



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 03:39 PM JST

PDB ID : 7EN2
EMDB ID : EMD-31200
Title : Pyochelin synthetase, a dimeric nonribosomal peptide synthetase elongation module-after-condensation, condensation
Authors : Wang, J.L.; Wang, Z.J.
Deposited on : 2021-04-15
Resolution : 3.78 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

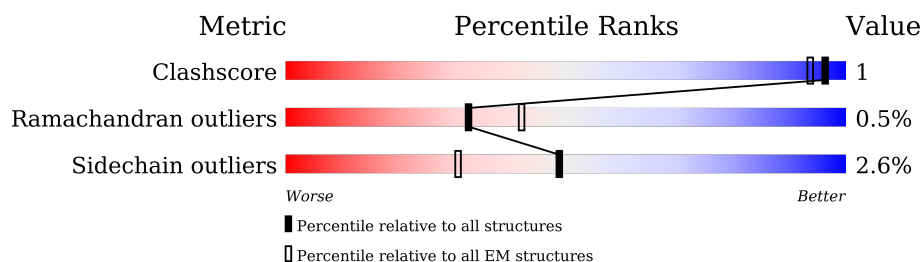
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.78 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	 7% 81% 8% • 9%
1	B	1455	 7% 86% 10% • •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 42083 atoms, of which 21074 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
1	A	1321	Total	C	H	N	O	S	0	0
			20290	6387	10167	1875	1830	31		
1	B	1410	Total	C	H	N	O	S	0	0
			21641	6808	10843	1994	1961	35		

There are 34 discrepancies between the modelled and reference sequences:

