Full wwPDB EM Validation Report ⓘ

Nov 23, 2022 – 12:28 PM JST

PDB ID	:	7VPK
EMDB ID	:	EMD-32068
Title	:	Cryo-EM structure of the human ATP13A2 (SPM-bound E2P state)
Authors	:	Tomita, A.; Yamashita, K.; Nishizawa, T.; Nureki, O.
Deposited on	:	2021-10-17
Resolution	:	3.50 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

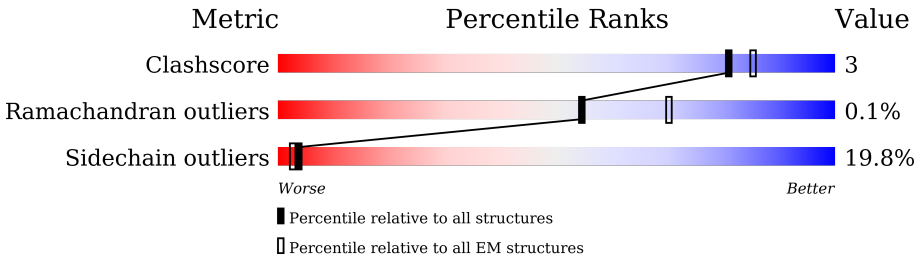
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.50 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	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	1184	32% 69% 18% • 11%
2	B	2	100% 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8197 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 Polyamine-transporting ATPase 13A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1055	Total	C	N	O	S	0	0
			8150	5269	1397	1430	54		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q9NQ11
A	-2	PRO	-	expression tag	UNP Q9NQ11
A	-1	SER	-	expression tag	UNP Q9NQ11
A	0	ARG	-	expression tag	UNP Q9NQ11

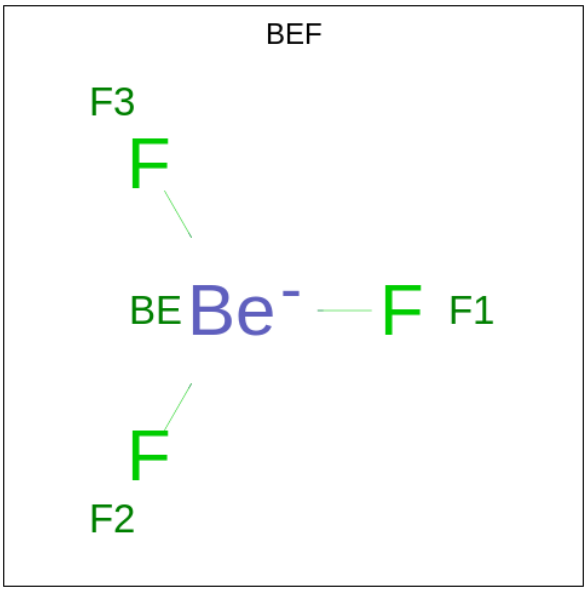
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

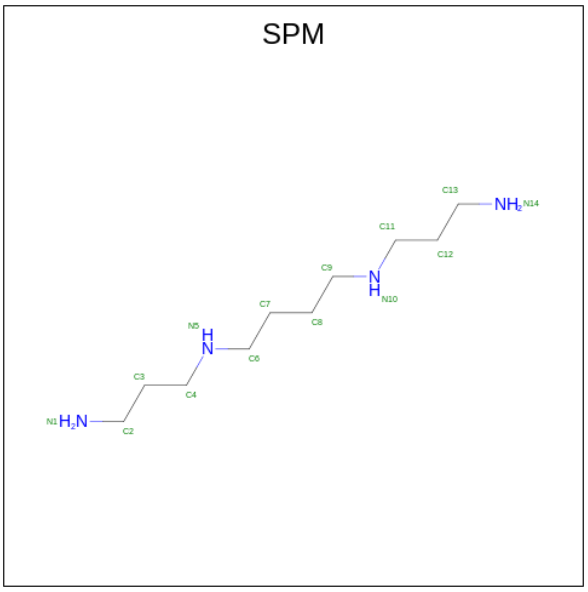
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Mg	0
			1	1	

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Be	F	
4	A	1	4	1	3	0

- Molecule 5 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$) (labeled as "Ligand of Interest" by depositor).



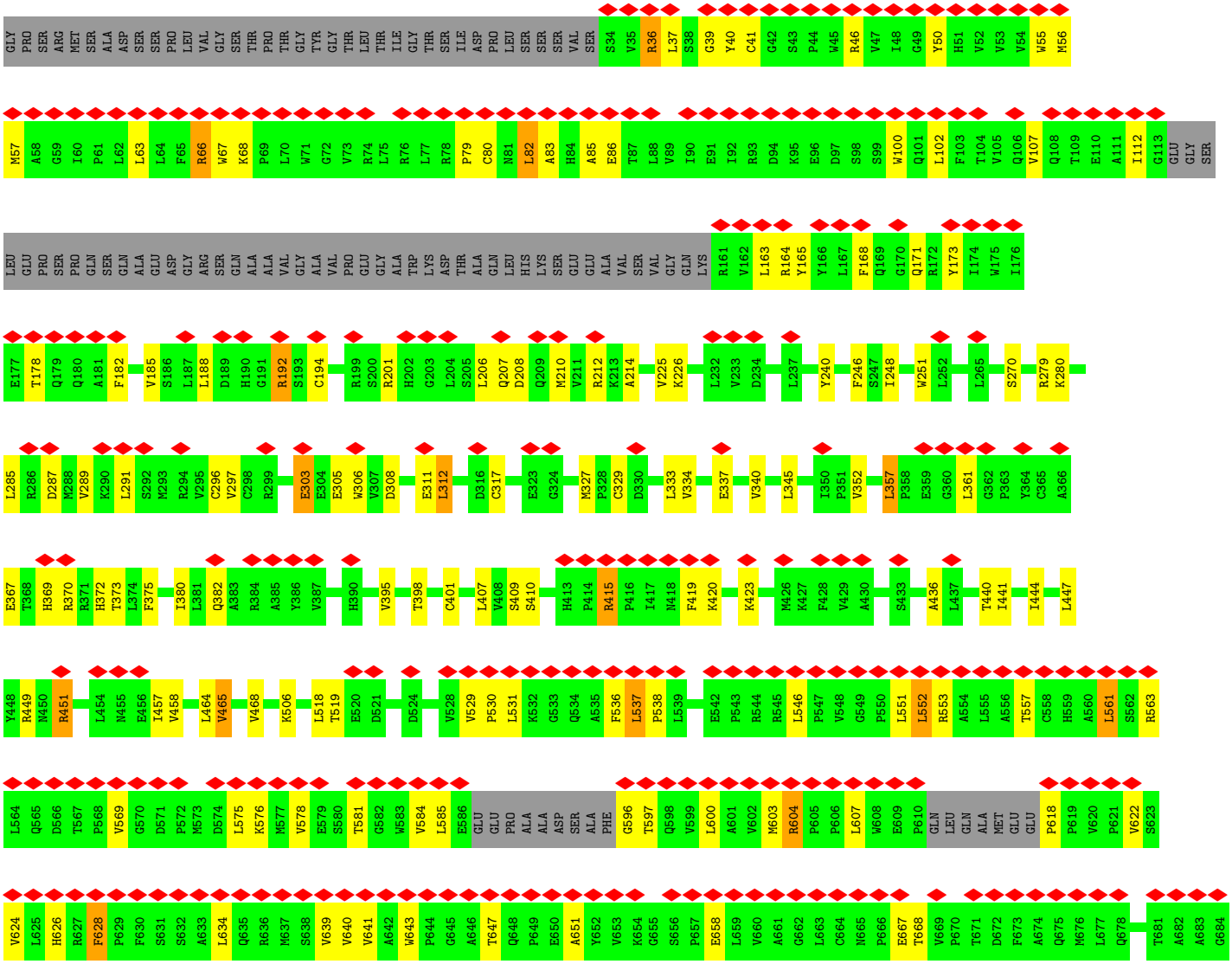
Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
5	A	1	14	10	4	0

