Full wwPDB EM Validation Report (i)

Dec 11, 2022 – 12:34 am GMT

PDB ID	:	6RAF
EMDB ID	:	EMD-4773
Title	:	Heterodimeric ABC exporter TmrAB in inward-facing narrow conformation under turnover conditions
Authors	:	Thomas, C.; Januliene, D.; Mehdipour, A.R.; Hofmann, S.; Hummer, G.; Moeller, A.; Tampe, R.
Deposited on	:	2019-04-06
Resolution	:	3.80 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 (i) symbol.

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

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

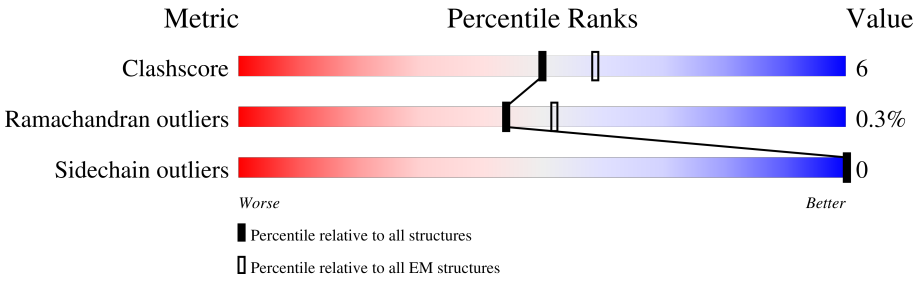
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.80 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	623	15% 82% 12% 6%
2	B	578	9% 87% 12% •
3	C	136	42% 71% 18% 11%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10174 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 Multidrug resistance ABC transporter ATP-binding and permease protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	588	4710	3069	818	815	8	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	601	LYS	-	expression tag	UNP Q72J05
A	602	LEU	-	expression tag	UNP Q72J05
A	603	GLY	-	expression tag	UNP Q72J05
A	604	GLY	-	expression tag	UNP Q72J05
A	605	GLY	-	expression tag	UNP Q72J05
A	606	GLY	-	expression tag	UNP Q72J05
A	607	GLU	-	expression tag	UNP Q72J05
A	608	ASN	-	expression tag	UNP Q72J05
A	609	LEU	-	expression tag	UNP Q72J05
A	610	TYR	-	expression tag	UNP Q72J05
A	611	PHE	-	expression tag	UNP Q72J05
A	612	GLN	-	expression tag	UNP Q72J05
A	613	GLY	-	expression tag	UNP Q72J05
A	614	HIS	-	expression tag	UNP Q72J05
A	615	HIS	-	expression tag	UNP Q72J05
A	616	HIS	-	expression tag	UNP Q72J05
A	617	HIS	-	expression tag	UNP Q72J05
A	618	HIS	-	expression tag	UNP Q72J05
A	619	HIS	-	expression tag	UNP Q72J05
A	620	HIS	-	expression tag	UNP Q72J05
A	621	HIS	-	expression tag	UNP Q72J05
A	622	HIS	-	expression tag	UNP Q72J05
A	623	HIS	-	expression tag	UNP Q72J05

- Molecule 2 is a protein called Multidrug resistance ABC transporter ATP-binding and permease protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	571	4508	2914	806	776	12	0	0

- Molecule 3 is a protein called Anti-vesicular stomatitis virus N VHH.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	121	897	560	159	173	5	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	MET	-	initiating methionine	UNP A0A192B6J5
C	0	ALA	-	expression tag	UNP A0A192B6J5
C	14	PRO	ALA	conflict	UNP A0A192B6J5
C	16	ASP	GLY	conflict	UNP A0A192B6J5
C	19	ARG	THR	conflict	UNP A0A192B6J5
C	23	ALA	VAL	conflict	UNP A0A192B6J5
C	24	VAL	ALA	conflict	UNP A0A192B6J5
C	27	SER	ARG	conflict	UNP A0A192B6J5
C	28	ALA	PRO	conflict	UNP A0A192B6J5
C	29	LEU	PHE	conflict	UNP A0A192B6J5
C	30	ASP	ARG	conflict	UNP A0A192B6J5
C	31	TYR	ASN	conflict	UNP A0A192B6J5
C	32	ASN	TYR	conflict	UNP A0A192B6J5
C	33	ALA	ARG	conflict	UNP A0A192B6J5
C	34	ILE	LEU	conflict	UNP A0A192B6J5
C	47	GLY	PHE	conflict	UNP A0A192B6J5
C	50	CYS	ALA	conflict	UNP A0A192B6J5
C	52	SER	ASN	conflict	UNP A0A192B6J5
C	53	LYS	TRP	conflict	UNP A0A192B6J5
C	54	ILE	GLY	conflict	UNP A0A192B6J5
C	55	THR	GLY	conflict	UNP A0A192B6J5
C	56	GLY	VAL	conflict	UNP A0A192B6J5
C	57	ASN	ILE	conflict	UNP A0A192B6J5
C	59	ALA	ASN	conflict	UNP A0A192B6J5
C	74	ASN	ASP	conflict	UNP A0A192B6J5
C	80	HIS	TYR	conflict	UNP A0A192B6J5
C	90	ASP	GLU	conflict	UNP A0A192B6J5
C	98	THR	ALA	conflict	UNP A0A192B6J5
C	99	VAL	PHE	conflict	UNP A0A192B6J5
C	100	THR	ASP	conflict	UNP A0A192B6J5
C	101	ALA	SER	conflict	UNP A0A192B6J5

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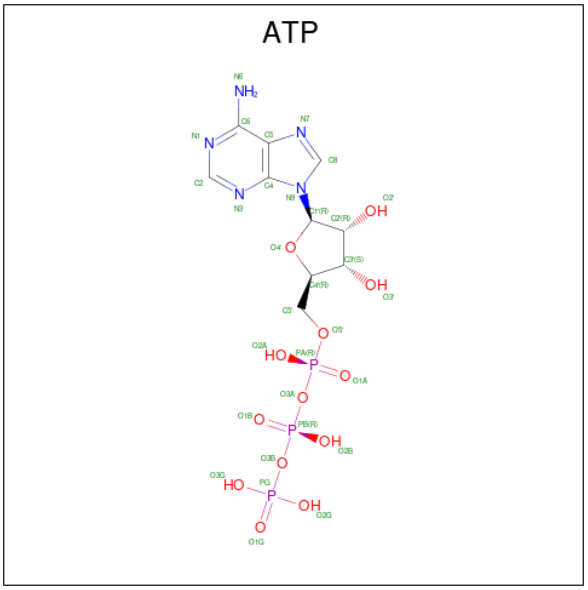
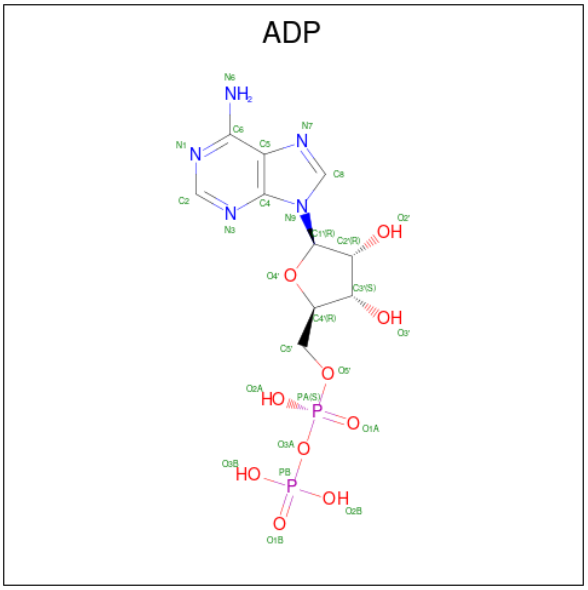
Chain	Residue	Modelled	Actual	Comment	Reference
C	102	VAL	THR	conflict	UNP A0A192B6J5
C	103	LEU	GLY	conflict	UNP A0A192B6J5
C	104	LEU	SER	conflict	UNP A0A192B6J5
C	106	GLY	ILE	conflict	UNP A0A192B6J5
C	107	ARG	VAL	conflict	UNP A0A192B6J5
C	108	CYS	ARG	conflict	UNP A0A192B6J5
C	109	VAL	ASP	conflict	UNP A0A192B6J5
C	110	PRO	ASN	conflict	UNP A0A192B6J5
C	111	GLY	TYR	conflict	UNP A0A192B6J5
C	112	LYS	GLU	conflict	UNP A0A192B6J5
C	119	PRO	GLN	conflict	UNP A0A192B6J5
C	125	HIS	-	expression tag	UNP A0A192B6J5
C	126	HIS	-	expression tag	UNP A0A192B6J5
C	127	HIS	-	expression tag	UNP A0A192B6J5
C	128	HIS	-	expression tag	UNP A0A192B6J5
C	129	HIS	-	expression tag	UNP A0A192B6J5
C	130	HIS	-	expression tag	UNP A0A192B6J5
C	131	GLU	-	expression tag	UNP A0A192B6J5
C	132	PRO	-	expression tag	UNP A0A192B6J5
C	133	GLU	-	expression tag	UNP A0A192B6J5
C	134	ALA	-	expression tag	UNP A0A192B6J5

