



Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 07:42 PM UTC

PDB ID : 7RZW / pdb_00007rzw
EMDB ID : EMD-24780
Title : CryoEM structure of Arabidopsis thaliana phytochrome B
Authors : Li, H.; Burgie, E.S.; Vierstra, R.D.; Li, H.
Deposited on : 2021-08-27
Resolution : 3.30 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

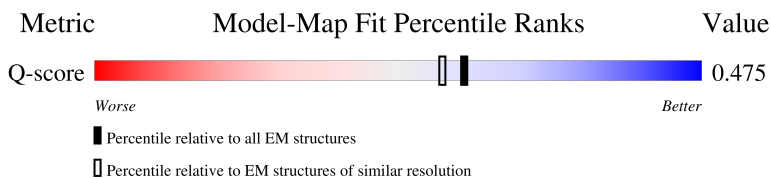
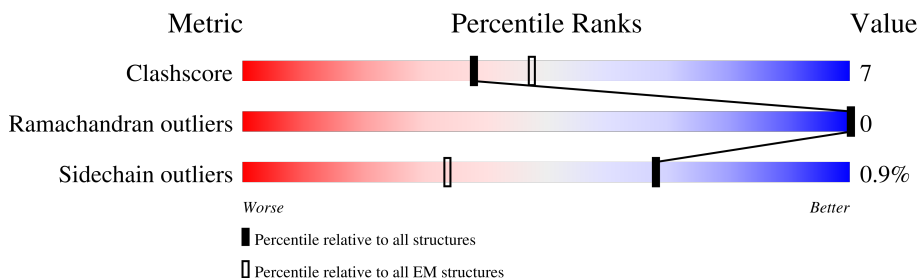
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	1172	 60% 13% 27%
1	B	1172	 59% 14% 26%

V1132	M983	L829	SER	Q611	M430	K277	VAL	TYR	MET
R1136	E986	T833	PRO	L612	M430	K277	PRO	THR	VAL
R1140	S987	V834	GLU	I613	K442	E282	THR	VAL	SER
L1144	I988	G835	LEU	E620	L445	V287	GLU	ALA	GLY
I1145	E989	E836	GLN	SER	M454	E296	LYS	ARG	GLY
L1147	D990	V837	LYS	GLU	L455	P304	PRO	LEU	SER
E1148	F993	S840	ALA	ALA	L456	E296	GLU	HIS	GLY
L1149	E999	L844	LEU	MET	R457	P304	LEU	VAL	GLY
P1150	A1013	K845	THR	SER	I463	S312	ARG	GLU	ARG
V1151	M1014	V837	VAL	LYS	I463	R313	GLN	GLY	GLY
PRO	M1014	A849	ASN	VAL	Q466	F314	SER	SER	GLY
ARG	L1017	M854	ALA	VAL	S467	L315	GLY	GLY	GLY
LYS	R1020	L857	CYS	GLY	P468	F316	ARG	SER	ARG
PRO	G1021	D867	SER	VAL	S468	K317	LYS	GLY	GLY
LEU	L1022	K868	LYS	ALA	I470	M323	LYS	GLY	GLY
SER	Q1023	P872	ASN	GLN	L473	T324	SER	LYS	GLY
THR	L1024	D875	LEU	VAL	A480	V325	ASP	THR	PRO
ALA	F1038	R876	ASN	CYS	E496	V347	THR	TYR	SER
SER	G1039	K879	LEU	ASP	I499	L351	SER	GLN	SER
GLY	T1044	V880	VAL	MET	D512	M362	THR	SER	HIS
ASP	L1048	F881	GLY	ALA	S813	S370	GLU	LEU	THR
MET	L1052	Q882	ASP	GLY	T514	I376	ASP	LYS	PRO
LEU	L1053	T886	ILE	ILE	S517	I377	PRO	THR	ASN
MET	R1057	Q905	LEU	ASP	L532	N378	ALA	THR	ASN
PRO	P1060	L911	ALA	LEU	V536	G379	LEU	TYR	ARG
TYR	I1067	V917	THR	ALA	C537	N380	GLU	GLY	ARG
	Q1075	R919	ASN	ALA	G538	GLU	ASP	SER	GLY
	M1076	T927	LYS	ALA	M639	ASP	ASP	VAL	ALA
	A1077	K930	LEU	ARG	A540	GLY	GLY	ALA	GLN
	D1078	Y934	ALA	VAL	V641	VAL	VAL	ILE	SER
	G1079	I939	LEU	VAL	A542	ALA	VAL	THR	GLY
	F1080	P942	ARG	LEU	I544	SER	ALA	LYS	LYS
	A1081	L943	GLY	ILE	B547	ARG	ALA	LEU	LEU
	A1082	M946	ASP	THR	D548	SER	GLY	ARG	ARG
	F1087	L958	GLU	THR	F549	S393	ARG	THR	SER
	R1088	I968	GLU	VAL	L550	H404	ALA	THR	ASN
	M1089	I976	LYS	PRO	P551	T410	VAL	THR	THR
	G1093	D982	ASN	ILE	M552	P413	V261	GLU	GLU
	L1096		VAL	PHE	F553	M40	V264	SER	MET
	L1100		GLU	ALA	R554	L414	T268	LYS	SER
	M1128		LYS	VAL	H569	R415	ALA	LYS	LYS
			LEU	ASP	E603	V416	ALA	ALA	ALA
			LYS	ALA		A417	GLY	PRO	ILE
			THR	GLY		F425	THR	GLN	GLN
			PHE	CYS			V273	SER	GLN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154901	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 ($e^-/\text{\AA}^2$)	54.4	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.167	Depositor
Minimum map value	-0.097	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	263.424, 263.424, 263.424	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.029, 1.029, 1.029	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: O6E

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	0.27	0/6881	0.59	0/9295
1	B	0.27	0/6914	0.59	0/9341
All	All	0.27	0/13795	0.59	0/18636

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

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	6749	0	6786	98	0
1	B	6781	0	6809	112	0
2	A	43	0	0	3	0
2	B	43	0	0	0	0
All	All	13616	0	13595	202	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 7.

