wwPDB EM Validation Summary Report (i)

Apr 1, 2025 – 10:52 pm BST

PDB ID	:	4CAK / pdb_00004cak
EMDB ID	:	EMD-2281
Title	:	Three-dimensional reconstruction of intact human integrin alphaIIbbeta3 in a phospholipid bilayer nanodisc
Authors	:	Choi, W.S.; Rice, W.J.; Stokes, D.L.; Coller, B.S.
Deposited on	:	2013-10-08
Resolution	:	20.50 Å(reported)
Based on initial model	:	3FCS

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:

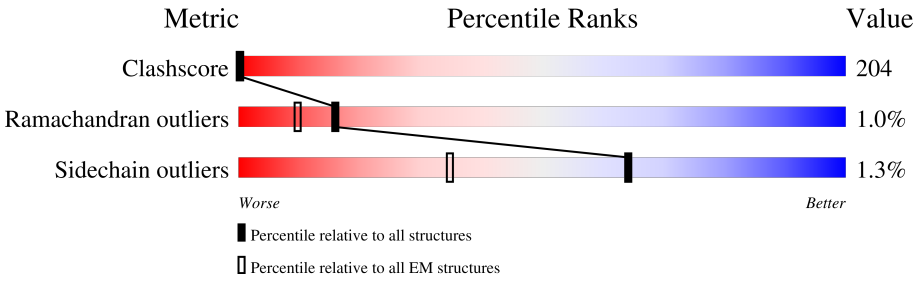
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 20.50 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	959	10% 50% 43% • 5%
2	B	690	15% 44% 54% •
3	C	2	50% 50% 50%
3	F	2	100%
4	D	4	75% 25%
5	E	3	33% 33% 67%
6	G	5	60% 40%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	F	1	-	-	X	-
3	NAG	F	2	-	-	X	-
4	NAG	D	1	-	-	X	-
4	NAG	D	2	-	-	X	-
4	BMA	D	3	-	-	X	-
4	MAN	D	4	-	-	X	-
5	NAG	E	1	-	-	X	-
6	NAG	G	2	-	-	X	-
6	MAN	G	4	-	-	X	-
6	MAN	G	5	-	-	X	-
7	NAG	A	3015	X	-	-	-
7	NAG	A	3570	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15960 atoms, of which 3296 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-IIb.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	913	Total	C	H	N	O	S	14	3
			10364	4466	3296	1236	1336	30		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	959	CYS	LEU	conflict	UNP P08514

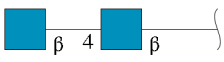
- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	680	Total	C	N	O	S	19	0
			5362	3294	913	1083	72		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	688	CYS	PRO	conflict	UNP P05106

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

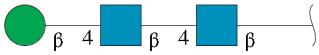


Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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.

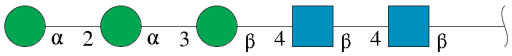
Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 5 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.



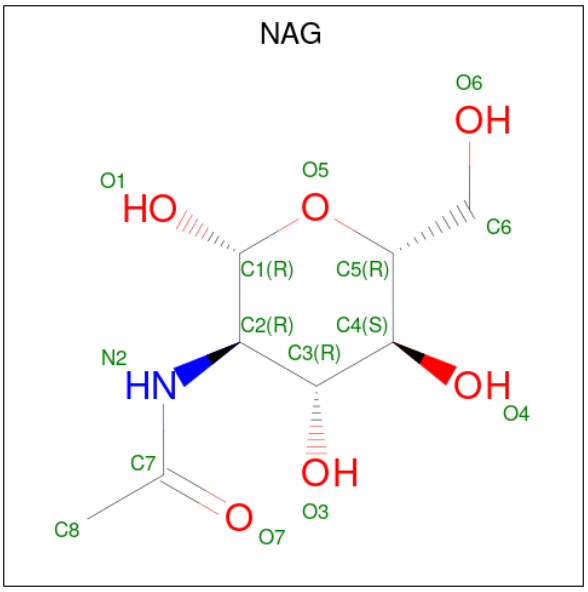
Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	3	Total	C	N	O	0	0
			39	22	2	15		

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



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

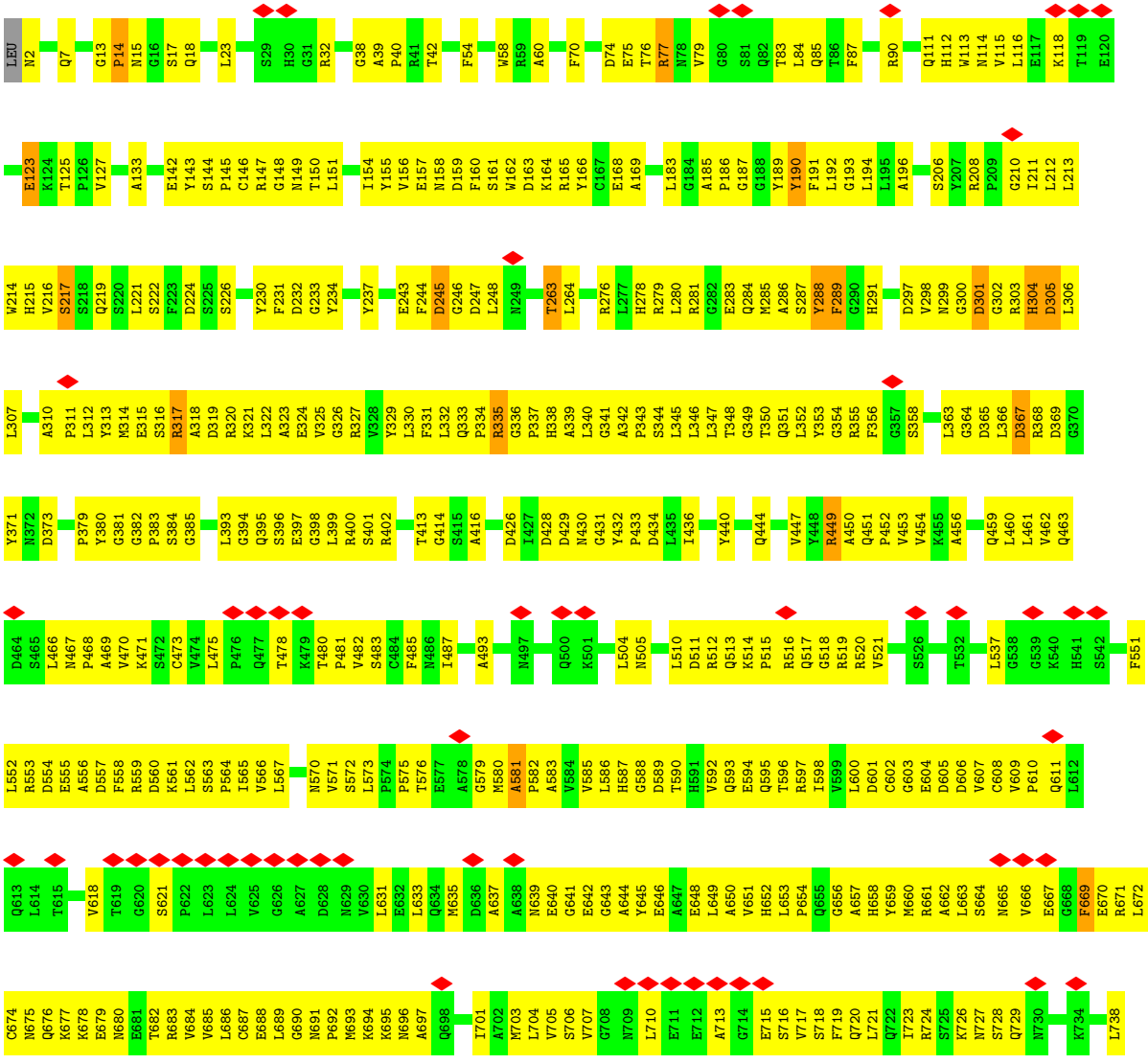


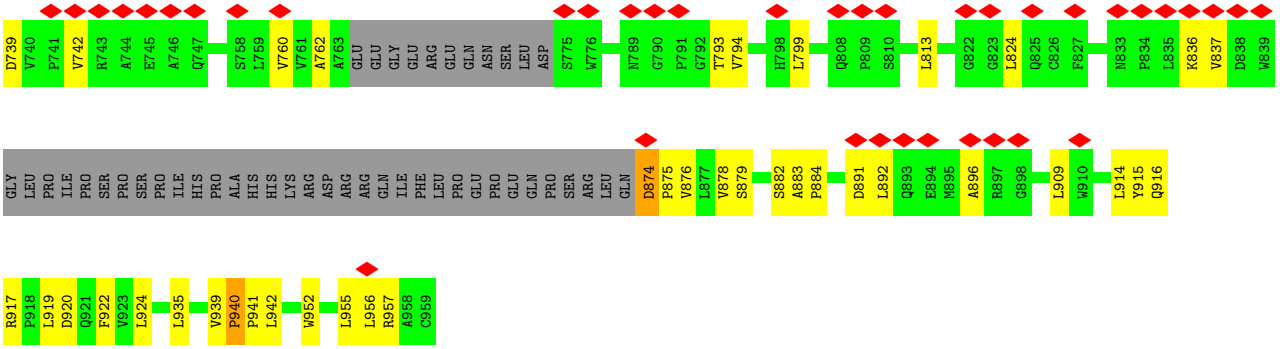
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	A	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

