



Full wwPDB EM Validation Report ⓘ

May 26, 2025 – 09:11 AM EDT

PDB ID : 6XG6 / pdb_00006xg6
EMDB ID : EMD-22174
Title : Full-length human mitochondrial Hsp90 (TRAP1) with ADP-BeF3
Authors : Liu, Y.X.; Wang, F.; Agard, D.A.
Deposited on : 2020-06-17
Resolution : 3.20 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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

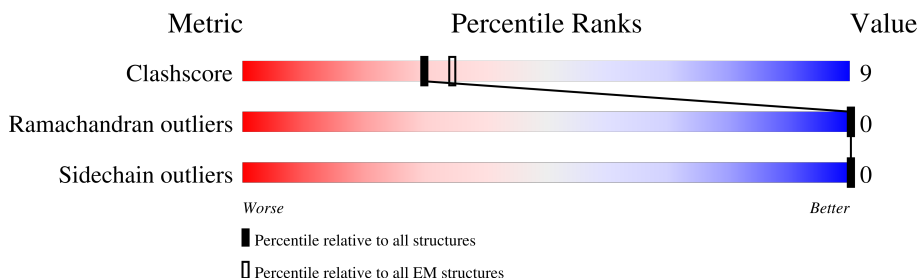
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	774	<div> <div>12%</div> <div>60%</div> <div>18%</div> <div>22%</div> </div>
1	B	774	<div> <div>14%</div> <div>62%</div> <div>17%</div> <div>21%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9825 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 Heat shock protein 75 kDa, mitochondrial, Fibronectin binding protein fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	607	Total	C	N	O	S	0	0
			4856	3077	845	913	21		
1	B	613	Total	C	N	O	S	0	0
			4903	3106	853	922	22		

There are 36 discrepancies between the modelled and reference sequences:

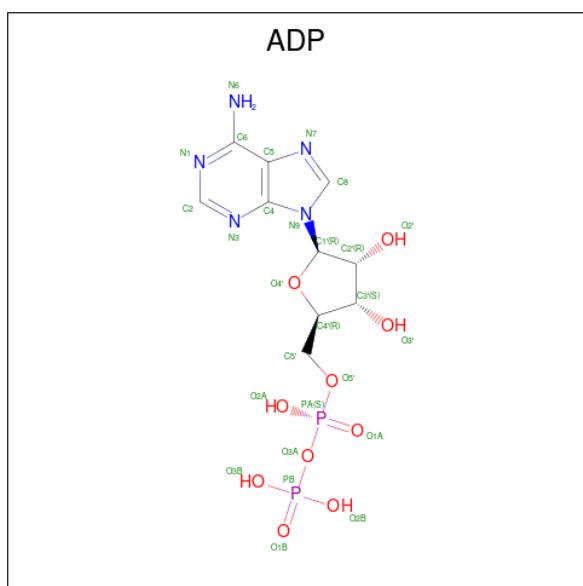
Chain	Residue	Modelled	Actual	Comment	Reference
A	54	GLY	-	expression tag	UNP Q12931
A	55	ILE	-	expression tag	UNP Q12931
A	56	ASP	-	expression tag	UNP Q12931
A	57	PRO	-	expression tag	UNP Q12931
A	58	PHE	-	expression tag	UNP Q12931
A	59	THR	-	expression tag	UNP Q12931
A	307	GLY	ARG	conflict	UNP Q12931
A	705	GLY	-	linker	UNP Q12931
A	706	GLY	-	linker	UNP Q12931
A	707	SER	-	linker	UNP Q12931
A	708	GLY	-	linker	UNP Q12931
A	709	SER	-	linker	UNP Q12931
A	710	GLY	-	linker	UNP Q12931
A	711	SER	-	linker	UNP Q12931
A	713	ALA	ARG	conflict	UNP Q8G9G1
A	714	MET	PRO	conflict	UNP Q8G9G1
A	748	GLU	ILE	conflict	UNP Q8G9G1
A	783	TYR	MET	conflict	UNP Q8G9G1
B	54	GLY	-	expression tag	UNP Q12931
B	55	ILE	-	expression tag	UNP Q12931
B	56	ASP	-	expression tag	UNP Q12931
B	57	PRO	-	expression tag	UNP Q12931
B	58	PHE	-	expression tag	UNP Q12931
B	59	THR	-	expression tag	UNP Q12931
B	307	GLY	ARG	conflict	UNP Q12931

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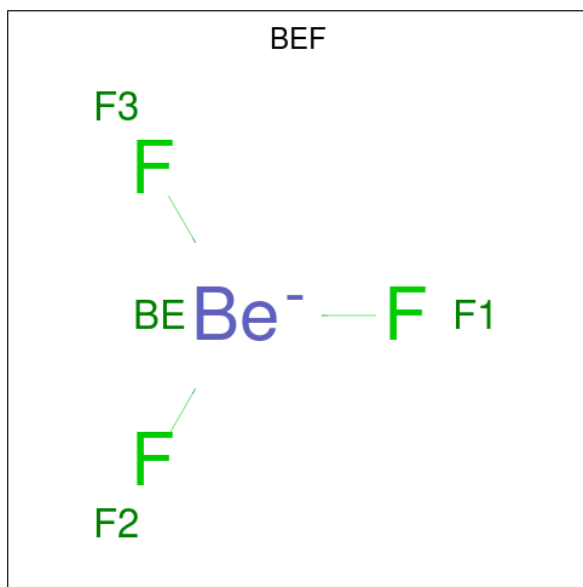
Chain	Residue	Modelled	Actual	Comment	Reference
B	705	GLY	-	linker	UNP Q12931
B	706	GLY	-	linker	UNP Q12931
B	707	SER	-	linker	UNP Q12931
B	708	GLY	-	linker	UNP Q12931
B	709	SER	-	linker	UNP Q12931
B	710	GLY	-	linker	UNP Q12931
B	711	SER	-	linker	UNP Q12931
B	713	ALA	ARG	conflict	UNP Q8G9G1
B	714	MET	PRO	conflict	UNP Q8G9G1
B	748	GLU	ILE	conflict	UNP Q8G9G1
B	783	TYR	MET	conflict	UNP Q8G9G1

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	K	0
			1	1	
5	B	1	Total	K	0
			1	1	

GLY	ILE	ASP	PRO	PHE	THR	SER	THR	GLN	THR	ALA	GLU	ASP	LYS	GLU	GLY	P70	L71	H72	S73	I74	I75	S76	S77	T78	E79	S80	V81	Q82	G83	S84	K87	F90	D99	I100	V101	A102	R103	S104	L105	E108	K109	E110	N119	R128	H129	K130	D134	G135	Q136	A137	L138										
M141	L145	Q146	E150	T155	I156	M163	E166	E167	M171	L172	G173	R177	S178	G179	A186	L187	Q188	N189	Q190	A191	E192	I197	I198	M210	V211	A212	E216	V217	R220	P224	G225	G228	W231	T241	R248	I253	I254	I255	D260	C261																					
K262	S265	R271	D272	V273	V274	T275	N279	F280	N288	M292	N293	T294	L295	Q296	A297	I298	W299	D302	P303	K304	D305	E308	W309	Q310	Y317	H322	Y327	H330	D334	A335	N338	I339	R340	S341	I342	V345	K349	P350	S351	M352	F353	D354	R357																		
E358	LEU	GLY	SER	S362	L365	R368	L371	I372	Q373	T374	K375	A376	T377	D378	L380	P381	T382	W383	L384	I387	E394	D395	I396	P397	L404	L405	Q406	E407	S408	A409	L410	I411	E450	Y470	E471	S472	L475	G478	Y486	M490	R491	A492	G493	T494	R495																
P503	N504	L507	K518	K519	K520	D521	T522	E523	V524	L525	F526	C527	D532	R540	E541	K544	K545	D557	HIS	TYR	LYS	GLU	GLY	LYS	PHE	GLU	ASP	ARG	SER	PRO	ALA	ALA	C573	L574	K577	E578	E581	L582	M583	A584	R587	N588	V589	L590	G591	S592	R593	V597													
L601	R602	L603	D604	M609	R619	H620	F621	L622	R623	L625	M624	Q625	Q626	LEU	ALA	LYS	THR	Q631	E632	E633	R634	A635	Q636	L637	L638	Q639	P640	T641	L642	E643	L650	K653	L654	R655	Q656	L657	R658	A659	S660	E661	P662	Q663	L664	A665	Q666	E674	N675	A680	G681	L682	V683	D684	D685								
P686	R687	A688	M689	V690	G691	R692	E695	V698	K699	A700	L701	E702	R703	H704	GLY	GLY	SER	GLY	SER	TRP	SER	ILE	SER	ASP	GLY	ALA	GLN	VAL	LYS	ASP	PHE	TYR	LEU	GLY	LEU	SER	PRO	GLY	LYS	THR	TYR	THR	PHE	VAL	GLU	THR	ALA	ALA	THR	HIS	ILE	LYS	PHE	SER	LYS	ARG	ASP				
GLU	ASP	GLY	LYS	GLU	LEU	ALA	GLY	ALA	ALA	THR	MET	GLY	LYS	LEU	ALA	THR	ARG	ASP	LYS	SER	GLY	ASP	GLY	LYS	THR	ILE	SER	ASP	GLY	ALA	GLN	VAL	LYS	ASP	PHE	TYR	LEU	GLY	LEU	TYR	PRO	GLY	LYS	THR	TYR	THR	PHE	VAL	GLU	THR	ALA	ALA	THR	HIS	ILE	LYS	PHE	SER	LYS	ARG	ASP
VAL	ASN	GLU	GLN	GLY	GLN	VAL	THR	VAL	VAL	ASN	GLY	LYS	ALA	THR	LYS	GLY	ASP	GLY	ASP	GLY	ASP	GLY	ASP	GLY	THR	ILE	SER	ASP	GLY	ALA	GLN	VAL	LYS	ASP	PHE	TYR	LEU	GLY	LEU	TYR	PRO	GLY	LYS	THR	TYR	THR	PHE	VAL	GLU	THR	ALA	ALA	THR	HIS	ILE	LYS	PHE	SER	LYS	ARG	ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	70998	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	69	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.058	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	260.48, 260.48, 260.48	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.814, 0.814, 0.814	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: K, MG, ADP, BEF

