	I	606	NAG	C1-O5-C5	2.22	115.16	112.19
9	E	601	NAG	C1-O5-C5	2.15	115.07	112.19

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	E	604	NAG	O5-C5-C6-O6
9	A	605	NAG	O5-C5-C6-O6
9	I	605	NAG	O5-C5-C6-O6
9	A	603	NAG	O5-C5-C6-O6
9	E	605	NAG	O5-C5-C6-O6
9	I	603	NAG	O5-C5-C6-O6
9	A	601	NAG	O5-C5-C6-O6
9	E	602	NAG	O5-C5-C6-O6
9	I	602	NAG	O5-C5-C6-O6
9	E	603	NAG	C4-C5-C6-O6
9	E	603	NAG	O5-C5-C6-O6
9	A	605	NAG	C1-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

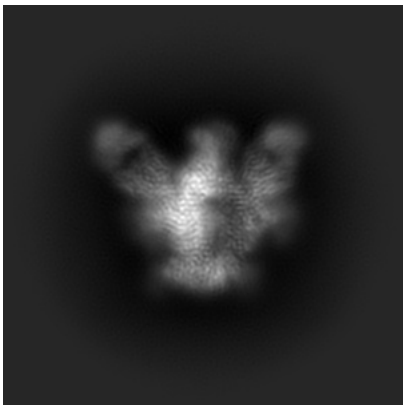
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-27624. These allow visual inspection of the internal detail of the map and identification of artifacts.

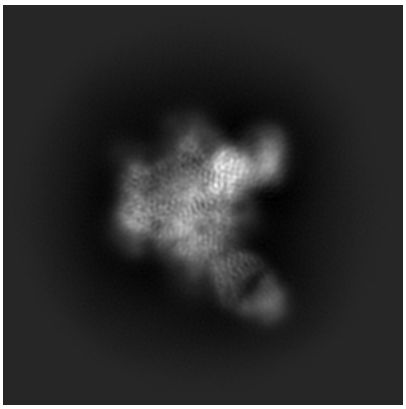
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

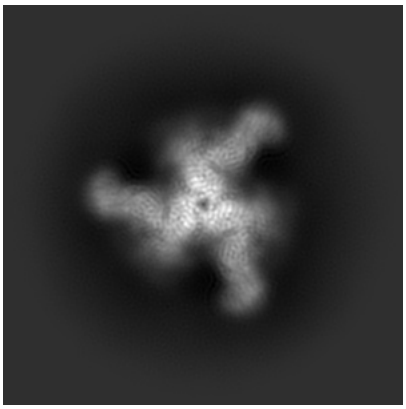
6.1.1 Primary map



X

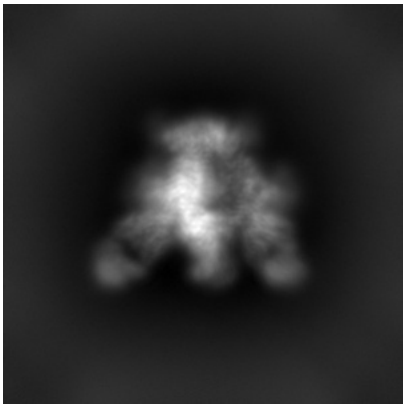


Y

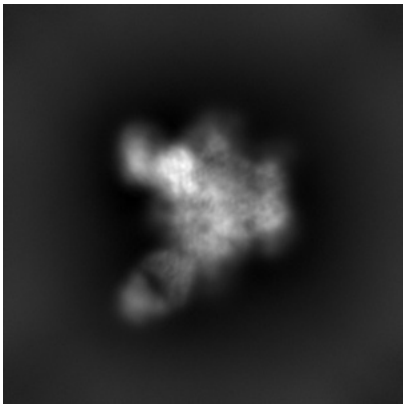


Z

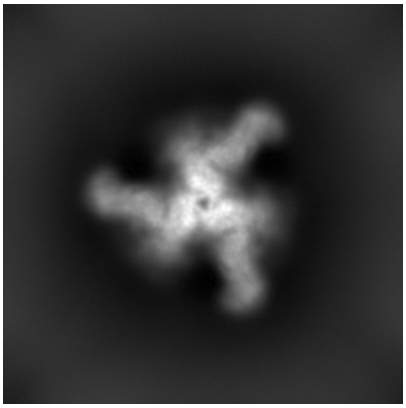
6.1.2 Raw map



X



Y

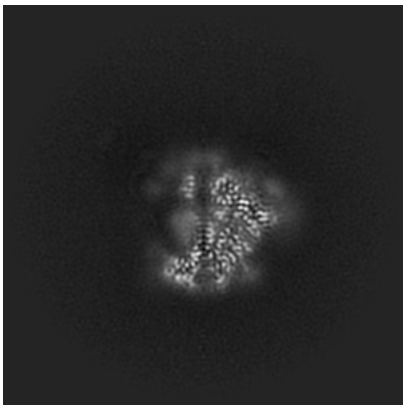


Z

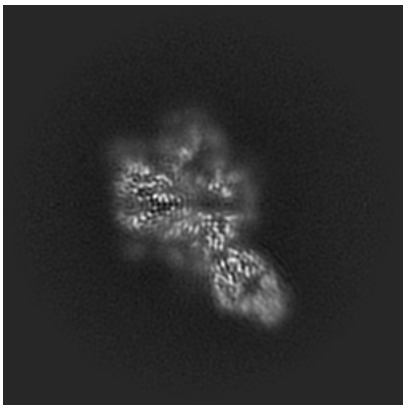
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