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	A	1	31	10	5	13	3	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
5	B	1	27	10	5	10	2	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

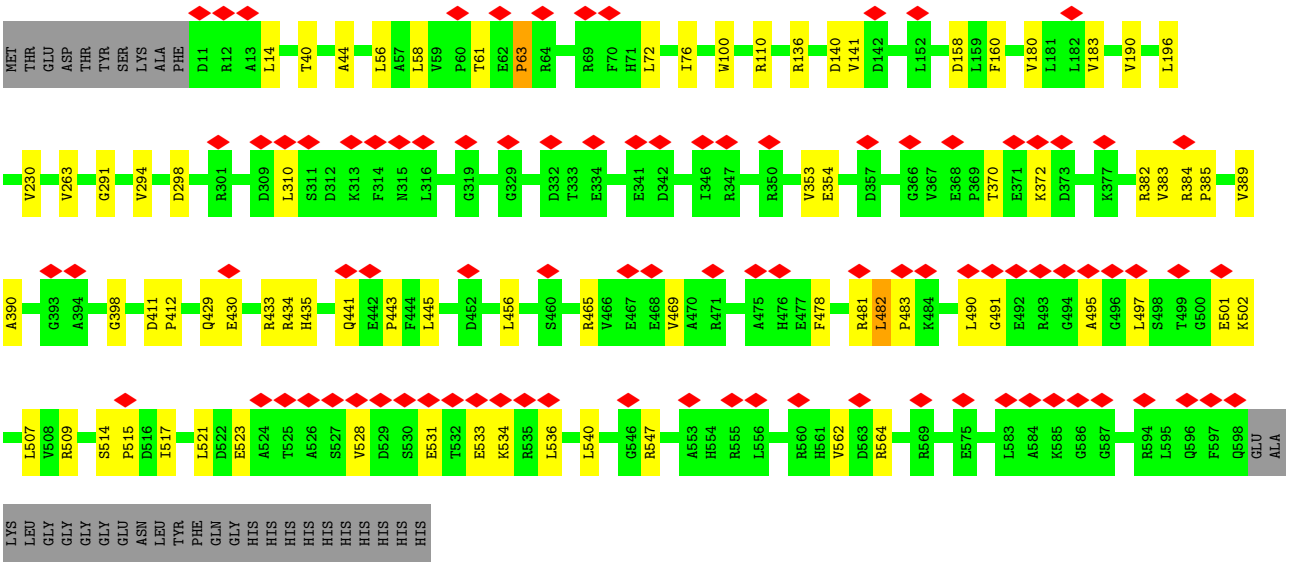
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	B	1	1	1	0

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.

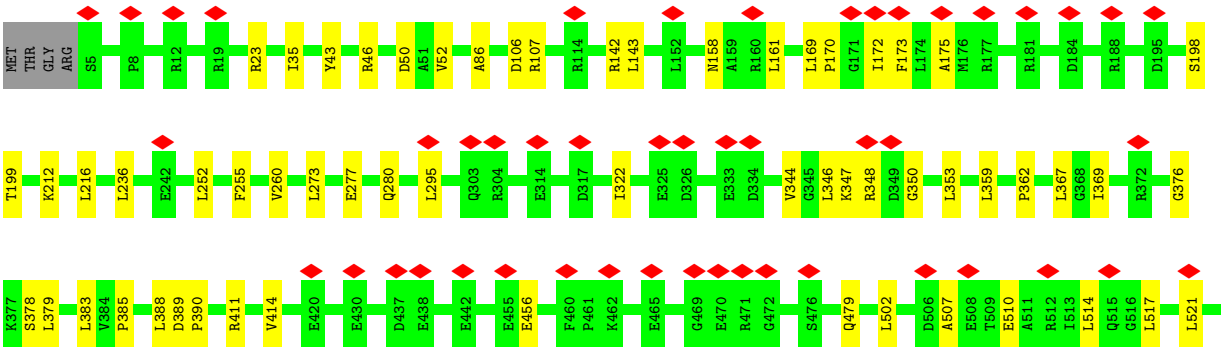
• Molecule 1: Multidrug resistance ABC transporter ATP-binding and permease protein

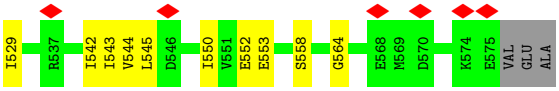
Chain A:



• Molecule 2: Multidrug resistance ABC transporter ATP-binding and permease protein

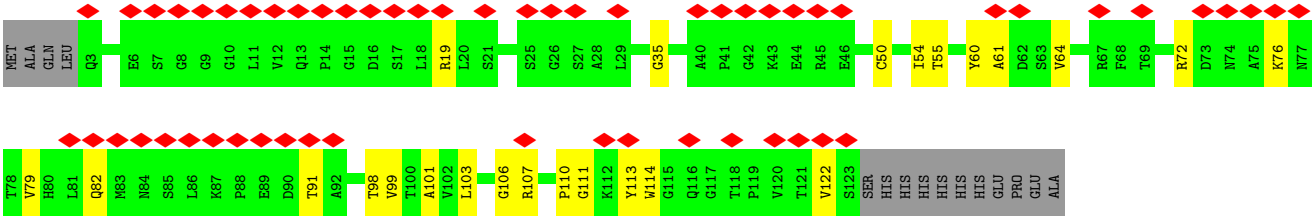
Chain B:





- Molecule 3: Anti-vesicular stomatitis virus N VHH

Chain C:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	133527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction was performed within 3D reconstruction in RELION-3	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	3.476	Depositor
Minimum map value	-2.426	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.57	Depositor
Map size (Å)	275.712, 275.712, 275.712	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.077, 1.077, 1.077	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: ATP, MG, ADP

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	0.40	0/4815	0.81	6/6531 (0.1%)
2	B	0.39	1/4597 (0.0%)	0.76	3/6224 (0.0%)
3	C	0.38	0/914	0.72	1/1242 (0.1%)
All	All	0.40	1/10326 (0.0%)	0.78	10/13997 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	170	PRO	N-CD	5.89	1.56	1.47

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	14	LEU	CA-CB-CG	7.93	133.54	115.30
2	B	521	LEU	CA-CB-CG	6.22	129.60	115.30
1	A	58	LEU	CA-CB-CG	6.18	129.52	115.30
2	B	50	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	507	LEU	CA-CB-CG	6.03	129.16	115.30
1	A	536	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	298	ASP	CB-CG-OD1	5.23	123.01	118.30
2	B	52	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	A	196	LEU	CB-CG-CD1	5.05	119.58	111.00
3	C	113	TYR	CB-CA-C	-5.04	100.33	110.40

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	4710	0	4837	54	0
2	B	4508	0	4673	60	0
3	C	897	0	887	21	0
4	A	31	0	12	1	0
5	B	27	0	12	4	0
6	B	1	0	0	0	0
All	All	10174	0	10421	123	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 6.

