



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:48 PM UTC

PDB ID : 7EMY / pdb_00007emy
EMDB ID : EMD-31198
Title : Pyochelin synthetase, a dimeric nonribosomal peptide synthetase elongation module
Authors : Wang, J.L.; Wang, Z.J.
Deposited on : 2021-04-15
Resolution : 2.97 Å(reported)

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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:

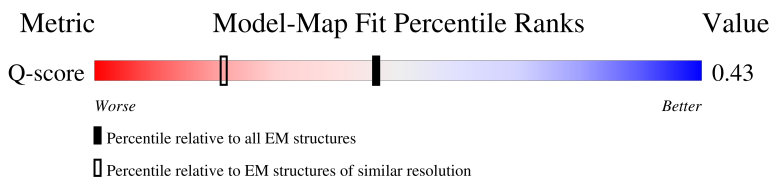
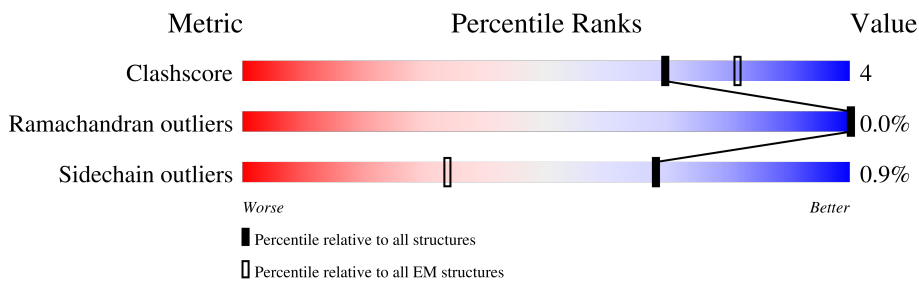
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.97 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	13205 (2.47 - 3.47)

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	1455	<p>9% (red), 57% (green), 32% (yellow), 8% (orange)</p>
1	B	1455	<p>9% (red), 57% (green), 31% (yellow), 8% (orange)</p>

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 41094 atoms, of which 20576 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 Dihydroaeruginosic acid synthetase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	1334	20444	6431	10245	1881	1854	33	0	0
1	B	1334	20444	6431	10245	1881	1854	33	0	0

There are 34 discrepancies between the modelled and reference sequences:

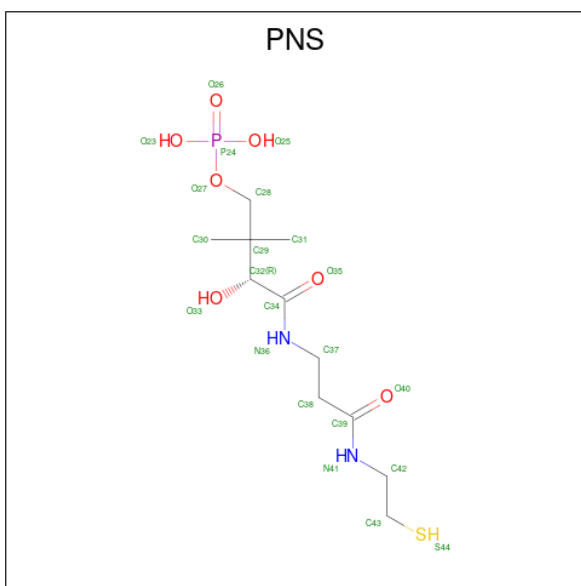
Chain	Residue	Modelled	Actual	Comment	Reference
A	1439	HIS	-	expression tag	UNP G3XCV2
A	1440	HIS	-	expression tag	UNP G3XCV2
A	1441	HIS	-	expression tag	UNP G3XCV2
A	1442	HIS	-	expression tag	UNP G3XCV2
A	1443	HIS	-	expression tag	UNP G3XCV2
A	1444	HIS	-	expression tag	UNP G3XCV2
A	1445	LEU	-	expression tag	UNP G3XCV2
A	1446	PRO	-	expression tag	UNP G3XCV2
A	1447	SER	-	expression tag	UNP G3XCV2
A	1448	TRP	-	expression tag	UNP G3XCV2
A	1449	SER	-	expression tag	UNP G3XCV2
A	1450	HIS	-	expression tag	UNP G3XCV2
A	1451	PRO	-	expression tag	UNP G3XCV2
A	1452	GLN	-	expression tag	UNP G3XCV2
A	1453	PHE	-	expression tag	UNP G3XCV2
A	1454	GLU	-	expression tag	UNP G3XCV2
A	1455	LYS	-	expression tag	UNP G3XCV2
B	1439	HIS	-	expression tag	UNP G3XCV2
B	1440	HIS	-	expression tag	UNP G3XCV2
B	1441	HIS	-	expression tag	UNP G3XCV2
B	1442	HIS	-	expression tag	UNP G3XCV2
B	1443	HIS	-	expression tag	UNP G3XCV2
B	1444	HIS	-	expression tag	UNP G3XCV2
B	1445	LEU	-	expression tag	UNP G3XCV2
B	1446	PRO	-	expression tag	UNP G3XCV2
B	1447	SER	-	expression tag	UNP G3XCV2

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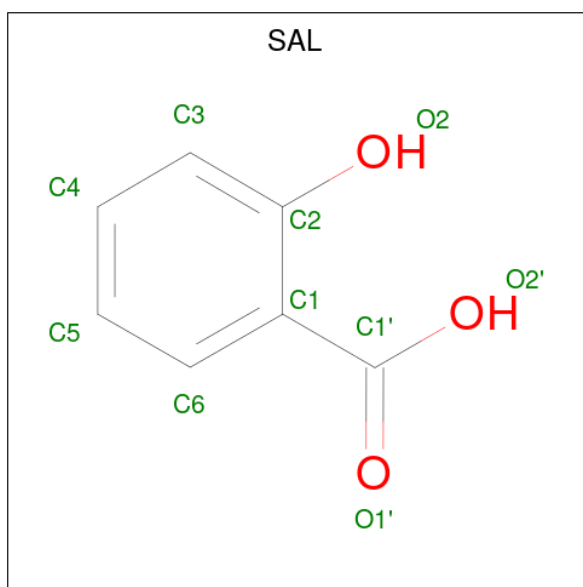
Chain	Residue	Modelled	Actual	Comment	Reference
B	1448	TRP	-	expression tag	UNP G3XCV2
B	1449	SER	-	expression tag	UNP G3XCV2
B	1450	HIS	-	expression tag	UNP G3XCV2
B	1451	PRO	-	expression tag	UNP G3XCV2
B	1452	GLN	-	expression tag	UNP G3XCV2
B	1453	PHE	-	expression tag	UNP G3XCV2
B	1454	GLU	-	expression tag	UNP G3XCV2
B	1455	LYS	-	expression tag	UNP G3XCV2

- Molecule 2 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							AltConf
			Total	C	H	N	O	P	S	
2	A	1	Total	C	H	N	O	P	S	0
			41	11	20	2	6	1	1	
2	B	1	Total	C	H	N	O	P	S	0
			41	11	20	2	6	1	1	

- Molecule 3 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: C₇H₆O₃).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	H	O	
3	A	1	14	7	5	2	0
3	B	1	14	7	5	2	0