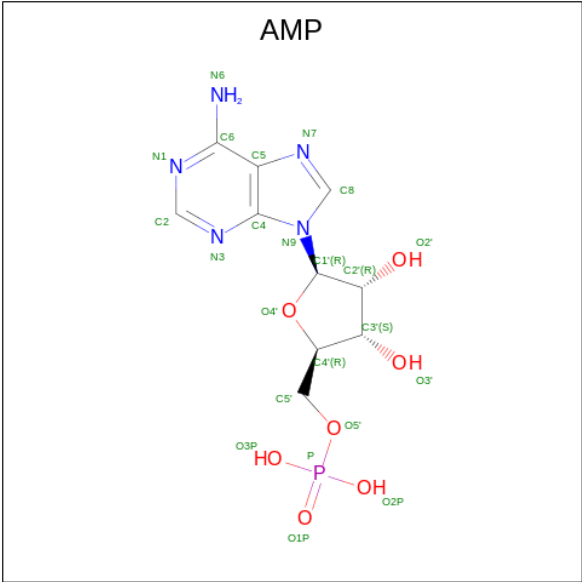
Chain	Residue	Modelled	Actual	Comment	Reference
A	1439	HIS	-	expression tag	UNP G3XCV2
A	1440	HIS	-	expression tag	UNP G3XCV2
A	1441	HIS	-	expression tag	UNP G3XCV2
A	1442	HIS	-	expression tag	UNP G3XCV2
A	1443	HIS	-	expression tag	UNP G3XCV2
A	1444	HIS	-	expression tag	UNP G3XCV2
A	1445	LEU	-	expression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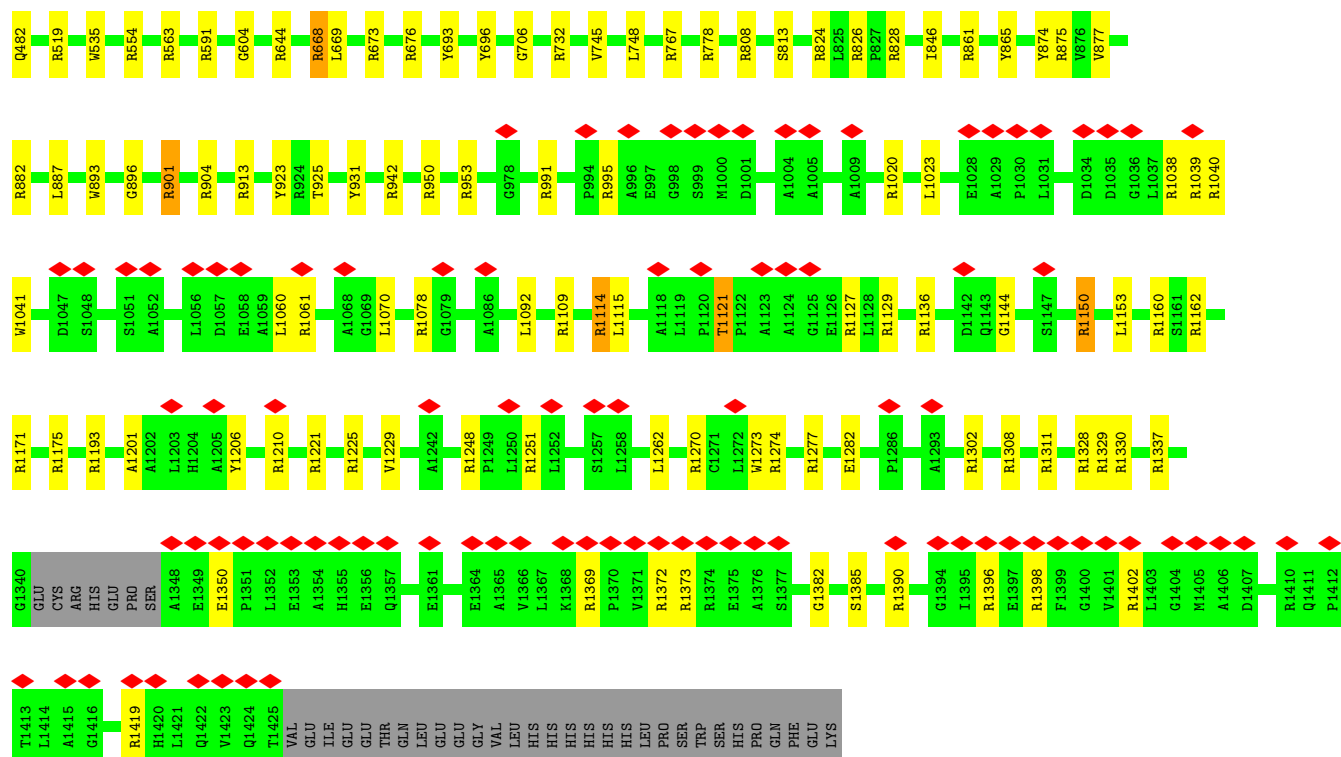
Chain	Residue	Modelled	Actual	Comment	Reference
B	1448	TRP	-	expression tag	UNP G3XCV2
B	1449	SER	-	expression tag	UNP G3XCV2
B	1450	HIS	-	expression tag	UNP G3XCV2
B	1451	PRO	-	expression tag	UNP G3XCV2
B	1452	GLN	-	expression tag	UNP G3XCV2
B	1453	PHE	-	expression tag	UNP G3XCV2
B	1454	GLU	-	expression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

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- The chemical structure represents a protein fragment (PNS) with a disulfide bond and a phosphate group. The structure is shown in a stick representation with atoms labeled by element type and carbon numbering. The phosphate group is attached to a carbon atom (C28) via an oxygen atom (O27). The disulfide bond is formed between the sulfur atoms of two cysteine residues (C43 and C44). The structure is colored by element type: carbon (grey), oxygen (red), nitrogen (blue), sulfur (yellow), and phosphorus (purple). The labels include O26, O25, O27, C28, C30, C29, C31, C32(R), C34, O33, N35, C37, C38, C39, O40, N41, C42, C43, C44, and S44.

