



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 07:56 PM UTC

PDB ID : 7VPI / pdb_00007vpi
EMDB ID : EMD-32066
Title : Cryo-EM structure of the human ATP13A2 (E1-ATP state)
Authors : Tomita, A.; Yamashita, K.; Nishizawa, T.; Nureki, O.
Deposited on : 2021-10-17
Resolution : 3.60 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

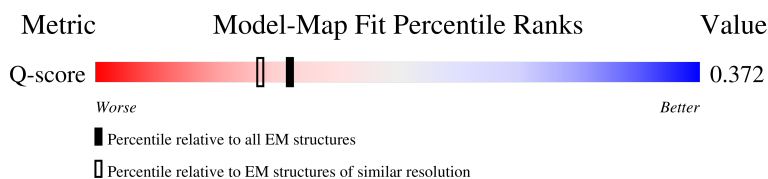
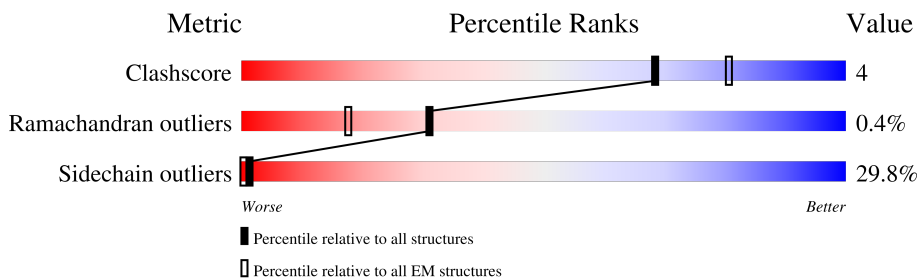
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	19% 54% 23% • 19%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7375 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.

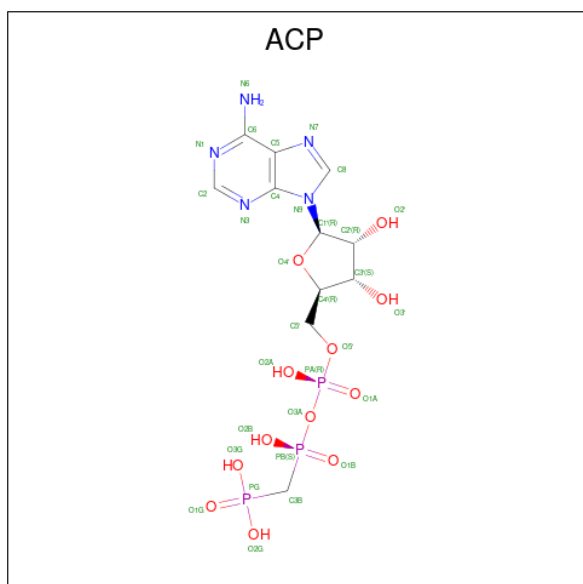
- Molecule 1 is a protein called Polyamine-transporting ATPase 13A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	959	7343	4738	1252	1303	50	0	0

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

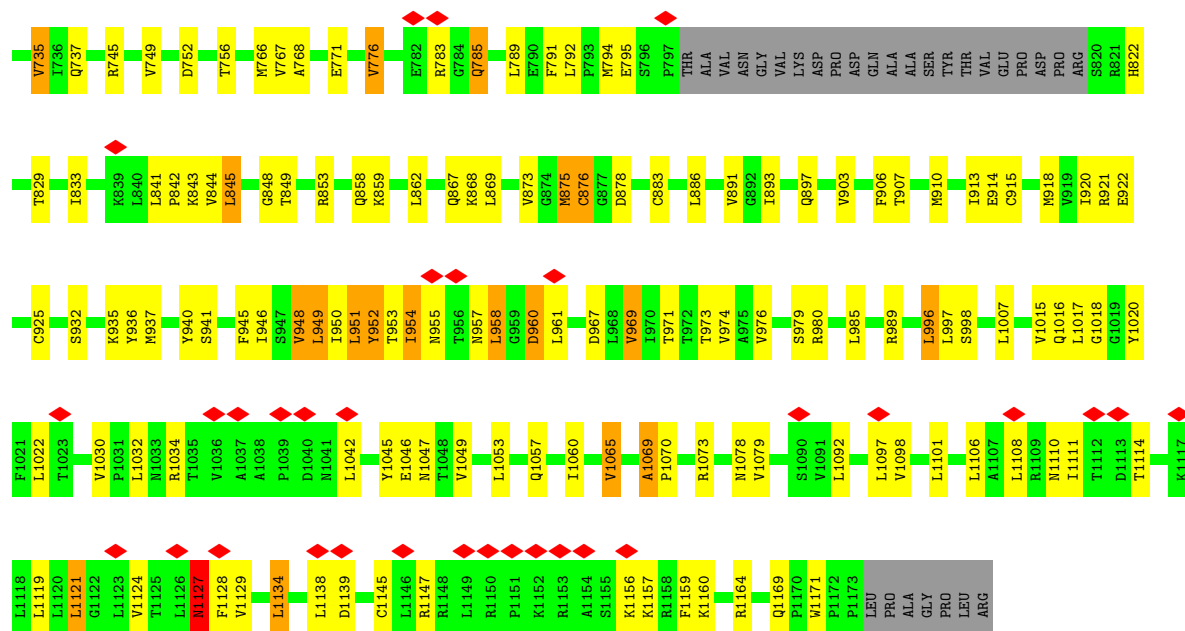
- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
2	A	1	31	11	5	12	3	0

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

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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3114	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 ($e^-/\text{\AA}^2$)	50	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	0.588	Depositor
Minimum map value	-0.414	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.0359	Depositor
Map size (Å)	179.08978, 179.08978, 179.08978	wwPDB
Map dimensions	118, 118, 118	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.51771, 1.51771, 1.51771	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: MG, ACP

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	1.31	3/7507 (0.0%)	1.93	47/10235 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	643	TRP	N-CA	5.24	1.50	1.45
1	A	413	HIS	N-CA	5.23	1.50	1.46
1	A	540	VAL	N-CA	5.02	1.50	1.46

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	785	GLN	CB-CA-C	6.72	117.58	109.31
1	A	313	VAL	N-CA-CB	6.40	116.58	109.99
1	A	288	MET	N-CA-CB	6.12	118.88	110.01
1	A	1018	GLY	CA-C-N	6.05	126.83	119.99
1	A	1018	GLY	C-N-CA	6.05	126.83	119.99
1	A	735	VAL	N-CA-CB	6.01	117.59	110.55
1	A	906	PHE	CA-CB-CG	5.95	119.75	113.80
1	A	1127	ASN	CA-CB-CG	5.91	118.51	112.60
1	A	998	SER	CA-C-N	5.90	125.05	120.33
1	A	998	SER	C-N-CA	5.90	125.05	120.33
1	A	1114	THR	CA-C-N	5.84	126.59	119.99
1	A	1114	THR	C-N-CA	5.84	126.59	119.99
1	A	513	ASP	CB-CA-C	5.79	119.35	109.80
1	A	370	ARG	CB-CG-CD	5.69	124.38	111.30
1	A	413	HIS	CB-CA-C	5.64	115.20	111.20
1	A	1129	VAL	CA-C-N	5.56	126.27	119.99
1	A	1129	VAL	C-N-CA	5.56	126.27	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	GLY	CA-C-N	5.52	126.21	120.03
1	A	504	GLY	C-N-CA	5.52	126.21	120.03
1	A	954	ILE	CB-CA-C	5.52	118.97	112.68
1	A	960	ASP	CA-CB-CG	5.50	118.10	112.60
1	A	513	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	1159	PHE	CA-CB-CG	5.40	119.20	113.80
1	A	566	ASP	CA-CB-CG	5.36	117.96	112.60
1	A	848	GLY	CA-C-O	-5.36	116.25	120.91
1	A	958	LEU	CA-C-N	5.35	126.86	121.35
1	A	958	LEU	C-N-CA	5.35	126.86	121.35
1	A	644	PRO	CA-C-N	5.34	126.01	120.03
1	A	644	PRO	C-N-CA	5.34	126.01	120.03
1	A	196	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	241	TYR	CA-C-N	5.28	125.80	119.94
1	A	241	TYR	C-N-CA	5.28	125.80	119.94
1	A	961	LEU	CA-C-N	5.21	127.52	120.38
1	A	961	LEU	C-N-CA	5.21	127.52	120.38
1	A	385	ALA	CA-C-N	5.19	127.55	120.54
1	A	385	ALA	C-N-CA	5.19	127.55	120.54
1	A	949	LEU	CA-C-O	-5.18	115.37	120.70
1	A	316	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	945	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	1078	ASN	CA-C-O	-5.15	115.40	121.07
1	A	451	ARG	CB-CG-CD	5.11	123.05	111.30
1	A	283	GLN	CA-C-O	-5.10	115.45	120.90
1	A	1121	LEU	CA-C-N	5.09	125.74	119.99
1	A	1121	LEU	C-N-CA	5.09	125.74	119.99
1	A	883	CYS	CA-C-N	5.07	125.72	119.99
1	A	883	CYS	C-N-CA	5.07	125.72	119.99

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	7343	0	7611	56	0
2	A	31	0	14	0	0
3	A	1	0	0	0	0
All	All	7375	0	7625	56	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 4.