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

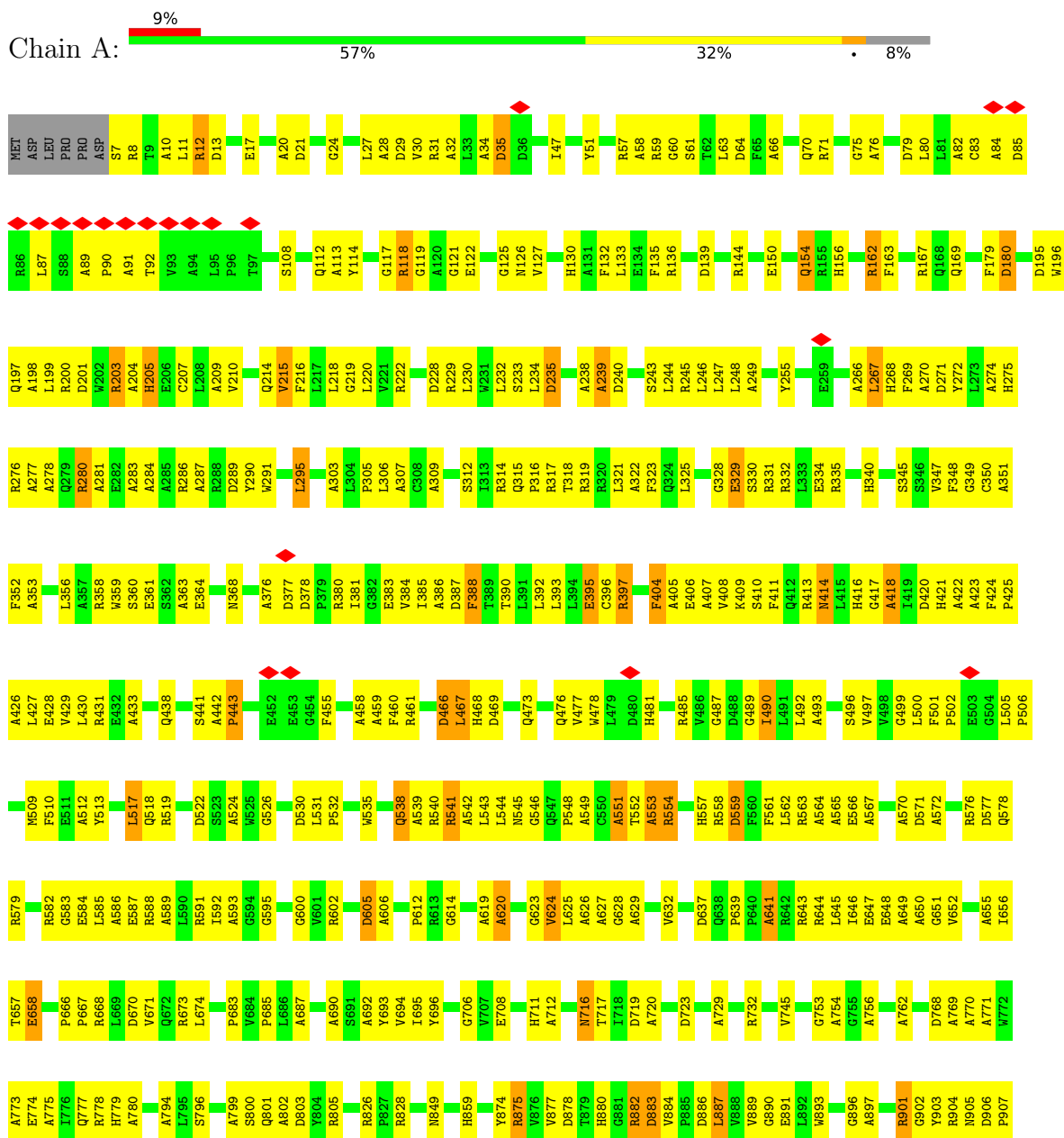
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	B	1	1	1	0

- Molecule 5 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dihydroaeruginosic acid synthetase



VAL	ARG	GLU	L1240	L1063	D927	V817	M716	Y621
ARG	LEU	CYS	G1241	L1056	I954	R828	T717	F622
LEU	GLY	HIS	A1242	D1057	C964	S848	I718	G623
GLY	MET	GLU	L1243	E1058	A965	N849	D719	V624
MET	ALA	PRO	L1244	R1061	Q866	P870	A720	L625
ALA	ASP	SER	L1245	Q1065	A967	Y874	L721	A626
ASP	PHE	ALA	D1246	Q1066	G978	R875	L722	A629
PHE	TYR	GLU	D1247	A1067	G979	A735	D723	A632
TYR	ARG	GLU	R1248	A1068	Y987	P639	A729	P633
ARG	GLN	PRO	P1249	T1071	P990	L748	R732	L634
GLN	ARG	LEU	L1250	A1076	R991	F749	L733	L635
ARG	LEU	ALA	R1251	L1077	G995	G750	L734	D635
LEU	ALA	ALA	E1254	A1082	L1002	R880	A735	I636
ALA	LEU	LEU	L1255	G1083	P1003	H881	A735	D637
LEU	ALA	ALA	P1256	E1084	A1004	D878	A735	A638
ALA	HIS	LEU	L1262	Q1085	A1005	T879	A735	P639
HIS	LEU	GLU	P1269	A1088	F1008	H880	A735	A641
LEU	GLN	TRP	S1275	G1089	A1009	G881	A735	R642
GLN	VAL	TRP	E1276	L1090	E1013	D882	A735	R643
VAL	THR	ALA	L1291	L1093	A1014	D883	A735	L644
THR	THR	ALA	D1292	D1093	E1015	D884	A735	L645
THR	VAL	VAL	A1293	P1094	L1105	D885	A735	I646
VAL	GLU	LEU	L1294	W1085	L1023	D886	A735	G647
GLU	LEU	PHE	L1295	L1105	L1026	L887	A735	E648
LEU	GLY	PHE	Q1296	E1110	L1027	A762	A735	A649
GLY	LEU	LEU	A1297	E1117	E1028	A766	A735	A650
LEU	LEU	SER	G1298	A1118	A1029	R767	A735	G651
LEU	LEU	THR	L1299	P1122	L1030	D768	A735	V652
LEU	LEU	ARG	E1300	A1123	L1031	A769	A735	T657
LEU	LEU	THR	Q1301	A1124	L1032	A770	A735	E658
LEU	LEU	ARG	L1311	A1146	L1033	A771	A735	L665
LEU	HIS	SER	R1311	L1181	D1034	A772	A735	P666
HIS	HIS	LEU	S1317	G1184	D1035	A773	A735	R668
HIS	HIS	LEU	L1318	L1185	R1038	A774	A735	L669
HIS	HIS	LEU	P1319	L1186	R1039	A775	A735	P685
HIS	HIS	LEU	L1320	P1187	R1040	A776	A735	L686
HIS	HIS	LEU	M1321	A1188	R1041	A777	A735	A687
HIS	HIS	LEU	K1325	L1188	L1042	A778	A735	A680
HIS	HIS	LEU	V1326	L1181	D1047	A779	A735	S691
HIS	HIS	LEU	D1327	L1181	S1048	A780	A735	A692
HIS	HIS	LEU	R1328	L1181	A1049	A780	A735	Y693
HIS	HIS	LEU	R1329	L1181	L1051	A780	A735	L695
HIS	HIS	LEU	R1330	L1181	D1052	A780	A735	Y696
HIS	HIS	LEU	L1331	L1181	D1053	A780	A735	T697
HIS	HIS	LEU	L1331	L1181	D1054	A780	A735	Y697
HIS	HIS	LEU	A1332	L1181	D1055	A780	A735	Y698
HIS	HIS	LEU	E1333	L1181	D1056	A780	A735	Y699
HIS	HIS	LEU	S1334	L1181	D1057	A780	A735	Y699
HIS	HIS	LEU	R1337	L1181	D1058	A780	A735	Y699
HIS	HIS	LEU	A1338	L1181	D1059	A780	A735	Y699
HIS	HIS	LEU	L1339	L1181	D1060	A780	A735	Y699
HIS	HIS	LEU	G1340	L1181	D1061	A780	A735	Y699
HIS	HIS	LEU		L1181	D1062	A780	A735	Y699
HIS	HIS	LEU		L1181	D1063	A780	A735	Y699
HIS	HIS	LEU		L1181	D1064	A780	A735	Y699
HIS	HIS	LEU		L1181	D1065	A780	A735	Y699
HIS	HIS	LEU		L1181	D1066	A780	A735	Y699
HIS	HIS	LEU		L1181	D1067	A780	A735	Y699
HIS	HIS	LEU		L1181	D1068	A780	A735	Y699
HIS	HIS	LEU		L1181	D1069	A780	A735	Y699
HIS	HIS	LEU		L1181	D1070	A780	A735	Y699
HIS	HIS	LEU		L1181	D1071	A780	A735	Y699
HIS	HIS	LEU		L1181	D1072	A780	A735	Y699
HIS	HIS	LEU		L1181	D1073	A780	A735	Y699
HIS	HIS	LEU		L1181	D1074	A780	A735	Y699
HIS	HIS	LEU		L1181	D1075	A780	A735	Y699
HIS	HIS	LEU		L1181	D1076	A780	A735	Y699
HIS	HIS	LEU		L1181	D1077	A780	A735	Y699
HIS	HIS	LEU		L1181	D1078	A780	A735	Y699
HIS	HIS	LEU		L1181	D1079	A780	A735	Y699
HIS	HIS	LEU		L1181	D1080	A780	A735	Y699
HIS	HIS	LEU		L1181	D1081	A780	A735	Y699
HIS	HIS	LEU		L1181	D1082	A780	A735	Y699
HIS	HIS	LEU		L1181	D1083	A780	A735	Y699
HIS	HIS	LEU		L1181	D1084	A780	A735	Y699
HIS	HIS	LEU		L1181	D1085	A780	A735	Y699
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HIS	HIS	LEU		L1181	D1088	A780	A735	Y699
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HIS	HIS	LEU		L1181	D1105	A780	A735	Y699
HIS	HIS	LEU		L1181	D1106	A780	A735	Y699
HIS	HIS	LEU		L1181	D1107	A780	A735	Y699
HIS	HIS	LEU		L1181	D1108	A780	A735	Y699
HIS	HIS	LEU		L1181	D1109	A780	A735	Y699
HIS	HIS	LEU		L1181	D1110	A780	A735	Y699
HIS	HIS	LEU		L1181	D1111	A780	A735	Y699
HIS	HIS	LEU		L1181	D1112	A780	A735	Y699
HIS	HIS	LEU		L1181	D1113	A780	A735	Y699
HIS	HIS	LEU		L1181	D1114	A780	A735	Y699
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HIS	HIS	LEU		L1181	D1120	A780	A735	Y699
HIS	HIS	LEU		L1181	D1121	A780	A735	Y699
HIS	HIS	LEU		L1181	D1122	A780	A735	Y699
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HIS	HIS	LEU		L1181	D1136	A780	A735	Y699
HIS	HIS	LEU		L1181	D1137	A780	A735	Y699
HIS	HIS	LEU		L1181	D1138	A780	A735	Y699
HIS	HIS	LEU		L1181	D1139	A780	A735	Y699
HIS	HIS	LEU		L1181	D1140	A780	A735	Y699
HIS	HIS	LEU		L1181	D1141	A780	A735	Y699
HIS	HIS	LEU		L1181	D1142	A780	A735	Y699
HIS	HIS	LEU		L1181	D1143	A780	A735	Y699
HIS	HIS	LEU		L1181	D1144	A780	A735	Y699
HIS	HIS	LEU		L1181	D1145	A780	A735	Y699
HIS	HIS	LEU		L1181	D1146	A780	A735	Y699
HIS	HIS	LEU		L1181	D1147	A780	A735	Y699
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HIS	HIS	LEU		L1181	D1154	A780	A735	Y699
HIS	HIS	LEU		L1181	D1155	A780	A735	Y699
HIS	HIS	LEU						