All (123) 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:482:LEU:HB3	1:A:483:PRO:HD2	1.17	1.13
1:A:482:LEU:HB3	1:A:483:PRO:CD	1.90	1.01
1:A:56:LEU:HB3	1:A:72:LEU:HD13	1.44	1.00
1:A:56:LEU:HD13	1:A:72:LEU:HD22	1.60	0.83
3:C:50:CYS:HB3	3:C:99:VAL:HG21	1.59	0.83
1:A:482:LEU:CB	1:A:483:PRO:HD2	2.07	0.82
2:B:543:ILE:HG23	2:B:550:ILE:HG23	1.63	0.80
1:A:514:SER:OG	1:A:515:PRO:HD2	1.82	0.79
3:C:98:THR:O	3:C:111:GLY:HA3	1.83	0.78
3:C:60:TYR:O	3:C:106:GLY:HA2	1.84	0.77
2:B:389:ASP:HB2	2:B:390:PRO:HD2	1.67	0.76
2:B:46:ARG:HD2	2:B:280:GLN:NE2	2.05	0.70
1:A:435:HIS:O	1:A:517:ILE:HG23	1.93	0.69
3:C:110:PRO:HB3	3:C:114:TRP:CZ2	2.29	0.68
2:B:46:ARG:HE	2:B:277:GLU:HG2	1.60	0.67
3:C:110:PRO:HB3	3:C:114:TRP:HZ2	1.59	0.66
1:A:491:GLY:H	1:A:495:ALA:HB2	1.60	0.65
3:C:50:CYS:CB	3:C:99:VAL:HG21	2.25	0.64
2:B:544:VAL:HG22	2:B:552:GLU:HB2	1.81	0.63
2:B:552:GLU:OE2	2:B:564:GLY:HA3	1.99	0.63
1:A:398:GLY:HA2	4:A:701:ATP:O1A	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ASP:HB3	1:A:412:PRO:HD2	1.80	0.63
1:A:389:VAL:HA	1:A:564:ARG:O	1.99	0.62
2:B:376:GLY:HA2	5:B:601:ADP:H4'	1.81	0.62
1:A:61:THR:O	1:A:63:PRO:HD3	2.00	0.62
3:C:91:THR:HG22	3:C:122:VAL:H	1.65	0.62
1:A:72:LEU:O	1:A:76:ILE:HG12	2.01	0.61
1:A:430:GLU:O	1:A:434:ARG:HG3	2.01	0.60
2:B:161:LEU:HD11	2:B:260:VAL:HA	1.85	0.58
1:A:429:GLN:HB3	1:A:433:ARG:HH12	1.68	0.58
1:A:370:THR:HG23	1:A:372:LYS:H	1.69	0.57
2:B:359:LEU:HD13	3:C:55:THR:HG22	1.87	0.57
2:B:107:ARG:HH21	2:B:388:LEU:HD11	1.70	0.56
2:B:514:LEU:HD23	2:B:517:LEU:HD12	1.86	0.56
1:A:158:ASP:HB3	1:A:310:LEU:HD12	1.87	0.56
2:B:543:ILE:HG21	2:B:550:ILE:HD13	1.89	0.55
2:B:378:SER:HB3	5:B:601:ADP:O2A	2.06	0.55
2:B:369:ILE:HB	2:B:529:ILE:HG12	1.89	0.55
2:B:558:SER:HB3	3:C:101:ALA:HB2	1.89	0.55
1:A:465:ARG:HH12	1:A:469:VAL:HB	1.72	0.54
1:A:429:GLN:HB3	1:A:433:ARG:NH1	2.23	0.54
1:A:443:PRO:HG2	1:A:502:LYS:HB3	1.88	0.54
1:A:353:VAL:HB	1:A:383:VAL:CG1	2.38	0.53
2:B:322:ILE:HD12	2:B:411:ARG:HH22	1.73	0.53
2:B:385:PRO:HG3	2:B:414:VAL:HG11	1.90	0.53
2:B:502:LEU:HD22	2:B:510:GLU:HA	1.91	0.53
3:C:19:ARG:NH1	3:C:82:GLN:OE1	2.42	0.52
1:A:456:LEU:HD22	2:B:216:LEU:HD11	1.92	0.52
1:A:478:PHE:HA	1:A:481:ARG:HE	1.73	0.52
2:B:456:GLU:HG2	2:B:479:GLN:HE22	1.75	0.52
2:B:346:LEU:HD23	2:B:379:LEU:HD23	1.91	0.52
2:B:558:SER:CB	3:C:101:ALA:HB2	2.40	0.52
1:A:110:ARG:HE	1:A:141:VAL:HG11	1.74	0.51
1:A:521:LEU:HD13	1:A:540:LEU:HD13	1.91	0.51
2:B:389:ASP:HB2	2:B:390:PRO:CD	2.36	0.51
2:B:542:ILE:O	2:B:553:GLU:HA	2.09	0.51
2:B:106:ASP:HB3	2:B:322:ILE:HG12	1.92	0.51
2:B:353:LEU:HD21	5:B:601:ADP:H1'	1.93	0.51
1:A:190:VAL:HG11	1:A:263:VAL:HG11	1.93	0.50
1:A:389:VAL:HG22	1:A:564:ARG:HB2	1.93	0.50
1:A:456:LEU:HD21	1:A:509:ARG:HD2	1.93	0.50
3:C:61:ALA:HB3	3:C:64:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:353:LEU:CD1	2:B:379:LEU:HD21	2.42	0.49
1:A:517:ILE:H	1:A:547:ARG:NH1	2.11	0.49
1:A:514:SER:H	1:A:517:ILE:HD11	1.78	0.49
2:B:367:LEU:HD11	2:B:543:ILE:HD12	1.94	0.49
3:C:103:LEU:HB2	3:C:107:ARG:HB3	1.95	0.49
2:B:545:LEU:HD21	2:B:550:ILE:HG12	1.96	0.48
1:A:40:THR:HG21	1:A:160:PHE:HB3	1.95	0.47
2:B:172:ILE:HD13	2:B:252:LEU:HD11	1.94	0.47
2:B:552:GLU:HG2	3:C:103:LEU:HG	1.96	0.47
1:A:531:GLU:HA	1:A:534:LYS:HE3	1.95	0.47
2:B:543:ILE:HG12	2:B:550:ILE:HG21	1.96	0.47
2:B:359:LEU:CD1	3:C:54:ILE:HG22	2.45	0.46
1:A:441:GLN:NE2	1:A:523:GLU:O	2.46	0.46
2:B:347:LYS:HE3	2:B:350:GLY:HA2	1.96	0.46
2:B:550:ILE:HD12	3:C:55:THR:CG2	2.46	0.46
1:A:456:LEU:HB3	2:B:216:LEU:HD21	1.98	0.45
1:A:180:VAL:O	1:A:183:VAL:HG22	2.16	0.45
1:A:443:PRO:CG	1:A:502:LYS:HB3	2.46	0.45
1:A:528:VAL:HG23	1:A:533:GLU:HB3	1.98	0.45
1:A:514:SER:O	1:A:517:ILE:CD1	2.65	0.45
2:B:172:ILE:HD13	2:B:252:LEU:CD1	2.47	0.45
2:B:172:ILE:HA	2:B:175:ALA:HB3	1.99	0.45
2:B:353:LEU:HD12	2:B:379:LEU:HD21	1.99	0.45
1:A:136:ARG:O	1:A:140:ASP:HB3	2.17	0.44
2:B:143:LEU:HD11	2:B:295:LEU:HB2	1.99	0.44
1:A:384:ARG:HB3	1:A:385:PRO:CD	2.47	0.44
2:B:169:LEU:O	2:B:173:PHE:N	2.50	0.44
1:A:291:GLY:HA2	1:A:294:VAL:HG22	2.00	0.44
2:B:353:LEU:HD22	5:B:601:ADP:O3'	2.17	0.44
1:A:56:LEU:HB3	1:A:72:LEU:CD1	2.32	0.43
2:B:507:ALA:HA	2:B:510:GLU:HG2	2.00	0.43
2:B:344:VAL:HG23	2:B:390:PRO:HB3	2.00	0.43
2:B:383:LEU:HD23	2:B:388:LEU:O	2.19	0.43
2:B:544:VAL:CG2	2:B:552:GLU:HB2	2.49	0.43
1:A:56:LEU:CB	1:A:72:LEU:HD13	2.31	0.43
1:A:354:GLU:CB	1:A:382:ARG:HG2	2.49	0.42
1:A:383:VAL:HG13	1:A:383:VAL:O	2.19	0.42
2:B:23:ARG:HD2	2:B:86:ALA:HB2	2.01	0.42
1:A:100:TRP:HD1	2:B:236:LEU:HD21	1.85	0.42
3:C:72:ARG:HB3	3:C:79:VAL:HG23	2.01	0.42
1:A:384:ARG:HB3	1:A:385:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:LEU:HD22	1:A:501:GLU:HB3	2.02	0.42
1:A:514:SER:O	1:A:517:ILE:HD11	2.20	0.41
1:A:40:THR:O	1:A:44:ALA:N	2.51	0.41
2:B:35:ILE:HD11	2:B:142:ARG:HG3	2.02	0.41
1:A:353:VAL:HB	1:A:383:VAL:HG12	2.01	0.41
2:B:389:ASP:N	2:B:389:ASP:OD1	2.52	0.41
2:B:543:ILE:CG2	2:B:550:ILE:HD13	2.50	0.41
2:B:543:ILE:HD13	2:B:550:ILE:HD13	2.03	0.41
2:B:550:ILE:HD12	3:C:55:THR:HG21	2.02	0.41
2:B:252:LEU:O	2:B:255:PHE:N	2.53	0.41
2:B:346:LEU:HD21	2:B:348:ARG:HE	1.86	0.41
3:C:76:LYS:HE2	3:C:76:LYS:HB2	1.77	0.41
1:A:433:ARG:HD3	2:B:212:LYS:O	2.21	0.41
2:B:158:ASN:ND2	2:B:273:LEU:HD21	2.36	0.40
1:A:390:ALA:HB2	1:A:562:VAL:HG21	2.03	0.40
2:B:198:SER:OG	2:B:199:THR:N	2.54	0.40
2:B:43:TYR:O	2:B:46:ARG:HB3	2.21	0.40
3:C:35:GLY:CA	3:C:50:CYS:HA	2.51	0.40
2:B:558:SER:HB3	3:C:101:ALA:CB	2.50	0.40
1:A:445:LEU:HB3	1:A:490:LEU:HD21	2.04	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	586/623 (94%)	563 (96%)	20 (3%)	3 (0%)	29	66
2	B	569/578 (98%)	547 (96%)	21 (4%)	1 (0%)	47	79
3	C	119/136 (88%)	116 (98%)	3 (2%)	0	100	100
All	All	1274/1337 (95%)	1226 (96%)	44 (4%)	4 (0%)	44	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
2	B	362	PRO
1	A	482	LEU
1	A	230	VAL

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	493/521 (95%)	493 (100%)	0	100	100
2	B	459/464 (99%)	459 (100%)	0	100	100
3	C	96/109 (88%)	96 (100%)	0	100	100
All	All	1048/1094 (96%)	1048 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	280	GLN
2	B	531	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)

There are no monosaccharides in this entry.

