



Full wwPDB EM Validation Report ⓘ

Sep 16, 2024 – 10:16 AM EDT

PDB ID : 8UPH
EMDB ID : EMD-42448
Title : Prf state of Stigmatella aurantiaca bacteriophytochrome 2
Authors : Malla, T.N.; Schmidt, M.; Stojkovic, E.A.
Deposited on : 2023-10-22
Resolution : 4.13 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:

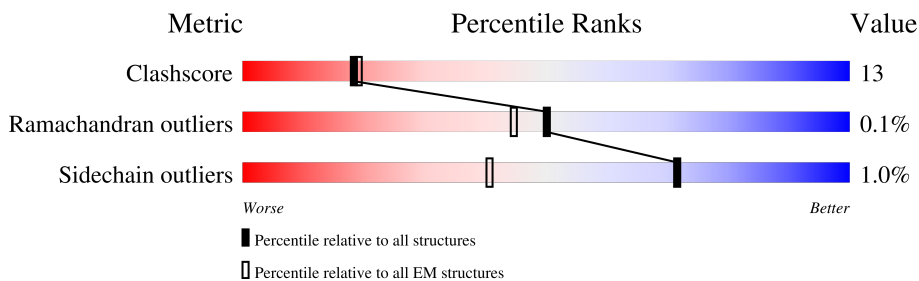
EMDB validation analysis : 0.0.1.dev112
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.3

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 4.13 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	747	
1	B	747	

2 Entry composition [i](#)

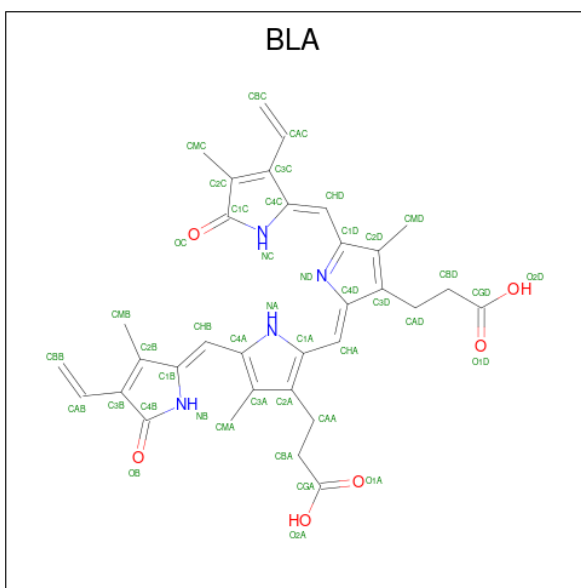
There are 2 unique types of molecules in this entry. The entry contains 8121 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bacteriophytochrome (Light-regulated signal transduction histidine kinase).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	538	4101	2591	746	754	10	0	0
1	B	516	3934	2483	719	723	9	1	0

- Molecule 2 is BILIVERDINE IX ALPHA (three-letter code: BLA) (formula: $C_{33}H_{34}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	43	33	4	6	0
2	B	1	43	33	4	6	0

R288	A289	C290	E291	T294	Q295	L299	Q300	L301	S302	R306	E309	R316	A317	A318	L319	P322	G331	T332	L333	E334	G352	L355	L356	L357	L363	R366	T367	M370	V373	W379	L380	F385	Q386	T387	Y398	L401	L411	V414	R415	L416																															
A417	R422	I423	A424	L425	W437	E448	R453	L454	H455	P456	G458	S459	F460	W463	K475	R476	A477	D478	A481	A482	E483	R486	S487	I490	V493	L494	R495	Q496	E499	R502	L503	S504	E505	A506	S508	R509	S510	N511	A512	E513	L514	D515	A516	F517	G518																										
H519	D524	LEU	LYS	GLU	PRO	LEU	ARG	GLY	ILE	GLN	GLN	TYR	ALA	GLY	PHE	VAL	MET	GLU	ASP	TYR	HIS	GLY	ALA	LEU	GLY	PRO	GLY	GLY	ARG	GLN	ARG	SER	LEU	MET	TRP	LEU	ALA	GLN	ASP	GLY	LEU	PHE	GLU	ASN	TYR	SER	ARG	ALA	GLY	ARG	VAL																				
ASP	LEU	ALA	TRP	GLY	VAL	ASN	MET	GLN	GLY	VAL	VAL	ASP	GLY	GLU	VAL	LEU	ALA	THR	LEU	SER	TYR	HIS	PHE	GLN	ALA	GLY	GLU	LYS	LEU	THR	VAL	ARG	MET	PRO	THR	THR	VAL	VAL	ARG	CYS	ASP	GLY	ILE	ARG	ILE	GLU	ALA	GLN	VAL	TRP	PHE	GLU	ALA	ASN	MET	PHE	LEU	LEU	ARG	VAL	VAL	ASN	ALA	ALA	SER	ALA	LYS	VAL			
TYR	GLN	GLU	GLY	PRO	GLY	THR	ARG	TRP	VAL	VAL	ALA	GLY	PHE	HIS	GLY	ARG	PRO	GLY	LEU	VAL	GLN	LEU	ARG	PRO	SER	GLY	GLY	ALA	ALA	ALA	TYR	VAL	VAL	PHE	VAL	TYR	PRO	GLY	ILE	ILE	GLY	ILE	ALA	PRO	PRO	PHE	HIS	HIS	GLU	GLU	ALA	ALA	ILE	PHE	GLU	ALA	ASN	MET	PHE	TYR	ARG	ARG	VAL	VAL	ASN	ALA	ALA	SER	ALA	LYS	ALA
LYS	ALA	TYR	GLY	GLY	THR	GLY	THR	GLY	VAL	LEU	ALA	ILE	ALA	ALA	ARG	ARG	LEU	GLN	LEU	HIS	HIS	GLY	GLY	ALA	ALA	LEU	TRP	VAL	VAL	ASP	SER	ALA	ALA	PRO	PRO	LYS	VAL	PHE	GLN	GLY	ALA	ALA	THR	PHE	TYR	PRO	PHE	THR	THR	LEU	GLY	ILE	ARG	GLY	PRO	PRO	GLY														

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	377549	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.39	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.353	Depositor
Minimum map value	-0.146	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	337.6, 337.6, 337.6	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.84400004, 0.84400004, 0.84400004	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: BLA

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	0.25	0/4191	0.54	0/5706
1	B	0.25	0/4020	0.55	0/5476
All	All	0.25	0/8211	0.54	0/11182

There are no bond length outliers.

There are no bond angle outliers.

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	4101	0	4125	109	0
1	B	3934	0	3962	105	0
2	A	43	0	30	7	0
2	B	43	0	31	9	0
All	All	8121	0	8148	210	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 13.

