wwPDB EM Validation Summary Report (i)

Sep 28, 2026 – 10:45 AM EDT

PDB ID	:	9YIW / pdb_00009yiw
EMDB ID	:	EMD-73000
Title	:	PC94-A.15 Fab in complex with BG505 SOSIP trimer and RM20A3 Fab
Authors	:	Phulera, S.; Omorodion, O.; Ward, A.B.; Ozorowski, G.
Deposited on	:	2025-10-02
Resolution	:	3.60 Å(reported)

This is a wwPDB EM Validation Summary 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:

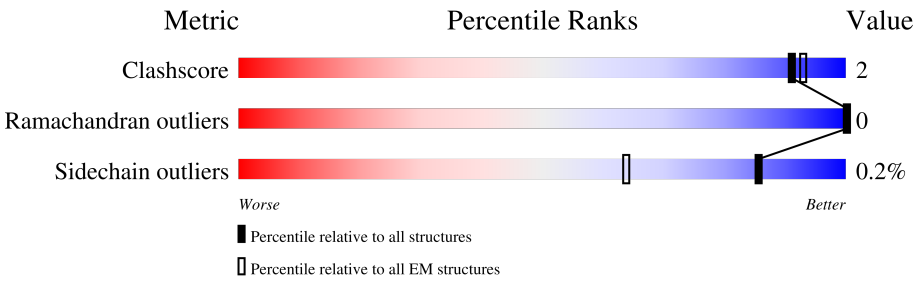
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

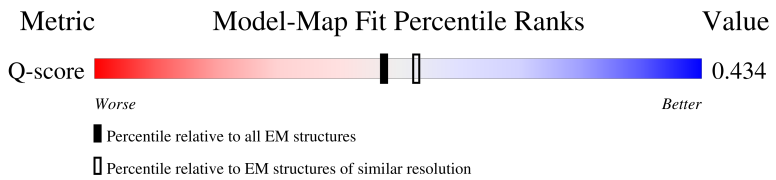
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	H	234	22% 50% • 46%
2	I	229	9% 53% • 46%
2	K	229	9% 52% • 46%
2	Q	229	10% 53% • 46%

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Mol	Chain	Length	Quality of chain
3	L	214	19% 44% 5% 50%
4	M	215	8% 49% 49%
4	O	215	13% 50% 49%
4	S	215	14% 49% 49%
5	A	516	7% 78% 7% 15%
5	C	516	8% 80% 16%
5	E	516	8% 79% 5% 16%
6	B	153	77% 20%
6	D	153	78% 20%
6	F	153	76% 20%
7	G	2	50% 100%
7	P	2	100% 100%
7	R	2	50% 100%
7	T	2	50% 100%
7	W	2	100% 100%
7	X	2	50% 100%
7	Y	2	50% 100%
7	b	2	50% 50% 50%
7	c	2	50% 100%
8	J	5	60% 20% 80%
9	N	10	10% 90%
10	U	4	25% 100%
10	Z	4	25% 25% 75%
11	V	3	33% 33% 67%
11	a	3	67% 33% 67%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 21564 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 PC94-A.15 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	H	126	985	620	168	190	7	0	0

- Molecule 2 is a protein called RM20A3 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	I	124	943	595	161	182	5	0	0
2	K	124	943	595	161	182	5	0	0
2	Q	124	943	595	161	182	5	0	0

- Molecule 3 is a protein called PC94-A.15 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	106	820	522	136	159	3	0	0

- Molecule 4 is a protein called RM20A3 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	109	811	505	136	167	3	0	0
4	O	109	811	505	136	167	3	0	0
4	S	109	811	505	136	167	3	0	0

- Molecule 5 is a protein called BG505 SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	437	3447	2167	610	642	28	0	0
5	C	436	3440	2162	609	641	28	0	0
5	E	436	3440	2162	609	641	28	0	0

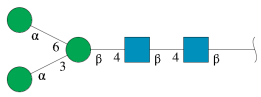
- Molecule 6 is a protein called BG505 SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	122	973	614	168	185	6	0	0
6	D	122	973	614	168	185	6	0	0
6	F	122	973	614	168	185	6	0	0

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

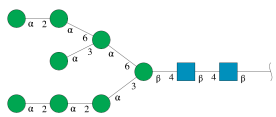
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	G	2	28	16	2	10	0	0
7	P	2	28	16	2	10	0	0
7	R	2	28	16	2	10	0	0
7	T	2	28	16	2	10	0	0
7	W	2	28	16	2	10	0	0
7	X	2	28	16	2	10	0	0
7	Y	2	28	16	2	10	0	0
7	b	2	28	16	2	10	0	0
7	c	2	28	16	2	10	0	0

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

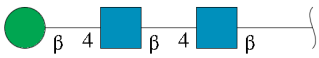


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	N	10	116	64	2	50	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

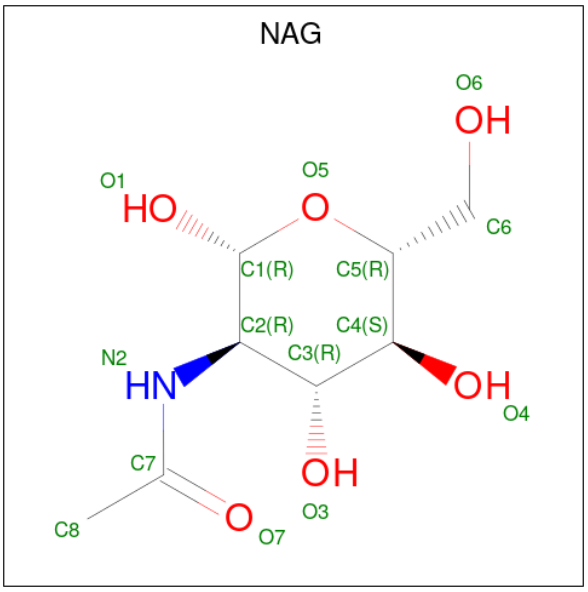
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
10	U	4	50	28	2	20	0	0
10	Z	4	50	28	2	20	0	0

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



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

- Molecule 12 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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

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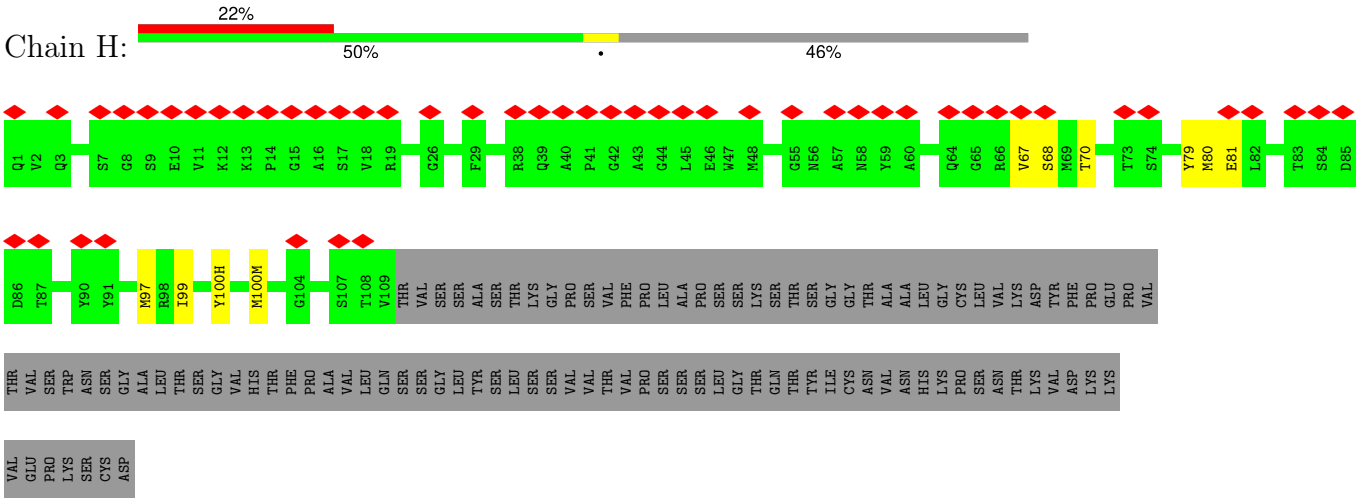
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
12	D	1	14	8	1	5	0
12	D	1	14	8	1	5	0
12	D	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	E	1	14	8	1	5	0
12	F	1	14	8	1	5	0
12	F	1	14	8	1	5	0
12	F	1	14	8	1	5	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.

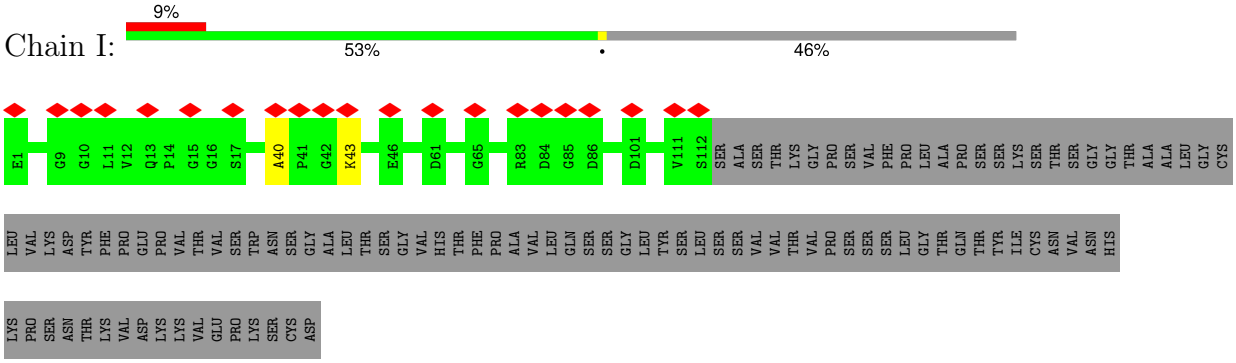
- Molecule 1: PC94-A.15 Fab heavy chain

Chain H:



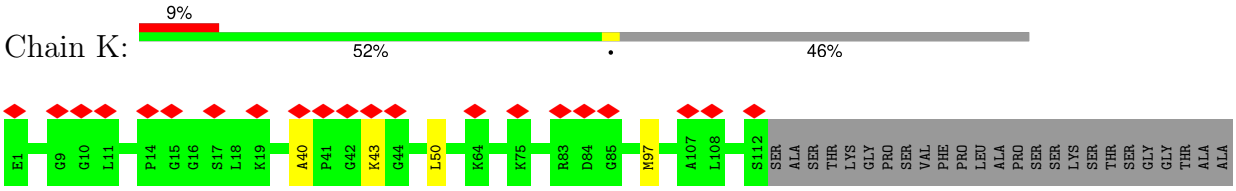
- Molecule 2: RM20A3 Fab heavy chain

Chain I:



- Molecule 2: RM20A3 Fab heavy chain

Chain K:



LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN

VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ASP

- Molecule 2: RM20A3 Fab heavy chain

Chain Q:

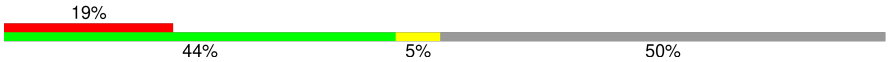
E1 V5 E6 T7 G8 G9 G10 L11 V12 Q13 P14 G15 G16 S17 A40 K43 G44 D61 G65 M82 R83 D84 G85 Q105 G106 T110 V111 S112 SER ALA SER THR LYS GLY PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR

ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU SER SER VAL VAL THR VAL PRO SER SER LEU GLY THR GLN THR TYR ILE

CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ASP

- Molecule 3: PC94-A.15 light chain

Chain L:



D1 S7 P8 S9 T10 L11 S12 A13 S14 V15 G16 D17 R18 V19 T20 I21 T22 L33 A34 W35 Y36 Q37 Q38 G41 K42 V43 L47 I48 H49 K50 L54 H55 I56 G57 S60 R61 F62 S63 T72 S76 S77 L78 Q79 P80 D81 D82 F83 A84 T85 T102 S103

V104 E105 A106 ASN ARG THR VAL ALA ALA PRO SER VAL PHE ILE PHE PRO PRO SER ASP GLU GLN LEU LYS SER GLY THR ALA SER VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL

THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR LEU THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL TYR ALA CYS GLU VAL THR HIS GLN GLY LEU SER SER PRO VAL THR LYS SER PHE ASN ARG GLY GLU CYS

- Molecule 4: RM20A3 light chain

Chain M:

A3 Q6 V11 S12 Q17 S18 V19 T20 S29 G41 D50 G57 V58 S59 G68 S76 G77 L78 Q79 A80 D81 D82 E83 Y87 G101 T105 V106 L107 GLY GLN PRO LYS ALA ALA PRO SER VAL THR LEU PHE PRO PRO SER SER GLU GLU LEU GLN

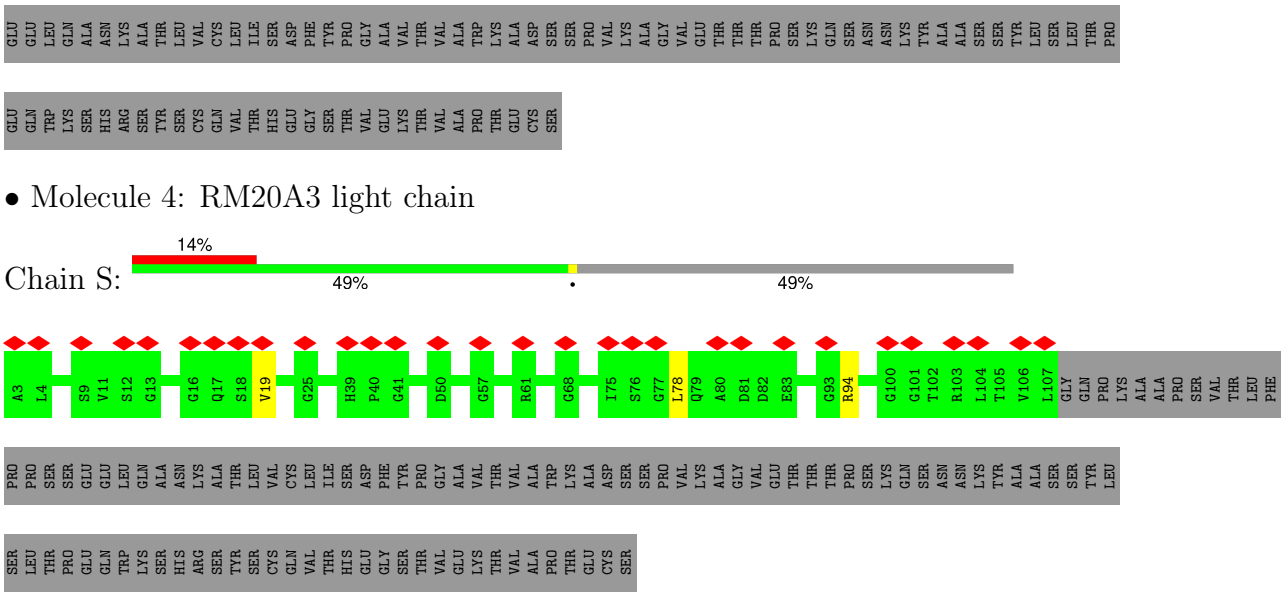
ALA ASN LYS ALA THR LEU VAL CYS LEU ILE SER ASP PHE TYR PRO GLY ALA VAL THR VAL ALA TRP LYS ALA ASP SER SER PRO VAL LYS ALA GLY VAL GLU THR THR THR PRO SER LYS GLN SER ASN ASN LYS TYR ALA ALA SER SER TYR LEU SER LEU THR PRO GLU GLN TRP LYS

SER HIS ARG SER TYR SER CYS GLN VAL THR HIS GLU GLY SER THR VAL GLU LYS THR VAL ALA PRO THR GLU CYS SER

- Molecule 4: RM20A3 light chain

Chain O:

A3 V11 S12 G13 S14 Q17 S18 V19 G25 G41 K42 R54 P55 S56 G57 K66 S67 G68 I75 S76 G77 L78 Q79 A80 D81 D82 E83 A84 G100 G101 T102 R103 L104 T105 V106 L107 GLY GLN PRO LYS ALA ALA PRO SER VAL THR LEU PHE PRO PRO SER SER

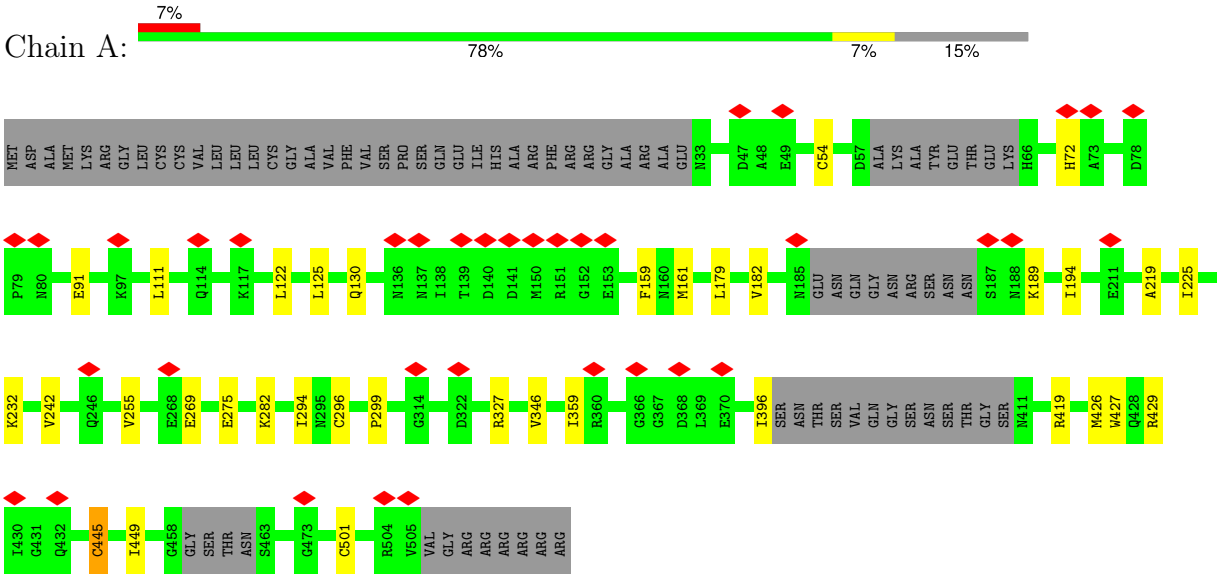


- Molecule 4: RM20A3 light chain

Chain S:

