wwPDB EM Validation Summary Report (i)

Dec 18, 2022 – 05:24 am GMT

PDB ID	:	7NWL
EMDB ID	:	EMD-12634
Title	:	Cryo-EM structure of human integrin alpha5beta1 (open form) in complex with fibronectin and TS2/16 Fv-clasp
Authors	:	Schumacher, S.; Dedden, D.; Vazquez Nunez, R.; Matoba, K.; Takagi, J.; Biertumpfel, C.; Mizuno, N.
Deposited on	:	2021-03-17
Resolution	:	3.10 Å(reported)
Based on initial models	:	3VI3, 5XCX, 4WK0, 1FNF

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 (i)) were used in the production of this report:

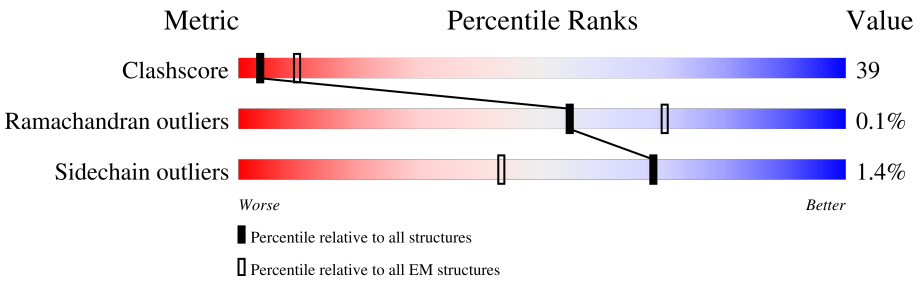
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1008	35% 25% 40%
2	B	778	30% 25% 43%
3	C	368	35% 47% 52%
4	D	172	28% 57% 42%
5	E	164	23% 60% 38%
6	F	3	33% 33% 67%
6	G	3	33% 67% 33%
6	K	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
6	M	3	67% 33% 33% 33%
7	H	2	50% 50%
7	L	2	50% 100%
7	O	2	100% 50% 50%
8	I	5	20% 40% 20% 40%
9	J	6	17% 33% 67%
10	N	4	75% 100%

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 13904 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	603	4583	2902	770	897	14	0	0

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	441	3430	2144	584	677	25	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	conflict	UNP P05556
B	195	THR	SER	conflict	UNP P05556

- Molecule 3 is a protein called Isoform 1 of Fibronectin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	368	2820	1765	480	573	2	0	0

- Molecule 4 is a protein called TS2/16 VH(S112C)-SARAH Chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	172	1362	859	224	269	10	0	0

- Molecule 5 is a protein called TS2/16 VL-SARAH(S37C) Chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	163	1276	805	212	251	8	0	0

- Molecule 6 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		
6	F	3	39	22	2	15	0	0
6	G	3	39	22	2	15	0	0
6	K	3	39	22	2	15	0	0
6	M	3	39	22	2	15	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	H	2	28	16	2	10	0	0
7	L	2	28	16	2	10	0	0
7	O	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	I	5	61	34	2	25	0	0

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-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
			Total	C	N	O		
9	J	6	75	42	3	30	0	0

- Molecule 10 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
			Total	C	N	O		
10	N	4	50	28	2	20	0	0

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

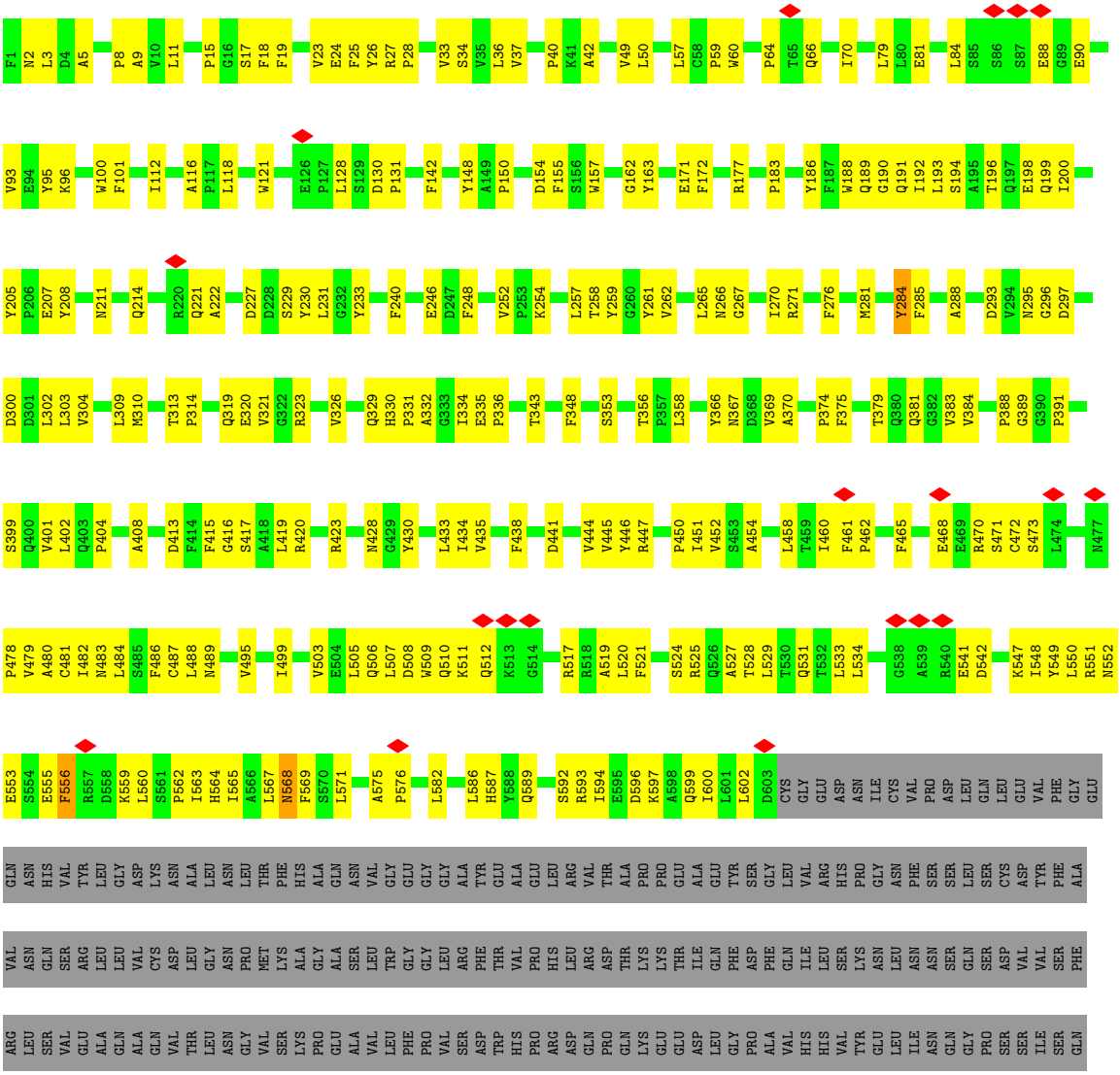
Mol	Chain	Residues	Atoms		AltConf
			Total	Mn	
11	A	4	4	4	0
11	B	3	3	3	0

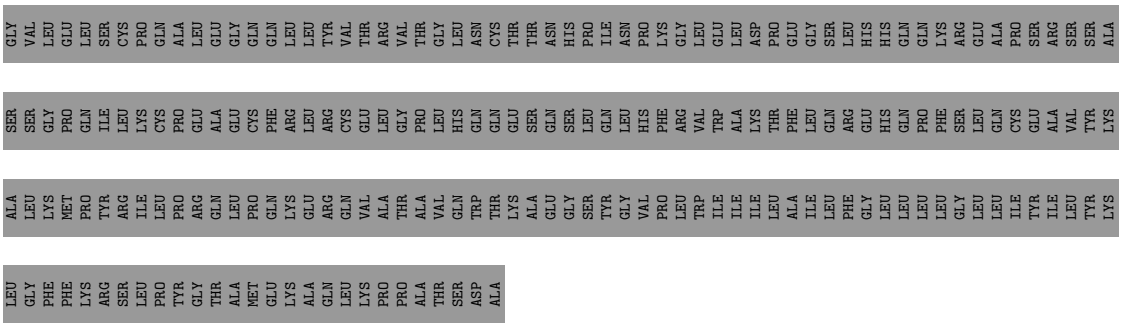
3 Residue-property plots (i)