All (56) 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:193:SER:HA	1:A:363:PRO:HA	1.64	0.79
1:A:383:ALA:HB1	1:A:391:VAL:HG21	1.72	0.72
1:A:523:LEU:HD11	1:A:573:MET:HA	1.72	0.71
1:A:193:SER:HA	1:A:363:PRO:CA	2.23	0.69
1:A:235:GLU:HB3	1:A:271:ILE:HD11	1.78	0.66
1:A:221:ILE:HG21	1:A:289:VAL:HB	1.76	0.66
1:A:425:SER:HB2	1:A:996:LEU:HD12	1.80	0.64
1:A:910:MET:HE1	1:A:918:MET:HE1	1.81	0.62
1:A:1007:LEU:HB3	1:A:1134:LEU:HD11	1.81	0.62
1:A:477:MET:HA	1:A:477:MET:HE2	1.83	0.61
1:A:876:CYS:O	1:A:876:CYS:SG	2.60	0.59
1:A:1060:ILE:HG21	1:A:1128:PHE:HA	1.84	0.59
1:A:523:LEU:HD13	1:A:724:MET:HB3	1.84	0.58
1:A:844:VAL:HG23	1:A:845:LEU:HD23	1.85	0.57
1:A:320:LEU:HD22	1:A:327:MET:HE1	1.87	0.56
1:A:493:ILE:HD11	1:A:918:MET:HE2	1.89	0.55
1:A:776:VAL:HG13	1:A:789:LEU:HD21	1.90	0.54
1:A:509:LEU:HD21	1:A:873:VAL:HG12	1.91	0.53
1:A:517:THR:HG21	1:A:876:CYS:O	2.08	0.53
1:A:1015:VAL:HG21	1:A:1127:ASN:HB3	1.91	0.52
1:A:622:VAL:HG12	1:A:643:TRP:HB3	1.91	0.52
1:A:989:ARG:O	1:A:989:ARG:NH1	2.43	0.51
1:A:686:ARG:NH1	1:A:752:ASP:OD2	2.44	0.50
1:A:1069:ALA:HB3	1:A:1070:PRO:HD3	1.93	0.49
1:A:386:TYR:HB2	1:A:598:GLN:HA	1.95	0.48
1:A:897:GLN:HB2	1:A:907:THR:HG23	1.96	0.48
1:A:893:ILE:HG21	1:A:915:CYS:SG	2.54	0.48
1:A:875:MET:HB3	1:A:886:LEU:HD23	1.96	0.47
1:A:523:LEU:HD12	1:A:523:LEU:O	2.13	0.47
1:A:452:VAL:HG23	1:A:457:ILE:HG22	1.97	0.46
1:A:842:PRO:HA	1:A:869:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:VAL:HG21	1:A:976:VAL:HG22	1.97	0.46
1:A:822:HIS:ND1	1:A:849:THR:HG21	2.30	0.46
1:A:415:ARG:NE	1:A:415:ARG:O	2.50	0.45
1:A:561:LEU:HD11	1:A:575:LEU:HA	1.97	0.45
1:A:520:GLU:O	1:A:726:ASN:ND2	2.50	0.45
1:A:948:VAL:HG22	1:A:958:LEU:HD22	1.98	0.45
1:A:460:ARG:HD3	1:A:952:TYR:CE1	2.52	0.44
1:A:446:ILE:HG13	1:A:953:THR:HG22	2.00	0.44
1:A:200:SER:HB2	1:A:394:VAL:HG21	2.00	0.43
1:A:336:GLY:HA3	1:A:391:VAL:HG12	2.00	0.43
1:A:845:LEU:HD13	1:A:862:LEU:HD12	2.00	0.43
1:A:451:ARG:HA	1:A:451:ARG:NH2	2.33	0.43
1:A:936:TYR:HB2	1:A:1065:VAL:HG11	1.99	0.43
1:A:193:SER:HA	1:A:363:PRO:CB	2.48	0.43
1:A:451:ARG:HA	1:A:451:ARG:CZ	2.48	0.43
1:A:969:VAL:O	1:A:973:THR:HB	2.19	0.42
1:A:517:THR:C	1:A:913:ILE:HD11	2.45	0.41
1:A:507:LEU:C	1:A:507:LEU:HD12	2.46	0.41
1:A:706:GLN:O	1:A:706:GLN:NE2	2.54	0.41
1:A:951:LEU:HB3	1:A:957:ASN:O	2.20	0.41
1:A:768:ALA:HB3	1:A:771:GLU:HG2	2.03	0.41
1:A:517:THR:HG23	1:A:878:ASP:HB3	2.02	0.40
1:A:320:LEU:HD21	1:A:393:ALA:HB3	2.03	0.40
1:A:383:ALA:HB1	1:A:391:VAL:CG2	2.47	0.40
1:A:201:ARG:HB2	1:A:334:VAL:HG21	2.02	0.40

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	951/1184 (80%)	909 (96%)	38 (4%)	4 (0%)	30 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	228	TYR
1	A	1079	VAL
1	A	1069	ALA
1	A	568	PRO

5.3.2 Protein sidechains ⓘ

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	819/1005 (82%)	575 (70%)	244 (30%)	0 2

All (244) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	PHE
1	A	184	GLN
1	A	190	HIS
1	A	194	CYS
1	A	195	ASP
1	A	197	VAL
1	A	201	ARG
1	A	204	LEU
1	A	206	LEU
1	A	207	GLN
1	A	208	ASP
1	A	213	LYS
1	A	216	TYR
1	A	223	ILE
1	A	226	LYS
1	A	230	GLN
1	A	232	LEU
1	A	233	VAL
1	A	234	ASP
1	A	244	GLN
1	A	246	PHE

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Mol	Chain	Res	Type
1	A	247	SER
1	A	252	LEU
1	A	257	TYR
1	A	262	CYS
1	A	265	LEU
1	A	273	LEU
1	A	274	SER
1	A	278	THR
1	A	280	LYS
1	A	281	GLN
1	A	283	GLN
1	A	288	MET
1	A	291	LEU
1	A	293	MET
1	A	294	ARG
1	A	299	ARG
1	A	303	GLU
1	A	304	GLU
1	A	307	VAL
1	A	308	ASP
1	A	313	VAL
1	A	316	ASP
1	A	319	VAL
1	A	327	MET
1	A	334	VAL
1	A	337	GLU
1	A	338	CYS
1	A	340	VAL
1	A	345	LEU
1	A	348	GLU
1	A	352	VAL
1	A	354	LYS
1	A	359	GLU
1	A	364	TYR
1	A	367	GLU
1	A	370	ARG
1	A	371	ARG
1	A	374	LEU
1	A	376	CYS
1	A	381	LEU
1	A	382	GLN
1	A	384	ARG

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Mol	Chain	Res	Type
1	A	386	TYR
1	A	387	VAL
1	A	390	HIS
1	A	392	LEU
1	A	396	THR
1	A	400	PHE
1	A	402	THR
1	A	404	LYS
1	A	415	ARG
1	A	417	ILE
1	A	418	ASN
1	A	420	LYS
1	A	421	PHE
1	A	423	LYS
1	A	432	LEU
1	A	438	LEU
1	A	445	PHE
1	A	446	ILE
1	A	447	LEU
1	A	451	ARG
1	A	452	VAL
1	A	454	LEU
1	A	457	ILE
1	A	460	ARG
1	A	464	LEU
1	A	468	VAL
1	A	469	VAL
1	A	482	LEU
1	A	486	SER
1	A	489	ARG
1	A	496	ILE
1	A	501	ILE
1	A	503	LEU
1	A	509	LEU
1	A	510	VAL
1	A	513	ASP
1	A	514	LYS
1	A	517	THR
1	A	518	LEU
1	A	520	GLU
1	A	523	LEU
1	A	526	MET