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	0.08	0/4941	0.23	0/6661
1	B	0.08	0/4988	0.24	1/6723 (0.0%)
All	All	0.08	0/9929	0.24	1/13384 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	662	PRO	CA-N-CD	-5.29	104.59	112.00

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	4856	0	4902	99	0
1	B	4903	0	4940	95	0
2	A	27	0	12	2	0
2	B	27	0	12	4	0
3	A	4	0	0	0	0
3	B	4	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	9825	0	9866	175	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 9.

All (175) 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:96:LYS:H	1:B:177:ARG:HH21	1.39	0.70
1:A:603:LEU:HD22	1:A:606:HIS:HB2	1.73	0.68
1:A:574:LEU:HB2	1:A:646:PRO:HB3	1.74	0.68
1:A:216:GLU:HB2	1:A:254:ILE:HB	1.77	0.67
1:A:687:ARG:HB3	1:B:507:LEU:HD11	1.78	0.65
1:B:220:ARG:HB3	1:B:228:GLY:HA2	1.78	0.65
1:A:218:TYR:HB2	1:A:252:LYS:HB3	1.78	0.65
1:B:146:GLN:NE2	1:B:288:ASN:OD1	2.31	0.64
1:B:146:GLN:HB3	1:B:155:THR:HB	1.80	0.63
1:B:217:VAL:HB	1:B:231:TRP:HB3	1.80	0.63
1:A:271:ARG:HD3	1:A:290:ARG:HH22	1.63	0.62
1:B:102:ALA:HA	1:B:210:MET:HG2	1.81	0.62
1:B:216:GLU:HB3	1:B:254:ILE:HB	1.82	0.62
1:A:662:PRO:O	1:A:666:GLN:NE2	2.33	0.61
1:A:119:ASN:ND2	2:A:901:ADP:O1A	2.34	0.61
1:A:629:LYS:HG2	1:B:504:ASN:HD21	1.66	0.60
1:A:685:ASP:OD2	1:A:687:ARG:NH1	2.35	0.60
1:A:607:PRO:HB2	1:A:672:ILE:HD11	1.84	0.59
1:A:142:GLU:HG2	1:A:284:PRO:HB2	1.85	0.59
1:A:146:GLN:HB3	1:A:155:THR:HB	1.85	0.59
1:A:339:ILE:HD13	1:A:393:SER:HB2	1.84	0.59
1:A:589:VAL:HG23	1:A:590:LEU:HG	1.84	0.58
1:A:469:ARG:HB3	1:A:480:LEU:HB3	1.85	0.58
1:A:125:GLU:HG2	1:A:196:LYS:HB2	1.86	0.58
1:A:185:ASP:O	1:A:188:GLN:NE2	2.37	0.58
1:B:275:THR:O	1:B:279:ASN:ND2	2.33	0.58
1:A:94:THR:HG21	1:B:90:PHE:HB3	1.85	0.57
1:B:296:GLN:NE2	1:B:310:GLN:OE1	2.37	0.57
1:B:119:ASN:ND2	2:B:901:ADP:O1A	2.36	0.57
1:A:107:SER:HB2	1:B:406:GLN:H	1.70	0.57
1:B:470:TYR:HB2	1:B:525:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:O	1:A:274:VAL:HG23	2.05	0.56
1:A:311:HIS:ND1	1:A:344:TYR:OH	2.35	0.56
1:B:330:HIS:HD2	1:B:342:ILE:HD12	1.71	0.55
1:B:491:ARG:HG3	1:B:493:GLY:H	1.71	0.55
1:B:490:MET:HE1	1:B:545:LYS:HG2	1.87	0.55
1:A:695:GLU:O	1:A:699:LYS:NZ	2.39	0.55
1:B:589:VAL:O	1:B:593:ARG:NH1	2.40	0.55
1:B:198:ILE:HG12	1:B:368:ARG:HB3	1.89	0.54
1:B:146:GLN:O	1:B:155:THR:N	2.33	0.54
1:B:171:ASN:HB3	2:B:901:ADP:H4'	1.90	0.54
1:B:186:ALA:O	1:B:188:GLN:NE2	2.41	0.54
1:B:334:ASP:OD1	1:B:340:ARG:NH2	2.41	0.54
1:B:275:THR:O	1:B:317:TYR:OH	2.26	0.53
1:B:351:SER:HB3	1:B:354:ASP:HB2	1.89	0.53
1:B:212:ALA:HB2	1:B:255:ILE:HG23	1.91	0.53
1:B:365:LEU:HG	1:B:372:ILE:HD13	1.91	0.52
1:B:472:SER:H	1:B:475:LEU:HD21	1.74	0.52
1:A:245:SER:HB2	1:B:82:GLN:HB2	1.91	0.52
1:A:95:LYS:NZ	1:A:236:SER:O	2.39	0.52
1:B:695:GLU:OE1	1:B:699:LYS:NZ	2.39	0.52
1:A:212:ALA:HB2	1:A:255:ILE:HG23	1.92	0.51
1:A:124:LEU:HD22	1:A:141:MET:HB2	1.92	0.51
1:A:579:THR:HG22	1:A:583:MET:HE3	1.91	0.51
1:B:179:GLY:N	2:B:901:ADP:O3'	2.40	0.51
1:A:365:LEU:HD13	1:A:379:ILE:HD13	1.93	0.51
1:A:574:LEU:HG	1:A:652:LYS:HG2	1.93	0.51
1:B:197:ILE:O	1:B:368:ARG:NH1	2.44	0.51
1:A:107:SER:HA	1:B:405:LEU:HD22	1.93	0.50
1:B:491:ARG:HE	1:B:492:ALA:H	1.58	0.50
1:A:408:SER:HB3	1:A:411:ILE:HG12	1.93	0.50
1:B:327:TYR:HB2	1:B:345:VAL:HB	1.94	0.50
1:B:637:LEU:O	1:B:639:GLN:NE2	2.44	0.50
1:A:146:GLN:HB2	1:B:75:ILE:HG13	1.94	0.50
1:A:217:VAL:HB	1:A:231:TRP:HB3	1.94	0.50
1:B:303:PRO:HG3	1:B:330:HIS:ND1	2.27	0.50
1:A:93:GLU:C	1:B:177:ARG:HH22	2.19	0.50
1:A:423:ILE:HG21	1:A:463:ASP:HB3	1.94	0.49
1:B:330:HIS:CD2	1:B:342:ILE:HD12	2.48	0.49
1:A:162:GLY:HA3	1:A:221:SER:HA	1.93	0.49
1:B:108:GLU:HB3	1:B:110:GLU:HG2	1.95	0.49
1:B:101:VAL:HG22	1:B:105:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:PRO:HG3	1:A:613:LEU:HG	1.95	0.48
1:B:272:ASP:OD1	1:B:273:VAL:N	2.46	0.48
1:B:382:LYS:NZ	1:B:450:GLU:OE2	2.44	0.48
1:B:701:LEU:HB2	1:B:704:HIS:CE1	2.48	0.48
1:B:128:ARG:HB2	1:B:141:MET:HE3	1.95	0.48
1:B:145:LEU:HD13	1:B:156:ILE:HG12	1.95	0.48
1:B:621:PHE:HD2	1:B:622:LEU:HD12	1.79	0.48
1:A:375:LYS:HG2	1:A:377:THR:HG23	1.96	0.48
1:B:674:GLU:OE2	1:B:692:ARG:NH1	2.47	0.48
1:A:275:THR:O	1:A:317:TYR:OH	2.31	0.48
1:A:681:GLY:HA2	1:B:687:ARG:HH22	1.79	0.48
1:A:165:GLN:HB2	1:A:229:TYR:CZ	2.49	0.48
1:A:603:LEU:HD12	1:A:645:ASN:HB3	1.96	0.48
1:A:75:ILE:HG21	1:B:146:GLN:HG2	1.96	0.47
1:A:382:LYS:O	1:A:385:ARG:NH2	2.46	0.47
1:A:381:PRO:HD2	1:A:384:LEU:HD12	1.95	0.47
1:B:262:LYS:O	1:B:265:SER:OG	2.31	0.47
1:A:108:GLU:OE1	1:A:110:GLU:HG3	2.14	0.47
1:A:101:VAL:HG11	1:A:206:TYR:HB2	1.95	0.47
1:A:153:THR:OG1	1:A:255:ILE:O	2.23	0.47
1:A:274:VAL:HG11	1:A:285:LEU:HD22	1.97	0.47
1:A:284:PRO:HB3	1:A:291:ARG:HD2	1.97	0.47
1:B:374:THR:HG21	1:B:404:LEU:HB3	1.96	0.47