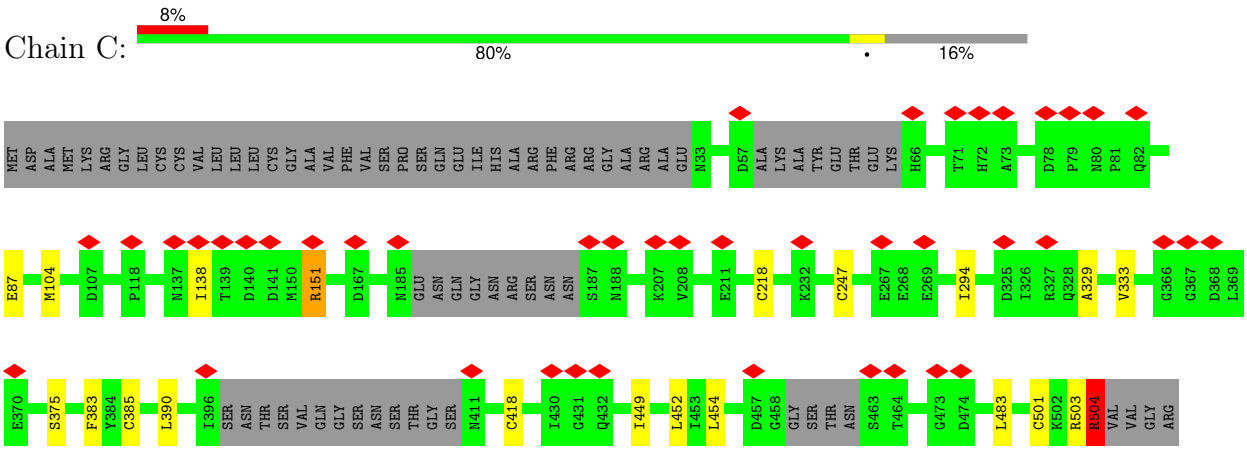
- Molecule 5: BG505 SOSIP.664 gp120

Chain A:



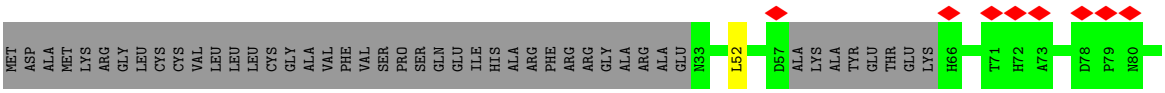
- Molecule 5: BG505 SOSIP.664 gp120

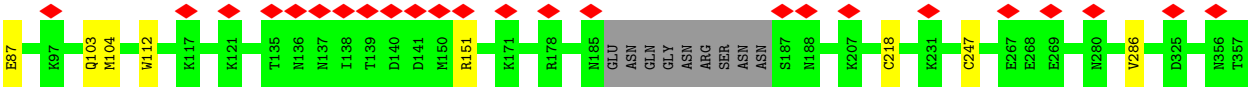
Chain C:

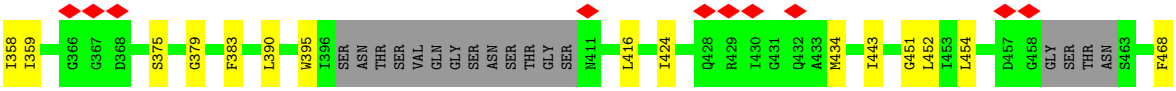


• Molecule 5: BG505 SOSIP.664 gp120

Chain E:

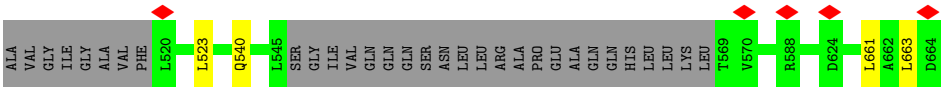






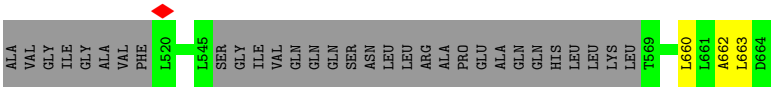
• Molecule 6: BG505 SOSIP.664 gp41

Chain B:



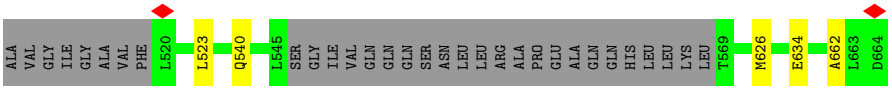
• Molecule 6: BG505 SOSIP.664 gp41

Chain D:



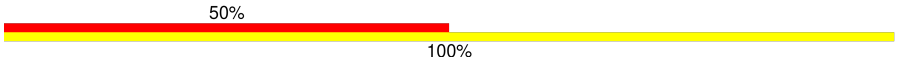
• Molecule 6: BG505 SOSIP.664 gp41

Chain F:



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

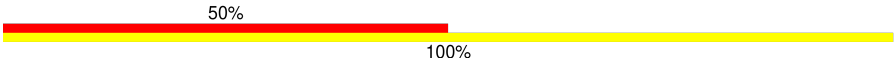
Chain G:



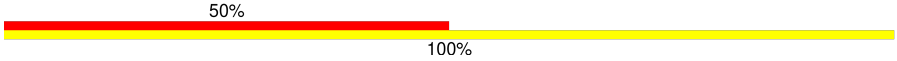
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:

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

Chain R: 

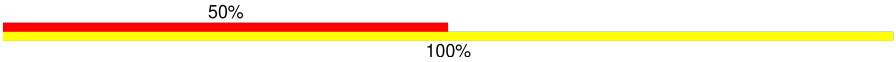
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T: 

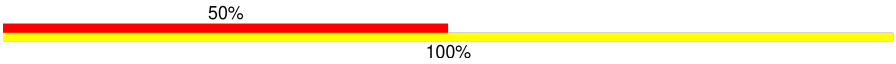
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:

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

Chain X: 

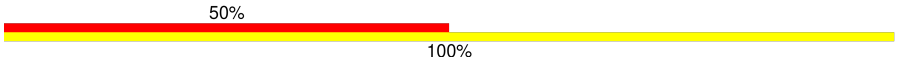
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y: 

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

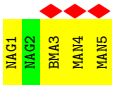
Chain b:

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

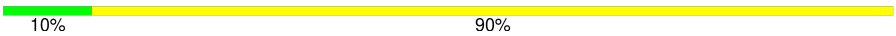
Chain c: 

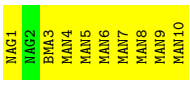
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

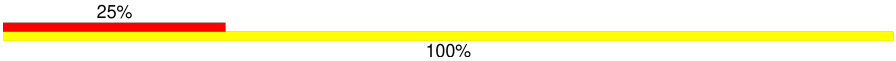


• Molecule 9: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N: 



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

Chain U: 

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

Chain Z:

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

Chain V:

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

Chain a:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16931	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1700	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	0.631	Depositor
Minimum map value	-0.303	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	413.56, 413.56, 413.56	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0339, 1.0339, 1.0339	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, NAG, 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	H	0.25	0/1009	0.64	0/1369
2	I	0.24	0/963	0.56	0/1300
2	K	0.24	0/963	0.56	0/1300
2	Q	0.24	0/963	0.56	0/1300
3	L	0.28	0/843	0.69	2/1148 (0.2%)
4	M	0.23	0/830	0.55	0/1129
4	O	0.24	0/830	0.57	0/1129
4	S	0.24	0/830	0.56	0/1129
5	A	0.28	0/3518	0.60	1/4775 (0.0%)
5	C	0.26	0/3511	0.55	0/4765
5	E	0.25	0/3511	0.55	0/4765
6	B	0.28	0/990	0.59	2/1343 (0.1%)
6	D	0.30	0/990	0.60	2/1343 (0.1%)
6	F	0.29	0/990	0.60	0/1343
All	All	0.26	0/20741	0.58	7/28138 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	C	0	3
5	E	0	2
All	All	0	5

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	663	LEU	CA-C-N	6.84	134.01	121.70
6	D	663	LEU	C-N-CA	6.84	134.01	121.70
5	A	445	CYS	CA-CB-SG	6.75	129.91	114.40
6	B	663	LEU	CA-C-N	5.36	131.35	121.70
6	B	663	LEU	C-N-CA	5.36	131.35	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	151	ARG	Sidechain
5	C	503	ARG	Sidechain
5	C	504	ARG	Sidechain
5	E	151	ARG	Sidechain
5	E	503	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	H	985	0	935	6	0
2	I	943	0	915	1	0
2	K	943	0	915	2	0
2	Q	943	0	915	1	0
3	L	820	0	791	5	0
4	M	811	0	767	2	0
4	O	811	0	767	1	0
4	S	811	0	767	2	0
5	A	3447	0	3386	20	0
5	C	3440	0	3378	12	0
5	E	3440	0	3378	15	0
6	B	973	0	949	1	0
6	D	973	0	949	1	0
6	F	973	0	949	3	0
7	G	28	0	25	0	0
7	P	28	0	25	0	0
7	R	28	0	25	0	0
7	T	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	W	28	0	25	0	0
7	X	28	0	25	0	0
7	Y	28	0	25	0	0
7	b	28	0	25	0	0
7	c	28	0	25	0	0
8	J	61	0	52	0	0
9	N	116	0	97	0	0
10	U	50	0	43	0	0
10	Z	50	0	43	0	0
11	V	39	0	34	0	0
11	a	39	0	34	0	0
12	A	182	0	169	1	0
12	B	42	0	39	0	0
12	C	168	0	156	1	0
12	D	42	0	39	0	0
12	E	168	0	156	1	0
12	F	42	0	39	0	0
All	All	21564	0	20887	69	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 2.

The worst 5 of 69 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)
5:A:346:VAL:HG13	5:A:359:ILE:HD12	1.79	0.64
3:L:22:THR:HG22	3:L:72:THR:HG22	1.82	0.61
6:B:523:LEU:HA	6:B:540:GLN:HE21	1.65	0.60
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.84	0.58
4:S:94:ARG:HH22	5:E:504:ARG:HH21	1.51	0.58

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	H	124/234 (53%)	123 (99%)	1 (1%)	0	100	100
2	I	122/229 (53%)	121 (99%)	1 (1%)	0	100	100
2	K	122/229 (53%)	120 (98%)	2 (2%)	0	100	100
2	Q	122/229 (53%)	122 (100%)	0	0	100	100
3	L	104/214 (49%)	101 (97%)	3 (3%)	0	100	100
4	M	107/215 (50%)	99 (92%)	8 (8%)	0	100	100
4	O	107/215 (50%)	99 (92%)	8 (8%)	0	100	100
4	S	107/215 (50%)	100 (94%)	7 (6%)	0	100	100
5	A	427/516 (83%)	413 (97%)	14 (3%)	0	100	100
5	C	426/516 (83%)	408 (96%)	18 (4%)	0	100	100
5	E	426/516 (83%)	414 (97%)	12 (3%)	0	100	100
6	B	118/153 (77%)	116 (98%)	2 (2%)	0	100	100
6	D	118/153 (77%)	116 (98%)	2 (2%)	0	100	100
6	F	118/153 (77%)	114 (97%)	4 (3%)	0	100	100
All	All	2548/3787 (67%)	2466 (97%)	82 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	H	103/197 (52%)	103 (100%)	0	100	100
2	I	101/192 (53%)	101 (100%)	0	100	100
2	K	101/192 (53%)	101 (100%)	0	100	100
2	Q	101/192 (53%)	101 (100%)	0	100	100
3	L	93/190 (49%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	M	89/180 (49%)	89 (100%)	0	100	100
4	O	89/180 (49%)	89 (100%)	0	100	100
4	S	89/180 (49%)	89 (100%)	0	100	100
5	A	392/456 (86%)	392 (100%)	0	100	100
5	C	391/456 (86%)	390 (100%)	1 (0%)	86	83
5	E	391/456 (86%)	389 (100%)	2 (0%)	81	80
6	B	105/129 (81%)	104 (99%)	1 (1%)	68	75
6	D	105/129 (81%)	104 (99%)	1 (1%)	68	75
6	F	105/129 (81%)	105 (100%)	0	100	100
All	All	2255/3258 (69%)	2250 (100%)	5 (0%)	85	85

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	661	LEU
5	C	504	ARG
6	D	660	LEU
5	E	503	ARG
5	E	504	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
5	E	103	GLN
6	F	543	ASN
4	S	95	GLN
5	A	72	HIS
5	A	130	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

47 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	NAG	G	1	5,7	14,14,15	0.73	0	17,19,21	1.23	2 (11%)
7	NAG	G	2	7	14,14,15	0.72	0	17,19,21	1.99	2 (11%)
8	NAG	J	1	5,8	14,14,15	0.76	0	17,19,21	1.32	1 (5%)
8	NAG	J	2	8	14,14,15	0.78	0	17,19,21	0.86	0
8	BMA	J	3	8	11,11,12	0.89	0	15,15,17	2.23	5 (33%)
8	MAN	J	4	8	11,11,12	0.71	0	15,15,17	1.29	1 (6%)
8	MAN	J	5	8	11,11,12	0.70	0	15,15,17	1.33	1 (6%)
9	NAG	N	1	9,5	14,14,15	0.82	0	17,19,21	1.40	2 (11%)
9	MAN	N	10	9	11,11,12	0.75	0	15,15,17	1.19	1 (6%)
9	NAG	N	2	9	14,14,15	0.83	0	17,19,21	0.90	0
9	BMA	N	3	9	11,11,12	0.89	0	15,15,17	1.73	5 (33%)
9	MAN	N	4	9	11,11,12	0.60	0	15,15,17	1.85	1 (6%)
9	MAN	N	5	9	11,11,12	0.70	0	15,15,17	1.44	1 (6%)
9	MAN	N	6	9	11,11,12	0.80	0	15,15,17	1.18	1 (6%)
9	MAN	N	7	9	11,11,12	0.82	0	15,15,17	1.22	1 (6%)
9	MAN	N	8	9	11,11,12	0.81	0	15,15,17	1.45	2 (13%)
9	MAN	N	9	9	11,11,12	0.86	1 (9%)	15,15,17	1.16	1 (6%)
7	NAG	P	1	5,7	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
7	NAG	P	2	7	14,14,15	0.67	0	17,19,21	0.93	1 (5%)
7	NAG	R	1	5,7	14,14,15	0.80	0	17,19,21	1.51	3 (17%)
7	NAG	R	2	7	14,14,15	0.78	0	17,19,21	1.95	4 (23%)
7	NAG	T	1	5,7	14,14,15	0.74	0	17,19,21	1.11	1 (5%)
7	NAG	T	2	7	14,14,15	0.72	0	17,19,21	1.84	2 (11%)
10	NAG	U	1	5,10	14,14,15	0.75	0	17,19,21	1.31	1 (5%)
10	NAG	U	2	10	14,14,15	0.74	0	17,19,21	0.90	1 (5%)
10	BMA	U	3	10	11,11,12	1.36	1 (9%)	15,15,17	2.58	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	MAN	U	4	10	11,11,12	0.69	0	15,15,17	1.19	1 (6%)
11	NAG	V	1	5,11	14,14,15	0.70	0	17,19,21	1.07	1 (5%)
11	NAG	V	2	11	14,14,15	0.75	0	17,19,21	0.99	0
11	BMA	V	3	11	11,11,12	0.97	0	15,15,17	2.09	5 (33%)
7	NAG	W	1	5,7	14,14,15	0.71	0	17,19,21	0.79	0
7	NAG	W	2	7	14,14,15	0.70	0	17,19,21	0.89	0
7	NAG	X	1	5,7	14,14,15	0.77	0	17,19,21	1.35	3 (17%)
7	NAG	X	2	7	14,14,15	0.82	1 (7%)	17,19,21	1.99	4 (23%)
7	NAG	Y	1	5,7	14,14,15	0.70	0	17,19,21	1.22	1 (5%)
7	NAG	Y	2	7	14,14,15	0.70	0	17,19,21	1.87	2 (11%)
10	NAG	Z	1	5,10	14,14,15	0.72	0	17,19,21	1.26	1 (5%)
10	NAG	Z	2	10	14,14,15	0.70	0	17,19,21	0.82	0
10	BMA	Z	3	10	11,11,12	1.24	1 (9%)	15,15,17	2.78	6 (40%)
10	MAN	Z	4	10	11,11,12	0.71	0	15,15,17	1.29	1 (6%)
11	NAG	a	1	5,11	14,14,15	0.74	0	17,19,21	1.05	1 (5%)
11	NAG	a	2	11	14,14,15	0.73	0	17,19,21	1.00	0
11	BMA	a	3	11	11,11,12	0.91	0	15,15,17	2.17	5 (33%)
7	NAG	b	1	5,7	14,14,15	0.72	0	17,19,21	0.75	0
7	NAG	b	2	7	14,14,15	0.74	0	17,19,21	0.91	1 (5%)
7	NAG	c	1	5,7	14,14,15	0.80	0	17,19,21	1.42	3 (17%)
7	NAG	c	2	7	14,14,15	0.75	0	17,19,21	2.05	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	G	1	5,7	-	3/6/23/26	0/1/1/1
7	NAG	G	2	7	-	2/6/23/26	0/1/1/1
8	NAG	J	1	5,8	-	2/6/23/26	0/1/1/1
8	NAG	J	2	8	-	0/6/23/26	0/1/1/1
8	BMA	J	3	8	-	0/2/19/22	0/1/1/1
8	MAN	J	4	8	-	2/2/19/22	0/1/1/1
8	MAN	J	5	8	-	0/2/19/22	0/1/1/1
9	NAG	N	1	9,5	-	2/6/23/26	0/1/1/1
9	MAN	N	10	9	-	2/2/19/22	0/1/1/1
9	NAG	N	2	9	-	1/6/23/26	0/1/1/1

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	U	3	BMA	C2-C3	3.28	1.57	1.52
10	Z	3	BMA	C2-C3	2.89	1.56	1.52
7	X	2	NAG	C1-C2	2.27	1.55	1.52
9	N	9	MAN	O5-C1	-2.18	1.40	1.43

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	Z	3	BMA	C1-O5-C5	8.01	122.92	112.19
10	U	3	BMA	C1-O5-C5	7.50	122.23	112.19
7	G	2	NAG	C2-N2-C7	6.56	131.69	122.90
9	N	4	MAN	C1-O5-C5	6.35	120.69	112.19
7	T	2	NAG	C2-N2-C7	6.09	131.06	122.90

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

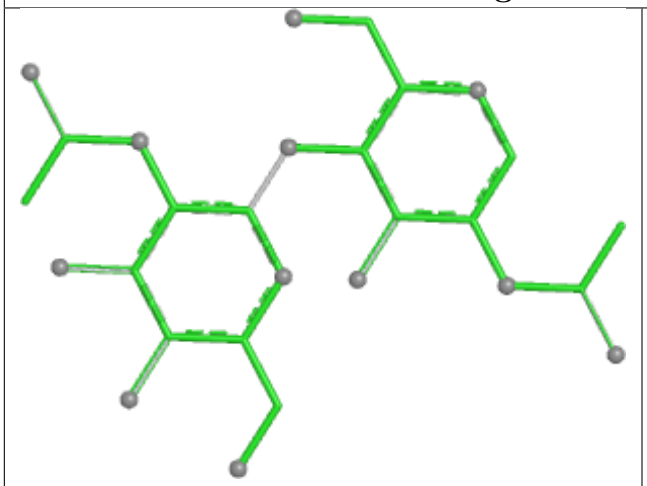
Mol	Chain	Res	Type	Atoms
7	G	2	NAG	C1-C2-N2-C7
7	T	2	NAG	C1-C2-N2-C7
7	Y	2	NAG	C1-C2-N2-C7
9	N	9	MAN	O5-C5-C6-O6
9	N	8	MAN	C4-C5-C6-O6

There are no ring outliers.