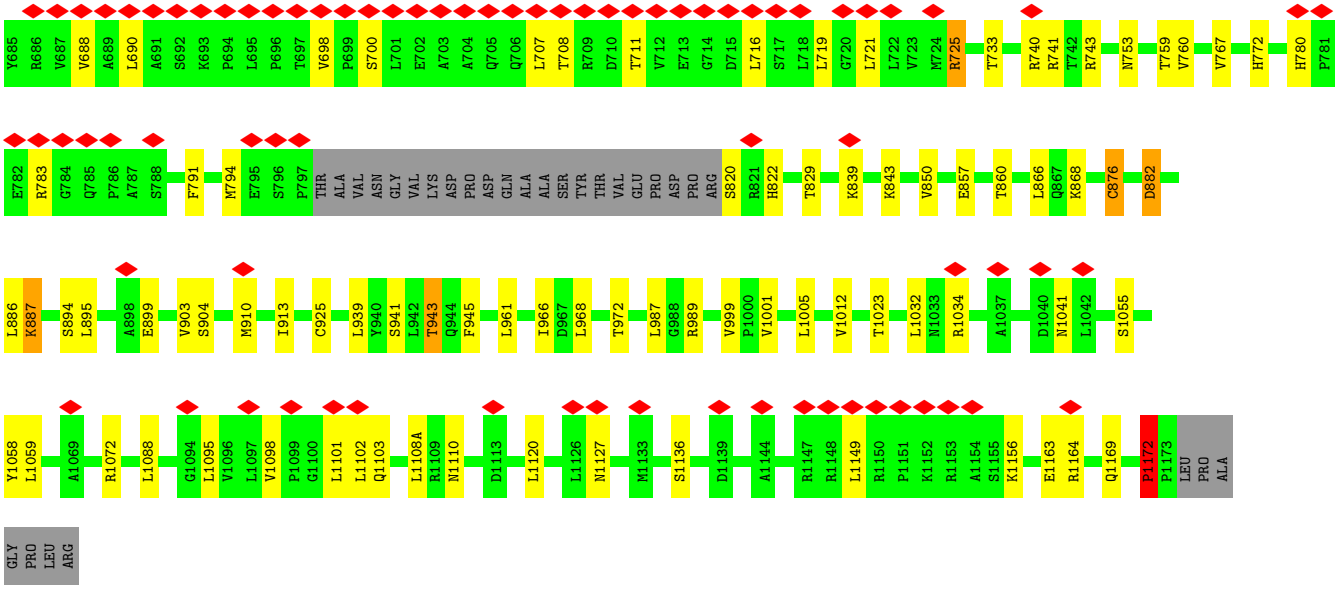
3 Residue-property plots (i)

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: Polyamine-transporting ATPase 13A2

Chain A:





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

Chain B:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3289	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.270	Depositor
Minimum map value	-0.166	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0438	Depositor
Map size (Å)	210.405, 210.405, 210.405	wwPDB
Map dimensions	156, 156, 156	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34875, 1.34875, 1.34875	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, SPM, BEF, 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	0.86	0/8338	1.10	11/11365 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1172	PRO	N-CA-CB	-8.77	92.78	103.30
1	A	66	ARG	CG-CD-NE	6.65	125.77	111.80
1	A	725	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	66	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	A	451	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	370	ARG	NE-CZ-NH2	5.37	122.98	120.30
1	A	415	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	36	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	628	PHE	CB-CG-CD1	5.16	124.41	120.80
1	A	604	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	563	ARG	NE-CZ-NH2	5.07	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	8150	0	8433	43	0
2	B	28	0	25	0	0
3	A	1	0	0	0	0
4	A	4	0	0	0	0
5	A	14	0	26	0	0
All	All	8197	0	8484	43	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 3.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLN:HE21	1:A:185:VAL:HG21	1.49	0.78
1:A:192:ARG:HA	1:A:192:ARG:CZ	2.23	0.68
1:A:171:GLN:HE22	1:A:401:CYS:HA	1.62	0.64
1:A:561:LEU:HD12	1:A:585:LEU:HD13	1.78	0.63
1:A:518:LEU:HD11	1:A:913:ILE:HD12	1.80	0.62
1:A:886:LEU:HD23	1:A:904:SER:HB3	1.82	0.62
1:A:39:GLY:HA2	1:A:85:ALA:HB2	1.83	0.60
1:A:192:ARG:HA	1:A:192:ARG:NE	2.17	0.60
1:A:40:TYR:HA	1:A:79:PRO:HA	1.83	0.60
1:A:536:PHE:CZ	1:A:721:LEU:HD23	2.39	0.58
1:A:163:LEU:HD22	1:A:165:TYR:CE1	2.41	0.55
1:A:887:LYS:HB2	1:A:903:VAL:HG12	1.90	0.54
1:A:82:LEU:HD22	1:A:82:LEU:H	1.73	0.53
1:A:882:ASP:N	1:A:882:ASP:OD1	2.42	0.53
1:A:537:LEU:HD13	1:A:538:PRO:HD2	1.90	0.53
1:A:596:GLY:N	1:A:700:SER:HG	2.06	0.52
1:A:640:VAL:HA	1:A:651:ALA:HA	1.90	0.52
1:A:444:ILE:HD13	1:A:457:ILE:HG22	1.90	0.52
1:A:876:CYS:SG	1:A:895:LEU:HD21	2.52	0.50
1:A:112:ILE:HG22	1:A:214:ALA:HB1	1.94	0.49
1:A:312:LEU:HD12	1:A:395:VAL:HG21	1.96	0.47
1:A:531:LEU:HD22	1:A:536:PHE:CE1	2.49	0.47
1:A:546:LEU:HD13	1:A:552:LEU:CD1	2.45	0.46
1:A:966:ILE:HD12	1:A:1058:TYR:CD2	2.51	0.46
1:A:83:ALA:O	1:A:164:ARG:NH2	2.49	0.45
1:A:311:GLU:N	1:A:311:GLU:OE2	2.50	0.45
1:A:340:VAL:HG12	1:A:380:ILE:HA	1.97	0.45
1:A:357:LEU:HD22	1:A:372:HIS:HB2	1.98	0.45
1:A:939:LEU:O	1:A:943:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:895:LEU:HD22	1:A:895:LEU:N	2.31	0.45
1:A:943:THR:HG23	1:A:1058:TYR:CE1	2.52	0.44
1:A:285:LEU:O	1:A:289:VAL:HG22	2.18	0.44
1:A:1103:GLN:HG2	1:A:1108(A):LEU:HD12	2.00	0.44
1:A:464:LEU:O	1:A:468:VAL:HG23	2.17	0.44
1:A:529:VAL:HB	1:A:721:LEU:HG	2.00	0.43
1:A:546:LEU:HD13	1:A:552:LEU:HD13	2.00	0.43
1:A:966:ILE:HD12	1:A:1058:TYR:CE2	2.54	0.43
1:A:436:ALA:HB1	1:A:465:VAL:HG22	2.00	0.42
1:A:468:VAL:HG22	1:A:945:PHE:CD1	2.54	0.42
1:A:530:PRO:HG2	1:A:537:LEU:HD12	2.02	0.42
1:A:85:ALA:O	1:A:107:VAL:HG21	2.19	0.42
1:A:297:VAL:O	1:A:303:GLU:HA	2.20	0.41
1:A:345:LEU:HD11	1:A:375:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1045/1184 (88%)	1003 (96%)	41 (4%)	1 (0%)	51 84

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1172	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	904/1005 (90%)	725 (80%)	179 (20%)	1 7

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	37	LEU
1	A	41	CYS
1	A	46	ARG
1	A	50	TYR
1	A	55	TRP
1	A	56	MET
1	A	57	MET
1	A	63	LEU
1	A	66	ARG
1	A	67	TRP
1	A	68	LYS
1	A	80	CYS
1	A	82	LEU
1	A	86	GLU
1	A	100	TRP
1	A	102	LEU
1	A	168	PHE
1	A	173	TYR
1	A	178	THR
1	A	182	PHE
1	A	188	LEU
1	A	192	ARG
1	A	194	CYS
1	A	201	ARG
1	A	206	LEU
1	A	207	GLN
1	A	208	ASP
1	A	210	MET
1	A	212	ARG
1	A	225	VAL
1	A	226	LYS
1	A	240	TYR
1	A	246	PHE