1:B:582:LEU:HA	1:B:658:ARG:HH22	1.79	0.47
1:A:678:ILE:HD13	1:B:689:MET:HE1	1.97	0.47
1:A:463:ASP:HA	1:A:466:LYS:HE2	1.97	0.47
1:B:368:ARG:HE	1:B:394:GLU:HB2	1.80	0.47
1:B:583:MET:HG3	1:B:587:ARG:HH21	1.80	0.47
1:A:491:ARG:NH2	1:A:521:ASP:HB3	2.31	0.46
1:B:503:PRO:HG2	1:B:507:LEU:HD13	1.97	0.46
1:B:163:MET:HE1	1:B:171:ASN:HB2	1.95	0.46
1:A:621:PHE:HE1	1:A:634:ARG:HB3	1.79	0.46
1:A:335:ALA:HB3	1:A:336:PRO:HD3	1.97	0.46
1:A:629:LYS:HD3	1:B:503:PRO:HB2	1.96	0.46
1:B:619:ARG:NE	1:B:680:ALA:O	2.32	0.46
1:B:475:LEU:H	1:B:475:LEU:HD23	1.81	0.45
1:A:231:TRP:HD1	1:A:241:ILE:HD12	1.80	0.45
1:B:299:TRP:HA	1:B:330:HIS:NE2	2.31	0.45
1:B:486:TYR:OH	1:B:523:GLU:O	2.30	0.45
1:A:205:PHE:N	2:A:901:ADP:O1A	2.49	0.45
1:B:217:VAL:HG22	1:B:253:ILE:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:ASP:HB3	1:B:305:ASP:CG	2.41	0.45
1:A:281:VAL:HG12	1:A:283:PHE:H	1.81	0.45
1:A:669:VAL:HA	1:A:672:ILE:HG22	1.99	0.45
1:A:110:GLU:HB3	1:A:264:PHE:HE1	1.82	0.45
1:A:336:PRO:HG3	1:A:417:VAL:HG21	1.99	0.45
1:A:94:THR:HB	1:A:98:LEU:HD23	1.99	0.44
1:A:189:ASN:OD1	1:A:190:GLN:N	2.50	0.44
1:A:97:LEU:HD13	1:A:175:ILE:HG21	1.99	0.44
1:B:397:PRO:HG2	1:B:405:LEU:HD12	1.99	0.44
1:B:101:VAL:HA	1:B:105:LEU:HB2	1.98	0.44
1:B:597:VAL:HA	1:B:642:LEU:O	2.17	0.44
1:B:99:ASP:O	1:B:103:ARG:HB2	2.17	0.44
1:B:503:PRO:HD2	1:B:507:LEU:HD22	1.99	0.44
1:A:604:ASP:OD1	1:A:604:ASP:N	2.51	0.43
1:B:603:LEU:HD23	1:B:603:LEU:HA	1.90	0.43
1:B:638:LEU:HD23	1:B:640:PRO:HG3	2.01	0.43
1:A:230:GLN:O	1:A:242:ALA:N	2.39	0.43
1:A:323:ASP:OD1	1:A:323:ASP:N	2.50	0.43
1:A:101:VAL:HG22	1:A:105:LEU:HD22	2.01	0.43
1:A:127:LEU:HD13	1:A:161:ILE:HA	2.00	0.43
1:A:458:GLN:NE2	1:A:462:GLU:OE2	2.47	0.43
1:B:379:ILE:HD11	1:B:411:ILE:HD11	2.01	0.43
1:A:679:ALA:HB2	1:B:690:VAL:HG21	2.01	0.42
1:B:338:ASN:OD1	1:B:340:ARG:NH2	2.52	0.42
1:A:583:MET:HA	1:A:586:MET:HB2	2.01	0.42
1:A:301:MET:HE2	1:A:306:VAL:HB	2.02	0.42
1:A:653:LYS:HE2	1:B:702:GLU:HA	2.02	0.42
2:B:901:ADP:O1B	3:B:902:BEF:F2	2.27	0.42
1:B:638:LEU:HD21	1:B:682:LEU:HD13	2.02	0.41
1:A:154:ILE:HG22	1:A:257:LEU:HD21	2.02	0.41
1:A:101:VAL:HA	1:A:105:LEU:HB2	2.02	0.41
1:A:325:PRO:HB3	1:A:344:TYR:HB3	2.03	0.41
1:B:527:CYS:HB3	1:B:532:ASP:HB3	2.02	0.41
1:A:105:LEU:HD11	1:A:400:LEU:HG	2.02	0.41
1:A:344:TYR:N	1:A:388:ARG:O	2.44	0.41
1:B:294:THR:O	1:B:295:LEU:HD23	2.21	0.41
1:B:384:LEU:O	1:B:387:ILE:HG12	2.20	0.41
1:A:70:PRO:HB2	1:A:71:LEU:H	1.63	0.41
1:A:91:GLN:N	1:B:173:GLY:O	2.49	0.41
1:B:371:LEU:HG	1:B:373:GLN:H	1.85	0.41
1:A:112:PHE:CZ	1:A:211:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:LEU:HD12	1:B:381:PRO:HD2	2.02	0.41
1:A:614:GLU:O	1:A:617:ALA:N	2.54	0.41
1:B:609:MET:HE3	1:B:609:MET:HB2	1.92	0.41
1:B:642:LEU:HD23	1:B:643:GLU:N	2.36	0.41
1:A:93:GLU:H	1:B:177:ARG:HH12	1.67	0.41
1:A:293:ASN:OD1	1:A:293:ASN:N	2.53	0.41
1:A:514:TYR:O	1:A:518:LYS:N	2.51	0.41
1:A:653:LYS:HD3	1:B:701:LEU:HG	2.03	0.41
1:A:287:LEU:HB3	1:A:292:MET:HE1	2.02	0.41
1:A:693:LEU:HD23	1:B:675:ASN:HD21	1.86	0.41
1:A:547:LEU:HD23	1:A:547:LEU:HA	1.90	0.40
1:A:598:LYS:HB2	1:A:598:LYS:HE3	1.87	0.40
1:B:653:LYS:HB3	1:B:653:LYS:HE3	1.65	0.40
1:A:88:HIS:HE1	1:B:241:ILE:HG22	1.87	0.40
1:A:213:ASP:N	1:A:213:ASP:OD1	2.52	0.40
1:B:271:ARG:HA	1:B:292:MET:HE1	2.03	0.40
1:B:280:PHE:HB3	1:B:297:ALA:HB2	2.03	0.40
1:B:354:ASP:OD1	1:B:357:ARG:NH2	2.50	0.40
1:A:108:GLU:CD	1:A:110:GLU:HG3	2.46	0.40
1:A:373:GLN:HG3	1:A:376:ALA:HB2	2.02	0.40
1:A:384:LEU:O	1:A:387:ILE:HG12	2.22	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	601/774 (78%)	578 (96%)	23 (4%)	0	100	100
1	B	605/774 (78%)	584 (96%)	21 (4%)	0	100	100
All	All	1206/1548 (78%)	1162 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	528/666 (79%)	528 (100%)	0	100	100
1	B	534/666 (80%)	534 (100%)	0	100	100
All	All	1062/1332 (80%)	1062 (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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	GLN
1	A	406	GLN
1	A	419	GLN
1	A	704	HIS
1	B	91	GLN
1	B	136	GLN
1	B	429	GLN
1	B	506	HIS
1	B	510	HIS
1	B	639	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	BEF	B	902	-	0,3,3	-	-	-		
2	ADP	A	901	5,4	24,29,29	0.92	1 (4%)	29,45,45	1.20	2 (6%)
2	ADP	B	901	5,4	24,29,29	0.92	0	29,45,45	1.19	2 (6%)
3	BEF	A	902	-	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
2	ADP	A	901	5,4	-	5/12/32/32	0/3/3/3
2	ADP	B	901	5,4	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	ADP	PA-O3A	2.02	1.61	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	ADP	N3-C2-N1	-3.68	123.68	128.67
2	B	901	ADP	N3-C2-N1	-3.66	123.70	128.67
2	A	901	ADP	C4-C5-N7	-2.61	106.58	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ADP	C4-C5-N7	-2.59	106.60	109.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