All (202) 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:975:GLN:O	1:A:979:ILE:HG13	1.76	0.86
1:A:352:ARG:HH22	2:A:1201:O6E:CAM	2.03	0.71
1:A:186:LEU:HD21	1:B:835:GLY:HA3	1.74	0.70
1:A:1035:ILE:HG12	1:A:1036:GLU:HG3	1.74	0.69
1:B:1087:PHE:HB2	1:B:1144:LEU:HD11	1.75	0.68
1:A:1116:LEU:HD11	1:B:930:LYS:HG3	1.75	0.67
1:B:813:TRP:HB3	1:B:825:ARG:HG3	1.78	0.65
1:B:808:THR:HG21	1:B:834:VAL:HG22	1.79	0.65
1:B:1136:ARG:HB3	1:B:1140:ARG:HH11	1.62	0.63
1:B:845:LYS:HB2	1:B:849:ALA:HB2	1.81	0.63
1:B:454:MET:HG2	1:B:457:ARG:HH21	1.64	0.63
1:A:804:ALA:HB2	1:A:833:ILE:HD12	1.80	0.62
1:B:378:ASN:O	1:B:430:ASN:ND2	2.33	0.61
1:B:1132:VAL:HG23	1:B:1144:LEU:HB3	1.82	0.61
1:B:514:THR:HG1	1:B:778:ASP:N	1.98	0.60
1:A:464:VAL:HG11	1:A:488:TYR:HB3	1.83	0.60
1:B:808:THR:HG22	1:B:808:THR:O	2.01	0.60
1:B:1144:LEU:HD12	1:B:1144:LEU:O	2.00	0.60
1:B:304:PRO:HA	1:B:568:HIS:HB2	1.83	0.59
1:B:1087:PHE:HB2	1:B:1144:LEU:CD1	2.32	0.59
1:A:352:ARG:NH2	2:A:1201:O6E:OBG	2.36	0.59
1:B:542:ALA:HB3	1:B:550:LEU:HB2	1.84	0.59
1:B:820:LEU:HD11	1:B:881:VAL:HG21	1.85	0.59
1:A:975:GLN:O	1:A:979:ILE:CG1	2.50	0.59
1:B:228:ILE:HG23	1:B:233:GLN:HB2	1.84	0.59
1:A:975:GLN:HG2	1:A:979:ILE:HD11	1.85	0.58
1:A:281:ASP:HB2	1:A:283:HIS:HD1	1.69	0.58
1:A:480:ALA:HB3	1:A:551:PHE:HB2	1.85	0.58
1:A:1087:PHE:HB2	1:A:1144:LEU:HB2	1.85	0.58
1:A:275:VAL:HG22	1:A:400:VAL:HG22	1.86	0.57
1:A:601:THR:O	1:A:605:ASP:HB2	2.04	0.57
1:B:271:ASP:HB2	1:B:404:HIS:HA	1.87	0.56
1:A:1068:HIS:HB3	1:A:1088:ARG:HB3	1.86	0.56
1:B:466:GLN:HG3	1:B:468:PRO:HD2	1.87	0.56
1:B:282:GLU:O	1:B:313:ARG:NH1	2.39	0.56
1:A:615:ARG:NH1	1:A:778:ASP:OD1	2.38	0.56
1:B:312:SER:HA	1:B:315:LEU:HD12	1.87	0.56
1:A:1022:LEU:HD22	1:A:1056:ILE:HG23	1.87	0.55
1:B:233:GLN:HA	1:B:236:LYS:HD2	1.86	0.55
1:A:868:LYS:O	1:A:919:ARG:NH1	2.38	0.55
1:A:1005:VAL:HG22	1:A:1041:GLN:HG3	1.88	0.55
1:B:108:ILE:HG21	1:B:315:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:LYS:HA	1:B:376:ILE:HD11	1.87	0.55
1:B:117:PHE:HB3	1:B:325:VAL:HG11	1.89	0.55
1:B:986:GLU:HG3	1:B:988:ILE:HG12	1.89	0.55
1:A:1027:ASP:N	1:A:1027:ASP:OD1	2.39	0.54
1:A:1047:LEU:HD22	1:A:1125:LEU:HG	1.89	0.54
1:A:921:GLN:NE2	1:A:924:GLU:OE1	2.39	0.53
1:B:272:ARG:NH2	1:B:296:GLU:O	2.40	0.53
1:B:138:ARG:HG2	1:B:157:LEU:HD13	1.91	0.53
1:A:164:ARG:HG2	1:A:172:SER:HB2	1.89	0.53
1:A:959:ASN:HB3	1:A:962:GLN:HB2	1.91	0.53
1:B:798:ILE:HD12	1:B:799:PRO:HD2	1.91	0.53
1:A:984:ASP:HB2	1:B:934:TYR:CE2	2.44	0.53
1:B:240:ARG:HH21	1:B:1100:LEU:HD12	1.74	0.52
1:B:537:CYS:SG	1:B:538:GLY:N	2.82	0.52
1:A:252:ASP:OD1	1:A:252:ASP:N	2.41	0.52
1:A:957:ASP:OD1	1:A:957:ASP:N	2.42	0.52
1:B:1082:ALA:HA	1:B:1149:LEU:HA	1.91	0.52
1:B:1020:ARG:HB3	1:B:1022:LEU:HD13	1.92	0.52
1:B:1077:ALA:HB3	1:B:1080:PHE:HB3	1.92	0.52
1:A:457:ARG:HH22	1:A:468:PRO:HG2	1.74	0.51
1:A:450:LEU:HD11	1:A:468:PRO:HB2	1.92	0.51
1:B:512:ASP:OD1	1:B:512:ASP:N	2.42	0.51
1:B:867:ASP:HA	1:B:886:THR:HG23	1.91	0.51
1:B:455:LEU:HD13	1:B:613:ILE:HB	1.92	0.51
1:A:369:ALA:HB3	1:A:404:HIS:HB3	1.93	0.50
1:A:975:GLN:HG2	1:A:979:ILE:CD1	2.42	0.50
1:A:1036:GLU:HB3	1:A:1151:VAL:HG22	1.93	0.50
1:B:990:ASP:N	1:B:990:ASP:OD1	2.44	0.50
1:B:834:VAL:HB	1:B:854:MET:HG2	1.94	0.50
1:B:999:GLU:HG3	1:B:1038:PHE:HB2	1.94	0.50
1:B:215:ASP:HB3	1:B:351:LEU:HD13	1.93	0.49
1:A:304:PRO:HG2	1:A:307:ASP:HB2	1.94	0.49
1:A:1060:PRO:HG2	1:A:1063:GLU:HG3	1.94	0.49
1:B:143:ILE:HG13	1:B:157:LEU:HD11	1.93	0.49
1:B:315:LEU:HD23	1:B:347:VAL:HG23	1.93	0.49
1:A:138:ARG:HA	1:A:143:ILE:HG22	1.94	0.49
1:B:544:ILE:HB	1:B:548:ASP:HB2	1.94	0.49
1:A:117:PHE:HB3	1:A:325:VAL:HG21	1.94	0.49
1:A:803:ALA:HB3	1:A:812:GLU:HB3	1.94	0.48
1:A:1067:ILE:HG13	1:A:1089:MET:HG2	1.94	0.48
1:B:532:LEU:HB3	1:B:536:VAL:HB	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HH21	1:A:157:LEU:HB3	1.78	0.48
1:A:834:VAL:HB	1:A:854:MET:HG2	1.95	0.48
1:A:837:VAL:HA	1:A:841:CYS:HB2	1.94	0.48
1:A:470:ILE:O	1:A:552:TRP:NE1	2.35	0.48
1:A:268:THR:O	1:A:408:ARG:NH1	2.47	0.48
1:B:1144:LEU:HD12	1:B:1144:LEU:C	2.39	0.48
1:A:1006:ILE:HA	1:A:1009:ILE:HG22	1.94	0.48
1:A:980:VAL:CG2	1:B:939:ILE:HD11	2.43	0.48
1:B:844:LEU:HD12	1:B:849:ALA:HB1	1.96	0.47
1:B:178:ALA:HA	1:B:187:LEU:HD22	1.96	0.47
1:B:1020:ARG:NH2	1:B:1057:ARG:O	2.47	0.47
1:A:403:HIS:NE2	2:A:1201:O6E:OAK	2.36	0.47
1:A:171:SER:HB3	1:A:192:ILE:HG12	1.96	0.47
1:B:209:ASP:N	1:B:209:ASP:OD1	2.46	0.47
1:B:264:VAL:O	1:B:268:THR:OG1	2.33	0.46
1:A:322:ARG:NH1	1:A:352:ARG:O	2.40	0.46
1:A:971:SER:O	1:A:1045:GLN:NE2	2.46	0.46
1:B:1096:LEU:HD21	1:B:1100:LEU:HD22	1.97	0.46
1:B:1128:MET:HE3	1:B:1146:ILE:HD11	1.96	0.46
1:B:875:ASP:OD1	1:B:879:LYS:N	2.48	0.46
1:B:868:LYS:O	1:B:919:ARG:NH2	2.48	0.46
1:A:346:LEU:H	1:A:346:LEU:HD23	1.79	0.46
1:A:1022:LEU:HD23	1:A:1065:VAL:HB	1.97	0.46
1:A:875:ASP:OD1	1:A:876:ARG:N	2.48	0.46
1:A:985:LEU:C	1:A:985:LEU:HD23	2.41	0.46
1:B:543:TYR:OH	1:B:547:ARG:NH1	2.47	0.46
1:B:473:LEU:HD22	1:B:610:LEU:HD22	1.97	0.46
1:B:480:ALA:HB3	1:B:551:PHE:HB2	1.96	0.46
1:B:801:ILE:HB	1:B:814:ASN:HB2	1.98	0.46
1:A:326:ASP:HB3	1:A:329:ALA:HB2	1.98	0.46
1:A:852:LYS:HB3	1:A:869:PHE:HZ	1.81	0.46
1:B:1013:ALA:HA	1:B:1053:LEU:HD21	1.97	0.45
1:A:492:VAL:HG11	1:A:1149:LEU:HD22	1.98	0.45
1:B:833:ILE:HA	1:B:837:VAL:HB	1.97	0.45
1:B:1052:LEU:HD12	1:B:1089:MET:HG2	1.98	0.45
1:A:292:ARG:NE	1:A:294:ASP:OD1	2.46	0.45
1:A:1104:MET:SD	1:A:1142:TYR:OH	2.68	0.45
1:B:1039:GLY:HA3	1:B:1148:GLU:HG2	1.98	0.45
1:A:207:ARG:HG2	1:A:212:VAL:HG12	1.99	0.45
1:B:277:LYS:HD3	1:B:287:VAL:HG11	1.97	0.45
1:A:786:ASP:N	1:A:786:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:GLN:NE2	1:B:1077:ALA:O	2.49	0.45
1:A:178:ALA:HA	1:A:187:LEU:HD13	1.98	0.45
1:A:875:ASP:HB3	1:A:879:LYS:H	1.81	0.45
1:A:1010:VAL:HG21	1:A:1026:ARG:HH12	1.82	0.45
1:B:517:SER:O	1:B:517:SER:OG	2.36	0.44
1:A:847:PRO:HB3	1:B:379:GLY:HA2	1.99	0.44
1:A:946:MET:HE3	1:A:946:MET:HB2	1.86	0.44
1:A:975:GLN:NE2	1:B:942:PRO:HG3	2.32	0.44
1:A:1066:GLU:O	1:A:1090:ALA:N	2.49	0.44
1:A:215:ASP:HB3	1:A:351:LEU:HD13	1.99	0.44
1:A:346:LEU:HD12	1:A:352:ARG:HB3	1.99	0.44
1:A:374:ALA:HA	1:A:399:LEU:HD23	2.00	0.44
1:B:540:ALA:HB3	1:B:552:TRP:HB2	2.00	0.44
1:B:1044:ILE:O	1:B:1048:LEU:HB2	2.17	0.44
1:A:970:VAL:O	1:A:974:LYS:HG3	2.18	0.44
1:B:261:VAL:HG12	1:B:273:VAL:HG12	2.00	0.44
1:B:943:LEU:HD11	1:B:976:ILE:HG22	1.99	0.44
1:A:404:HIS:CD2	1:A:408:ARG:HB2	2.53	0.44
1:A:975:GLN:HA	1:A:1042:ILE:HG23	2.00	0.44
1:B:1060:PRO:HG3	1:B:1093:GLY:HA3	2.00	0.44
1:B:463:ILE:HG22	1:B:470:ILE:HB	2.00	0.44
1:B:872:PRO:HA	1:B:882:GLN:HA	2.00	0.44
1:A:949:ALA:O	1:A:953:LEU:HB2	2.18	0.43
1:B:442:LYS:HG3	1:B:911:LEU:HD11	1.98	0.43
1:A:517:SER:HB2	1:A:604:MET:HE2	2.00	0.43
1:A:336:GLN:HE22	1:A:344:MET:HB2	1.84	0.43
1:A:818:GLU:HG3	1:A:824:SER:HA	2.01	0.43
1:A:1009:ILE:HD12	1:A:1009:ILE:HA	1.78	0.43
1:A:143:ILE:HD13	1:A:157:LEU:HB2	2.01	0.43
1:A:516:LEU:HB3	1:A:541:VAL:HG12	2.01	0.43
1:B:808:THR:CG2	1:B:834:VAL:HG22	2.47	0.43
1:B:946:MET:HE2	1:B:946:MET:HB2	1.84	0.43
1:B:122:ALA:N	1:B:132:GLY:O	2.44	0.42
1:A:1136:ARG:HG2	1:A:1140:ARG:HG3	2.00	0.42
1:A:559:LYS:HZ3	1:A:561:ILE:HD11	1.84	0.42
1:B:268:THR:HG22	1:B:410:ILE:HD13	2.00	0.42
1:B:836:GLU:HA	1:B:840:SER:HB3	2.01	0.42
1:B:189:PRO:HG3	1:B:413:PRO:HD3	2.02	0.42
1:B:445:LEU:HD22	1:B:905:GLN:HB3	2.02	0.42
1:A:917:VAL:HA	1:B:917:VAL:HG12	2.01	0.42
1:B:323:MET:HE2	1:B:323:MET:HB3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:983:MET:HA	1:B:990:ASP:HB2	2.02	0.42
1:B:1014:MET:HA	1:B:1017:LEU:HD12	2.01	0.42
1:B:140:MET:O	1:B:199:LYS:NZ	2.44	0.41
1:A:911:LEU:HD12	1:A:914:ALA:HB3	2.01	0.41
1:B:234:SER:HB3	1:B:413:PRO:HA	2.02	0.41
1:B:829:ILE:HD12	1:B:829:ILE:HA	1.92	0.41
1:A:189:PRO:HG3	1:A:413:PRO:HD3	2.02	0.41
1:A:882:GLN:O	1:A:912:GLN:NE2	2.54	0.41
1:A:1010:VAL:HG21	1:A:1026:ARG:HH22	1.84	0.41
1:B:393:SER:O	1:B:393:SER:OG	2.33	0.41
1:B:496:GLU:HA	1:B:499:ILE:HG22	2.02	0.41
1:B:930:LYS:O	1:B:934:TYR:HB3	2.21	0.41
1:A:188:ASN:HA	1:A:189:PRO:HA	1.79	0.41
1:A:514:THR:HB	1:A:611:GLN:HE22	1.85	0.41
1:A:543:TYR:O	1:A:611:GLN:NE2	2.43	0.41
1:B:927:THR:HA	1:B:930:LYS:HD3	2.03	0.41
1:B:1024:LEU:HD11	1:B:1067:ILE:HD11	2.03	0.41
1:B:256:LEU:HG	1:B:425:PHE:HE1	1.86	0.41
1:B:362:MET:HE3	1:B:370:SER:HB3	2.03	0.41
1:B:554:ARG:NH1	1:B:603:GLU:OE1	2.54	0.41
1:B:834:VAL:HG13	1:B:857:LEU:HD23	2.02	0.41
1:A:609:SER:HB3	1:A:797:LEU:H	1.85	0.41
1:B:217:GLU:OE2	1:B:415:ARG:NH2	2.39	0.41
1:B:240:ARG:HD2	1:B:240:ARG:HA	1.87	0.41
1:B:378:ASN:OD1	1:B:378:ASN:N	2.53	0.41
1:A:276:TYR:CZ	1:A:284:GLY:HA3	2.56	0.41
1:B:1087:PHE:CD2	1:B:1144:LEU:HD11	2.56	0.41
1:A:323:MET:HE3	1:A:323:MET:HB2	1.88	0.40
1:A:855:ILE:HG12	1:B:242:ILE:HG21	2.02	0.40
1:B:238:ALA:HB2	1:B:417:ALA:HB1	2.04	0.40
1:B:248:LEU:HA	1:B:249:PRO:HD3	1.96	0.40
1:B:808:THR:HG21	1:B:834:VAL:CG2	2.48	0.40
1:A:805:ASP:HB3	1:A:811:LEU:HD11	2.01	0.40
1:B:1053:LEU:HD23	1:B:1053:LEU:HA	1.97	0.40
1:A:801:ILE:HG12	1:A:903:PHE:HB3	2.04	0.40
1:A:1088:ARG:HA	1:A:1088:ARG:HD2	1.82	0.40
1:B:823:TRP:HA	1:B:876:ARG:HH11	1.86	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	847/1172 (72%)	795 (94%)	52 (6%)	0	100	100
1	B	854/1172 (73%)	808 (95%)	46 (5%)	0	100	100
All	All	1701/2344 (73%)	1603 (94%)	98 (6%)	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	739/994 (74%)	734 (99%)	5 (1%)	76	80
1	B	742/994 (75%)	734 (99%)	8 (1%)	65	76
All	All	1481/1988 (74%)	1468 (99%)	13 (1%)	68	78