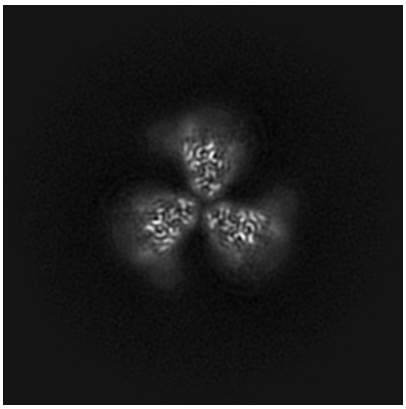
6.2.1 Primary map



X Index: 160

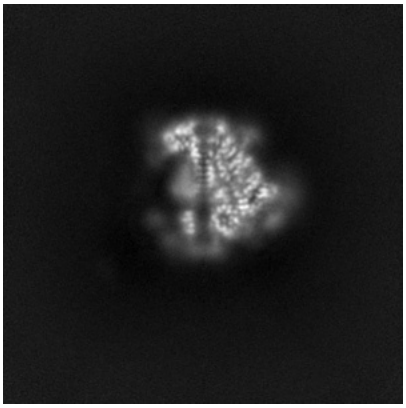


Y Index: 160

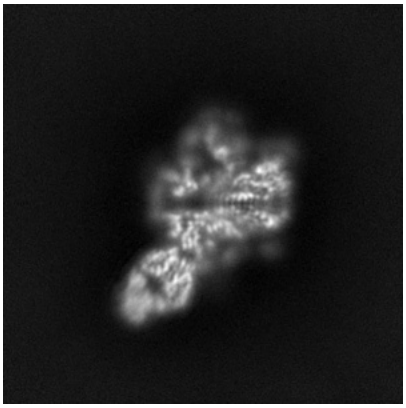


Z Index: 160

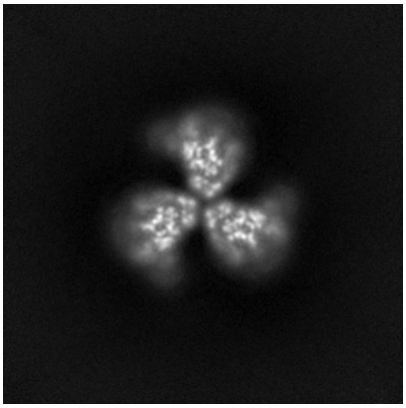
6.2.2 Raw map



X Index: 160



Y Index: 160

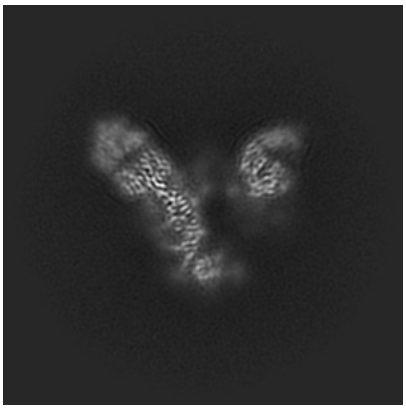


Z Index: 160

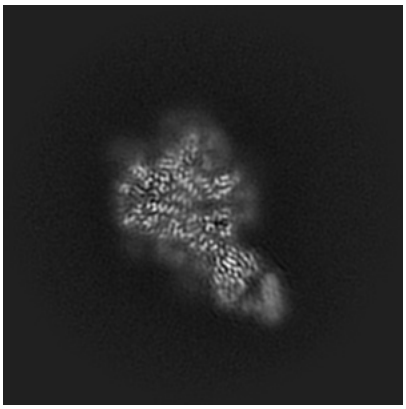
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