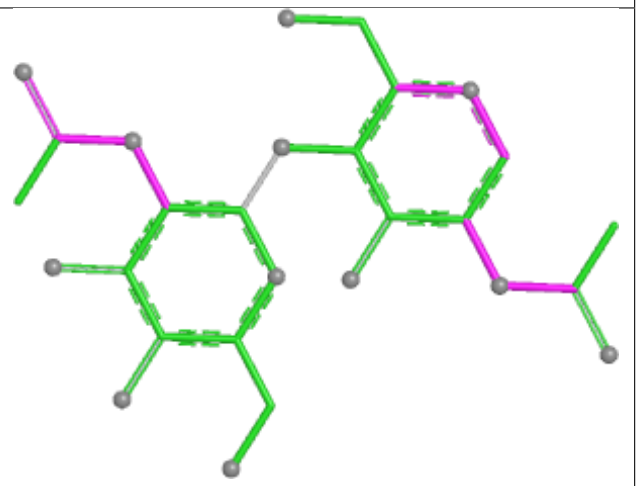
No monomer is involved in short contacts.

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

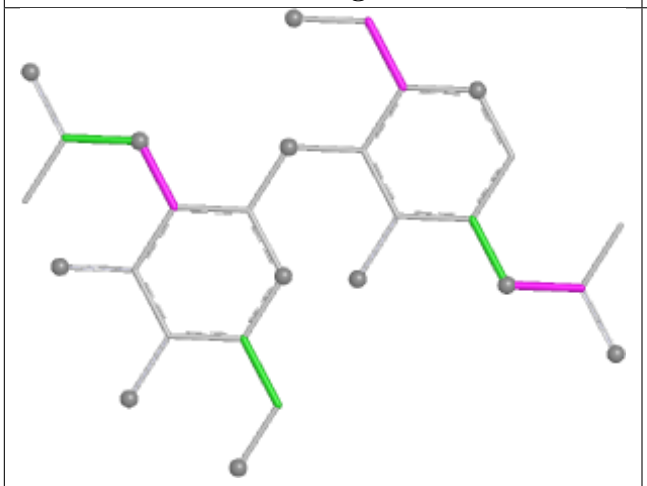
Oligosaccharide Chain G



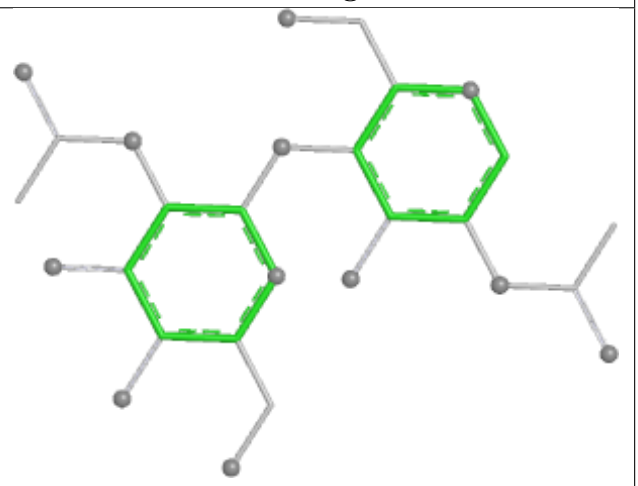
Bond lengths



Bond angles

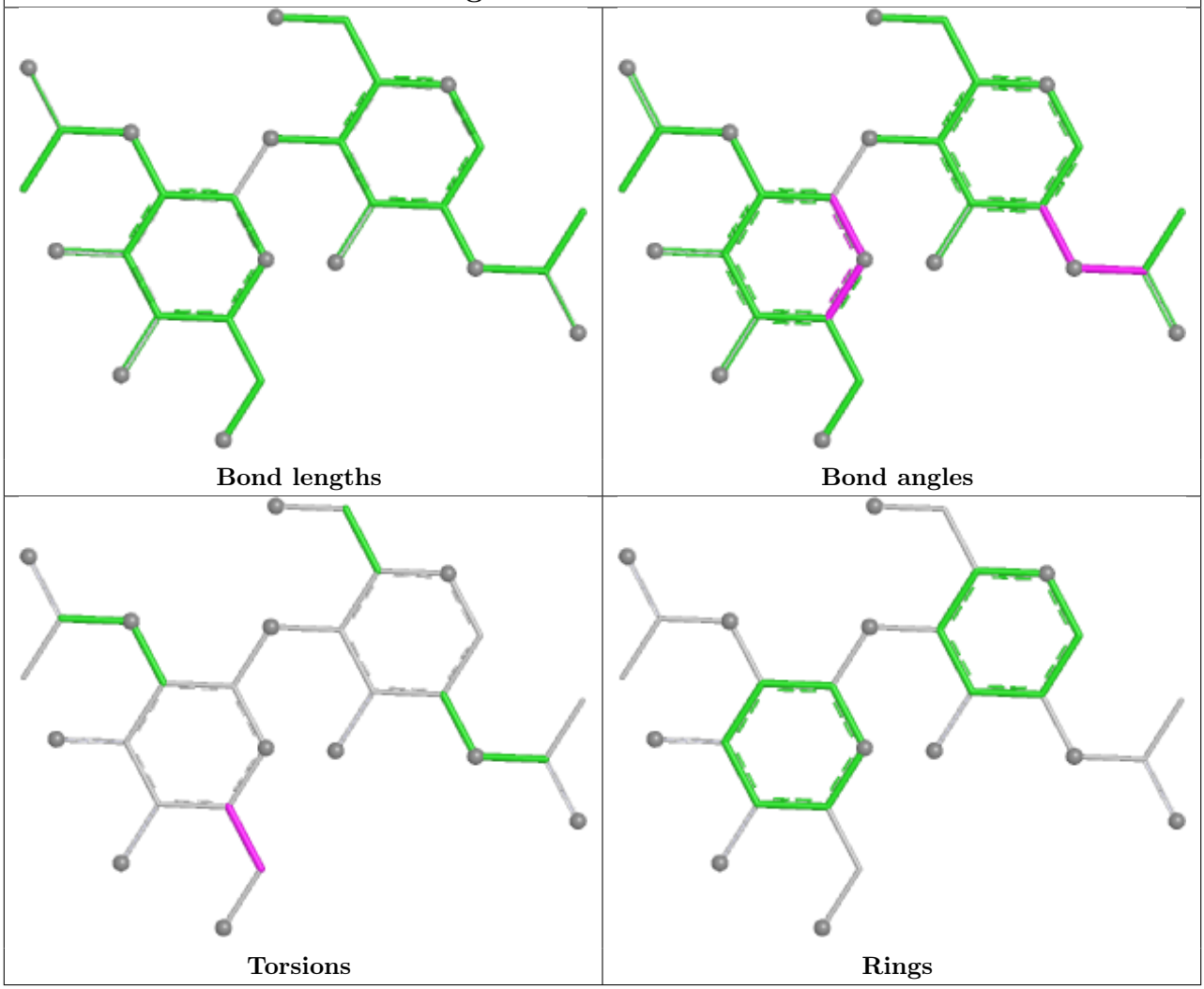


Torsions

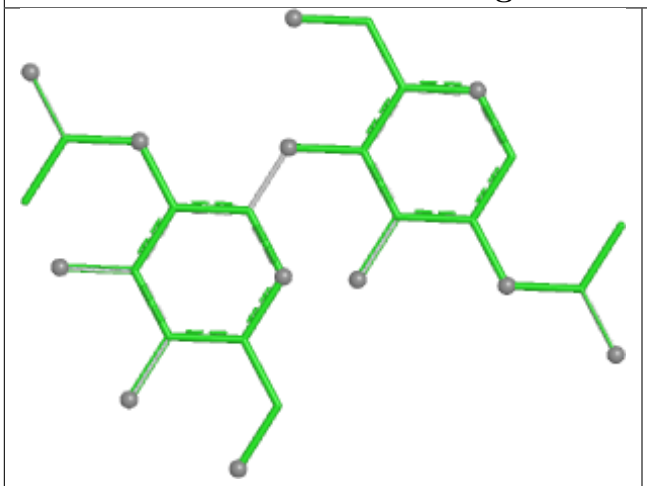


Rings

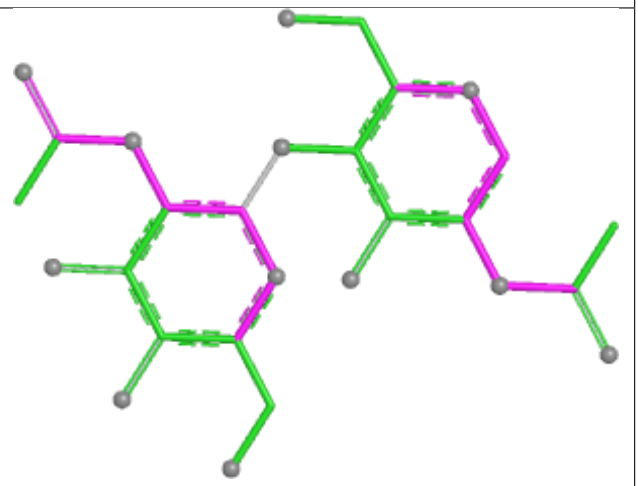
Oligosaccharide Chain P



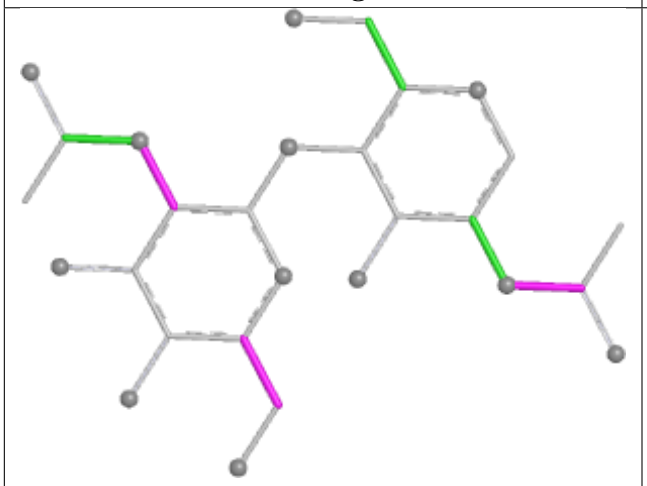
Oligosaccharide Chain R



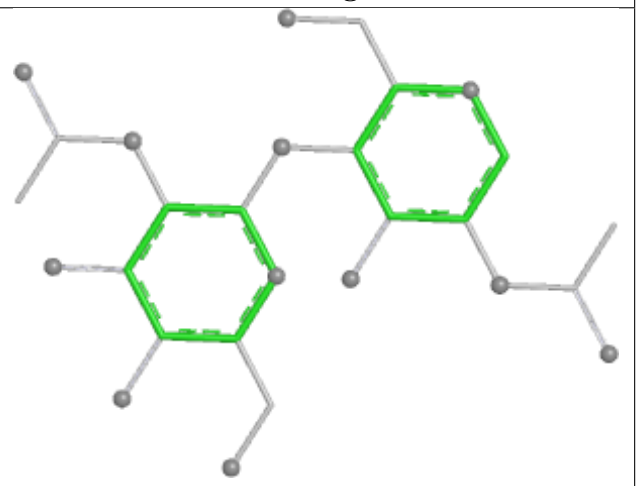
Bond lengths



Bond angles

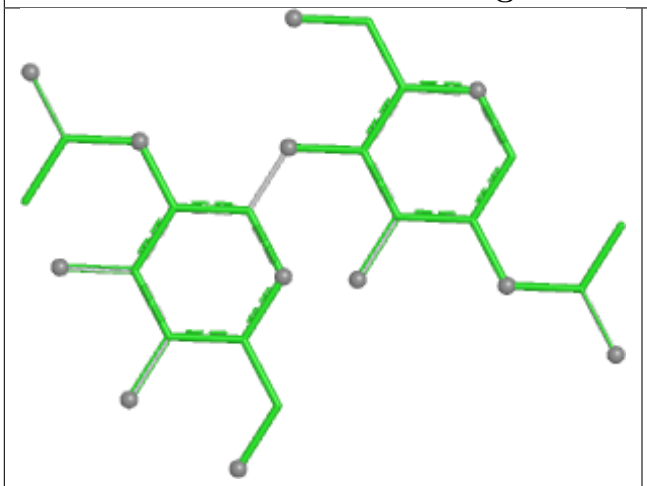


Torsions

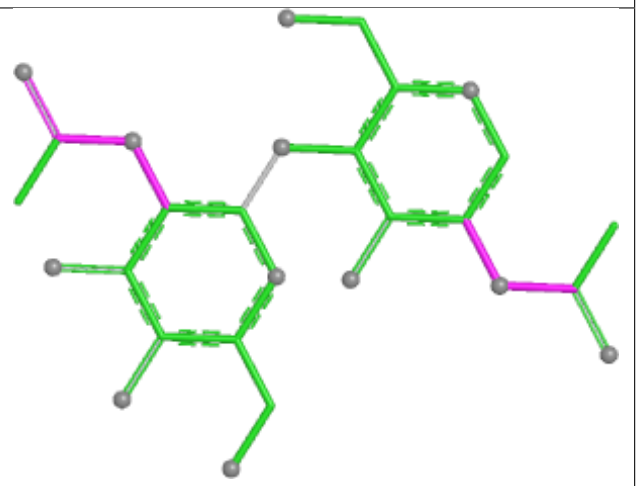


Rings

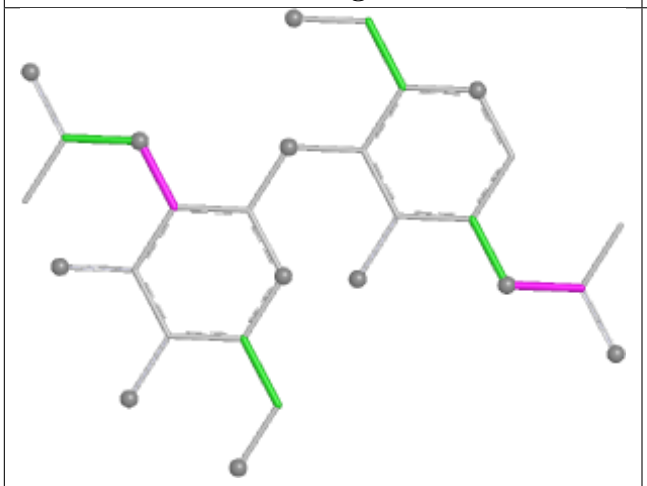
Oligosaccharide Chain T