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	ADP	B	601	6	24,29,29	0.82	0	29,45,45	1.47	3 (10%)
4	ATP	A	701	-	26,33,33	0.96	1 (3%)	31,52,52	1.77	5 (16%)

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	ADP	B	601	6	-	2/12/32/32	0/3/3/3
4	ATP	A	701	-	-	0/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	ATP	C5-C4	2.38	1.47	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	ADP	PA-O3A-PB	-5.33	114.53	132.83
4	A	701	ATP	PB-O3B-PG	-4.51	117.34	132.83
4	A	701	ATP	PA-O3A-PB	-4.26	118.21	132.83
4	A	701	ATP	C3'-C2'-C1'	3.57	106.35	100.98
4	A	701	ATP	N3-C2-N1	-3.45	123.29	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	ADP	N3-C2-N1	-3.05	123.91	128.68
4	A	701	ATP	C4-C5-N7	-2.43	106.87	109.40
5	B	601	ADP	C5-C6-N6	2.09	123.52	120.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	601	ADP	C5'-O5'-PA-O1A
5	B	601	ADP	O4'-C4'-C5'-O5'

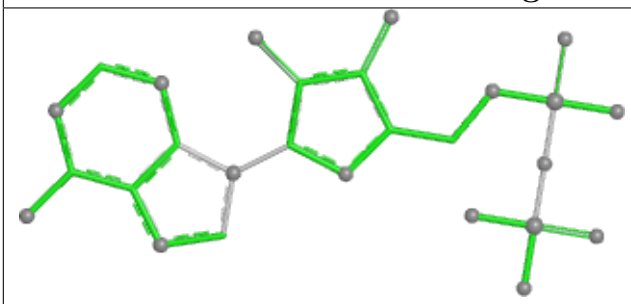
There are no ring outliers.

2 monomers are involved in 5 short contacts:

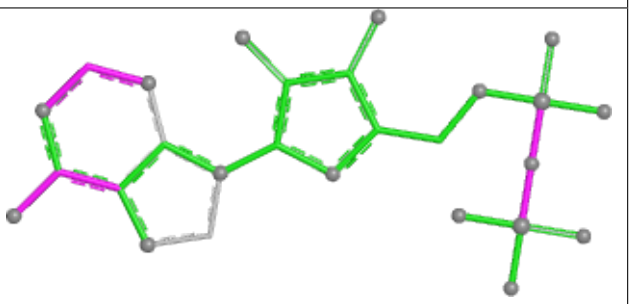
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	601	ADP	4	0
4	A	701	ATP	1	0

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

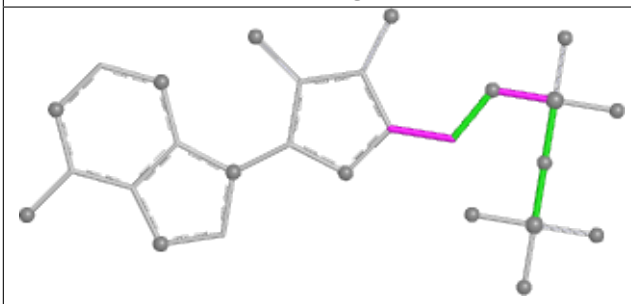
Ligand ADP B 601



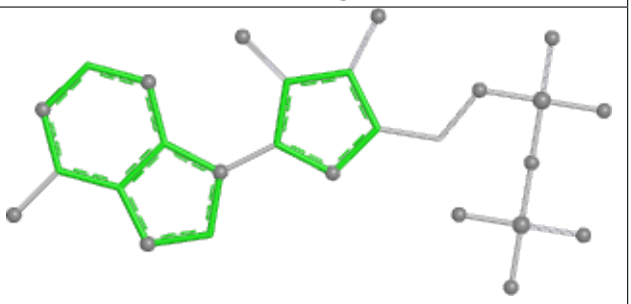
Bond lengths



Bond angles

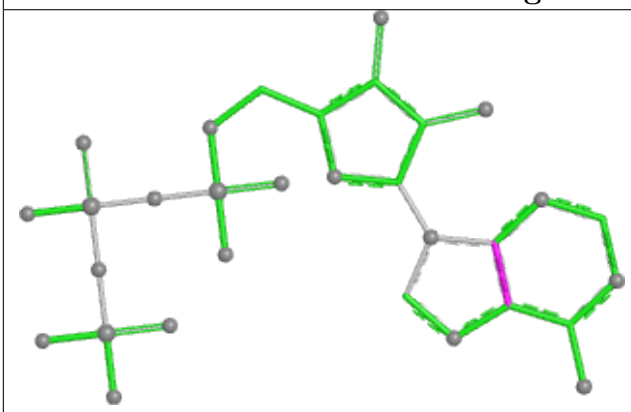


Torsions

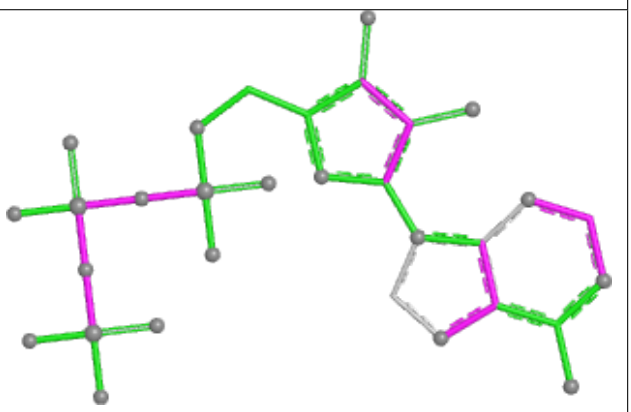


Rings

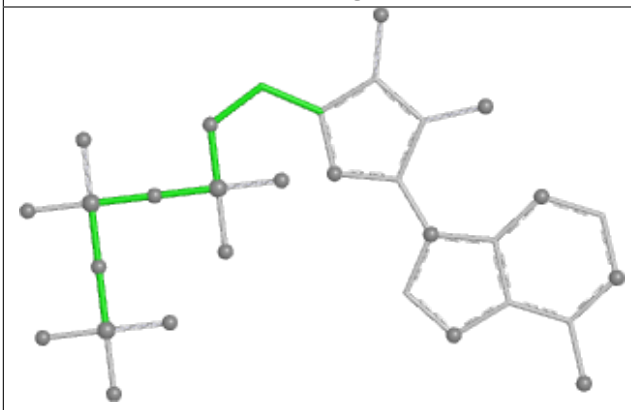
Ligand ATP A 701



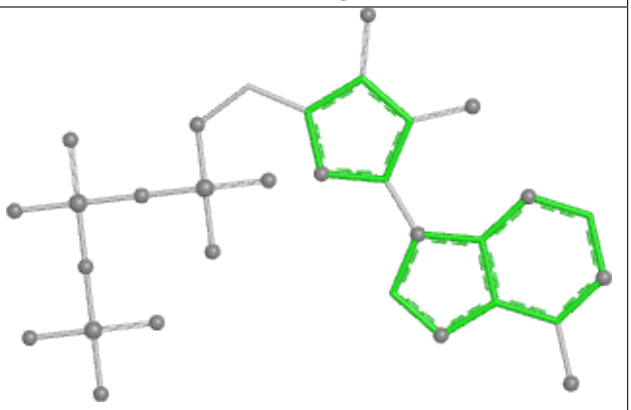
Bond lengths



Bond angles



Torsions



Rings

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)

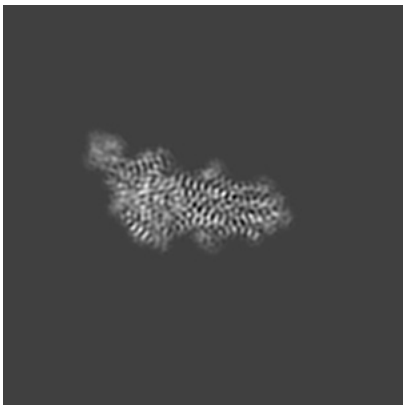
This section contains visualisations of the EMDB entry EMD-4773. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