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: Integrin alpha-5

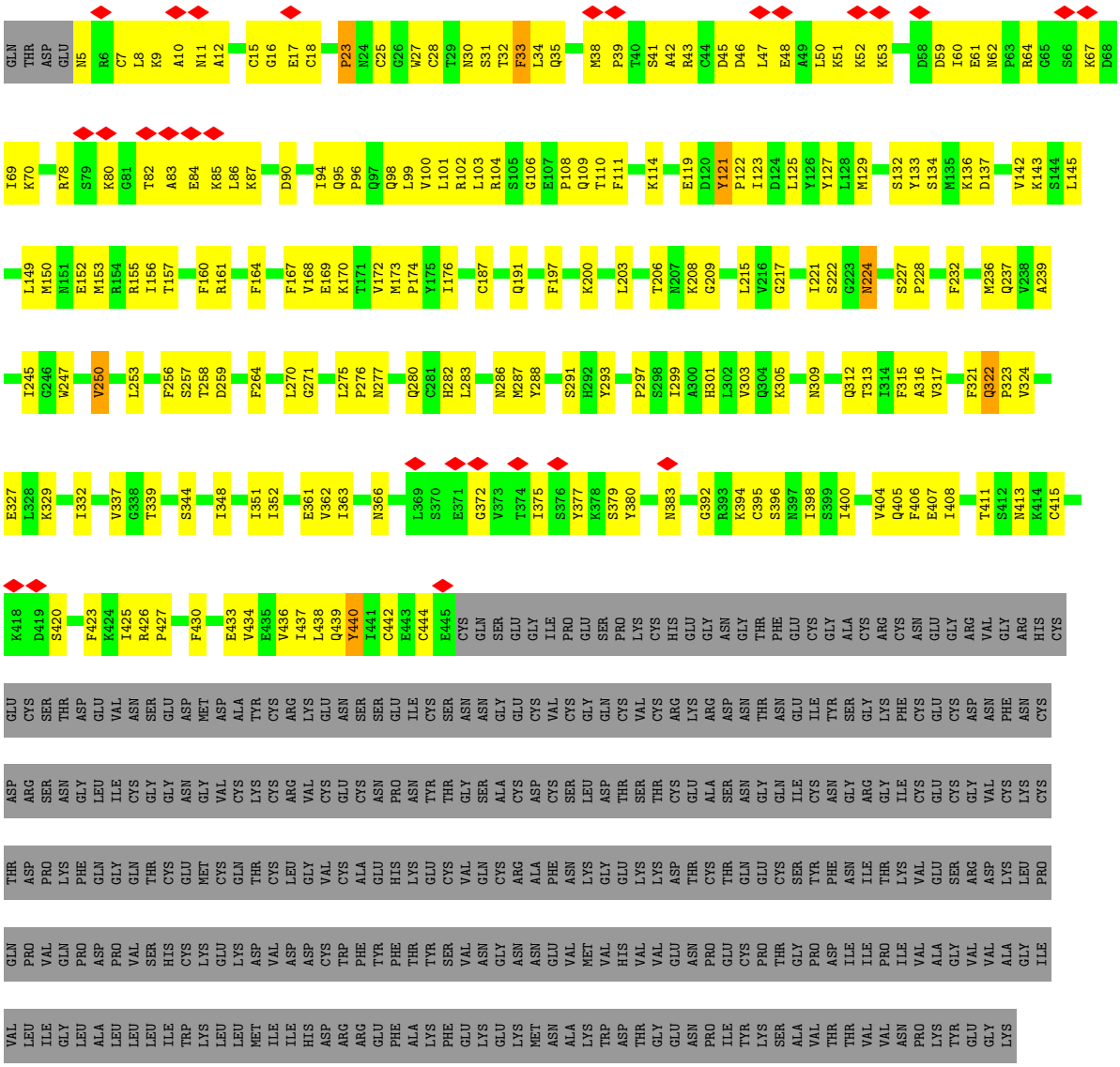
Chain A: 35% 25% 40%





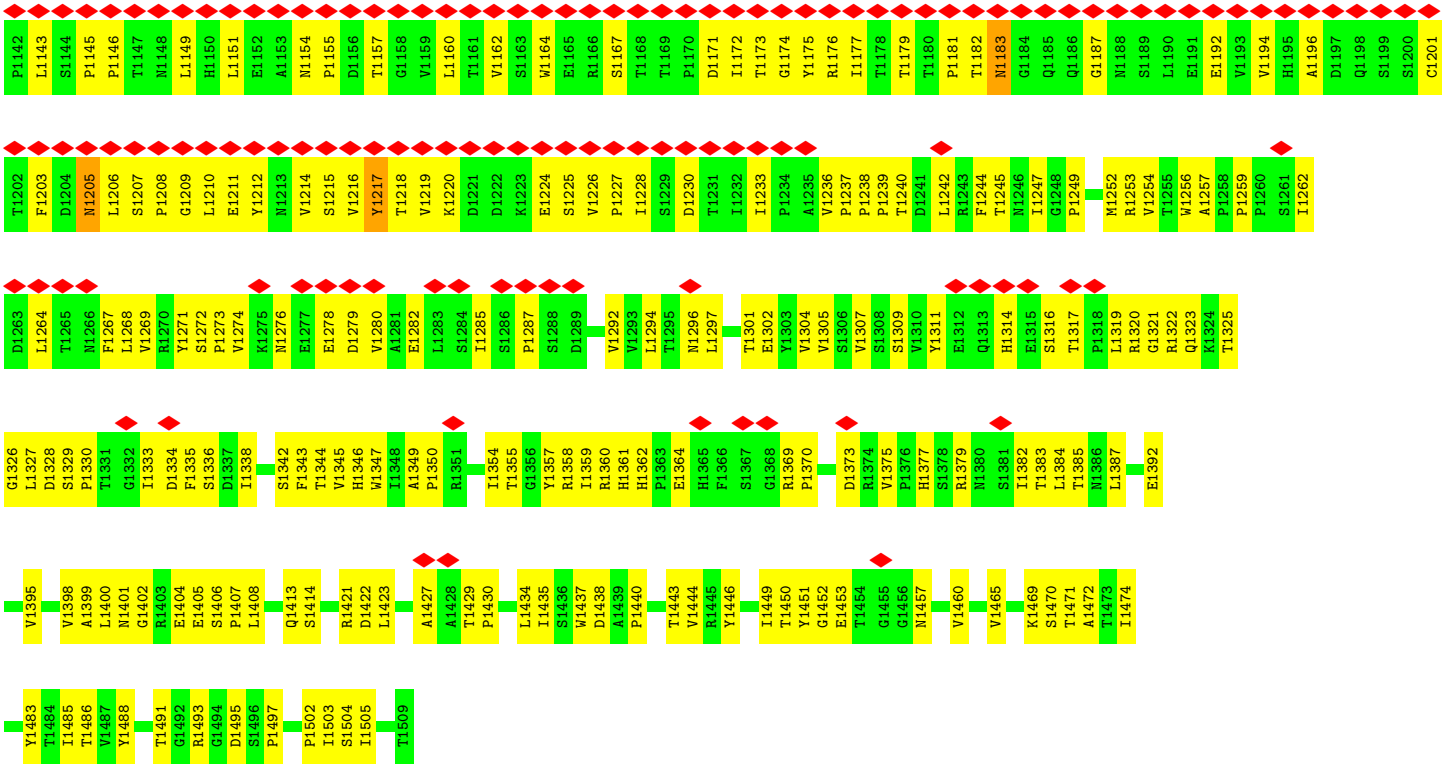
- Molecule 2: Integrin beta-1

Chain B:



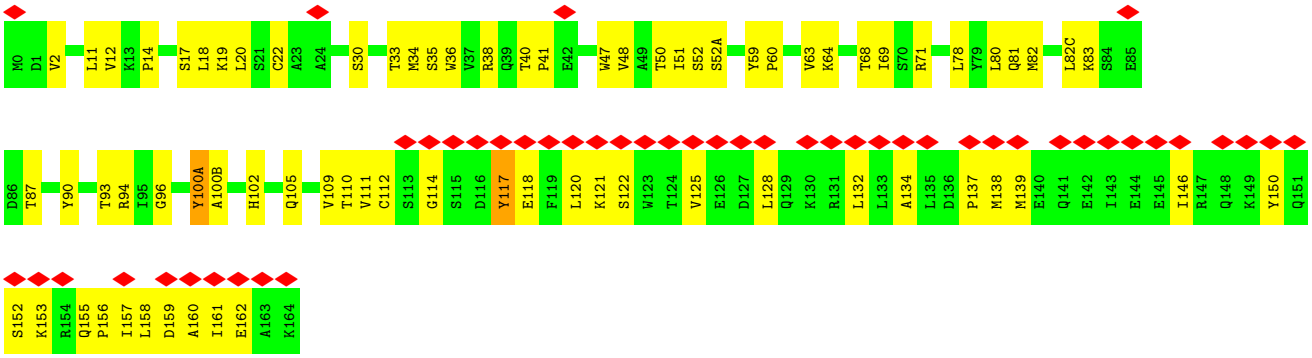
- Molecule 3: Isoform 1 of Fibronectin

Chain C:



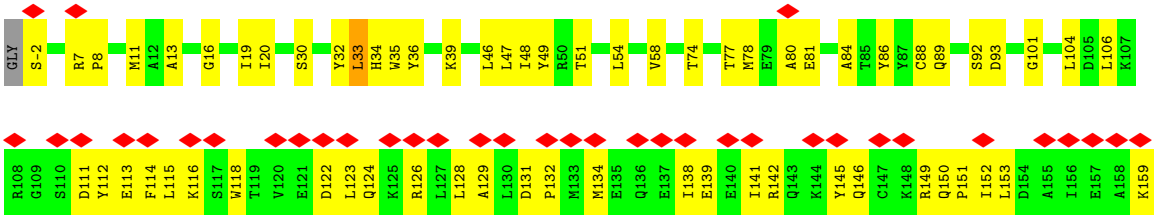
- Molecule 4: TS2/16 VH(S112C)-SARAH Chimera

Chain D:



- Molecule 5: TS2/16 VL-SARAH(S37C) Chimera

Chain E:



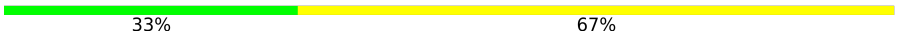
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

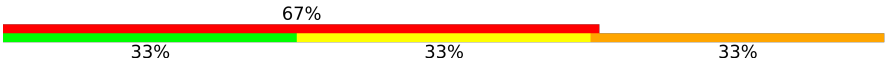
• Molecule 6: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

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

Chain K: 

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

Chain M: 

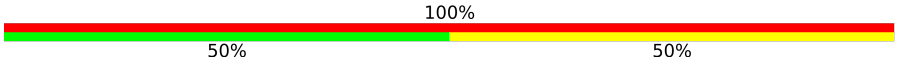
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

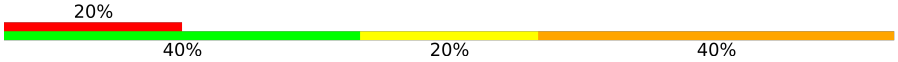
• Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

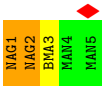
Chain L:

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

Chain O: 

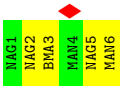
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 



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



• Molecule 10: 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:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	680610	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 ($e^-/Å^2$)	59.7	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.159	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0292	Depositor
Map size (Å)	498.24, 498.24, 498.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.384, 1.384, 1.384	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, BMA, MN, NAG

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	0.66	0/4700	0.62	0/6396
2	B	0.66	0/3490	0.62	0/4711
3	C	0.66	0/2891	0.62	0/3974
4	D	0.66	0/1390	0.62	0/1873
5	E	0.66	0/1302	0.63	0/1760
All	All	0.66	0/13773	0.62	0/18714

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4583	0	4379	301	0
2	B	3430	0	3375	253	0
3	C	2820	0	2754	340	0
4	D	1362	0	1332	131	0
5	E	1276	0	1271	120	0
6	F	39	0	34	3	0
6	G	39	0	34	1	0
6	K	39	0	34	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	39	0	34	1	0
7	H	28	0	25	3	0
7	L	28	0	25	0	0
7	O	28	0	25	1	0
8	I	61	0	52	2	0
9	J	75	0	64	4	0
10	N	50	0	43	0	0
11	A	4	0	0	0	0
11	B	3	0	0	0	0
All	All	13904	0	13481	1080	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 39.

The worst 5 of 1080 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:B:33:PHE:CE1	2:B:53:LYS:HD3	1.45	1.51
4:D:120:LEU:CD1	5:E:152:ILE:HA	1.48	1.41
3:C:1429:THR:HG22	3:C:1430:PRO:CD	1.51	1.41
3:C:1252:MET:HG2	3:C:1297:LEU:CD1	1.54	1.37
1:A:462:PRO:HG2	1:A:482:ILE:CG2	1.58	1.32

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	601/1008 (60%)	593 (99%)	8 (1%)	0	100 100
2	B	439/778 (56%)	424 (97%)	14 (3%)	1 (0%)	47 79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	366/368 (100%)	361 (99%)	5 (1%)	0	100	100
4	D	170/172 (99%)	169 (99%)	1 (1%)	0	100	100
5	E	161/164 (98%)	156 (97%)	5 (3%)	0	100	100
All	All	1737/2490 (70%)	1703 (98%)	33 (2%)	1 (0%)	54	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	23	PRO

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	488/837 (58%)	480 (98%)	8 (2%)	62	84
2	B	391/688 (57%)	385 (98%)	6 (2%)	65	85
3	C	328/328 (100%)	324 (99%)	4 (1%)	71	88
4	D	149/149 (100%)	147 (99%)	2 (1%)	69	87
5	E	144/144 (100%)	143 (99%)	1 (1%)	84	93
All	All	1500/2146 (70%)	1479 (99%)	21 (1%)	68	86

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1183	ASN
3	C	1296	ASN
5	E	33	LEU
4	D	100(A)	TYR
3	C	1217	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	1457	ASN
5	E	150	GLN
3	C	1461	GLN
5	E	31	ASN
2	B	263	HIS

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)