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Mol	Chain	Res	Type
1	A	248	ILE
1	A	251	TRP
1	A	270	SER
1	A	279	ARG
1	A	280	LYS
1	A	287	ASP
1	A	291	LEU
1	A	296	CYS
1	A	303	GLU
1	A	305	GLU
1	A	306	TRP
1	A	308	ASP
1	A	312	LEU
1	A	317	CYS
1	A	327	MET
1	A	329	CYS
1	A	333	LEU
1	A	334	VAL
1	A	337	GLU
1	A	352	VAL
1	A	357	LEU
1	A	361	LEU
1	A	367	GLU
1	A	369	HIS
1	A	373	THR
1	A	382	GLN
1	A	398	THR
1	A	407	LEU
1	A	409	SER
1	A	410	SER
1	A	415	ARG
1	A	419	PHE
1	A	420	LYS
1	A	423	LYS
1	A	440	THR
1	A	441	ILE
1	A	447	LEU
1	A	449	ARG
1	A	451	ARG
1	A	458	VAL
1	A	465	VAL
1	A	506	LYS

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Mol	Chain	Res	Type
1	A	519	THR
1	A	537	LEU
1	A	551	LEU
1	A	552	LEU
1	A	553	ARG
1	A	557	THR
1	A	561	LEU
1	A	569	VAL
1	A	575	LEU
1	A	576	LYS
1	A	578	VAL
1	A	581	THR
1	A	584	VAL
1	A	597	THR
1	A	600	LEU
1	A	603	MET
1	A	604	ARG
1	A	607	LEU
1	A	618	PRO
1	A	622	VAL
1	A	624	VAL
1	A	626	HIS
1	A	628	PHE
1	A	634	LEU
1	A	639	VAL
1	A	641	VAL
1	A	643	TRP
1	A	647	THR
1	A	658	GLU
1	A	667	GLU
1	A	668	THR
1	A	688	VAL
1	A	690	LEU
1	A	698	VAL
1	A	707	LEU
1	A	708	THR
1	A	711	THR
1	A	716	LEU
1	A	719	LEU
1	A	725	ARG
1	A	733	THR
1	A	740	ARG

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Mol	Chain	Res	Type
1	A	741	ARG
1	A	743	ARG
1	A	753	ASN
1	A	759	THR
1	A	760	VAL
1	A	767	VAL
1	A	772	HIS
1	A	780	HIS
1	A	783	ARG
1	A	791	PHE
1	A	794	MET
1	A	820	SER
1	A	822	HIS
1	A	829	THR
1	A	839	LYS
1	A	843	LYS
1	A	850	VAL
1	A	857	GLU
1	A	860	THR
1	A	866	LEU
1	A	868	LYS
1	A	876	CYS
1	A	882	ASP
1	A	887	LYS
1	A	894	SER
1	A	899	GLU
1	A	910	MET
1	A	925	CYS
1	A	941	SER
1	A	943	THR
1	A	961	LEU
1	A	968	LEU
1	A	972	THR
1	A	987	LEU
1	A	989	ARG
1	A	999	VAL
1	A	1001	VAL
1	A	1005	LEU
1	A	1012	VAL
1	A	1023	THR
1	A	1032	LEU
1	A	1034	ARG

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Mol	Chain	Res	Type
1	A	1041	ASN
1	A	1055	SER
1	A	1059	LEU
1	A	1072	ARG
1	A	1088	LEU
1	A	1095	LEU
1	A	1098	VAL
1	A	1101	LEU
1	A	1102	LEU
1	A	1110	ASN
1	A	1120	LEU
1	A	1127	ASN
1	A	1136	SER
1	A	1149	LEU
1	A	1156	LYS
1	A	1163	GLU
1	A	1164	ARG
1	A	1169	GLN
1	A	1172	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	230	GLN
1	A	382	GLN
1	A	847	GLN
1	A	1044	ASN
1	A	1169	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)

2 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	$\#\|Z\| > 2$
2	NAG	B	1	1,2	14,14,15	0.61	0	17,19,21	1.18	1 (5%)
2	NAG	B	2	2	14,14,15	0.47	0	17,19,21	1.14	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
2	NAG	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1	NAG	C1-O5-C5	3.17	116.49	112.19
2	B	2	NAG	C2-N2-C7	2.16	125.98	122.90
2	B	2	NAG	C1-O5-C5	2.10	115.04	112.19

There are no chirality outliers.

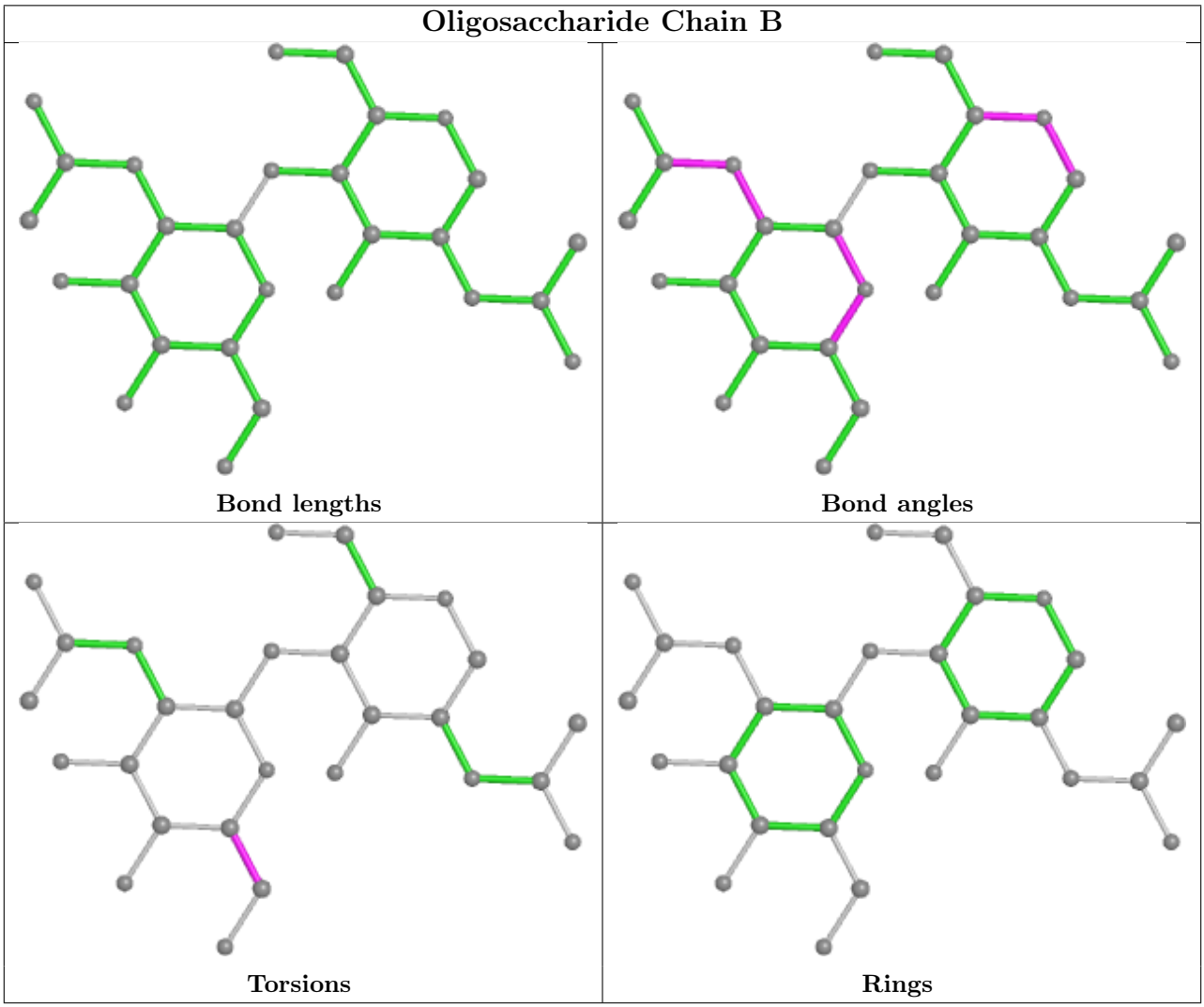
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-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.



5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SPM	A	1203	-	13,13,13	0.19	0	12,12,12	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	BEF	A	1202	1	0,3,3	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SPM	A	1203	-	-	4/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

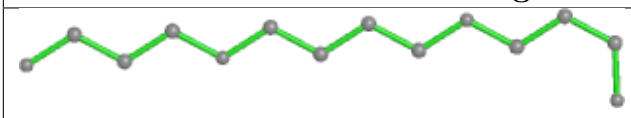
Mol	Chain	Res	Type	Atoms
5	A	1203	SPM	N5-C6-C7-C8
5	A	1203	SPM	N1-C2-C3-C4
5	A	1203	SPM	C11-C12-C13-N14
5	A	1203	SPM	C3-C4-N5-C6

There are no ring outliers.