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Mol	Chain	Res	Type
1	A	529	VAL
1	A	531	LEU
1	A	532	LYS
1	A	534	GLN
1	A	537	LEU
1	A	540	VAL
1	A	542	GLU
1	A	544	ARG
1	A	545	ARG
1	A	546	LEU
1	A	558	CYS
1	A	561	LEU
1	A	563	ARG
1	A	564	LEU
1	A	567	THR
1	A	573	MET
1	A	576	LYS
1	A	579	GLU
1	A	600	LEU
1	A	604	ARG
1	A	607	LEU
1	A	631	SER
1	A	634	LEU
1	A	636	ARG
1	A	658	GLU
1	A	663	LEU
1	A	668	THR
1	A	672	ASP
1	A	678	GLN
1	A	681	THR
1	A	693	LYS
1	A	698	VAL
1	A	702	GLU
1	A	705	GLN
1	A	706	GLN
1	A	707	LEU
1	A	708	THR
1	A	709	ARG
1	A	717	SER
1	A	719	LEU
1	A	724	MET
1	A	726	ASN

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Mol	Chain	Res	Type
1	A	727	LEU
1	A	731	GLN
1	A	735	VAL
1	A	737	GLN
1	A	745	ARG
1	A	749	VAL
1	A	756	THR
1	A	766	MET
1	A	767	VAL
1	A	776	VAL
1	A	783	ARG
1	A	785	GLN
1	A	791	PHE
1	A	792	LEU
1	A	794	MET
1	A	795	GLU
1	A	829	THR
1	A	833	ILE
1	A	841	LEU
1	A	843	LYS
1	A	845	LEU
1	A	853	ARG
1	A	858	GLN
1	A	859	LYS
1	A	867	GLN
1	A	868	LYS
1	A	875	MET
1	A	876	CYS
1	A	891	VAL
1	A	903	VAL
1	A	914	GLU
1	A	920	ILE
1	A	921	ARG
1	A	922	GLU
1	A	925	CYS
1	A	932	SER
1	A	935	LYS
1	A	937	MET
1	A	940	TYR
1	A	941	SER
1	A	946	ILE
1	A	948	VAL

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Mol	Chain	Res	Type
1	A	949	LEU
1	A	950	ILE
1	A	951	LEU
1	A	952	TYR
1	A	954	ILE
1	A	955	ASN
1	A	960	ASP
1	A	967	ASP
1	A	969	VAL
1	A	971	THR
1	A	974	VAL
1	A	979	SER
1	A	980	ARG
1	A	985	LEU
1	A	996	LEU
1	A	997	LEU
1	A	1016	GLN
1	A	1017	LEU
1	A	1020	TYR
1	A	1022	LEU
1	A	1030	VAL
1	A	1032	LEU
1	A	1034	ARG
1	A	1042	LEU
1	A	1045	TYR
1	A	1046	GLU
1	A	1047	ASN
1	A	1049	VAL
1	A	1053	LEU
1	A	1057	GLN
1	A	1065	VAL
1	A	1073	ARG
1	A	1092	LEU
1	A	1097	LEU
1	A	1098	VAL
1	A	1101	LEU
1	A	1106	LEU
1	A	1108	LEU
1	A	1110	ASN
1	A	1111	ILE
1	A	1119	LEU
1	A	1121	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1124	VAL
1	A	1127	ASN
1	A	1134	LEU
1	A	1138	LEU
1	A	1139	ASP
1	A	1145	CYS
1	A	1147	ARG
1	A	1156	LYS
1	A	1157	LYS
1	A	1160	LYS
1	A	1164	ARG
1	A	1169	GLN
1	A	1171	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	322	GLN
1	A	382	GLN
1	A	418	ASN
1	A	534	GLN
1	A	635	GLN
1	A	648	GLN
1	A	678	GLN
1	A	706	GLN
1	A	726	ASN
1	A	731	GLN
1	A	858	GLN
1	A	957	ASN
1	A	962	GLN
1	A	1016	GLN
1	A	1140	GLN
1	A	1169	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
2	ACP	A	1201	3	31,33,33	0.73	1 (3%)	47,52,52	0.69	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
2	ACP	A	1201	3	-	7/19/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ACP	PB-O2B	-2.28	1.50	1.56

There are no bond angle outliers.

There are no chirality outliers.

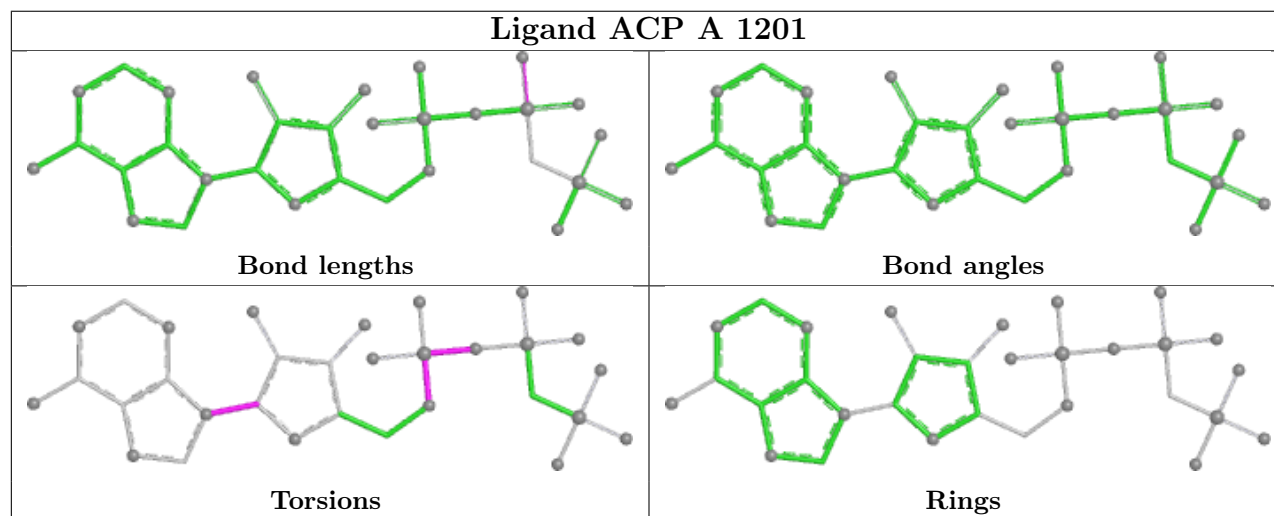
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ACP	C5'-O5'-PA-O1A
2	A	1201	ACP	C5'-O5'-PA-O2A
2	A	1201	ACP	C5'-O5'-PA-O3A
2	A	1201	ACP	C2'-C1'-N9-C8
2	A	1201	ACP	C2'-C1'-N9-C4
2	A	1201	ACP	PB-O3A-PA-O5'
2	A	1201	ACP	O4'-C1'-N9-C8

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32066. These allow visual inspection of the internal detail of the map and identification of artifacts.