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms						AltConf
3	A	1	Total	C	H	N	O	P	0
			35	10	12	5	7	1	
3	B	1	Total	C	H	N	O	P	0
			35	10	12	5	7	1	



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	19661	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.046	Depositor
Minimum map value	-0.016	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.006	Depositor
Map size (Å)	250.0, 250.0, 250.0	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, 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	0.69	0/10337	1.19	90/14076 (0.6%)
1	B	0.69	0/11021	1.21	107/15008 (0.7%)
All	All	0.69	0/21358	1.20	197/29084 (0.7%)

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	11
1	B	0	11
All	All	0	22

There are no bond length outliers.

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1251	ARG	NE-CZ-NH1	10.92	125.76	120.30
1	B	200	ARG	NE-CZ-NH1	9.75	125.18	120.30
1	B	942	ARG	NE-CZ-NH1	9.56	125.08	120.30
1	A	1160	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	B	824	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	A	397	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	B	882	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	194	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	A	953	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	B	435	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	A	435	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	B	644	ARG	NE-CZ-NH1	8.35	124.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	824	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	882	ARG	NE-CZ-NH1	8.21	124.41	120.30
1	A	591	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	185	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	B	808	ARG	NE-CZ-NH1	8.01	124.30	120.30
1	B	167	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	203	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	136	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	995	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	B	222	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	185	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	222	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	114	TYR	CB-CG-CD2	-7.68	116.39	121.00
1	B	331	ARG	NE-CZ-NH1	7.65	124.13	120.30
1	B	431	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	B	950	ARG	NE-CZ-NH1	7.63	124.12	120.30
1	A	901	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	B	203	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	397	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	B	461	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	200	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	1329	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	194	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	B	380	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	319	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	519	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	B	1372	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	B	591	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	B	374	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	B	1038	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	1221	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	A	1329	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	808	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	1221	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	B	1162	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	12	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	331	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	431	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	1398	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	1150	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	1248	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	953	ARG	NE-CZ-NH1	6.90	123.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1337	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	245	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	1396	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	B	1020	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	B	55	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	668	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	B	1078	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	1270	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	563	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	317	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	A	1196	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	942	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	A	1369	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	B	1129	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	913	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	B	1302	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	673	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	B	317	ARG	NE-CZ-NH1	6.61	123.61	120.30
1	B	1390	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	245	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	B	1040	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	229	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	B	138	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	826	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	913	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	167	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	1396	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	953	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	B	1419	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	B	1171	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	1193	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	1330	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	1410	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	1061	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	865	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	435	ARG	NH1-CZ-NH2	-6.27	112.50	119.40
1	A	1129	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	413	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	563	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	B	229	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	1127	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	118	ARG	NE-CZ-NH1	6.20	123.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	767	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	B	1150	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	1039	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	1162	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	1277	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	B	673	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	767	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	144	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	276	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	1020	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	931	TYR	CB-CG-CD1	-5.95	117.43	121.00
1	A	642	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	434	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	1409	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	B	280	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	676	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	1039	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	1078	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	991	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	991	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	136	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	276	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	440	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	288	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	1274	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	1114	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	B	101	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	1302	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	1193	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	57	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	203	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	1390	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	461	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	1225	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	101	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	1273	TRP	CA-CB-CG	5.74	124.61	113.70
1	A	931	TYR	CB-CG-CD1	-5.74	117.56	121.00
1	B	732	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	828	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	1277	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	A	1109	ARG	NE-CZ-NH1	5.69	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	778	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	1038	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	904	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	882	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	380	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	114	TYR	CB-CG-CD1	5.59	124.35	121.00
1	A	904	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	431	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	434	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	904	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	1251	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	222	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	A	380	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	861	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	245	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	1104	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	222	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	260	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	294	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	B	1398	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	540	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	925	THR	CA-CB-CG2	5.34	119.88	112.40
1	B	1328	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	314	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	319	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	B	1160	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	240	ASP	N-CA-CB	-5.32	101.03	110.60
1	A	805	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	B	1302	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	B	826	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	1210	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	A	1248	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	144	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	B	1136	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	554	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	A	930	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	1330	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	1160	ARG	NH1-CZ-NH2	-5.21	113.67	119.40
1	B	1311	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	B	875	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	1221	ARG	NE-CZ-NH2	-5.20	117.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	991	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	882	ARG	CD-NE-CZ	5.18	130.85	123.60
1	B	435	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	A	732	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	260	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	865	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	875	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	1373	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	1369	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	461	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	B	294	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	1373	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	435	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
1	A	676	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	828	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	A	1274	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	B	136	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1104	ARG	Sidechain
1	A	114	TYR	Sidechain
1	A	314	ARG	Sidechain
1	A	435	ARG	Sidechain
1	A	440	ARG	Sidechain
1	A	540	ARG	Sidechain
1	A	644	ARG	Sidechain
1	A	676	ARG	Sidechain
1	A	874	TYR	Sidechain
1	A	904	ARG	Sidechain
1	A	913	ARG	Sidechain
1	B	1150	ARG	Sidechain
1	B	1206	TYR	Sidechain
1	B	1270	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	200	ARG	Sidechain
1	B	374	ARG	Sidechain
1	B	48	ARG	Sidechain
1	B	51	TYR	Sidechain
1	B	57	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	874	TYR	Sidechain
1	B	901	ARG	Sidechain