33 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	$\#\|Z\| > 2$
6	NAG	F	1	1,6	14,14,15	0.33	0	17,19,21	0.54	0
6	NAG	F	2	6	14,14,15	0.31	0	17,19,21	0.70	0
6	BMA	F	3	6	11,11,12	0.22	0	15,15,17	0.66	0
6	NAG	G	1	1,6	14,14,15	0.37	0	17,19,21	0.67	0
6	NAG	G	2	6	14,14,15	0.31	0	17,19,21	0.57	0
6	BMA	G	3	6	11,11,12	0.23	0	15,15,17	0.66	0
7	NAG	H	1	1,7	14,14,15	0.31	0	17,19,21	1.29	3 (17%)
7	NAG	H	2	7	14,14,15	0.26	0	17,19,21	0.85	0
8	NAG	I	1	1,8	14,14,15	0.29	0	17,19,21	0.94	1 (5%)
8	NAG	I	2	8	14,14,15	0.42	0	17,19,21	1.28	1 (5%)
8	BMA	I	3	8	11,11,12	0.26	0	15,15,17	1.17	2 (13%)
8	MAN	I	4	8	11,11,12	0.23	0	15,15,17	0.87	0
8	MAN	I	5	8	11,11,12	0.24	0	15,15,17	0.87	0
9	NAG	J	1	9,1	14,14,15	0.30	0	17,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NAG	J	2	9	14,14,15	0.31	0	17,19,21	0.89	0
9	BMA	J	3	9	11,11,12	0.48	0	15,15,17	1.32	2 (13%)
9	MAN	J	4	9	11,11,12	0.26	0	15,15,17	0.83	0
9	NAG	J	5	9	14,14,15	0.31	0	17,19,21	0.79	0
9	MAN	J	6	9	11,11,12	0.23	0	15,15,17	0.97	1 (6%)
6	NAG	K	1	1,6	14,14,15	0.27	0	17,19,21	0.62	0
6	NAG	K	2	6	14,14,15	0.27	0	17,19,21	0.77	0
6	BMA	K	3	6	11,11,12	0.24	0	15,15,17	0.84	0
7	NAG	L	1	7,2	14,14,15	0.27	0	17,19,21	0.59	0
7	NAG	L	2	7	14,14,15	0.28	0	17,19,21	0.72	0
6	NAG	M	1	6,2	14,14,15	0.34	0	17,19,21	1.49	2 (11%)
6	NAG	M	2	6	14,14,15	0.32	0	17,19,21	0.77	1 (5%)
6	BMA	M	3	6	11,11,12	0.25	0	15,15,17	0.83	0
10	NAG	N	1	2,10	14,14,15	0.27	0	17,19,21	0.61	0
10	NAG	N	2	10	14,14,15	0.28	0	17,19,21	0.62	0
10	BMA	N	3	10	11,11,12	0.22	0	15,15,17	0.86	0
10	MAN	N	4	10	11,11,12	0.24	0	15,15,17	0.85	0
7	NAG	O	1	7,2	14,14,15	0.32	0	17,19,21	0.86	0
7	NAG	O	2	7	14,14,15	0.32	0	17,19,21	0.73	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
6	NAG	F	1	1,6	-	4/6/23/26	0/1/1/1
6	NAG	F	2	6	-	3/6/23/26	0/1/1/1
6	BMA	F	3	6	-	0/2/19/22	0/1/1/1
6	NAG	G	1	1,6	-	3/6/23/26	0/1/1/1
6	NAG	G	2	6	-	4/6/23/26	0/1/1/1
6	BMA	G	3	6	-	0/2/19/22	0/1/1/1
7	NAG	H	1	1,7	-	5/6/23/26	0/1/1/1
7	NAG	H	2	7	-	4/6/23/26	0/1/1/1
8	NAG	I	1	1,8	-	4/6/23/26	0/1/1/1
8	NAG	I	2	8	-	1/6/23/26	0/1/1/1
8	BMA	I	3	8	-	1/2/19/22	0/1/1/1
8	MAN	I	4	8	-	0/2/19/22	0/1/1/1
8	MAN	I	5	8	-	0/2/19/22	0/1/1/1
9	NAG	J	1	9,1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

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

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	1	NAG	C1-O5-C5	5.09	119.09	112.19
8	I	2	NAG	C1-O5-C5	3.31	116.67	112.19
7	H	1	NAG	C1-O5-C5	3.01	116.28	112.19
8	I	3	BMA	O5-C1-C2	-2.75	106.53	110.77
9	J	3	BMA	O3-C3-C4	2.68	116.55	110.35

There are no chirality outliers.

5 of 67 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	2	NAG	C8-C7-N2-C2
6	F	2	NAG	O7-C7-N2-C2
6	G	1	NAG	C8-C7-N2-C2
6	G	1	NAG	O7-C7-N2-C2
6	G	2	NAG	C8-C7-N2-C2

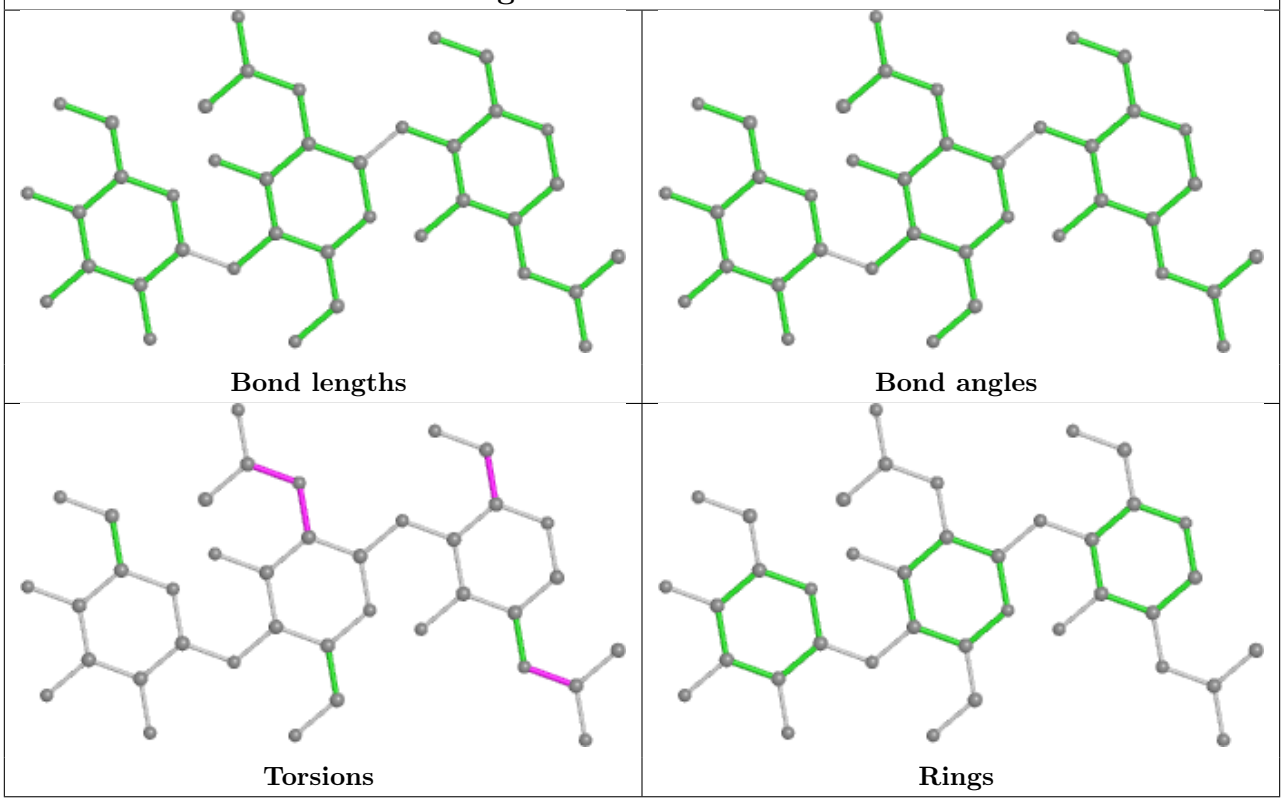
There are no ring outliers.

13 monomers are involved in 17 short contacts:

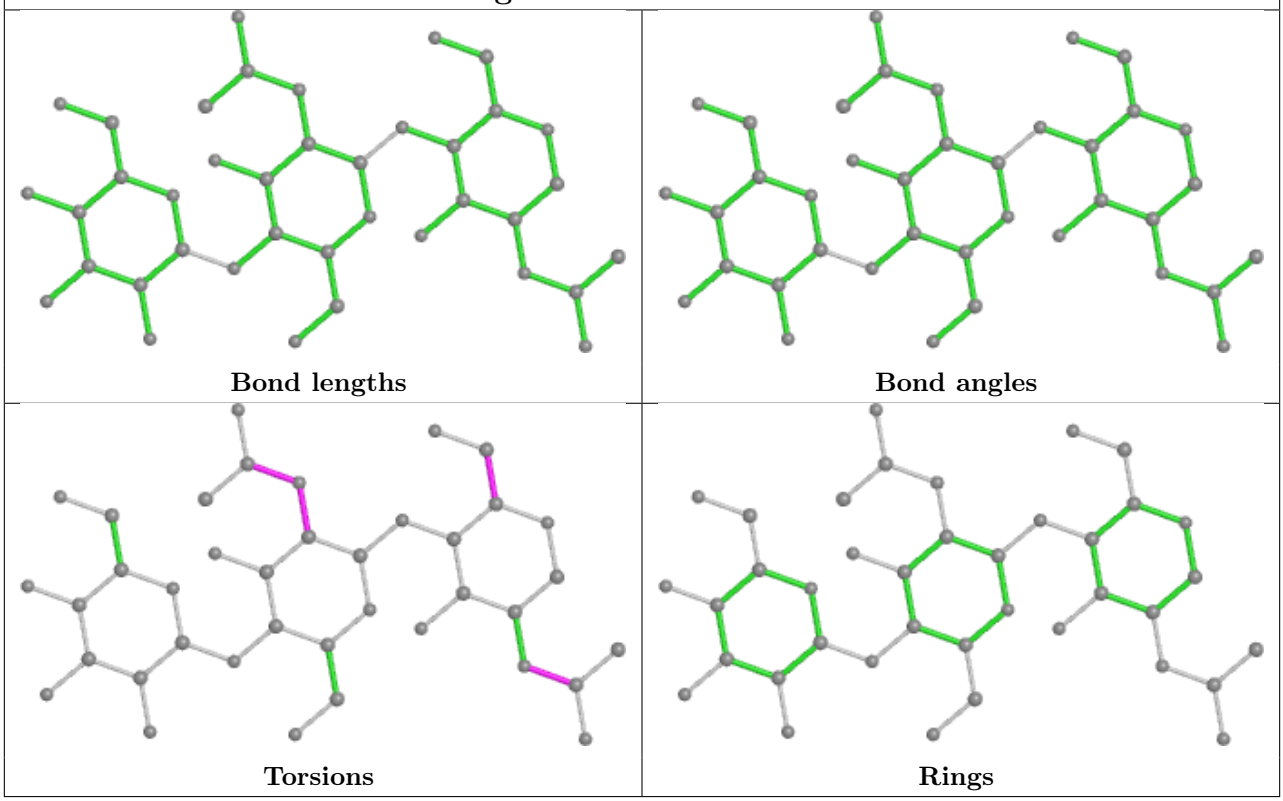
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	G	2	NAG	1	0
9	J	5	NAG	3	0
6	F	2	NAG	2	0
6	F	1	NAG	1	0
7	H	1	NAG	2	0
8	I	2	NAG	1	0
6	K	1	NAG	2	0
6	M	2	NAG	1	0
7	H	2	NAG	1	0
9	J	2	NAG	1	0
7	O	2	NAG	1	0
8	I	1	NAG	2	0
6	K	2	NAG	1	0