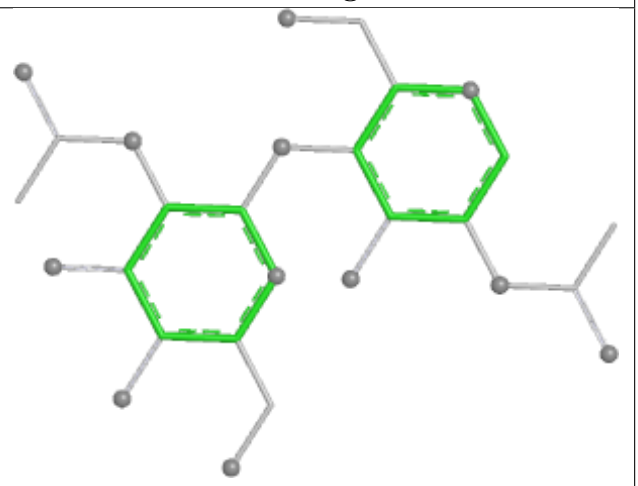
Bond lengths



Bond angles

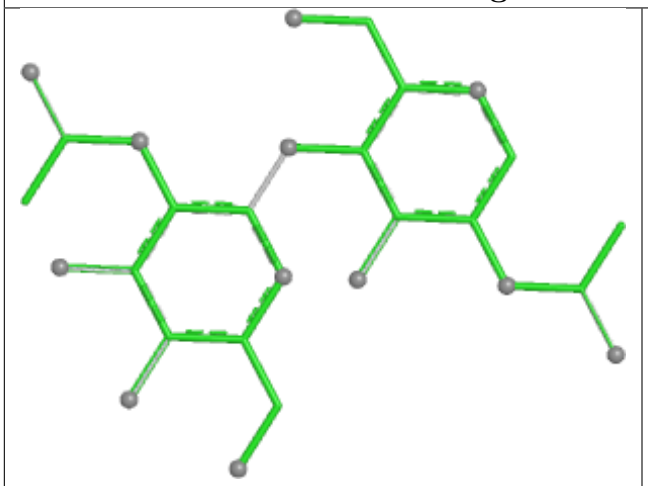


Torsions

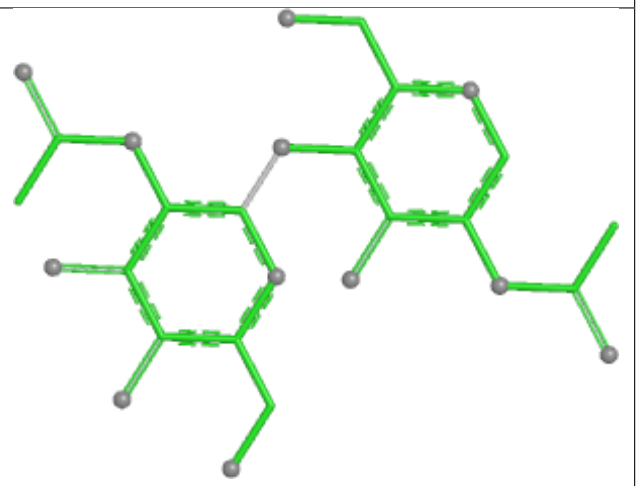


Rings

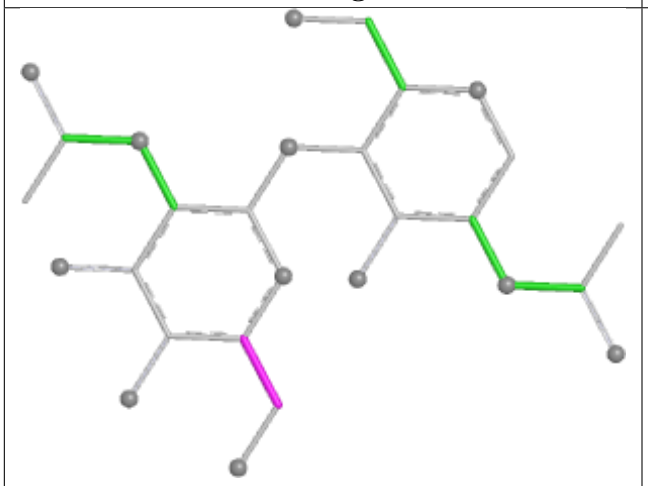
Oligosaccharide Chain W



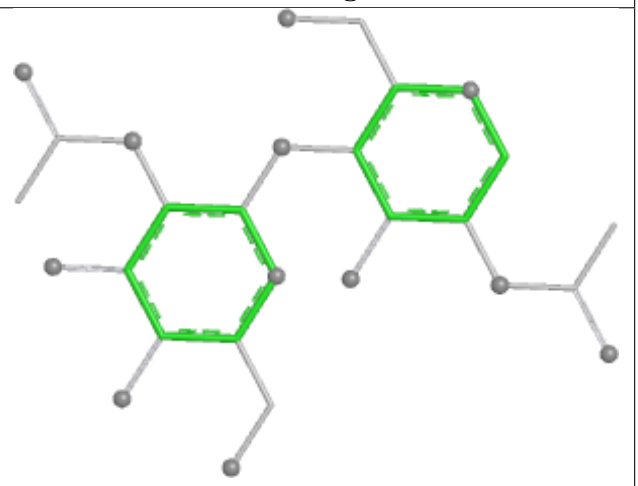
Bond lengths



Bond angles

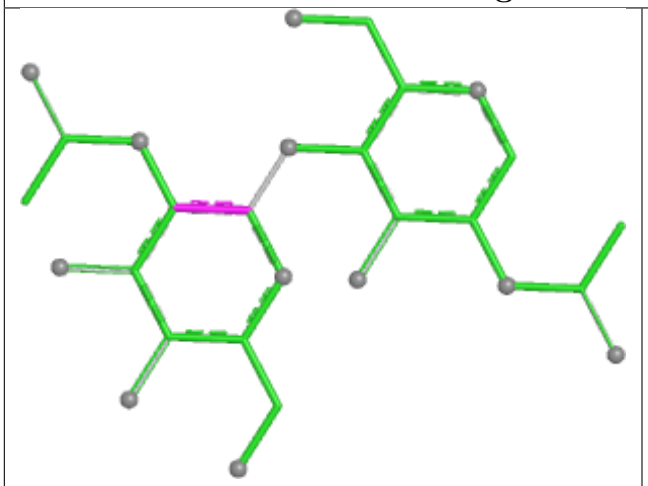


Torsions

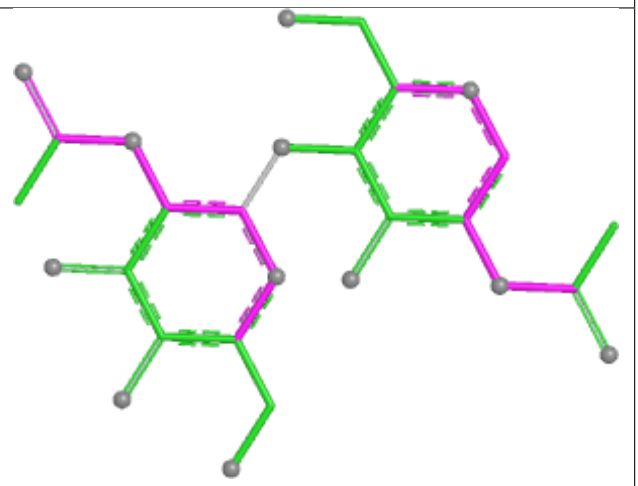


Rings

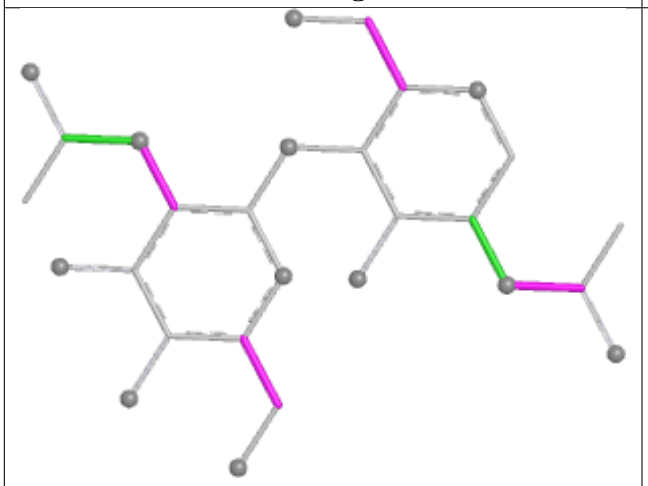
Oligosaccharide Chain X



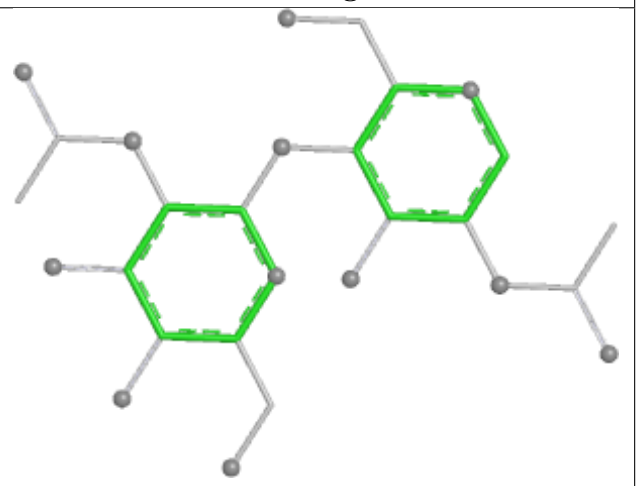
Bond lengths



Bond angles

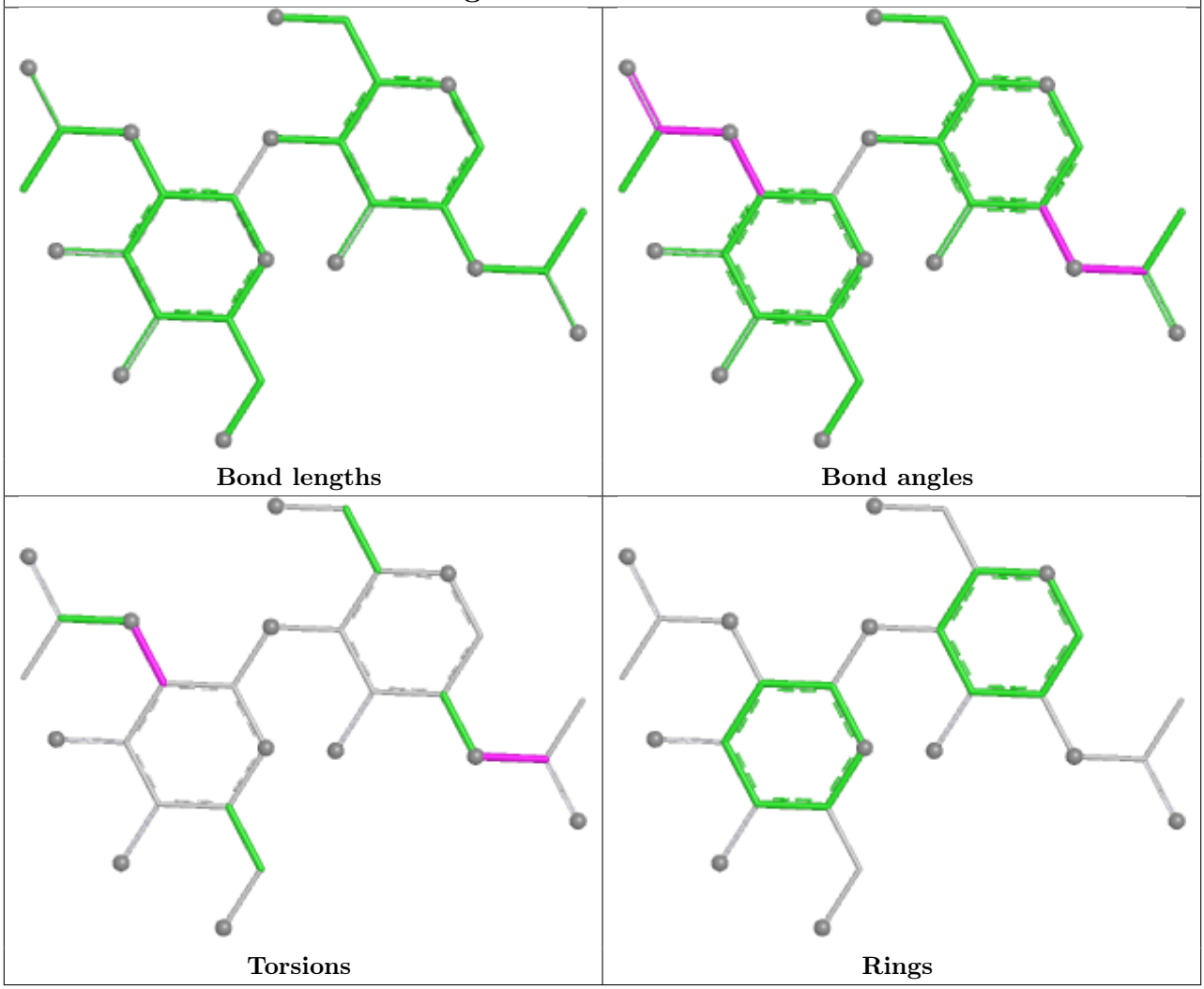


Torsions

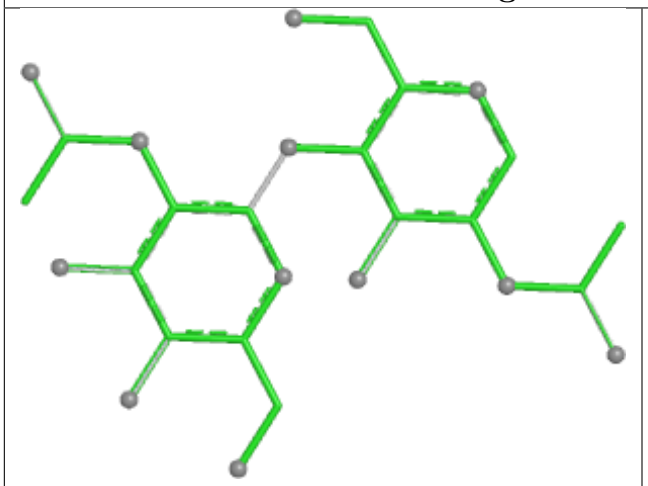


Rings

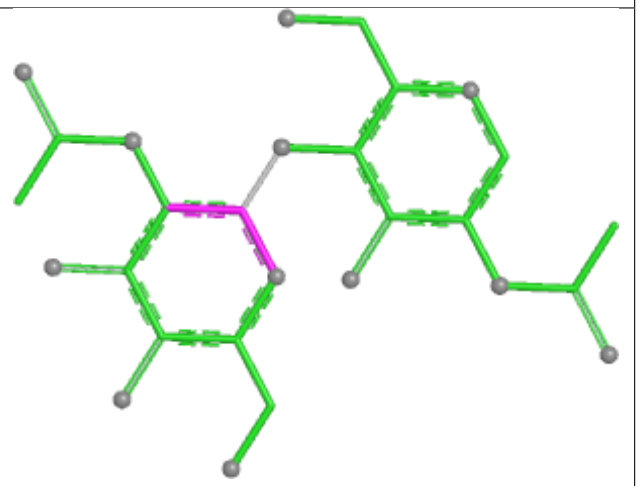
Oligosaccharide Chain Y



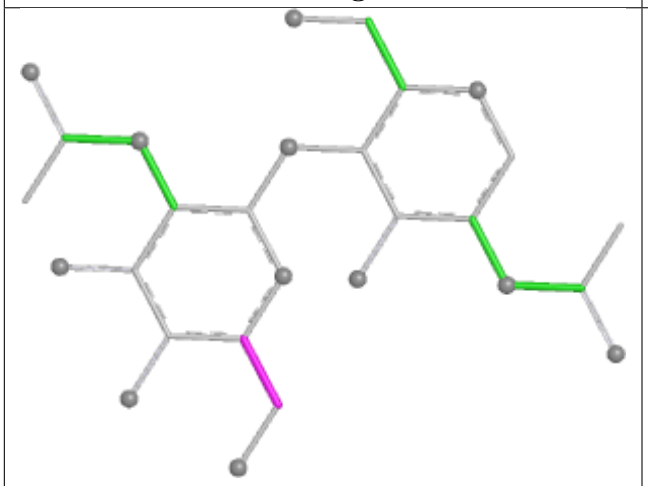
Oligosaccharide Chain b