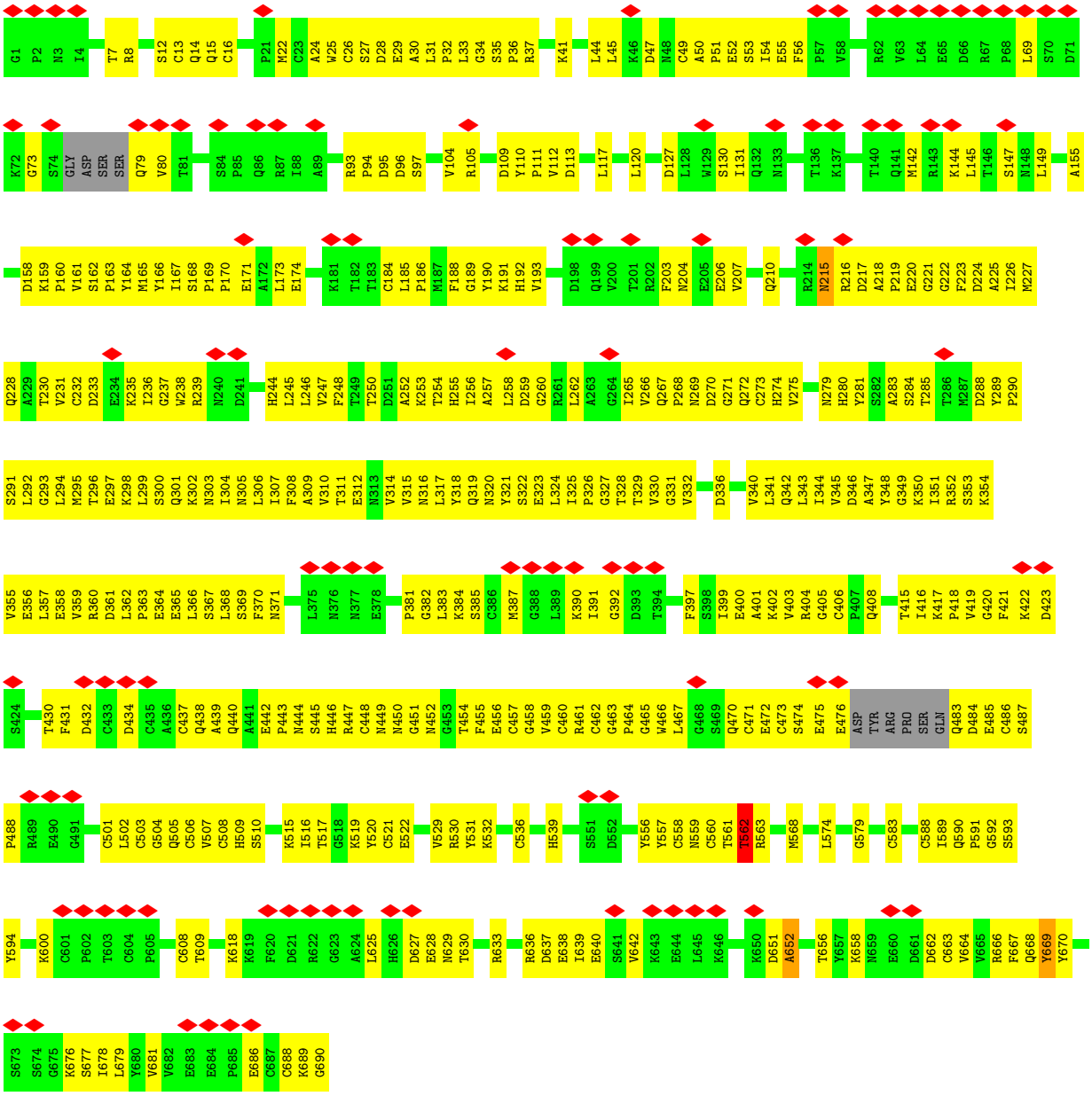
- Molecule 1: Integrin alpha-IIb





• Molecule 2: Integrin beta-3

Chain B:

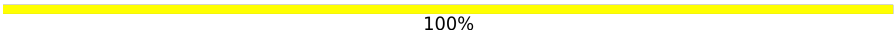


• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

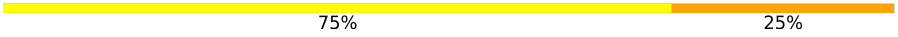
• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:



• Molecule 4: 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 D:

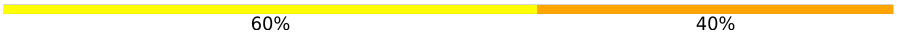


• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 6: alpha-D-mannopyranose-(1-2)-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 G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	25008	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/Å^2$)	13	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	50592	Depositor
Image detector	GENERIC TVIPS (4k x 4k)	Depositor
Maximum map value	0.288	Depositor
Minimum map value	-0.124	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	402.56, 402.56, 402.56	wwPDB
Map dimensions	136, 136, 136	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.96, 2.96, 2.96	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.65	1/7233 (0.0%)	1.09	16/9839 (0.2%)
2	B	0.45	2/5447 (0.0%)	0.63	6/7341 (0.1%)
All	All	0.57	3/12680 (0.0%)	0.92	22/17180 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	PRO	C-N	27.97	1.98	1.34
2	B	562[A]	THR	C-N	-20.14	0.87	1.34
2	B	562[B]	THR	C-N	-20.14	0.87	1.34

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	PRO	CA-C-N	-50.09	7.00	117.20
1	A	14	PRO	C-N-CA	-39.38	23.26	121.70
2	B	562[A]	THR	O-C-N	-24.32	83.80	122.70
2	B	562[B]	THR	O-C-N	-24.32	83.80	122.70
2	B	562[A]	THR	C-N-CA	-11.36	93.29	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	562[A]	THR	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7068	3296	6699	3511	0
2	B	5362	0	4912	3094	0
3	C	28	0	25	1	0
3	F	28	0	17	74	0
4	D	50	0	40	75	0
5	E	39	0	31	17	0
6	G	61	0	44	45	0
7	A	28	0	23	38	0
All	All	12664	3296	11791	4980	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 204.

The worst 5 of 4980 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:254:THR:HG21	2:B:308:PHE:CD1	1.25	1.68
1:A:351:GLN:HE21	2:B:230:THR:CG2	1.05	1.67
1:A:331:PHE:CE2	1:A:661:ARG:HG3	1.17	1.65
1:A:592:VAL:CG2	1:A:727:ASN:HA	1.17	1.65
1:A:156:VAL:CG1	1:A:190:TYR:CD1	1.77	1.65

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	901/959 (94%)	818 (91%)	71 (8%)	12 (1%)	10 43
2	B	669/690 (97%)	610 (91%)	55 (8%)	4 (1%)	22 60
All	All	1570/1649 (95%)	1428 (91%)	126 (8%)	16 (1%)	16 49

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	837	VAL
1	A	940	PRO
1	A	190	TYR
1	A	263	THR
1	A	581	ALA

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	767/799 (96%)	755 (98%)	12 (2%)	58 73
2	B	620/612 (101%)	614 (99%)	6 (1%)	73 82
All	All	1387/1411 (98%)	1369 (99%)	18 (1%)	64 77

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	423	ASP
2	B	669	TYR
2	B	651	ASP
1	A	444	GLN
2	B	215	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	215	ASN
2	B	449	ASN
2	B	668	GLN
2	B	408	GLN
1	A	517	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)