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	10123	10167	10164	19	0
1	B	10798	10843	10840	18	0
2	A	21	20	21	0	0
2	B	21	20	21	0	0
3	A	23	12	12	0	0
3	B	23	12	12	0	0
All	All	21009	21074	21070	34	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 1.

All (34) 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:240:ASP:H	1:A:387:ASP:HA	1.65	0.61
1:B:846:ILE:H	1:B:846:ILE:HD12	1.68	0.58
1:A:1111:ALA:HB1	1:A:1229:VAL:HG11	1.86	0.58
1:A:1229:VAL:HG12	1:A:1280:LEU:HA	1.85	0.58
1:B:1023:LEU:HD23	1:B:1041:TRP:CE3	2.42	0.54
1:A:513:TYR:CZ	1:A:517:LEU:HD11	2.45	0.52
1:A:877:VAL:HG21	1:A:893:TRP:CE2	2.46	0.50
1:B:1060:LEU:HD22	1:B:1070:LEU:HD21	1.94	0.49
1:B:128:SER:HB2	1:B:130:HIS:HB3	1.96	0.48
1:B:877:VAL:HG21	1:B:893:TRP:CE2	2.49	0.47
1:A:896:GLY:HA2	1:B:535:TRP:CD2	2.50	0.46
1:A:234:LEU:HD21	1:A:239:ALA:HB3	1.97	0.46
1:A:693:TYR:CZ	1:A:745:VAL:HG21	2.53	0.44
1:A:923:TYR:CE2	1:A:925:THR:HA	2.53	0.44
1:A:1121:THR:HG23	1:A:1122:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1201:ALA:H	1:B:1229:VAL:HG23	1.83	0.44
1:A:359:TRP:CD2	1:A:885:PRO:HG2	2.52	0.43
1:A:359:TRP:HA	1:A:888:VAL:HG21	1.99	0.43
1:B:693:TYR:CE2	1:B:745:VAL:HG11	2.53	0.43
1:A:326:SER:HB3	1:B:604:GLY:HA3	2.00	0.43
1:A:232:LEU:C	1:A:232:LEU:HD12	2.39	0.43
1:B:696:TYR:CZ	1:B:706:GLY:HA3	2.54	0.42
1:B:1350:GLU:CD	1:B:1350:GLU:H	2.23	0.42
1:A:535:TRP:CE3	1:B:896:GLY:HA2	2.54	0.42
1:A:846:ILE:H	1:A:846:ILE:HD12	1.84	0.42
1:B:923:TYR:CE2	1:B:925:THR:HA	2.55	0.42
1:B:1262:LEU:C	1:B:1262:LEU:HD23	2.41	0.41
1:B:149:ALA:HB1	1:B:178:CYS:SG	2.60	0.41
1:A:1350:GLU:H	1:A:1350:GLU:CD	2.24	0.41
1:B:668:ARG:C	1:B:669:LEU:HD12	2.41	0.41
1:B:1121:THR:HG21	1:B:1153:LEU:HD12	2.03	0.40
1:A:203:ARG:HD3	1:A:231:TRP:CH2	2.56	0.40
1:B:385:ILE:HG22	1:B:385:ILE:O	2.21	0.40
1:A:392:LEU:HD11	1:A:418:ALA:HB1	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1317/1455 (90%)	1219 (93%)	90 (7%)	8 (1%)	25	61
1	B	1404/1455 (96%)	1293 (92%)	105 (8%)	6 (0%)	34	69
All	All	2721/2910 (94%)	2512 (92%)	195 (7%)	14 (0%)	32	65