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	LEU
1	A	245	LEU
1	A	470	ILE
1	A	965	LEU
1	A	1072	LEU
1	B	220	ARG
1	B	234	SER
1	B	370	SER

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Mol	Chain	Res	Type
1	B	536	VAL
1	B	611	GLN
1	B	917	VAL
1	B	1048	LEU
1	B	1149	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	302	HIS
1	A	318	GLN
1	A	355	HIS
1	A	360	GLN
1	A	448	GLN
1	A	859	ASN
1	A	912	GLN
1	A	937	GLN
1	A	959	ASN
1	A	1012	GLN
1	B	380	ASN
1	B	580	HIS
1	B	1012	GLN
1	B	1133	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	O6E	A	1201	1	46,46,46	2.00	13 (28%)	62,67,67	1.37	9 (14%)
2	O6E	B	1201	1	46,46,46	2.03	14 (30%)	62,67,67	1.28	5 (8%)

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	O6E	A	1201	1	-	7/26/74/74	0/4/4/4
2	O6E	B	1201	1	-	9/26/74/74	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	O6E	CAO-CBO	5.71	1.53	1.40
2	B	1201	O6E	CAP-CBL	5.54	1.53	1.40
2	B	1201	O6E	CAO-CBO	5.22	1.52	1.40
2	A	1201	O6E	CAP-CBL	5.04	1.52	1.40
2	A	1201	O6E	CAQ-CAY	4.52	1.50	1.40
2	B	1201	O6E	CAQ-CAY	4.45	1.50	1.40
2	B	1201	O6E	CAV-NAE	3.46	1.46	1.38
2	A	1201	O6E	CAV-CBB	3.44	1.51	1.45
2	B	1201	O6E	CAV-CBB	3.43	1.51	1.45
2	A	1201	O6E	CAV-NAE	3.20	1.45	1.38
2	B	1201	O6E	CAW-NAJ	3.11	1.43	1.37
2	A	1201	O6E	CAW-NAJ	3.09	1.43	1.37
2	A	1201	O6E	CAY-NAN	2.88	1.42	1.37
2	B	1201	O6E	CAF-CAL	2.85	1.57	1.50
2	A	1201	O6E	CBL-CBH	2.82	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	O6E	CBL-CBH	2.82	1.51	1.45
2	B	1201	O6E	CAI-CAM	2.80	1.57	1.50
2	A	1201	O6E	CBO-NAN	2.71	1.42	1.37
2	A	1201	O6E	CAI-CAM	2.68	1.56	1.50
2	A	1201	O6E	CAF-CAL	2.65	1.56	1.50
2	B	1201	O6E	CAY-NAN	2.60	1.42	1.37
2	B	1201	O6E	CBK-CBE	2.44	1.45	1.38
2	B	1201	O6E	CBO-NAN	2.43	1.42	1.37
2	A	1201	O6E	CBK-CBE	2.31	1.44	1.38
2	B	1201	O6E	CBJ-CBN	2.22	1.55	1.50
2	B	1201	O6E	CBN-NBP	2.17	1.41	1.37
2	A	1201	O6E	CAW-CBC	-2.08	1.41	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	O6E	CAQ-CBN-NBP	3.43	129.91	125.63
2	A	1201	O6E	CBM-CBI-CBC	2.94	111.70	107.92
2	A	1201	O6E	CBD-CAX-NBP	2.88	110.69	108.29
2	A	1201	O6E	CAS-CBC-CAW	2.88	127.66	124.16
2	B	1201	O6E	CBD-CAX-NBP	2.86	110.66	108.29
2	B	1201	O6E	CBD-CBJ-CBN	2.82	105.56	101.34
2	B	1201	O6E	CBM-CBI-CBC	2.81	111.54	107.92
2	B	1201	O6E	CAS-CBC-CAW	2.67	127.40	124.16
2	B	1201	O6E	CAQ-CBN-NBP	2.66	128.95	125.63
2	A	1201	O6E	CAQ-CAY-CBE	-2.33	121.81	127.53
2	A	1201	O6E	CAQ-CAY-NAN	2.31	130.50	125.29
2	A	1201	O6E	CAT-CBD-CAX	-2.16	107.74	112.40
2	A	1201	O6E	CBD-CBJ-CBN	2.16	104.58	101.34
2	A	1201	O6E	CBB-CAV-NAE	-2.16	106.99	110.04

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	O6E	CBL-CAP-CAW-CBC
2	B	1201	O6E	CAW-CAP-CBL-NAE
2	B	1201	O6E	CBL-CAP-CAW-CBC
2	A	1201	O6E	CBL-CAP-CAW-NAJ
2	B	1201	O6E	CBL-CAP-CAW-NAJ
2	A	1201	O6E	CAW-CAP-CBL-NAE
2	A	1201	O6E	CAW-CAP-CBL-CBH