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

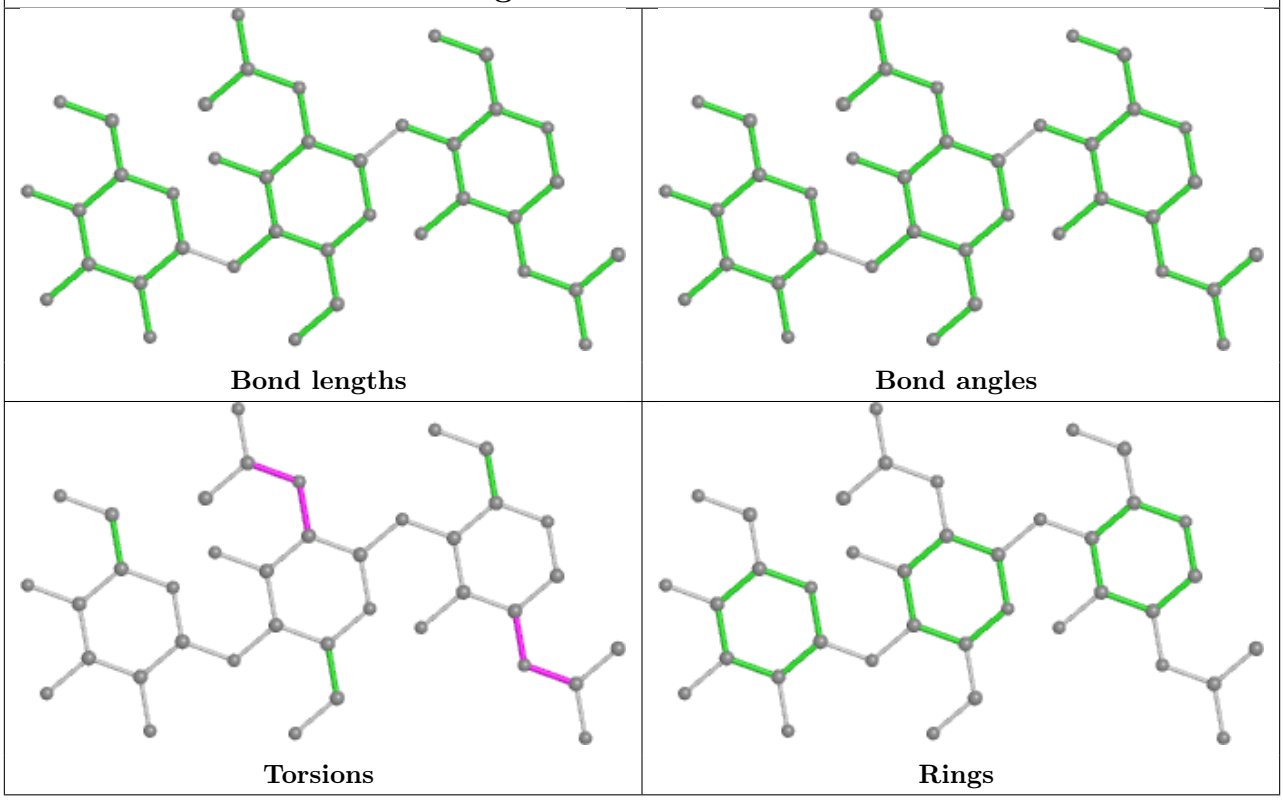
Oligosaccharide Chain F

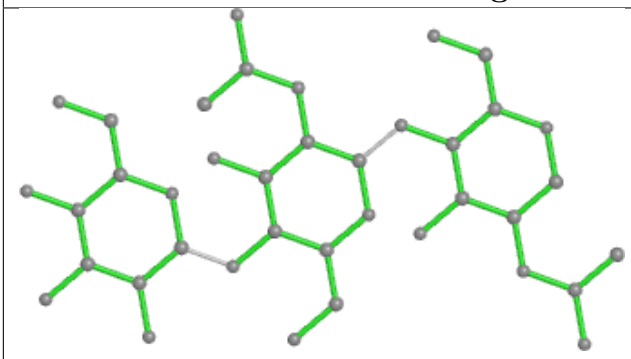
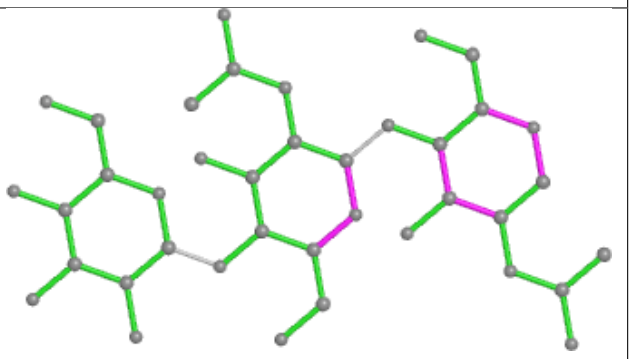
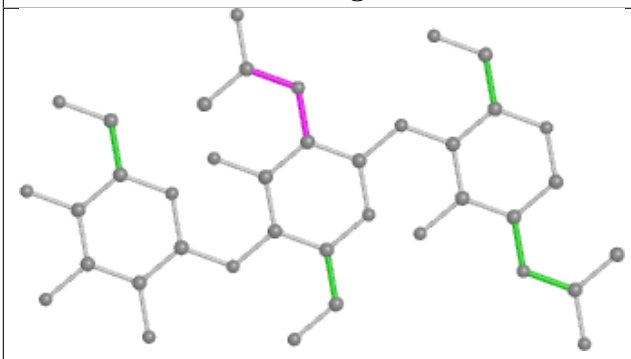
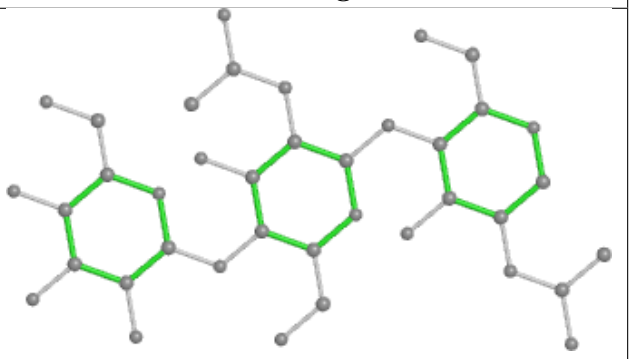


Oligosaccharide Chain G

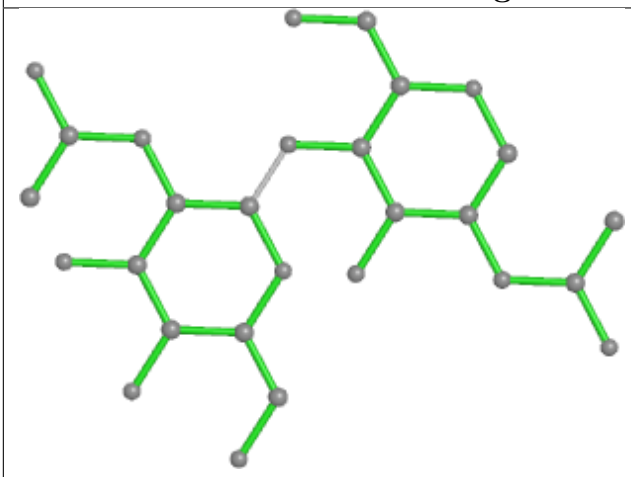


Oligosaccharide Chain K

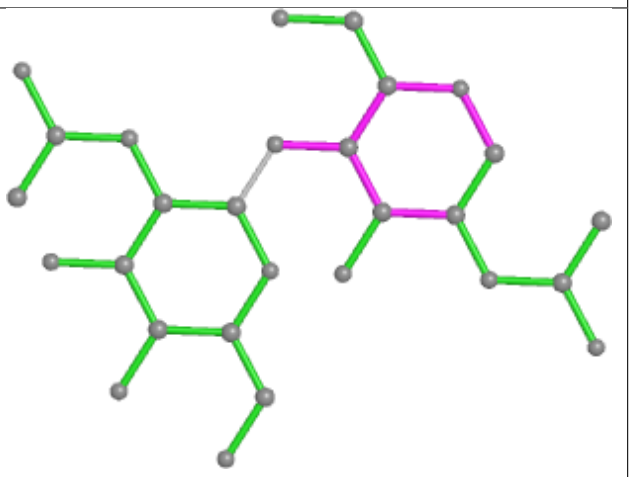


Oligosaccharide Chain M	
 Bond lengths	 Bond angles
 Torsions	 Rings

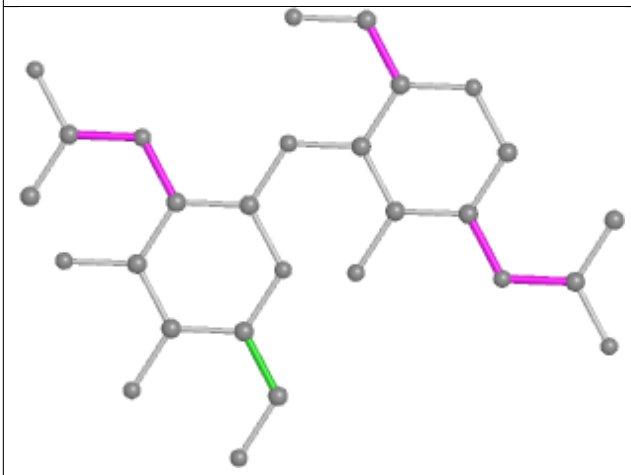
Oligosaccharide Chain H



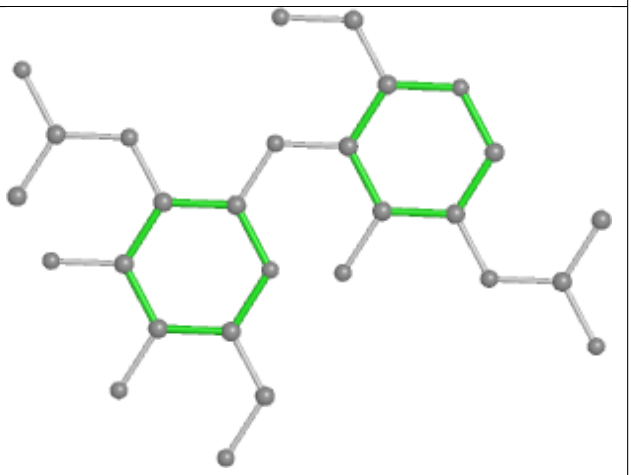
Bond lengths



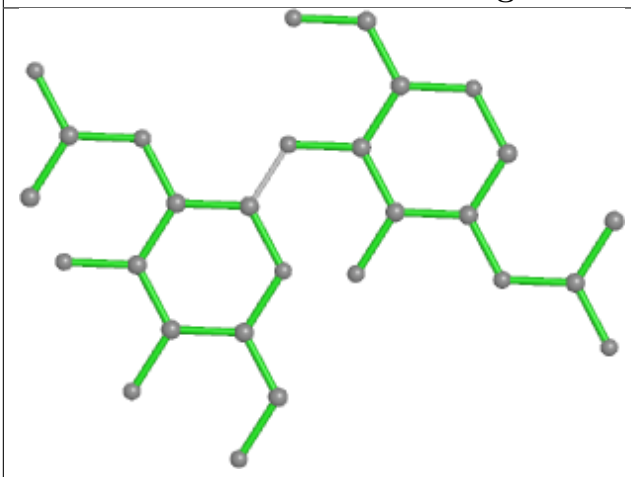
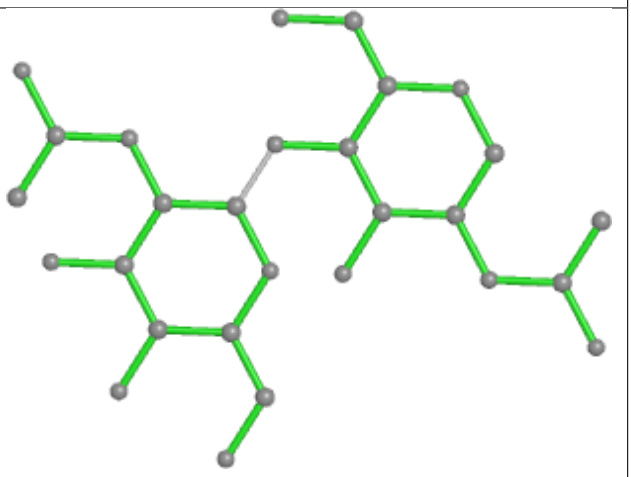
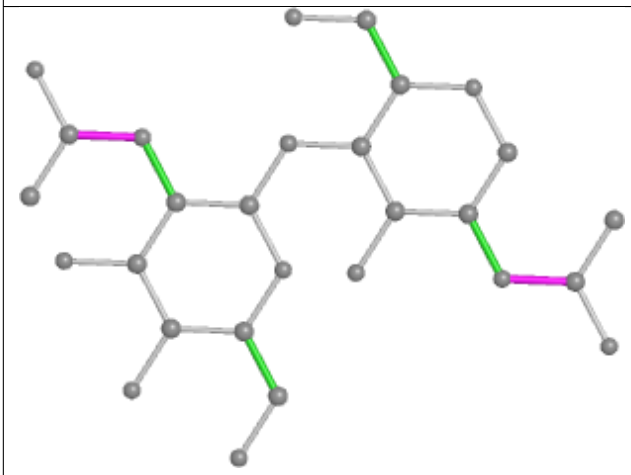
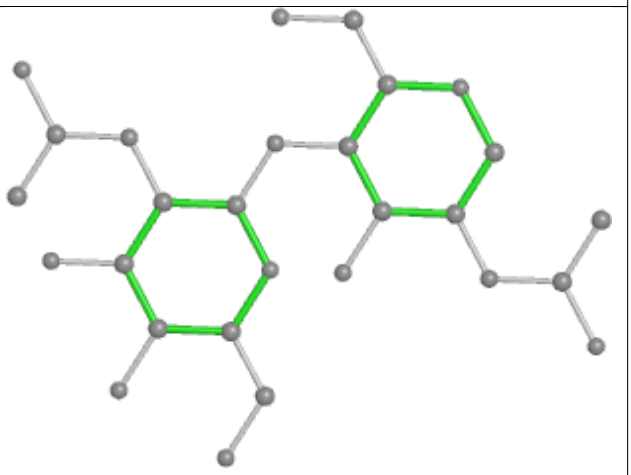
Bond angles