16 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	$\#\|Z\| > 2$
3	NAG	C	1	2,3	14,14,15	0.62	0	17,19,21	1.14	1 (5%)
3	NAG	C	2	3	14,14,15	0.60	0	17,19,21	0.95	1 (5%)
4	NAG	D	1	2,4	14,14,15	0.50	0	17,19,21	0.71	0
4	NAG	D	2	4	14,14,15	0.55	0	17,19,21	0.69	0
4	BMA	D	3	4	11,11,12	0.61	0	15,15,17	0.68	0
4	MAN	D	4	4	11,11,12	0.51	0	15,15,17	2.54	3 (20%)
5	NAG	E	1	2,5	14,14,15	0.64	0	17,19,21	0.69	0
5	NAG	E	2	5	14,14,15	0.51	0	17,19,21	0.82	0
5	BMA	E	3	5	11,11,12	0.65	0	15,15,17	0.61	0
3	NAG	F	1	2,3	14,14,15	0.67	0	17,19,21	0.88	0
3	NAG	F	2	3	14,14,15	0.53	0	17,19,21	0.66	0
6	NAG	G	1	2,6	14,14,15	0.63	0	17,19,21	0.91	1 (5%)
6	NAG	G	2	6	14,14,15	0.48	0	17,19,21	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	BMA	G	3	6	11,11,12	0.57	0	15,15,17	0.95	1 (6%)
6	MAN	G	4	6	11,11,12	0.57	0	15,15,17	0.72	0
6	MAN	G	5	6	11,11,12	0.62	0	15,15,17	0.74	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
3	NAG	C	1	2,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	0/6/23/26	0/1/1/1
4	NAG	D	1	2,4	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
4	BMA	D	3	4	-	0/2/19/22	0/1/1/1
4	MAN	D	4	4	-	2/2/19/22	0/1/1/1
5	NAG	E	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	4/6/23/26	0/1/1/1
5	BMA	E	3	5	-	2/2/19/22	0/1/1/1
3	NAG	F	1	2,3	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
6	NAG	G	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	G	2	6	-	0/6/23/26	0/1/1/1
6	BMA	G	3	6	-	2/2/19/22	0/1/1/1
6	MAN	G	4	6	-	0/2/19/22	0/1/1/1
6	MAN	G	5	6	-	2/2/19/22	0/1/1/1

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})
4	D	4	MAN	C1-O5-C5	7.31	122.10	112.19
4	D	4	MAN	C1-C2-C3	4.62	115.34	109.67
4	D	4	MAN	O5-C1-C2	4.15	117.17	110.77
3	C	1	NAG	C4-C3-C2	3.47	116.11	111.02
3	C	2	NAG	C4-C3-C2	2.35	114.47	111.02

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	3	BMA	O5-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	D	4	MAN	O5-C5-C6-O6
6	G	5	MAN	O5-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6

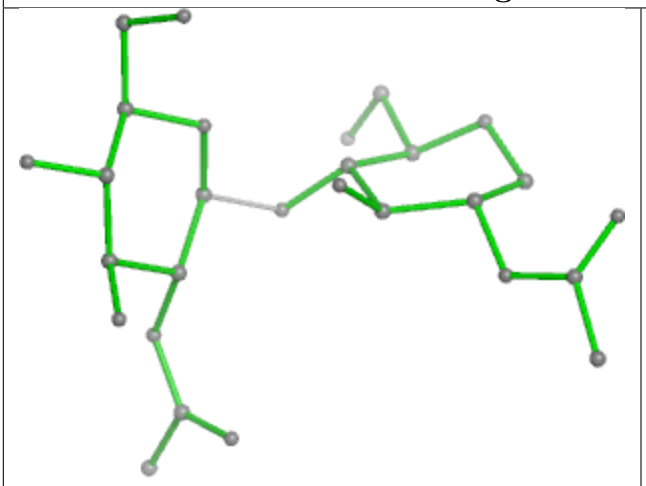
There are no ring outliers.

14 monomers are involved in 211 short contacts:

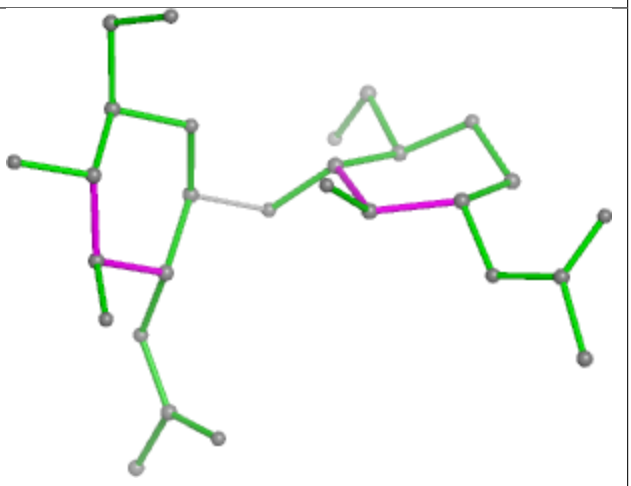
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1	NAG	15	0
6	G	2	NAG	9	0
3	C	1	NAG	1	0
3	F	2	NAG	37	0
5	E	2	NAG	2	0
4	D	2	NAG	11	0
3	F	1	NAG	37	0
6	G	4	MAN	23	0
6	G	3	BMA	5	0
6	G	1	NAG	3	0
4	D	3	BMA	10	0
4	D	1	NAG	42	0
6	G	5	MAN	6	0
4	D	4	MAN	12	0