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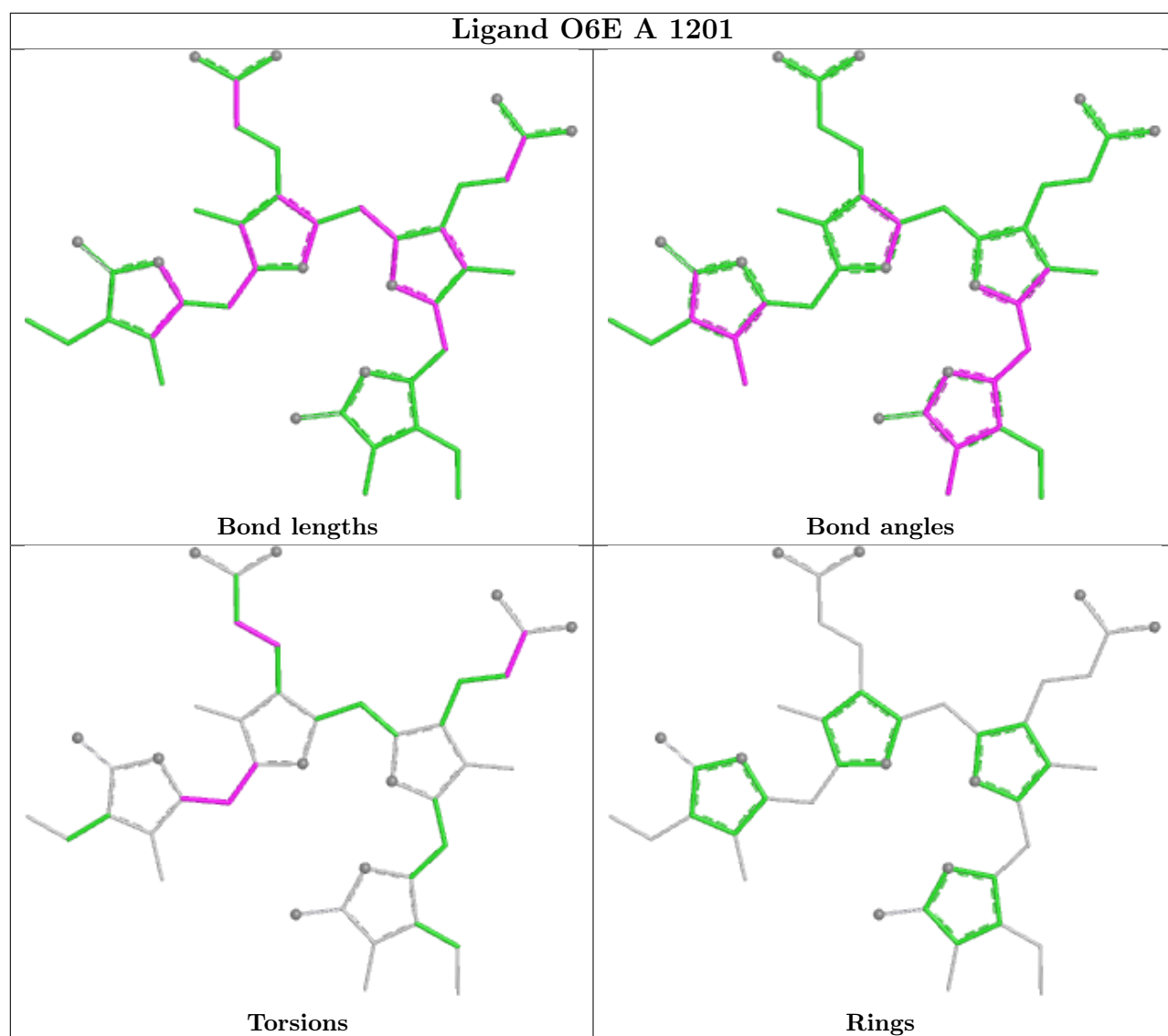
Mol	Chain	Res	Type	Atoms
2	B	1201	O6E	CAW-CAP-CBL-CBH
2	A	1201	O6E	CBB-CAA-CAF-CAL
2	B	1201	O6E	CAH-CAC-CBJ-CBN
2	B	1201	O6E	CBB-CAA-CAF-CAL
2	B	1201	O6E	CAH-CAC-CBJ-CBD
2	B	1201	O6E	CAD-CAI-CAM-OBG
2	B	1201	O6E	CAD-CAI-CAM-OBA
2	A	1201	O6E	CAD-CAI-CAM-OBA
2	A	1201	O6E	CAD-CAI-CAM-OBG

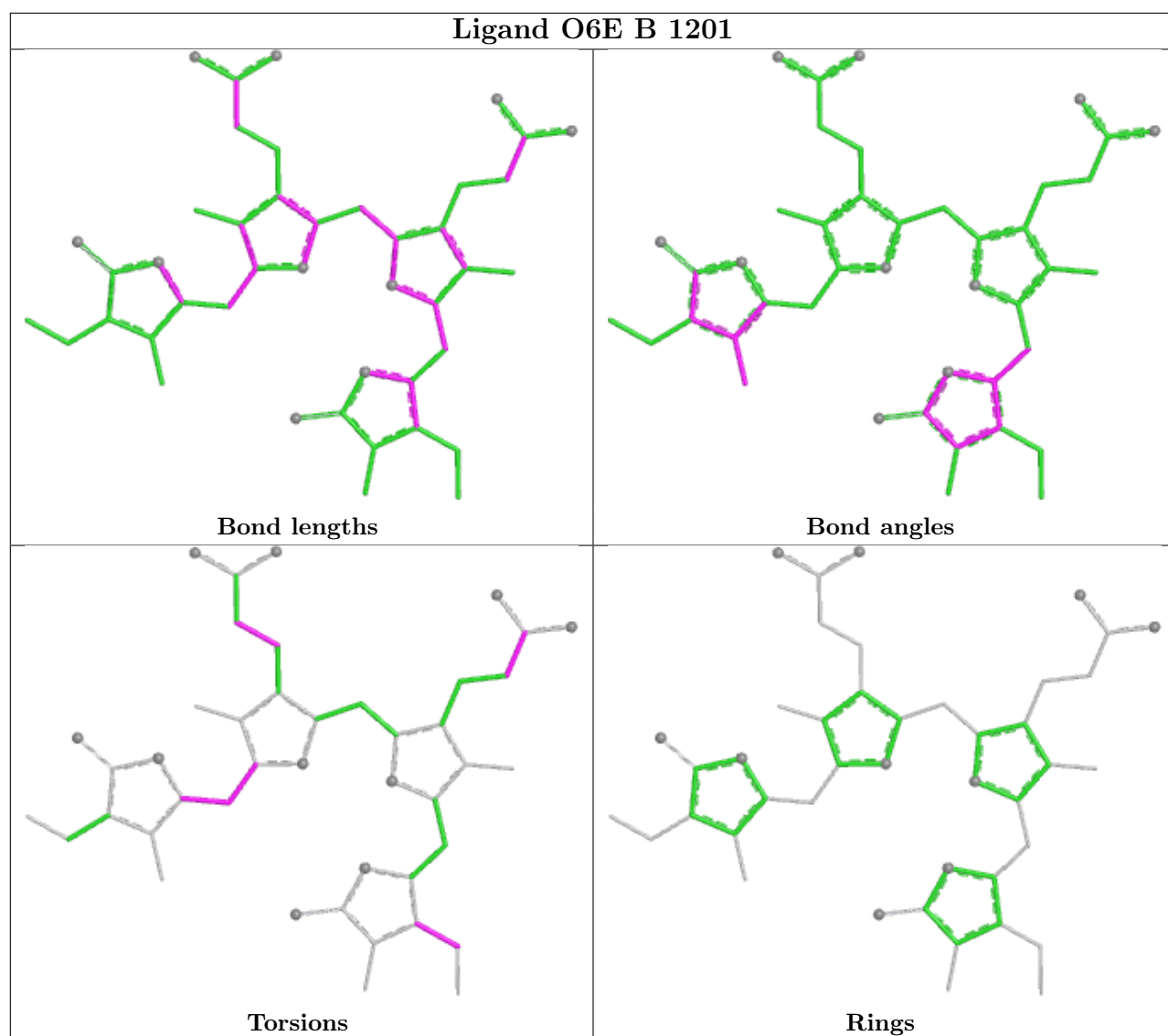
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	O6E	3	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.

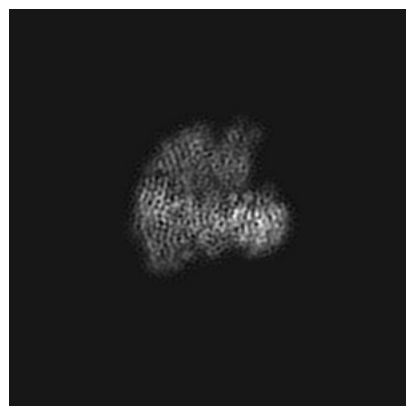
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24780. These allow visual inspection of the internal detail of the map and identification of artifacts.

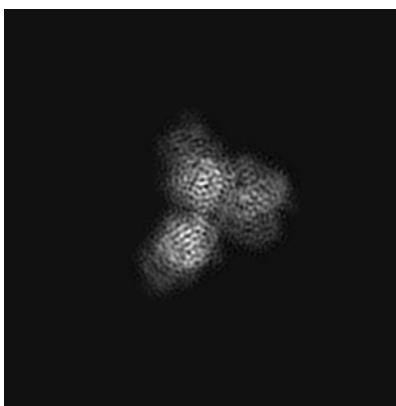
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