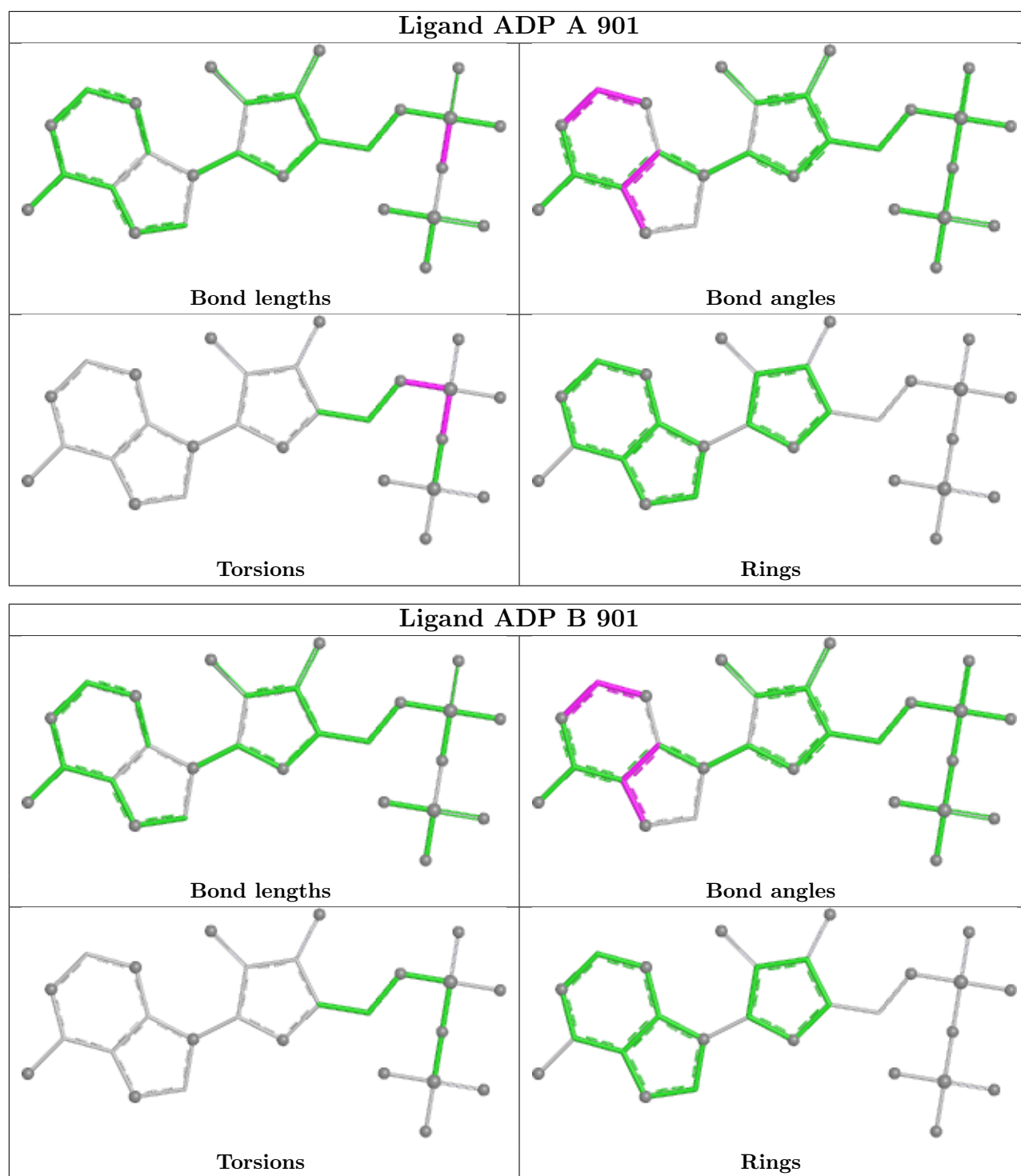
Mol	Chain	Res	Type	Atoms
2	A	901	ADP	C5'-O5'-PA-O2A
2	A	901	ADP	PB-O3A-PA-O5'
2	A	901	ADP	C5'-O5'-PA-O1A
2	A	901	ADP	C5'-O5'-PA-O3A
2	A	901	ADP	PB-O3A-PA-O2A

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	BEF	1	0
2	A	901	ADP	2	0
2	B	901	ADP	4	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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

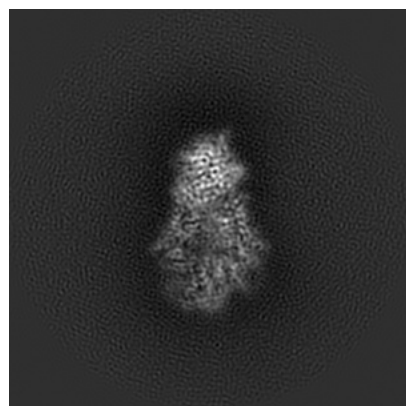
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22174. These allow visual inspection of the internal detail of the map and identification of artifacts.

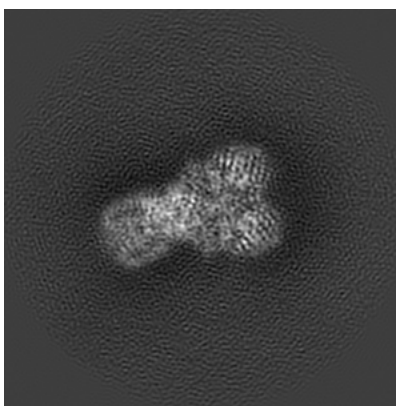
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

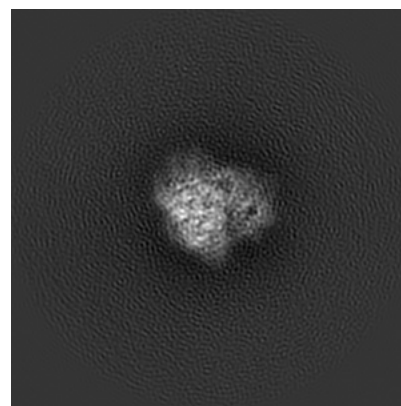
6.1.1 Primary map



X

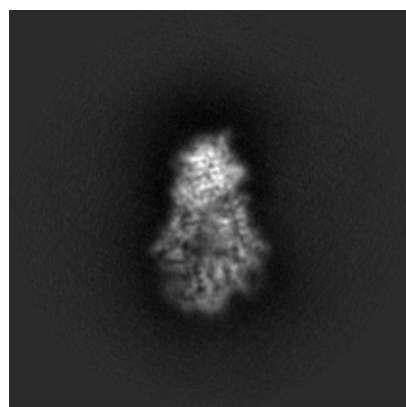


Y

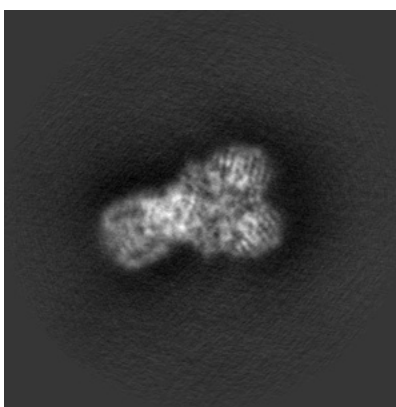


Z

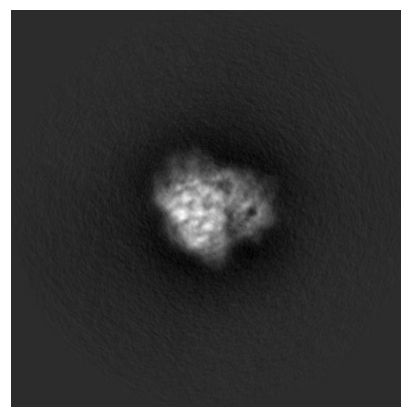
6.1.2 Raw map



X



Y

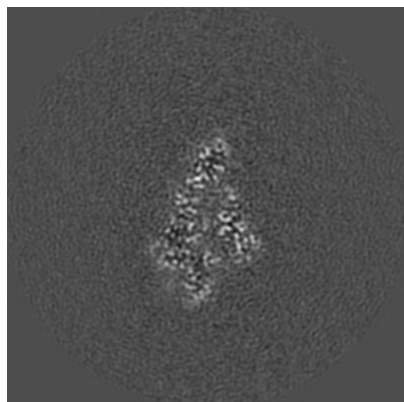


Z

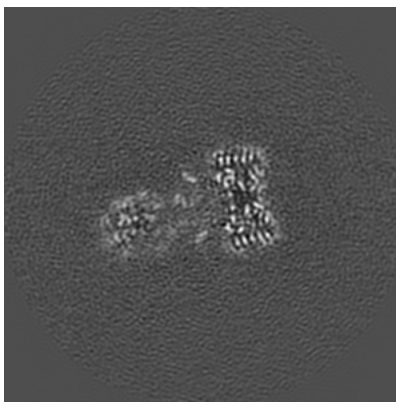
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