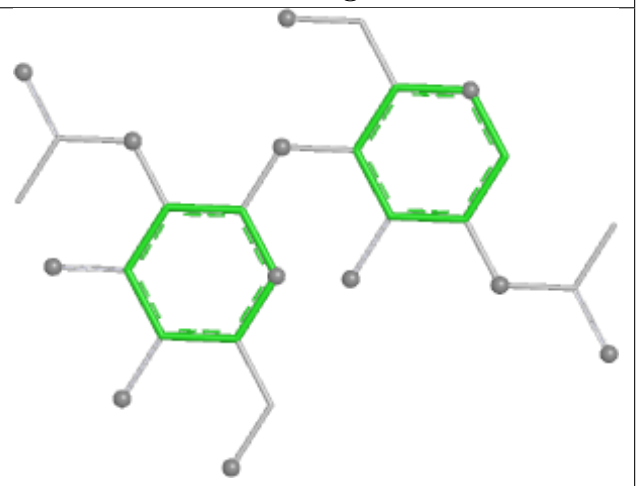
Bond lengths



Bond angles

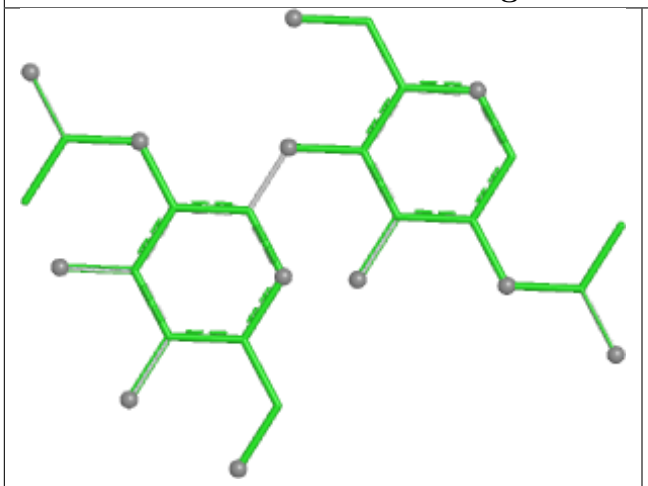


Torsions

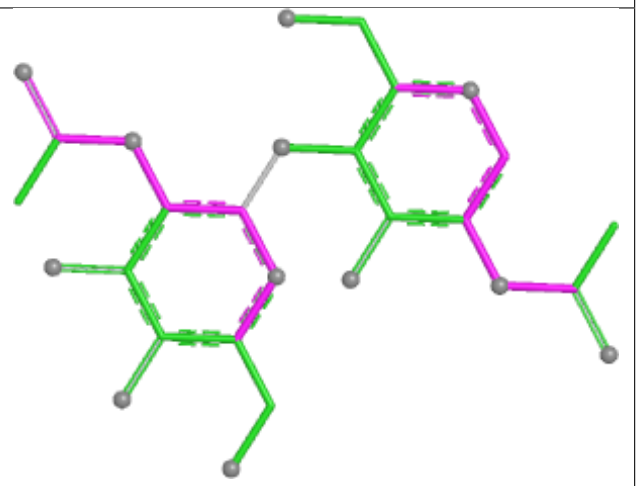


Rings

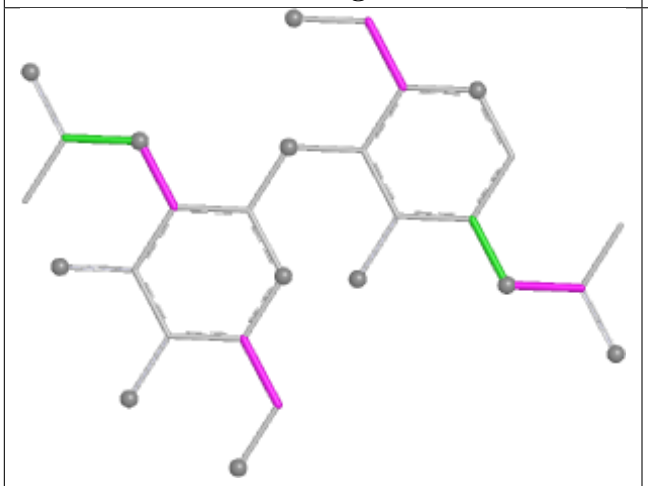
Oligosaccharide Chain c



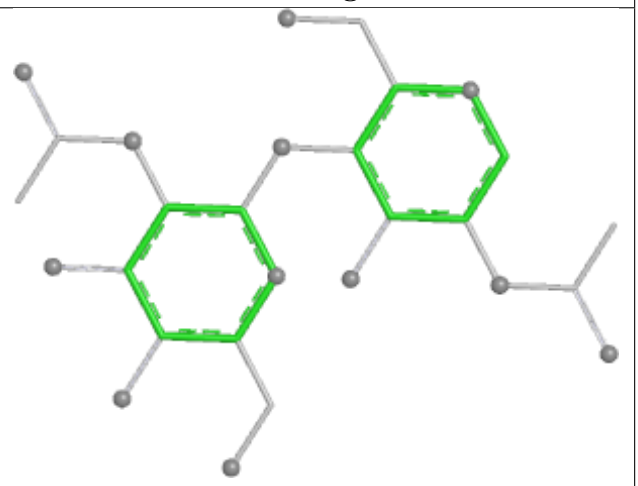
Bond lengths



Bond angles

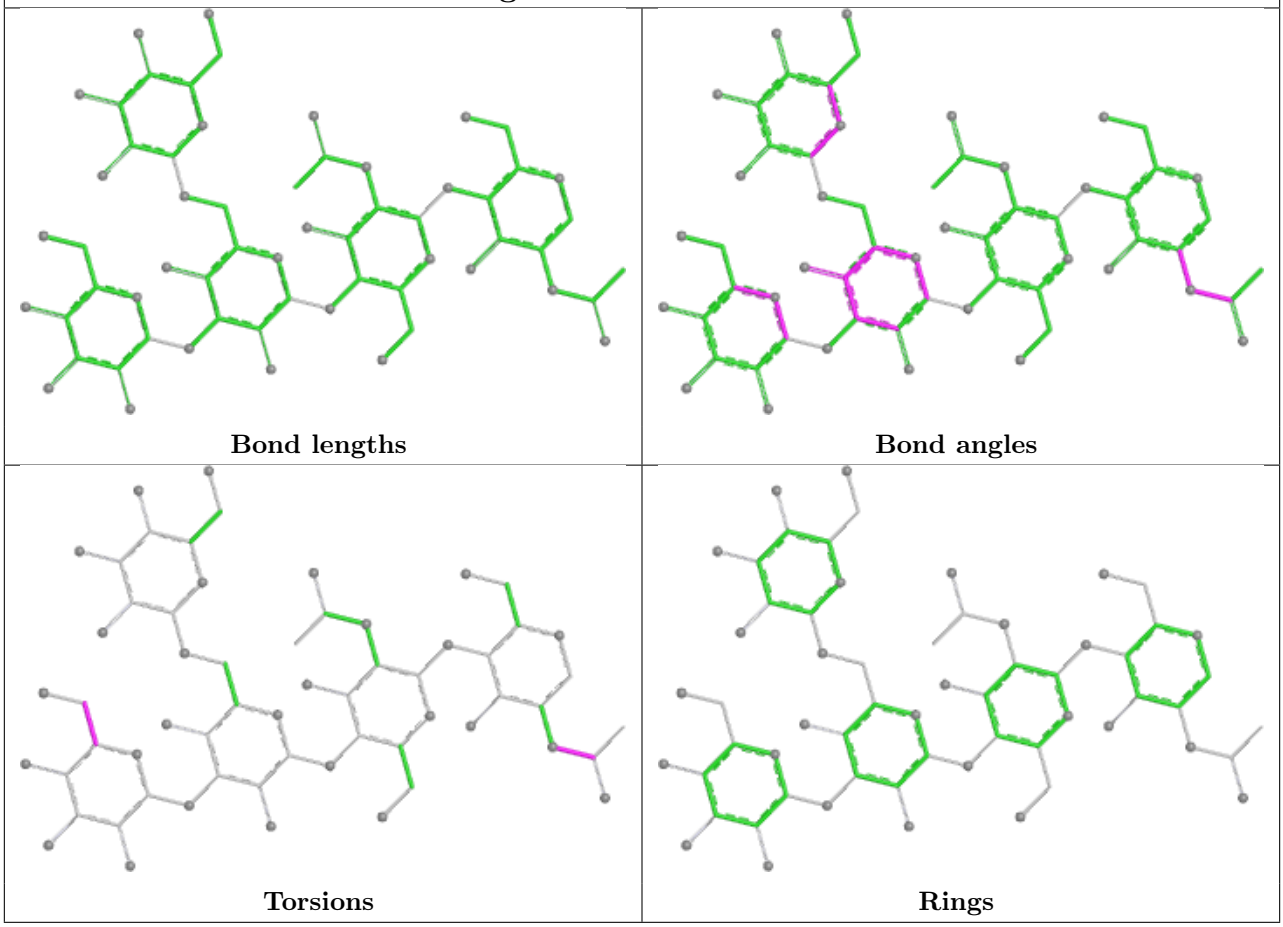


Torsions

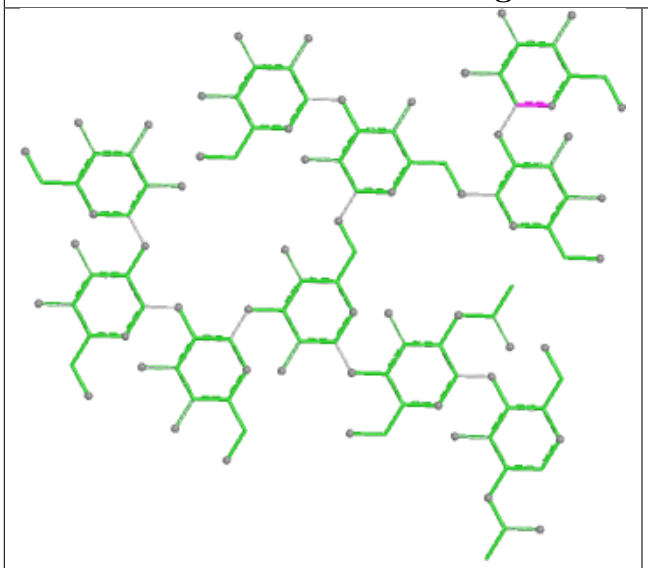


Rings

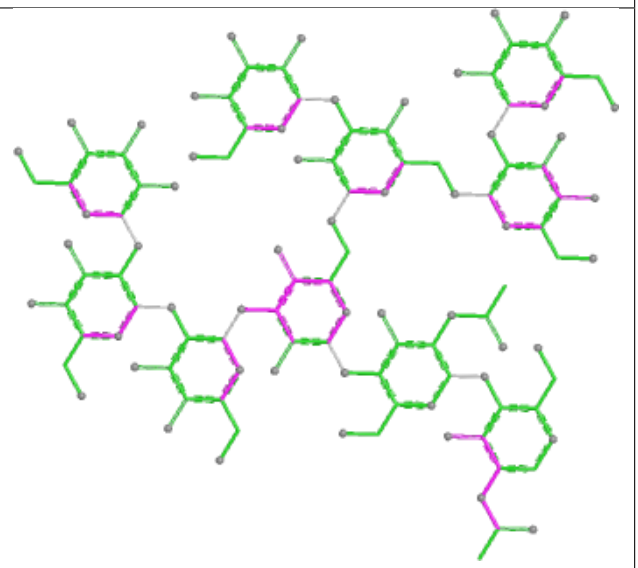
Oligosaccharide Chain J



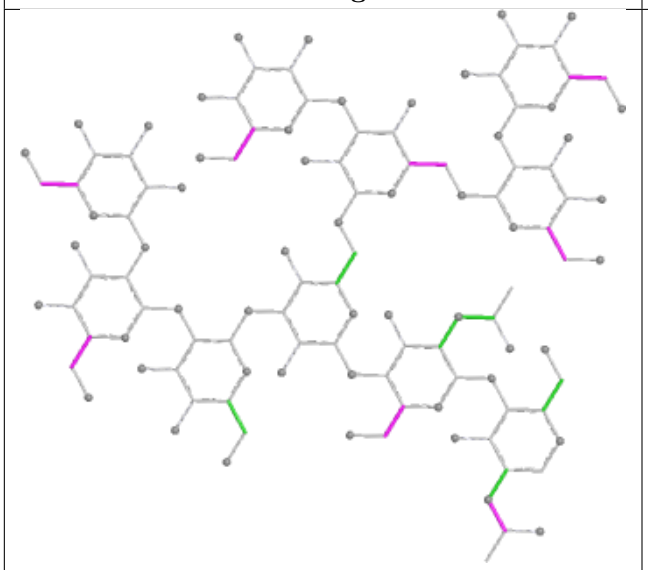
Oligosaccharide Chain N



Bond lengths



Bond angles



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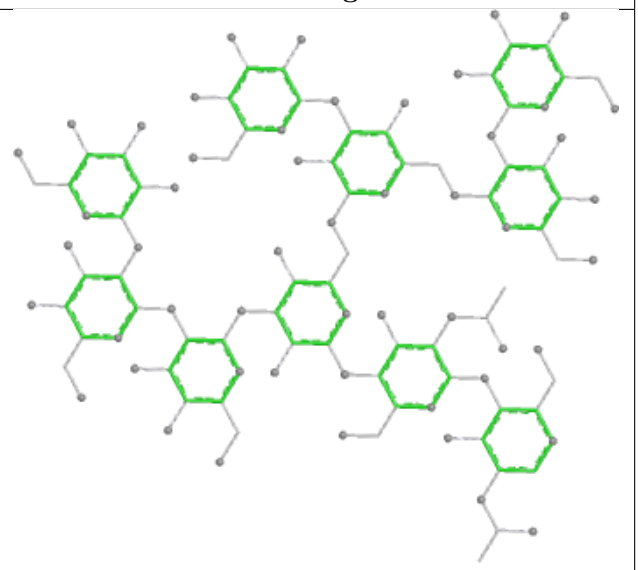
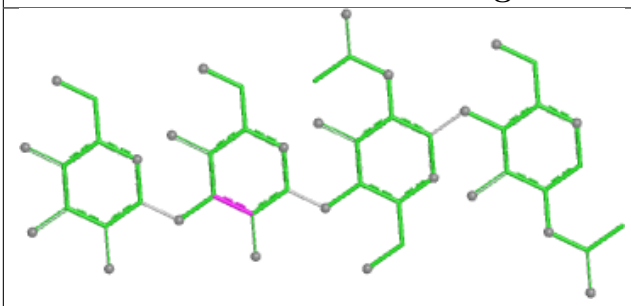
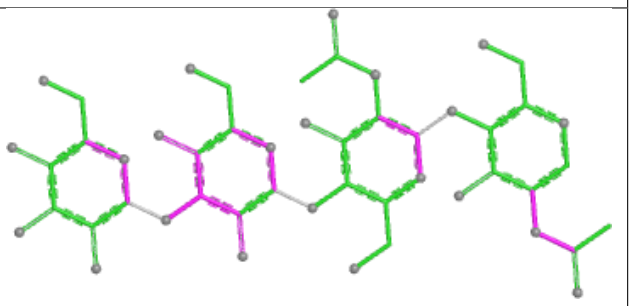