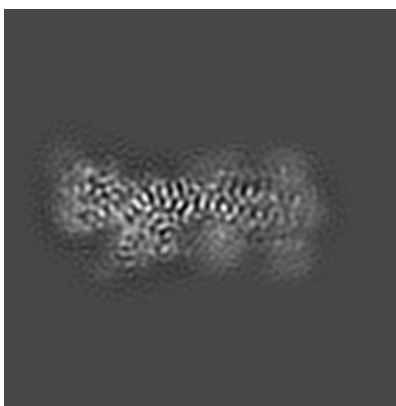
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

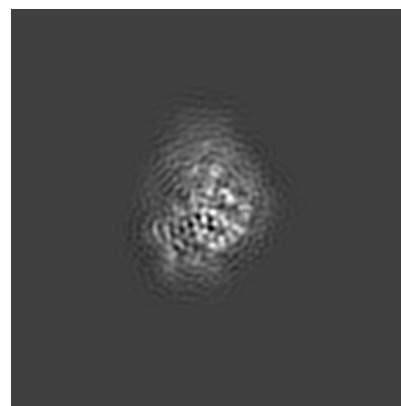
6.1.1 Primary map



X

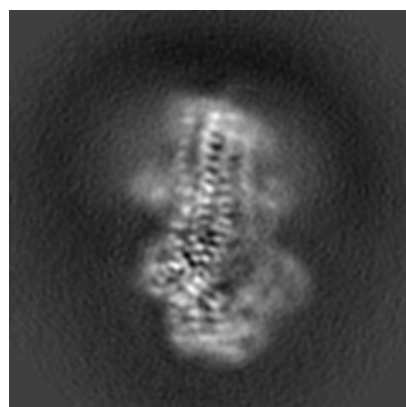


Y

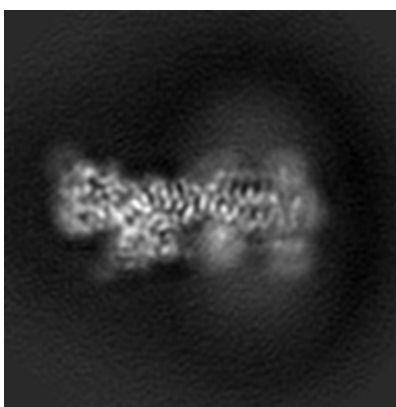


Z

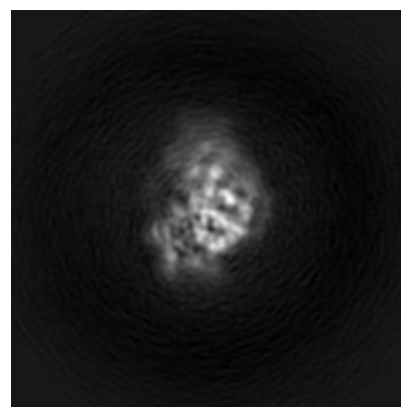
6.1.2 Raw map



X



Y



Z

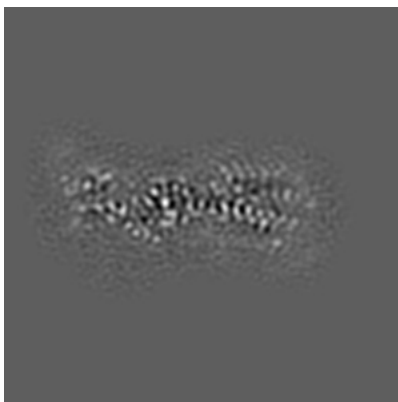
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

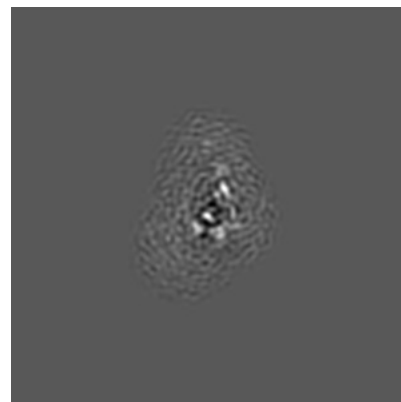
6.2.1 Primary map



X Index: 59

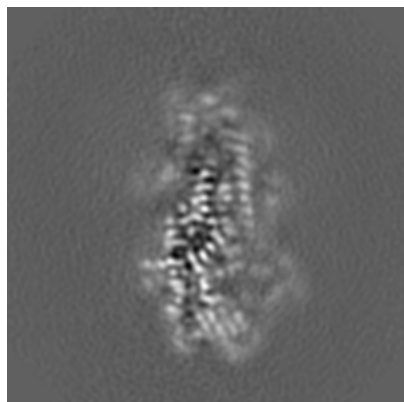


Y Index: 59

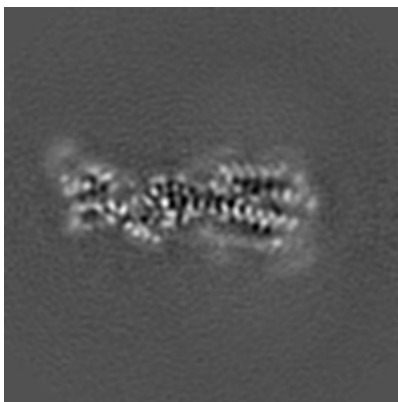


Z Index: 59

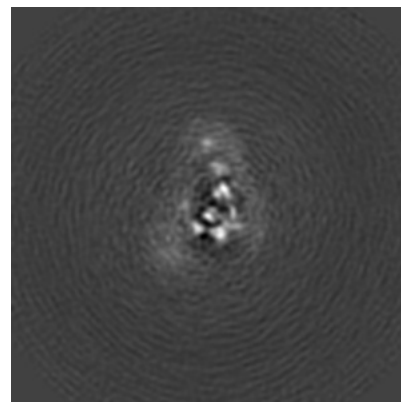
6.2.2 Raw map



X Index: 59



Y Index: 59

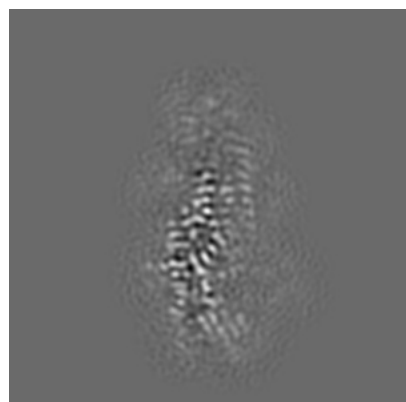


Z Index: 59

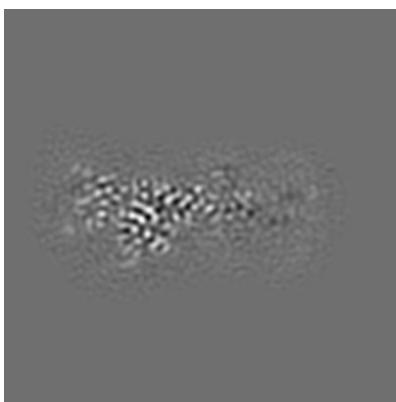
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

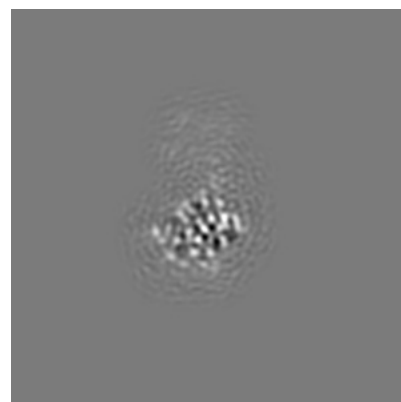
6.3.1 Primary map



X Index: 59

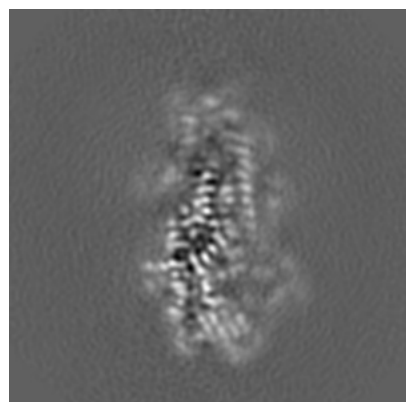


Y Index: 55

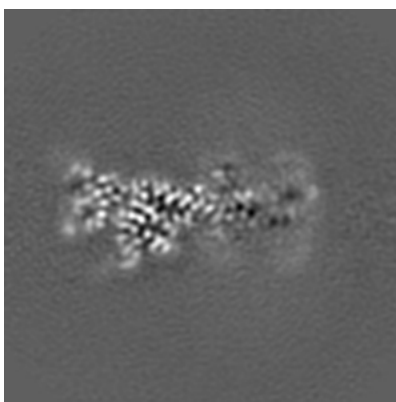


Z Index: 41

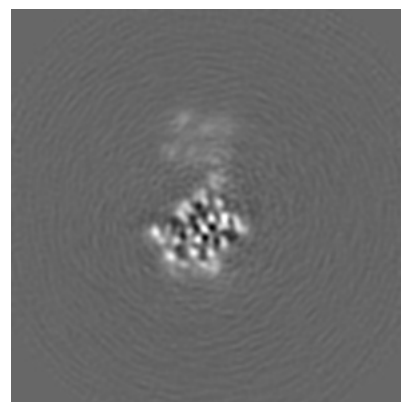
6.3.2 Raw map



X Index: 59



Y Index: 55

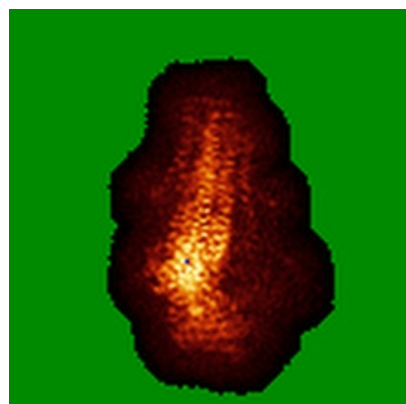


Z Index: 41

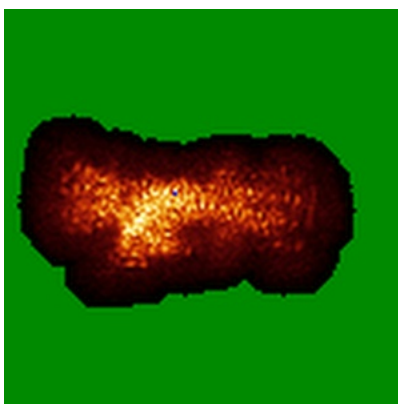
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