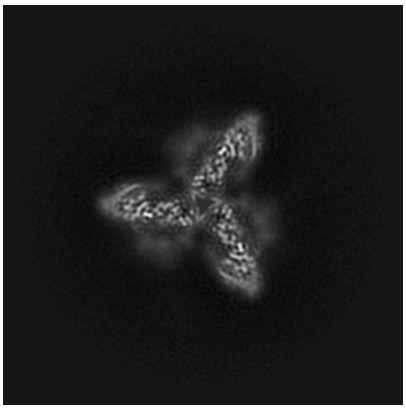
6.3.1 Primary map



X Index: 189

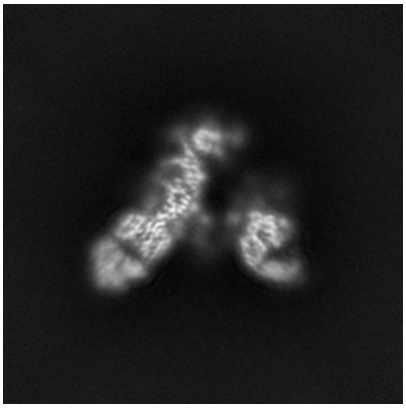


Y Index: 155

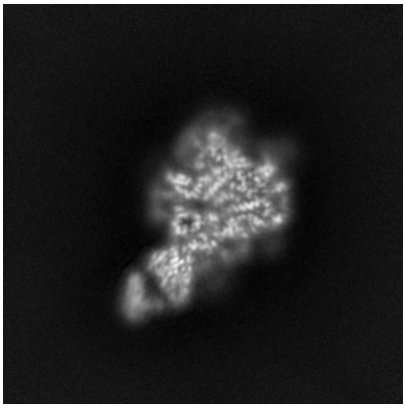


Z Index: 175

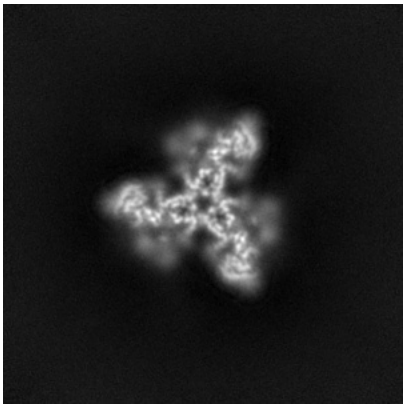
6.3.2 Raw map



X Index: 189



Y Index: 154



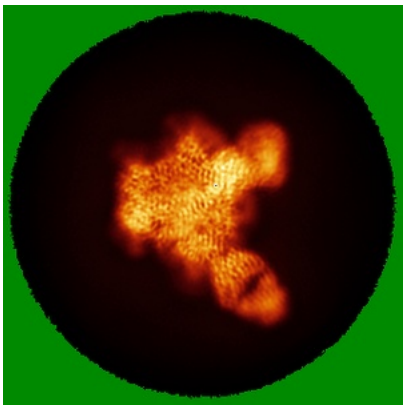
Z Index: 148

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

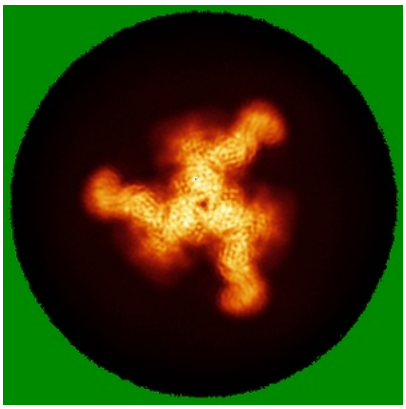
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map