Rings

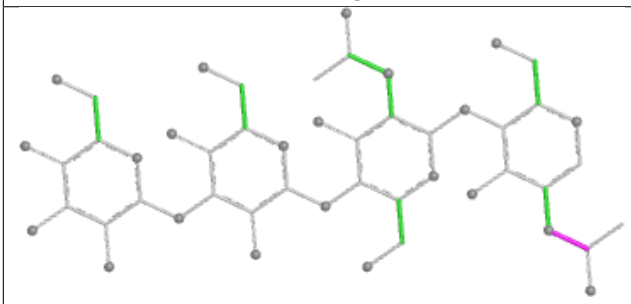
Oligosaccharide Chain U



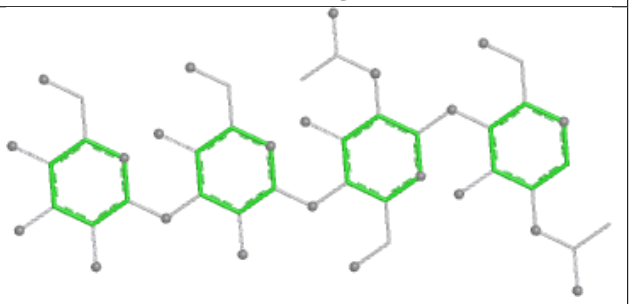
Bond lengths



Bond angles

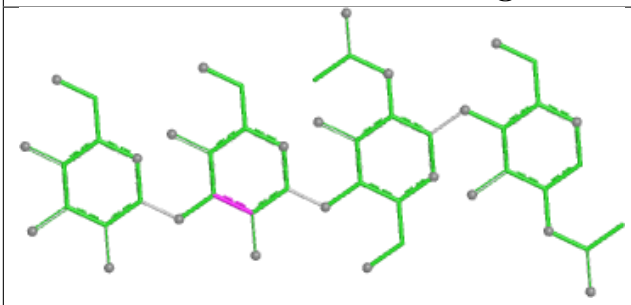


Torsions

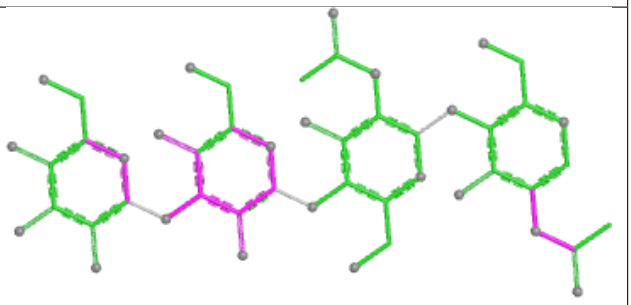


Rings

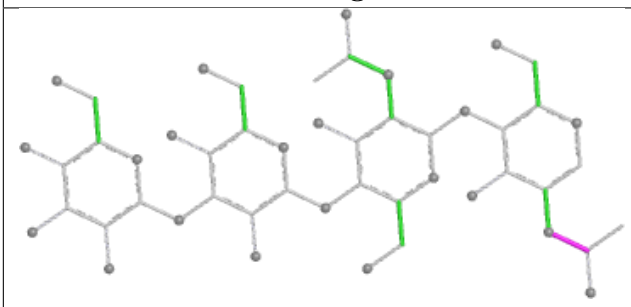
Oligosaccharide Chain Z



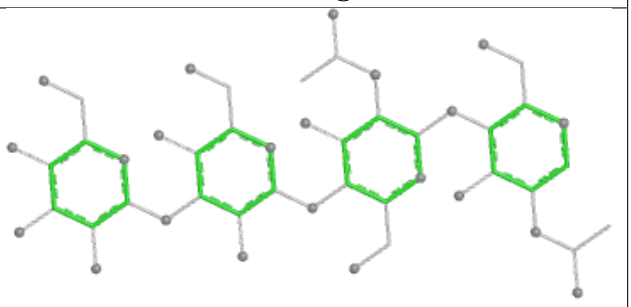
Bond lengths



Bond angles

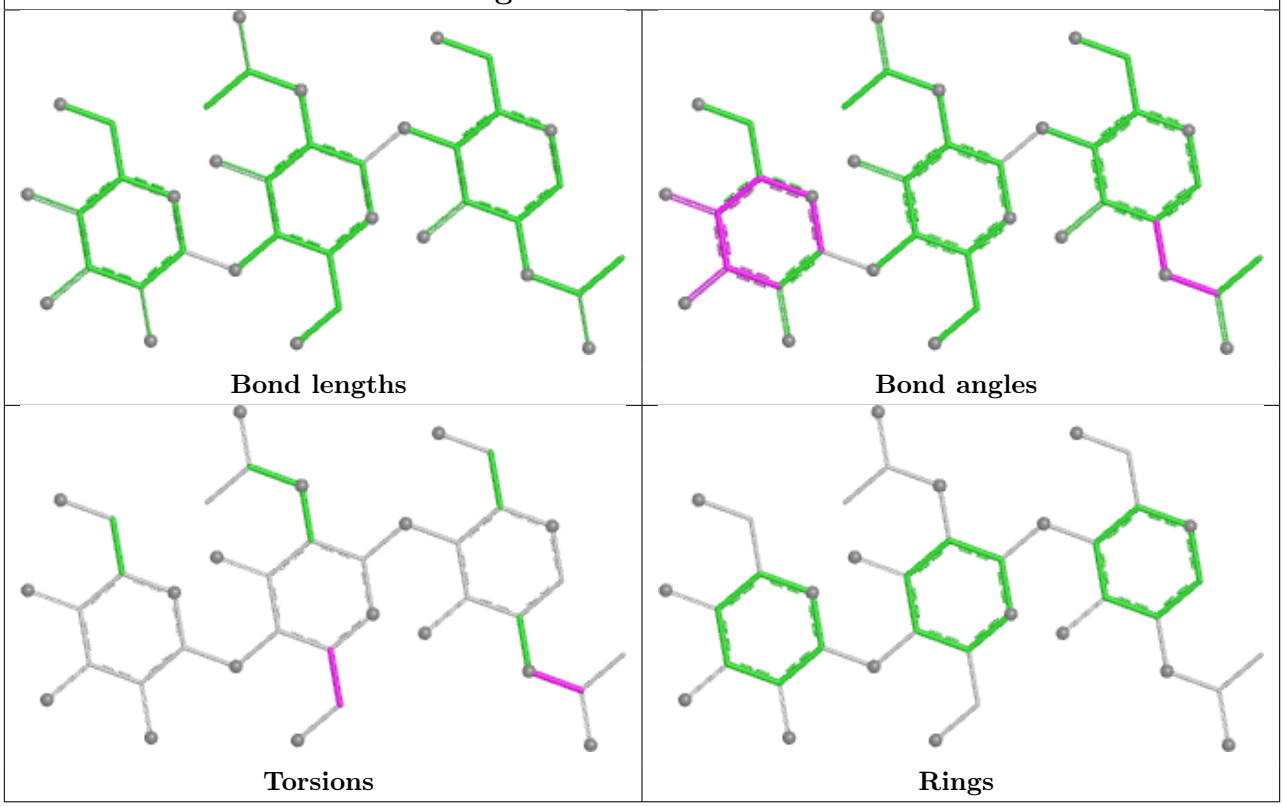


Torsions

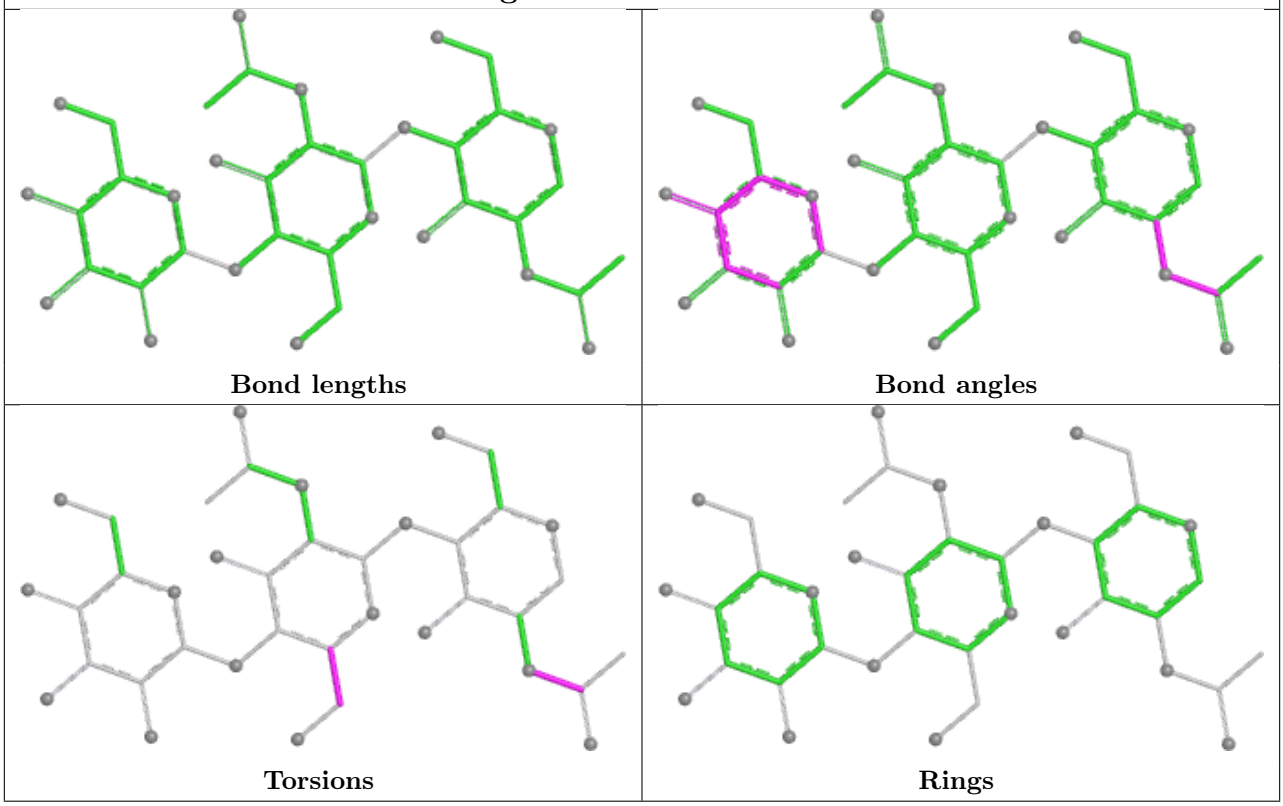


Rings

Oligosaccharide Chain V



Oligosaccharide Chain a



5.6 Ligand geometry (i)

46 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	$\#\|Z\| > 2$
12	NAG	B	703	6	14,14,15	0.72	0	17,19,21	0.87	0
12	NAG	D	702	6	14,14,15	0.76	0	17,19,21	1.39	1 (5%)
12	NAG	E	601	5	14,14,15	0.73	0	17,19,21	0.84	0
12	NAG	B	701	6	14,14,15	0.70	0	17,19,21	1.33	1 (5%)
12	NAG	C	608	5	14,14,15	0.70	0	17,19,21	0.80	0
12	NAG	A	608	5	14,14,15	0.71	0	17,19,21	1.04	1 (5%)
12	NAG	E	602	5	14,14,15	0.71	0	17,19,21	0.84	0
12	NAG	C	602	5	14,14,15	0.70	0	17,19,21	0.89	1 (5%)
12	NAG	A	612	5	14,14,15	0.71	0	17,19,21	1.90	3 (17%)
12	NAG	A	610	5	14,14,15	0.73	0	17,19,21	1.11	1 (5%)
12	NAG	B	702	6	14,14,15	0.68	0	17,19,21	1.33	2 (11%)
12	NAG	C	605	5	14,14,15	0.75	0	17,19,21	0.77	0
12	NAG	E	609	5	14,14,15	0.71	0	17,19,21	2.26	4 (23%)
12	NAG	F	701	6	14,14,15	0.68	0	17,19,21	1.19	2 (11%)
12	NAG	D	703	6	14,14,15	0.73	0	17,19,21	0.76	0
12	NAG	A	605	5	14,14,15	0.70	0	17,19,21	0.74	0
12	NAG	C	601	5	14,14,15	0.74	0	17,19,21	0.80	0
12	NAG	C	609	5	14,14,15	0.71	0	17,19,21	2.17	3 (17%)
12	NAG	E	604	5	14,14,15	0.67	0	17,19,21	1.31	2 (11%)
12	NAG	C	604	5	14,14,15	0.66	0	17,19,21	1.25	2 (11%)
12	NAG	A	607	5	14,14,15	0.73	0	17,19,21	1.05	1 (5%)
12	NAG	E	606	5	14,14,15	0.71	0	17,19,21	0.92	0
12	NAG	F	703	6	14,14,15	0.73	0	17,19,21	0.85	0
12	NAG	A	603	5	14,14,15	0.83	1 (7%)	17,19,21	2.28	4 (23%)
12	NAG	E	607	5	14,14,15	0.75	0	17,19,21	0.85	1 (5%)
12	NAG	A	602	5	14,14,15	0.70	0	17,19,21	0.90	0
12	NAG	A	611	5	14,14,15	0.71	0	17,19,21	1.14	1 (5%)
12	NAG	C	607	5	14,14,15	0.73	0	17,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	NAG	E	612	5	14,14,15	0.69	0	17,19,21	1.87	3 (17%)
12	NAG	C	612	5	14,14,15	0.69	0	17,19,21	1.88	3 (17%)
12	NAG	D	701	6	14,14,15	0.68	0	17,19,21	1.32	1 (5%)
12	NAG	C	610	5	14,14,15	0.70	0	17,19,21	1.12	1 (5%)
12	NAG	E	608	5	14,14,15	0.73	0	17,19,21	0.82	0
12	NAG	E	610	5	14,14,15	0.70	0	17,19,21	1.15	1 (5%)
12	NAG	E	603	5	14,14,15	0.71	0	17,19,21	1.16	1 (5%)
12	NAG	C	603	5	14,14,15	0.76	0	17,19,21	1.28	1 (5%)
12	NAG	E	611	5	14,14,15	0.67	0	17,19,21	1.13	1 (5%)
12	NAG	C	611	5	14,14,15	0.72	0	17,19,21	1.23	1 (5%)
12	NAG	A	609	5	14,14,15	0.68	0	17,19,21	1.84	3 (17%)
12	NAG	A	606	5	14,14,15	0.69	0	17,19,21	0.93	0
12	NAG	E	605	5	14,14,15	0.71	0	17,19,21	0.82	1 (5%)
12	NAG	F	702	6	14,14,15	0.74	0	17,19,21	1.44	2 (11%)
12	NAG	A	601	5	14,14,15	0.73	0	17,19,21	0.96	1 (5%)
12	NAG	C	606	5	14,14,15	0.69	0	17,19,21	0.87	0
12	NAG	A	604	5	14,14,15	0.73	0	17,19,21	1.41	2 (11%)
12	NAG	A	613	5	14,14,15	0.71	0	17,19,21	0.84	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
12	NAG	B	703	6	-	1/6/23/26	0/1/1/1
12	NAG	D	702	6	-	2/6/23/26	0/1/1/1
12	NAG	E	601	5	-	0/6/23/26	0/1/1/1
12	NAG	B	701	6	-	2/6/23/26	0/1/1/1
12	NAG	C	608	5	-	0/6/23/26	0/1/1/1
12	NAG	A	608	5	-	1/6/23/26	0/1/1/1
12	NAG	E	602	5	-	0/6/23/26	0/1/1/1
12	NAG	C	602	5	-	0/6/23/26	0/1/1/1
12	NAG	A	612	5	-	2/6/23/26	0/1/1/1
12	NAG	A	610	5	-	2/6/23/26	0/1/1/1
12	NAG	B	702	6	-	2/6/23/26	0/1/1/1
12	NAG	C	605	5	-	0/6/23/26	0/1/1/1
12	NAG	E	609	5	-	3/6/23/26	0/1/1/1

Continued on next page...

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	NAG	F	701	6	-	2/6/23/26	0/1/1/1
12	NAG	D	703	6	-	0/6/23/26	0/1/1/1
12	NAG	A	605	5	-	0/6/23/26	0/1/1/1
12	NAG	C	601	5	-	0/6/23/26	0/1/1/1
12	NAG	C	609	5	-	2/6/23/26	0/1/1/1
12	NAG	E	604	5	-	3/6/23/26	0/1/1/1
12	NAG	C	604	5	-	3/6/23/26	0/1/1/1
12	NAG	A	607	5	-	1/6/23/26	0/1/1/1
12	NAG	E	606	5	-	1/6/23/26	0/1/1/1
12	NAG	F	703	6	-	0/6/23/26	0/1/1/1
12	NAG	A	603	5	-	2/6/23/26	0/1/1/1
12	NAG	E	607	5	-	0/6/23/26	0/1/1/1
12	NAG	A	602	5	-	0/6/23/26	0/1/1/1
12	NAG	A	611	5	-	2/6/23/26	0/1/1/1
12	NAG	C	607	5	-	0/6/23/26	0/1/1/1
12	NAG	E	612	5	-	2/6/23/26	0/1/1/1
12	NAG	C	612	5	-	2/6/23/26	0/1/1/1
12	NAG	D	701	6	-	2/6/23/26	0/1/1/1
12	NAG	C	610	5	-	2/6/23/26	0/1/1/1
12	NAG	E	608	5	-	0/6/23/26	0/1/1/1
12	NAG	E	610	5	-	2/6/23/26	0/1/1/1
12	NAG	E	603	5	-	3/6/23/26	0/1/1/1
12	NAG	C	603	5	-	3/6/23/26	0/1/1/1
12	NAG	E	611	5	-	2/6/23/26	0/1/1/1
12	NAG	C	611	5	-	2/6/23/26	0/1/1/1
12	NAG	A	609	5	-	2/6/23/26	0/1/1/1
12	NAG	A	606	5	-	1/6/23/26	0/1/1/1
12	NAG	E	605	5	-	0/6/23/26	0/1/1/1
12	NAG	F	702	6	-	2/6/23/26	0/1/1/1
12	NAG	A	601	5	-	0/6/23/26	0/1/1/1
12	NAG	C	606	5	-	1/6/23/26	0/1/1/1
12	NAG	A	604	5	-	3/6/23/26	0/1/1/1
12	NAG	A	613	5	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	603	NAG	C1-C2	2.15	1.55	1.52

The worst 5 of 53 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	E	609	NAG	C2-N2-C7	7.44	132.88	122.90
12	A	603	NAG	C2-N2-C7	7.25	132.62	122.90
12	C	609	NAG	C2-N2-C7	7.06	132.37	122.90
12	E	612	NAG	C2-N2-C7	5.79	130.66	122.90
12	A	609	NAG	C2-N2-C7	5.55	130.33	122.90

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	609	NAG	C1-C2-N2-C7
12	E	609	NAG	C1-C2-N2-C7
12	E	612	NAG	C1-C2-N2-C7
12	E	609	NAG	O5-C5-C6-O6
12	E	609	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	601	NAG	1	0
12	C	601	NAG	1	0
12	A	609	NAG	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

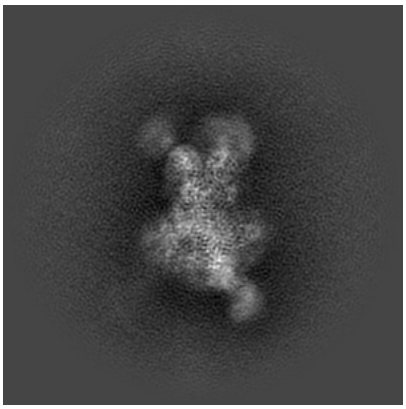
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-73000. These allow visual inspection of the internal detail of the map and identification of artifacts.

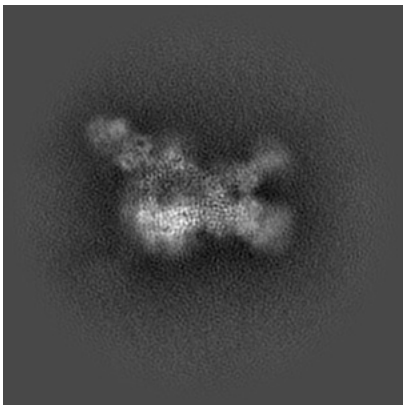
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

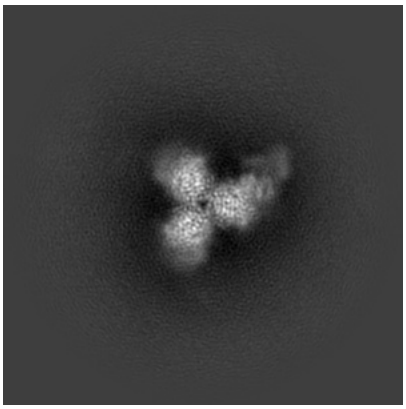
6.1.1 Primary map



X

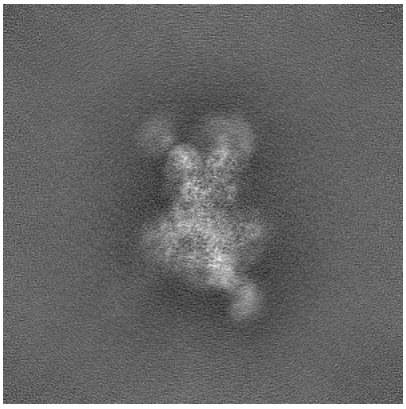


Y

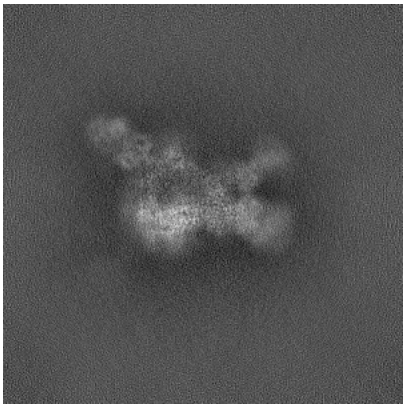


Z

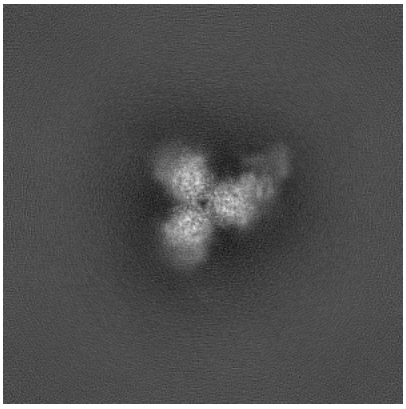
6.1.2 Raw map



X



Y

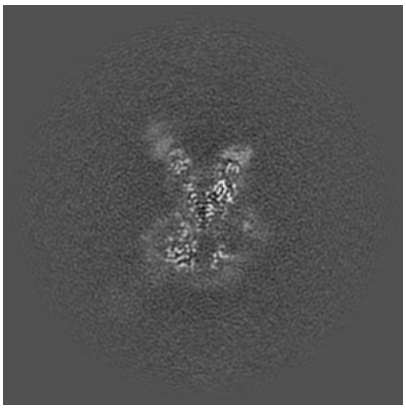


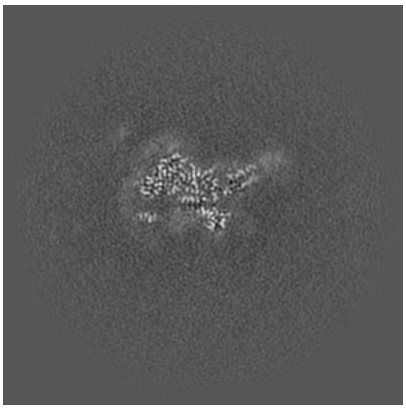
Z

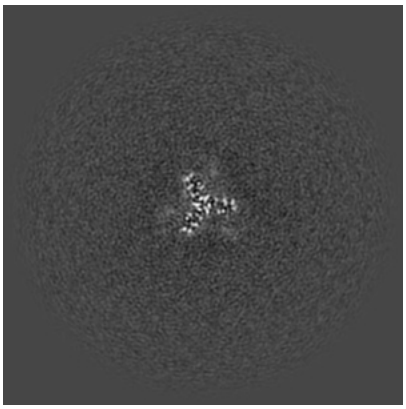
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