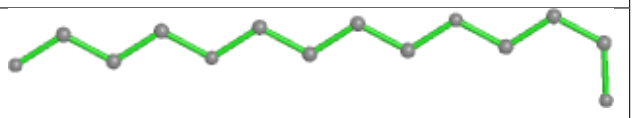
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

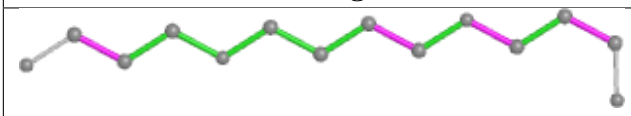
Ligand SPM A 1203



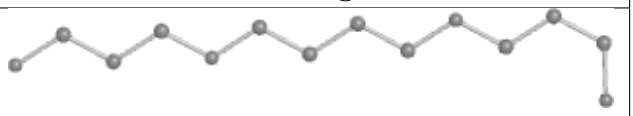
Bond lengths



Bond angles

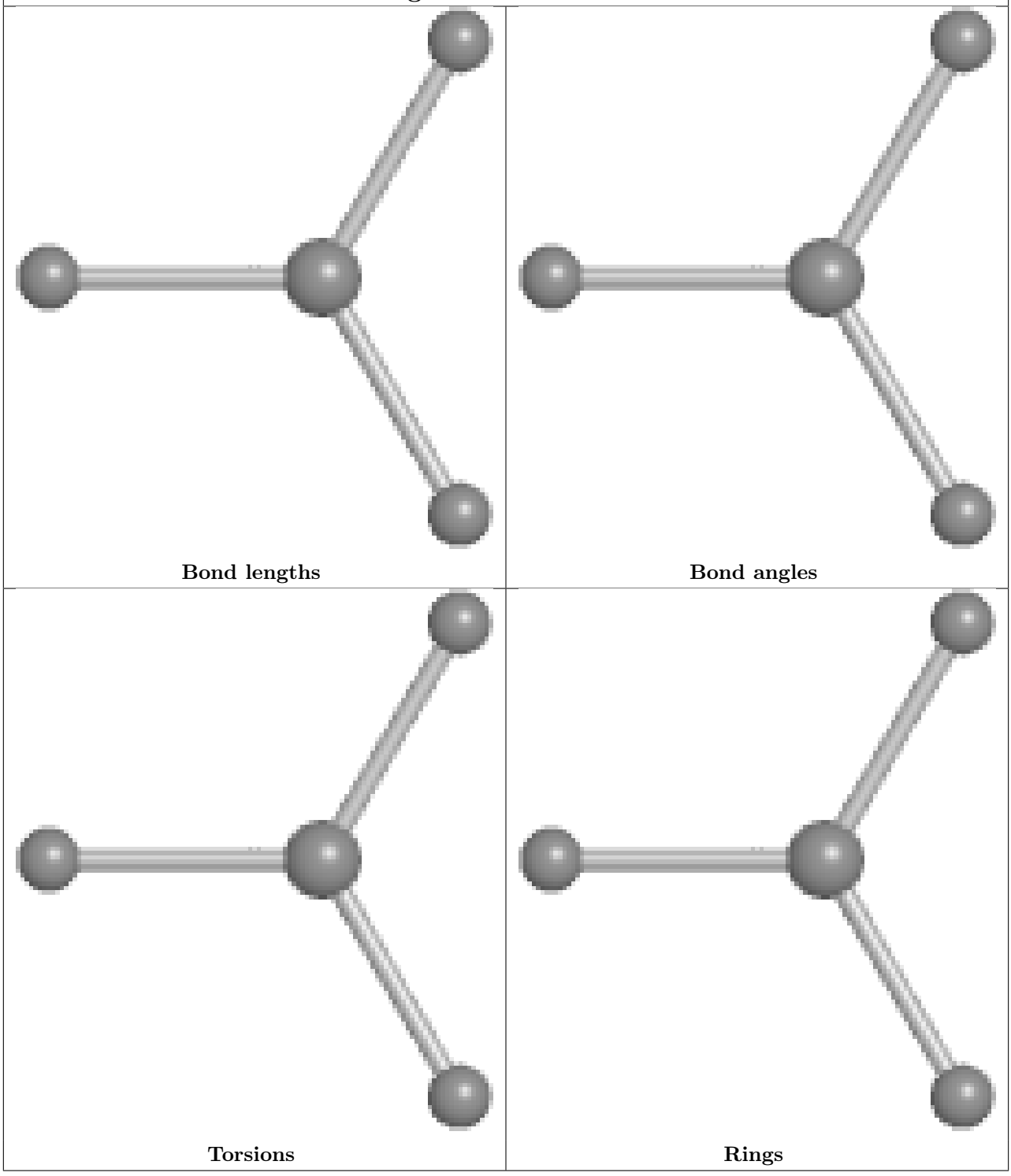


Torsions



Rings

Ligand BEF A 1202



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

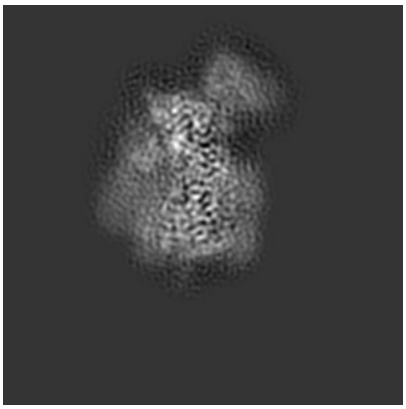
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32068. These allow visual inspection of the internal detail of the map and identification of artifacts.

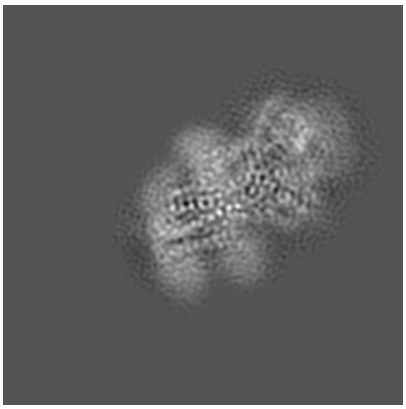
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