All (210) 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:126:ARG:HD3	1:B:288:ARG:HH21	1.49	0.78
1:B:83:ALA:HB1	1:B:94:ARG:HH22	1.52	0.74
1:B:309:GLU:HB2	1:B:476:ARG:HH21	1.56	0.70
1:A:516:ALA:HA	1:A:519:HIS:CE1	2.26	0.70
1:A:112:GLU:HG3	1:A:114:GLN:H	1.55	0.70
1:B:483:GLU:HA	1:B:486:ARG:HD3	1.72	0.70
1:A:330:GLY:O	1:A:495:ARG:NH1	2.25	0.69
1:A:417:ALA:HB2	1:B:494:LEU:HD22	1.75	0.68
1:A:490:ILE:HG21	1:B:486:ARG:HB3	1.76	0.68
1:B:385:PHE:O	1:B:415:ARG:NH1	2.27	0.68
1:A:490:ILE:HD13	1:B:490:ILE:HB	1.76	0.67
1:B:262:LEU:HD11	1:B:272:ILE:HG12	1.76	0.67
1:B:57:ALA:O	1:B:61:LYS:NZ	2.28	0.66
1:A:526:LYS:HA	1:A:529:LEU:HD13	1.77	0.66
1:B:194:PRO:HG3	2:B:801:BLA:HMD3	1.78	0.65
1:B:32:ALA:HB1	1:B:103:LEU:HD21	1.77	0.65
1:B:166:ASP:OD1	1:B:168:HIS:ND1	2.29	0.65
1:B:66:VAL:HG23	1:B:67:LEU:HD12	1.78	0.65
1:B:516:ALA:HA	1:B:519:HIS:CD2	2.32	0.64
1:A:77:LEU:HD12	1:A:81:ARG:HH12	1.63	0.63
1:A:536:ALA:O	1:A:539:VAL:HG12	1.99	0.63
1:A:487:SER:O	1:B:486:ARG:NH2	2.32	0.63
1:A:170:GLU:OE1	1:A:187:HIS:NE2	2.32	0.63
1:B:53:ARG:NH2	1:B:66:VAL:O	2.32	0.63
1:B:331:GLY:O	1:B:495:ARG:NH1	2.33	0.62
1:B:34:ARG:HB3	1:B:39:ARG:HB2	1.82	0.61
1:A:284:TYR:HA	1:A:287:ARG:HE	1.65	0.61
1:A:385:PHE:O	1:A:415:ARG:NH2	2.34	0.61
1:A:422:ARG:HG3	1:B:494:LEU:HD21	1.83	0.61
1:A:380:LEU:HD23	1:A:423:LEU:HD13	1.83	0.60
1:A:299:LEU:HD21	1:B:299:LEU:HB3	1.82	0.60
1:A:487:SER:O	1:A:490:ILE:HG22	2.02	0.59
1:B:20:LEU:HD12	1:B:230:PRO:HD2	1.85	0.59
1:A:61:LYS:HD3	1:A:62:THR:H	1.67	0.59
1:A:323:LEU:HD12	1:A:343:ARG:HB3	1.85	0.59
1:A:502:ARG:O	1:A:505:GLU:HG3	2.03	0.59
1:B:207:ARG:HD2	2:B:801:BLA:HBA2	1.85	0.58
1:A:94:ARG:HD3	1:A:284:TYR:HB3	1.84	0.58
1:A:150:ARG:NH2	1:A:175:SER:O	2.36	0.58
1:B:363:LEU:HB2	1:B:367:THR:HG21	1.84	0.57
1:A:33:PHE:HB2	1:A:104:THR:HB	1.87	0.57
1:A:540:MET:O	1:A:544:HIS:ND1	2.29	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:LEU:HD11	1:B:424:ALA:HB2	1.85	0.56
1:A:74:GLN:HB3	1:A:77:LEU:HD21	1.87	0.56
1:A:211:ASN:OD1	1:A:214:ALA:N	2.39	0.56
1:B:161:TYR:CZ	1:B:169:GLY:HA3	2.40	0.56
1:A:127:ARG:O	1:A:130:SER:OG	2.24	0.56
2:A:801:BLA:HMD3	2:A:801:BLA:HAC	1.88	0.56
1:A:523:HIS:HA	1:A:526:LYS:HG2	1.88	0.55
1:A:130:SER:HB2	1:A:133:ALA:HB2	1.88	0.55
1:B:211:ASN:OD1	1:B:214:ALA:N	2.37	0.54
1:B:475:LYS:HG3	1:B:476:ARG:H	1.72	0.54
1:B:291:GLU:OE2	1:B:295:GLN:NE2	2.36	0.54
1:B:302:SER:O	1:B:306:ARG:HG2	2.07	0.54
1:B:506:ALA:HA	1:B:509:ARG:HB3	1.88	0.54
1:A:201:TYR:OH	2:A:801:BLA:HAD2	2.07	0.54
1:B:147:ASN:OD1	1:B:148:THR:N	2.40	0.54
1:B:284:TYR:HA	1:B:287:ARG:HE	1.73	0.54
1:A:12:GLN:NE2	1:A:451:HIS:O	2.35	0.54
1:A:150:ARG:NH2	1:A:156:ASP:O	2.40	0.54
1:B:84:LEU:O	1:B:94:ARG:NH1	2.42	0.53
1:A:58:LEU:HD12	1:A:66:VAL:HG22	1.89	0.53
1:A:489:LEU:O	1:A:493:VAL:HG23	2.09	0.53
1:B:379:TRP:HE3	1:B:380:LEU:HD22	1.74	0.53
1:A:32:ALA:HB3	1:A:42:VAL:HB	1.90	0.53
1:A:428:ARG:HH11	1:A:472:PRO:HG2	1.73	0.53
1:A:202:THR:HA	1:A:268:LEU:HD21	1.90	0.52
1:B:239:ARG:HH12	2:B:801:BLA:CGD	2.23	0.52
1:B:512:ALA:O	1:B:516:ALA:HB2	2.09	0.52
1:A:159:MET:HB2	1:A:273:ALA:HB3	1.91	0.52
1:A:61:LYS:HD3	1:A:62:THR:N	2.23	0.52
1:B:67:LEU:HB3	1:B:71:LEU:HD21	1.91	0.52
1:A:505:GLU:HA	1:A:508:SER:HB2	1.92	0.52
1:A:192:ASP:HA	2:A:801:BLA:OC	2.10	0.52
1:A:262:LEU:HD12	1:A:270:GLY:HA3	1.92	0.52
1:A:420:SER:OG	1:A:421:SER:N	2.43	0.51
1:A:155:PHE:HE1	1:A:282:LEU:HD11	1.74	0.51
1:A:328:GLY:O	1:A:495:ARG:NH2	2.43	0.51
1:A:96:LEU:O	1:A:107:GLU:N	2.41	0.51
1:B:241:VAL:HA	2:B:801:BLA:O2D	2.10	0.51
1:A:114:GLN:NE2	1:A:116:ASP:OD1	2.34	0.51
1:B:490:ILE:HA	1:B:493:VAL:HG12	1.93	0.50
1:A:323:LEU:HD13	1:A:347:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HD21	1:B:210:ALA:HB2	1.94	0.50
1:B:192:ASP:OD2	2:B:801:BLA:HBB	2.11	0.50
1:A:258:PHE:HB3	1:A:274:CYS:HB2	1.94	0.49
1:B:208:LEU:HD11	1:B:282:LEU:HB3	1.94	0.49
1:B:282:LEU:HD21	1:B:286:ARG:HB3	1.93	0.49
1:A:140:GLU:OE1	1:A:140:GLU:N	2.35	0.49
1:A:33:PHE:HD2	1:A:38:ARG:HB3	1.78	0.49
1:A:392:GLU:OE2	1:A:393:ARG:NH1	2.45	0.49
1:A:394:LEU:HB3	1:A:401:LEU:HD11	1.94	0.49
1:B:502:ARG:O	1:B:505:GLU:HG3	2.13	0.49
1:B:437:TRP:N	1:B:463:TRP:O	2.39	0.49
1:A:30:LEU:HD12	1:A:31:LEU:N	2.28	0.49
1:A:506:ALA:O	1:A:509:ARG:HG3	2.13	0.49
1:A:532:ILE:HA	1:A:535:TYR:HB3	1.94	0.49
1:B:505:GLU:O	1:B:508:SER:OG	2.25	0.48
1:A:85:ARG:NH1	1:A:86:VAL:O	2.46	0.48
1:B:232:ASP:OD1	1:B:233:LEU:N	2.46	0.48
1:B:448:GLU:OE1	1:B:455:HIS:NE2	2.46	0.48
1:A:352:GLY:O	1:A:427:PHE:N	2.44	0.48
2:A:801:BLA:HMC1	2:A:801:BLA:CBC	2.44	0.48
1:B:355:LEU:HD13	1:B:357:LEU:HD13	1.95	0.48
1:A:398:TYR:CD2	1:A:400:PRO:HD2	2.48	0.48
1:A:523:HIS:CG	1:A:526:LYS:HZ3	2.31	0.48
1:A:61:LYS:NZ	1:A:65:GLN:HG2	2.29	0.48
1:B:459:SER:OG	1:B:460:PHE:N	2.47	0.47
1:A:53:ARG:HE	1:A:58:LEU:HD11	1.79	0.47
1:A:516:ALA:HA	1:A:519:HIS:ND1	2.29	0.47
1:B:516:ALA:HA	1:B:519:HIS:NE2	2.29	0.47
1:A:155:PHE:CD2	1:A:276:HIS:HB2	2.50	0.47
1:B:499:GLU:HA	1:B:502:ARG:HD3	1.97	0.47
1:A:30:LEU:HD12	1:A:31:LEU:H	1.79	0.47
1:A:371:ASP:OD1	1:A:371:ASP:N	2.48	0.47
1:B:74:GLN:HB3	1:B:84:LEU:HD22	1.95	0.46
1:A:379:TRP:O	1:A:382:PRO:HD2	2.15	0.46
1:A:385:PHE:CE2	1:A:415:ARG:HB2	2.51	0.46
1:A:181:ASP:OD1	1:A:182:GLY:N	2.48	0.46
1:B:256:ALA:HB3	1:B:276:HIS:HB3	1.97	0.46
1:A:132:LEU:HD11	1:A:135:ALA:HB2	1.98	0.46
1:B:141:LEU:HD21	1:B:300:GLN:HB3	1.97	0.46
1:A:204:ASN:ND2	1:A:234:SER:O	2.48	0.46
1:B:414:VAL:HG21	1:B:486:ARG:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLU:OE1	1:B:70:GLU:N	2.46	0.46
1:B:239:ARG:NH1	2:B:801:BLA:O2D	2.49	0.45
1:A:14:ASP:O	1:A:196:GLN:NE2	2.50	0.45
1:B:177:ARG:NH1	1:B:180:MET:HE3	2.32	0.45
1:A:475:LYS:NZ	1:A:477:ALA:HB3	2.32	0.45
1:B:499:GLU:HA	1:B:502:ARG:CD	2.45	0.45
1:B:69:ALA:HA	1:B:72:TRP:HZ3	1.80	0.45
1:B:13:CYS:HA	2:B:801:BLA:HBC2	1.58	0.45
1:A:486:ARG:HA	1:A:489:LEU:HB3	1.99	0.45
1:A:540:MET:SD	1:A:540:MET:N	2.90	0.45
1:A:147:ASN:OD1	1:A:148:THR:N	2.50	0.45
1:A:264:LYS:HG3	1:A:265:ASP:H	1.82	0.44
1:A:516:ALA:O	1:A:520:THR:OG1	2.26	0.44
1:A:142:LEU:HD13	1:A:297:LEU:HD21	2.00	0.44
1:B:84:LEU:H	1:B:94:ARG:HH12	1.65	0.44
1:A:142:LEU:HD21	1:A:301:LEU:HD11	2.00	0.44
2:A:801:BLA:HMA1	2:A:801:BLA:C1B	2.46	0.44
1:B:94:ARG:HA	1:B:94:ARG:HD2	1.79	0.44
1:B:514:LEU:HA	1:B:517:PHE:CE2	2.52	0.44
1:A:244:ILE:HG13	1:A:245:HIS:N	2.32	0.44
1:B:370:MET:O	1:B:373:VAL:HG12	2.18	0.44
1:B:97:LEU:HD12	1:B:98:HIS:N	2.32	0.44
1:B:209:ILE:HD11	1:B:241:VAL:HG13	1.99	0.44
1:B:284:TYR:HB2	1:B:287:ARG:HH21	1.83	0.43
1:A:121:ALA:O	1:A:125:VAL:HG23	2.18	0.43
1:B:398:TYR:CE2	1:B:401:LEU:HG	2.53	0.43
1:B:478:ASP:HA	1:B:481:ALA:HB3	2.00	0.43
1:A:479:LEU:HD23	1:A:479:LEU:HA	1.84	0.43
1:B:386:GLN:HG2	1:B:387:THR:HG23	1.98	0.43
1:B:496:GLN:NE2	1:B:499:GLU:OE2	2.51	0.43
1:A:542:ASP:OD1	1:A:543:TYR:N	2.52	0.43
1:B:194:PRO:HG2	1:B:197:ALA:HB2	2.01	0.43
1:B:386:GLN:OE1	1:B:386:GLN:N	2.51	0.43
1:B:67:LEU:HD23	1:B:71:LEU:HD11	2.00	0.43
1:B:411:LEU:HD23	1:B:425:LEU:HD12	2.00	0.43
1:A:526:LYS:O	1:A:529:LEU:HB2	2.19	0.43
1:A:33:PHE:CD2	1:A:38:ARG:HB3	2.52	0.43
1:A:39:ARG:HH21	1:A:63:ALA:H	1.65	0.43
1:A:485:PHE:O	1:A:489:LEU:HB2	2.19	0.43
1:A:245:HIS:ND1	2:A:801:BLA:ND	2.67	0.43
1:B:155:PHE:CD1	1:B:276:HIS:HB2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:ASN:HA	1:B:514:LEU:HD12	2.00	0.43
1:B:318:ALA:O	1:B:322:PRO:HD3	2.19	0.43
1:A:213:ARG:HG3	1:A:250:ARG:HH21	1.84	0.42
1:A:320:LEU:HD21	1:A:484:GLY:O	2.19	0.42
1:A:251:ASN:ND2	1:A:457:ARG:O	2.51	0.42
1:B:69:ALA:HA	1:B:72:TRP:CZ3	2.55	0.42
1:B:316:ARG:HD3	1:B:316:ARG:HA	1.70	0.42
1:B:192:ASP:OD1	1:B:457:ARG:NH2	2.52	0.42
1:A:319:LEU:O	1:A:322:PRO:HD2	2.19	0.42
1:A:335:GLU:OE1	1:A:335:GLU:N	2.45	0.42
1:B:333:LEU:HD12	1:B:334:GLU:N	2.35	0.42
1:A:232:ASP:OD1	1:A:233:LEU:N	2.52	0.42
1:A:501:GLU:HA	1:A:504:SER:HB2	2.02	0.42
1:B:245:HIS:CE1	2:B:801:BLA:O1A	2.72	0.42
1:A:71:LEU:HD21	1:A:88:LEU:HD21	2.02	0.42
1:A:211:ASN:OD1	1:A:213:ARG:N	2.53	0.42
1:B:417:ALA:HB3	1:B:422:ARG:HB2	2.02	0.41
1:A:33:PHE:N	1:A:104:THR:O	2.47	0.41
1:B:142:LEU:HD23	1:B:160:VAL:HG11	2.01	0.41
1:B:290:CYS:O	1:B:294:THR:HG23	2.20	0.41
1:B:39:ARG:HH21	1:B:62:THR:N	2.19	0.41
1:B:93:TYR:HD2	1:B:108:LEU:HB3	1.85	0.41
1:B:141:LEU:HA	1:B:144:THR:HG22	2.02	0.41
1:B:487:SER:HA	1:B:490:ILE:HG22	2.02	0.41
1:A:492:VAL:HA	1:A:495:ARG:HB3	2.03	0.41
1:A:493:VAL:HG21	1:B:490:ILE:HD13	2.01	0.41
1:B:150:ARG:NH1	1:B:176:LYS:O	2.54	0.41
1:B:319:LEU:O	1:B:322:PRO:HD2	2.21	0.41
1:A:245:HIS:CE1	2:A:801:BLA:NA	2.89	0.41
1:A:421:SER:OG	1:A:422:ARG:NH2	2.54	0.41
1:B:84:LEU:H	1:B:94:ARG:NH1	2.18	0.41
1:A:468:ARG:HD2	1:A:468:ARG:HA	1.93	0.41
1:A:363:LEU:HD22	1:A:367:THR:HG21	2.04	0.41
1:B:107:GLU:OE1	1:B:107:GLU:N	2.54	0.41
1:B:398:TYR:HE2	1:B:401:LEU:HG	1.86	0.41
1:A:264:LYS:HG3	1:A:265:ASP:N	2.36	0.40
1:A:33:PHE:HE2	1:A:63:ALA:HB1	1.85	0.40
1:B:27:TYR:CE2	1:B:210:ALA:HB3	2.56	0.40
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.97	0.40
1:B:53:ARG:HH22	1:B:66:VAL:HA	1.87	0.40
1:B:352:GLY:HA3	1:B:366:ARG:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:LEU:HA	1:B:506:ALA:HB3	2.02	0.40
2:B:801:BLA:C1B	2:B:801:BLA:HMA1	2.52	0.40
1:B:88:LEU:HD23	1:B:88:LEU:HA	1.94	0.40
1:B:150:ARG:HD2	1:B:175:SER:O	2.22	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	536/747 (72%)	523 (98%)	12 (2%)	1 (0%)	44 77
1	B	515/747 (69%)	503 (98%)	12 (2%)	0	100 100
All	All	1051/1494 (70%)	1026 (98%)	24 (2%)	1 (0%)	50 82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	SER