X

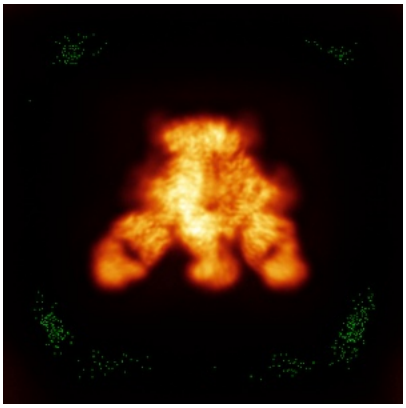


Y

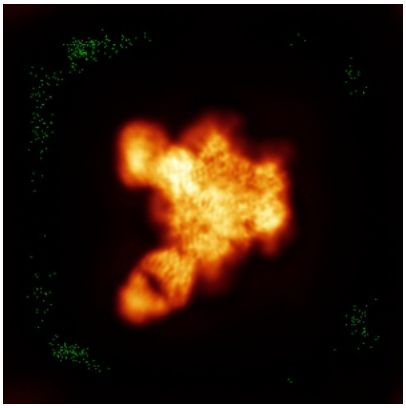


Z

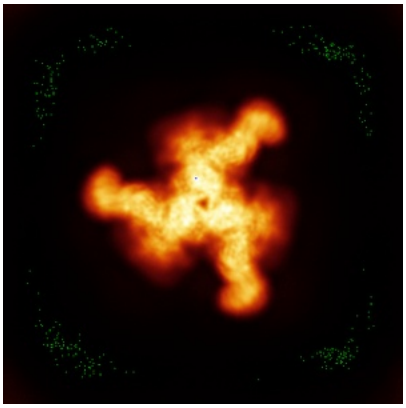
6.4.2 Raw map



X



Y

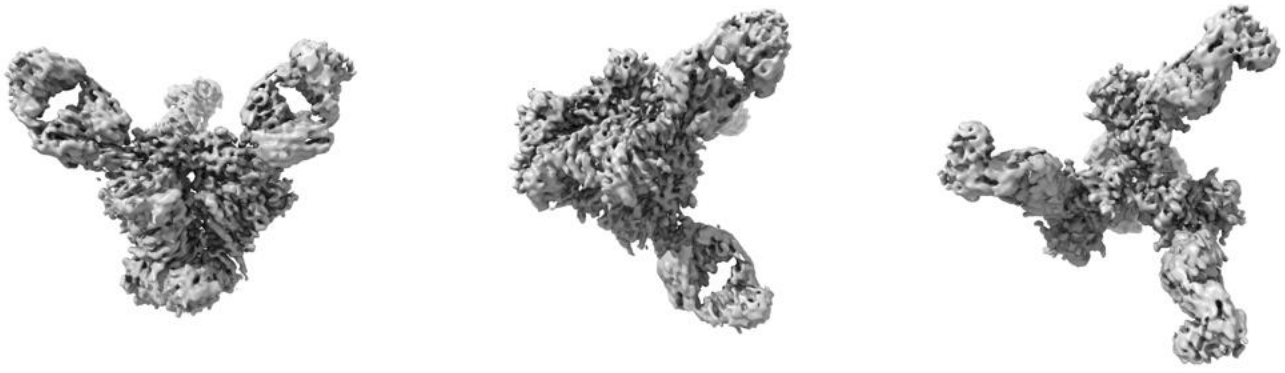


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

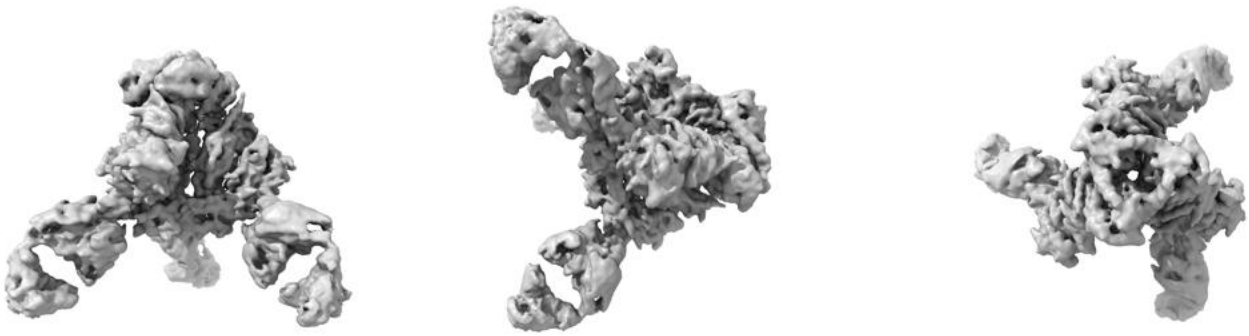
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.9. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

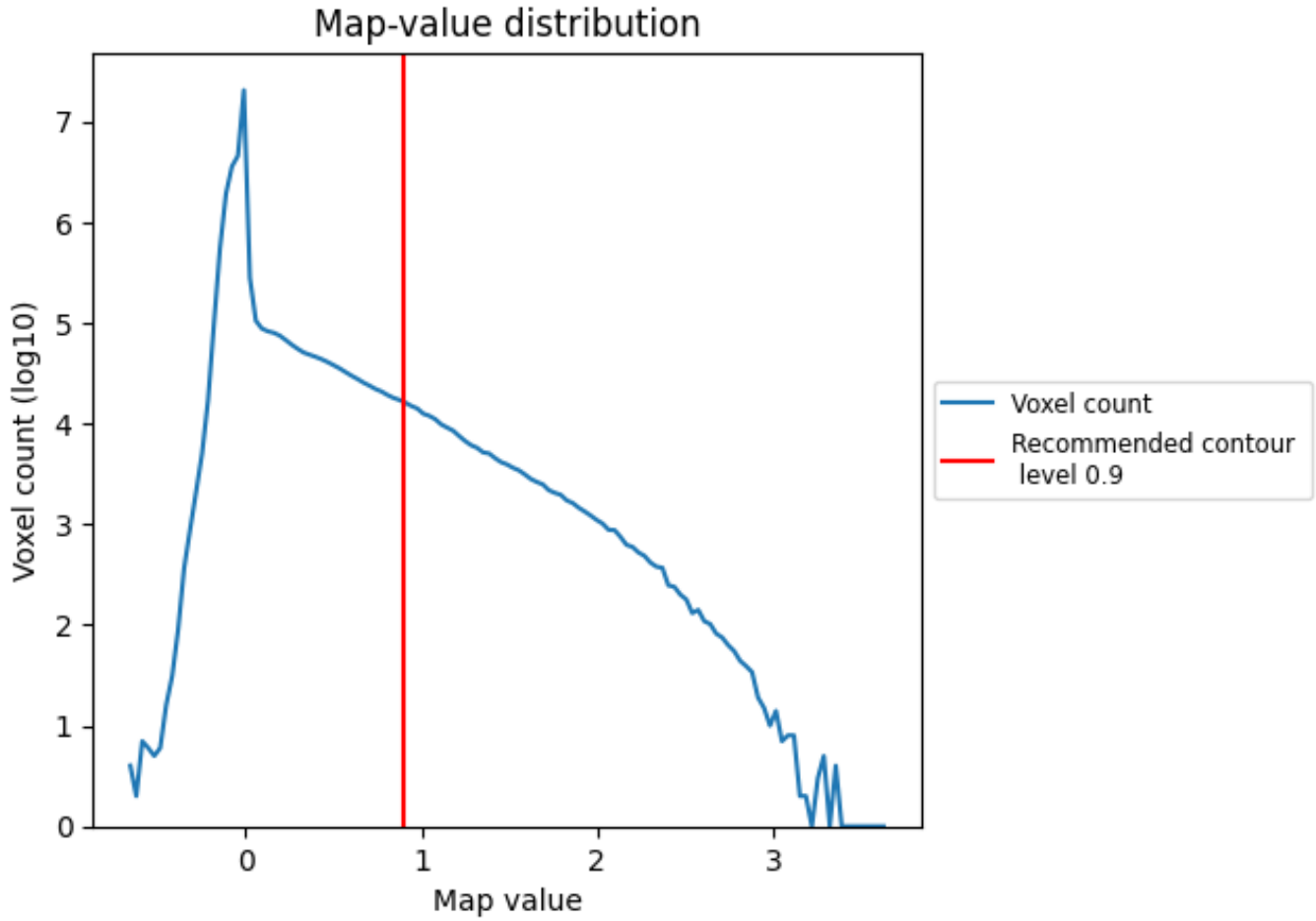
6.6 Mask visualisation (i)