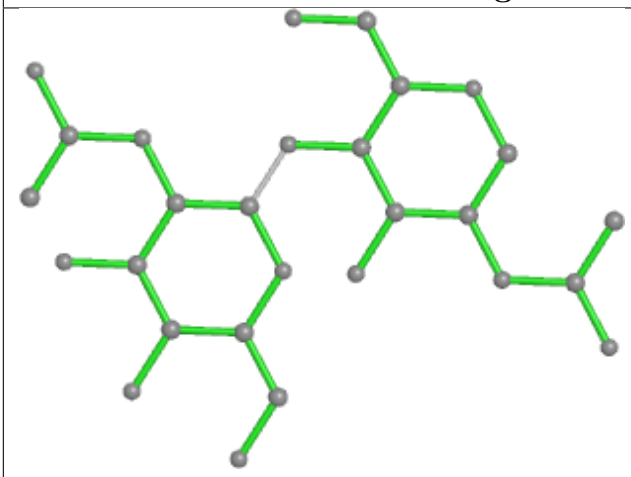
Torsions



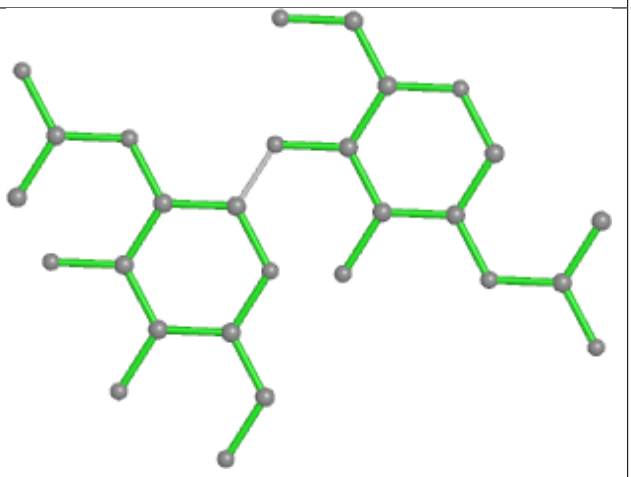
Rings

Oligosaccharide Chain L	
 Bond lengths	 Bond angles
 Torsions	 Rings

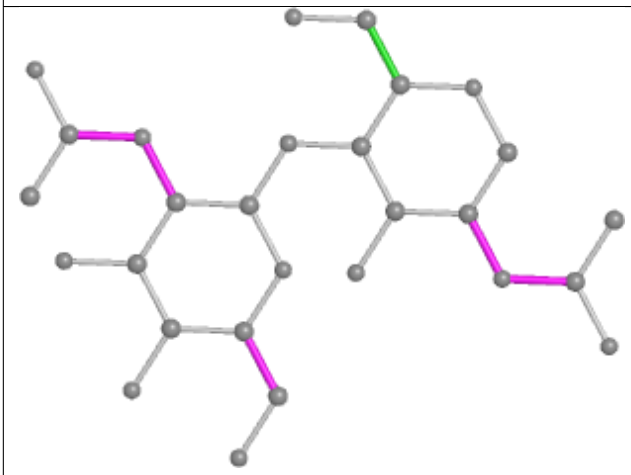
Oligosaccharide Chain O



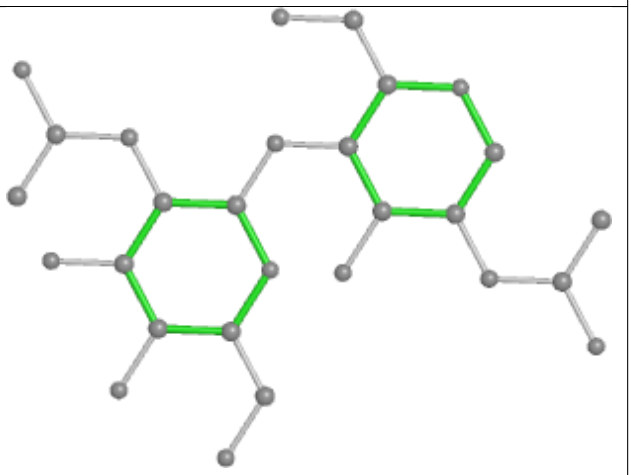
Bond lengths



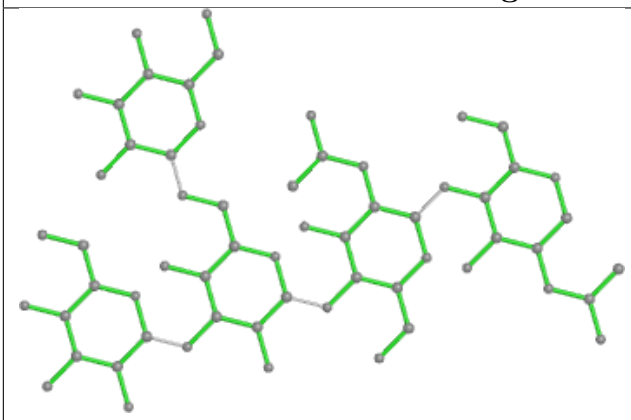
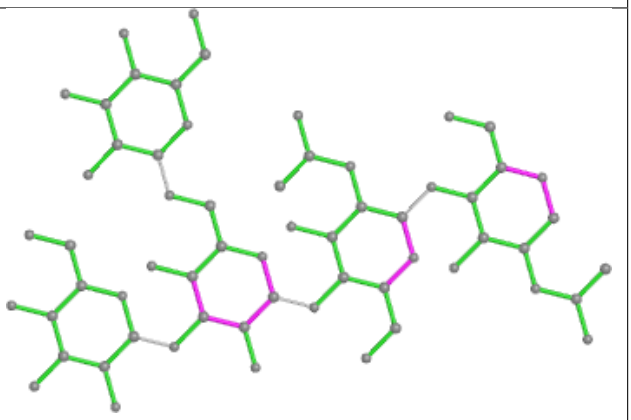
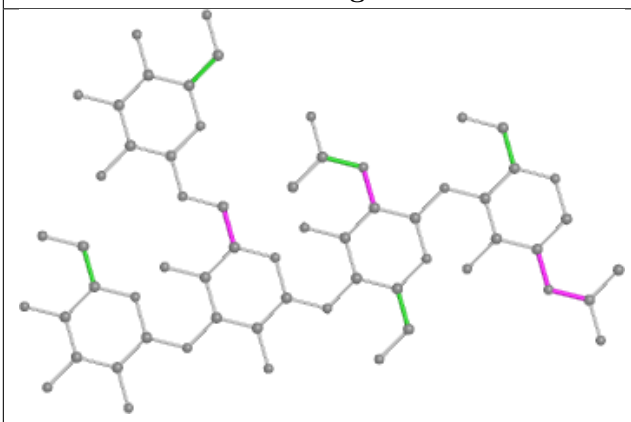
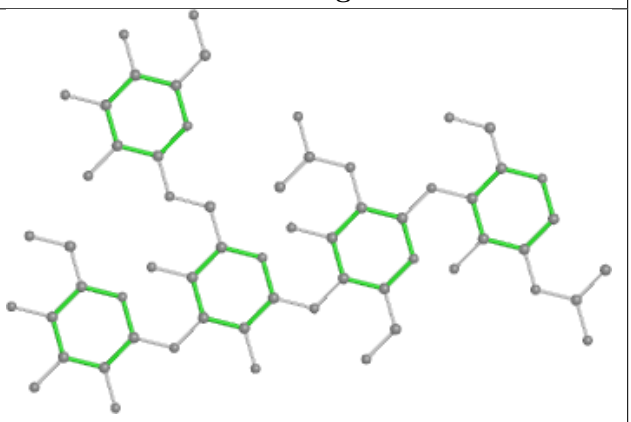
Bond angles

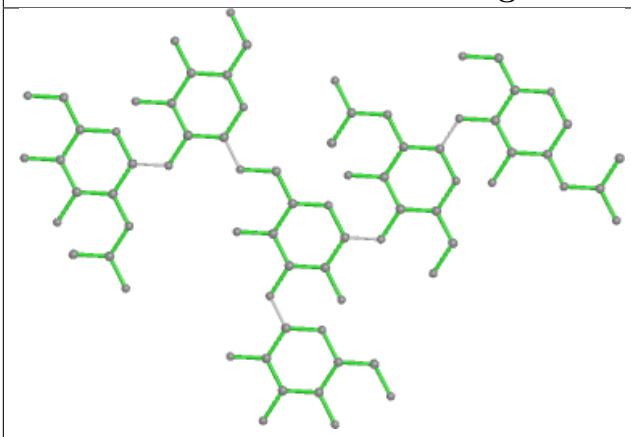
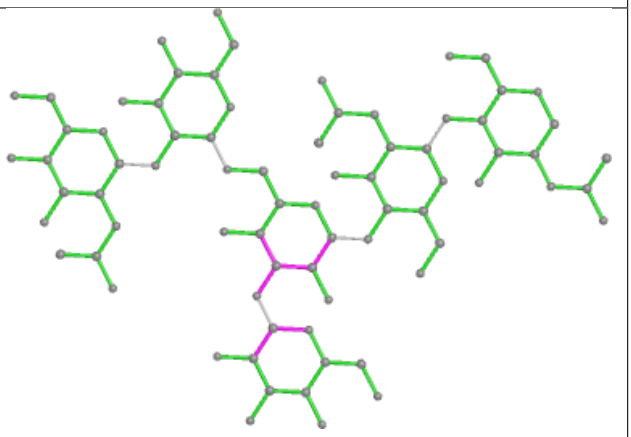
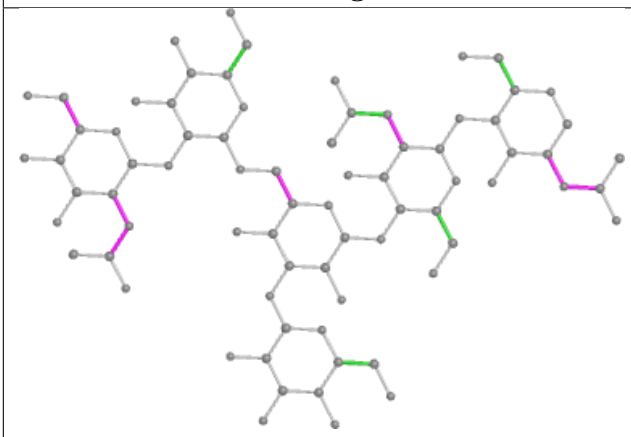
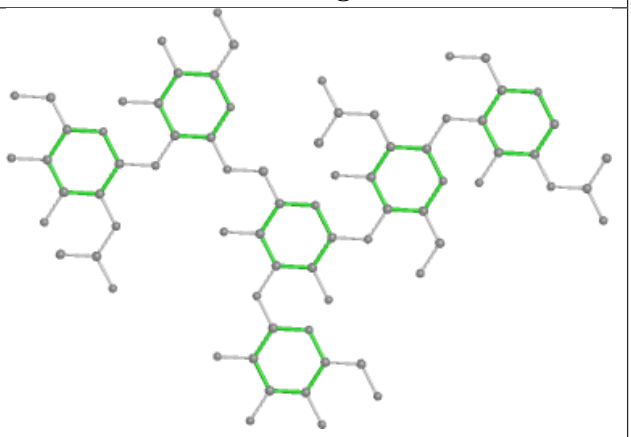