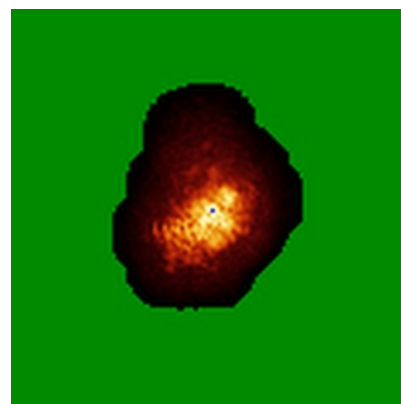
6.4.1 Primary map



X

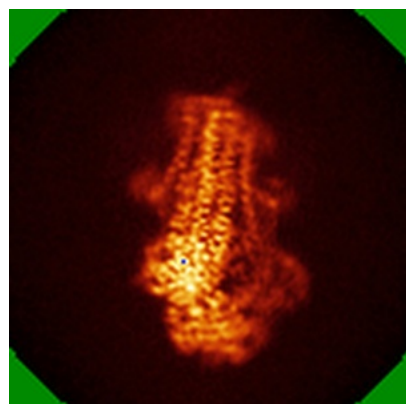


Y

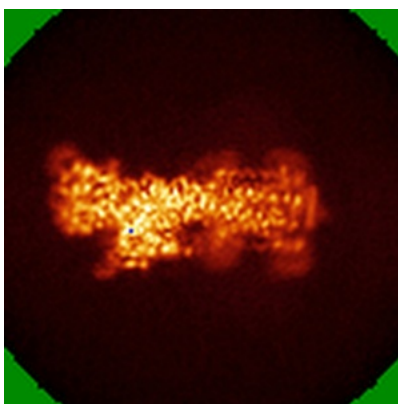


Z

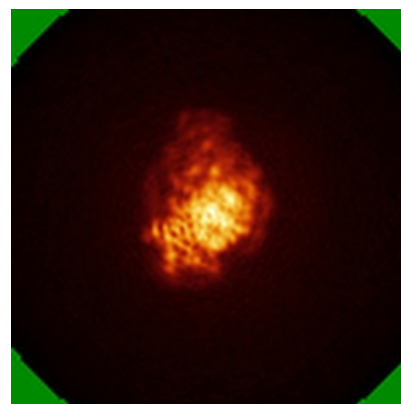
6.4.2 Raw map



X



Y

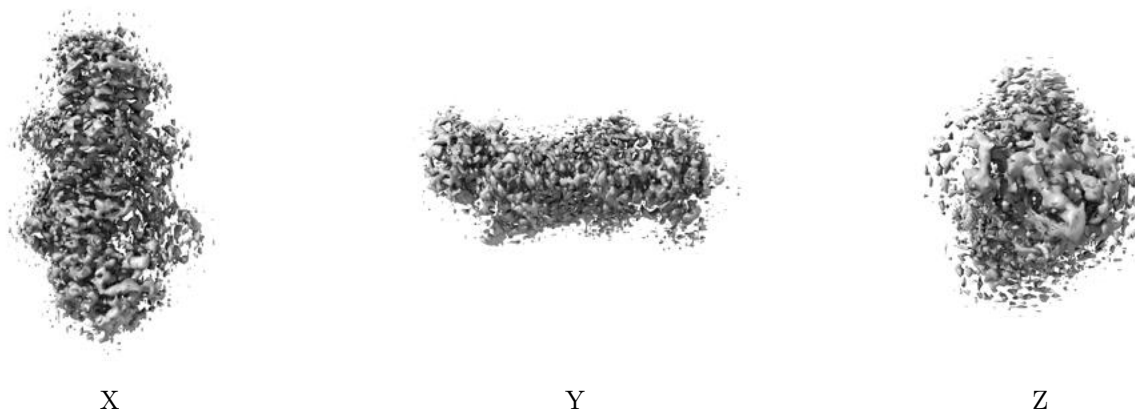


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

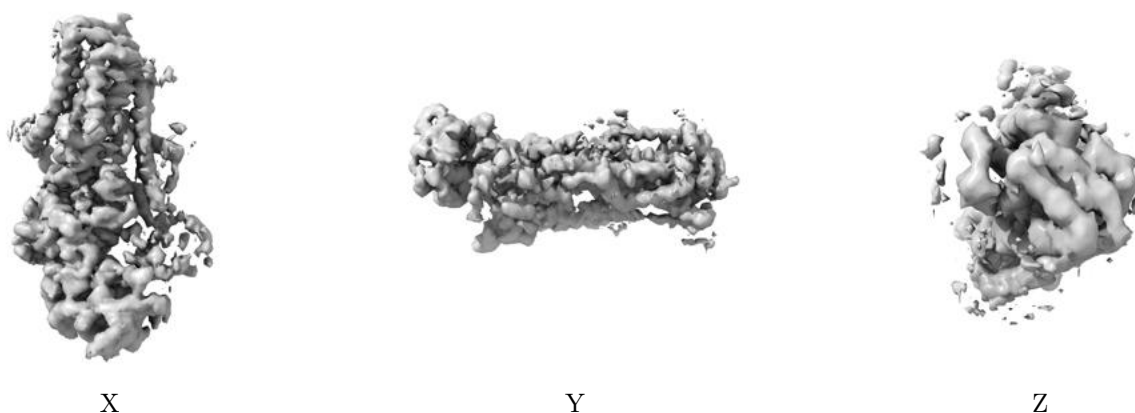
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0359. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

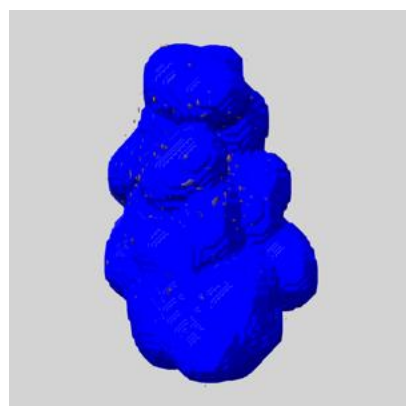
6.6 Mask visualisation [i](#)

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

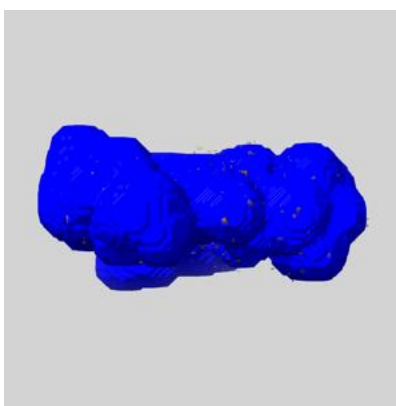
A mask typically either:

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

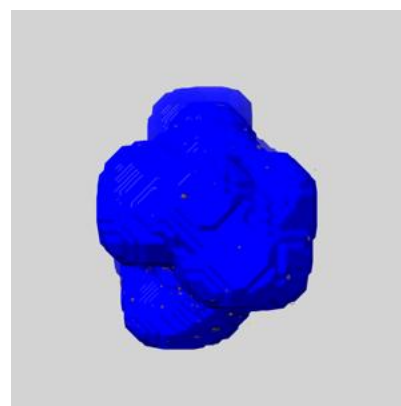
6.6.1 emd_32066_msk_1.map [i](#)