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	219049	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 ($e^-/\text{\AA}^2$)	60.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.073	Depositor
Minimum map value	-0.032	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (\AA)	250.0, 250.0, 250.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0, 1.0, 1.0	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: SAL, AMP, MG, PNS

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	2.11	321/10412 (3.1%)	2.01	612/14189 (4.3%)
1	B	2.07	297/10412 (2.9%)	1.97	581/14189 (4.1%)
All	All	2.09	618/20824 (3.0%)	1.99	1193/28378 (4.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

The worst 5 of 618 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	442	ALA	CA-CB	-9.53	1.42	1.53
1	A	442	ALA	CA-CB	-9.46	1.42	1.53
1	B	481	HIS	ND1-CE1	-8.90	1.23	1.32
1	B	156	HIS	ND1-CE1	-8.90	1.23	1.32
1	B	880	HIS	ND1-CE1	-8.89	1.23	1.32

The worst 5 of 1193 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	ASP	CA-CB-CG	7.33	119.94	112.60
1	B	70	GLN	CA-C-N	7.32	131.09	122.89
1	B	70	GLN	C-N-CA	7.32	131.09	122.89
1	B	605	ASP	CA-CB-CG	7.22	119.82	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	368	ASN	CA-CB-CG	7.19	119.79	112.60

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	51	TYR	Sidechain
1	A	696	TYR	Sidechain
1	A	923	TYR	Sidechain
1	B	374	ARG	Sidechain
1	B	696	TYR	Sidechain

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	10199	10245	10243	72	0
1	B	10199	10245	10243	78	0
2	A	21	20	20	0	0
2	B	21	20	20	0	0
3	A	9	5	4	0	0
3	B	9	5	4	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	23	12	12	0	0
5	B	23	12	12	1	0
6	A	6	6	4	0	0
6	B	6	6	4	0	0
All	All	20518	20576	20566	147	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 147 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:B:1242:ALA:O	1:B:1246:ASP:N	2.19	0.76
1:A:602:ARG:NH1	1:A:605:ASP:OD2	2.18	0.76
1:A:1242:ALA:O	1:A:1246:ASP:N	2.19	0.75
1:B:602:ARG:NH1	1:B:605:ASP:OD2	2.18	0.75
1:A:358:ARG:NH1	1:A:531:LEU:O	2.20	0.74

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	1332/1455 (92%)	1273 (96%)	59 (4%)	0	100	100
1	B	1332/1455 (92%)	1270 (95%)	61 (5%)	1 (0%)	48	78
All	All	2664/2910 (92%)	2543 (96%)	120 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	748	LEU

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	1019/1122 (91%)	1010 (99%)	9 (1%)	70	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1019/1122 (91%)	1010 (99%)	9 (1%)	70 85
All	All	2038/2244 (91%)	2020 (99%)	18 (1%)	68 85

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	295	LEU
1	B	954	ILE
1	B	717	THR
1	A	954	ILE
1	B	280	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	945	GLN
1	B	859	HIS
1	B	368	ASN
1	A	851	GLN
1	B	851	GLN

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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PNS	A	1501	3,1	14,20,21	1.01	0	18,26,29	0.85	1 (5%)
5	AMP	B	1504	6,4	25,25,25	1.14	1 (4%)	37,38,38	1.54	7 (18%)
3	SAL	A	1502	2	9,9,10	0.64	0	11,11,13	0.74	0
6	CYS	B	1505	5	4,5,6	0.81	0	1,5,7	1.57	0
2	PNS	B	1501	3,1	14,20,21	1.02	0	18,26,29	0.85	0
3	SAL	B	1502	2	9,9,10	0.64	0	11,11,13	0.68	0
6	CYS	A	1505	5	4,5,6	0.83	0	1,5,7	0.91	0
5	AMP	A	1504	6,4	25,25,25	1.14	1 (4%)	37,38,38	1.53	8 (21%)

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	PNS	A	1501	3,1	-	6/24/26/27	-
5	AMP	B	1504	6,4	-	8/10/26/26	0/3/3/3
3	SAL	A	1502	2	-	2/2/2/4	0/1/1/1
6	CYS	B	1505	5	-	0/1/4/6	-
2	PNS	B	1501	3,1	-	5/24/26/27	-
3	SAL	B	1502	2	-	2/2/2/4	0/1/1/1
6	CYS	A	1505	5	-	0/1/4/6	-
5	AMP	A	1504	6,4	-	8/10/26/26	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1504	AMP	C5-C4	-2.62	1.34	1.39
5	A	1504	AMP	C5-C4	-2.56	1.34	1.39

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1504	AMP	O5'-P-O1P	3.35	115.50	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1504	AMP	O5'-P-O1P	3.29	115.32	106.44
5	A	1504	AMP	C5-C4-N3	-3.27	122.22	126.72
5	B	1504	AMP	C5-C4-N3	-3.21	122.29	126.72
5	A	1504	AMP	C4-C5-N7	2.69	113.66	110.58