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

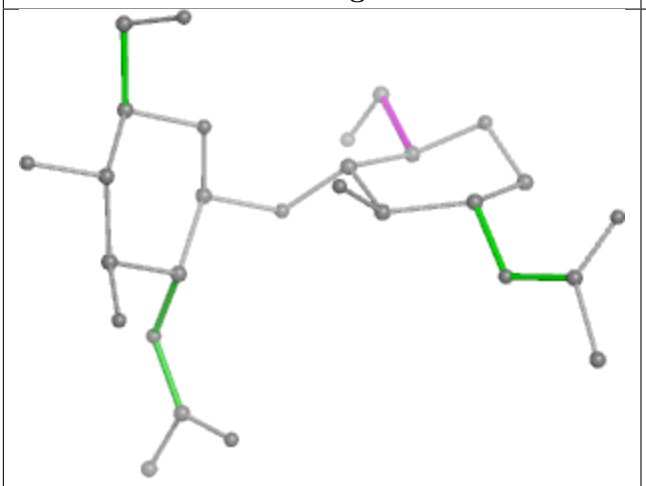
Oligosaccharide Chain C



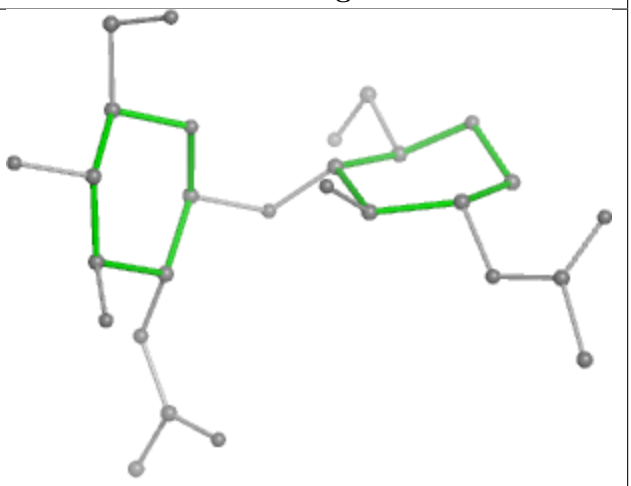
Bond lengths



Bond angles

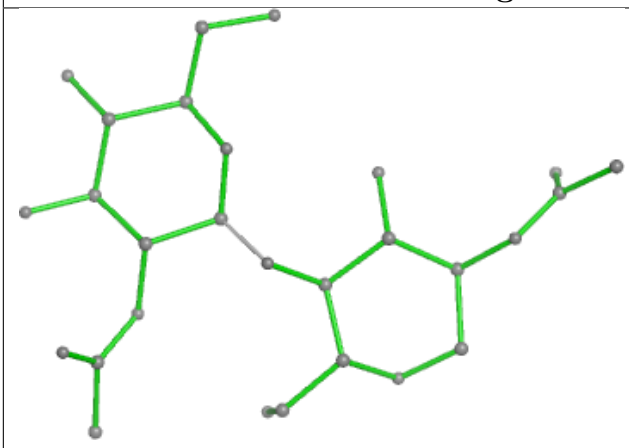


Torsions

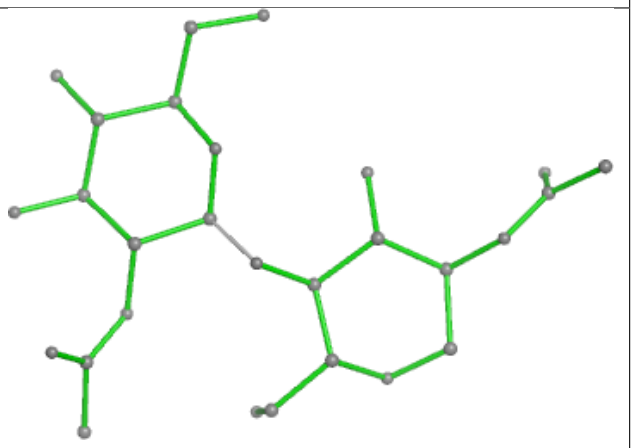


Rings

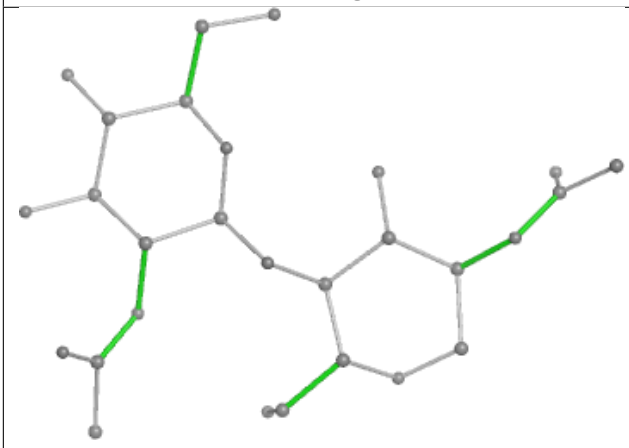
Oligosaccharide Chain F



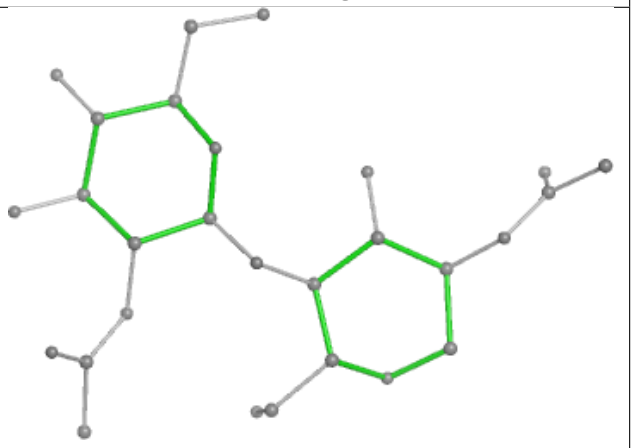
Bond lengths



Bond angles

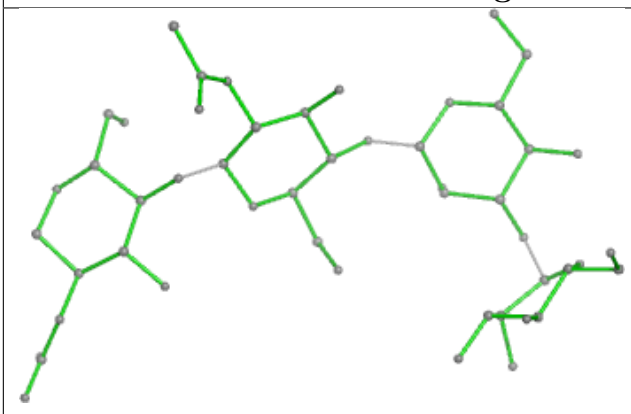


Torsions

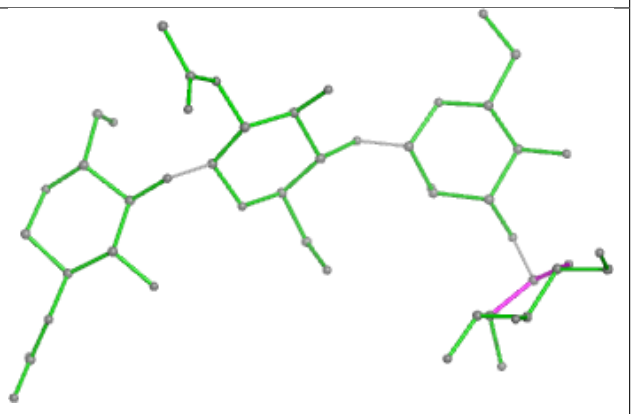


Rings

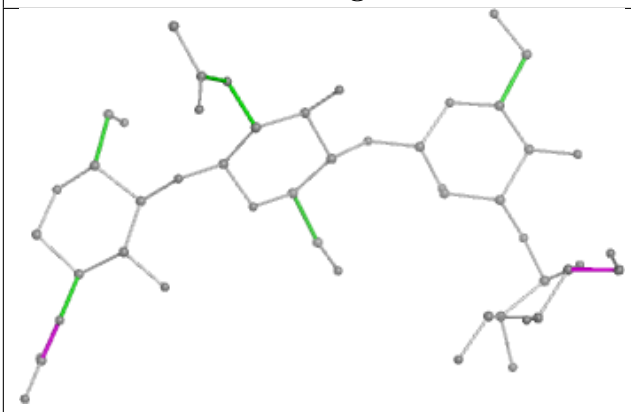
Oligosaccharide Chain D



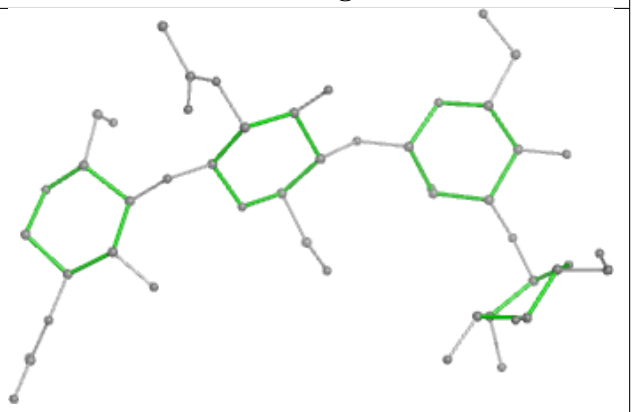
Bond lengths



Bond angles

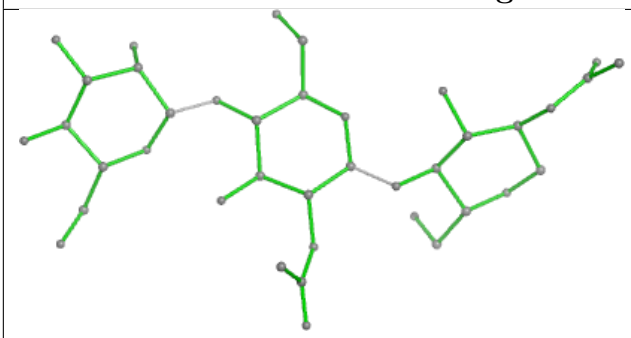


Torsions

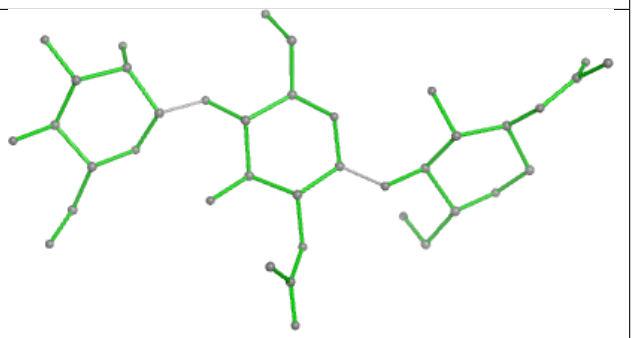


Rings

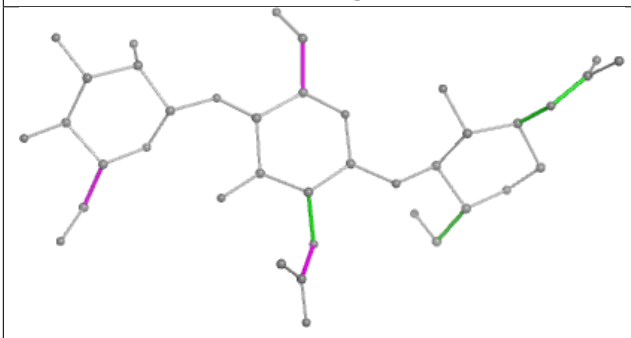
Oligosaccharide Chain E



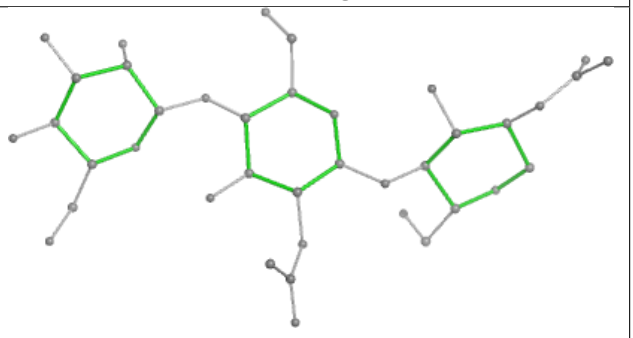
Bond lengths



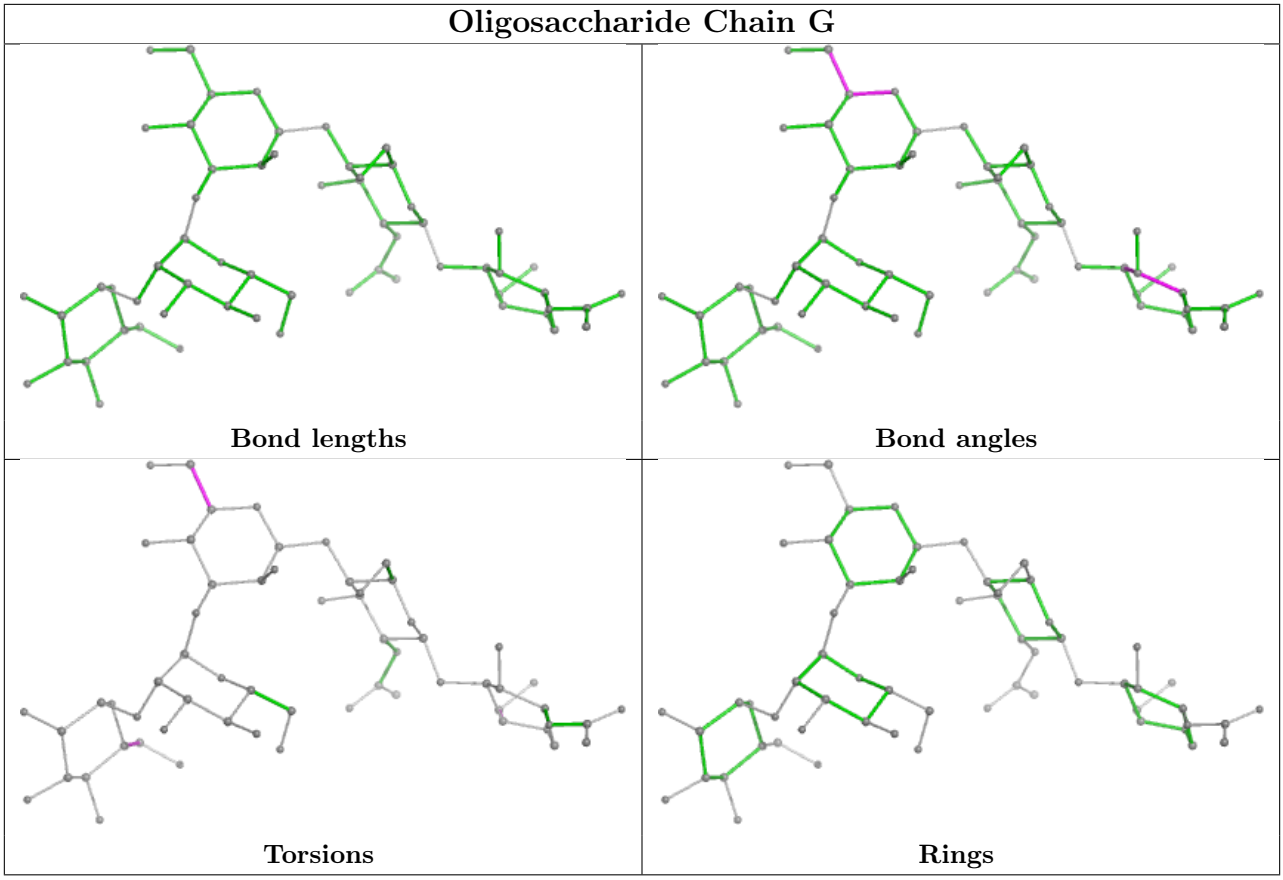
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
7	NAG	A	3015	1	14,14,15	0.49	0	17,19,21	0.73	0
7	NAG	A	3570	1	14,14,15	0.66	0	17,19,21	1.60	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	A	3015	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	A	3570	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	3570	NAG	C1-O5-C5	5.42	119.53	112.19