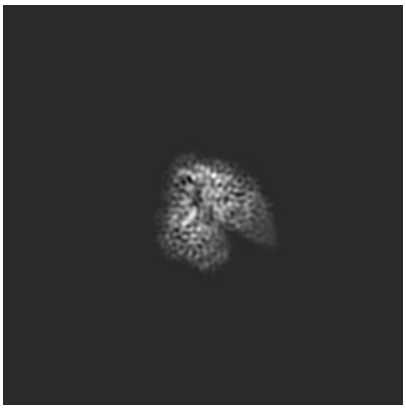
6.1 Orthogonal projections (i)

6.1.1 Primary map

X

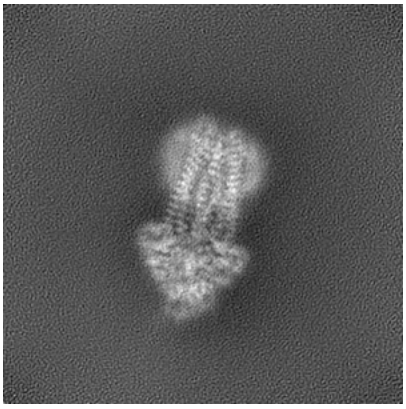


Y

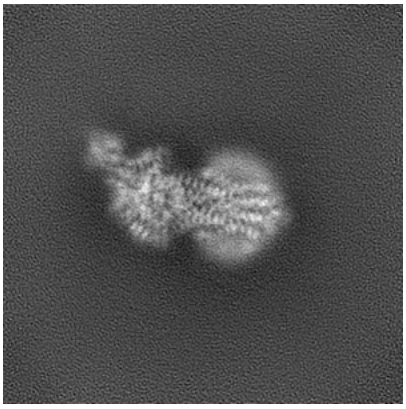


Z

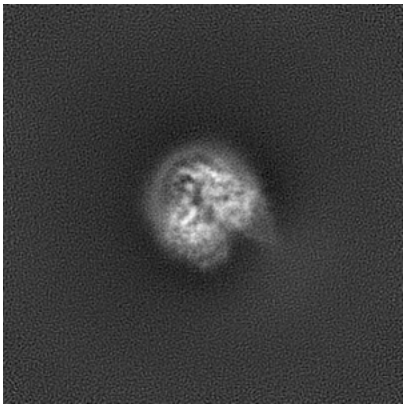
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

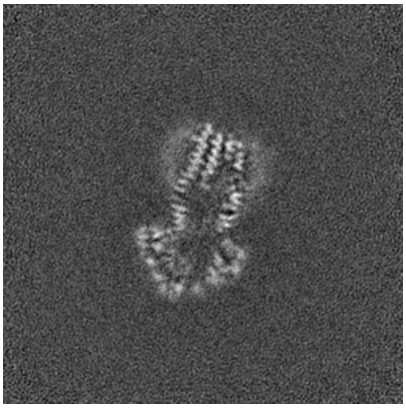
6.2.1 Primary map

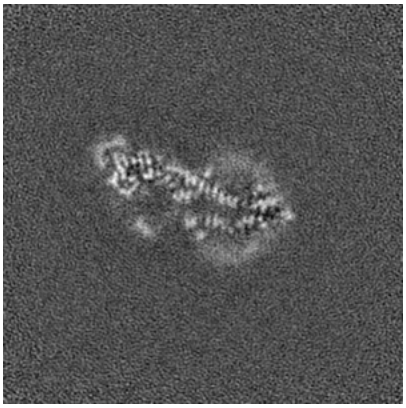
X Index: 128

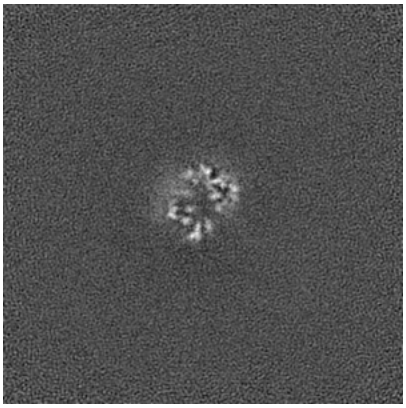
Y Index: 128

Z Index: 128

6.2.2 Raw map


X Index: 128

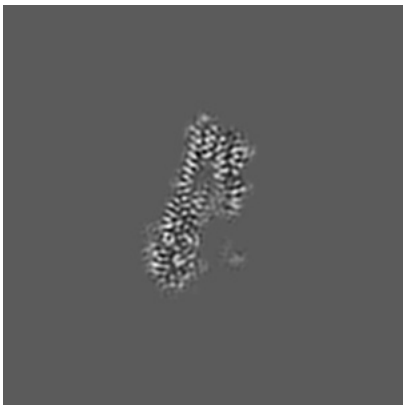

Y Index: 128


Z Index: 128

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

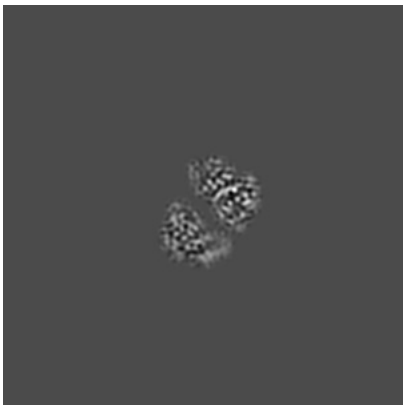
6.3 Largest variance slices (i)

6.3.1 Primary map



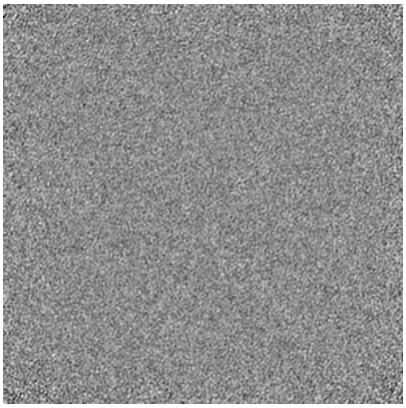
X Index: 119

Y Index: 146

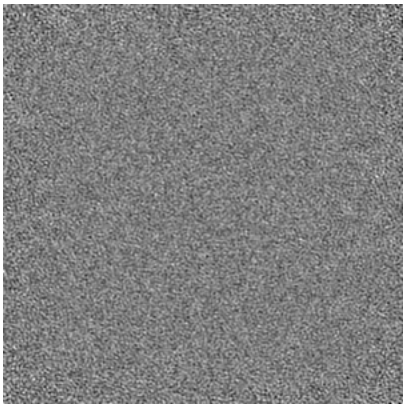


Z Index: 92

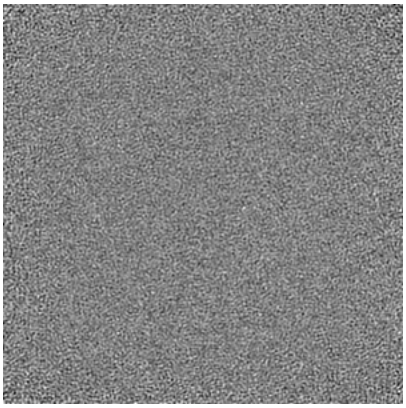
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

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

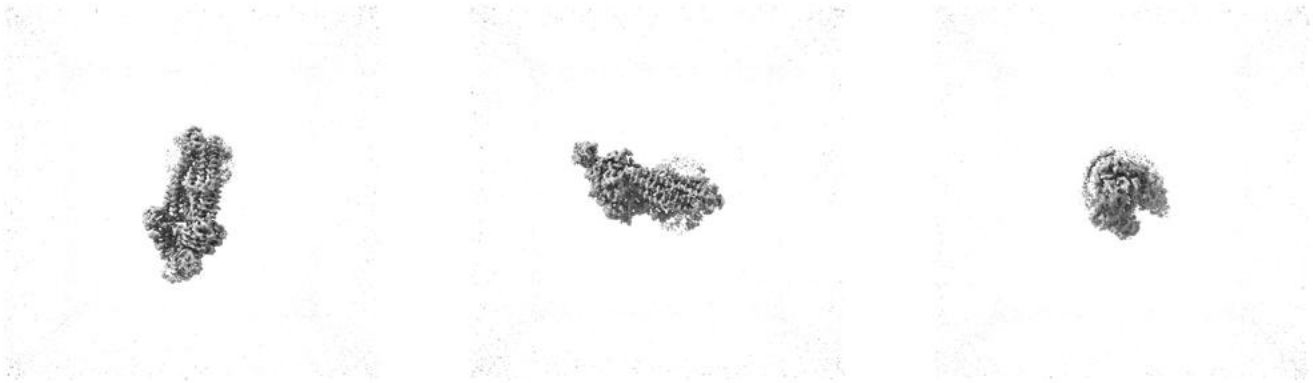
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.57. 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.