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	415/574 (72%)	411 (99%)	4 (1%)	73 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	399/574 (70%)	395 (99%)	4 (1%)	73	81
All	All	814/1148 (71%)	806 (99%)	8 (1%)	71	81

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	ARG
1	A	213	ARG
1	A	287	ARG
1	A	475	LYS
1	B	13	CYS
1	B	53	ARG
1	B	453	ARG
1	B	502	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	245	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BLA	A	801	1	42,46,46	1.42	5 (11%)	54,67,67	1.47	6 (11%)
2	BLA	B	801	1	42,46,46	1.30	5 (11%)	54,67,67	1.34	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BLA	A	801	1	-	19/26/74/74	0/4/4/4
2	BLA	B	801	1	-	17/26/74/74	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	BLA	C3C-C4C	-4.22	1.37	1.45
2	A	801	BLA	CAC-C3C	-4.08	1.36	1.47
2	B	801	BLA	C3C-C4C	-3.49	1.39	1.45
2	B	801	BLA	CAB-C3B	-3.36	1.38	1.47
2	A	801	BLA	CAB-C3B	-3.36	1.38	1.47
2	B	801	BLA	CAC-C3C	-3.27	1.38	1.47
2	A	801	BLA	CHD-C1D	-2.66	1.34	1.40
2	B	801	BLA	CHD-C1D	-2.65	1.34	1.40
2	A	801	BLA	C1B-C2B	-2.14	1.41	1.45
2	B	801	BLA	O2A-CGA	-2.00	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	BLA	CHA-C4D-ND	-4.40	122.78	128.76
2	A	801	BLA	CMC-C2C-C1C	4.34	130.29	121.21
2	A	801	BLA	C1A-CHA-C4D	-4.00	123.38	128.73
2	B	801	BLA	CMC-C2C-C1C	3.80	129.15	121.21
2	B	801	BLA	CHA-C4D-ND	-3.68	123.77	128.76
2	B	801	BLA	C1A-CHA-C4D	-3.59	123.92	128.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	BLA	CMB-C2B-C1B	3.33	128.21	124.16
2	A	801	BLA	CMB-C2B-C1B	3.12	127.95	124.16
2	A	801	BLA	C4C-NC-C1C	-3.05	106.92	110.66
2	B	801	BLA	C4C-NC-C1C	-2.71	107.33	110.66
2	A	801	BLA	CHD-C4C-NC	2.28	130.91	126.06
2	B	801	BLA	C4B-C3B-C2B	-2.08	105.26	107.92

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	BLA	ND-C4D-CHA-C1A
2	A	801	BLA	C3D-C4D-CHA-C1A
2	A	801	BLA	NA-C4A-CHB-C1B
2	A	801	BLA	C3A-C4A-CHB-C1B
2	A	801	BLA	NB-C1B-CHB-C4A
2	A	801	BLA	C2B-C1B-CHB-C4A
2	A	801	BLA	NC-C4C-CHD-C1D
2	A	801	BLA	C3C-C4C-CHD-C1D
2	A	801	BLA	ND-C1D-CHD-C4C
2	A	801	BLA	C2D-C1D-CHD-C4C
2	B	801	BLA	NA-C1A-CHA-C4D
2	B	801	BLA	C2A-C1A-CHA-C4D
2	B	801	BLA	ND-C4D-CHA-C1A
2	B	801	BLA	C3D-C4D-CHA-C1A
2	B	801	BLA	NB-C1B-CHB-C4A
2	B	801	BLA	C2B-C1B-CHB-C4A
2	B	801	BLA	C2B-C3B-CAB-CBB
2	B	801	BLA	C4B-C3B-CAB-CBB
2	B	801	BLA	ND-C1D-CHD-C4C
2	B	801	BLA	C2D-C1D-CHD-C4C
2	B	801	BLA	C3C-C4C-CHD-C1D
2	B	801	BLA	NC-C4C-CHD-C1D
2	A	801	BLA	C2A-CAA-CBA-CGA
2	B	801	BLA	C2A-CAA-CBA-CGA
2	B	801	BLA	C2C-C3C-CAC-CBC
2	B	801	BLA	C4C-C3C-CAC-CBC
2	A	801	BLA	C4D-C3D-CAD-CBD
2	A	801	BLA	C2B-C3B-CAB-CBB
2	A	801	BLA	C2D-C3D-CAD-CBD
2	A	801	BLA	CAA-CBA-CGA-O1A
2	B	801	BLA	CAA-CBA-CGA-O2A