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

7 Map analysis

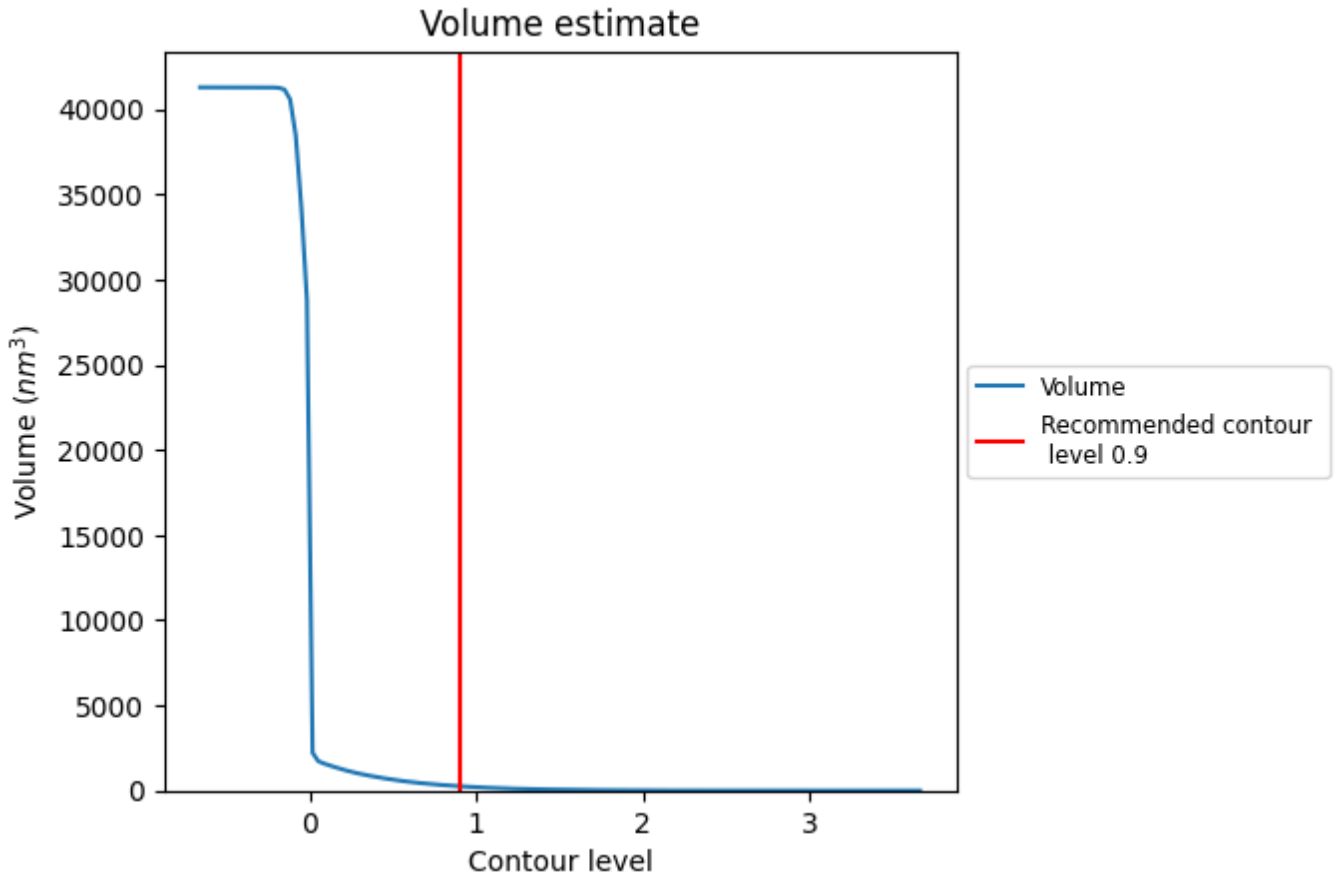
This section contains the results of statistical analysis of the map.

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.