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1274	ARG
1	B	451	GLY
1	B	748	LEU
1	B	1382	GLY
1	A	109	SER
1	A	1051	SER
1	A	1160	ARG
1	B	61	SER
1	A	275	HIS
1	A	1382	GLY
1	A	385	ILE
1	A	604	GLY
1	B	96	PRO
1	B	1144	GLY

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	1008/1122 (90%)	983 (98%)	25 (2%)	47	70
1	B	1078/1122 (96%)	1049 (97%)	29 (3%)	44	69
All	All	2086/2244 (93%)	2032 (97%)	54 (3%)	49	70

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	TYR
1	A	162	ARG
1	A	194	ARG
1	A	232	LEU
1	A	240	ASP
1	A	311	GLU
1	A	314	ARG
1	A	317	ARG
1	A	518	GLN
1	A	531	LEU

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Mol	Chain	Res	Type
1	A	571	ASP
1	A	757	SER
1	A	953	ARG
1	A	970	GLU
1	A	973	CYS
1	A	1006	GLN
1	A	1018	LEU
1	A	1105	LEU
1	A	1109	ARG
1	A	1175	ARG
1	A	1207	GLU
1	A	1273	TRP
1	A	1276	GLU
1	A	1305	GLN
1	A	1384	ASP
1	B	48	ARG
1	B	53	GLN
1	B	137	THR
1	B	138	ARG
1	B	158	MET
1	B	194	ARG
1	B	235	ASP
1	B	245	ARG
1	B	280	ARG
1	B	374	ARG
1	B	381	ILE
1	B	402	VAL
1	B	471	LEU
1	B	474	THR
1	B	482	GLN
1	B	813	SER
1	B	887	LEU
1	B	901	ARG
1	B	1092	LEU
1	B	1109	ARG
1	B	1114	ARG
1	B	1115	LEU
1	B	1121	THR
1	B	1175	ARG
1	B	1273	TRP
1	B	1282	GLU
1	B	1308	ARG

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Mol	Chain	Res	Type
1	B	1385	SER
1	B	1402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	PNS	A	1501	1	13,20,21	0.92	0	18,26,29	1.04	0
3	AMP	B	1502	-	22,25,25	1.30	4 (18%)	25,38,38	1.85	9 (36%)
3	AMP	A	1502	-	22,25,25	1.25	4 (18%)	25,38,38	1.89	6 (24%)
2	PNS	B	1501	-	13,20,21	0.87	0	18,26,29	0.94	1 (5%)