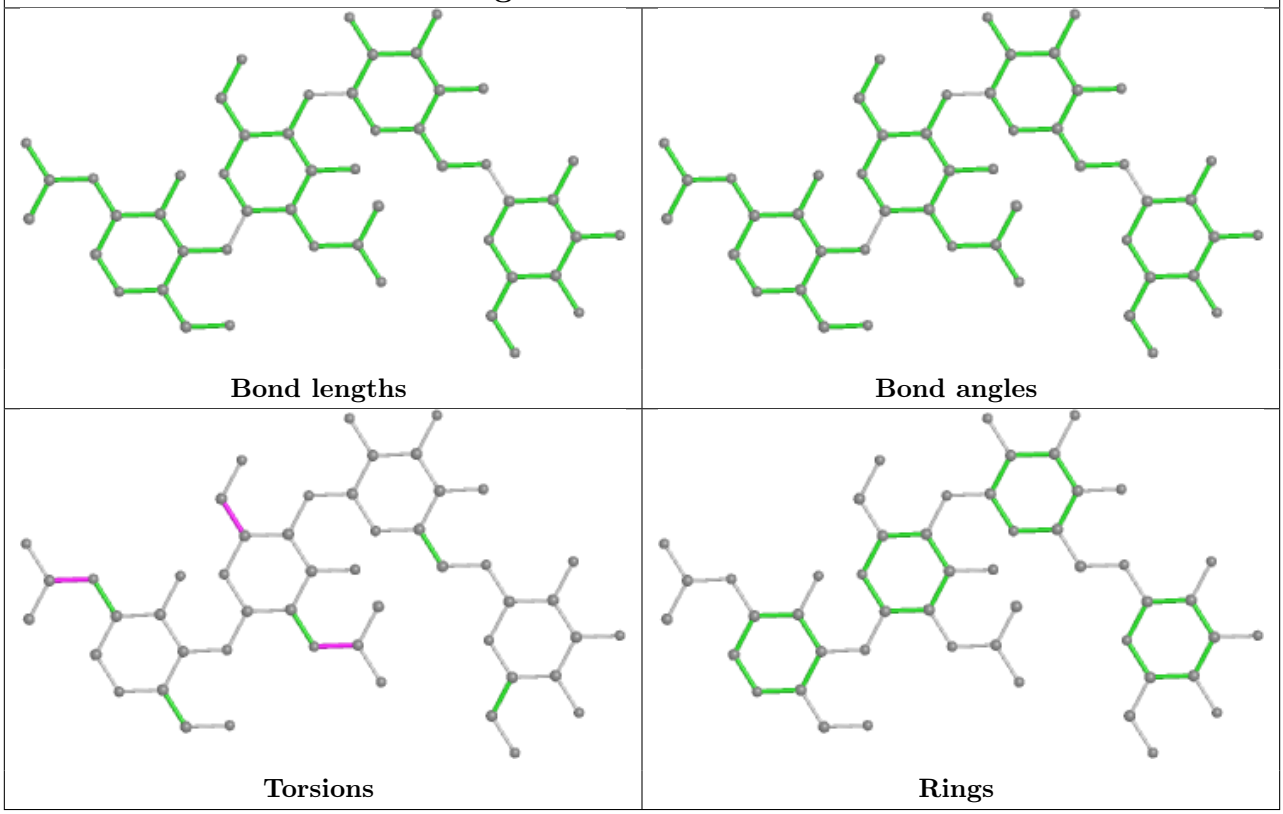
Torsions



Rings

Oligosaccharide Chain I	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain J	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain N	
	
Bond lengths	Bond angles
Torsions	Rings

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 (i)

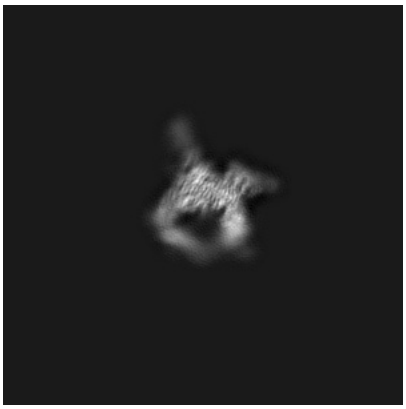
This section contains visualisations of the EMDB entry EMD-12634. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

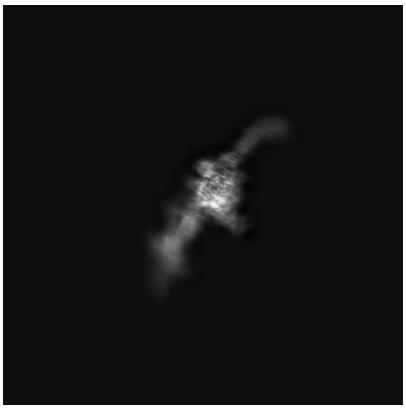
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

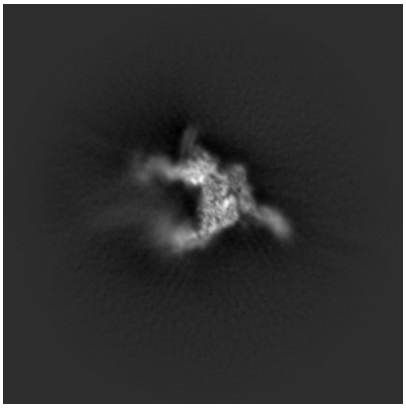


Y

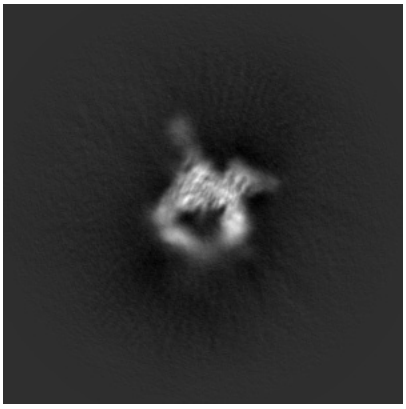


Z

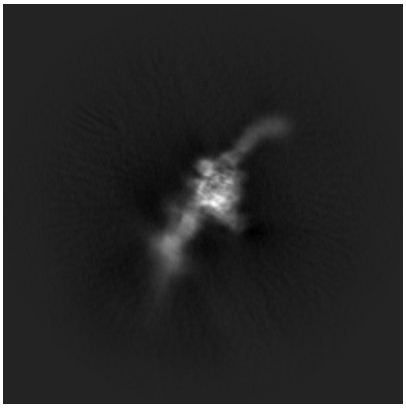
6.1.2 Raw map



X



Y

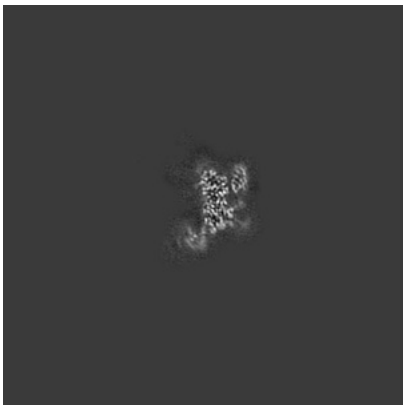


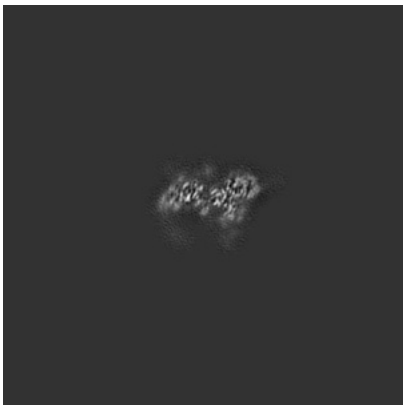
Z

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

6.2 Central slices (i)

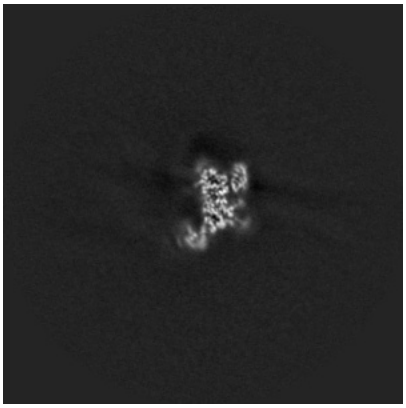
6.2.1 Primary map

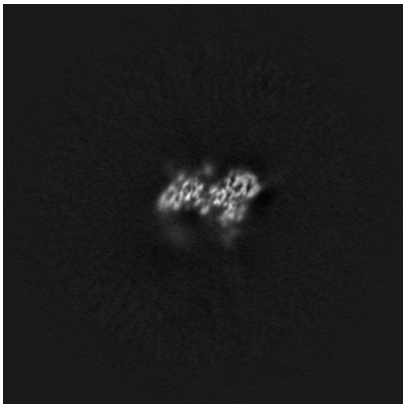

X Index: 180

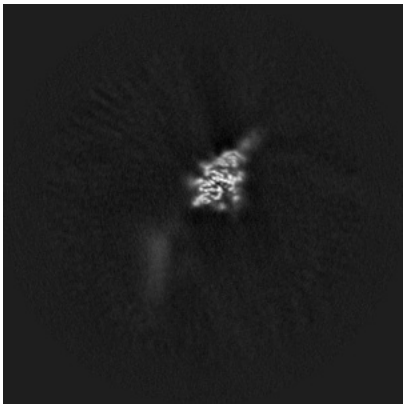

Y Index: 180

Z Index: 180

6.2.2 Raw map


X Index: 180


Y Index: 180

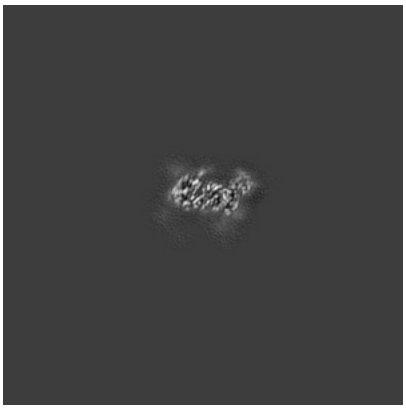

Z Index: 180

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

6.3 Largest variance slices (i)

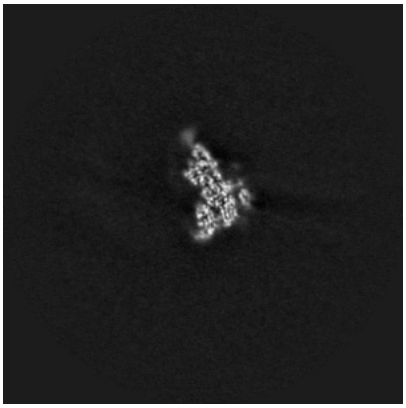
6.3.1 Primary map

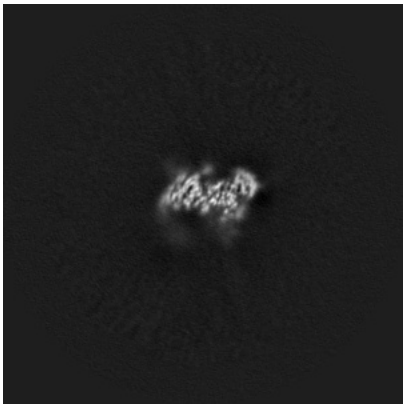
X Index: 193

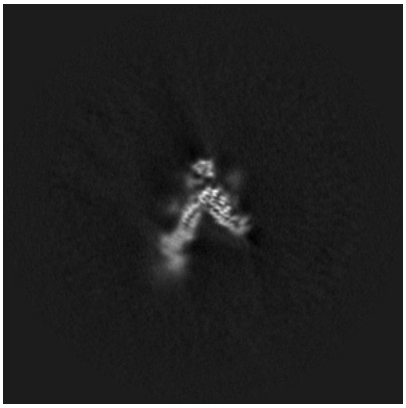

Y Index: 186

Z Index: 201

6.3.2 Raw map


X Index: 193


Y Index: 182


Z Index: 208

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0292. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

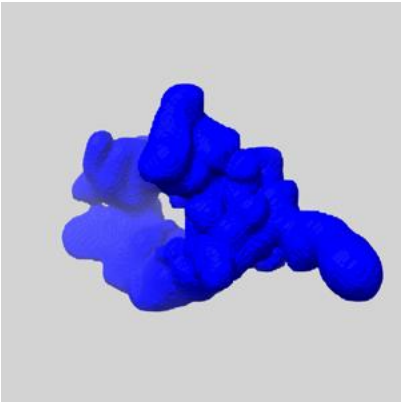
6.5 Mask visualisation (i)