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

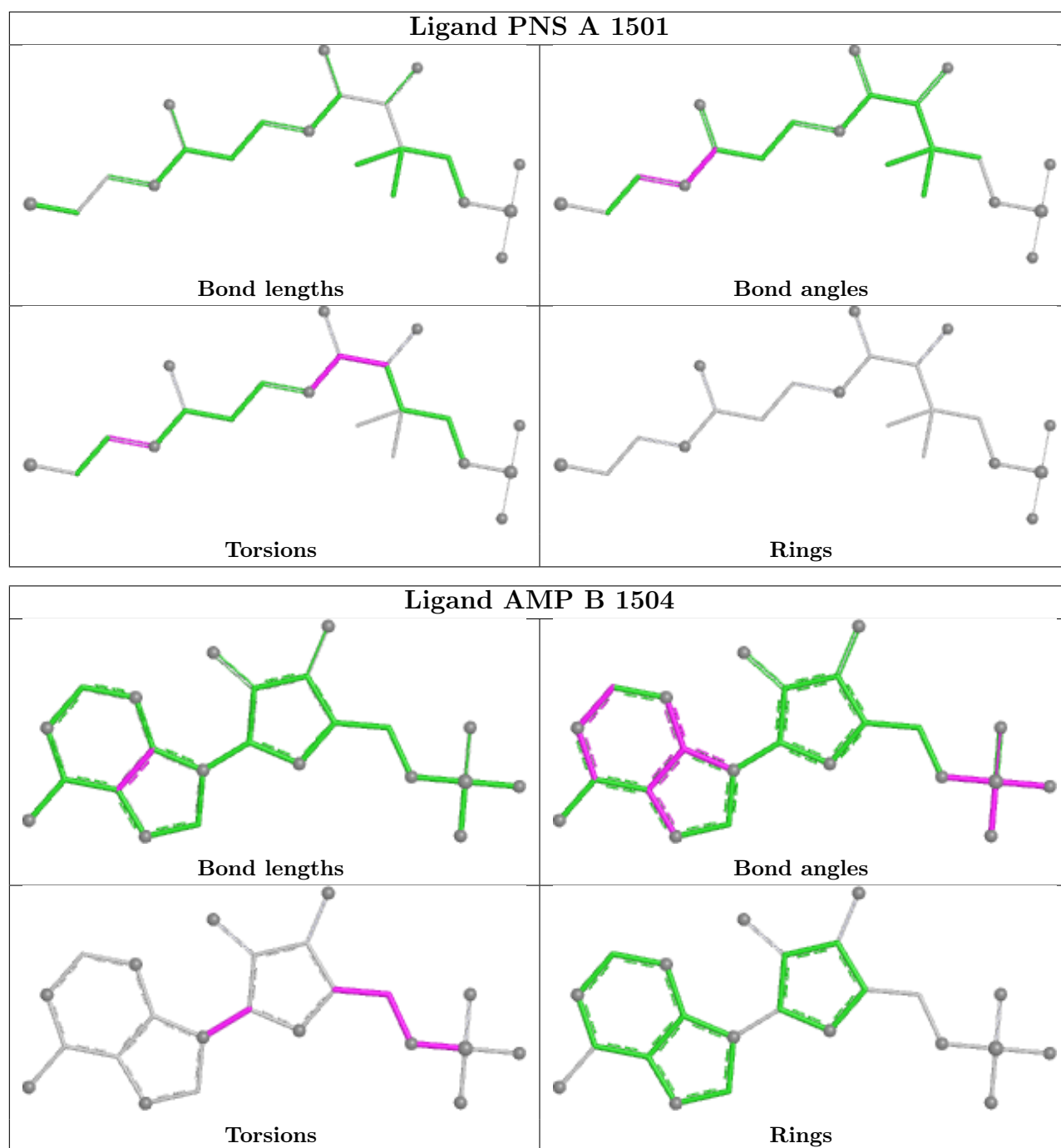
Mol	Chain	Res	Type	Atoms
2	A	1501	PNS	O33-C32-C34-O35
2	A	1501	PNS	O33-C32-C34-N36
2	A	1501	PNS	C43-C42-N41-C39
2	B	1501	PNS	O33-C32-C34-O35
2	B	1501	PNS	O33-C32-C34-N36

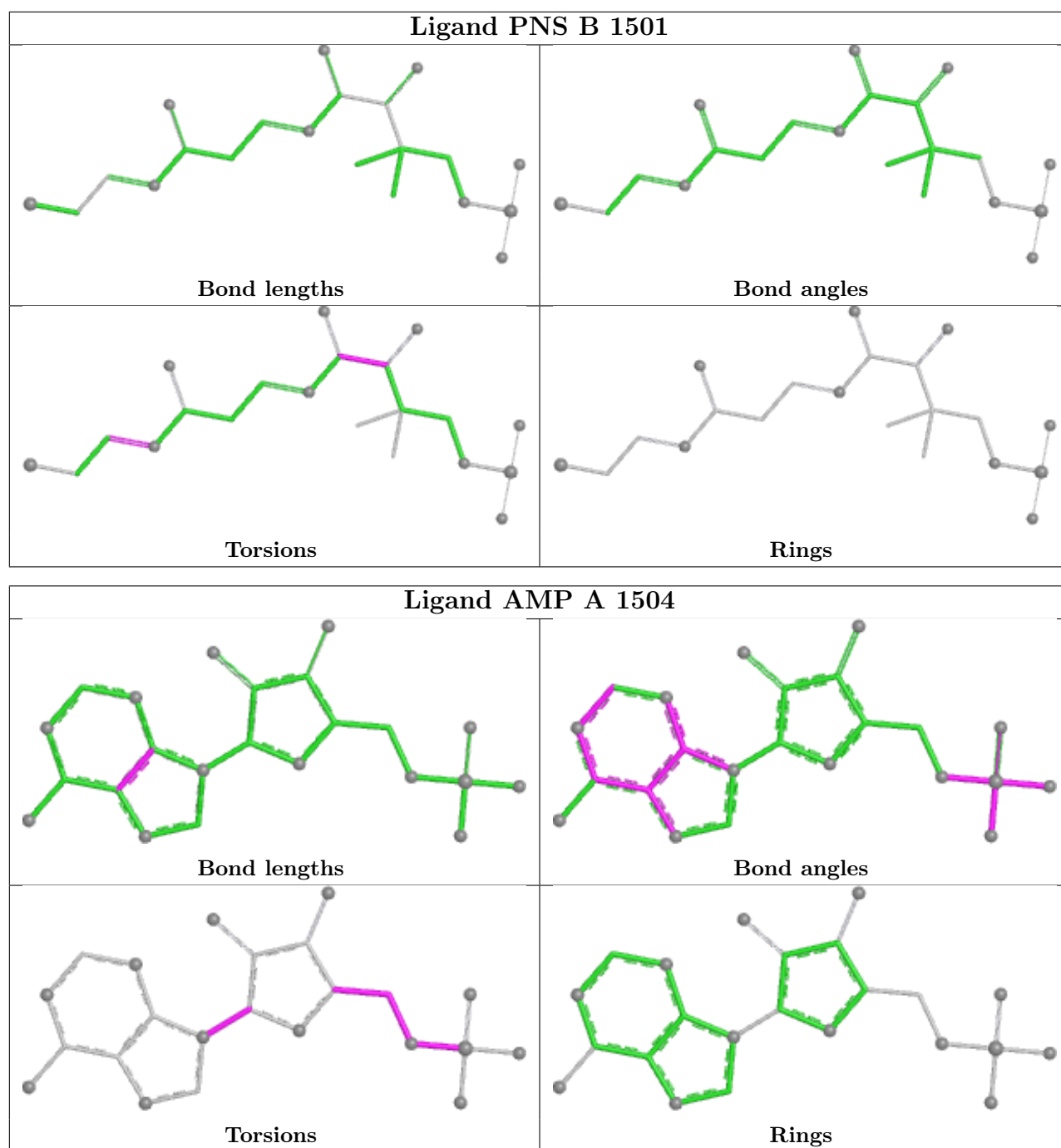
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1504	AMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

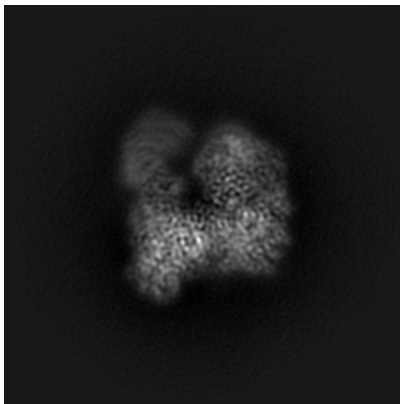
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31198. These allow visual inspection of the internal detail of the map and identification of artifacts.