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	1	-	4/24/26/27	-
3	AMP	B	1502	-	-	3/6/26/26	0/3/3/3
3	AMP	A	1502	-	-	3/6/26/26	0/3/3/3
2	PNS	B	1501	-	-	4/24/26/27	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1502	AMP	O4'-C1'	2.29	1.44	1.41
3	B	1502	AMP	P-O1P	2.25	1.57	1.50
3	B	1502	AMP	C5-C4	-2.21	1.35	1.40
3	A	1502	AMP	C5-C4	-2.20	1.35	1.40
3	A	1502	AMP	C4-N3	-2.19	1.32	1.35
3	B	1502	AMP	O4'-C1'	2.11	1.44	1.41
3	A	1502	AMP	P-O2P	-2.04	1.47	1.54
3	B	1502	AMP	P-O2P	-2.01	1.47	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1502	AMP	C4-C5-N7	4.48	114.07	109.40
3	B	1502	AMP	C4-C5-N7	3.94	113.51	109.40
3	A	1502	AMP	O3P-P-O5'	-3.80	96.63	106.73
3	B	1502	AMP	O5'-P-O1P	-3.71	96.07	106.47
3	A	1502	AMP	O2P-P-O5'	2.69	113.89	106.73
3	B	1502	AMP	O3P-P-O5'	2.67	113.83	106.73
3	B	1502	AMP	N6-C6-N1	-2.51	113.37	118.57
2	B	1501	PNS	C42-N41-C39	2.44	127.37	122.84
3	A	1502	AMP	C3'-C2'-C1'	2.41	104.61	100.98
3	B	1502	AMP	C3'-C2'-C1'	2.33	104.49	100.98
3	B	1502	AMP	C5-C6-N6	2.28	123.82	120.35
3	A	1502	AMP	N6-C6-N1	-2.26	113.89	118.57
3	A	1502	AMP	C2-N1-C6	-2.23	114.95	118.75
3	B	1502	AMP	O2P-P-O5'	2.20	112.59	106.73
3	B	1502	AMP	O4'-C1'-C2'	-2.12	103.83	106.93
3	B	1502	AMP	C2-N1-C6	-2.05	115.24	118.75

There are no chirality outliers.