X



Y

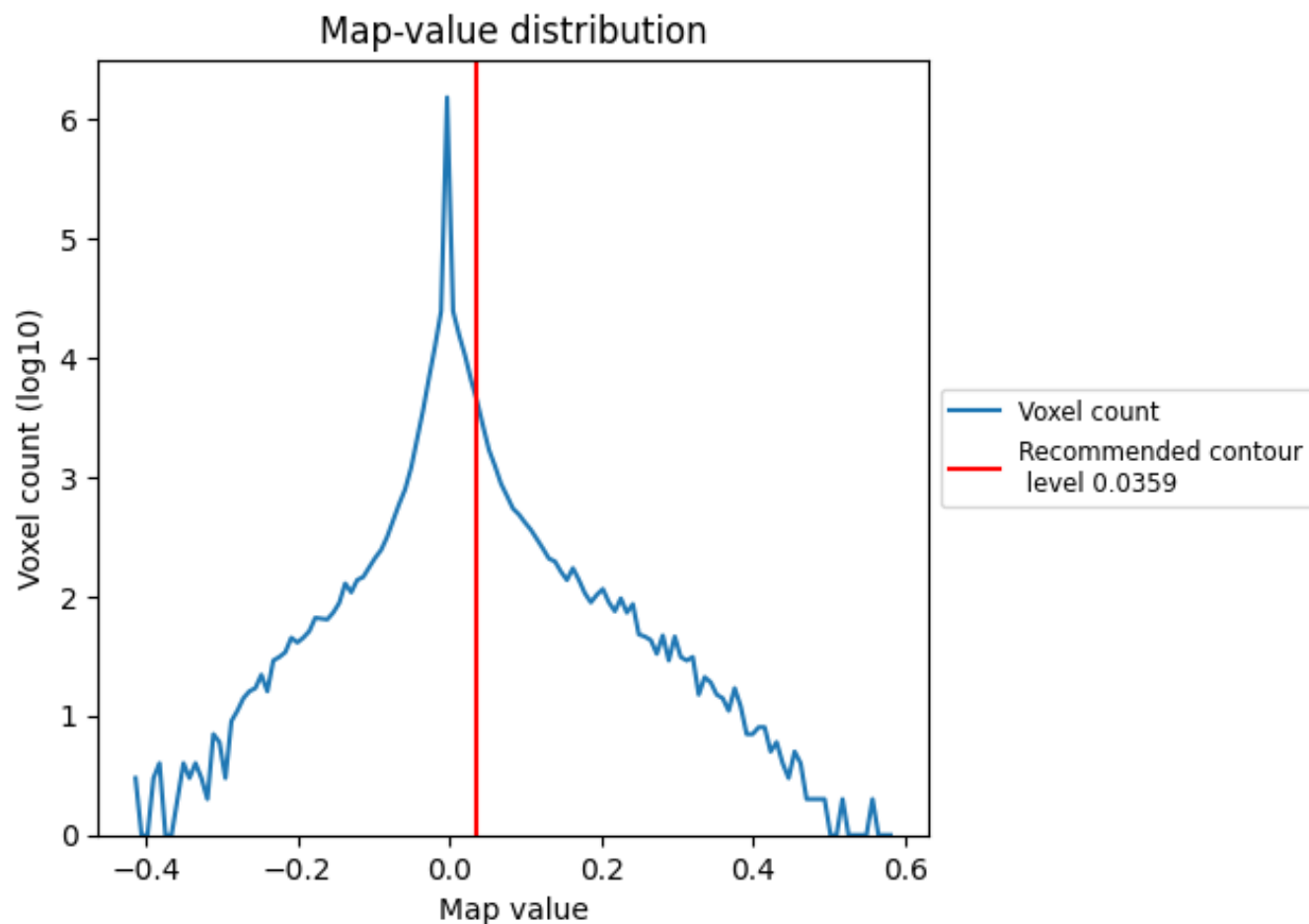


Z

7 Map analysis [i](#)

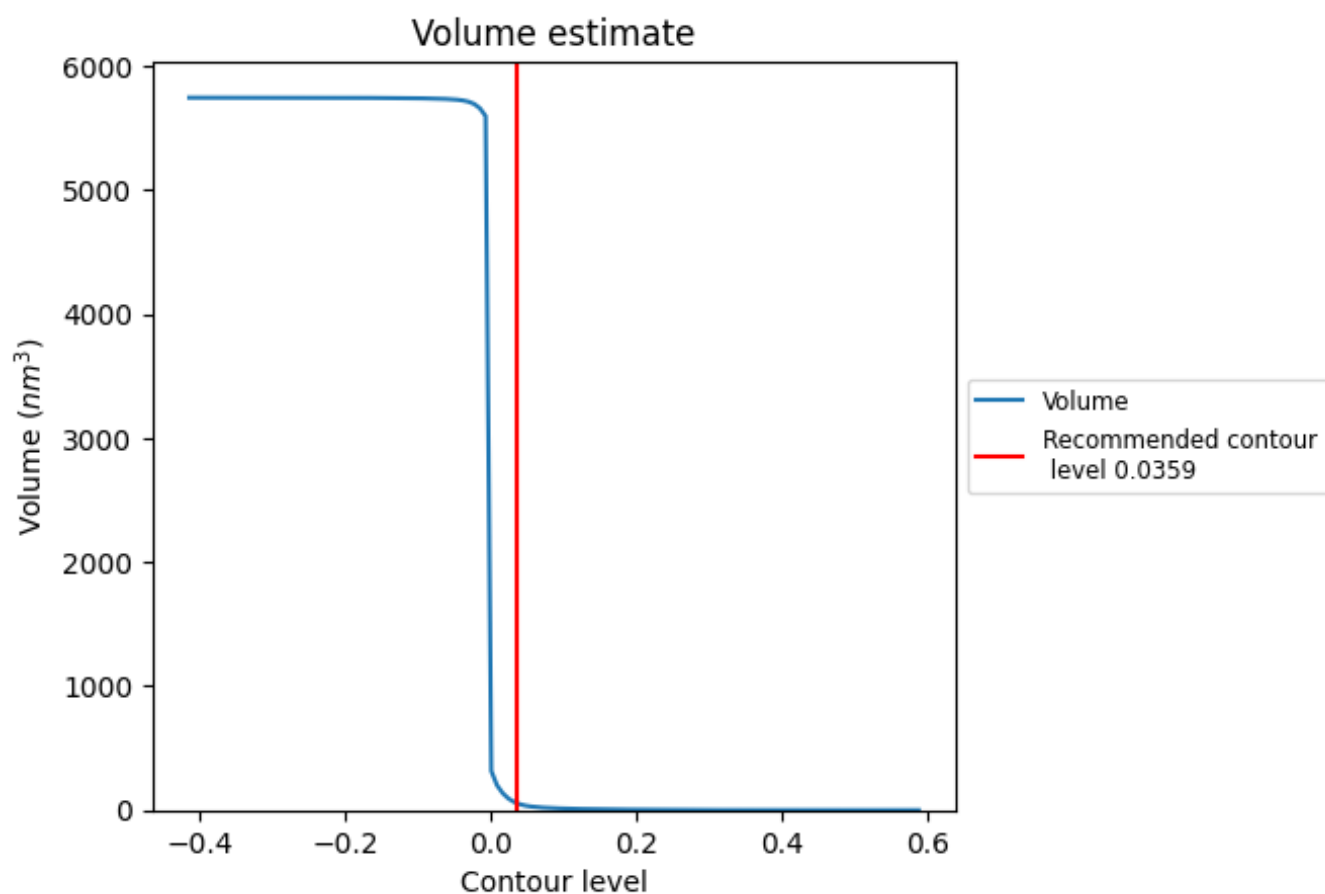
This section contains the results of statistical analysis of the map.

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.