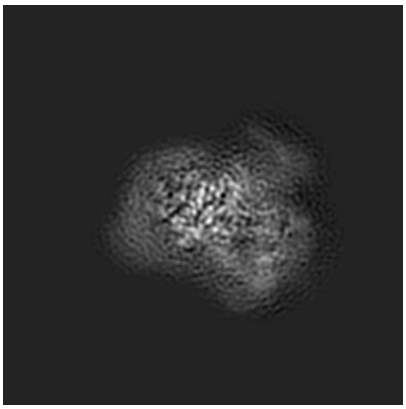
6.1.1 Primary map



X

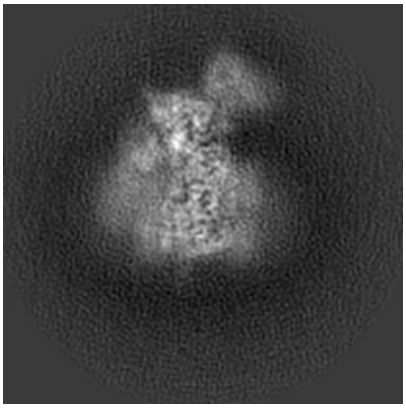


Y

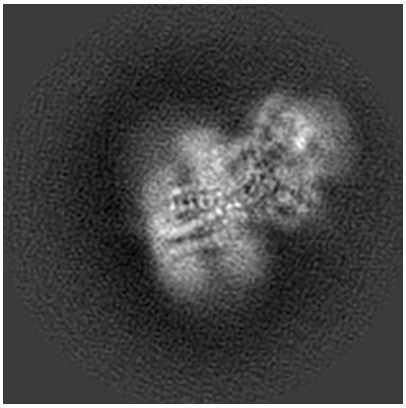


Z

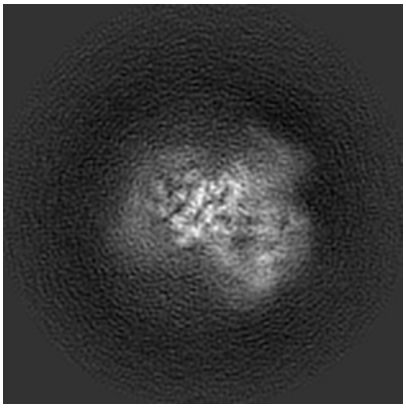
6.1.2 Raw map



X



Y



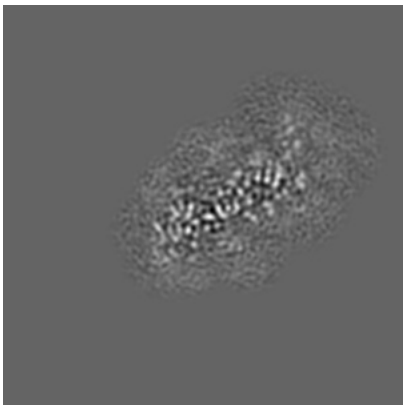
Z

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

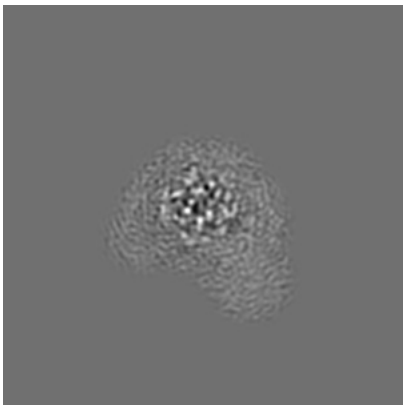
6.2 Central slices (i)

6.2.1 Primary map

X Index: 78

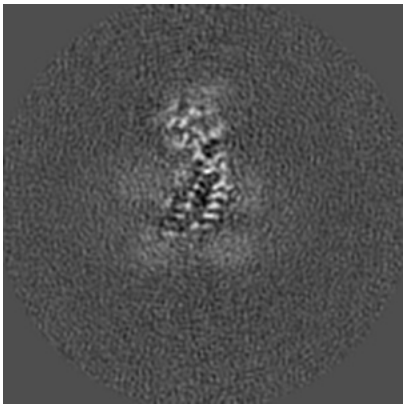


Y Index: 78

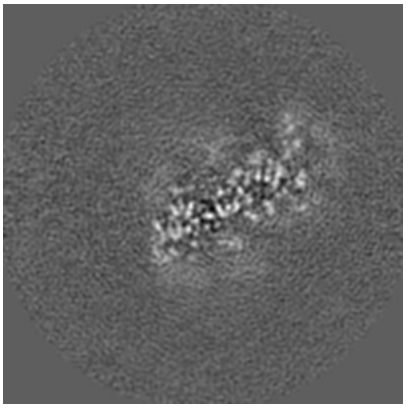


Z Index: 78

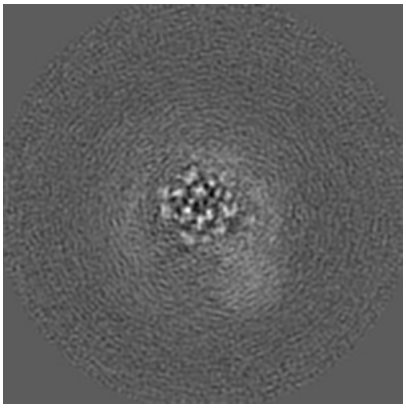
6.2.2 Raw map



X Index: 78



Y Index: 78

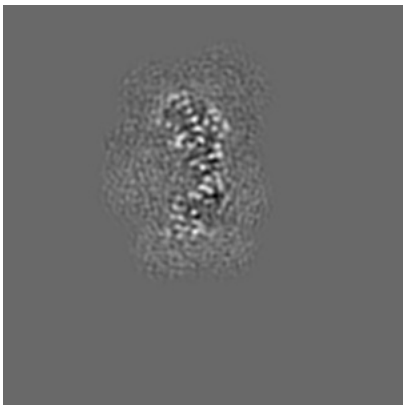


Z Index: 78

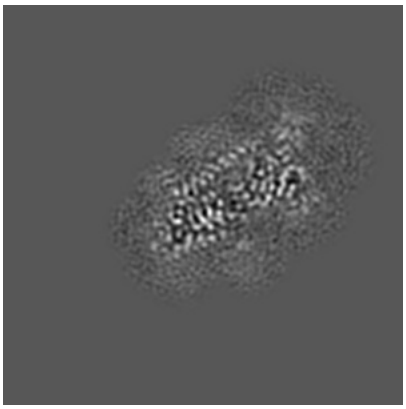
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

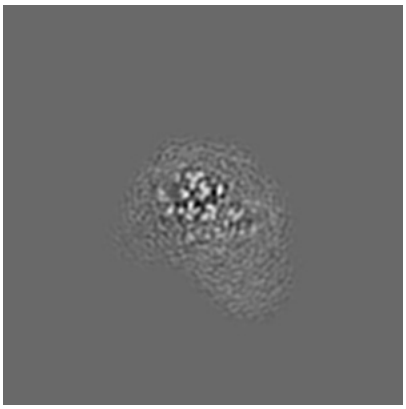
6.3.1 Primary map



X Index: 82

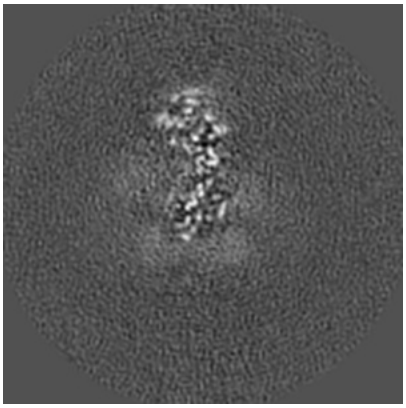


Y Index: 75

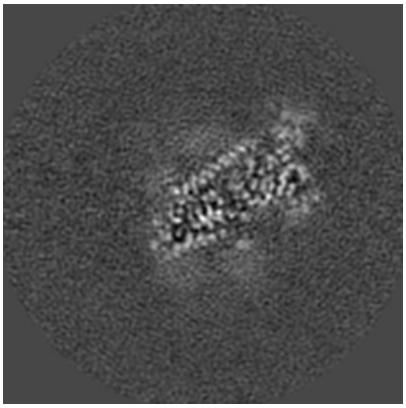


Z Index: 81

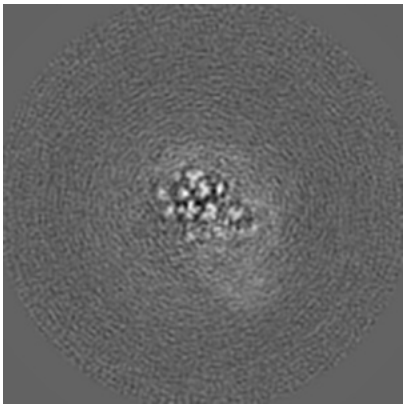
6.3.2 Raw map



X Index: 80



Y Index: 75



Z Index: 81

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 0.0438. 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.

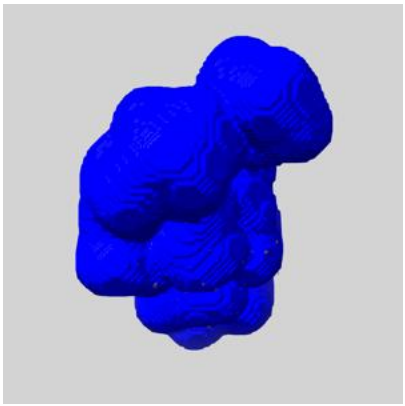
6.5 Mask visualisation (i)

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

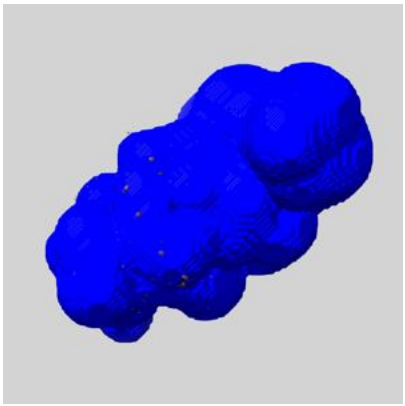
A mask typically either:

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

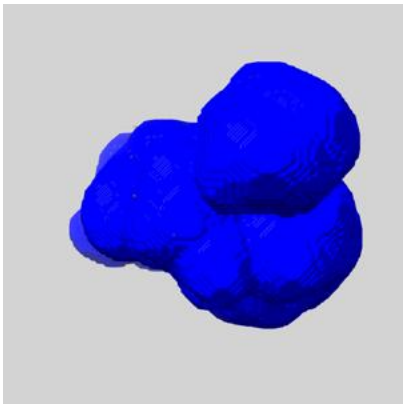
6.5.1 emd_32068_msk_1.map (i)



X



Y

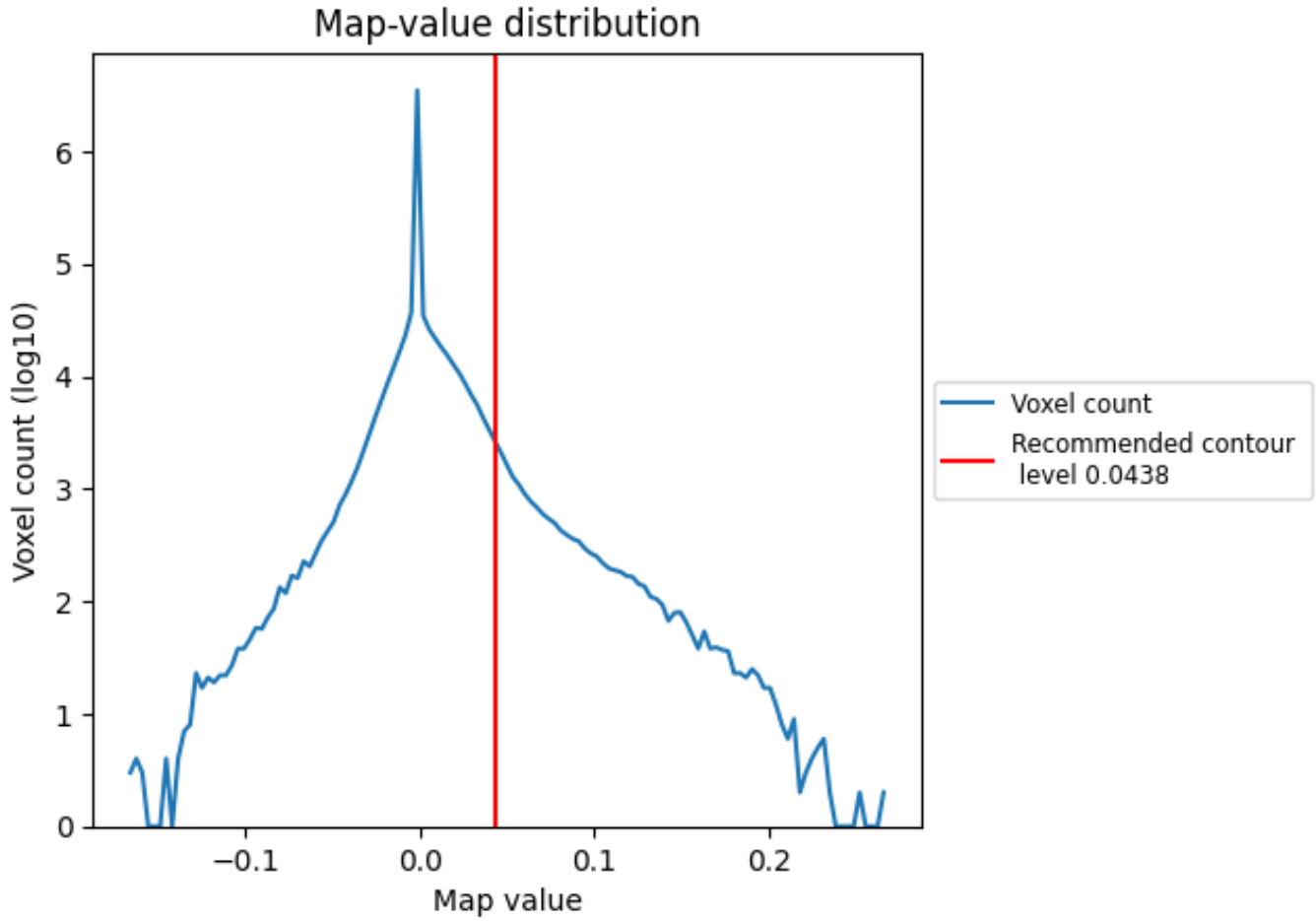


Z

7 Map analysis

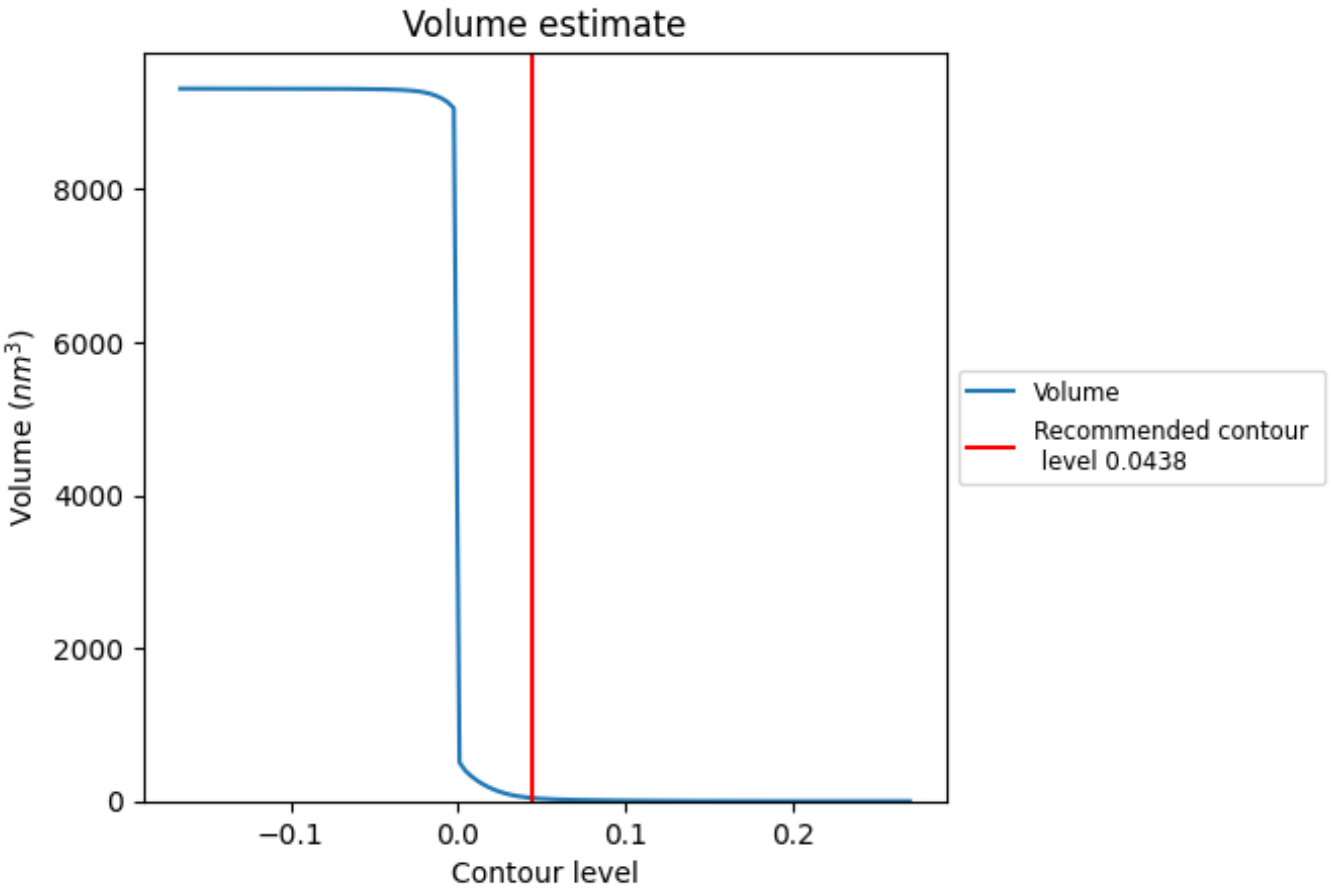
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