7	A	3570	NAG	O5-C1-C2	2.70	115.55	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	3015	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	3570	NAG	O5-C5-C6-O6
7	A	3570	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3570	NAG	38	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	16
1	A	14

The worst 5 of 30 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	433:CYS	C	434:ASP	N	30.92
1	B	56:PHE	C	57:PRO	N	30.36
1	A	744:ALA	C	745:GLU	N	21.99
1	B	600:LYS	C	601:CYS	N	20.54
1	A	601:ASP	C	602:CYS	N	19.21

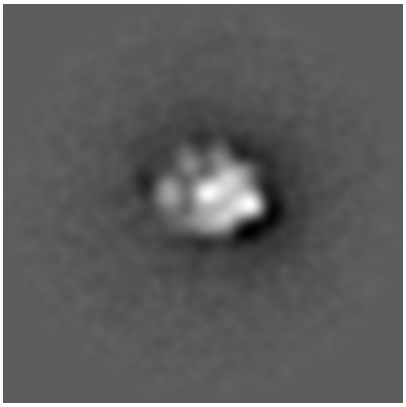
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-2281. These allow visual inspection of the internal detail of the map and identification of artifacts.

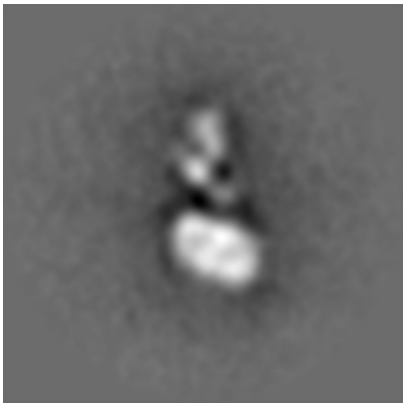
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

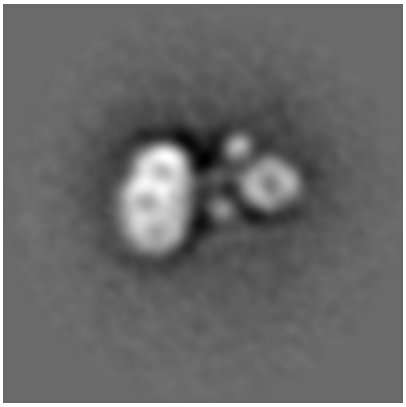
6.1.1 Primary map



X



Y

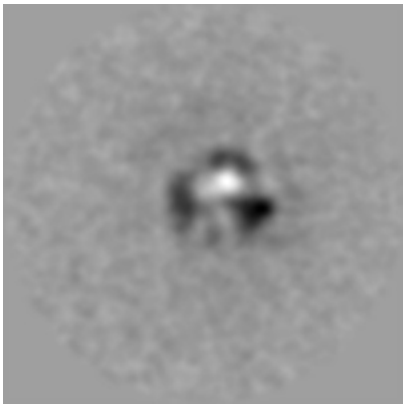


Z

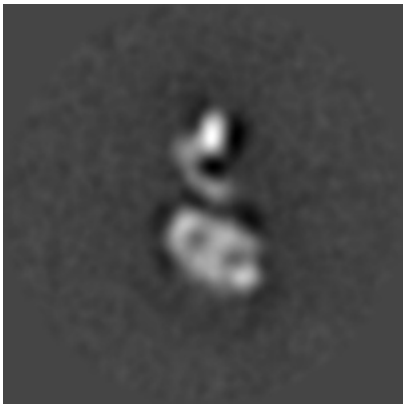
The images above show the map projected in three orthogonal directions.