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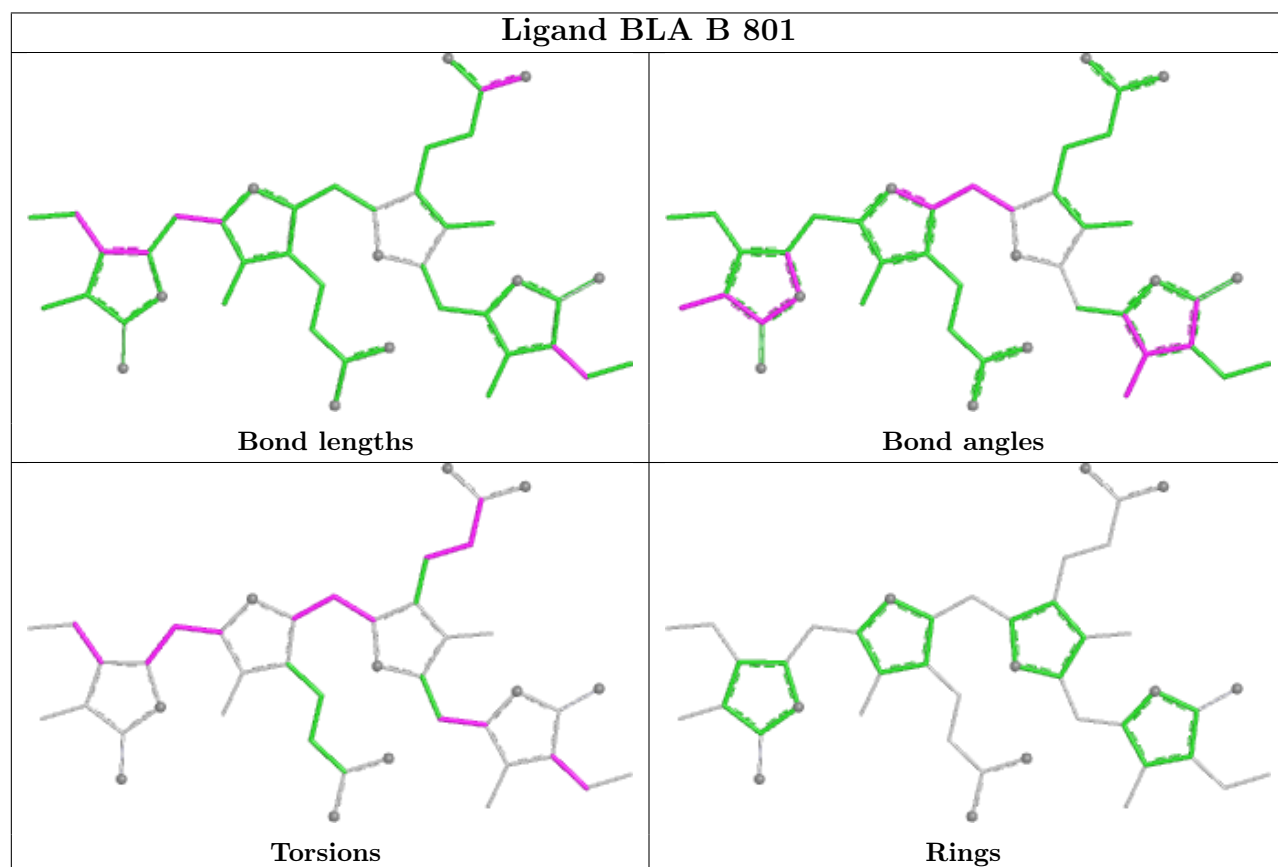
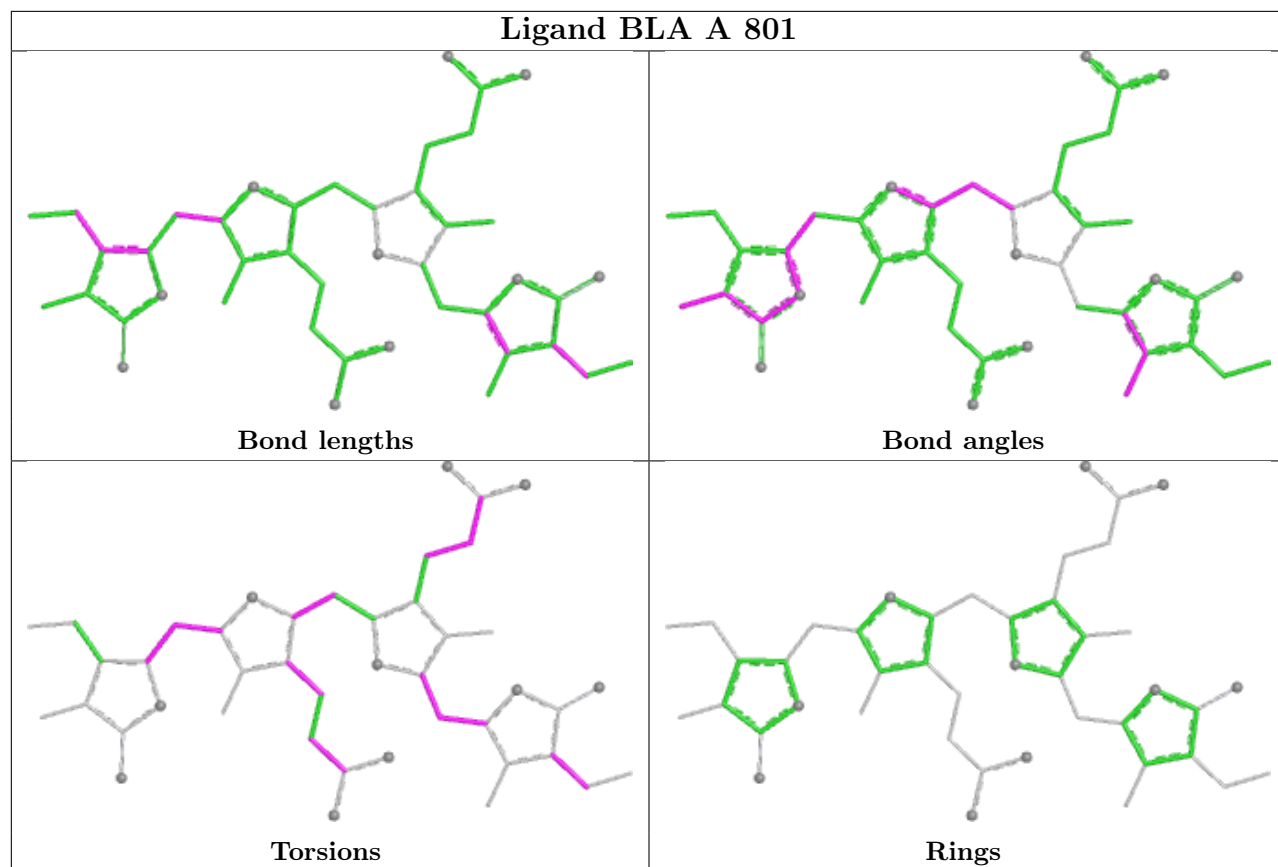
Mol	Chain	Res	Type	Atoms
2	A	801	BLA	CAA-CBA-CGA-O2A
2	B	801	BLA	CAA-CBA-CGA-O1A
2	A	801	BLA	C4B-C3B-CAB-CBB
2	A	801	BLA	CAD-CBD-CGD-O2D
2	A	801	BLA	CAD-CBD-CGD-O1D

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BLA	7	0
2	B	801	BLA	9	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

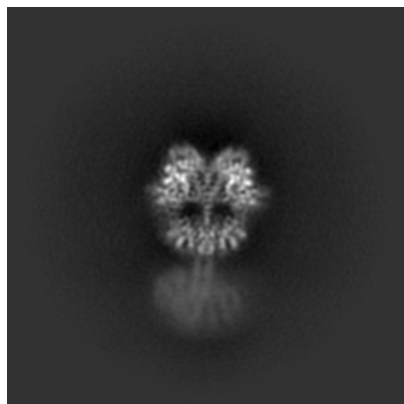
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42448. These allow visual inspection of the internal detail of the map and identification of artifacts.

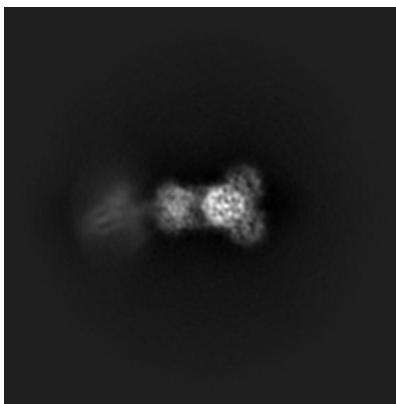
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

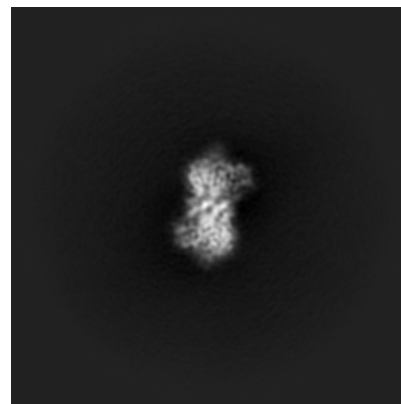
6.1.1 Primary map



X

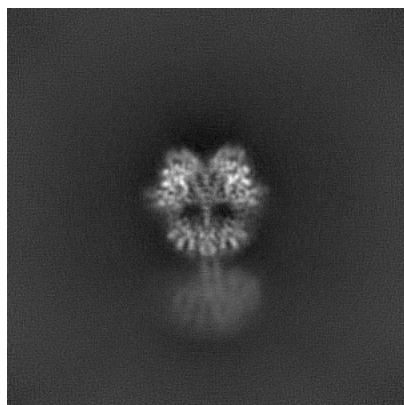


Y

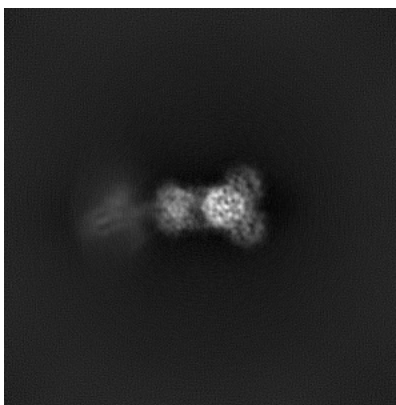


Z

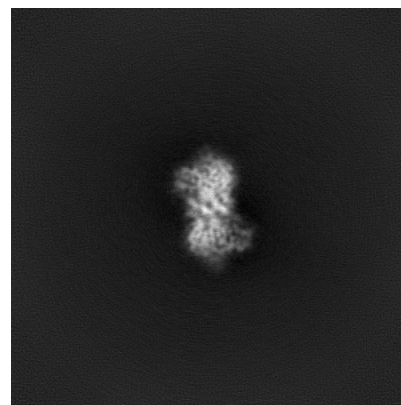
6.1.2 Raw map



X



Y

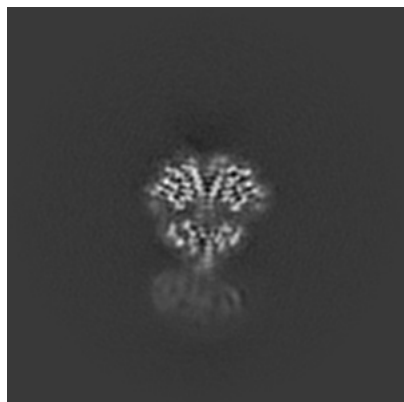


Z

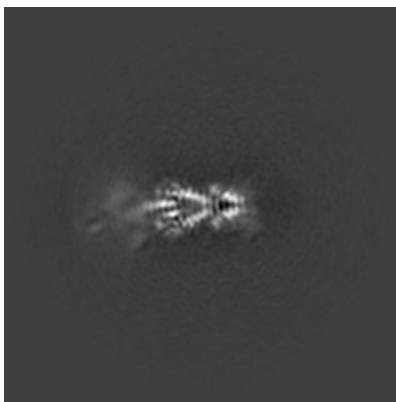
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