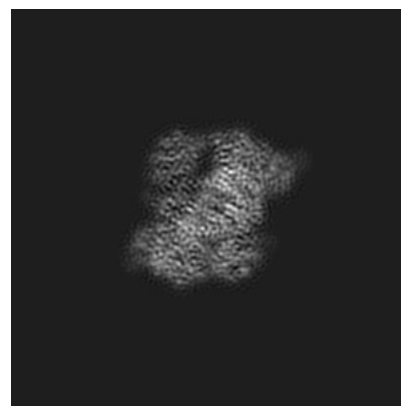
6.1.1 Primary map



X

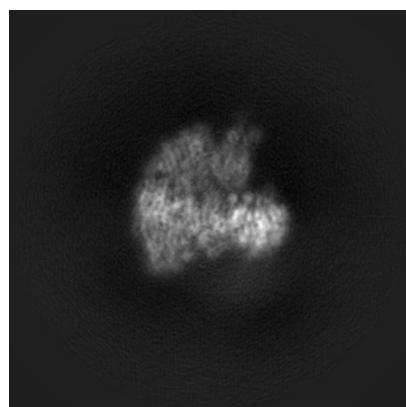


Y

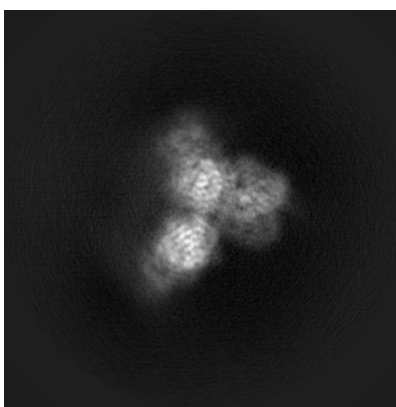


Z

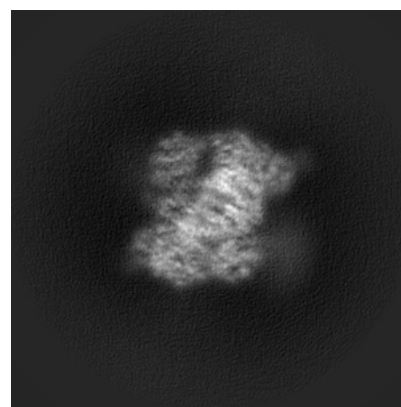
6.1.2 Raw map



X



Y

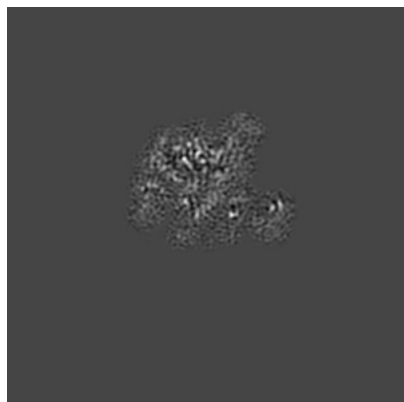


Z

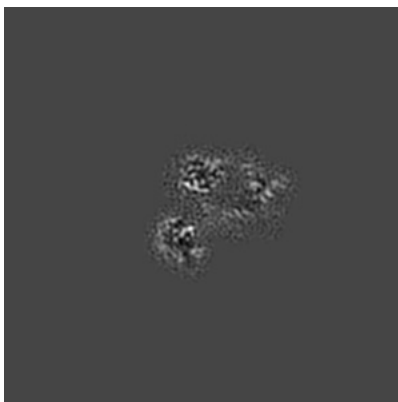
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

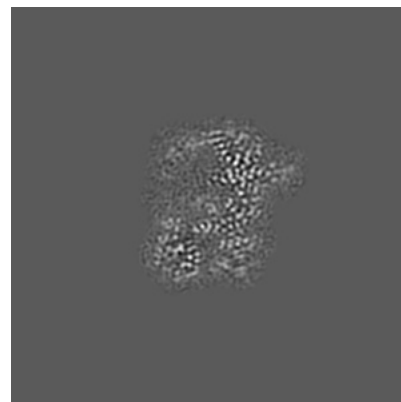
6.2.1 Primary map



X Index: 128

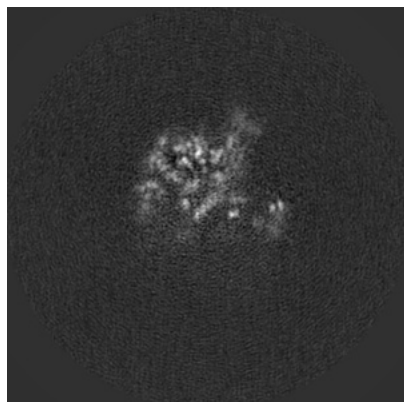


Y Index: 128

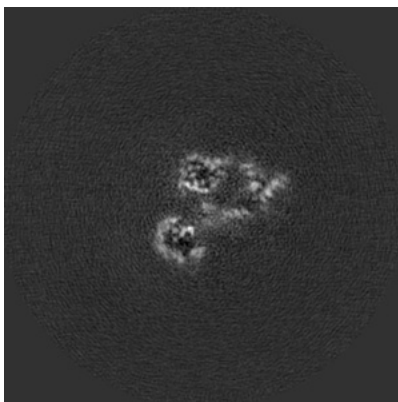


Z Index: 128

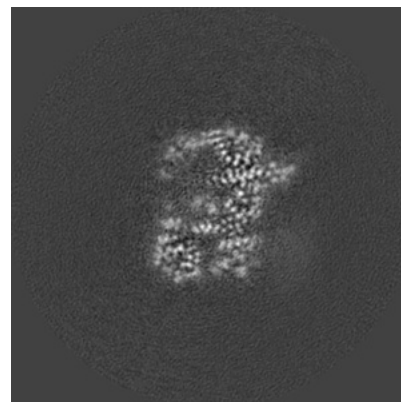
6.2.2 Raw map



X Index: 128



Y Index: 128

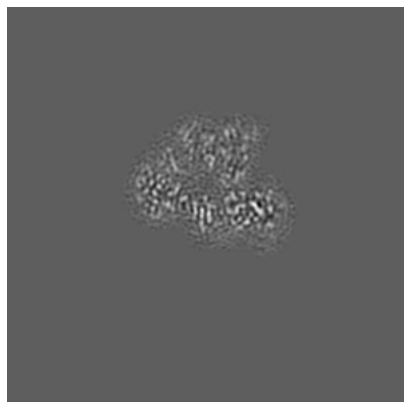


Z Index: 128

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

6.3 Largest variance slices [i](#)

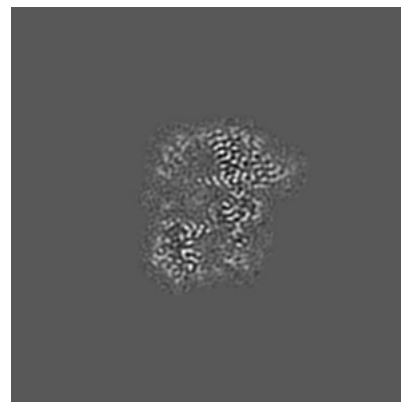
6.3.1 Primary map



X Index: 139

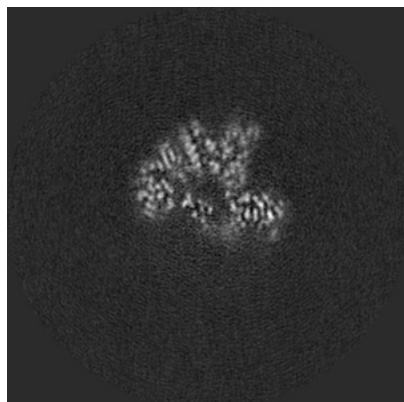


Y Index: 144

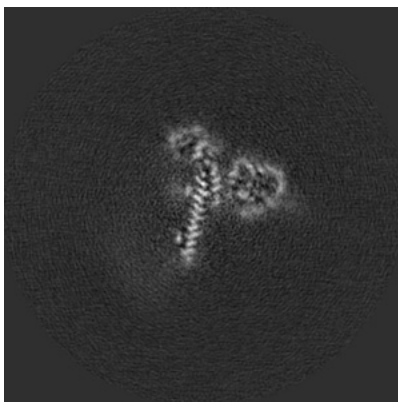


Z Index: 126

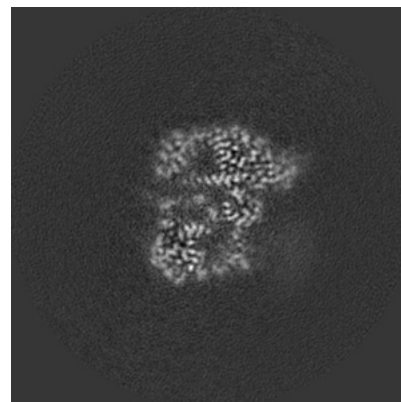
6.3.2 Raw map



X Index: 136



Y Index: 144

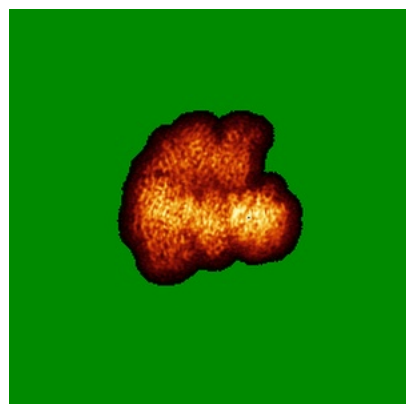


Z Index: 125

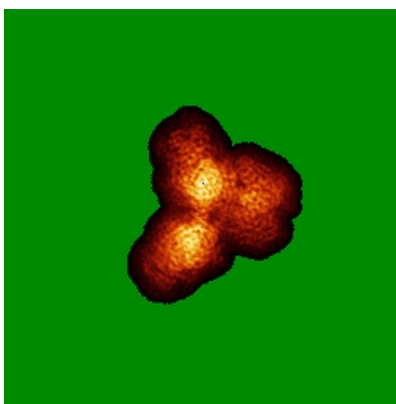
The images above show the largest variance slices of the map in three orthogonal directions.