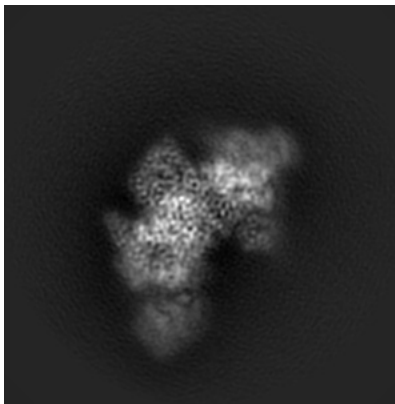
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

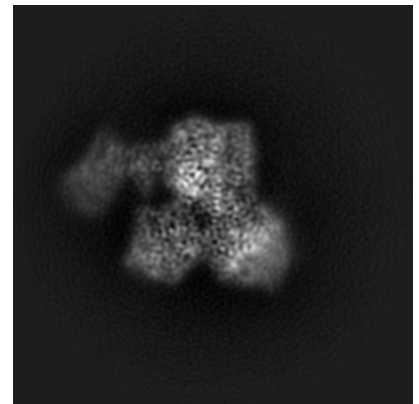
6.1.1 Primary map



X

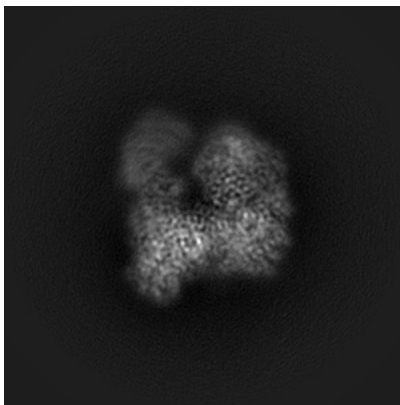


Y

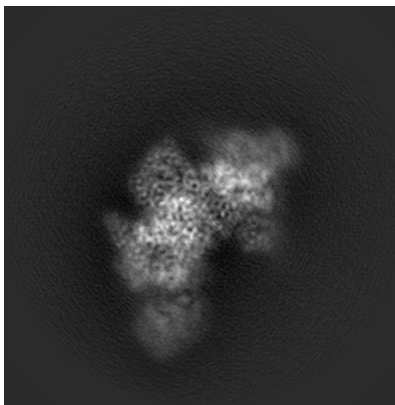


Z

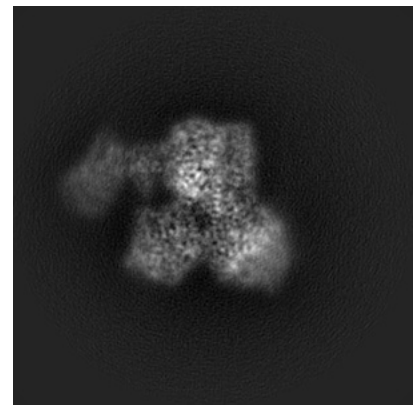
6.1.2 Raw map



X



Y

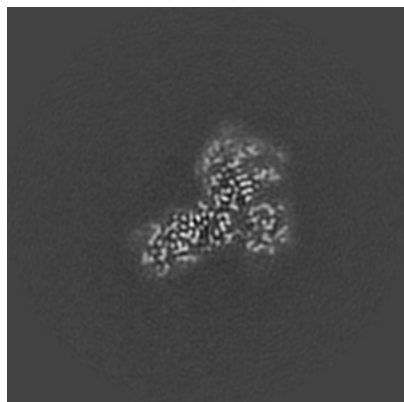


Z

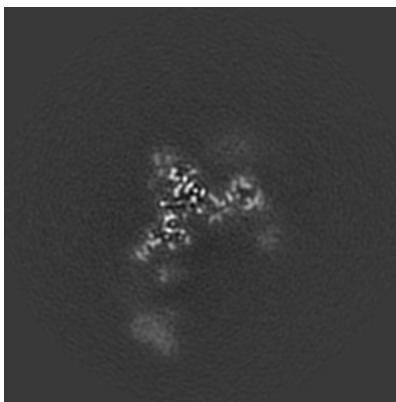
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

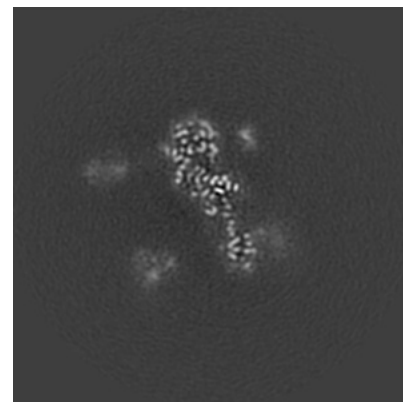
6.2.1 Primary map



X Index: 125

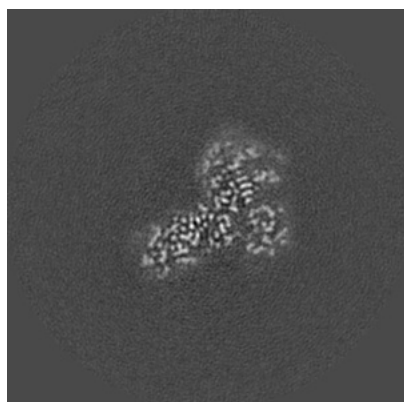


Y Index: 125

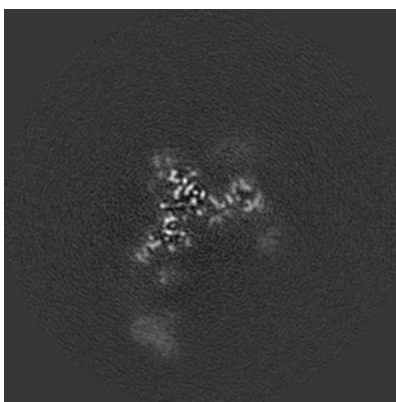


Z Index: 125

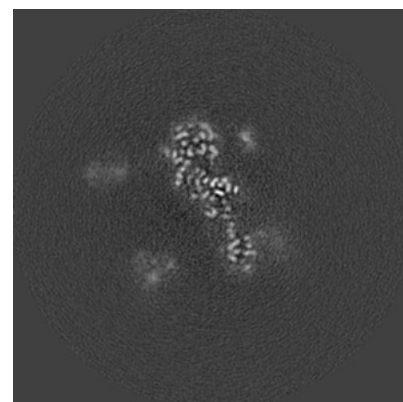
6.2.2 Raw map



X Index: 125



Y Index: 125

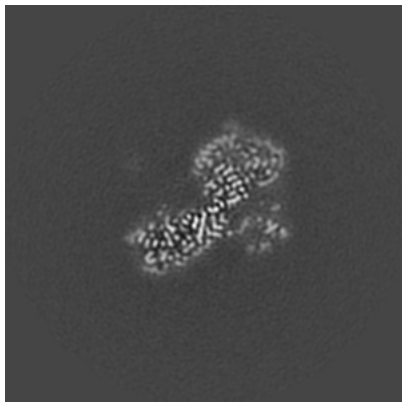


Z Index: 125

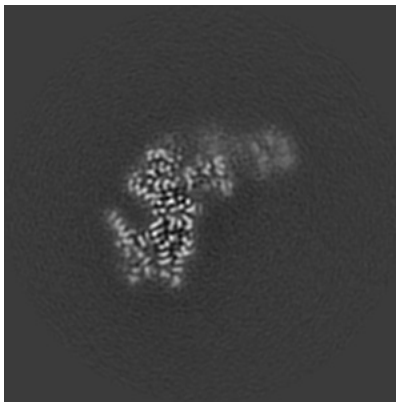
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