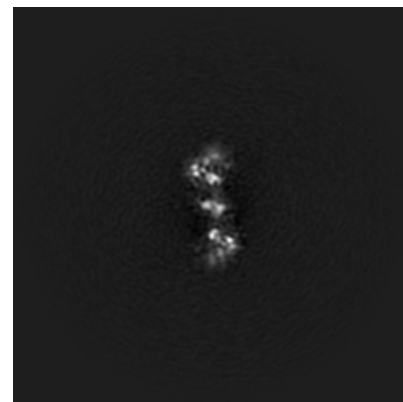
6.2.1 Primary map



X Index: 200

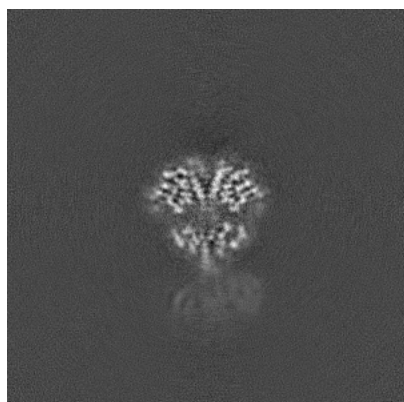


Y Index: 200

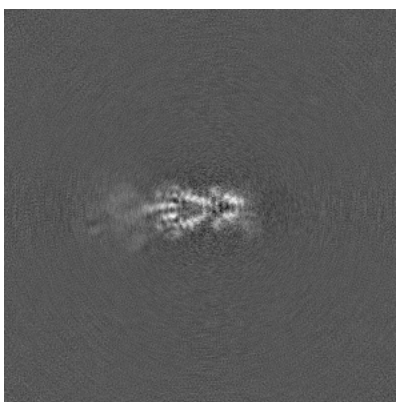


Z Index: 200

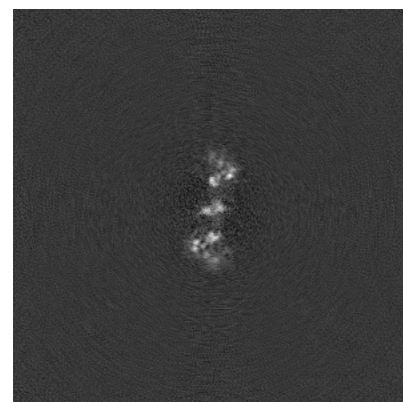
6.2.2 Raw map



X Index: 200



Y Index: 200

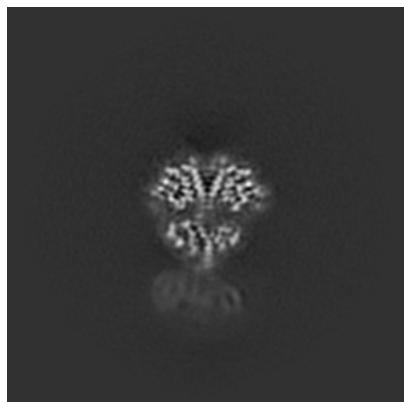


Z Index: 200

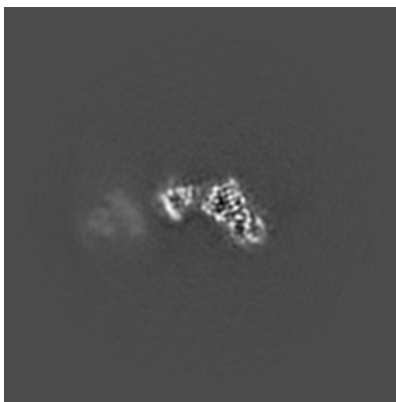
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