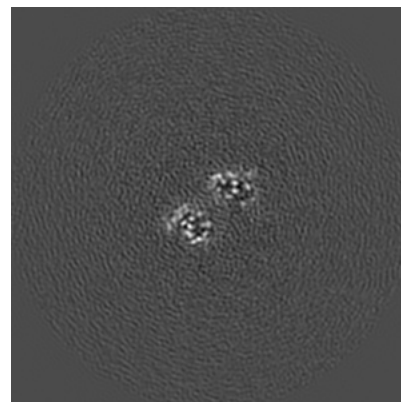
6.2.1 Primary map



X Index: 160

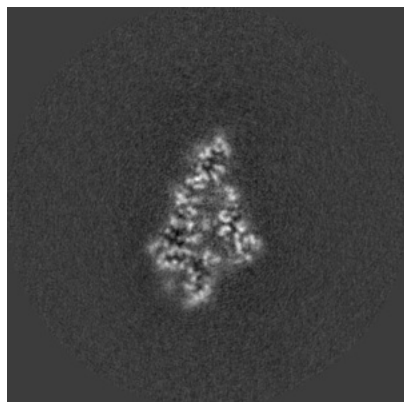


Y Index: 160

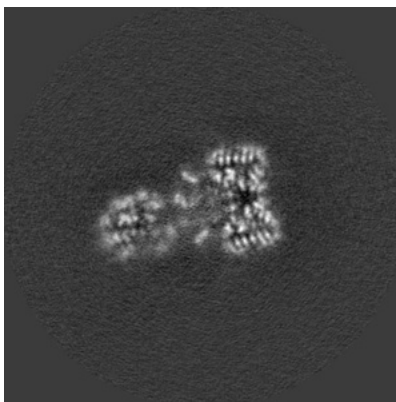


Z Index: 160

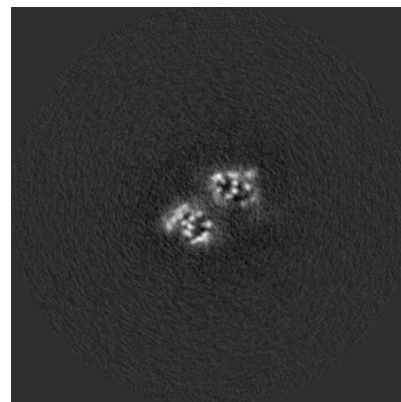
6.2.2 Raw map



X Index: 160



Y Index: 160

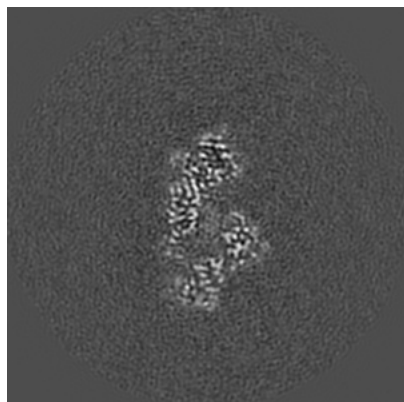


Z Index: 160

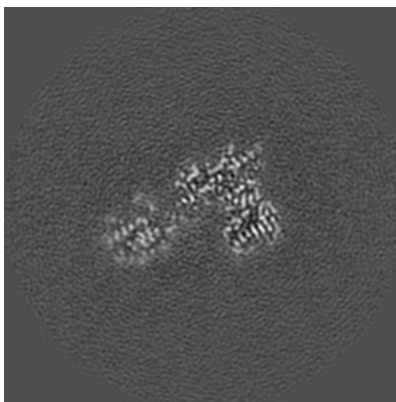
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

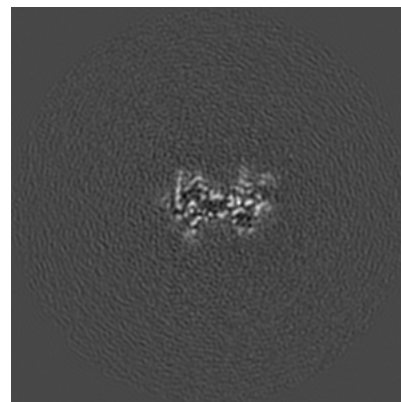
6.3.1 Primary map



X Index: 148

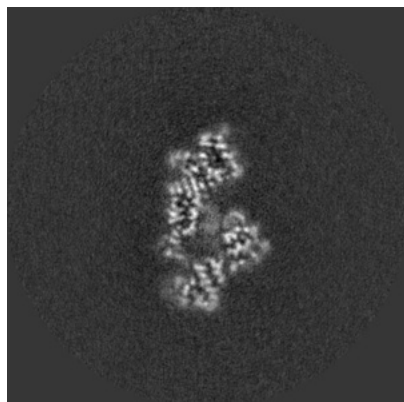


Y Index: 168

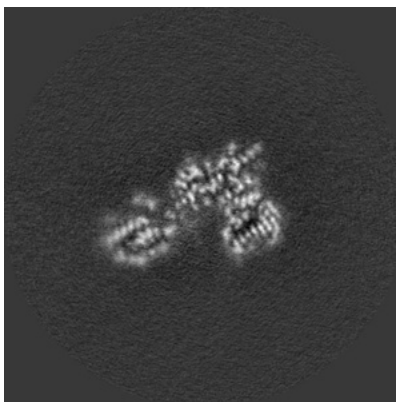


Z Index: 191

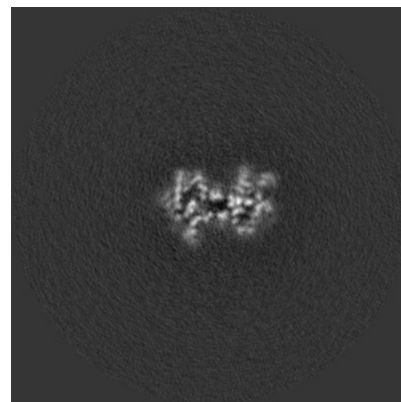
6.3.2 Raw map



X Index: 148



Y Index: 169

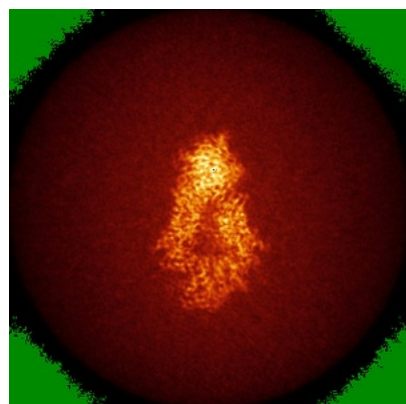


Z Index: 191

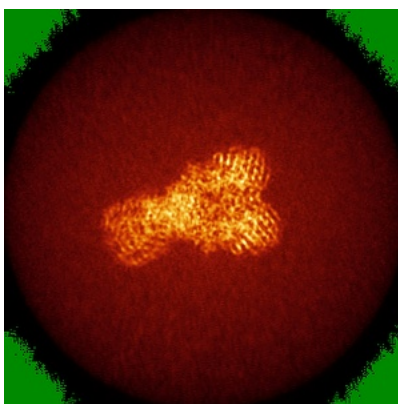
The images above show the largest variance slices of the map in three orthogonal directions.

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

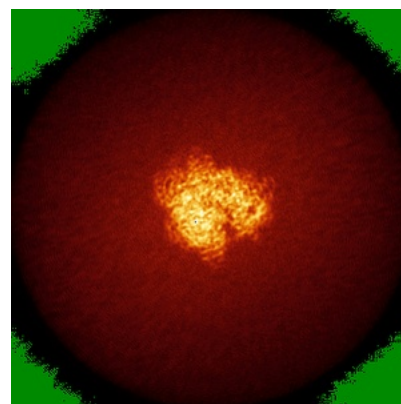
6.4.1 Primary map



X

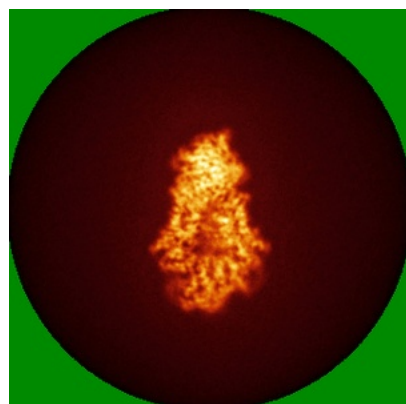


Y

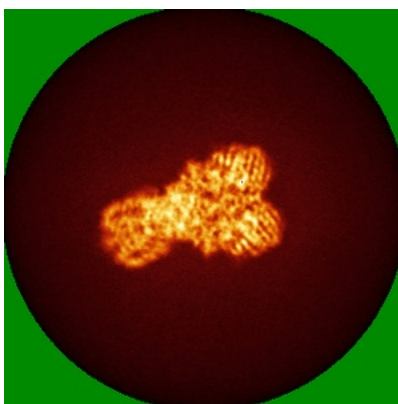


Z

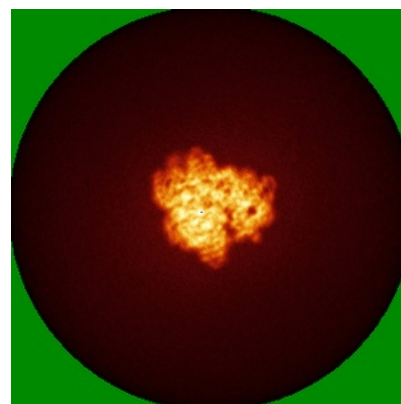
6.4.2 Raw map



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](#)

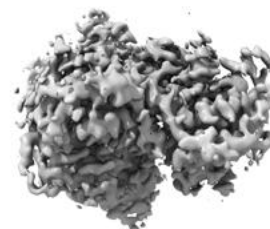
6.5.1 Primary map



X



Y



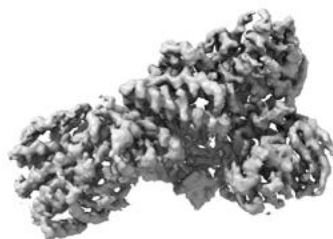
Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. 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



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.