6.2 Central slices

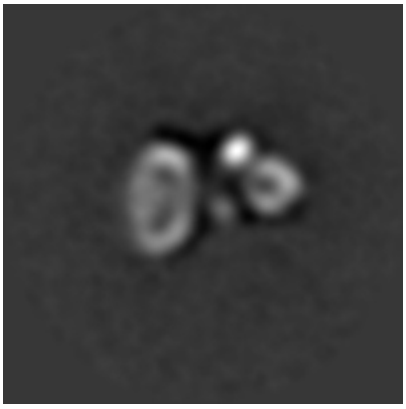
6.2.1 Primary map



X Index: 68



Y Index: 68

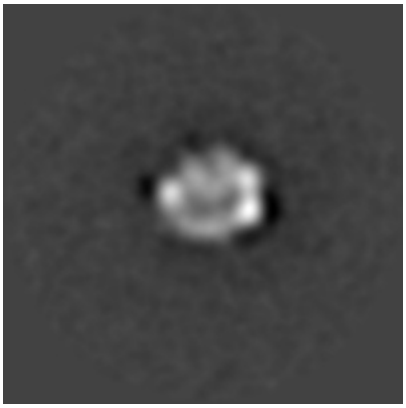


Z Index: 68

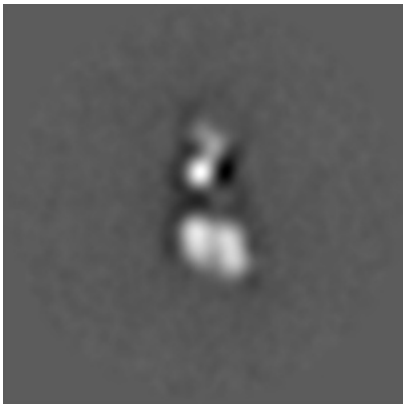
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 57



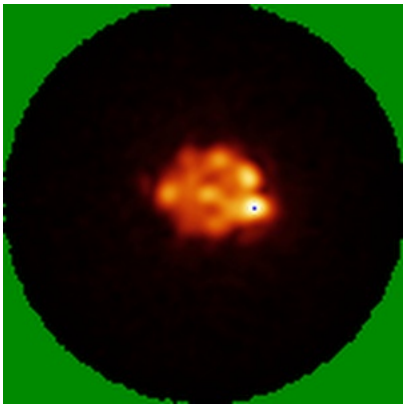
Y Index: 83

Z Index: 67

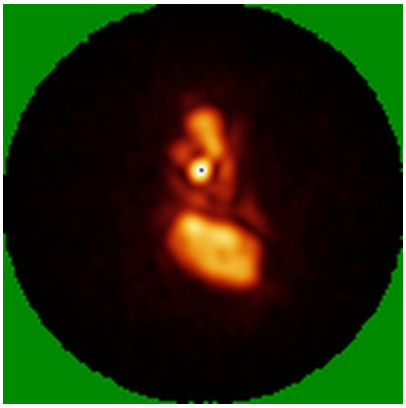
The images above show the largest variance slices of the map in three orthogonal directions.

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

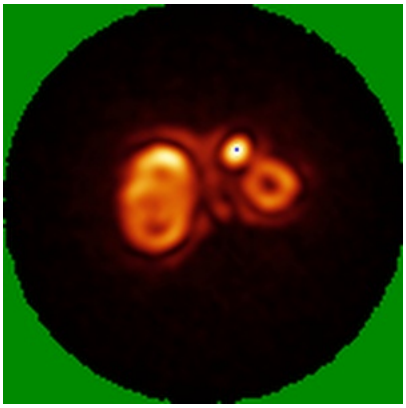
6.4.1 Primary map



X



Y

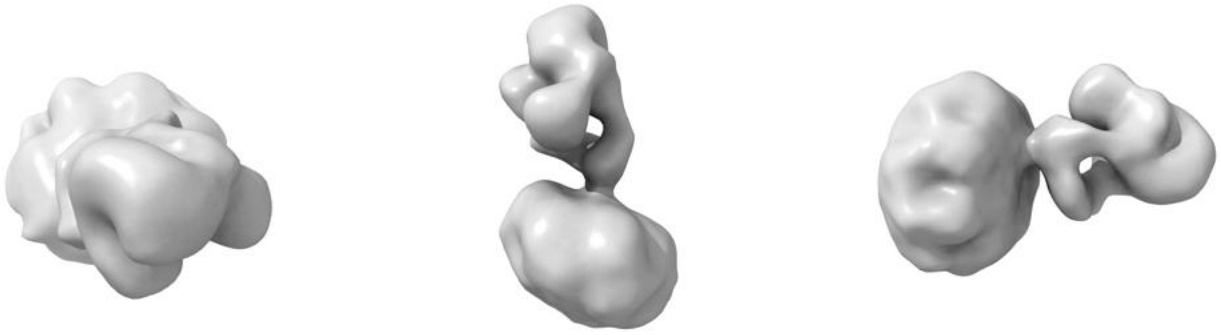


Z

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 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

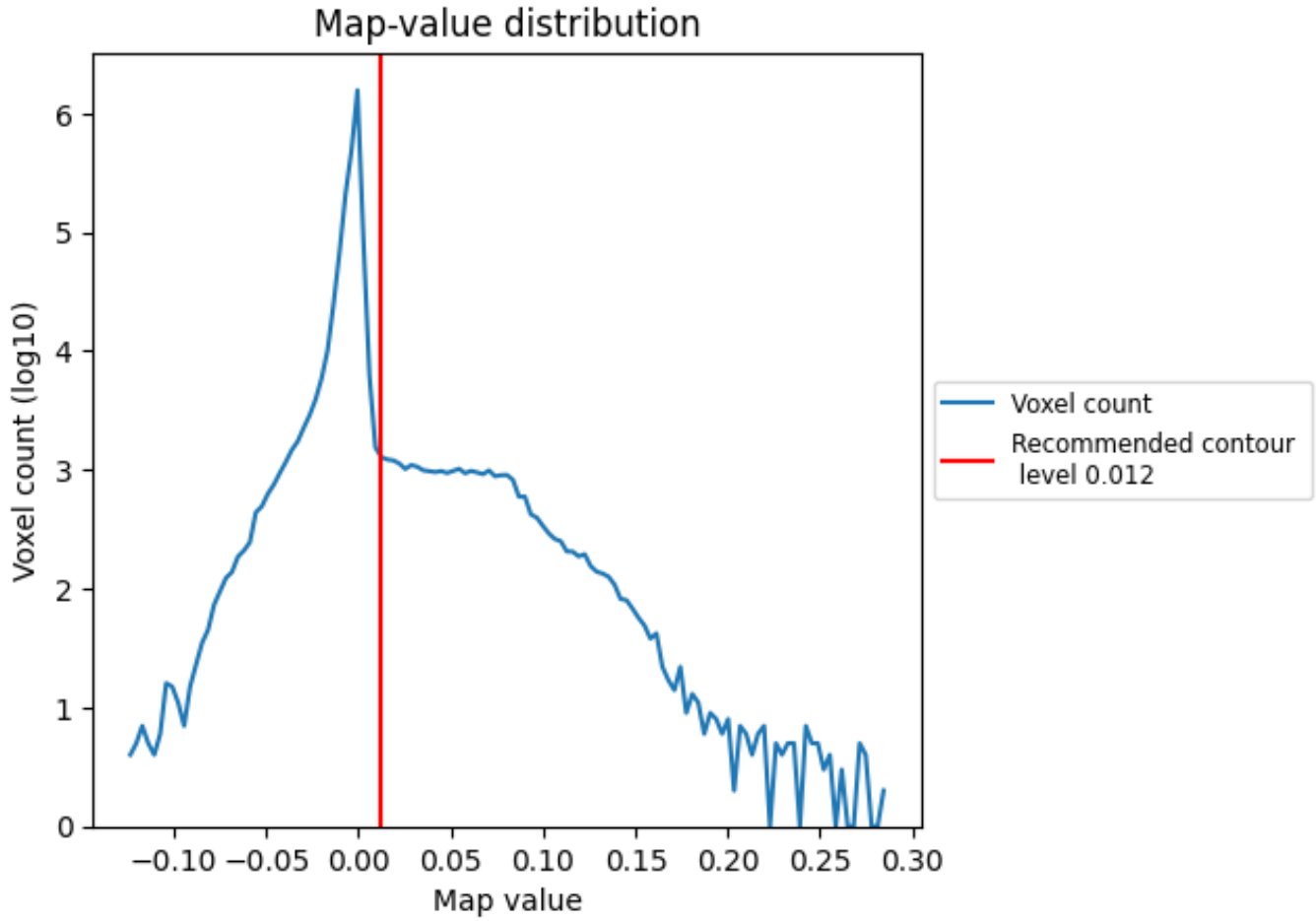
6.6 Mask visualisation (i)