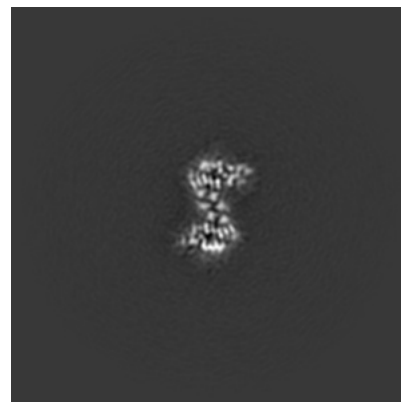
6.3.1 Primary map



X Index: 201

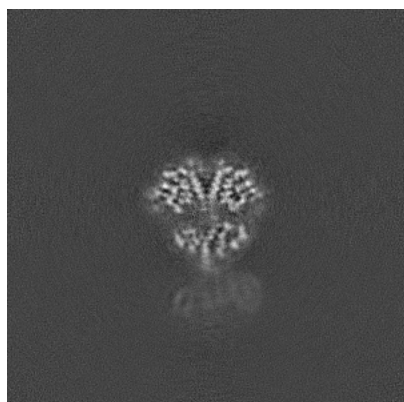


Y Index: 173

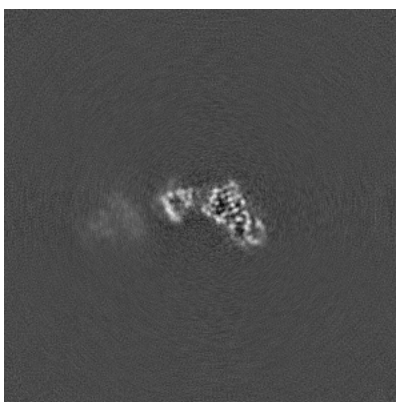


Z Index: 225

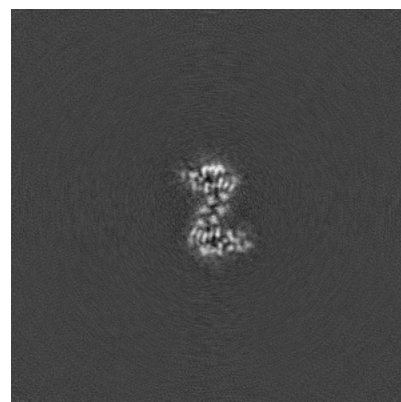
6.3.2 Raw map



X Index: 201



Y Index: 226

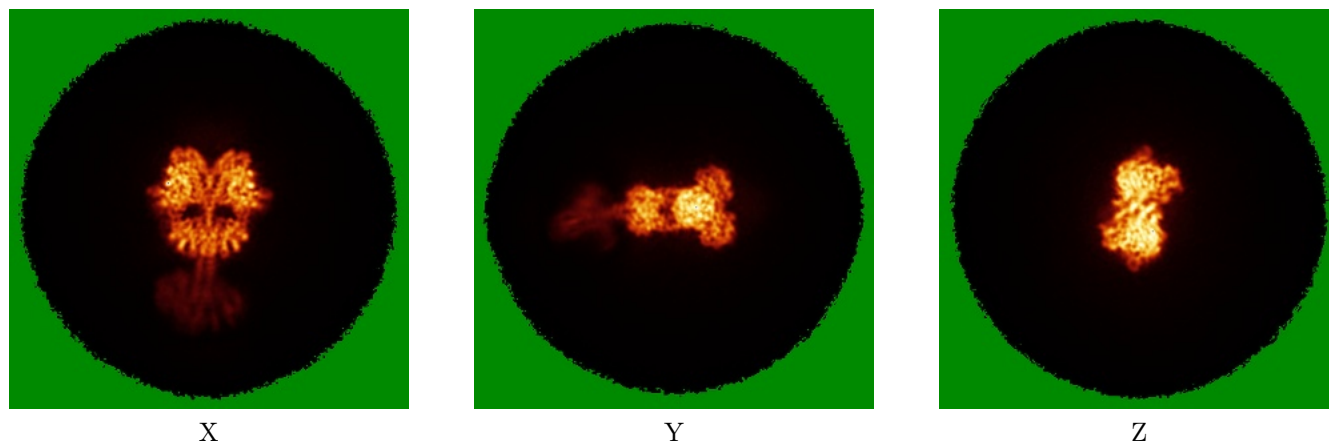


Z Index: 225

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

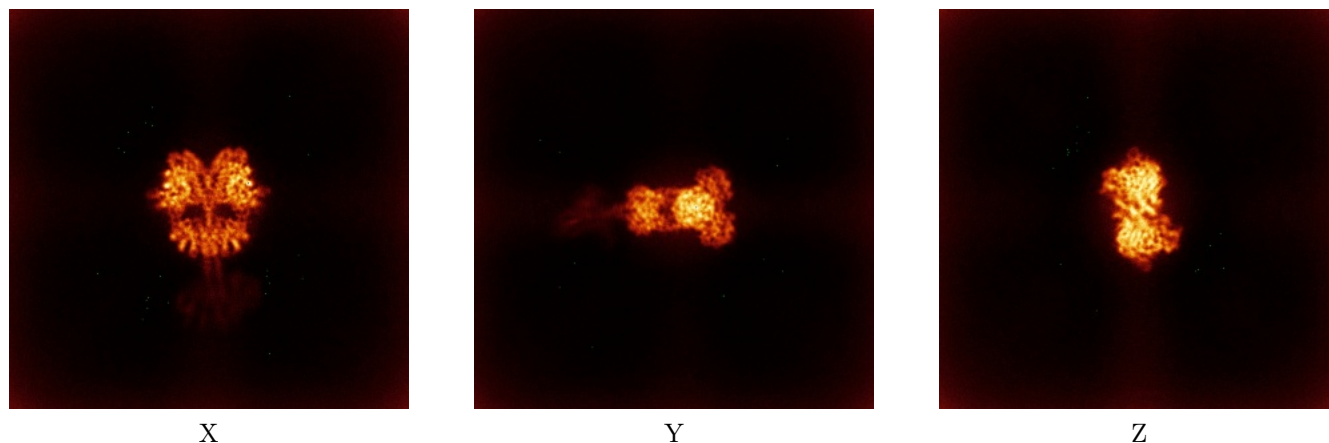


X

Y

Z

6.4.2 Raw map



X

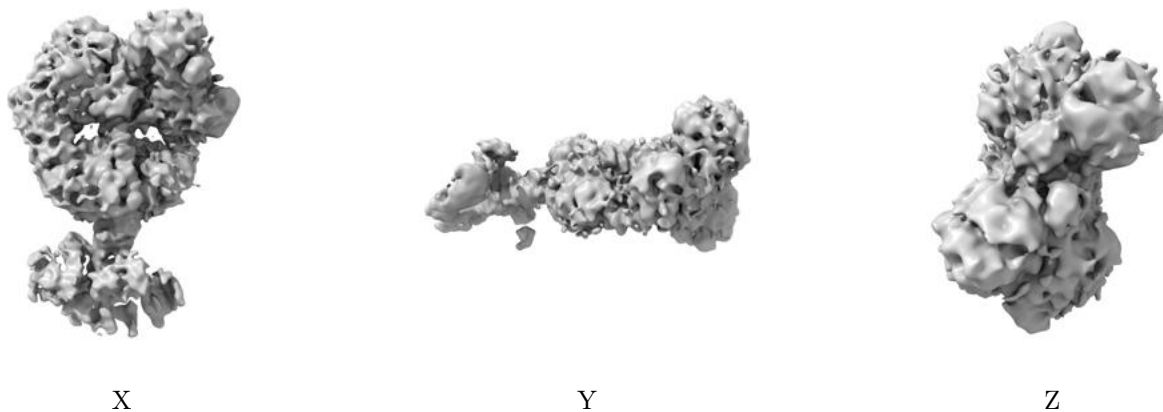
Y

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.

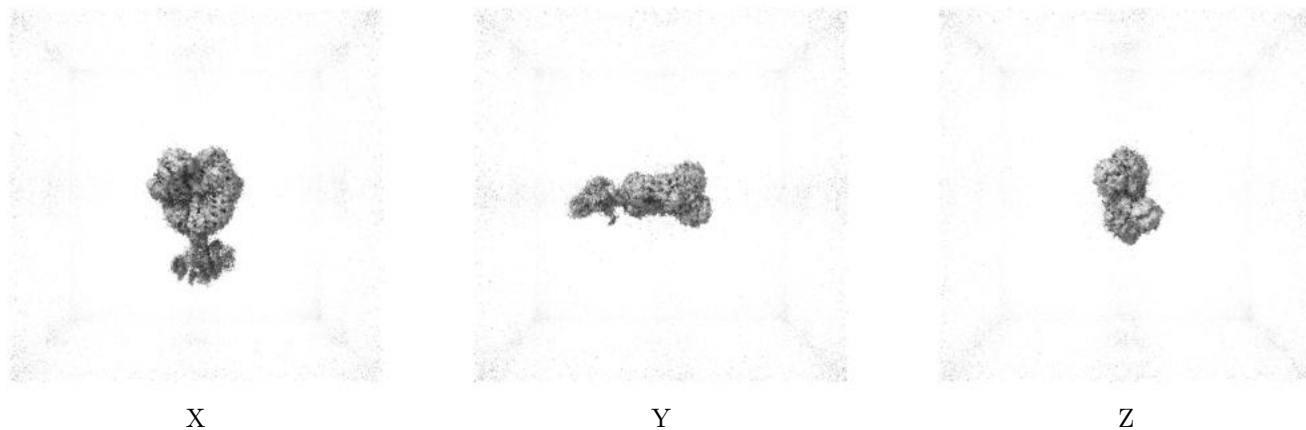
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

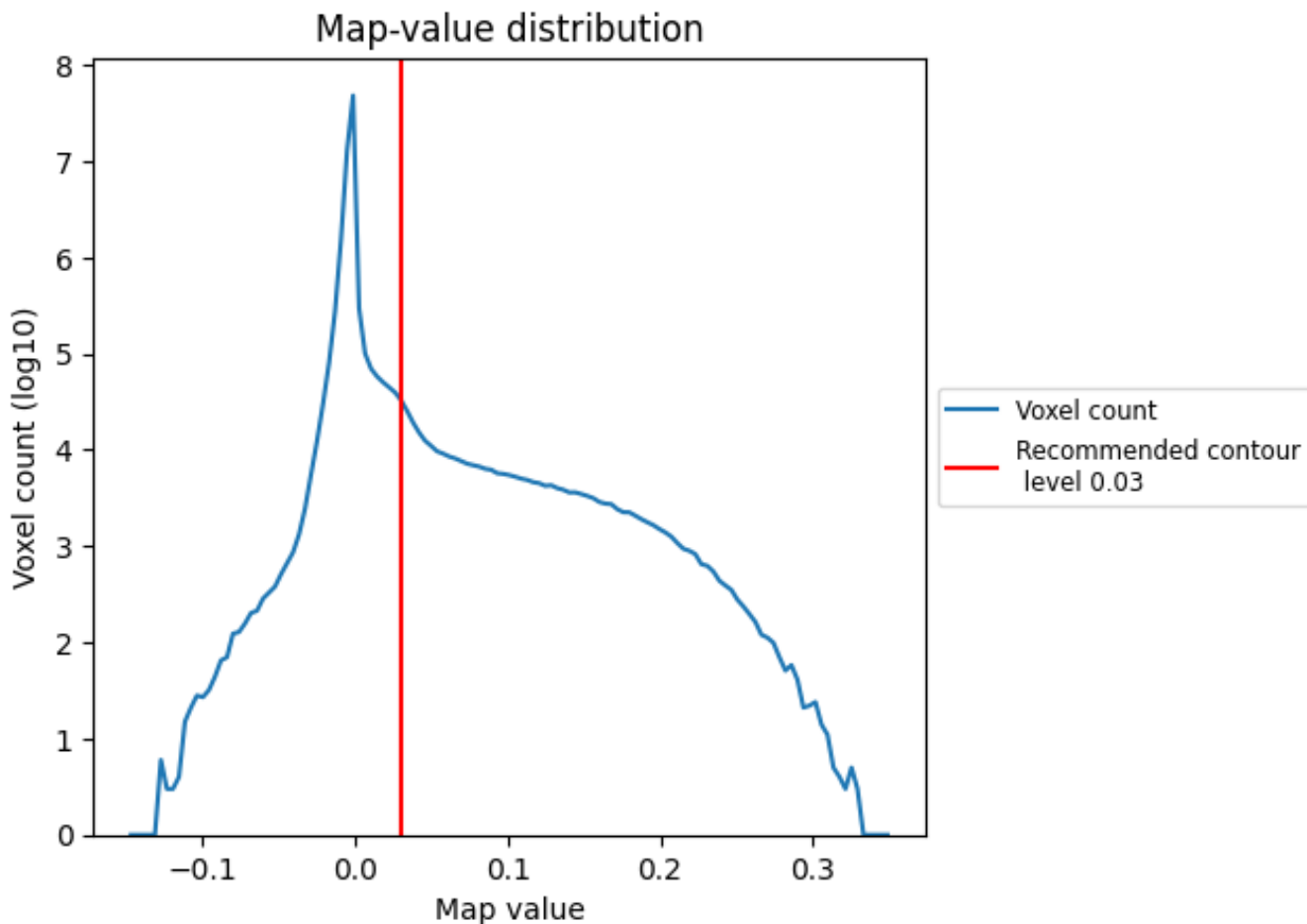
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