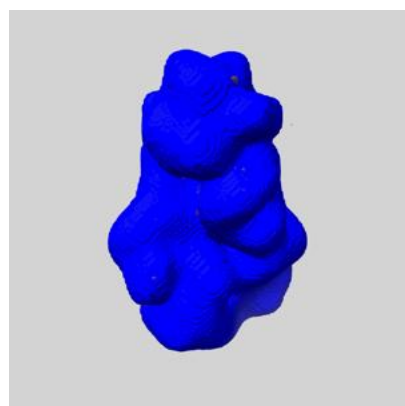
6.6 Mask visualisation [i](#)

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

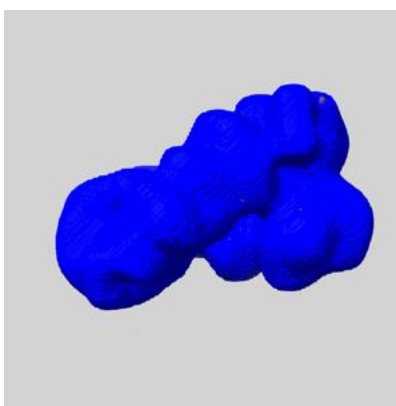
A mask typically either:

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

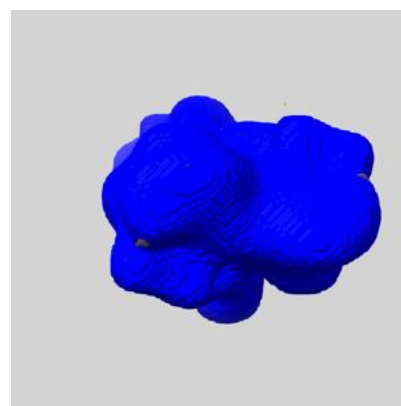
6.6.1 emd_22174_msk_1.map [i](#)



X



Y

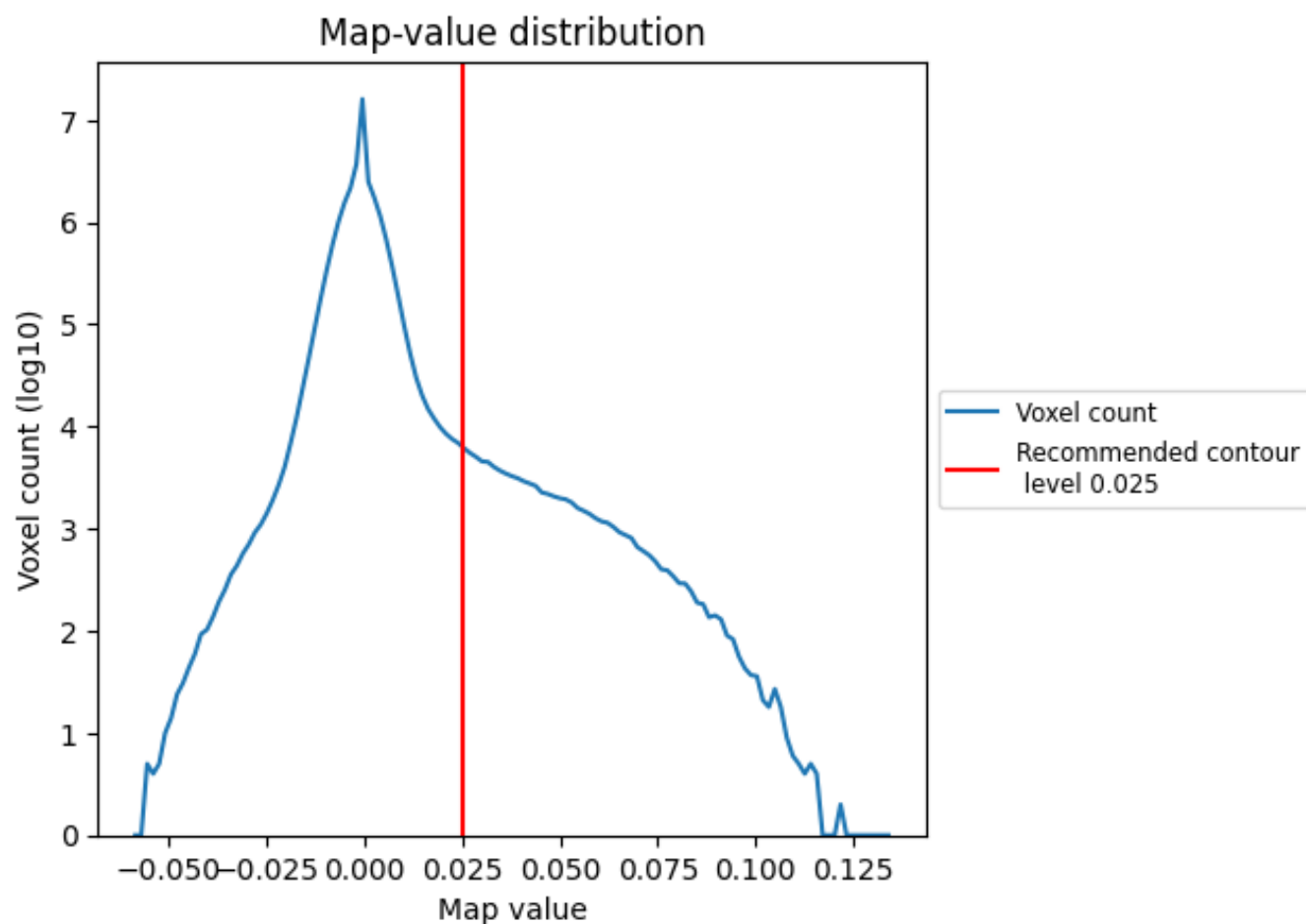


Z

7 Map analysis [i](#)

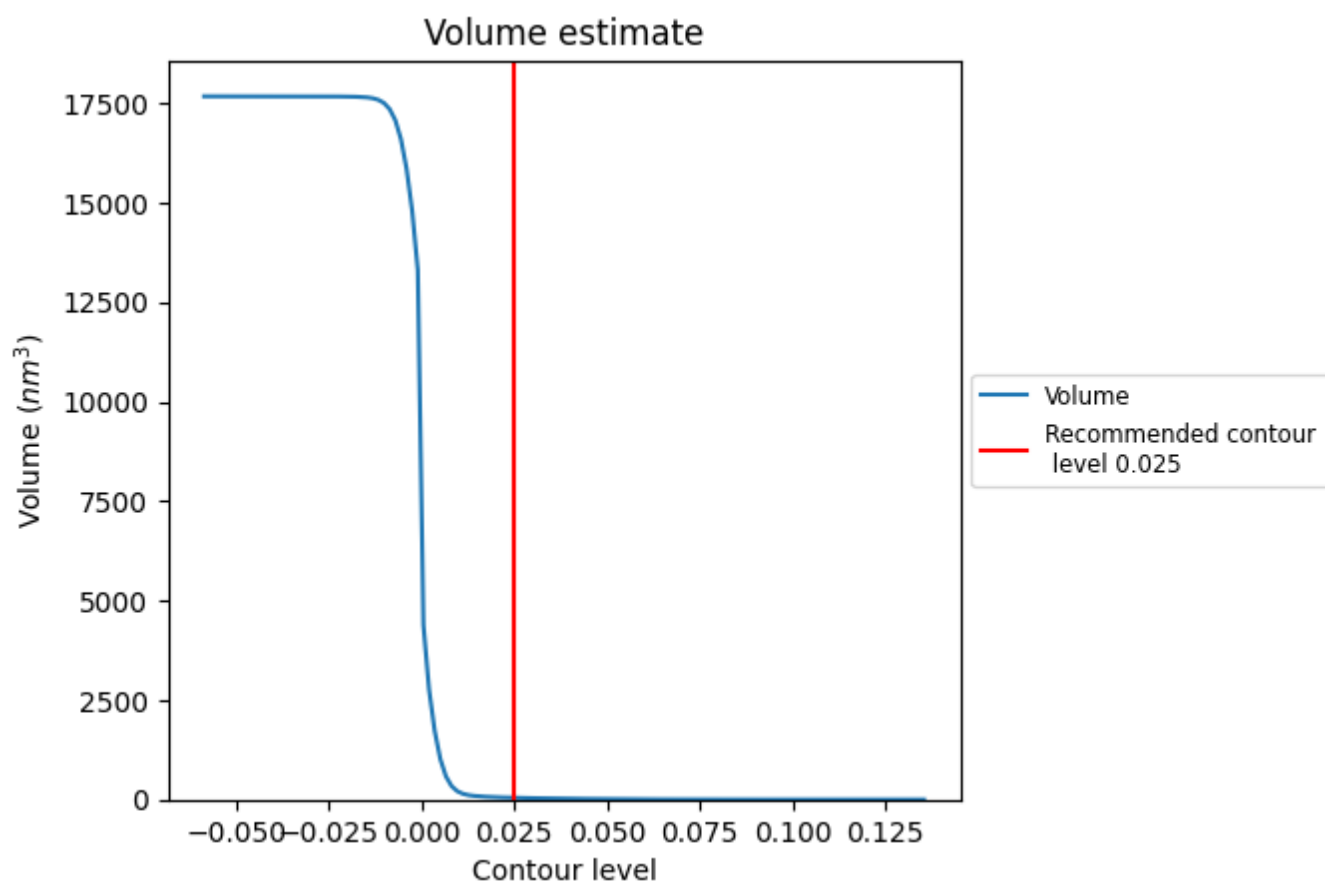
This section contains the results of statistical analysis of the map.