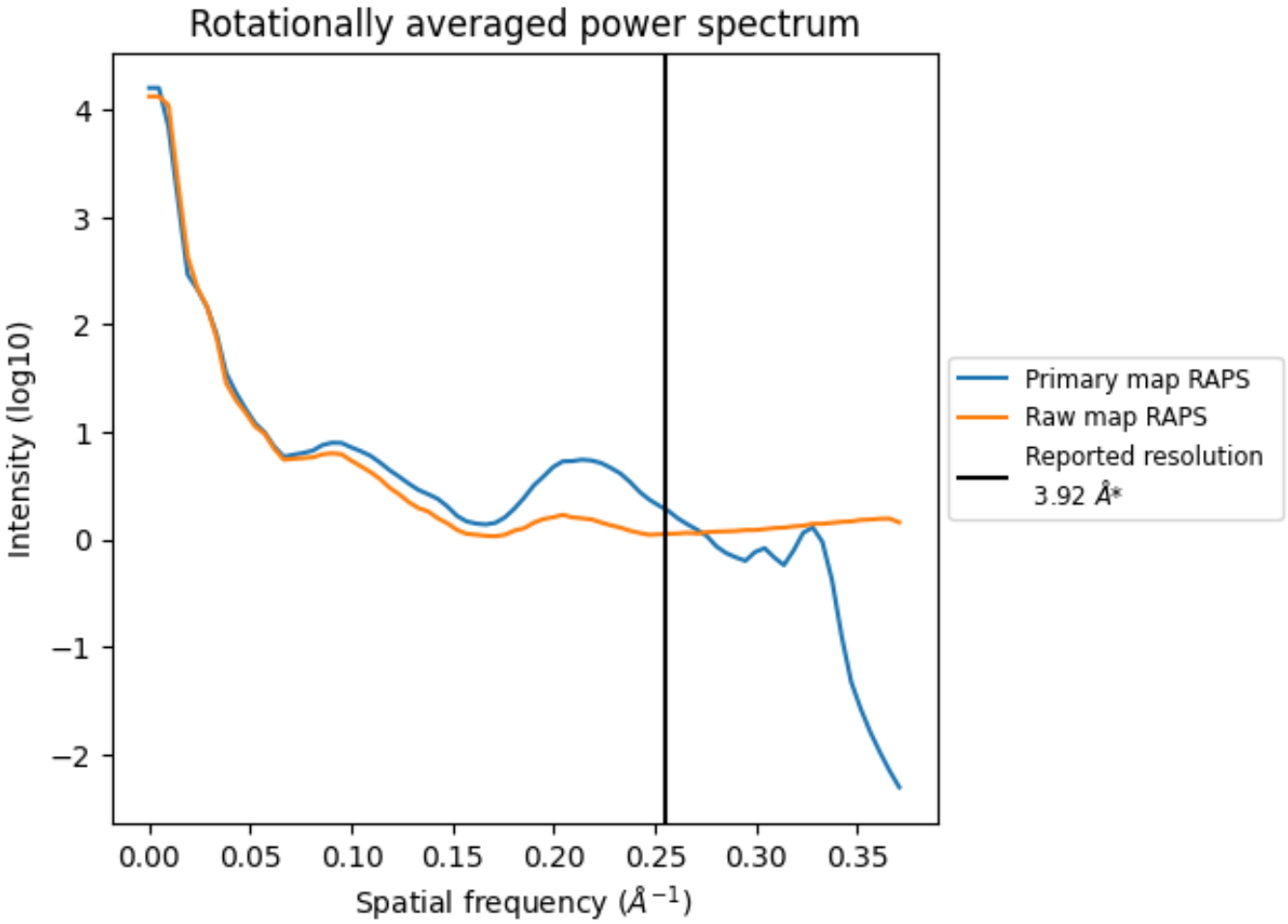
7.2 Volume estimate



The volume at the recommended contour level is 42 nm^3; this corresponds to an approximate mass of 38 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)

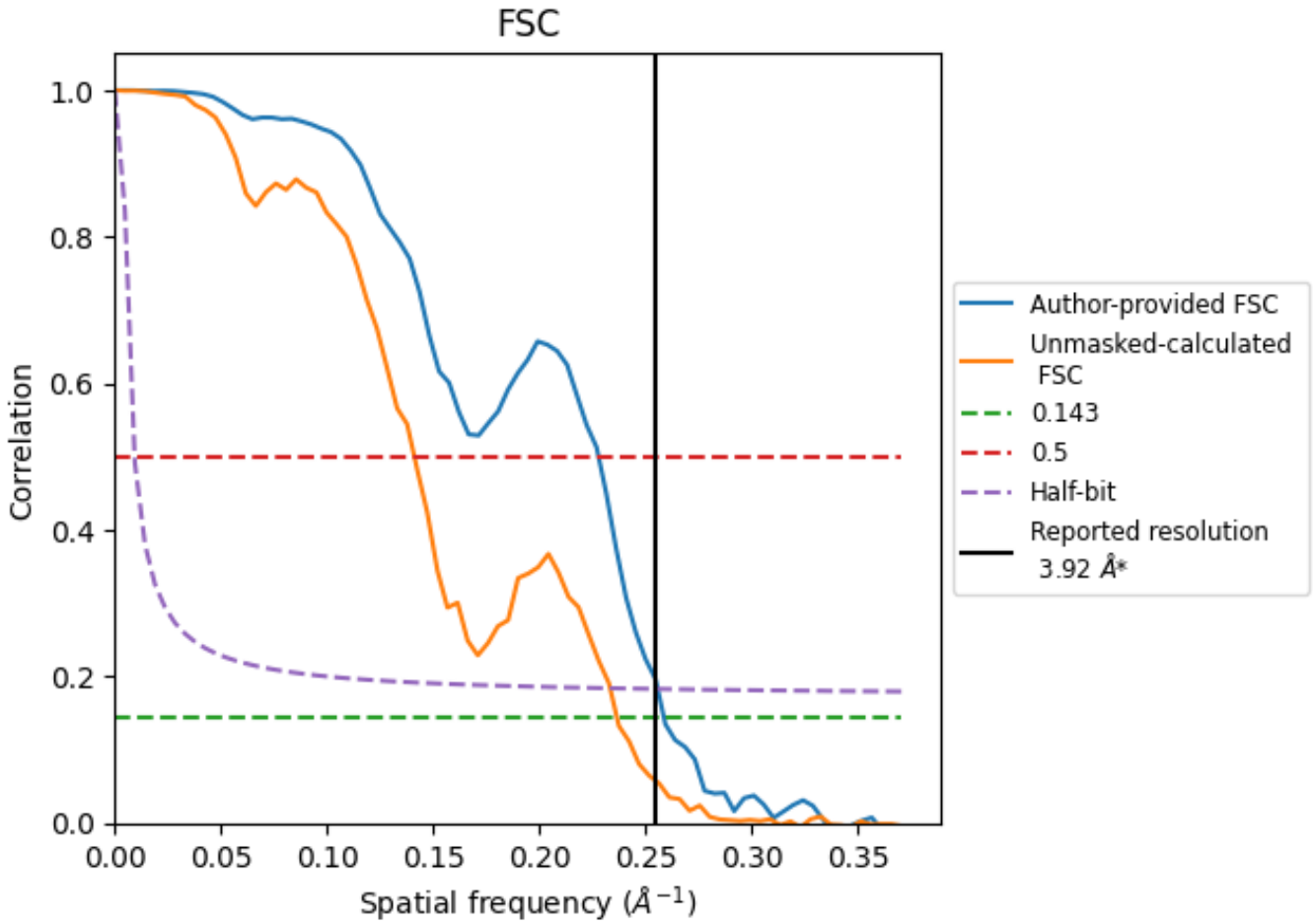


*Reported resolution corresponds to spatial frequency of 0.255 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.255 Å^{-1}

8.2 Resolution estimates (i)

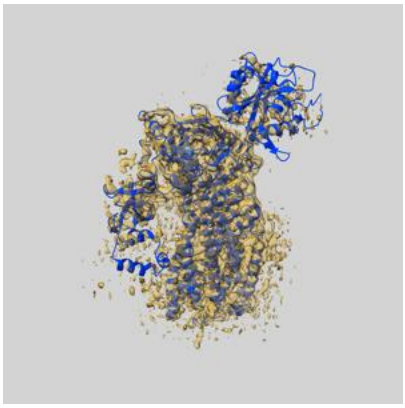
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.92	-	-
Author-provided FSC curve	3.86	4.39	3.91
Unmasked-calculated*	4.22	7.08	4.28

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

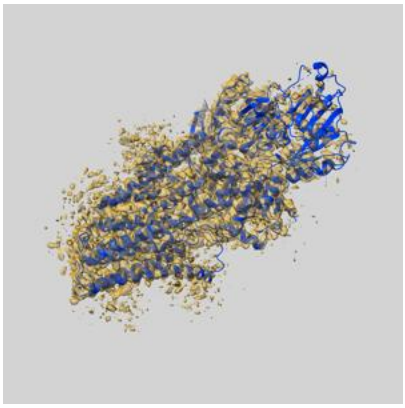
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32068 and PDB model 7VPK. Per-residue inclusion information can be found in section 3 on page 5.