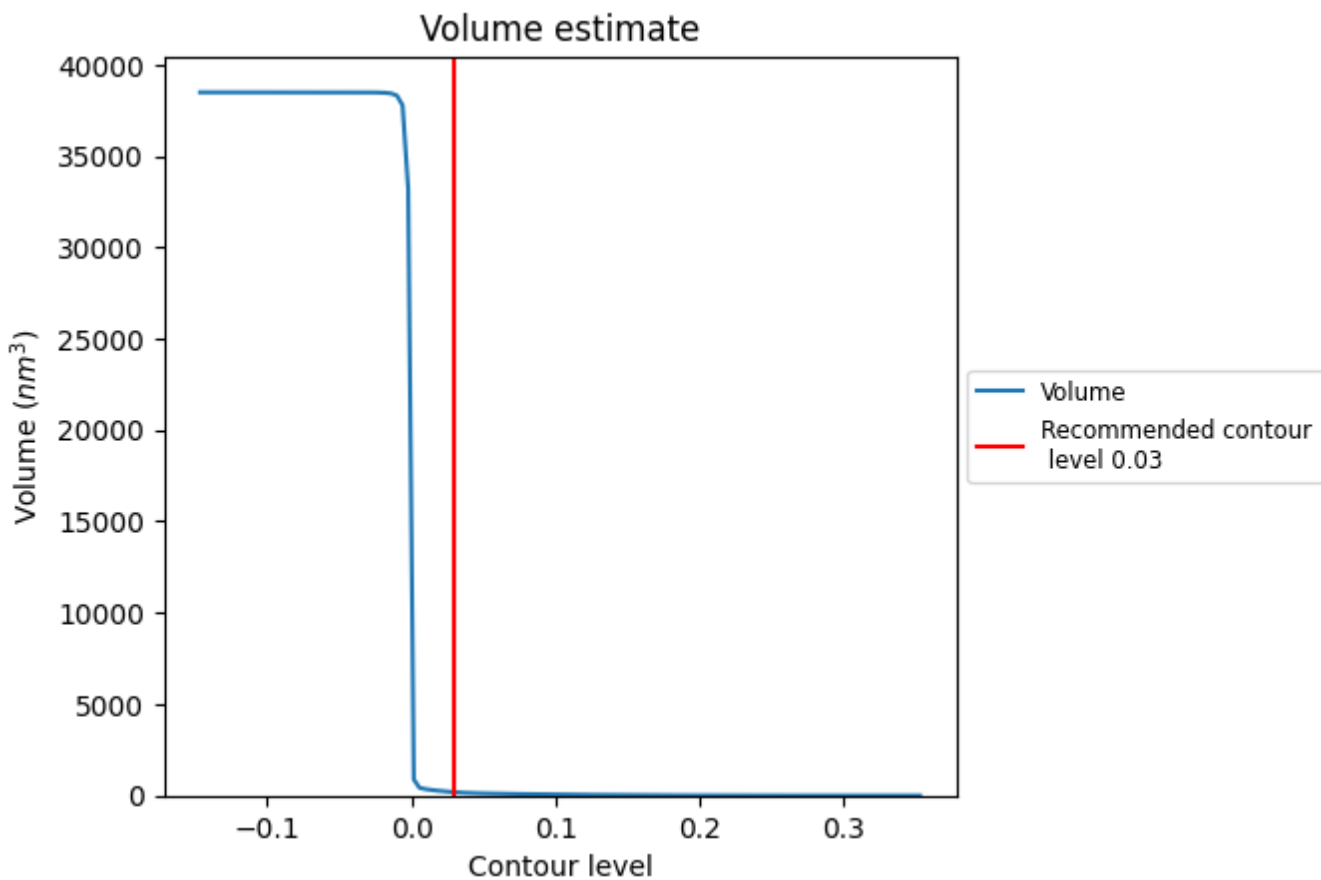
This section contains the results of statistical analysis of the map.

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.

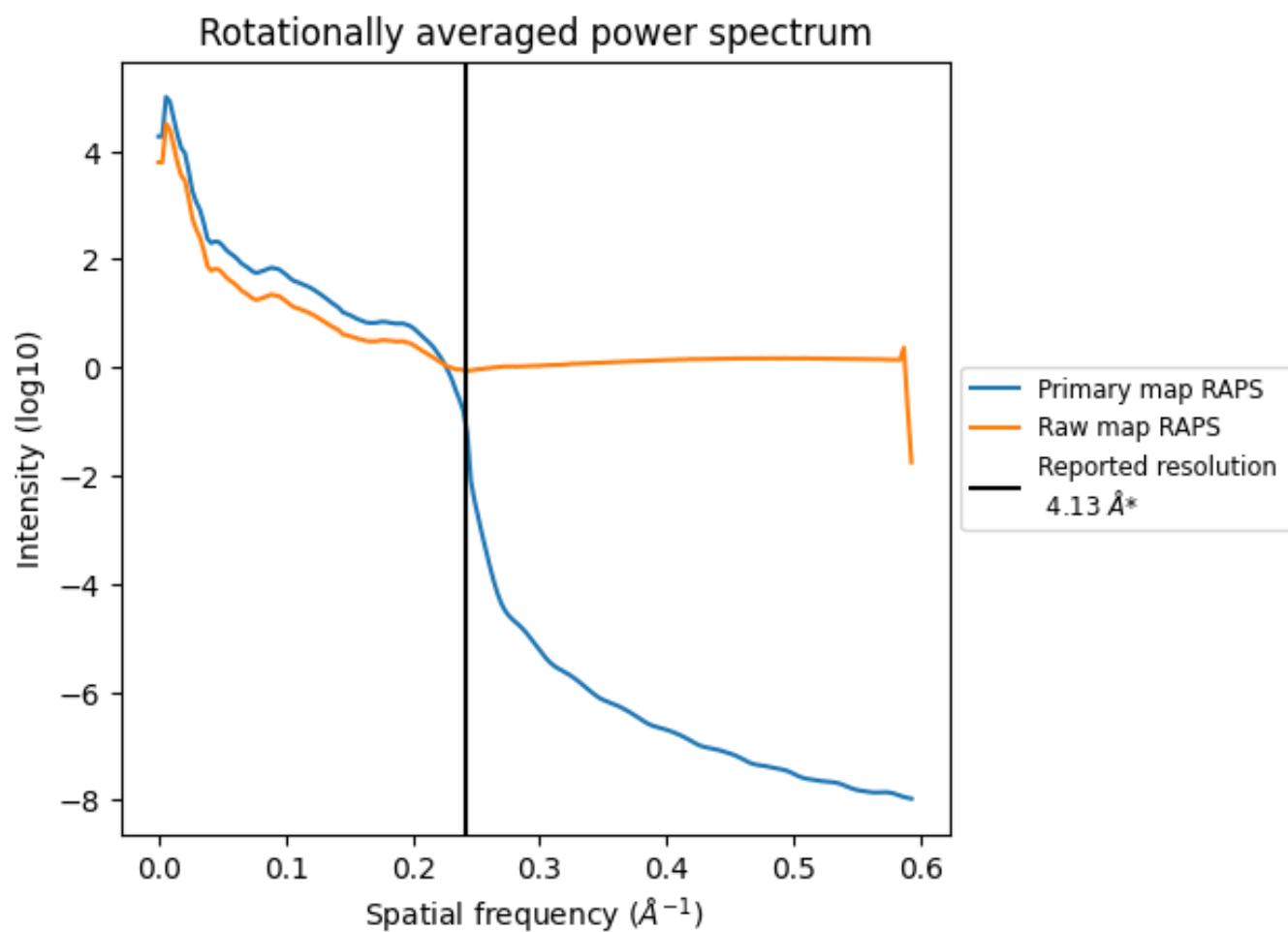
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm³; this corresponds to an approximate mass of 167 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