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

7 Map analysis

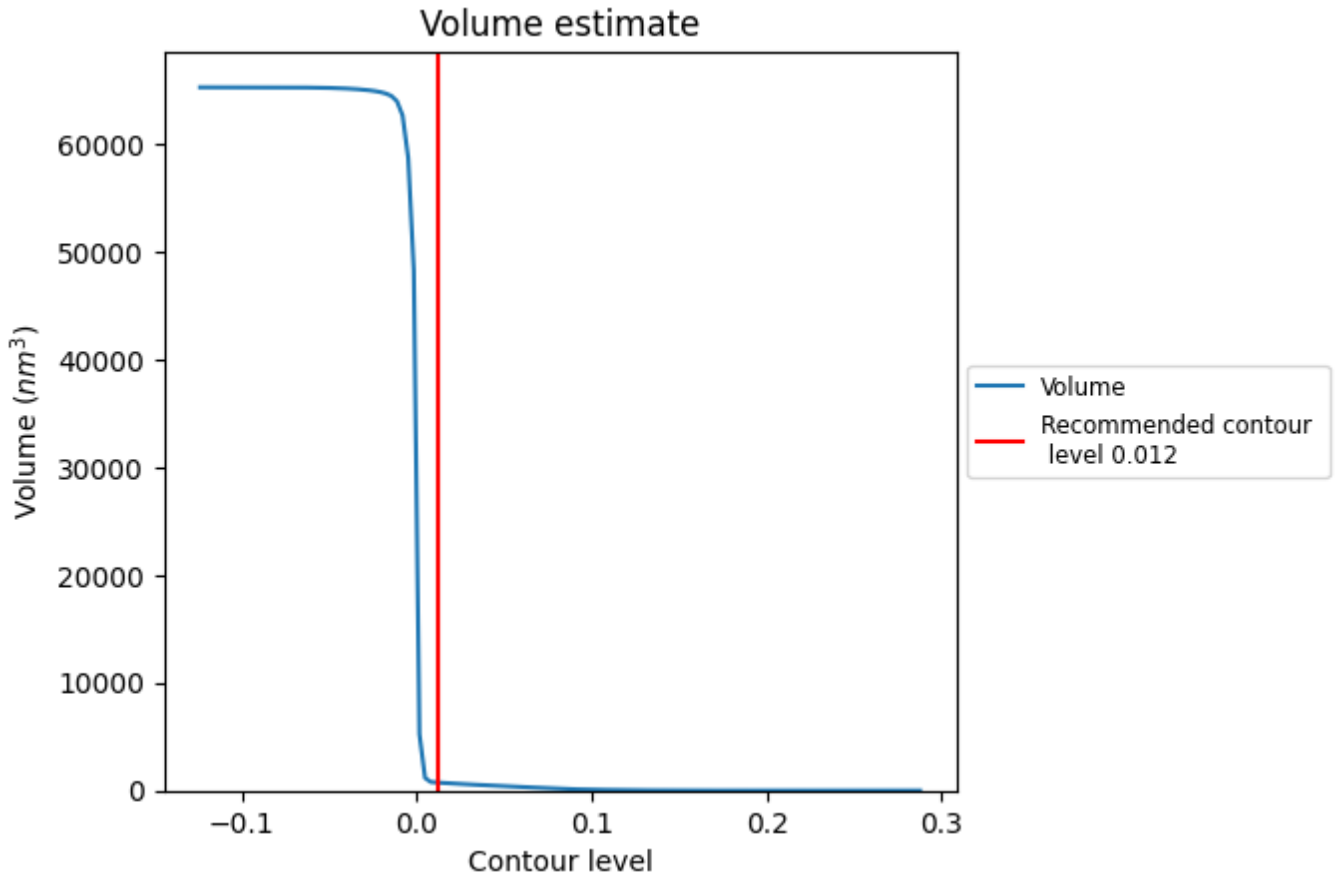
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

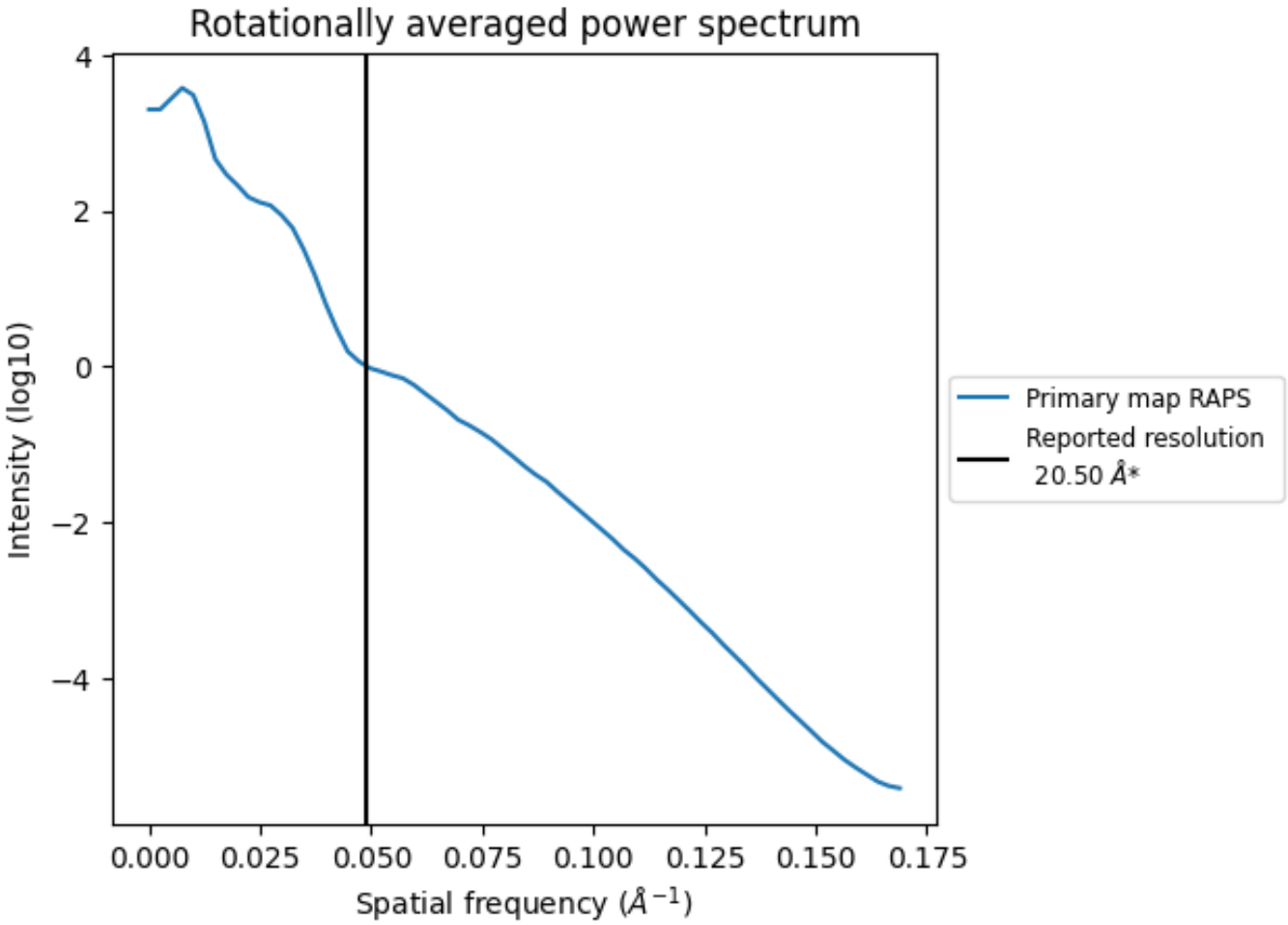
7.2 Volume estimate (i)



The volume at the recommended contour level is 741 nm^3; this corresponds to an approximate mass of 670 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 0.049 Å^{-1}

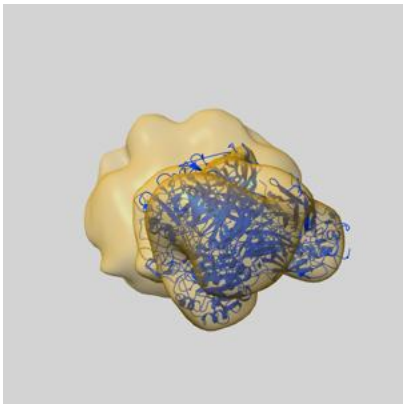
8 Fourier-Shell correlation (i)

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

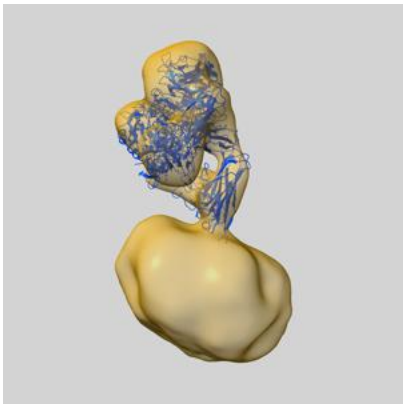
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-2281 and PDB model 4CAK. Per-residue inclusion information can be found in section 3 on page 7.