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

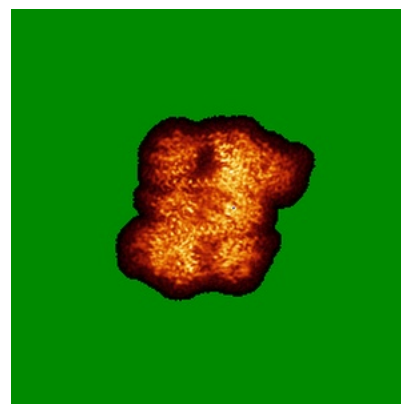
6.4.1 Primary map



X

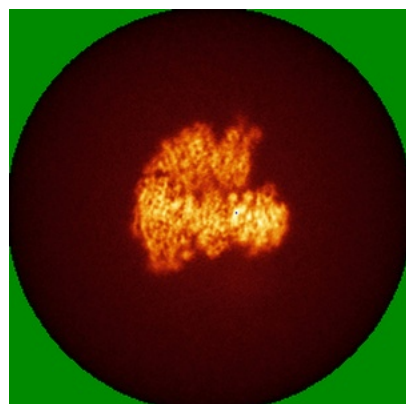


Y

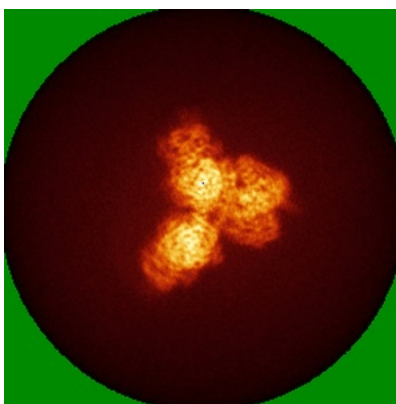


Z

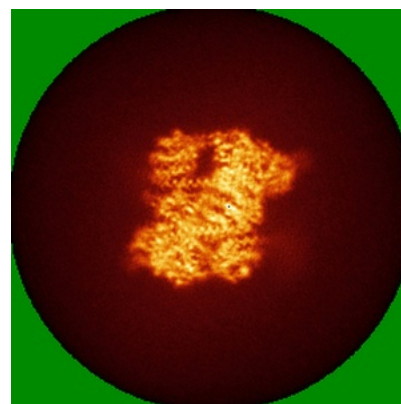
6.4.2 Raw map



X



Y

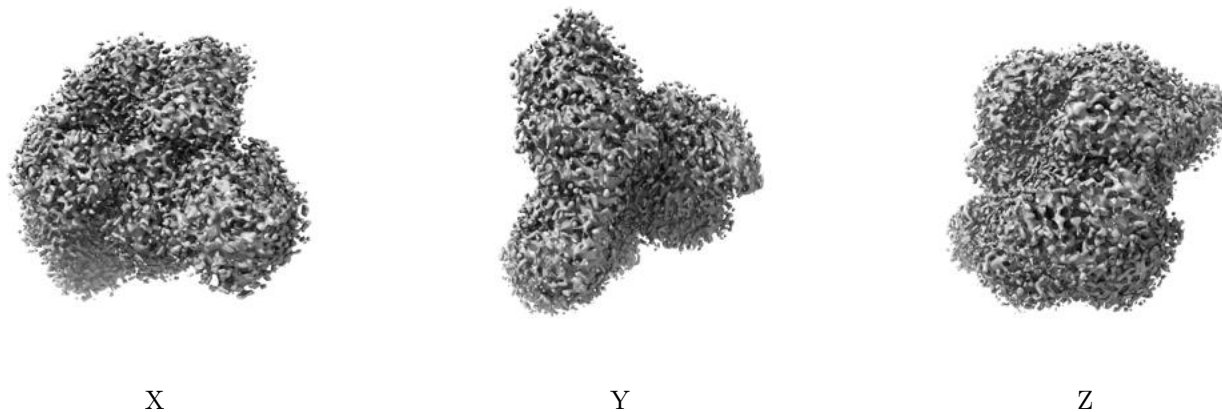


Z

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.

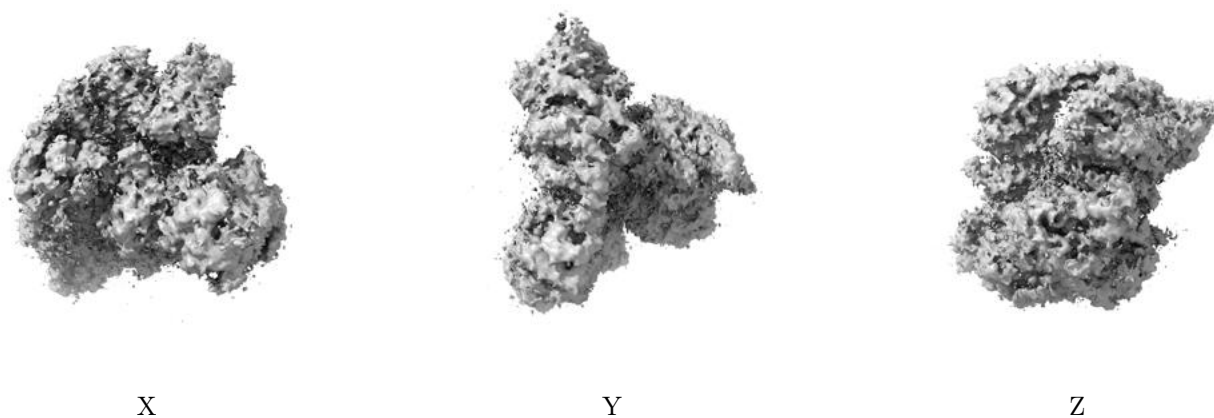
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

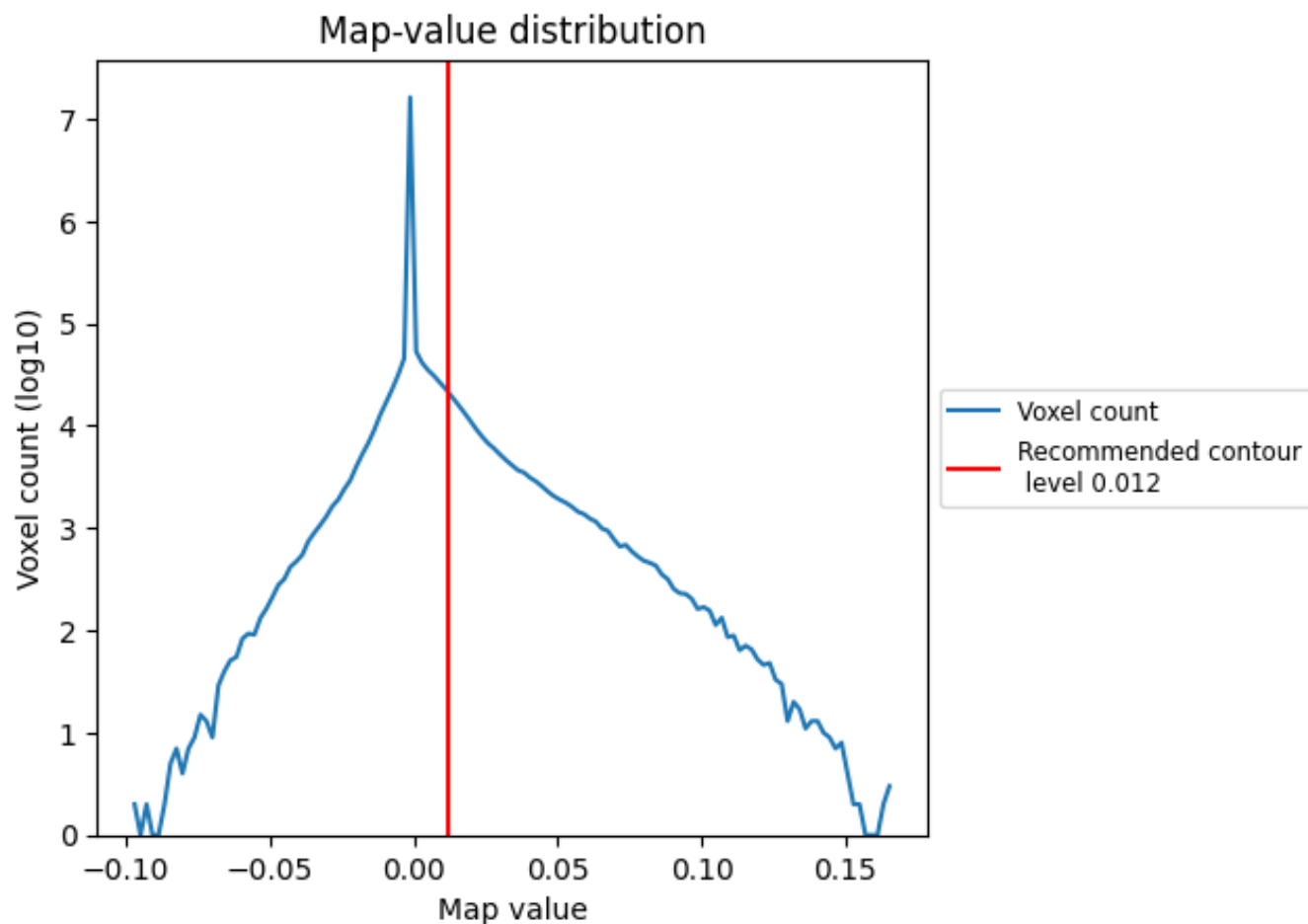
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