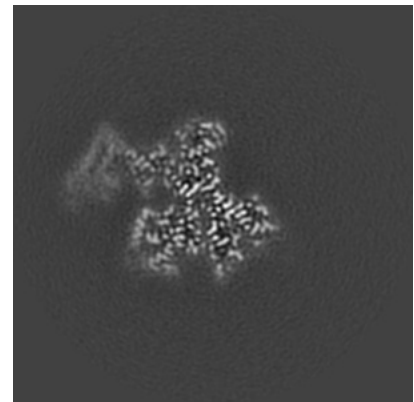
6.3.1 Primary map



X Index: 128

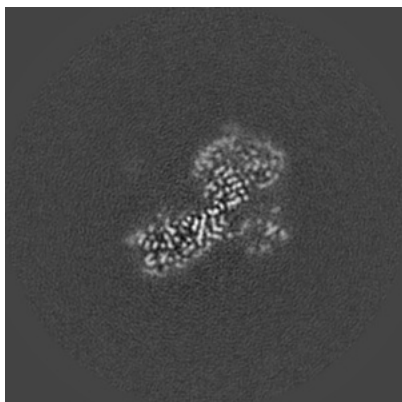


Y Index: 106

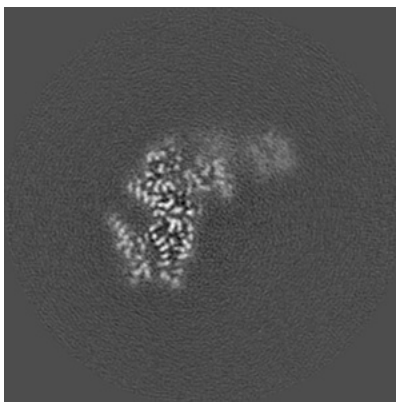


Z Index: 107

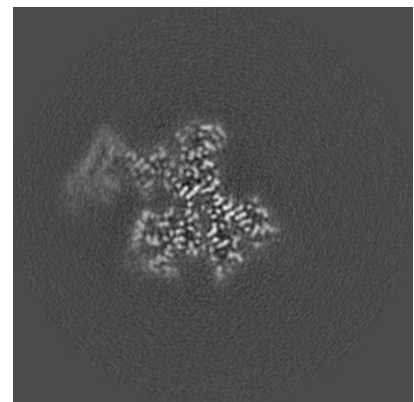
6.3.2 Raw map



X Index: 128



Y Index: 107

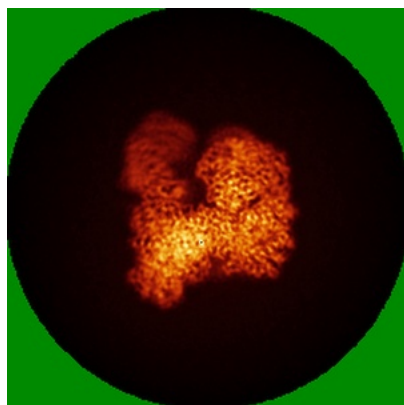


Z Index: 107

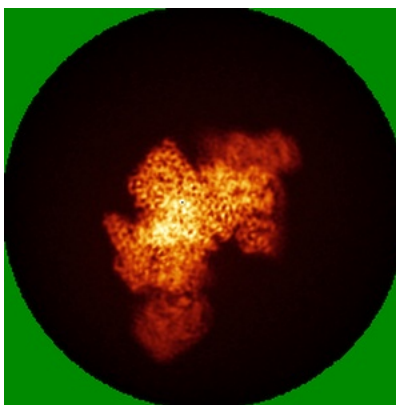
The images above show the largest variance slices of the map in three orthogonal directions.

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

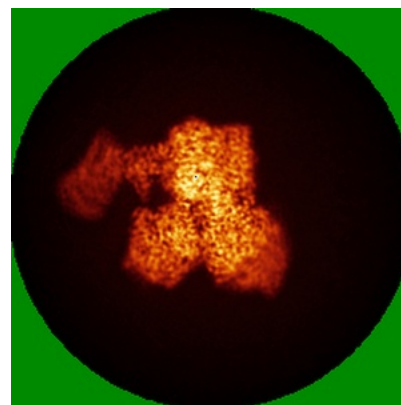
6.4.1 Primary map



X

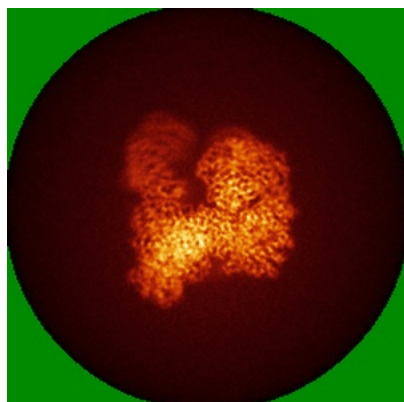


Y

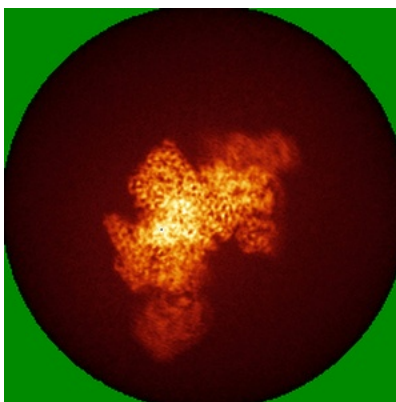


Z

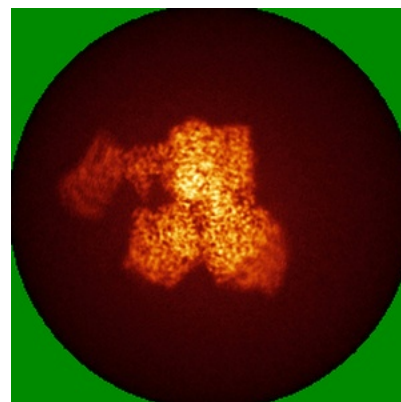
6.4.2 Raw map



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](#)

This section was not generated.

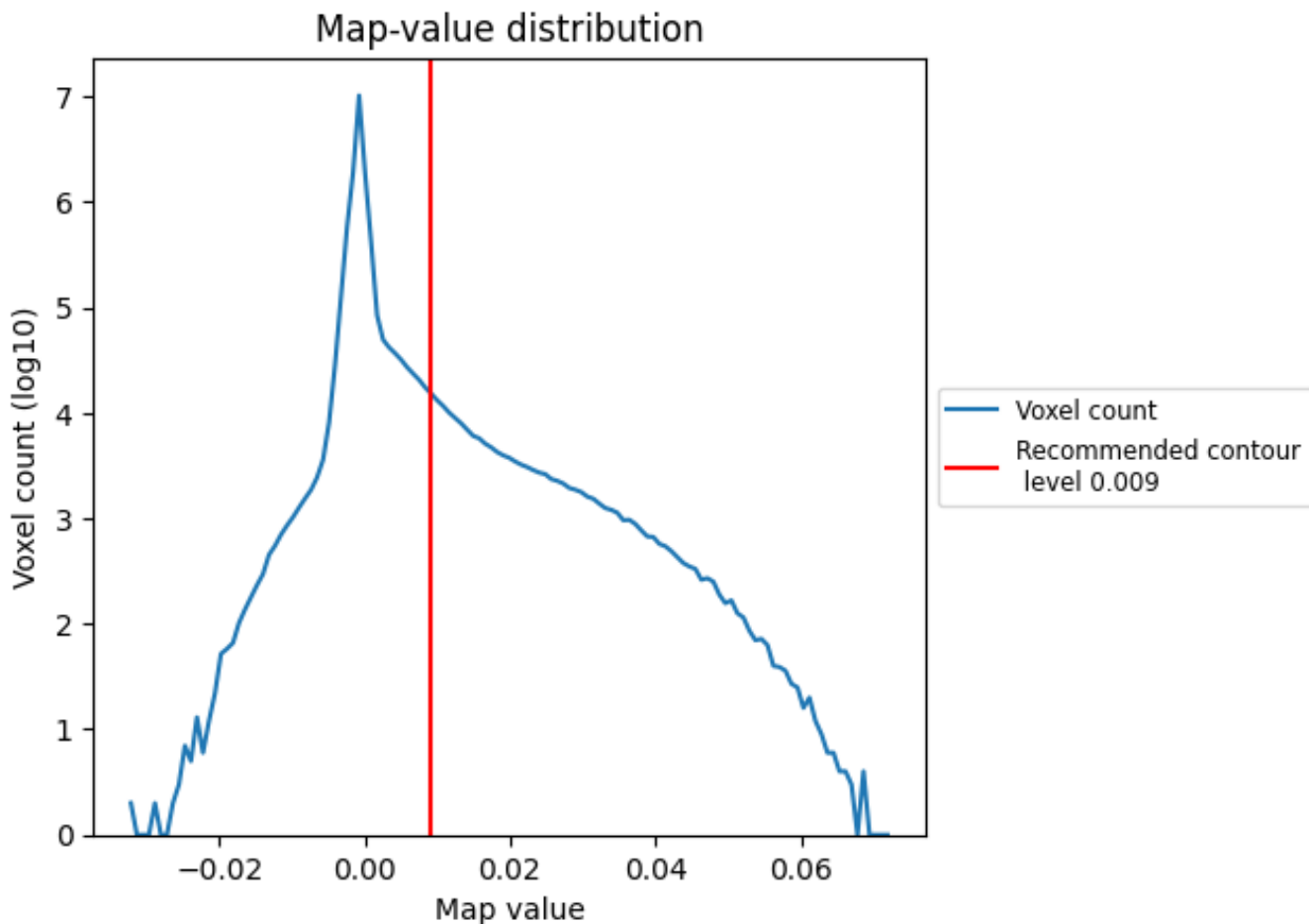
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