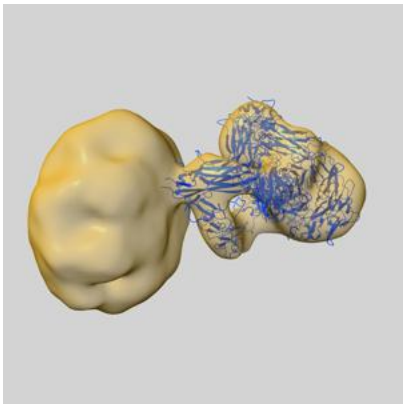
9.1 Map-model overlay



X



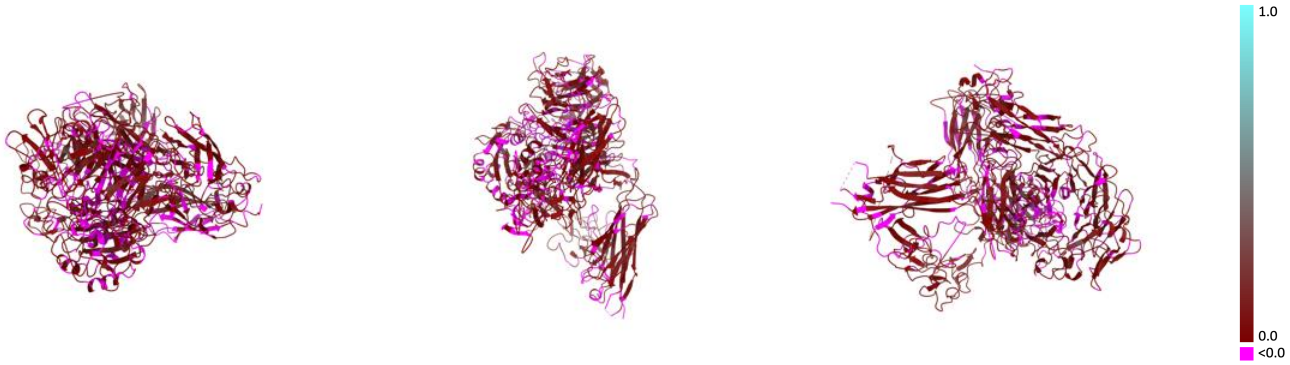
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 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.

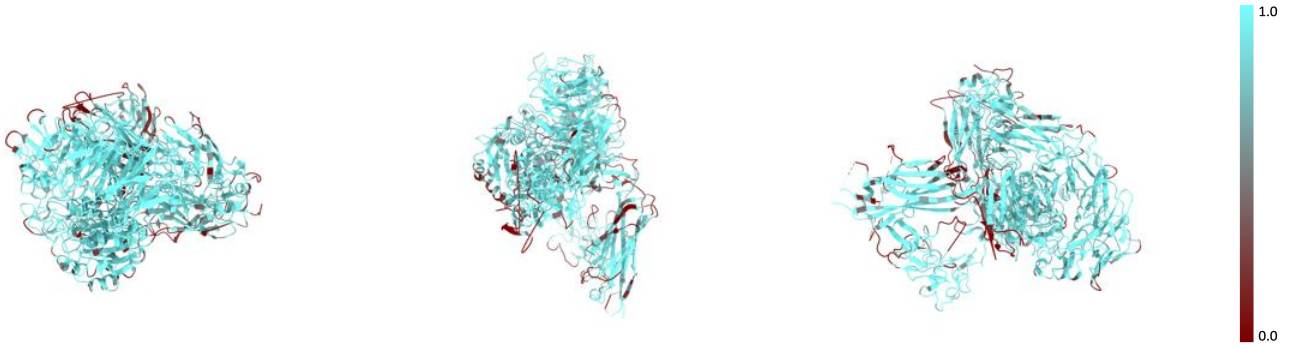
9.2 Q-score mapped to coordinate model



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.

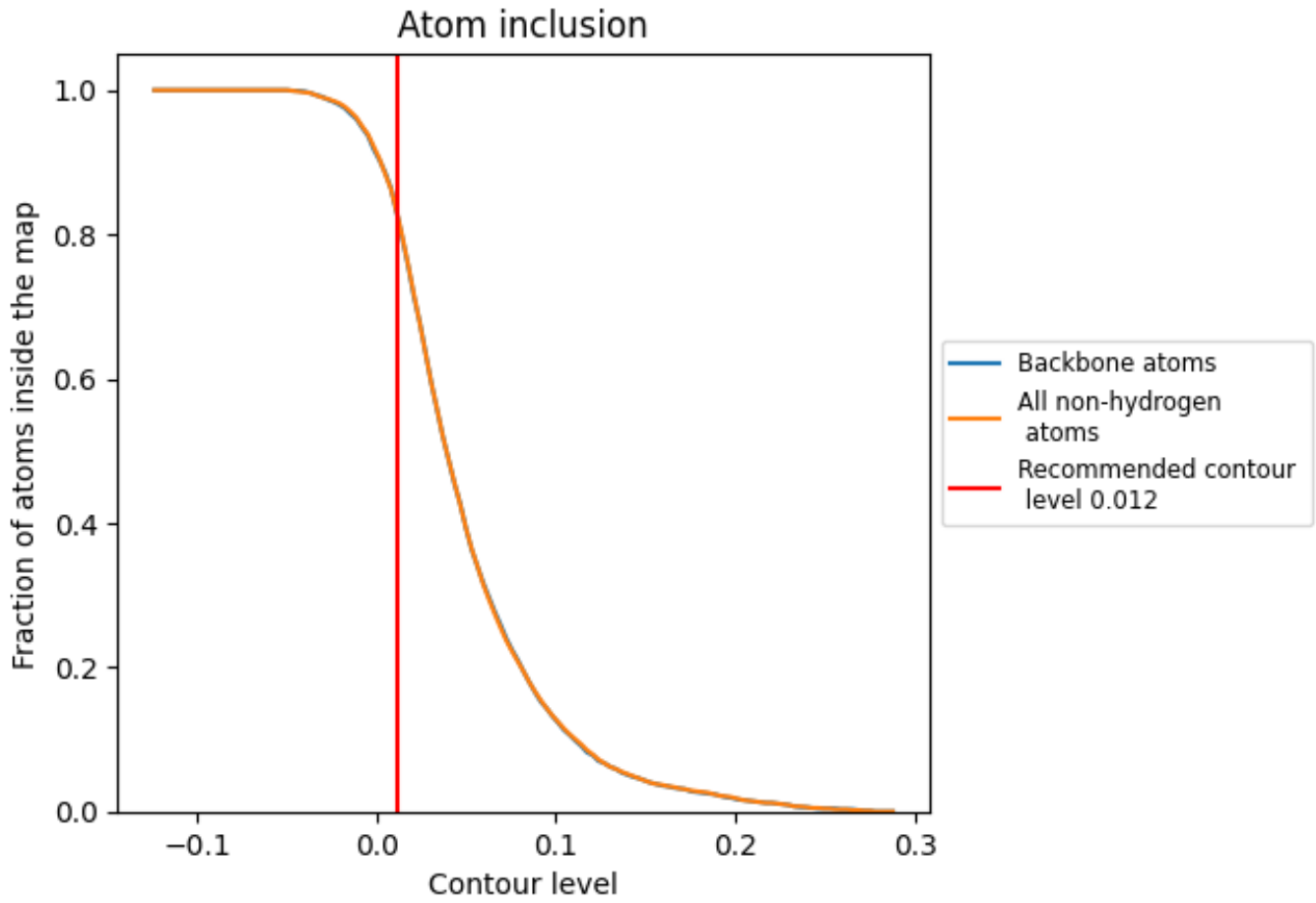
9.3 Atom inclusion mapped to coordinate model



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 (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8240	0.0490
A	0.8650	0.0530
B	0.8000	0.0440
C	0.6070	0.0590
D	0.8200	0.0620
E	0.7440	0.0490
F	0.7500	0.0300
G	0.8850	0.0850