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.

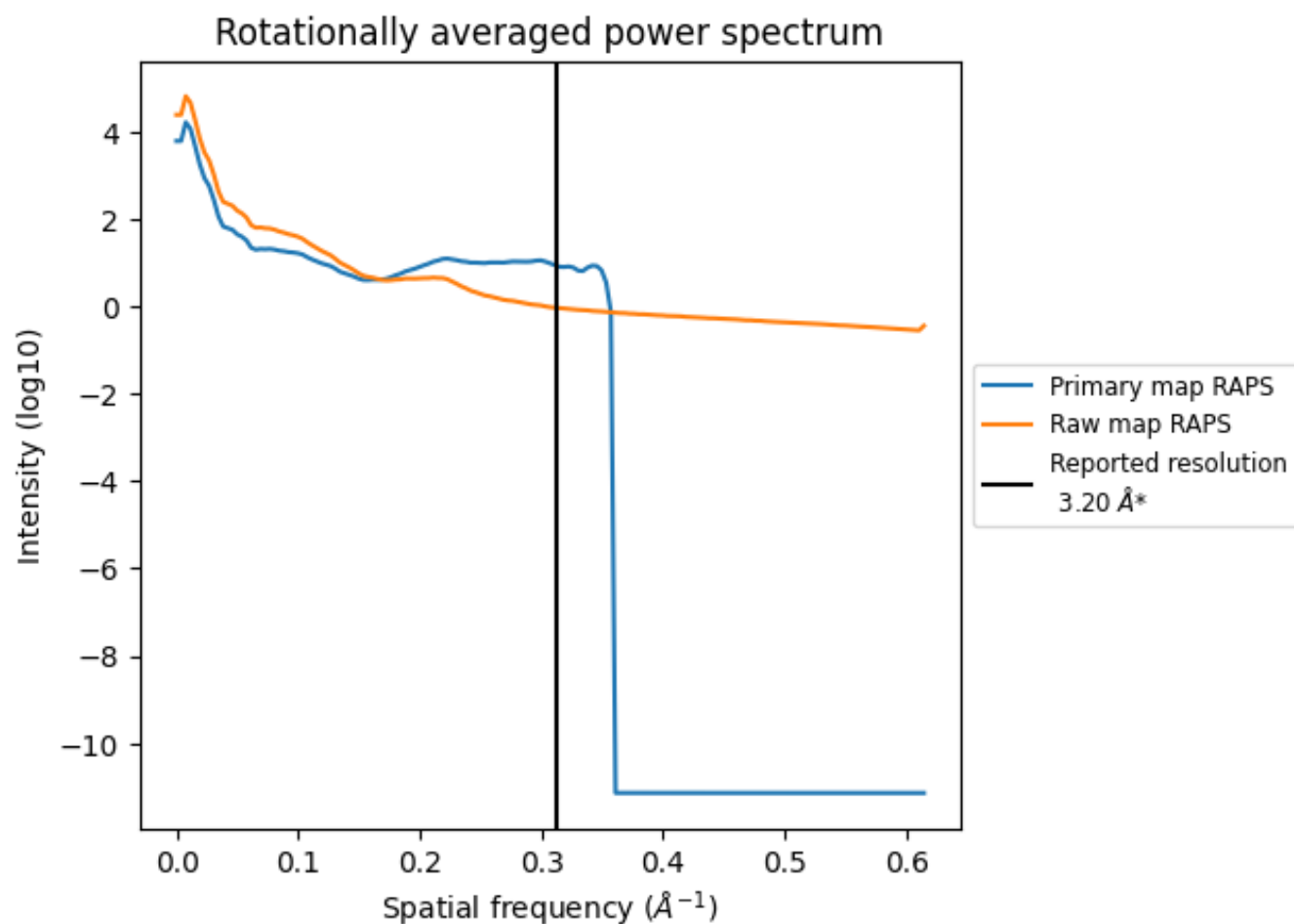
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 45 nm³; this corresponds to an approximate mass of 41 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 ⓘ

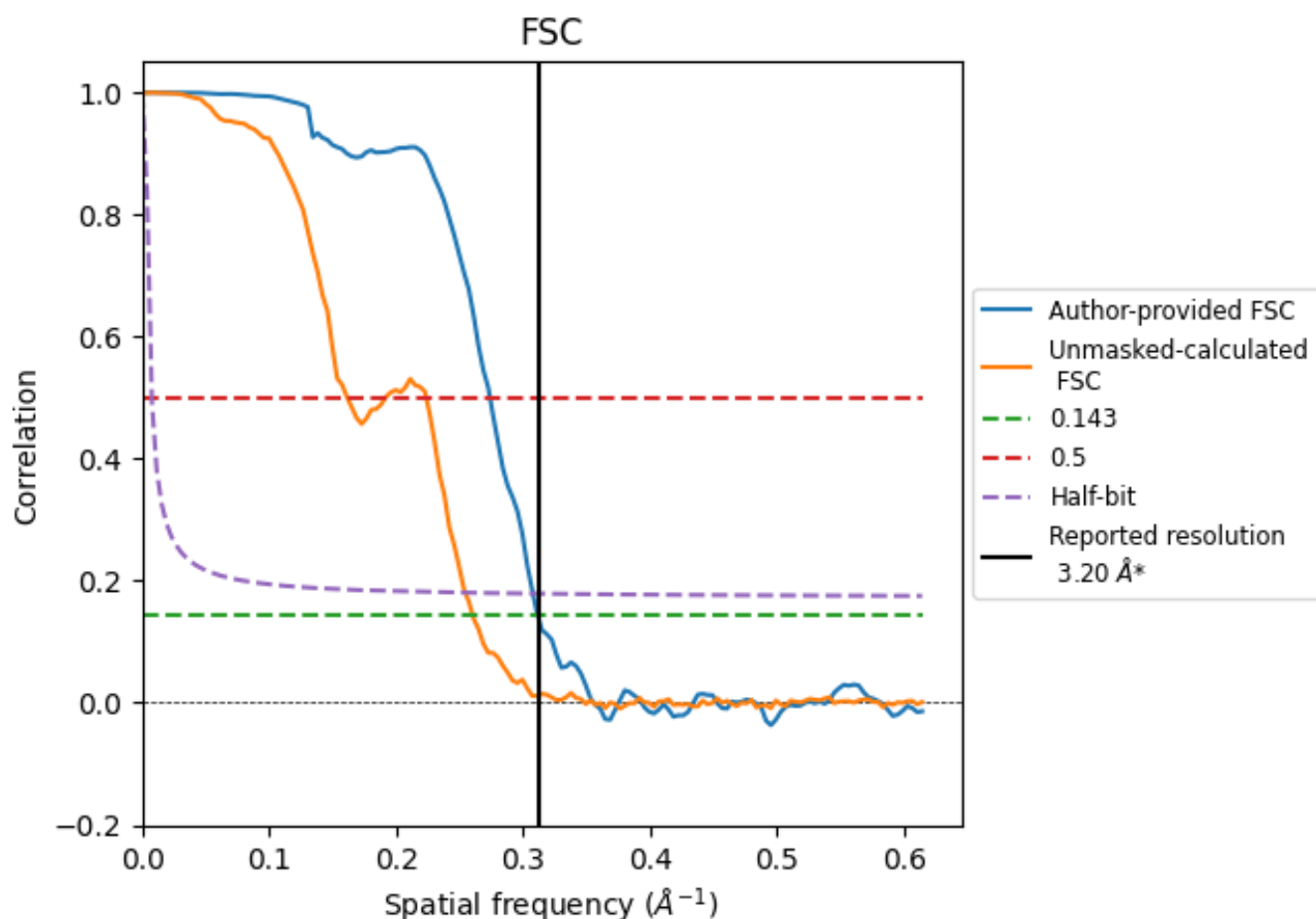


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 \AA^{-1}

8.2 Resolution estimates [i](#)

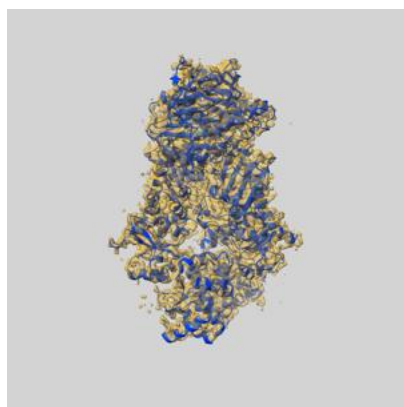
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.21	3.65	3.25
Unmasked-calculated*	3.84	6.19	3.93