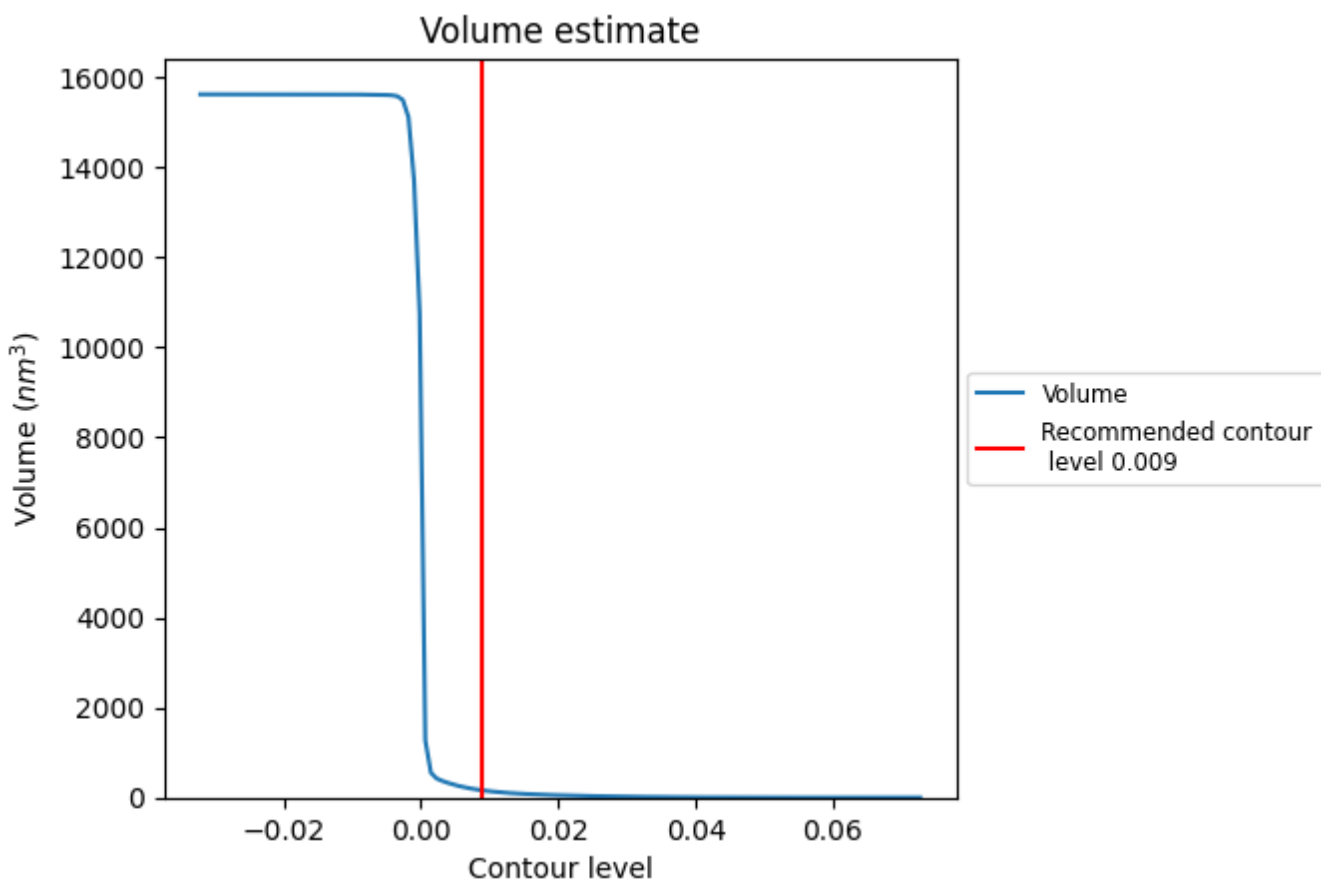
This section contains the results of statistical analysis of the map.

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.

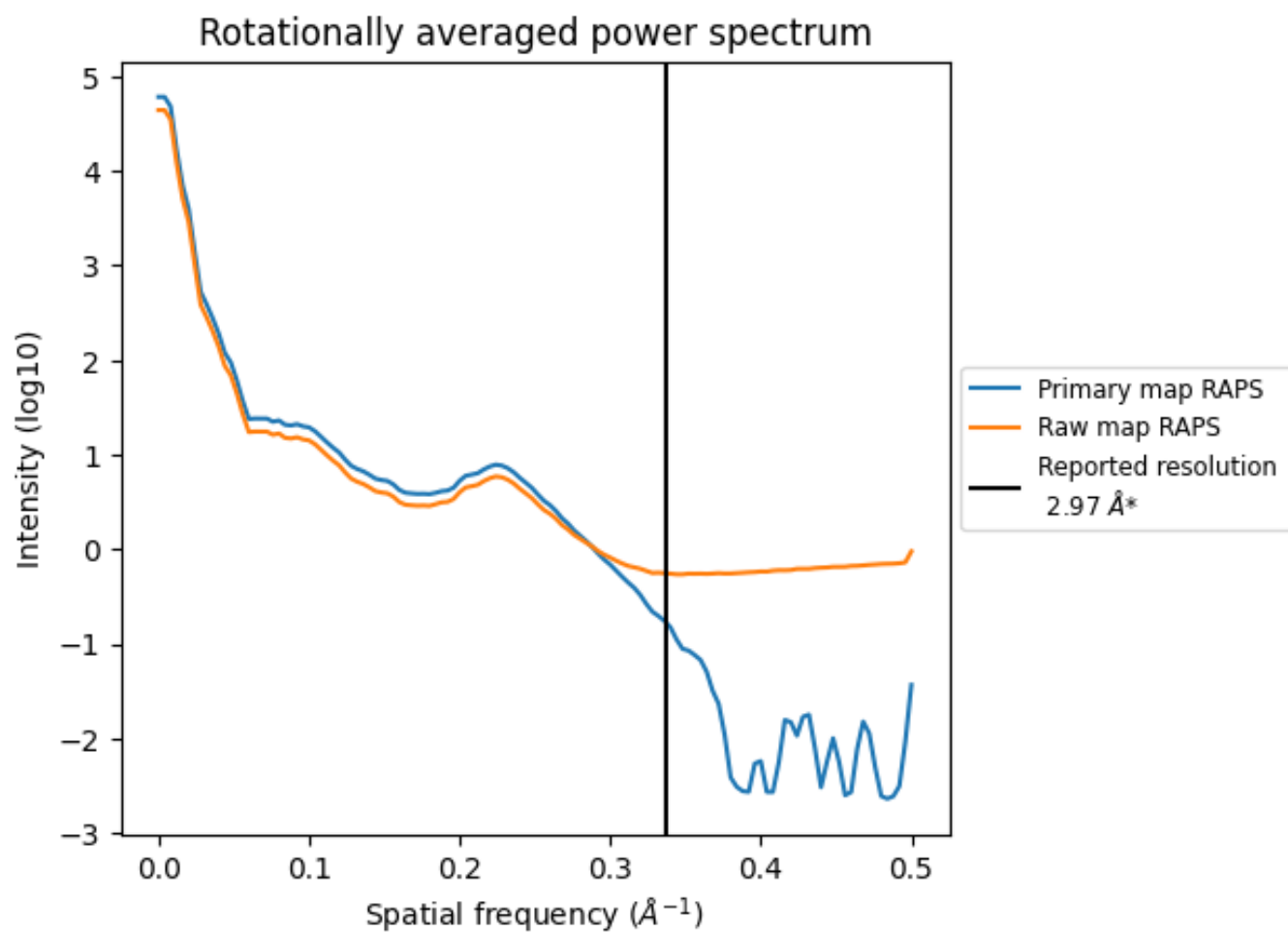
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 160 nm³; this corresponds to an approximate mass of 144 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