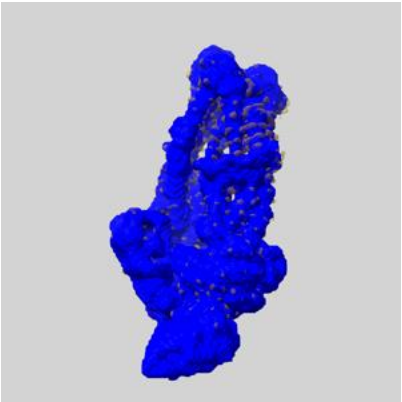
6.5 Mask visualisation (i)

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

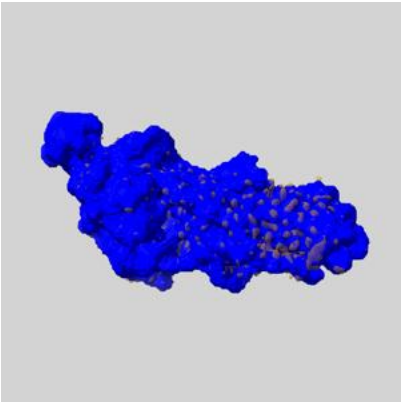
A mask typically either:

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

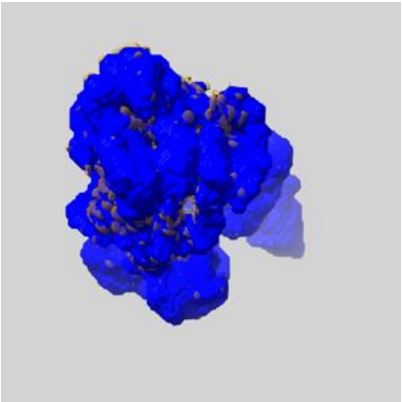
6.5.1 emd_4773_msk_1.map (i)



X



Y

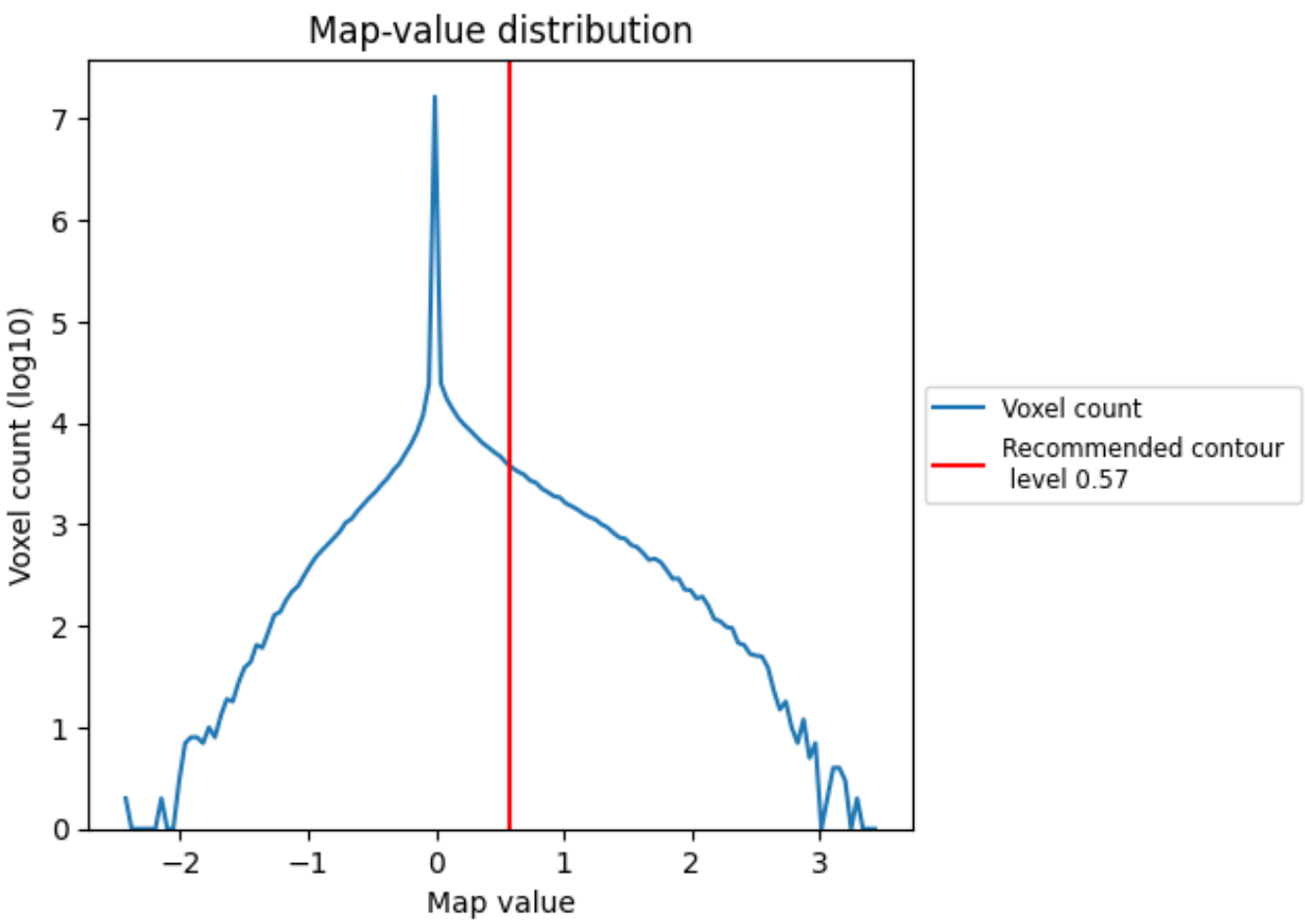


Z

7 Map analysis (i)

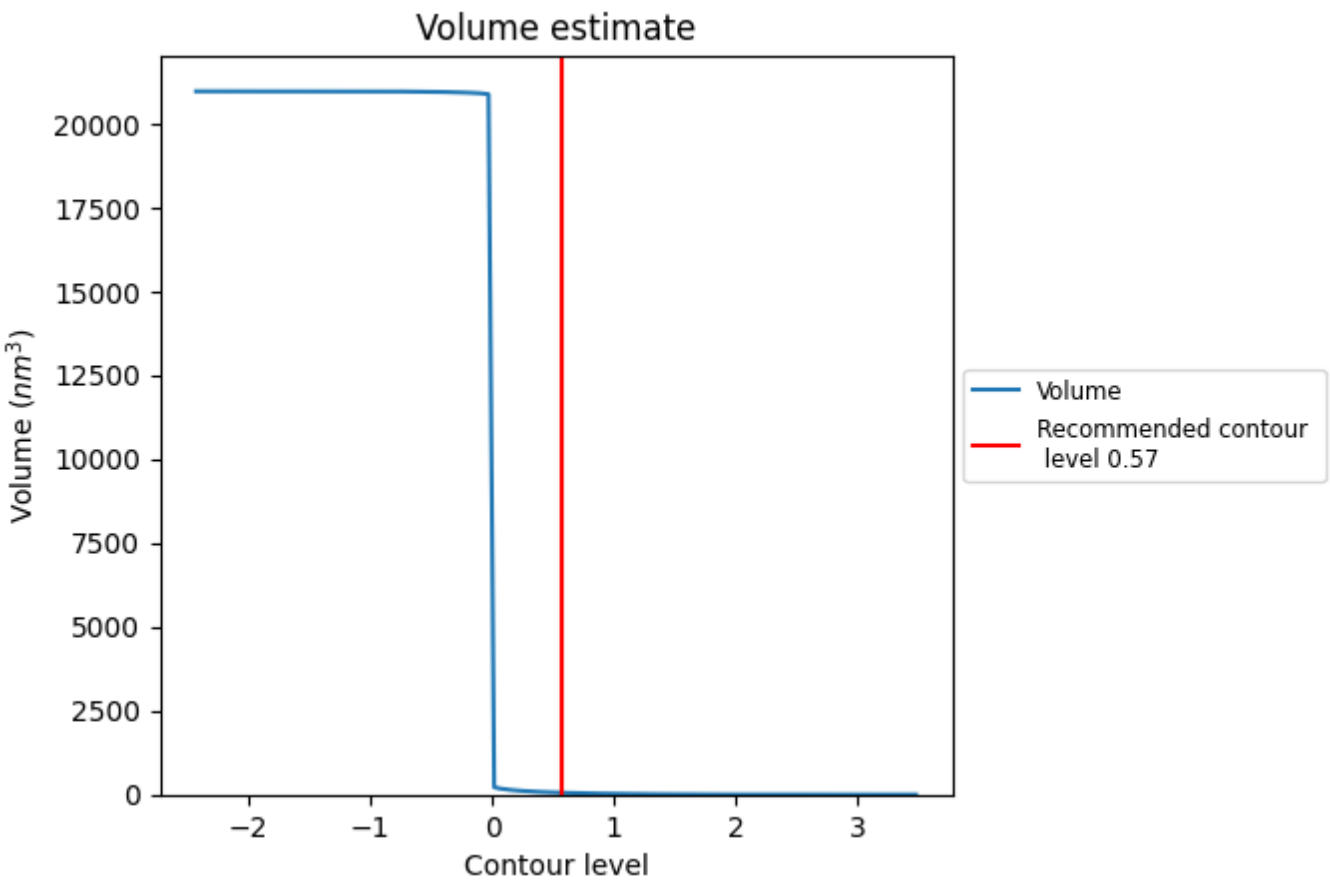
This section contains the results of statistical analysis of the map.