*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 3.84 differs from the reported value 3.2 by more than 10 %

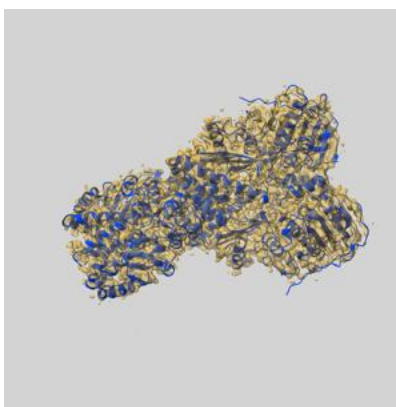
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22174 and PDB model 6XG6. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

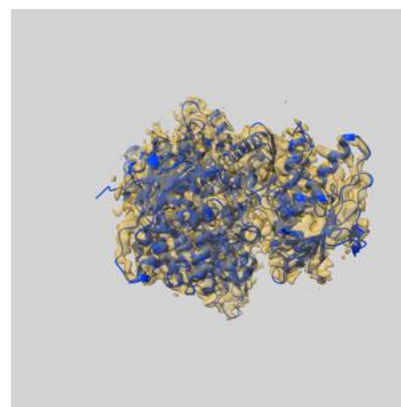
9.1 Map-model overlay [i](#)



X



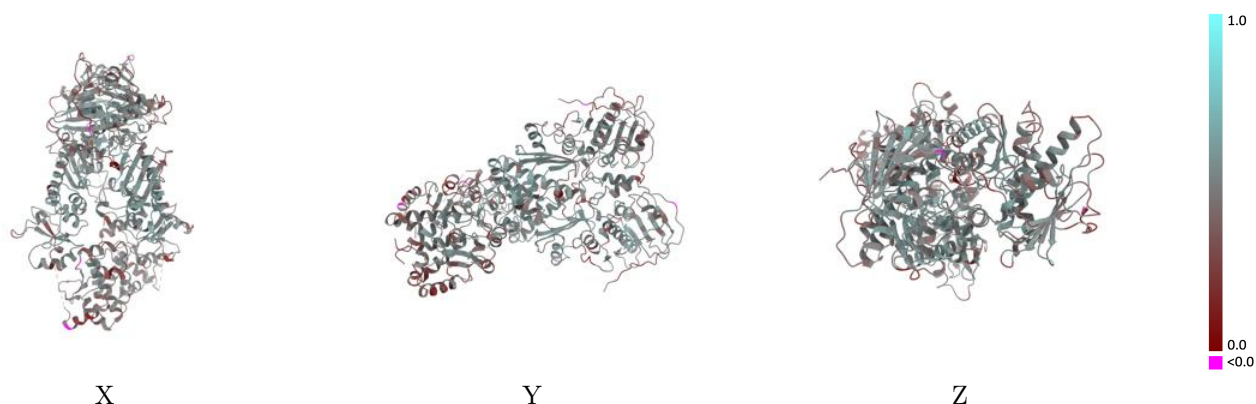
Y



Z

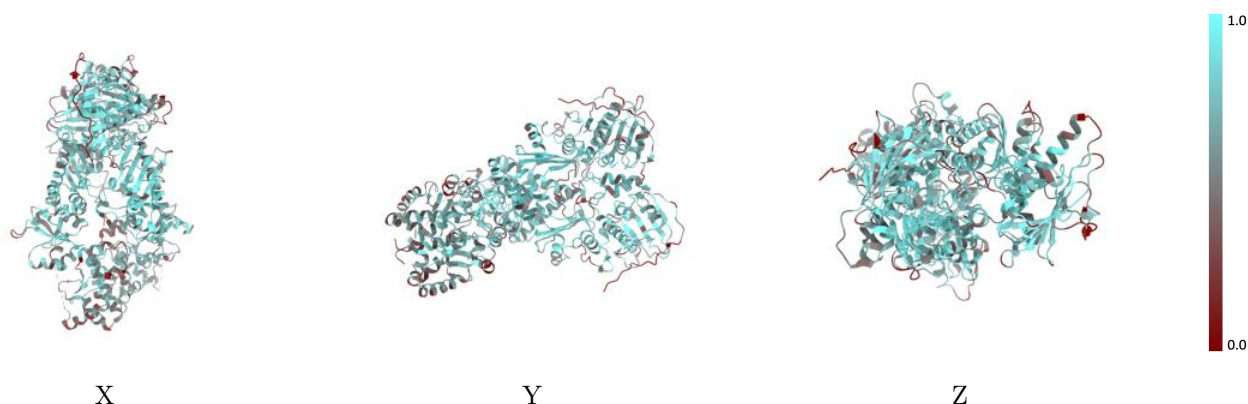
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



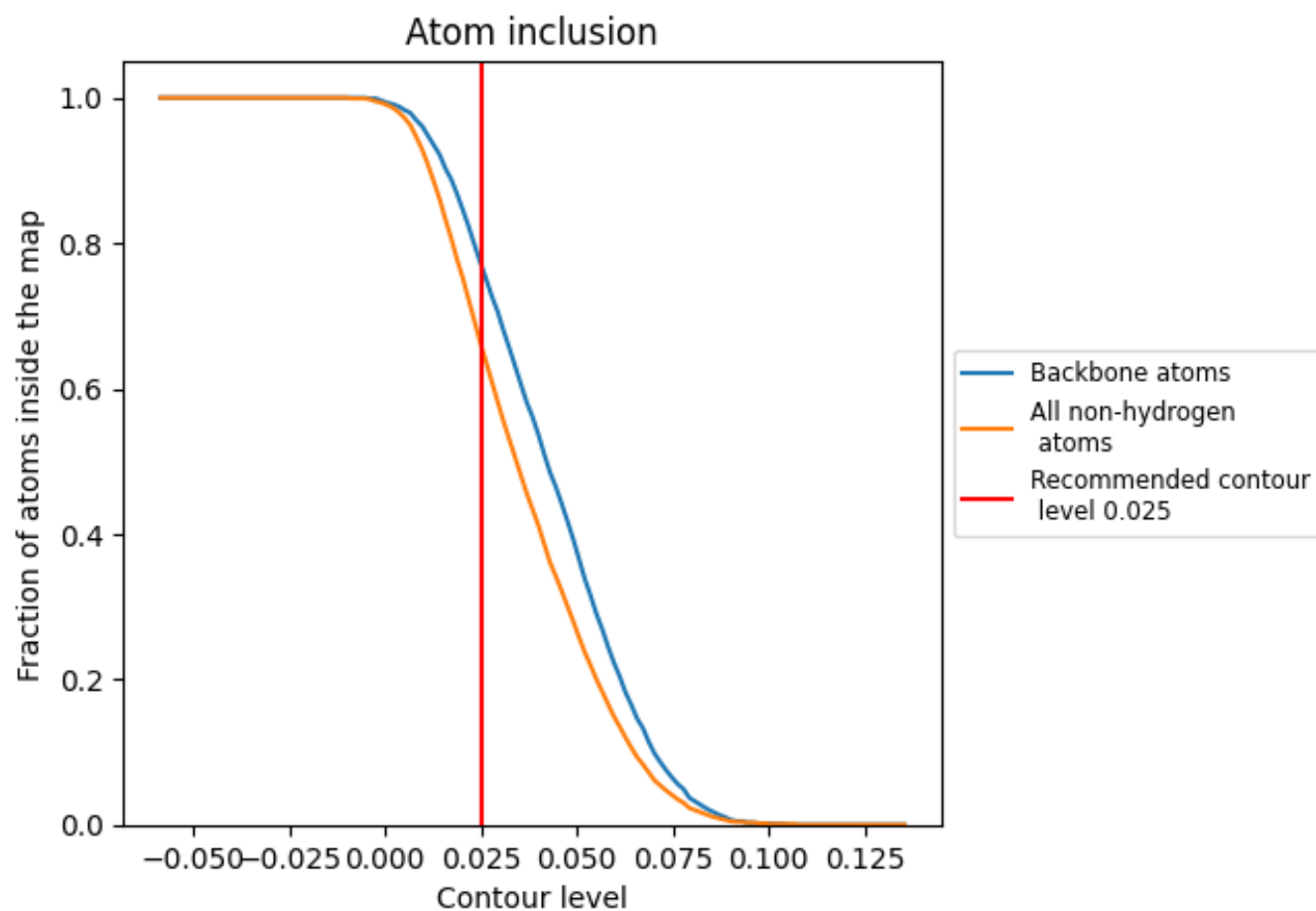
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.025).

9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 66% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6610	<div></div> 0.4670
A	<div></div> 0.6650	<div></div> 0.4690
B	<div></div> 0.6560	<div></div> 0.4640