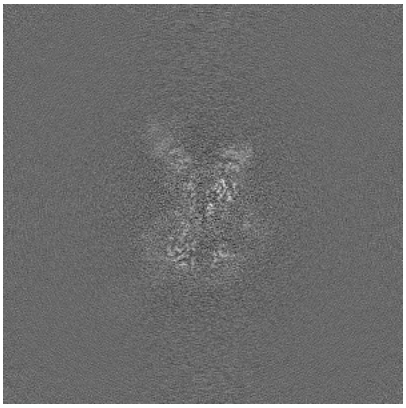
6.2.1 Primary map

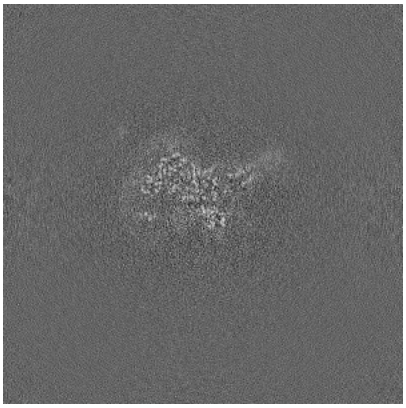

X Index: 200

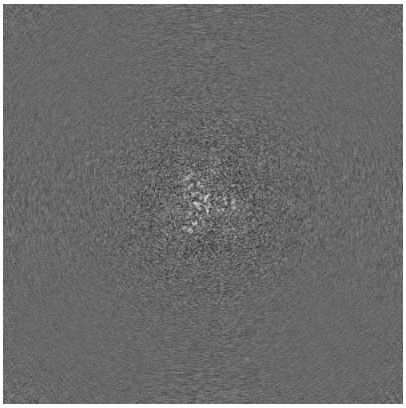

Y Index: 200


Z Index: 200

6.2.2 Raw map


X Index: 200

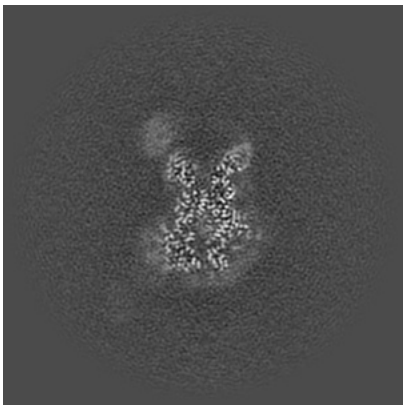

Y Index: 200


Z Index: 200

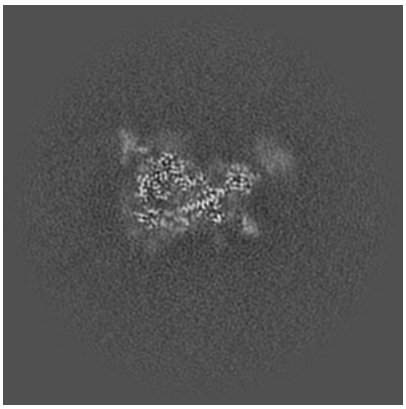
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

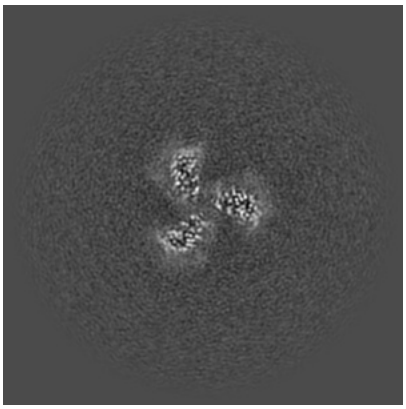
6.3.1 Primary map



X Index: 193

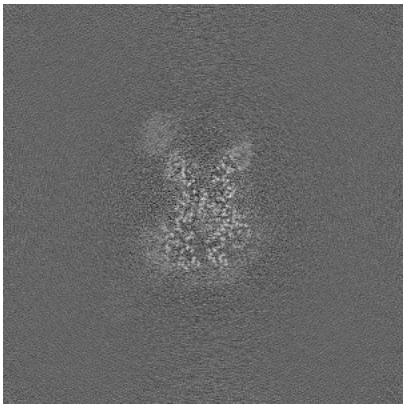


Y Index: 206

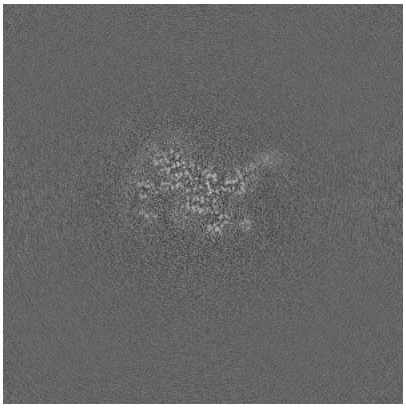


Z Index: 169

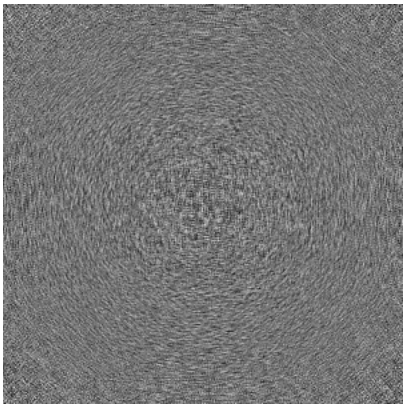
6.3.2 Raw map



X Index: 193



Y Index: 197

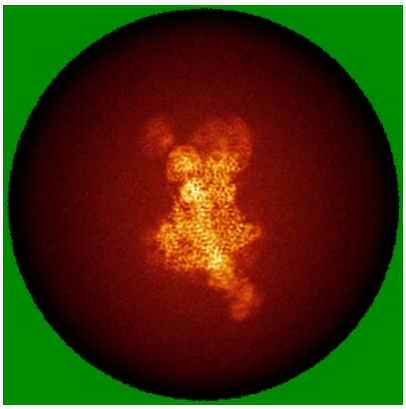


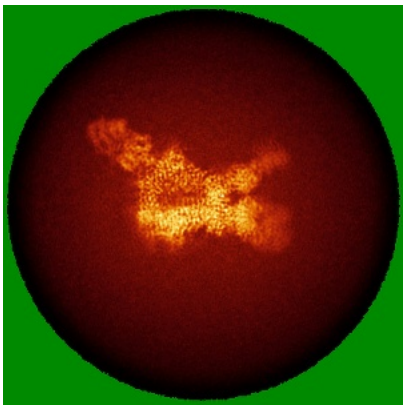
Z Index: 0

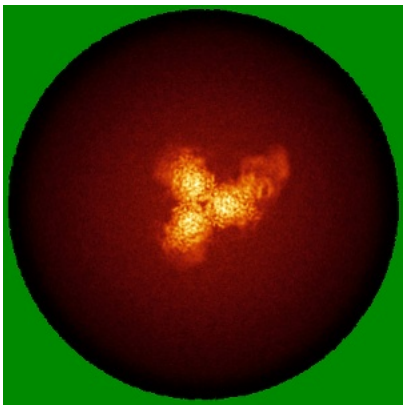
The images above show the largest variance slices of the map in three orthogonal directions.

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

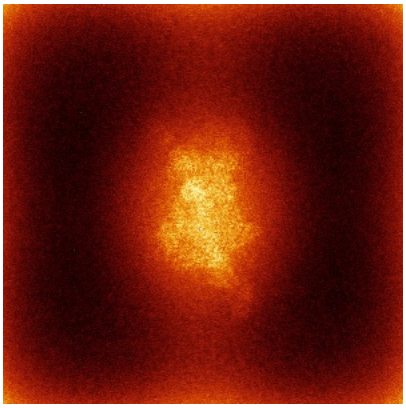
6.4.1 Primary map

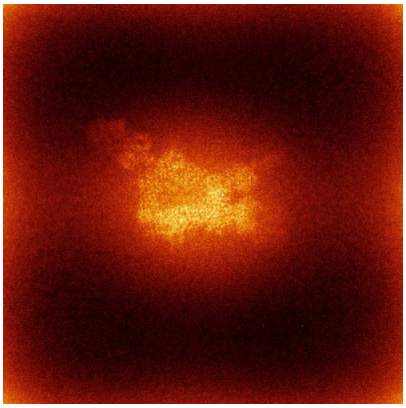

X

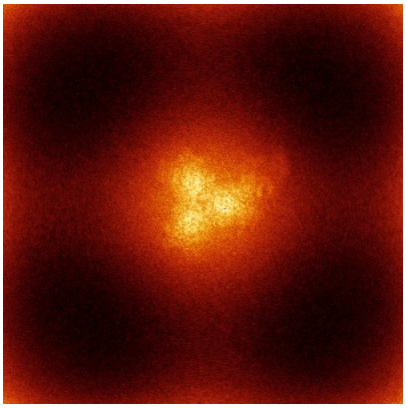

Y


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 0.15. 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.

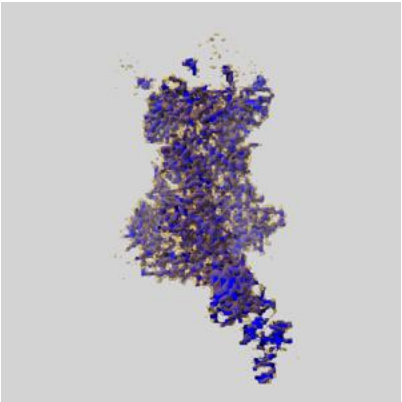
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

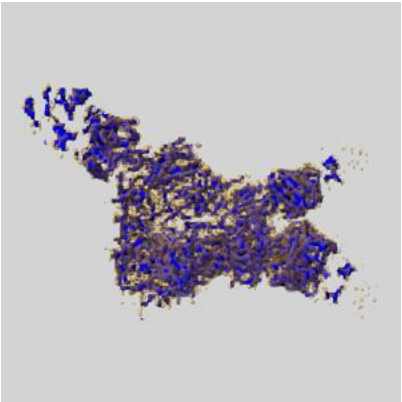
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

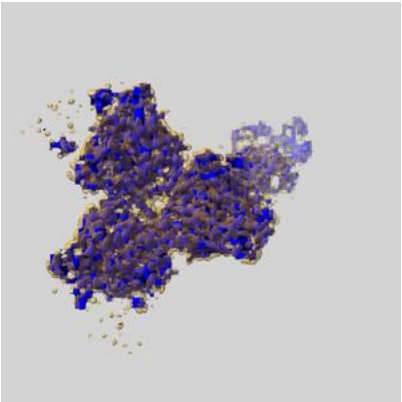
6.6.1 emd_73000_msk_1.map (i)



X



Y

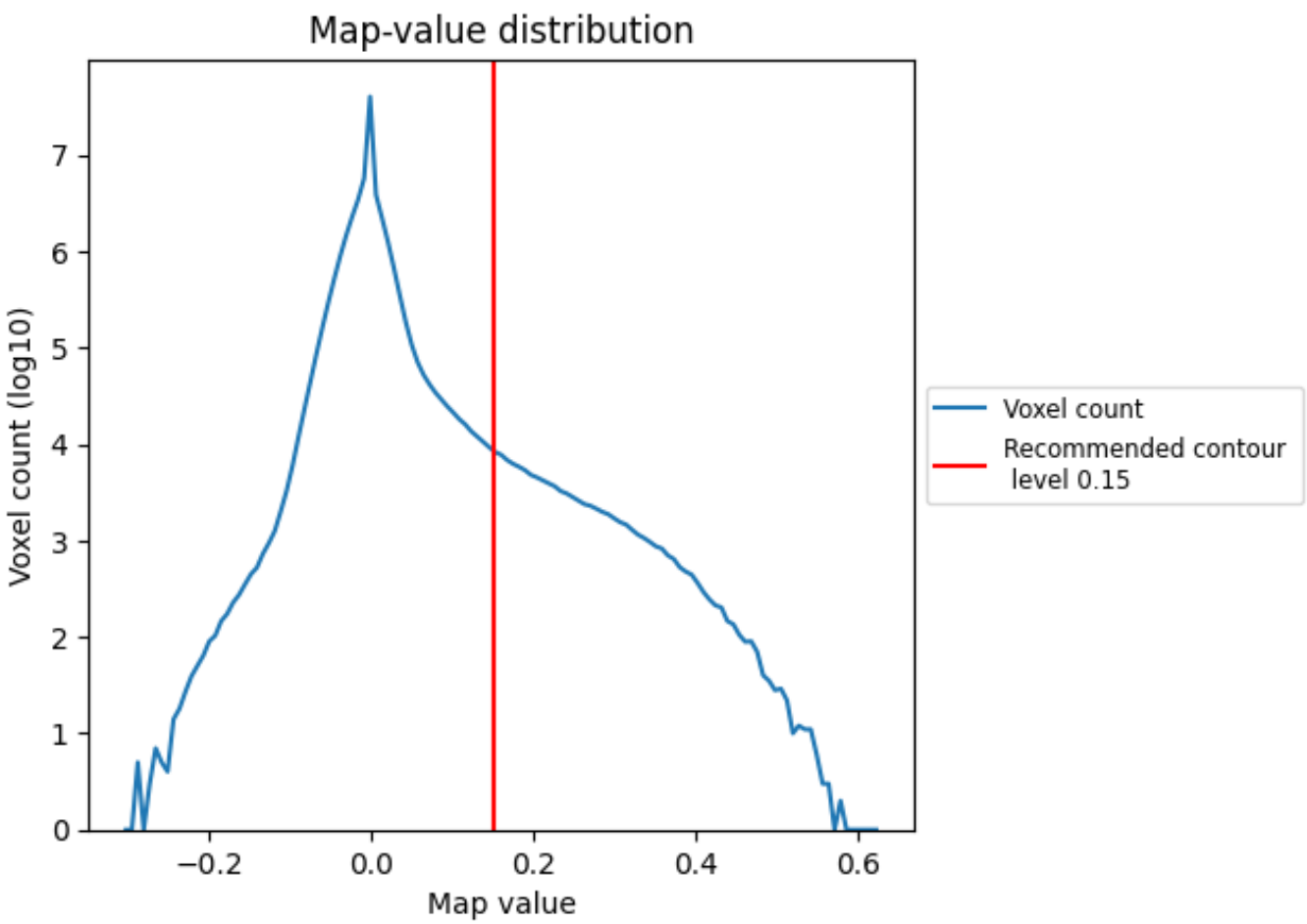


Z

7 Map analysis (i)

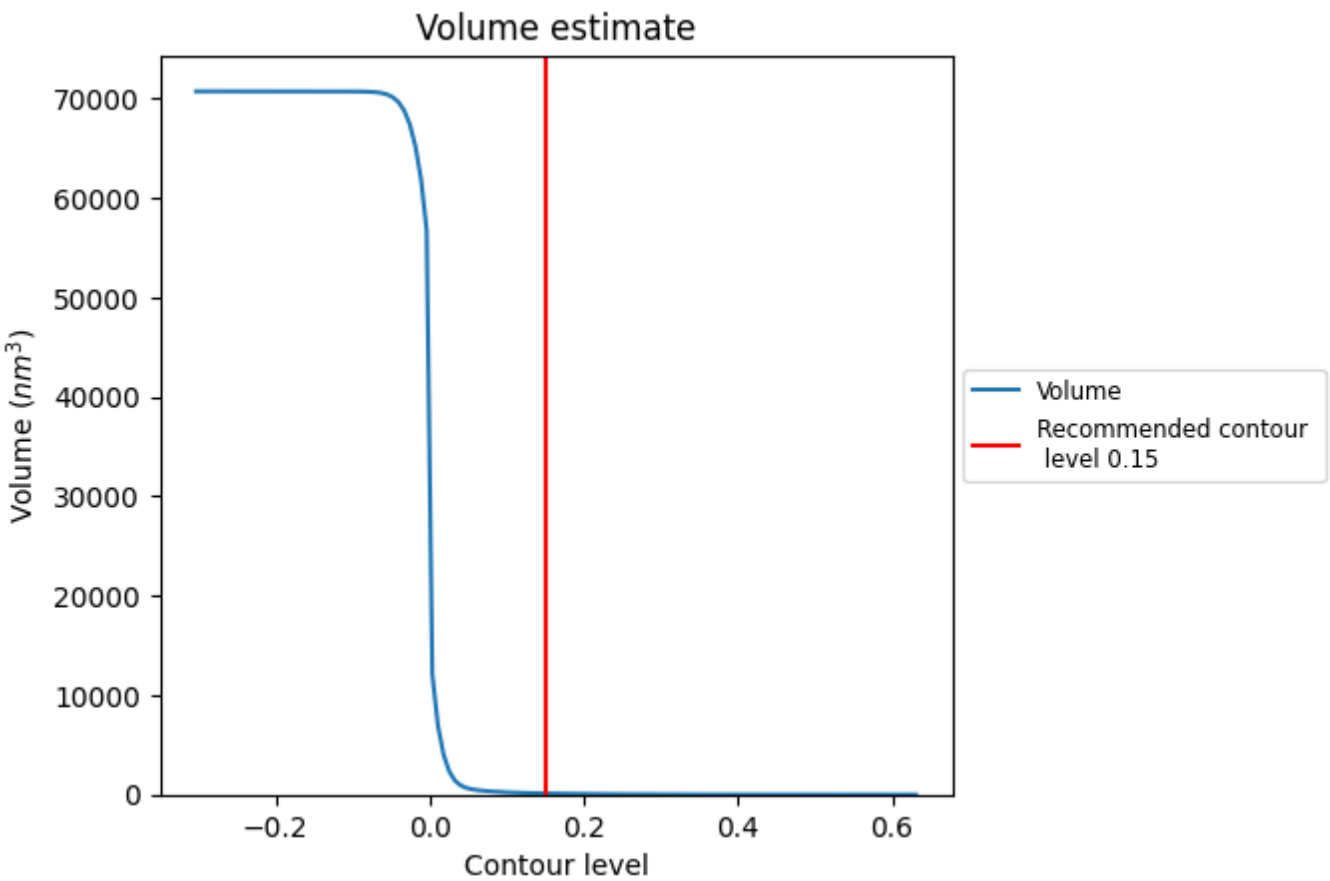
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