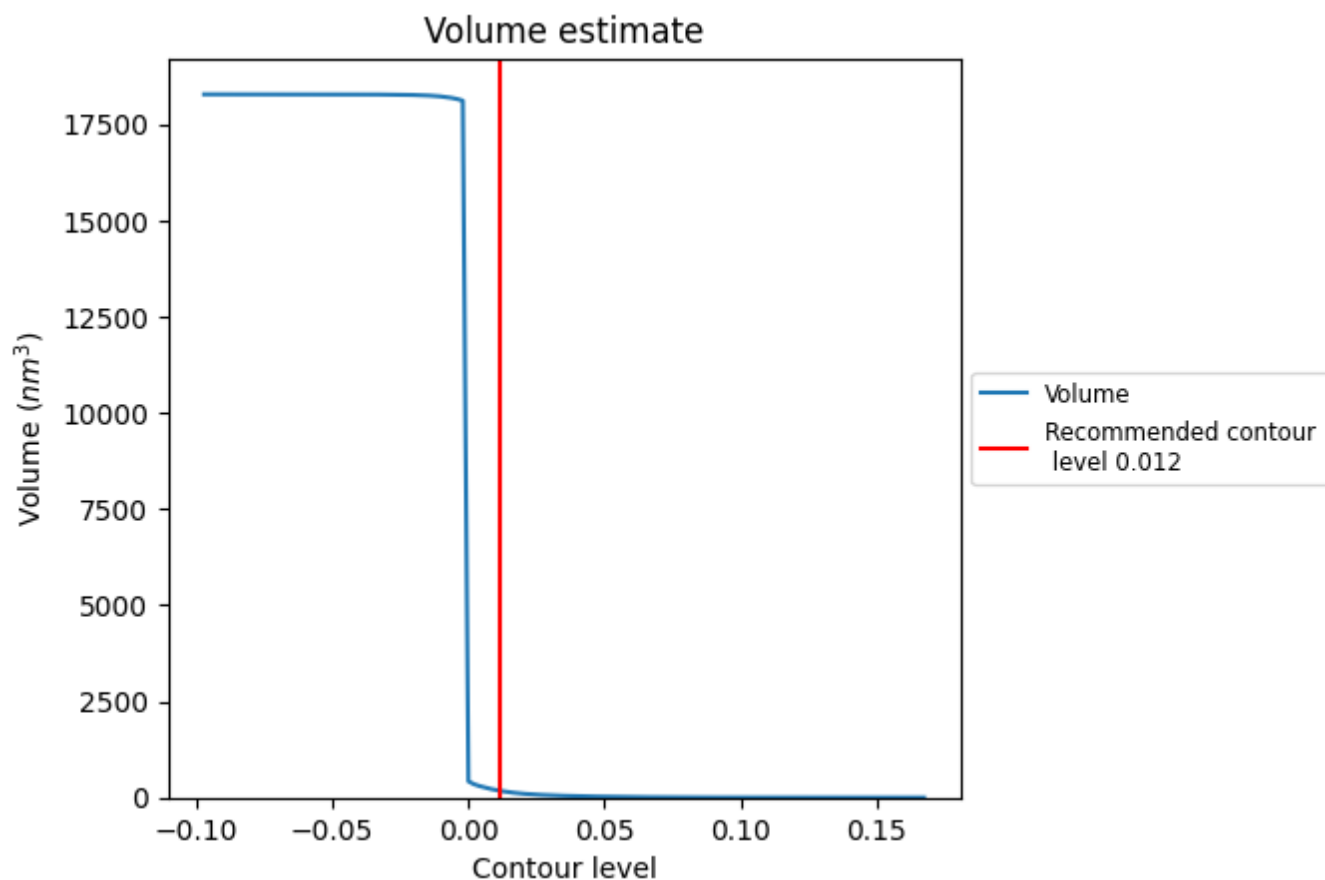
This section contains the results of statistical analysis of the map.

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.

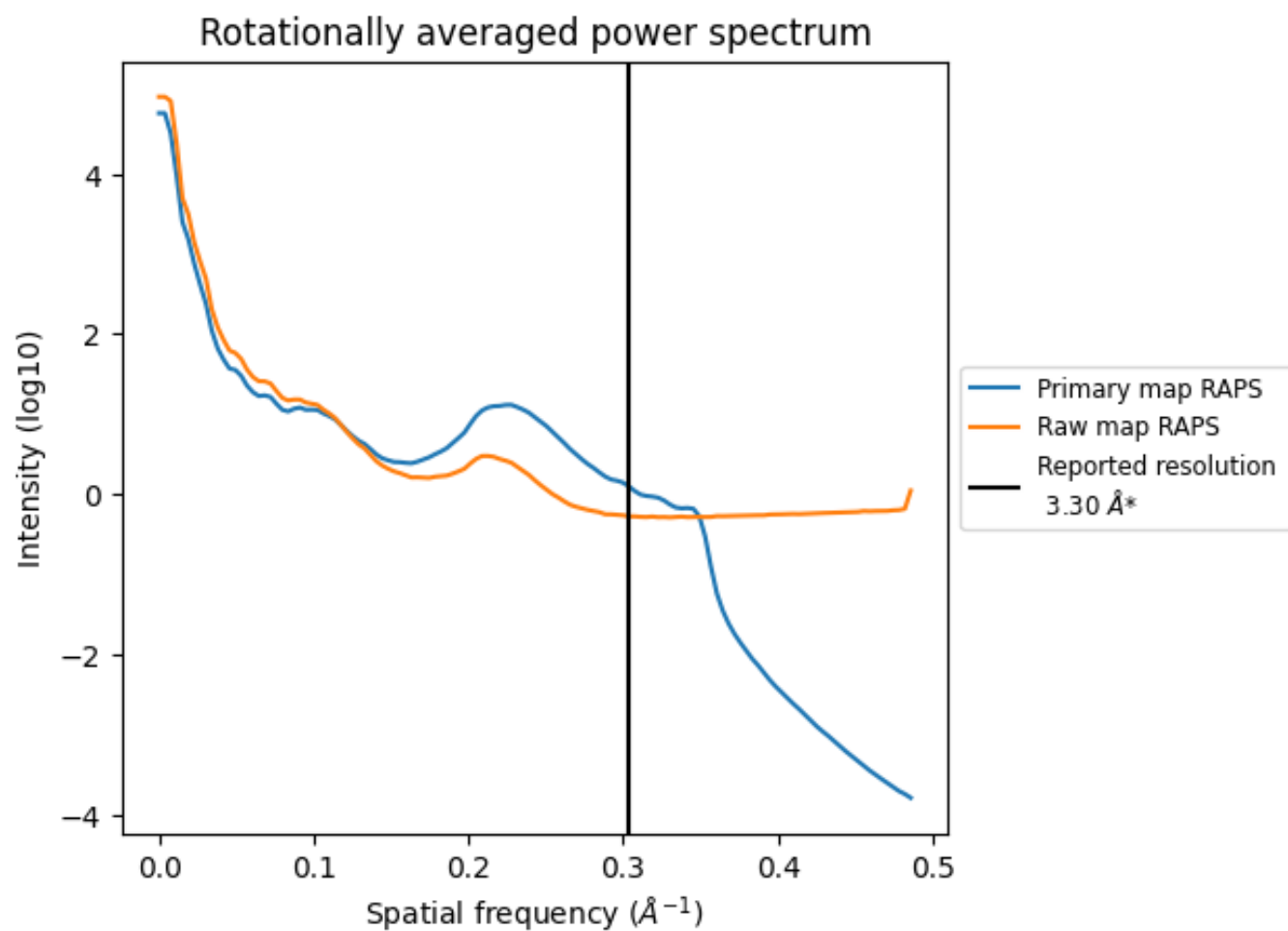
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 173 nm^3 ; this corresponds to an approximate mass of 157 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 ⓘ