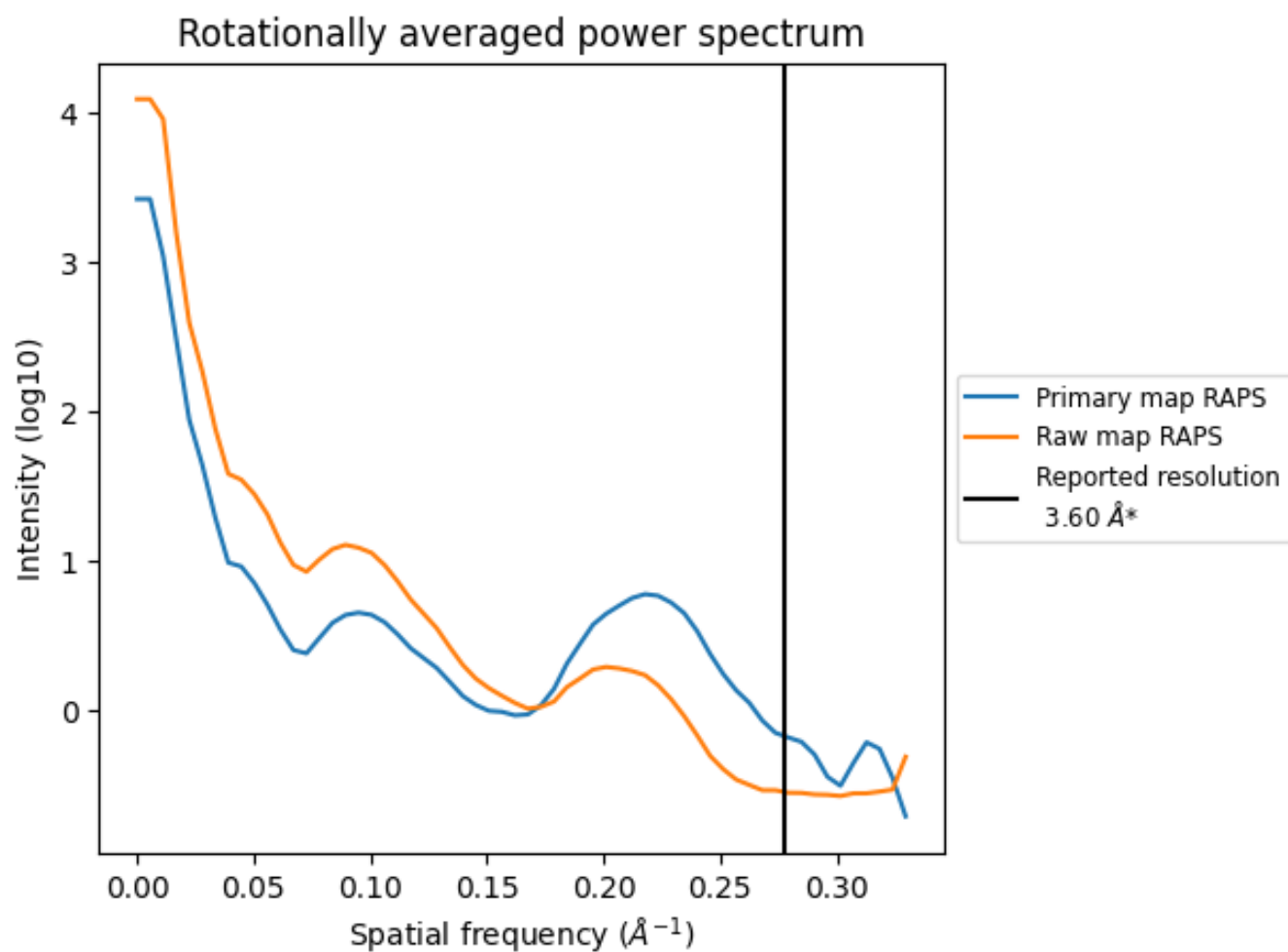
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 58 nm³; this corresponds to an approximate mass of 53 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 ⓘ

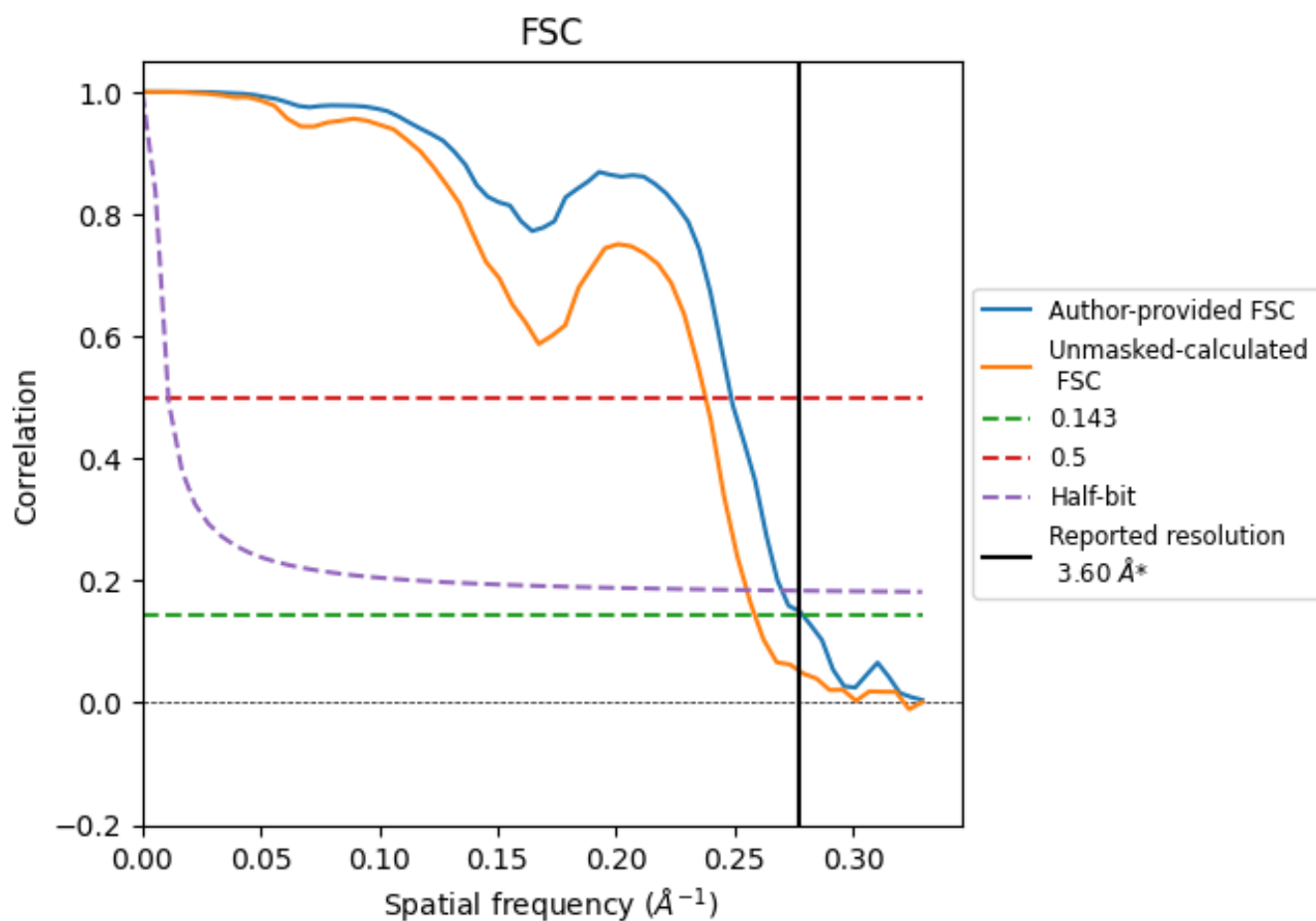


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

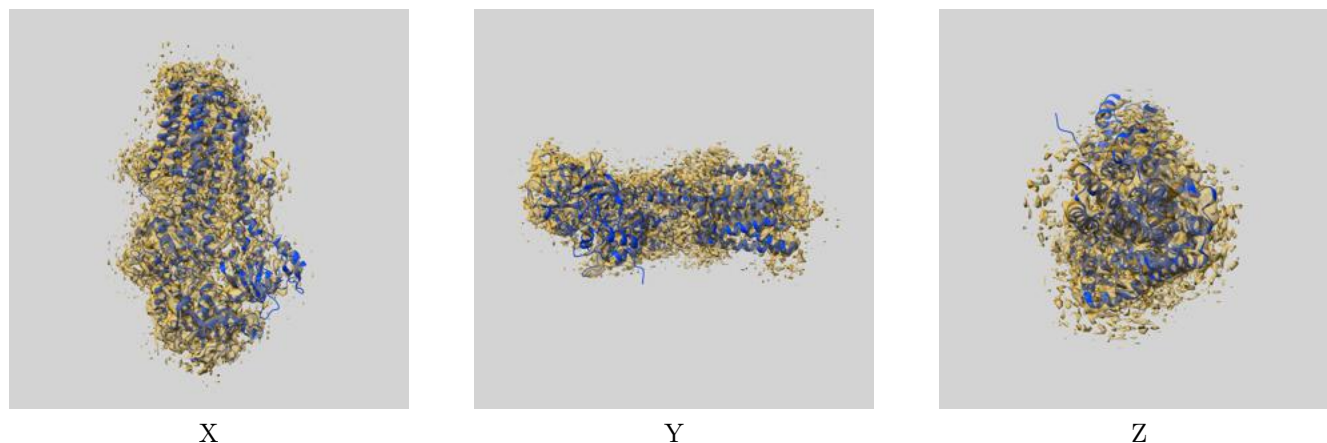
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.02	3.70
Unmasked-calculated*	3.86	4.20	3.92