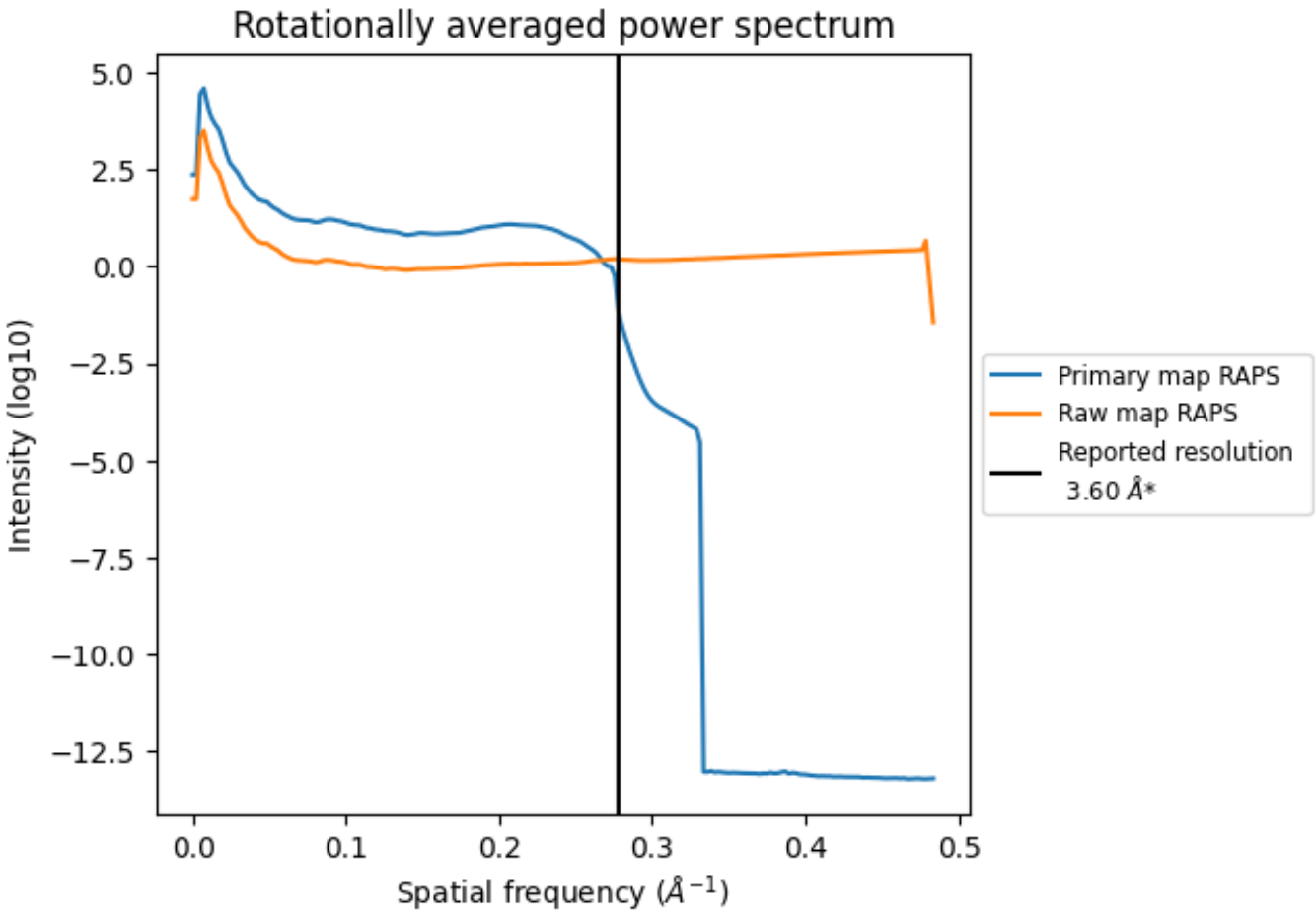
7.2 Volume estimate (i)



The volume at the recommended contour level is 114 nm^3; this corresponds to an approximate mass of 103 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)

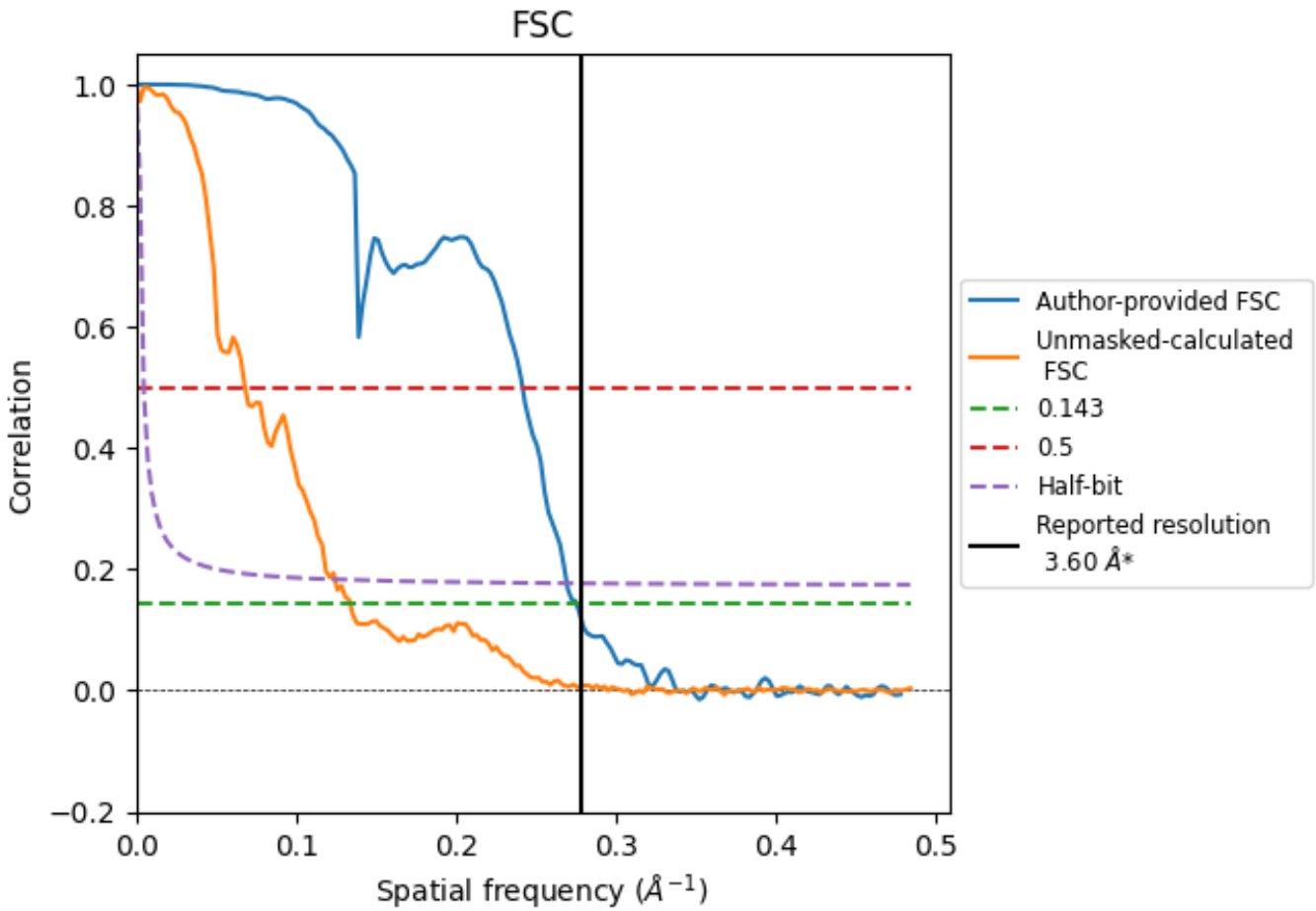


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation (i)

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 (i)



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

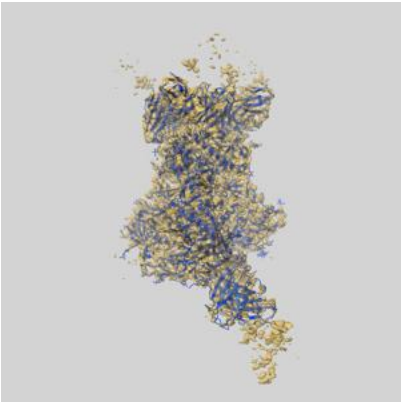
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.64	4.14	3.72
Unmasked-calculated*	7.49	14.71	8.05

*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 7.49 differs from the reported value 3.6 by more than 10 %

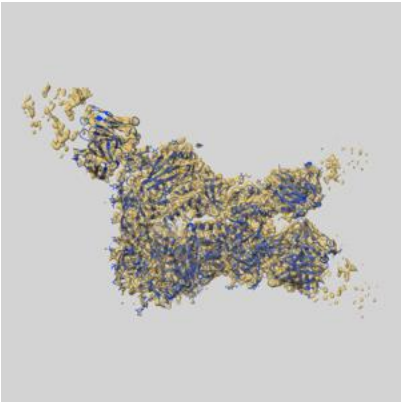
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-73000 and PDB model 9YIW. Per-residue inclusion information can be found in section 3 on page 10.

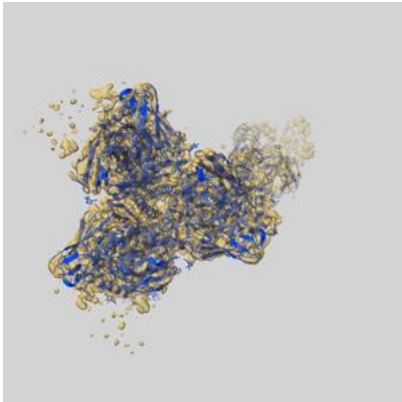
9.1 Map-model overlay (i)



X



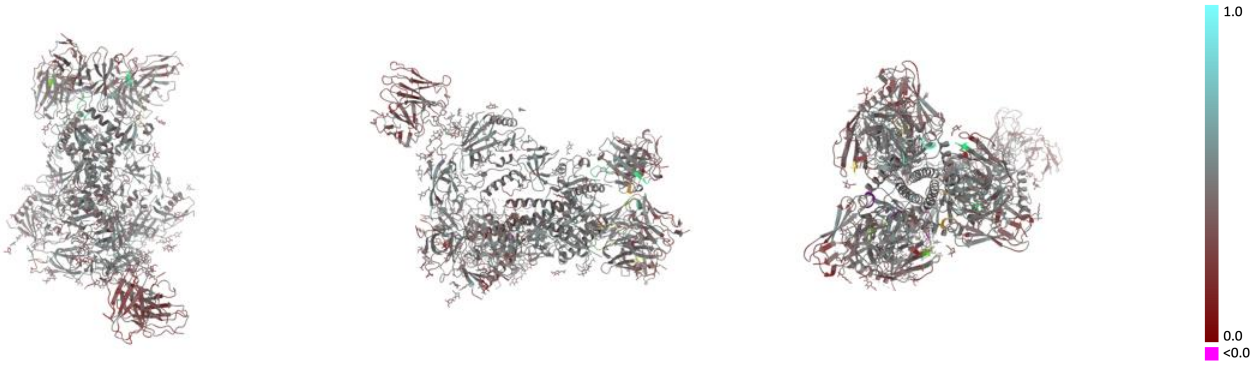
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

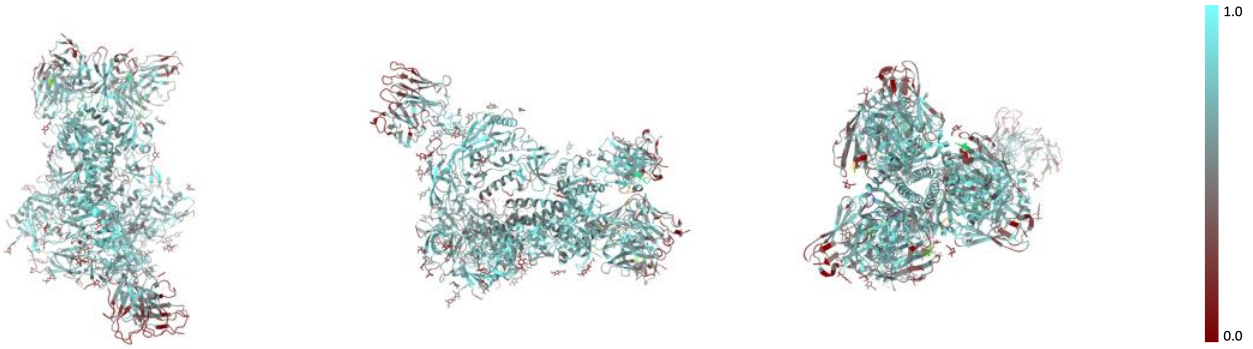
9.2 Q-score mapped to coordinate model (i)



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.

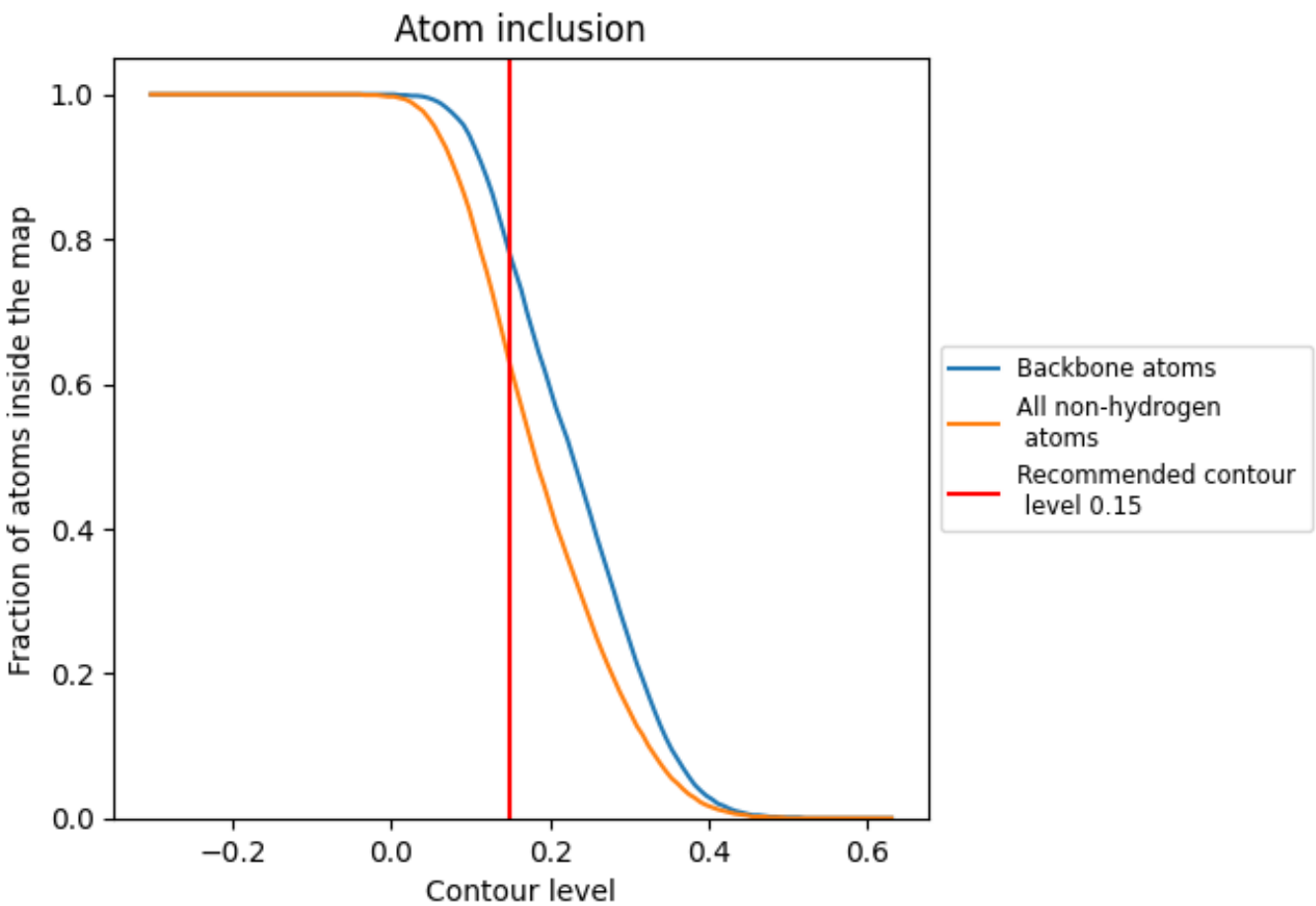
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6250	0.4340
A	0.6710	0.4700
B	0.7000	0.4610
C	0.6520	0.4460
D	0.7060	0.4670
E	0.6410	0.4450
F	0.7090	0.4710
G	0.4290	0.4620
H	0.4580	0.3170
I	0.6270	0.4330
J	0.4920	0.4620
K	0.6220	0.4280
L	0.4540	0.3340
M	0.5970	0.4100
N	0.6550	0.4300
O	0.5490	0.4020
P	0.1790	0.2640
Q	0.6160	0.4260
R	0.4640	0.3730
S	0.5470	0.4020
T	0.3570	0.3710
U	0.4400	0.3460
V	0.4870	0.4330
W	0.1790	0.2120
X	0.5000	0.4040
Y	0.3930	0.3830
Z	0.4600	0.4360
a	0.3590	0.3340
b	0.2860	0.2990
c	0.3930	0.3060