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

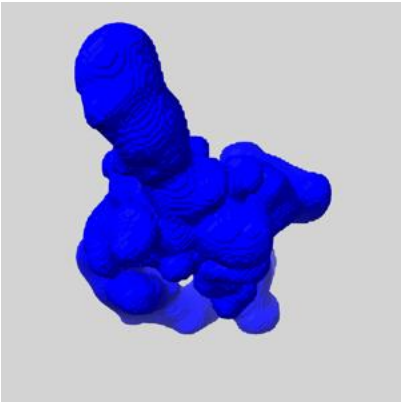
A mask typically either:

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

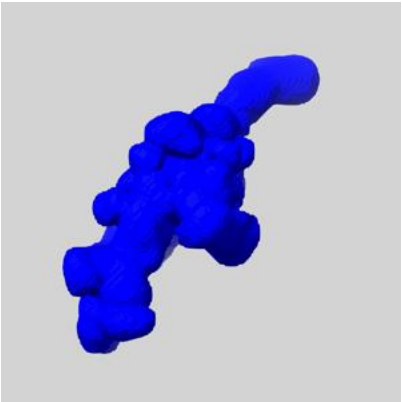
6.5.1 emd_12634_msk_1.map (i)



X



Y

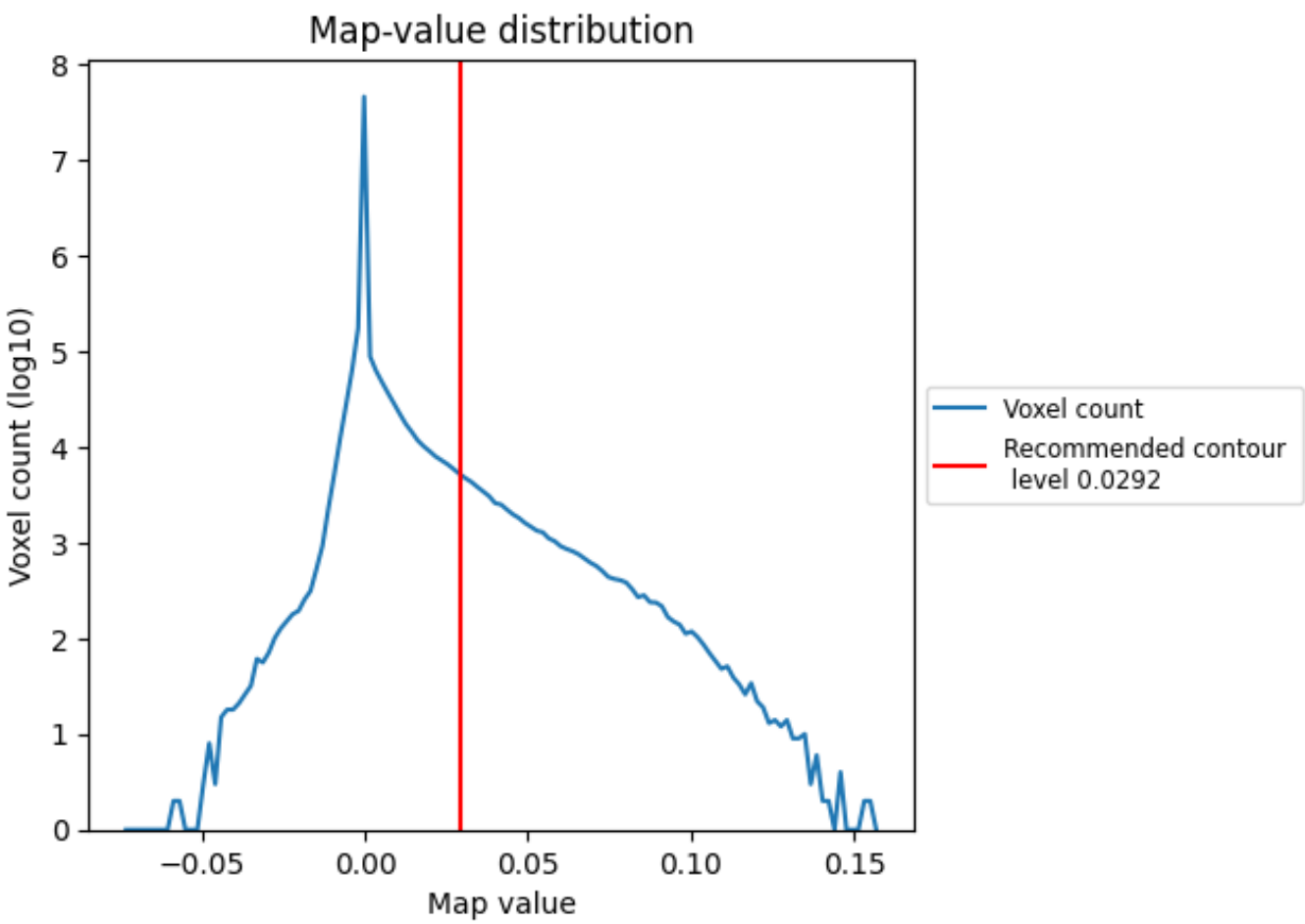


Z

7 Map analysis (i)

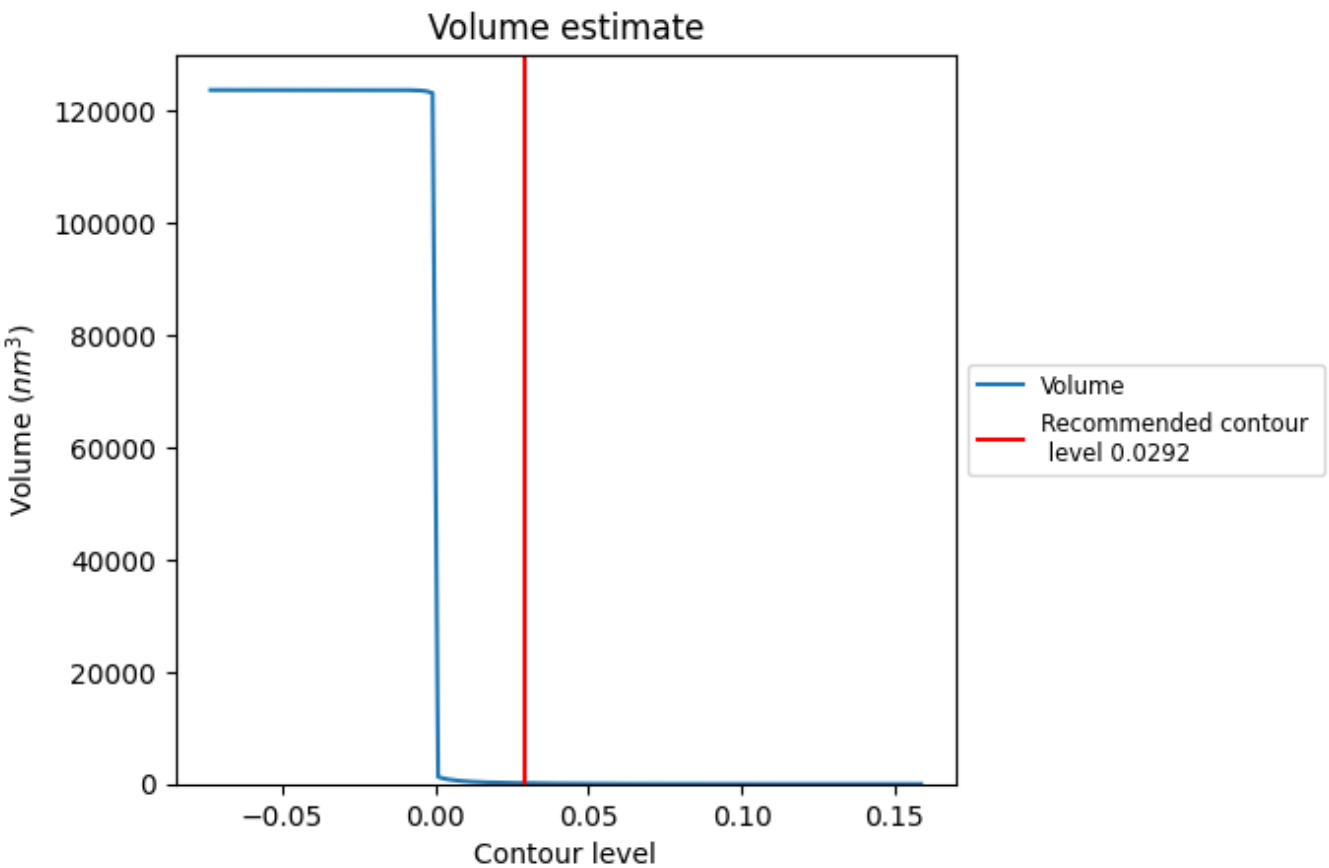
This section contains the results of statistical analysis of the map.

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.

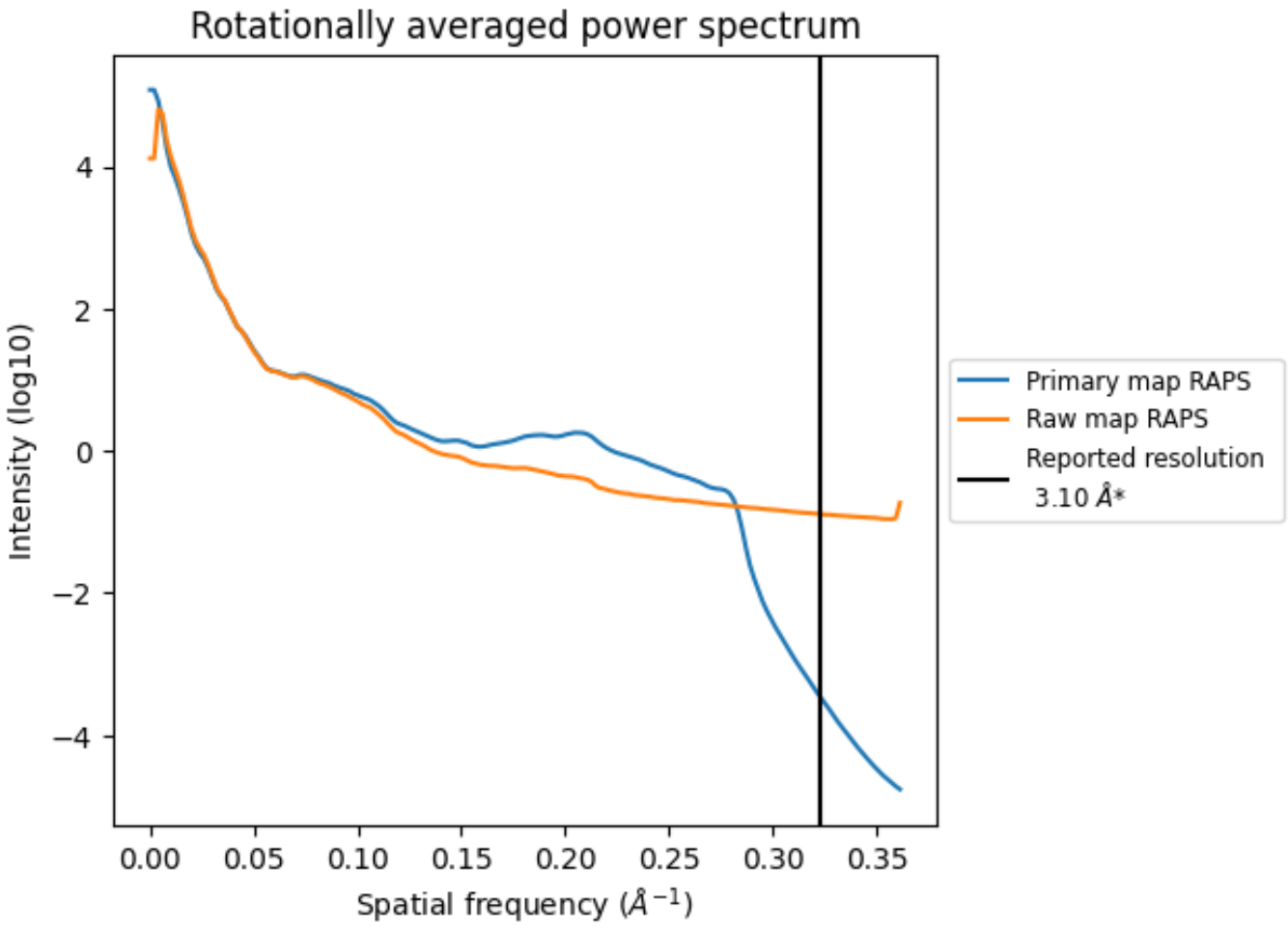
7.2 Volume estimate (i)