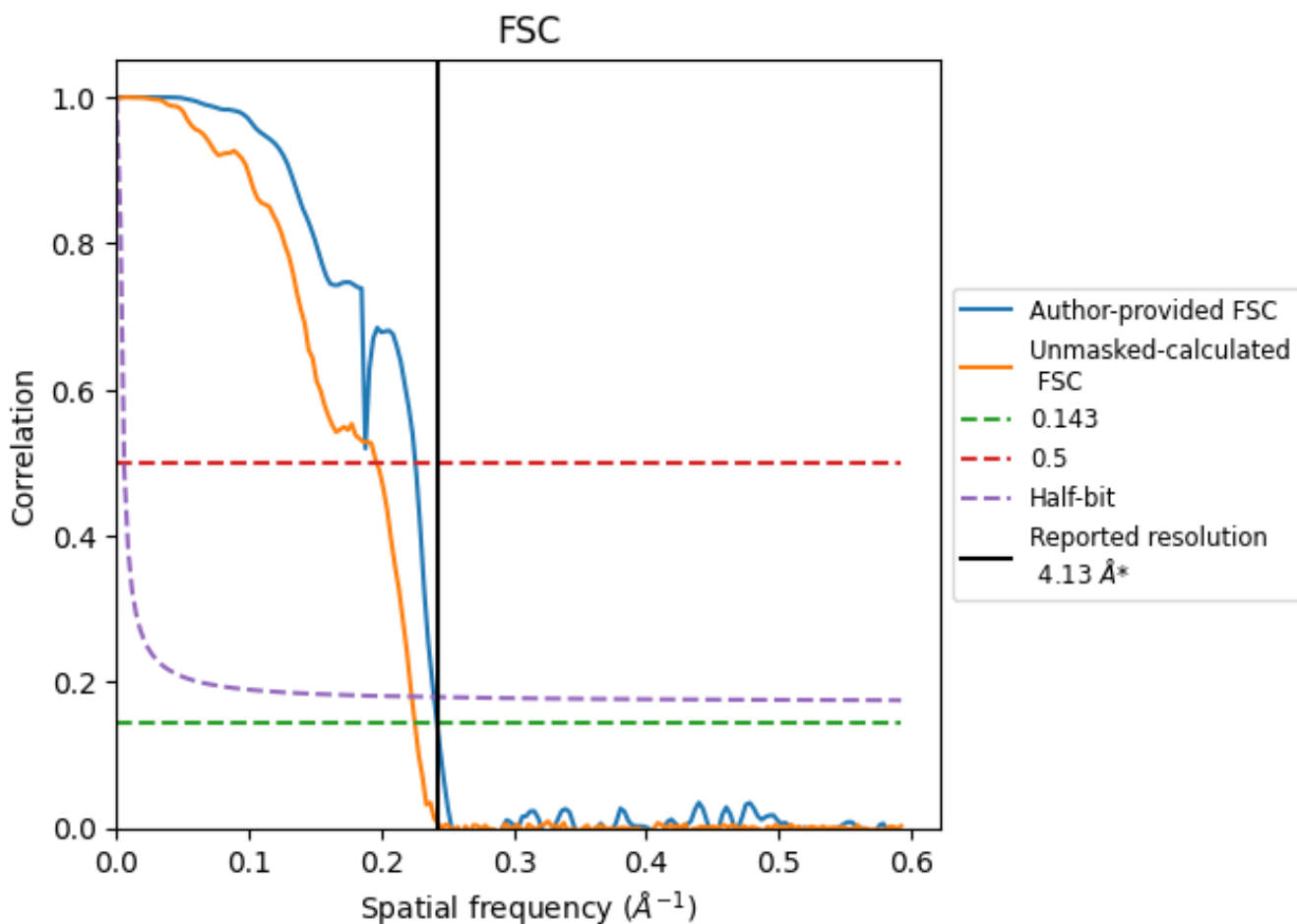


*Reported resolution corresponds to spatial frequency of 0.242 Å⁻¹

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 0.242 Å⁻¹

8.2 Resolution estimates [i](#)

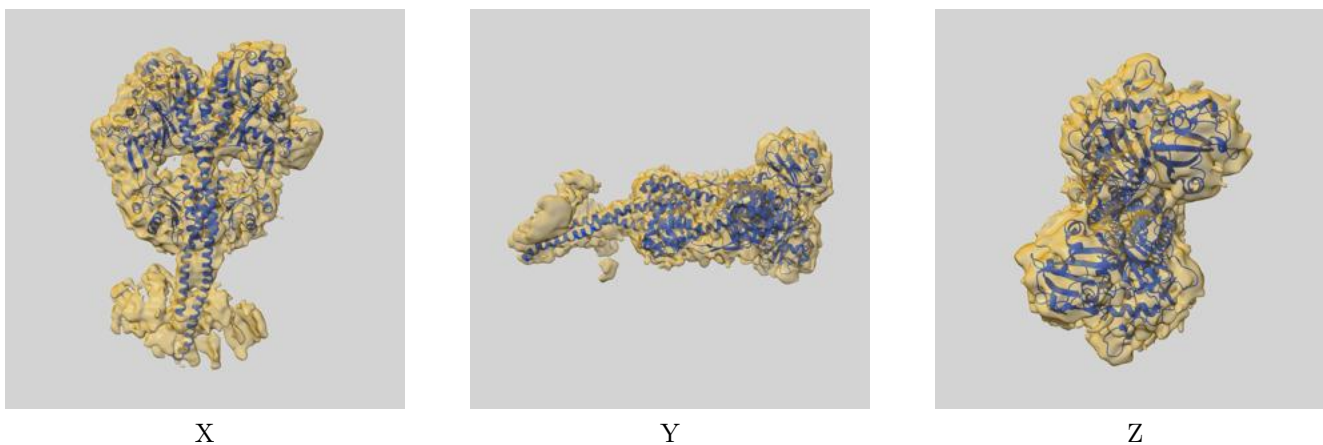
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.13	-	-
Author-provided FSC curve	4.13	4.43	4.17
Unmasked-calculated*	4.44	5.09	4.49

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

9 Map-model fit [i](#)

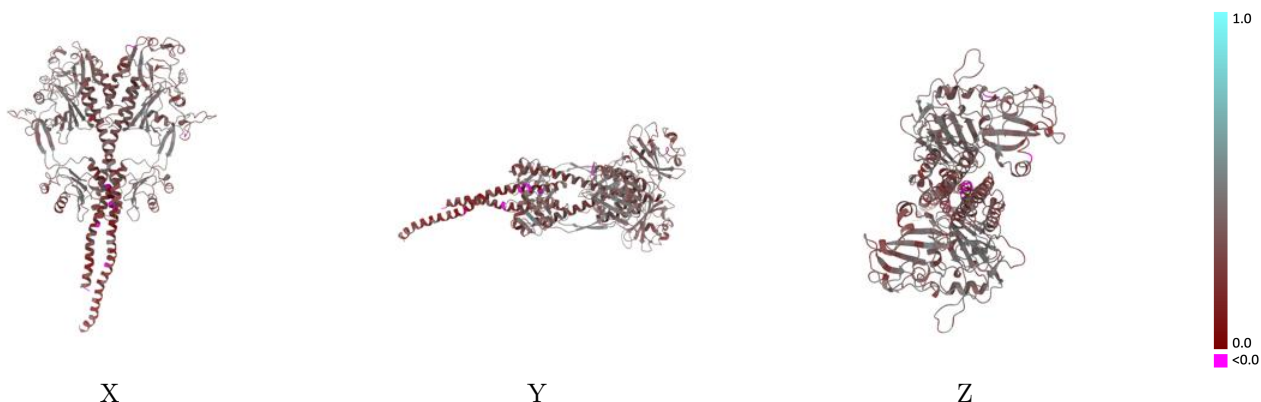
This section contains information regarding the fit between EMDB map EMD-42448 and PDB model 8UPH. Per-residue inclusion information can be found in section 3 on page 4.

9.1 Map-model overlay [i](#)



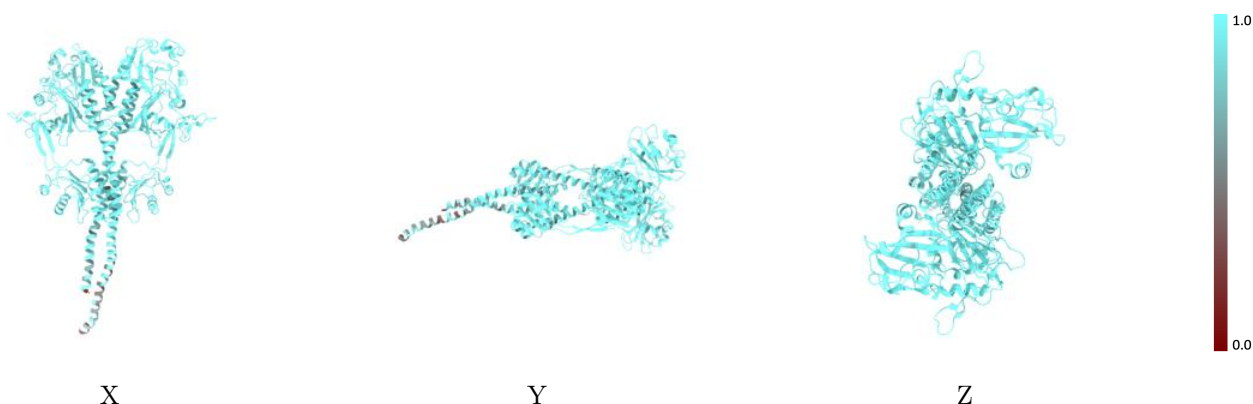
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



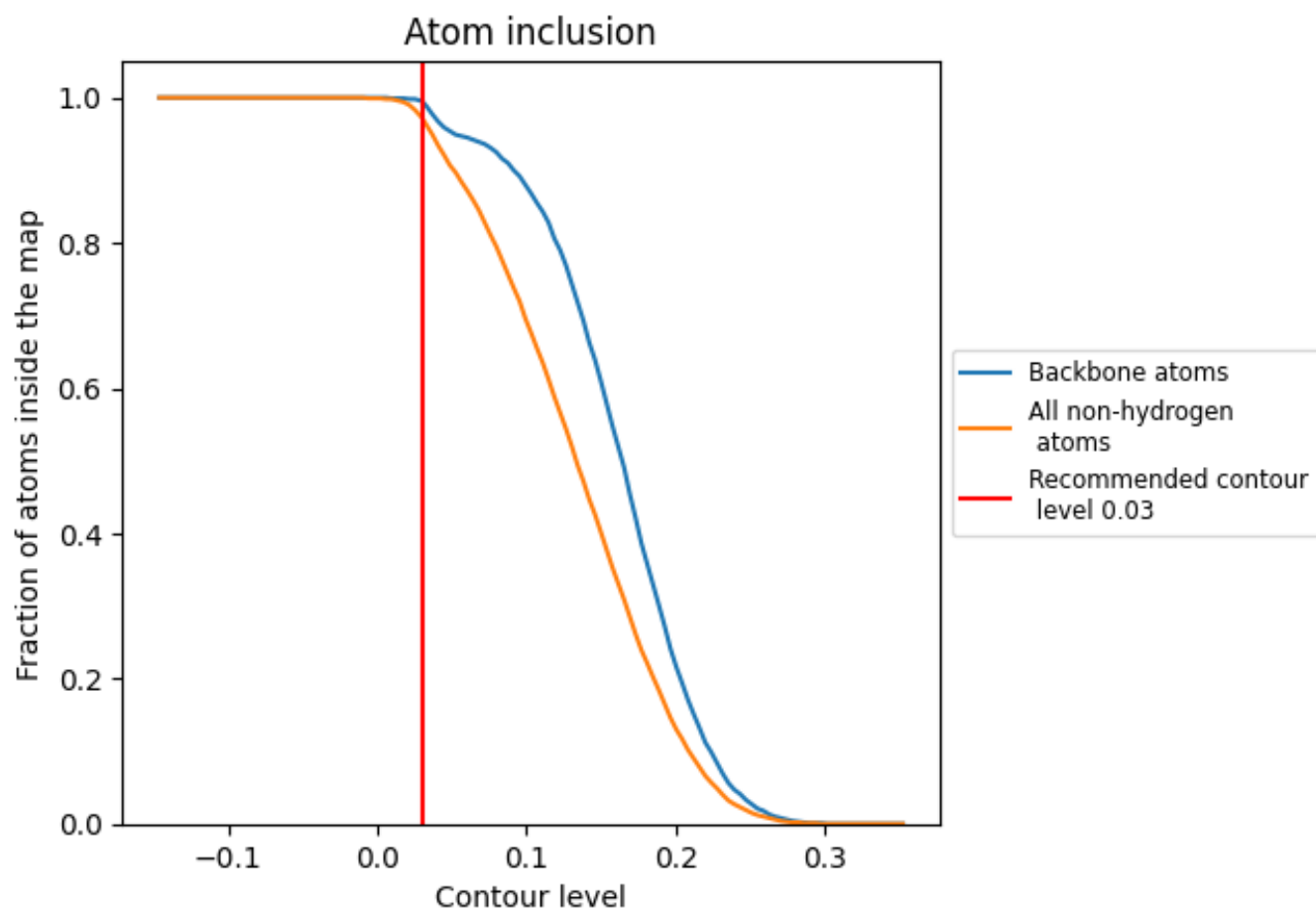
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).



9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 97% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9720	 0.3530
A	 0.9660	 0.3480
B	 0.9780	 0.3580