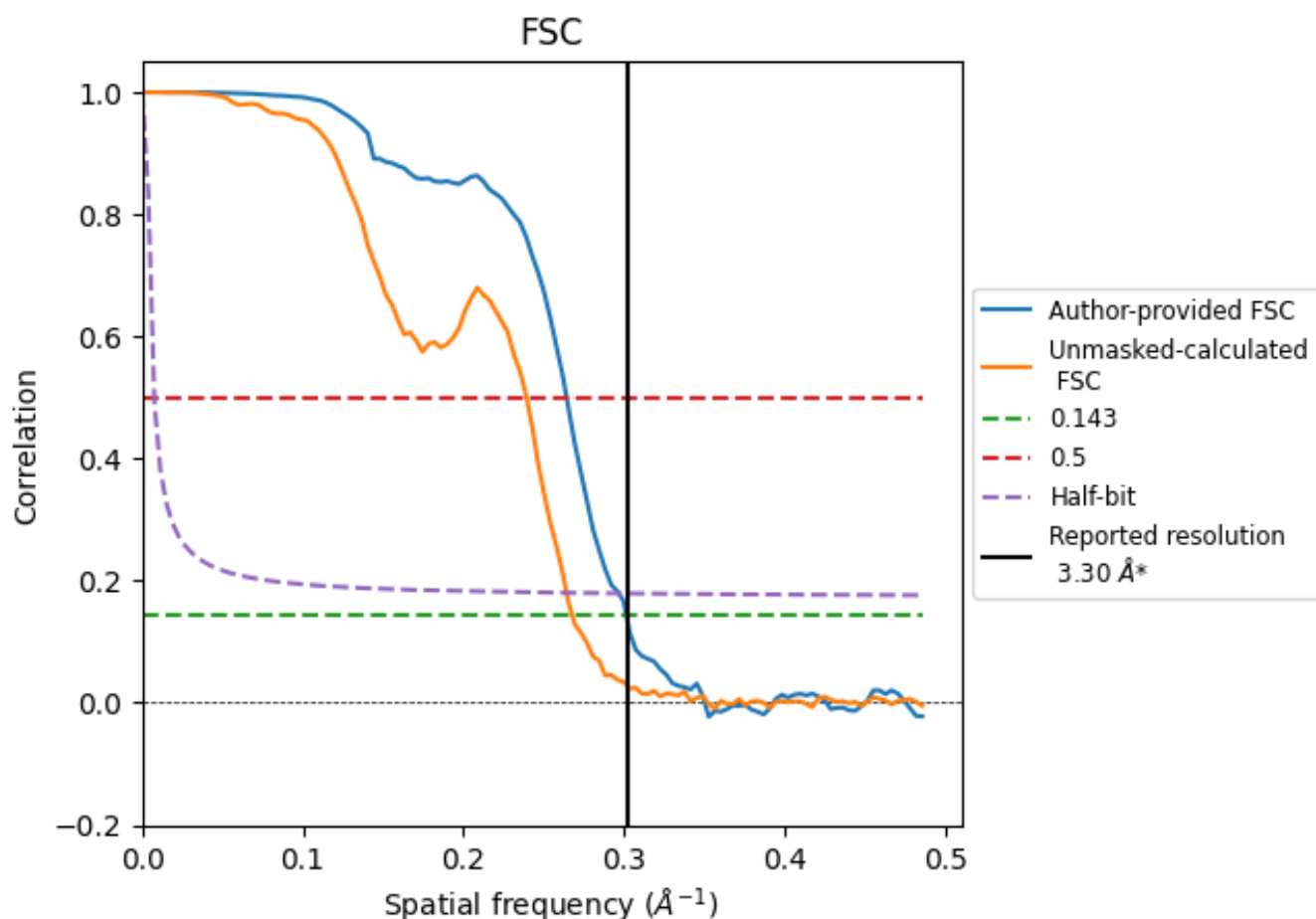


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

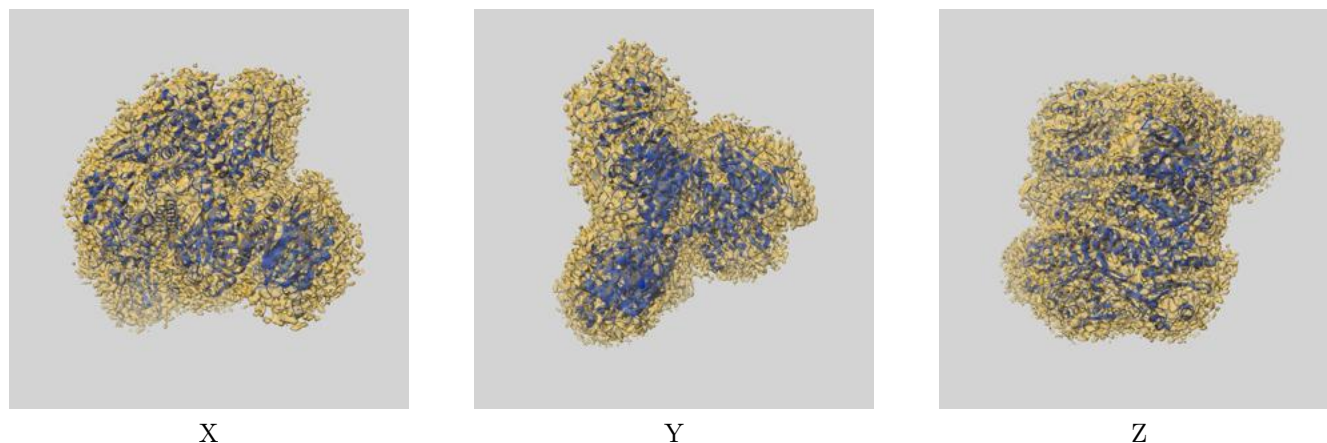
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.32	3.78	3.37
Unmasked-calculated*	3.73	4.18	3.78

*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 3.73 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

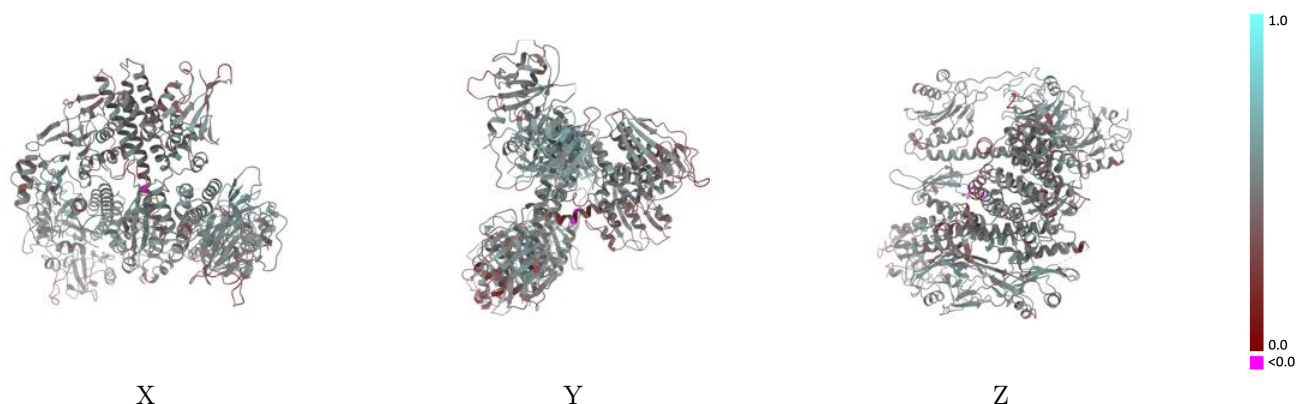
This section contains information regarding the fit between EMDB map EMD-24780 and PDB model 7RZW. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

9.1 Map-model overlay [i](#)



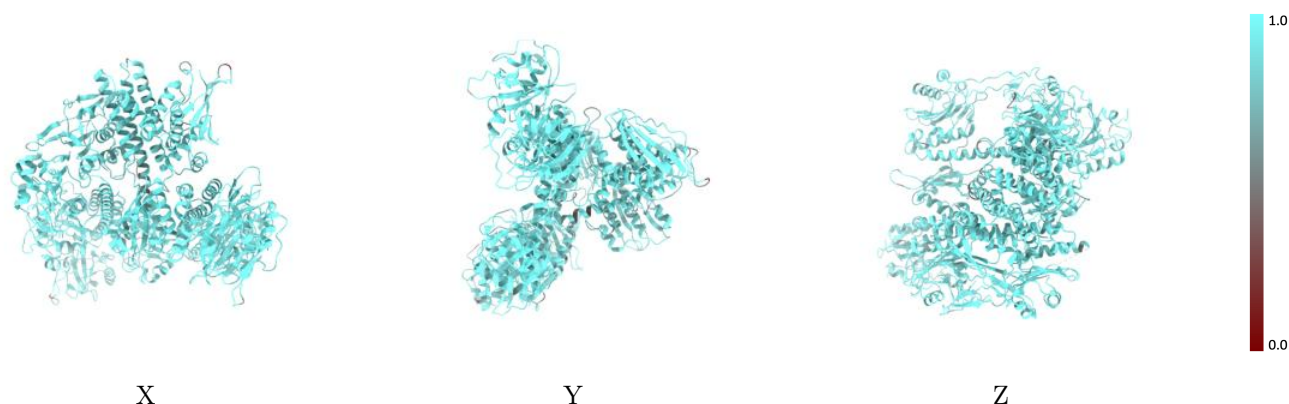
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



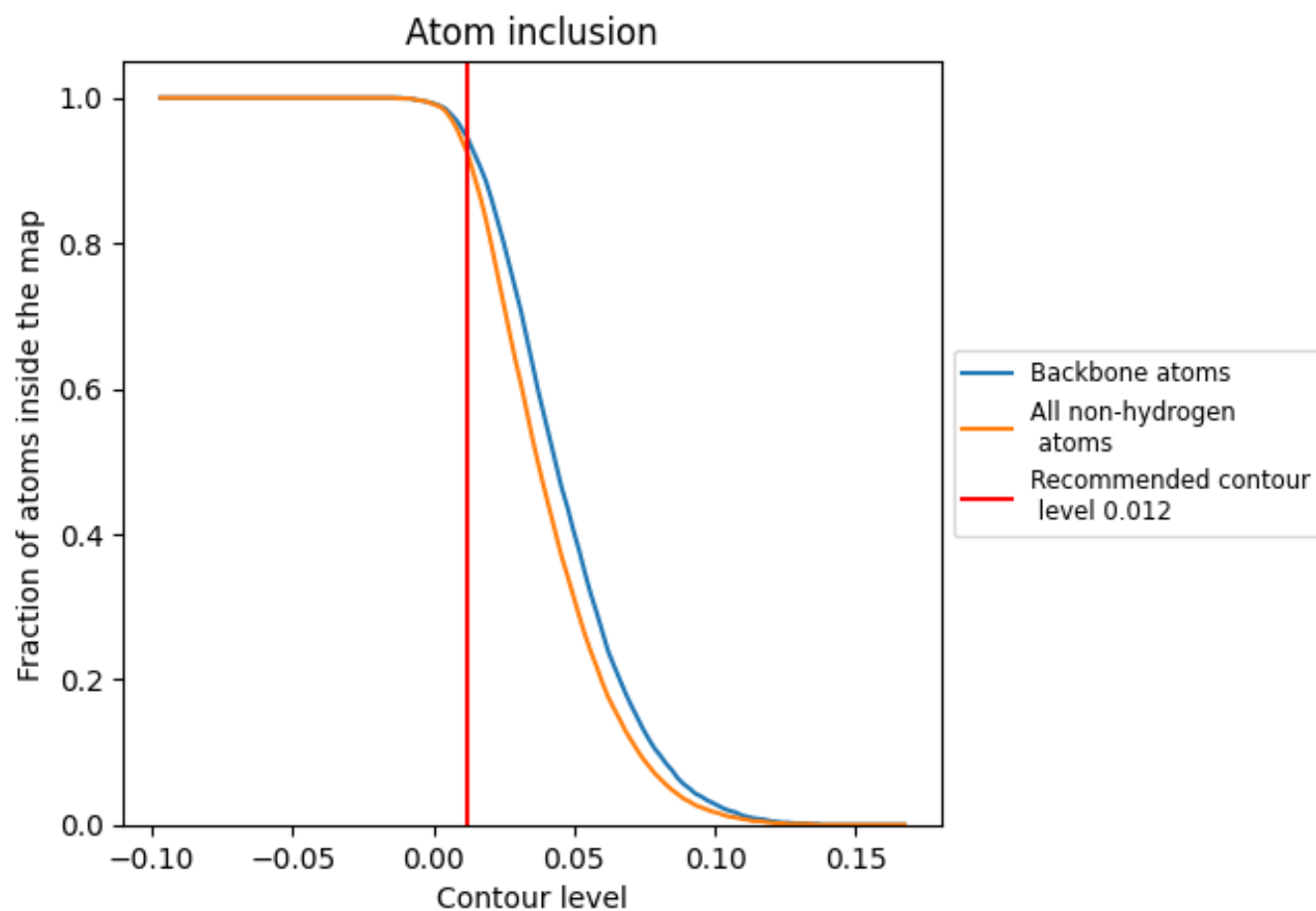
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 92% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9250	0.4750
A	0.9310	0.4780
B	0.9180	0.4710