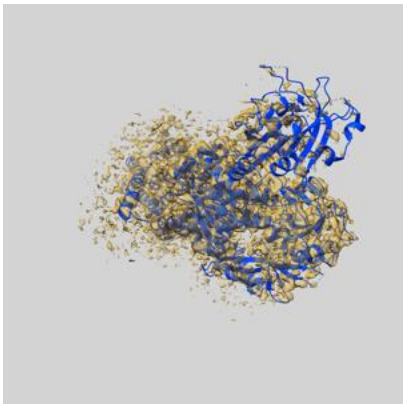
9.1 Map-model overlay



X



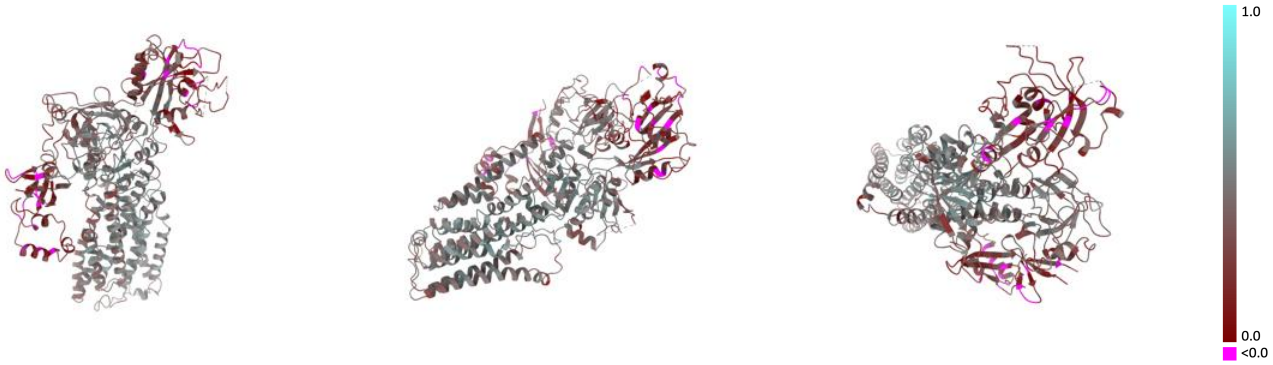
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0438 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.

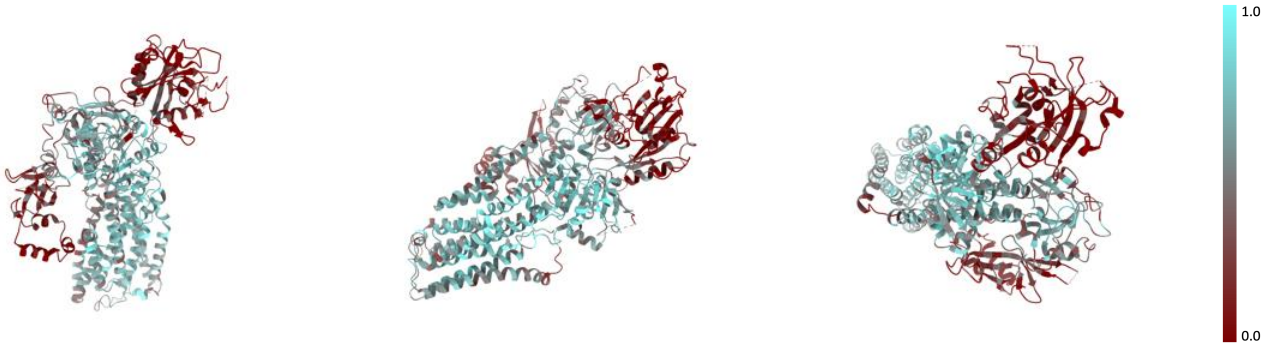
9.2 Q-score mapped to coordinate model (i)



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.

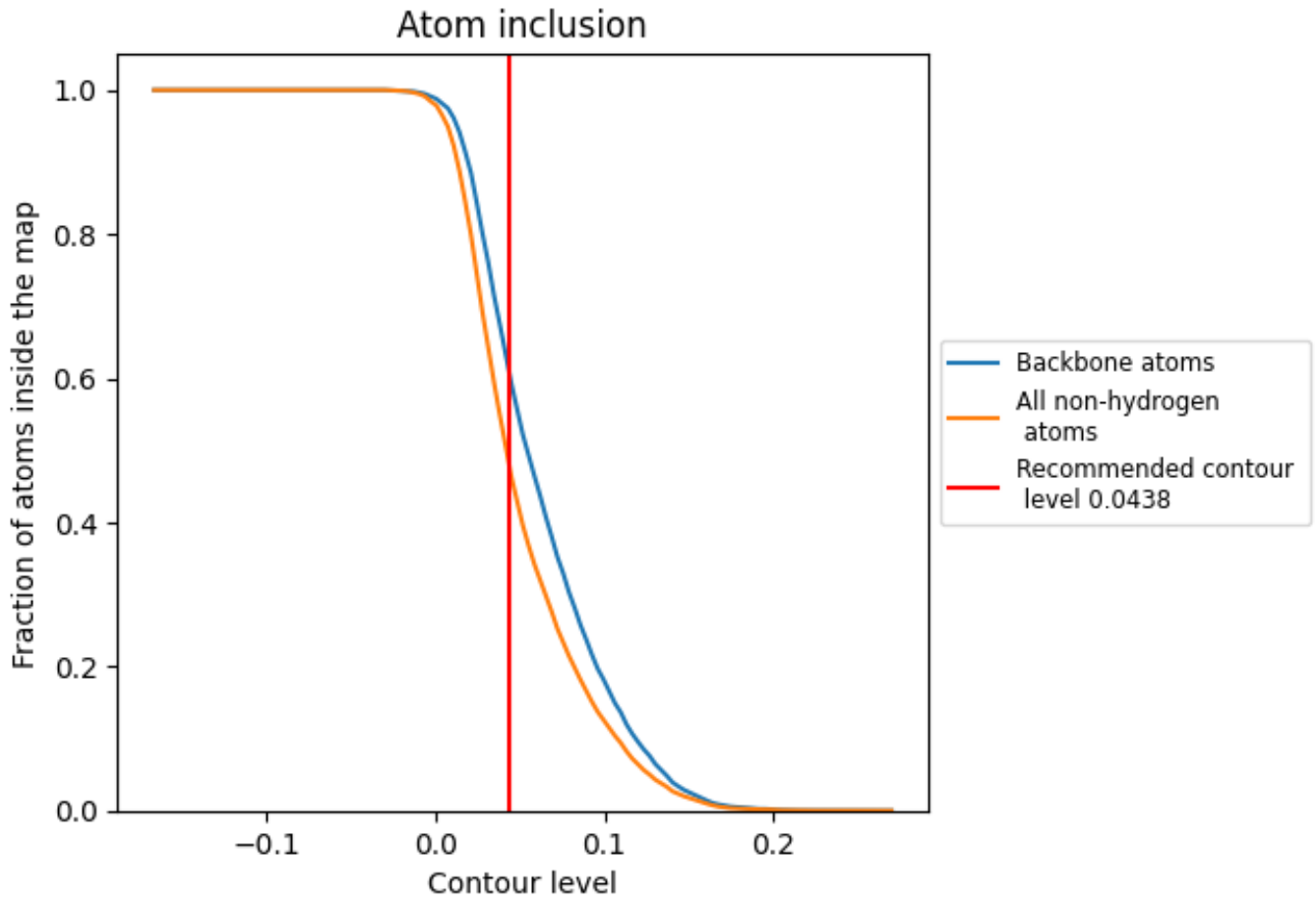
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0438).

9.4 Atom inclusion (i)



At the recommended contour level, 61% of all backbone atoms, 48% 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 (0.0438) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4778	0.3690
A	0.4787	0.3690
B	0.2143	0.2210