The volume at the recommended contour level is 141 nm^3; this corresponds to an approximate mass of 128 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)

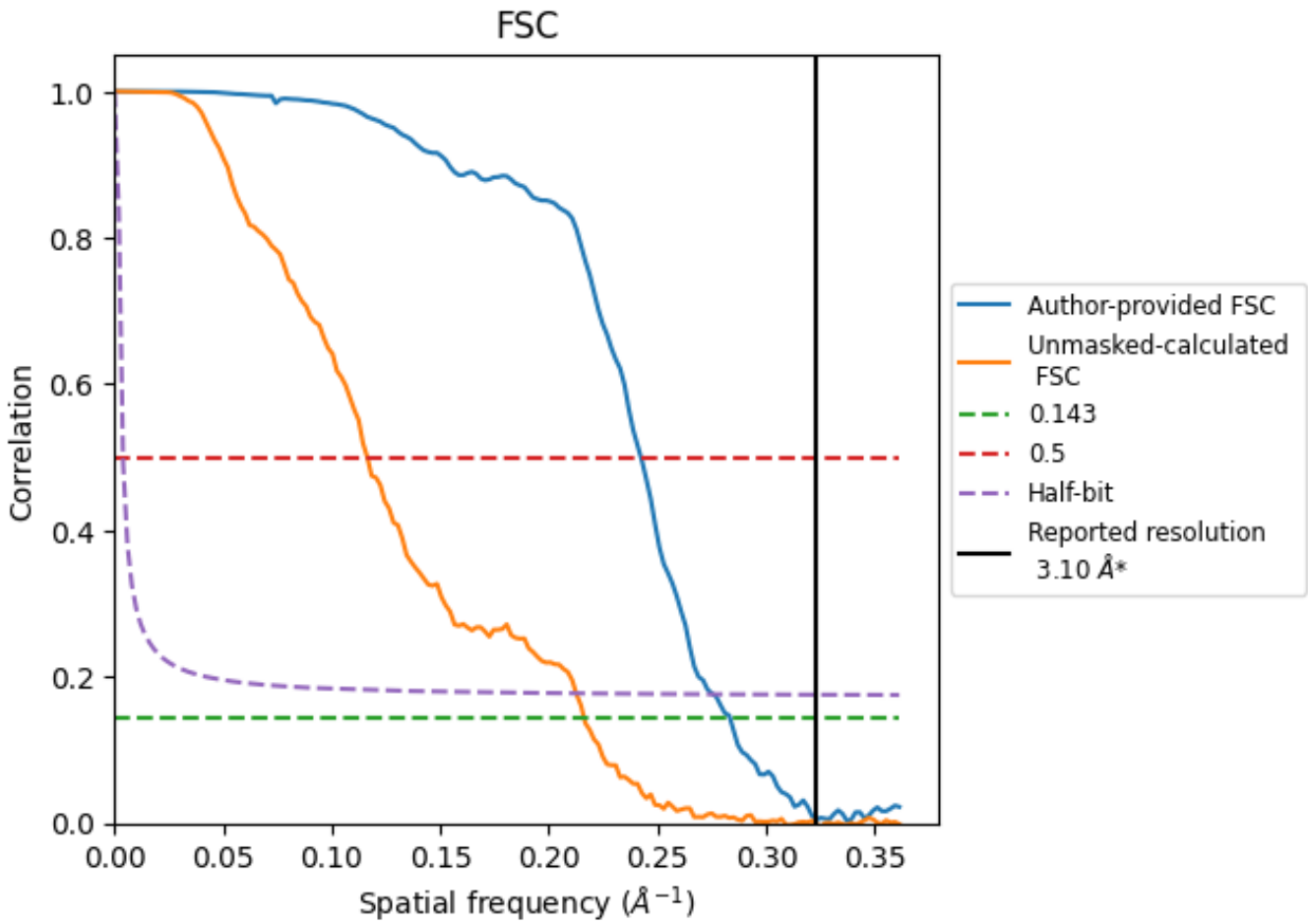


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.53	4.13	3.63
Unmasked-calculated*	4.63	8.59	4.70

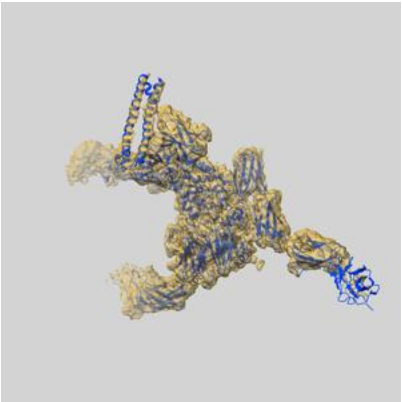
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 3.1 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.63 differs from the reported value 3.1 by more than 10 %

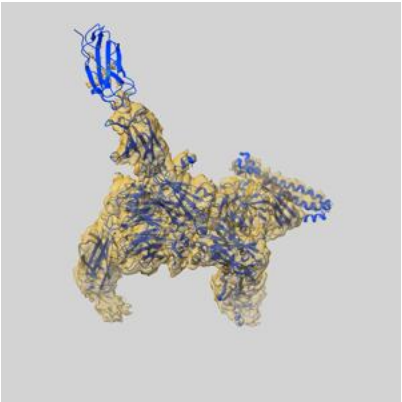
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-12634 and PDB model 7NWL. Per-residue inclusion information can be found in section 3 on page 7.

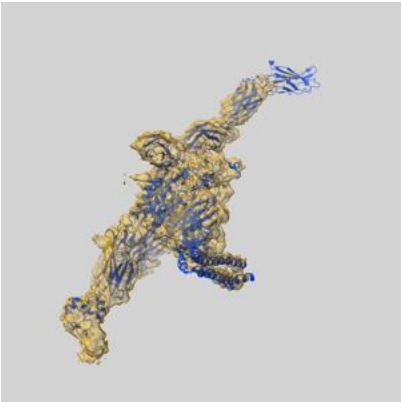
9.1 Map-model overlay (i)



X



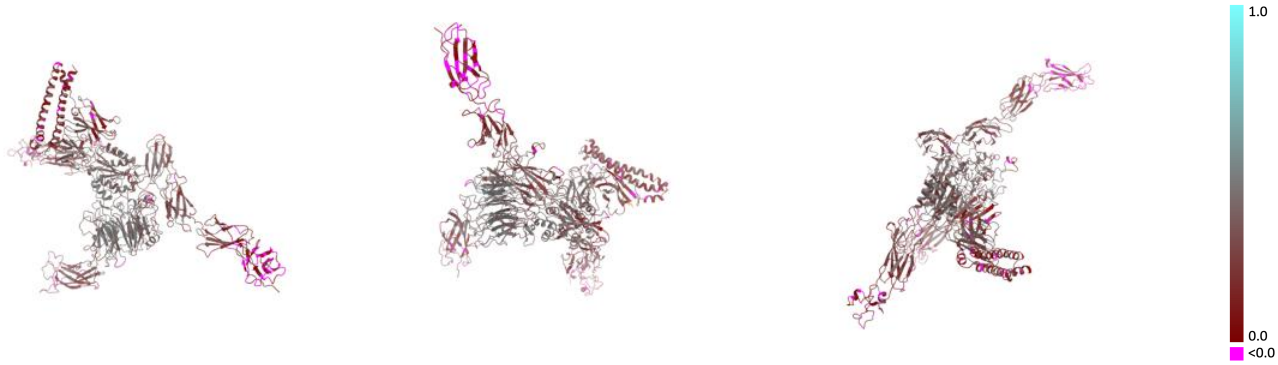
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0292 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

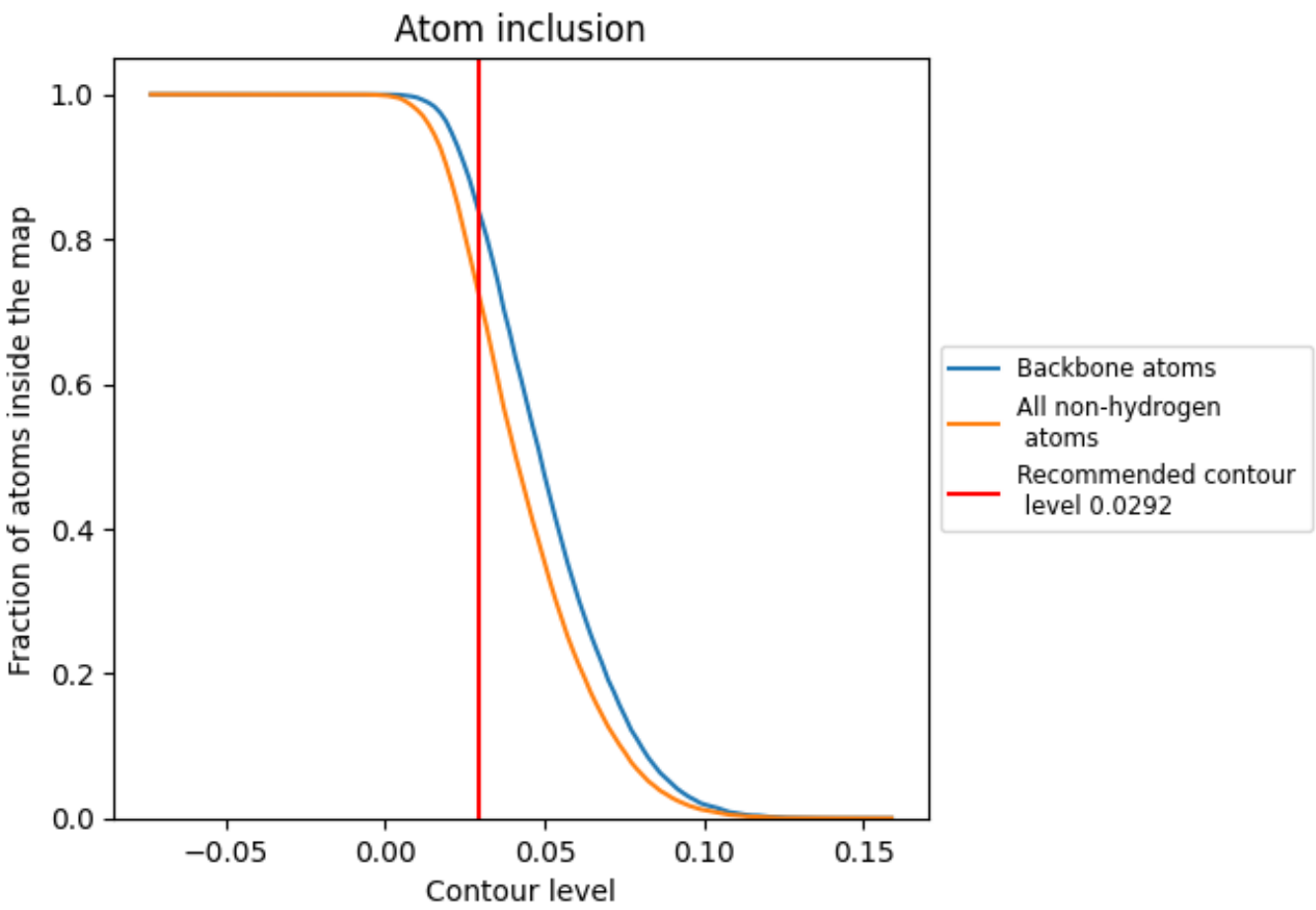
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0292).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 73% 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 (0.0292) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7257	0.2960
A	0.8564	0.3600
B	0.8026	0.2920
C	0.5485	0.2210
D	0.5890	0.2400
E	0.6446	0.2960
F	0.7179	0.3970
G	0.6410	0.3490
H	0.6429	0.2600
I	0.5574	0.3200
J	0.7600	0.3250
K	0.6923	0.4370
L	0.2500	0.3750
M	0.4615	0.3030
N	0.3000	0.1880
O	0.1786	0.1890