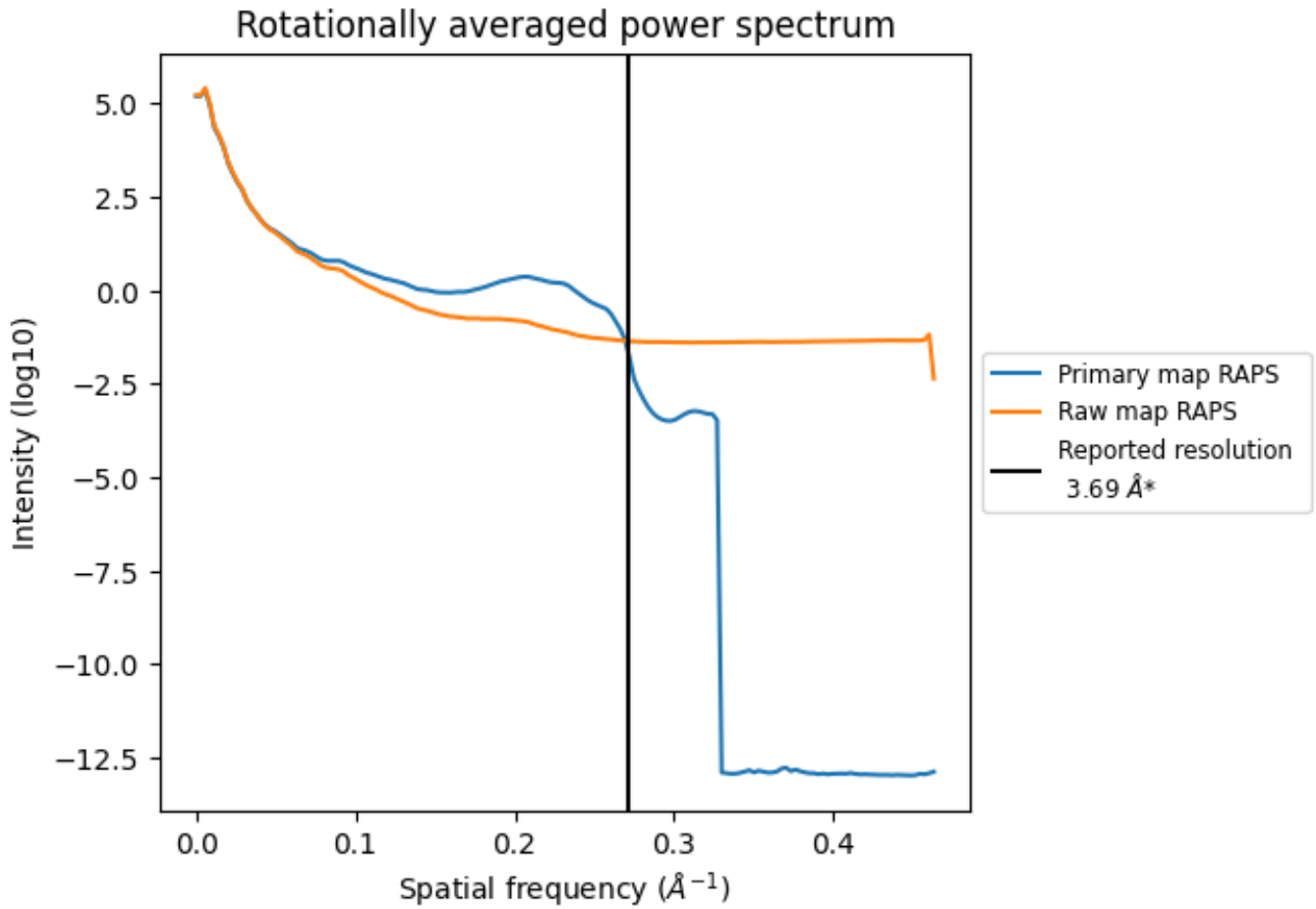
7.2 Volume estimate



The volume at the recommended contour level is 255 nm^3; this corresponds to an approximate mass of 231 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)