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.

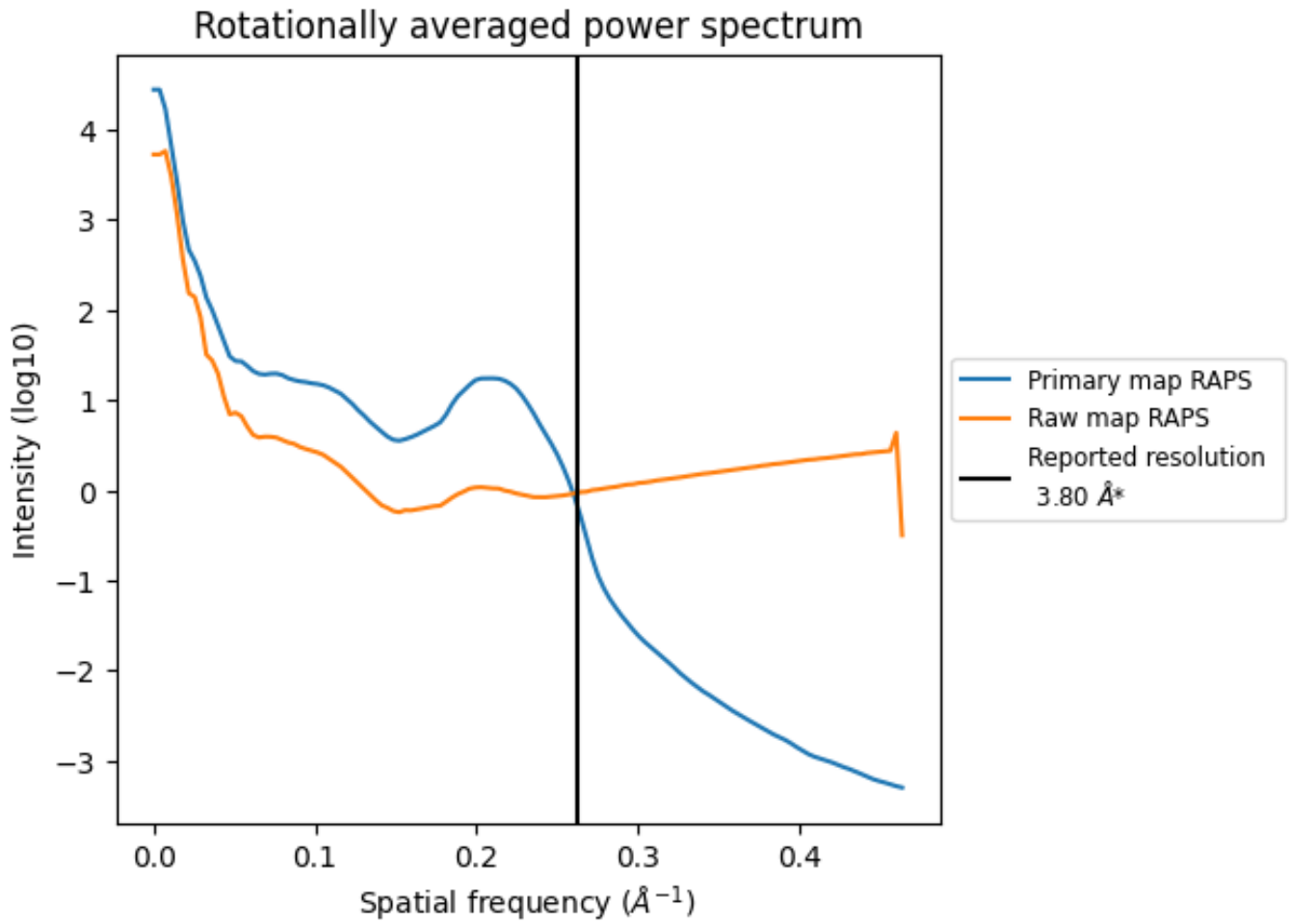
7.2 Volume estimate (i)



The volume at the recommended contour level is 55 nm^3; this corresponds to an approximate mass of 49 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)

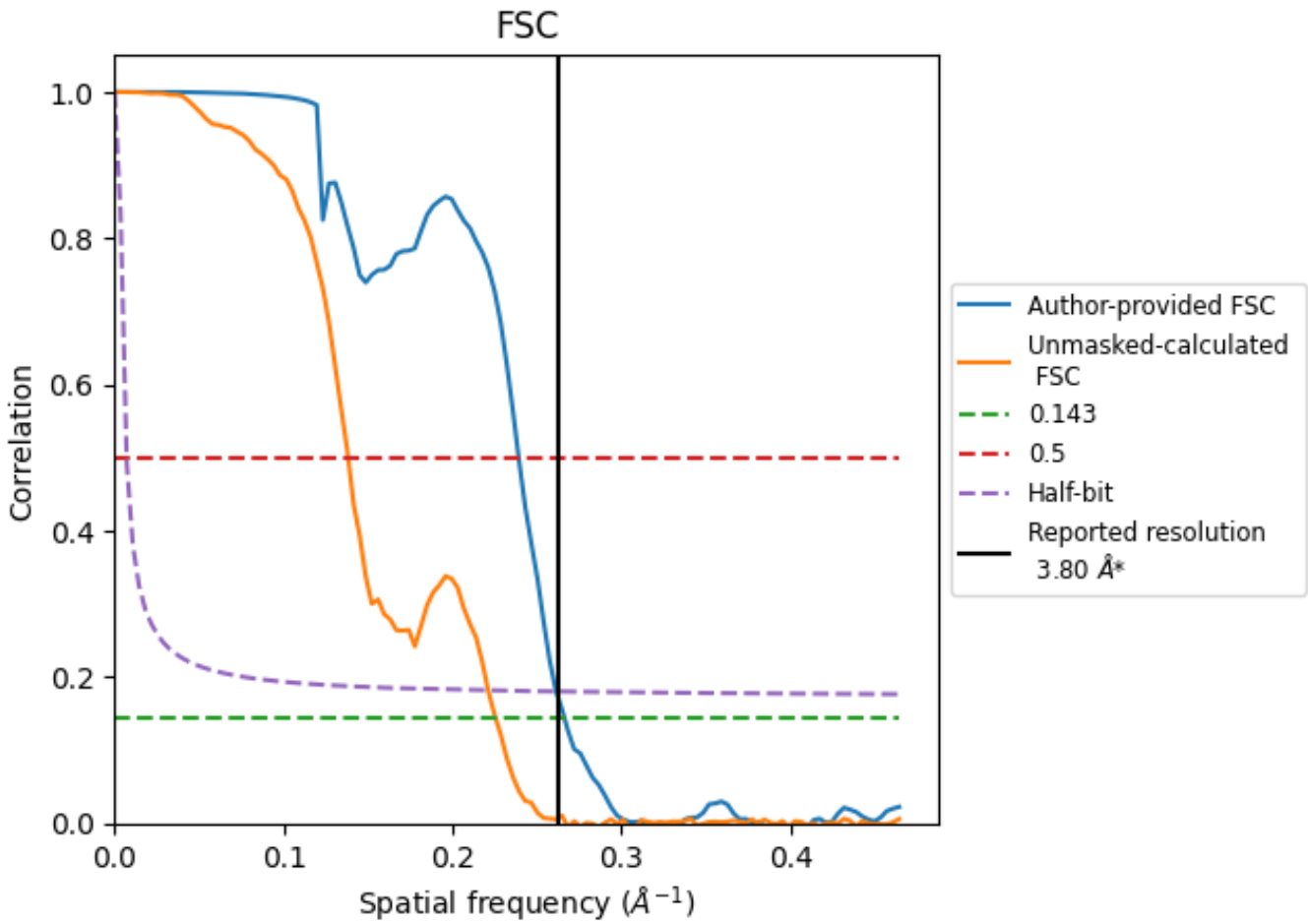


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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 0.263 Å^{-1}

8.2 Resolution estimates (i)

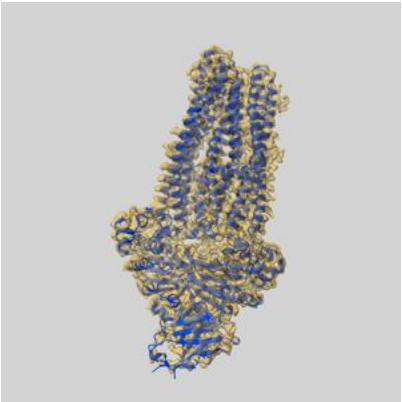
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.18	3.83
Unmasked-calculated*	4.43	7.23	4.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.43 differs from the reported value 3.8 by more than 10 %

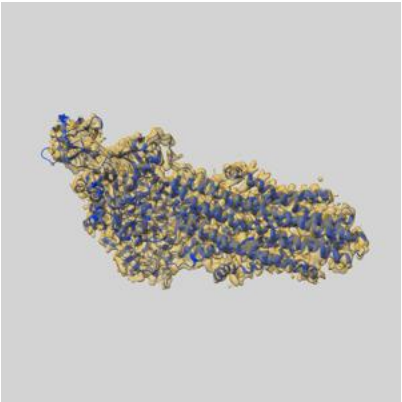
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4773 and PDB model 6RAF. Per-residue inclusion information can be found in section 3 on page 7.