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

9 Map-model fit [i](#)

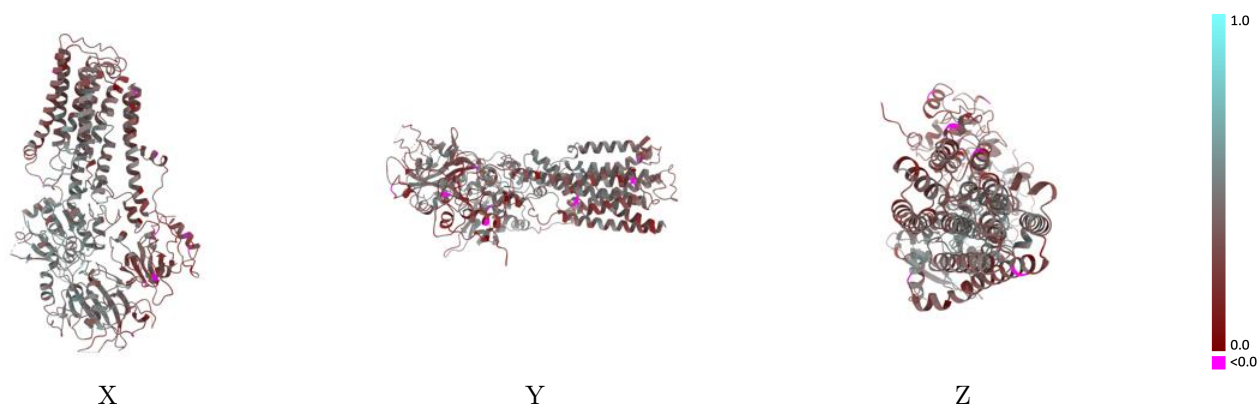
This section contains information regarding the fit between EMDB map EMD-32066 and PDB model 7VPI. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



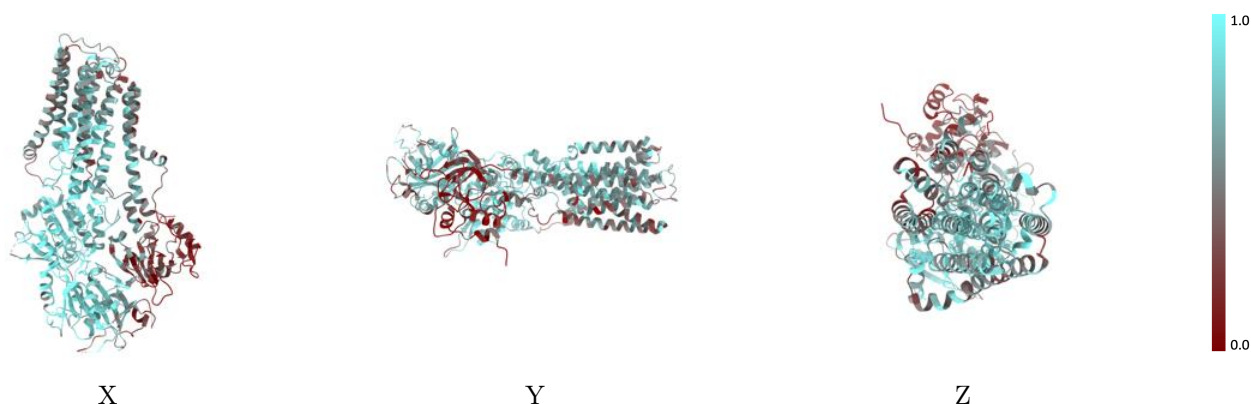
The images above show the 3D surface view of the map at the recommended contour level 0.0359 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



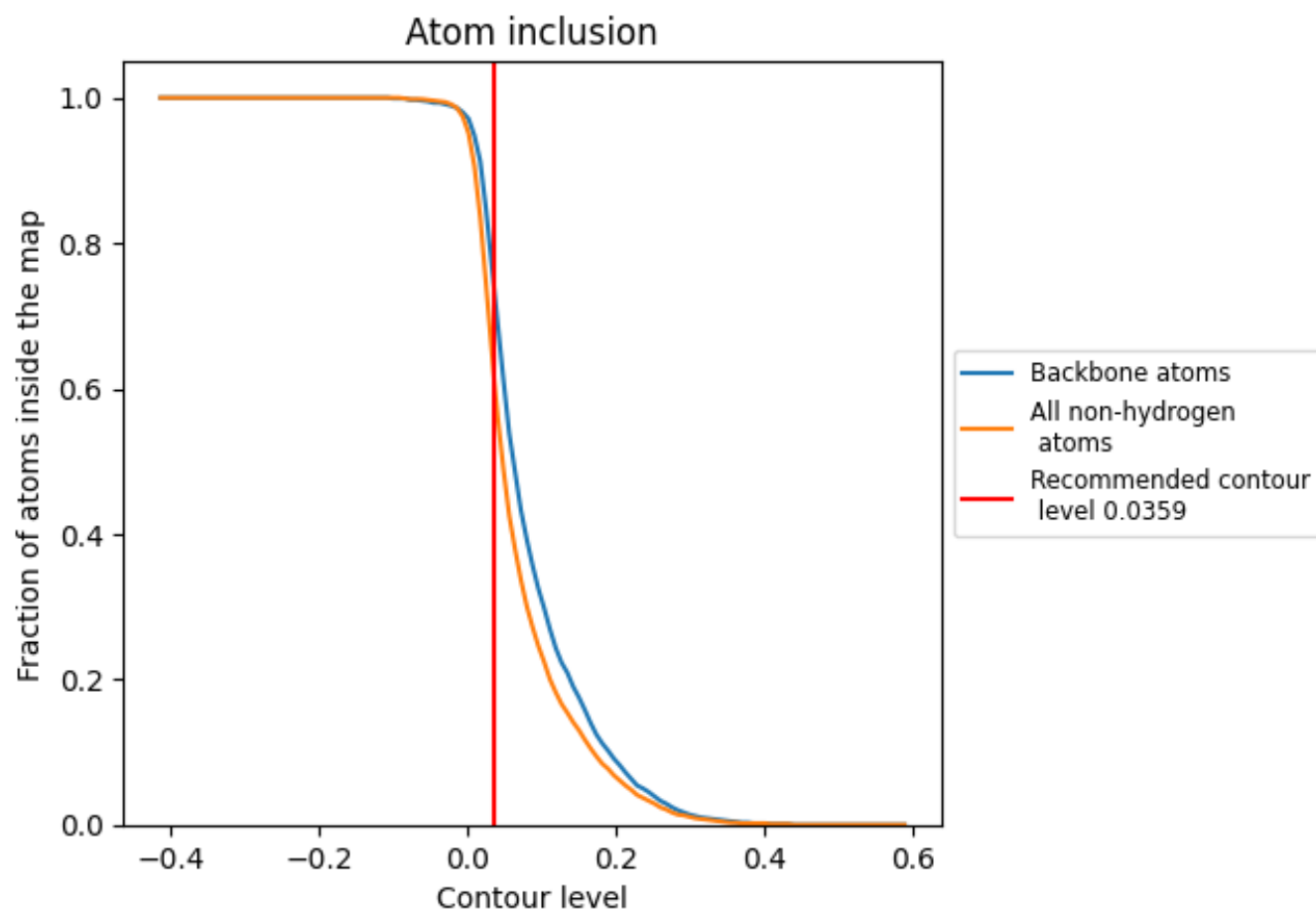
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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 (0.0359).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 61% 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 (0.0359) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6100	0.3720
A	0.6100	0.3720