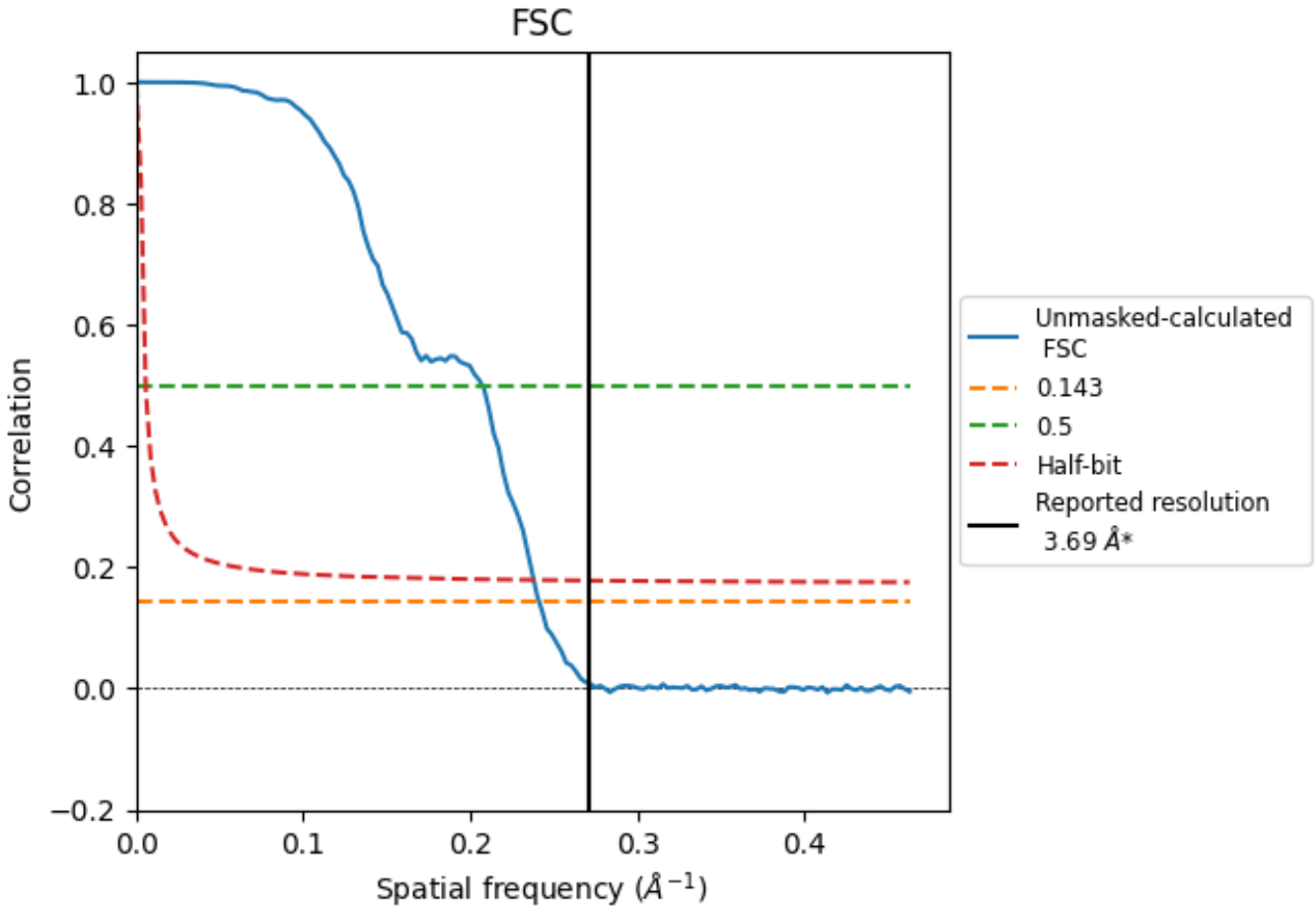


*Reported resolution corresponds to spatial frequency of 0.271 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.271 Å^{-1}

8.2 Resolution estimates (i)

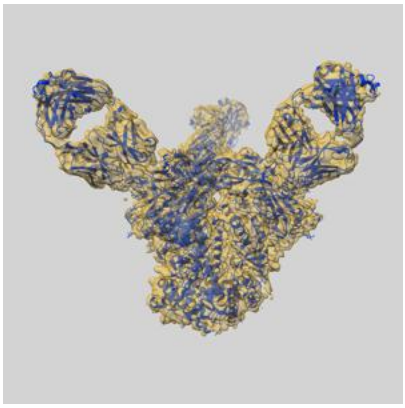
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.69	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.15	4.83	4.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.15 differs from the reported value 3.69 by more than 10 %

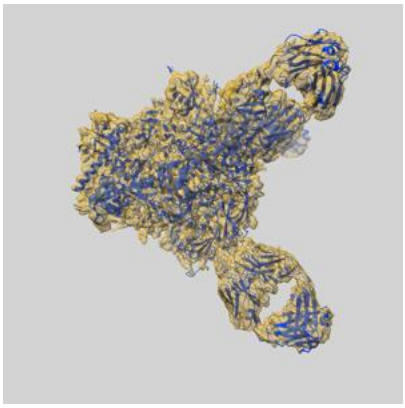
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-27624 and PDB model 8DOW. Per-residue inclusion information can be found in section 3 on page 10.

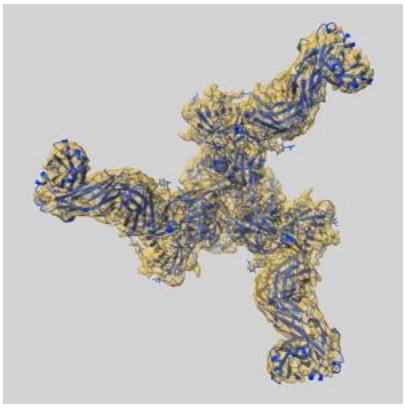
9.1 Map-model overlay



X



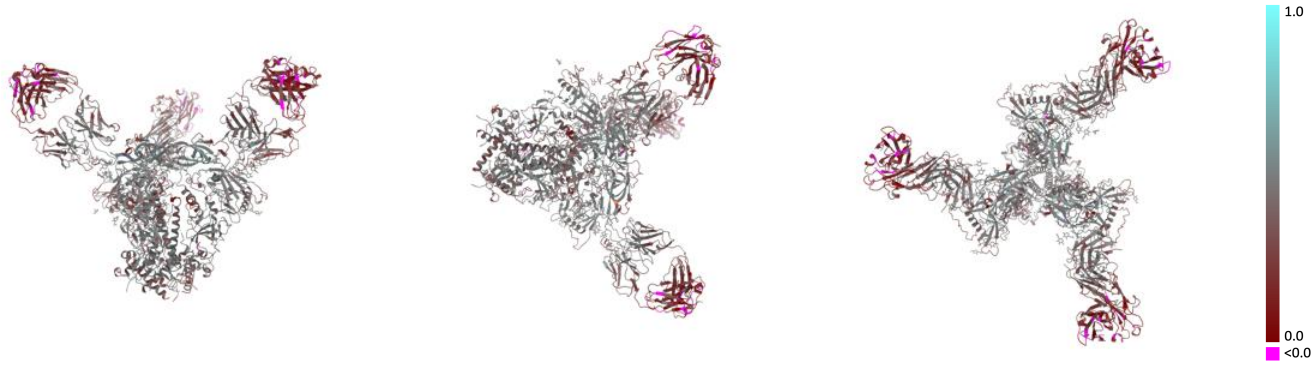
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.9 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.

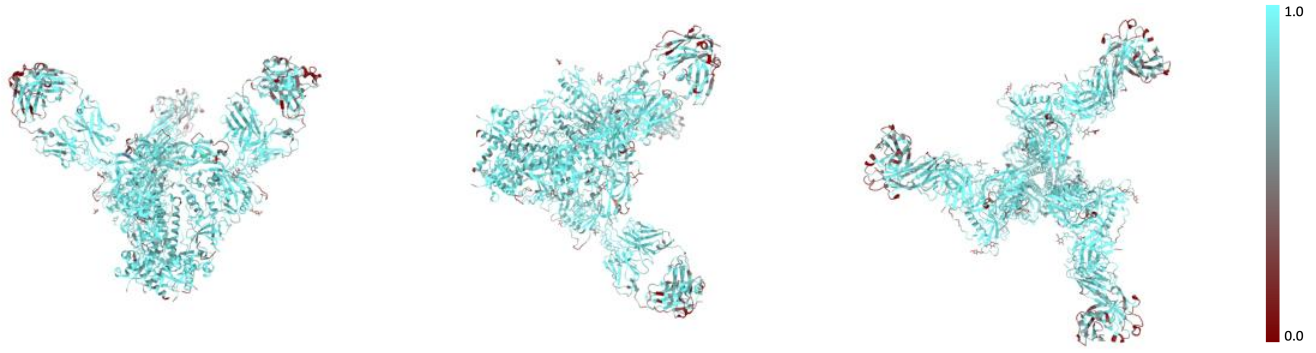
9.2 Q-score mapped to coordinate model (i)



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.