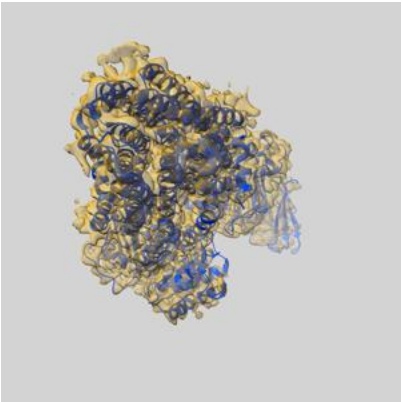
9.1 Map-model overlay (i)



X



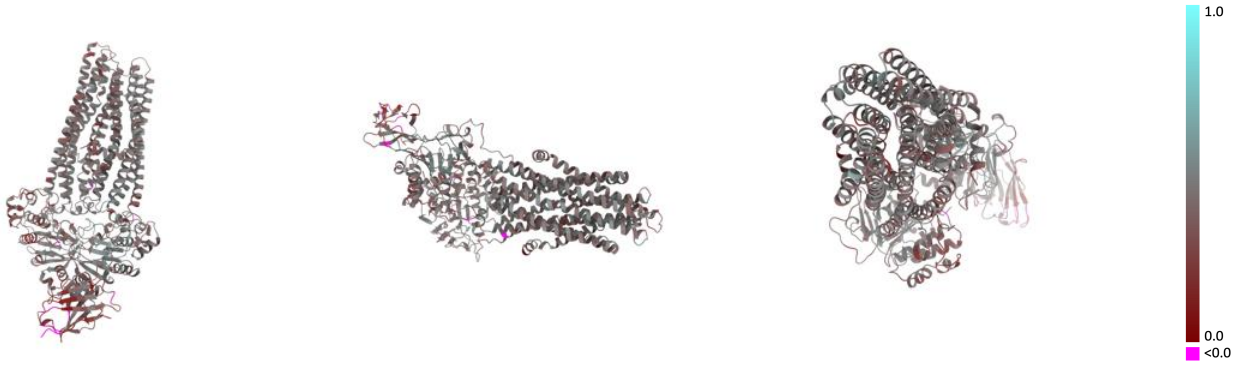
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.57 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.

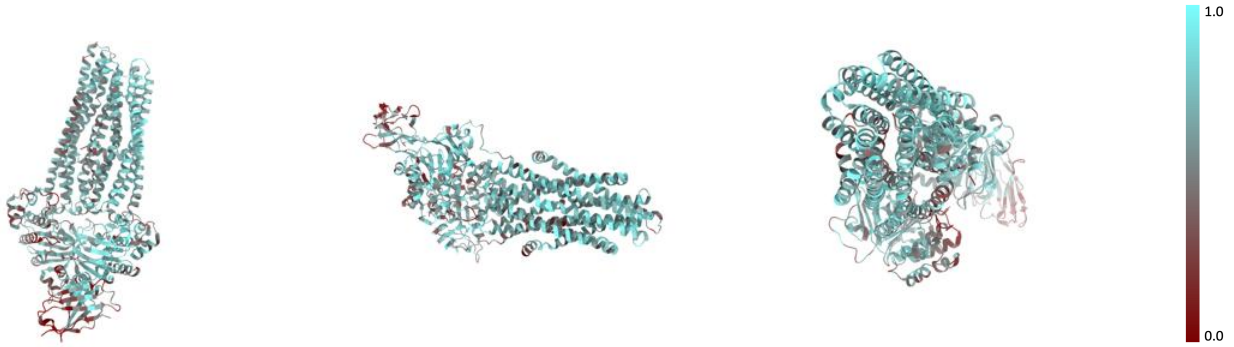
9.2 Q-score mapped to coordinate model (i)



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.

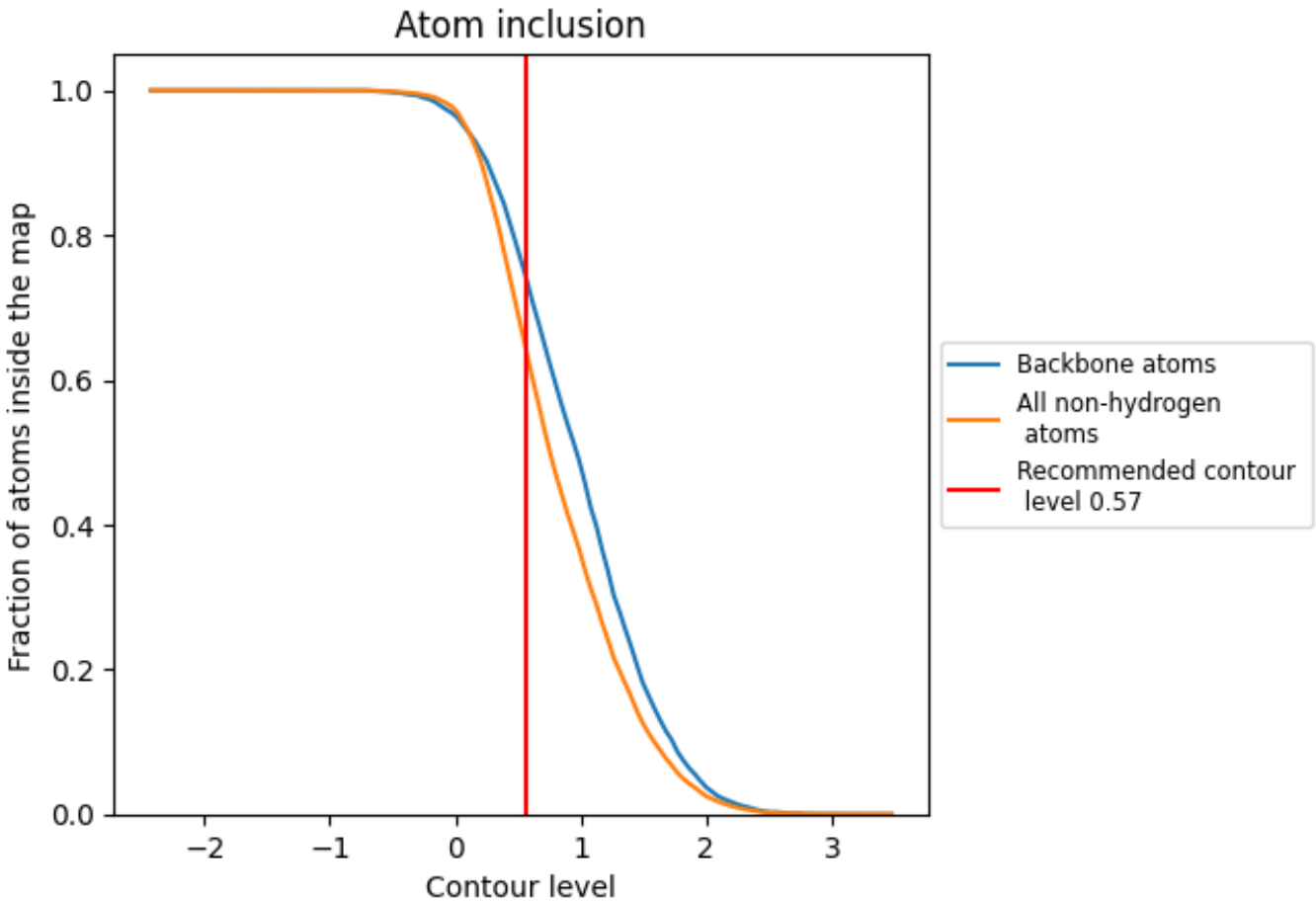
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.57).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 64% 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 (0.57) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6373	0.4070
A	0.6418	0.4100
B	0.6768	0.4290
C	0.4157	0.2790