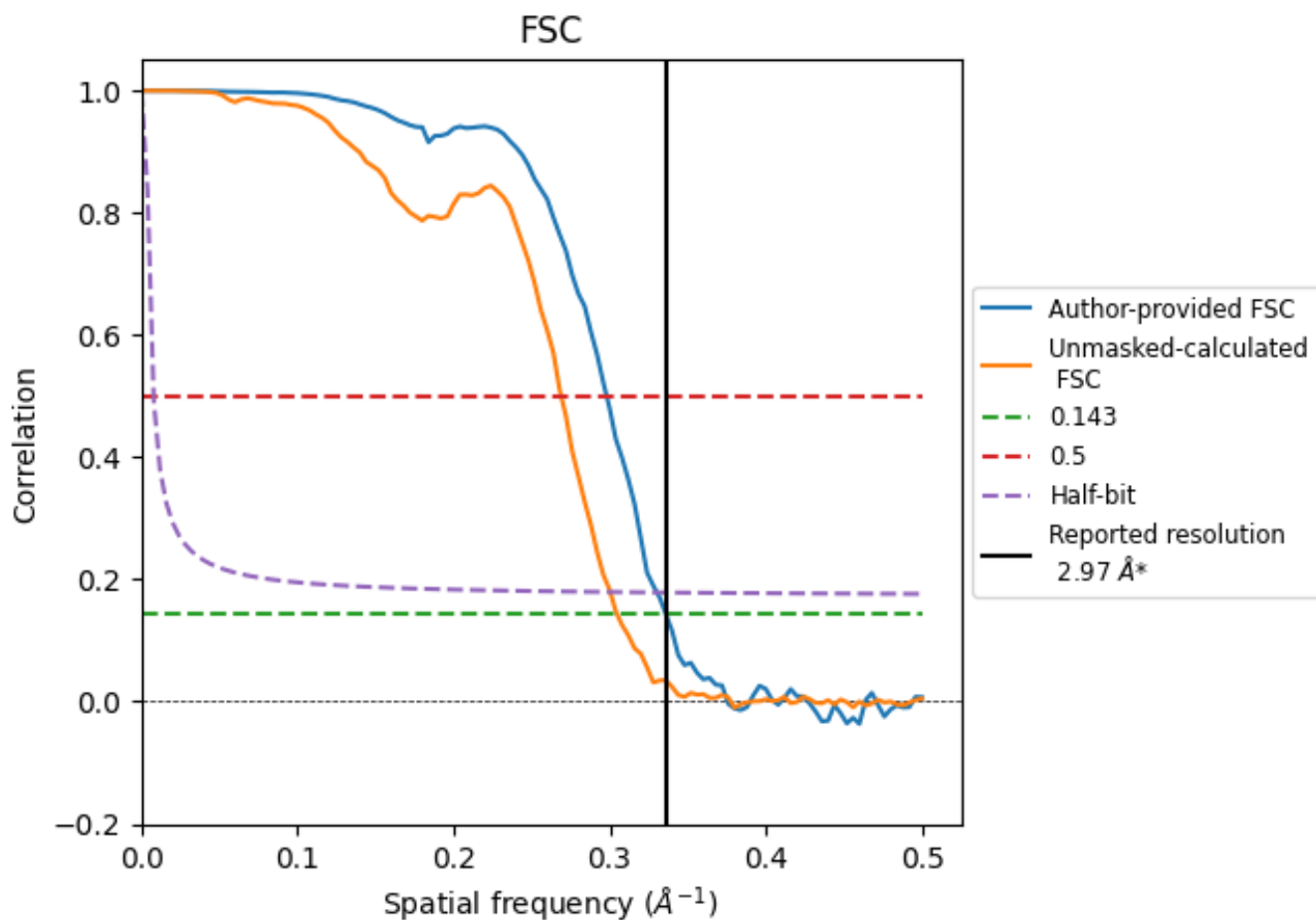


*Reported resolution corresponds to spatial frequency of 0.337 \AA^{-1}

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 0.337\AA^{-1}

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.98	3.35	3.03
Unmasked-calculated*	3.28	3.72	3.33

*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 3.28 differs from the reported value 2.97 by more than 10 %

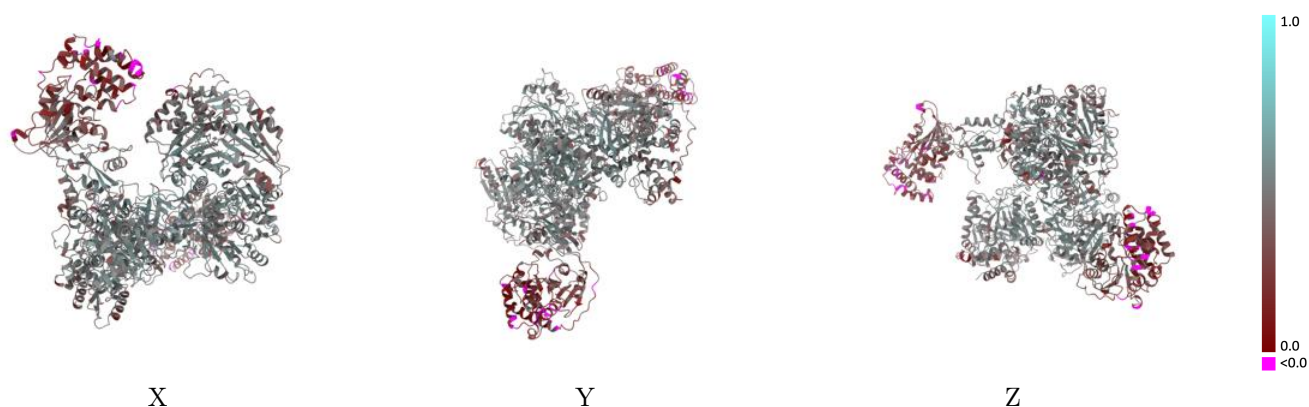
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31198 and PDB model 7EMY. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)

This section was not generated.

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

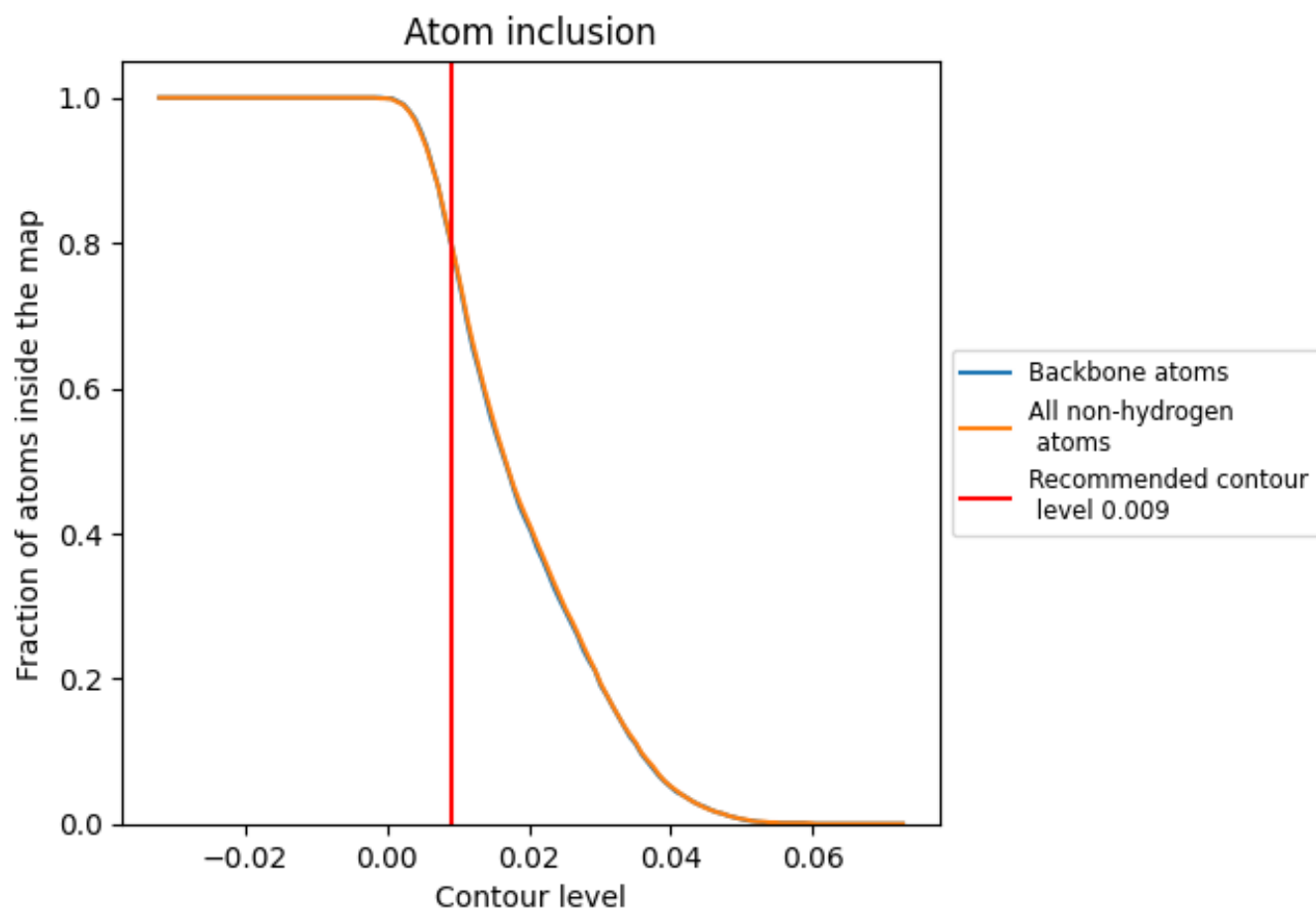


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.


9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 80% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8030	 0.4300
A	 0.7900	 0.4220
B	 0.8520	 0.4380