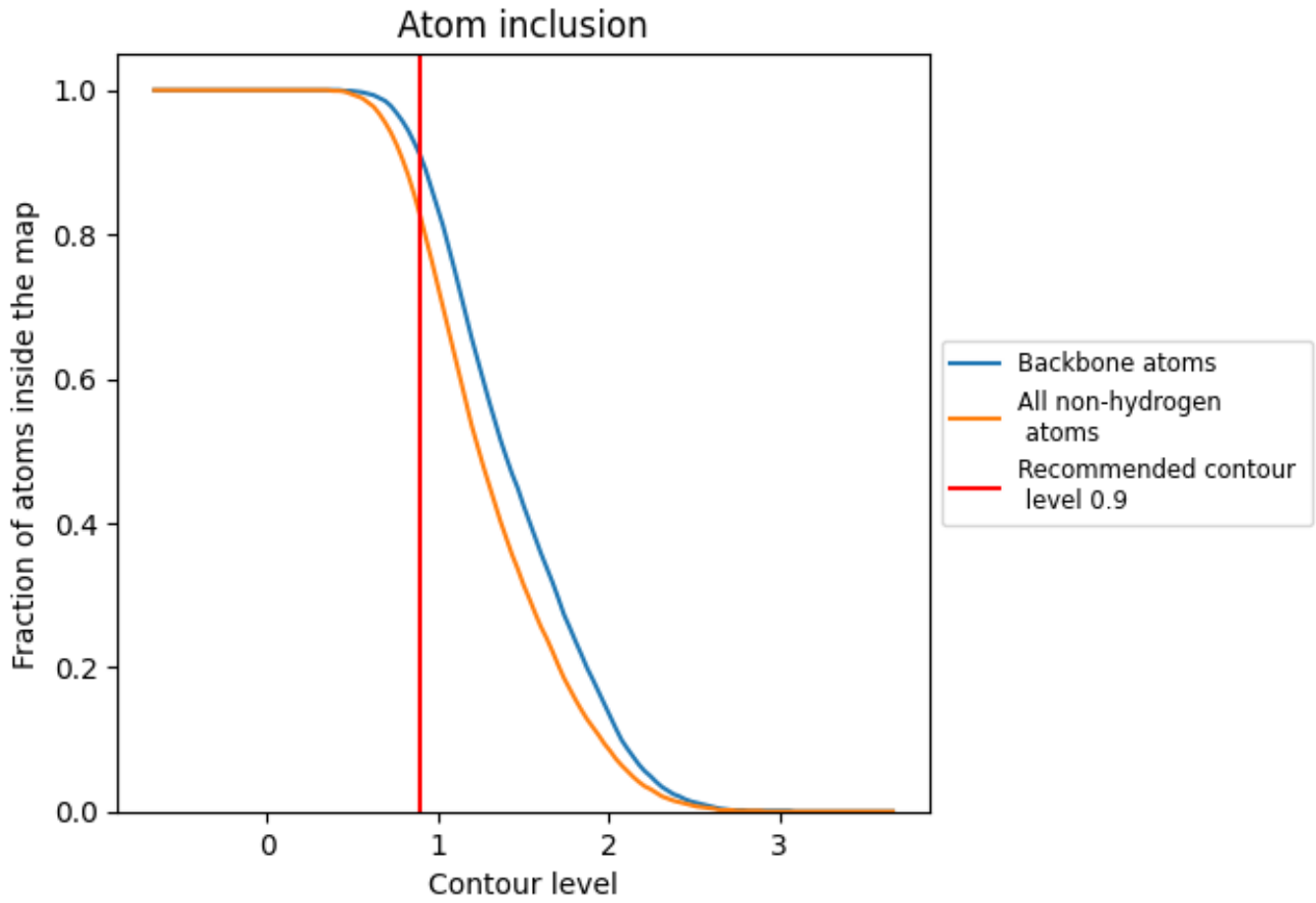
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.9).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 82% 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 (0.9) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.3870
A	0.8740	0.4400
B	0.8510	0.4110
C	0.7920	0.3450
D	0.7460	0.2930
E	0.8690	0.4400
F	0.8580	0.4120
G	0.7910	0.3450
H	0.7490	0.2930
I	0.8690	0.4420
J	0.8550	0.4090
K	0.7920	0.3440
L	0.7450	0.2910
M	0.5000	0.4330
N	0.9580	0.4190
O	0.8200	0.4790
P	0.5710	0.3810
Q	0.6430	0.4820
R	0.5710	0.4190
S	0.9310	0.4170
T	0.5710	0.4240
U	0.6790	0.4760
V	0.8400	0.4830
W	0.9580	0.4260
X	0.5710	0.4260
Y	0.6790	0.4500
Z	0.6070	0.3600
a	0.8200	0.4520
b	0.4620	0.4660