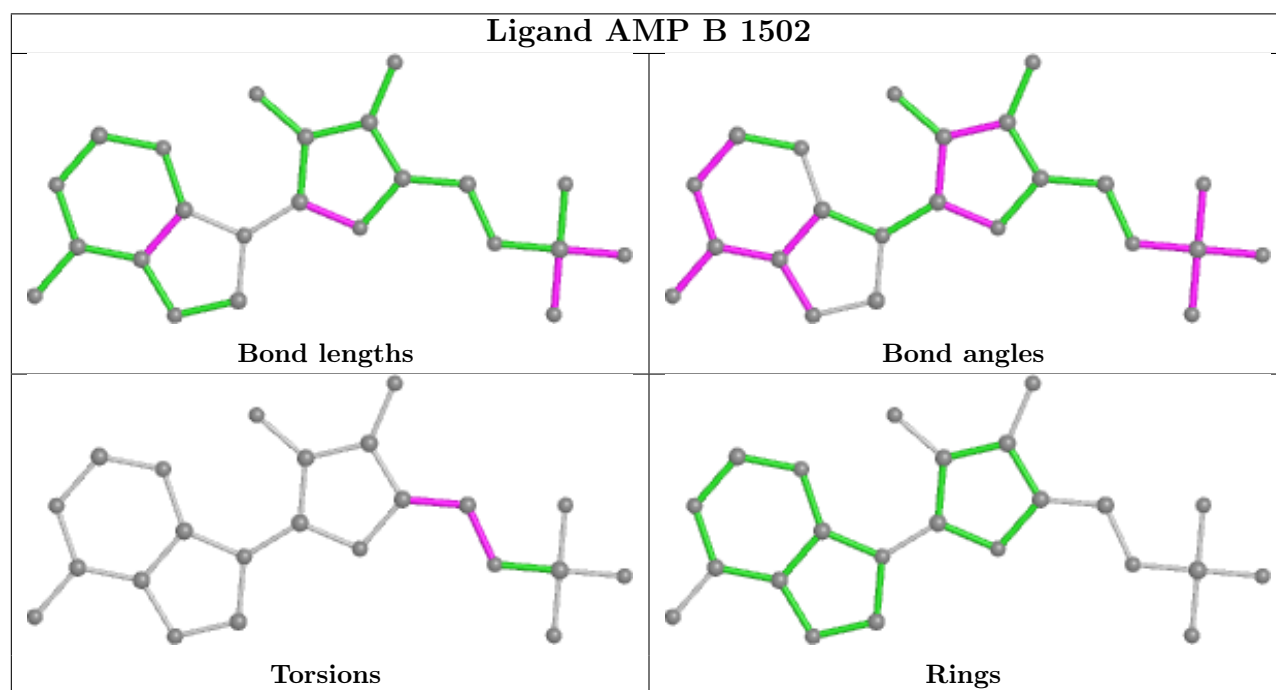
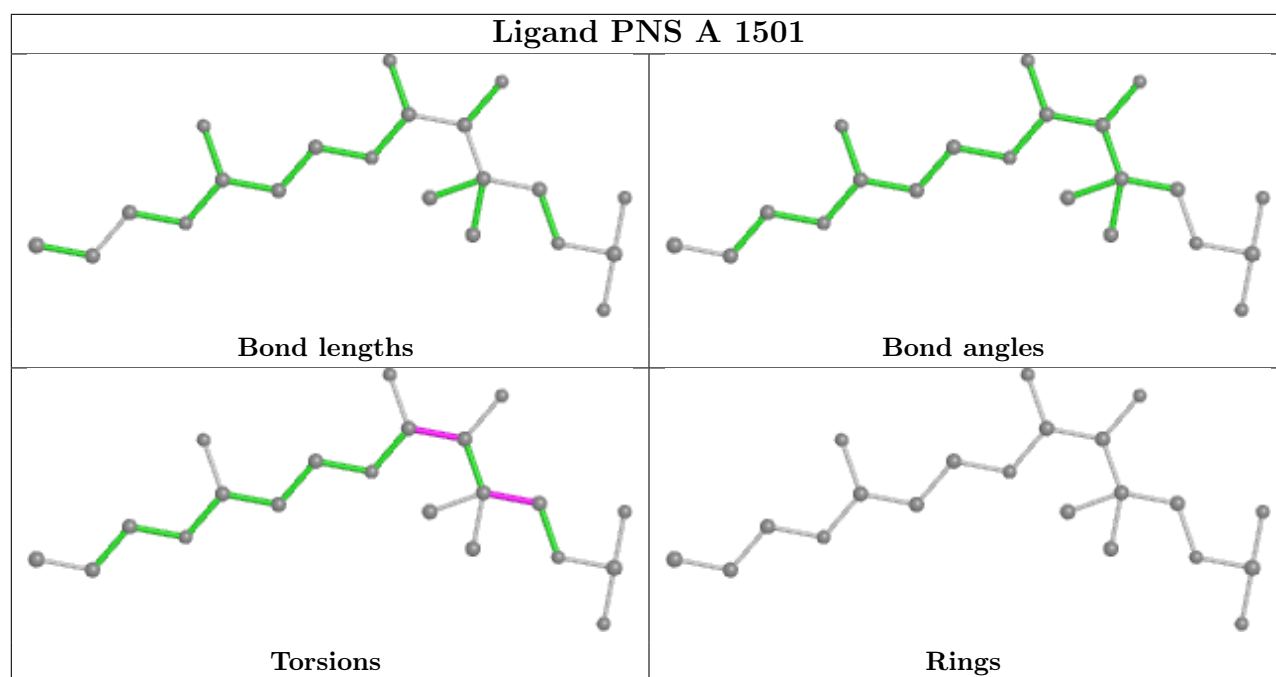
All (14) torsion outliers are listed below:

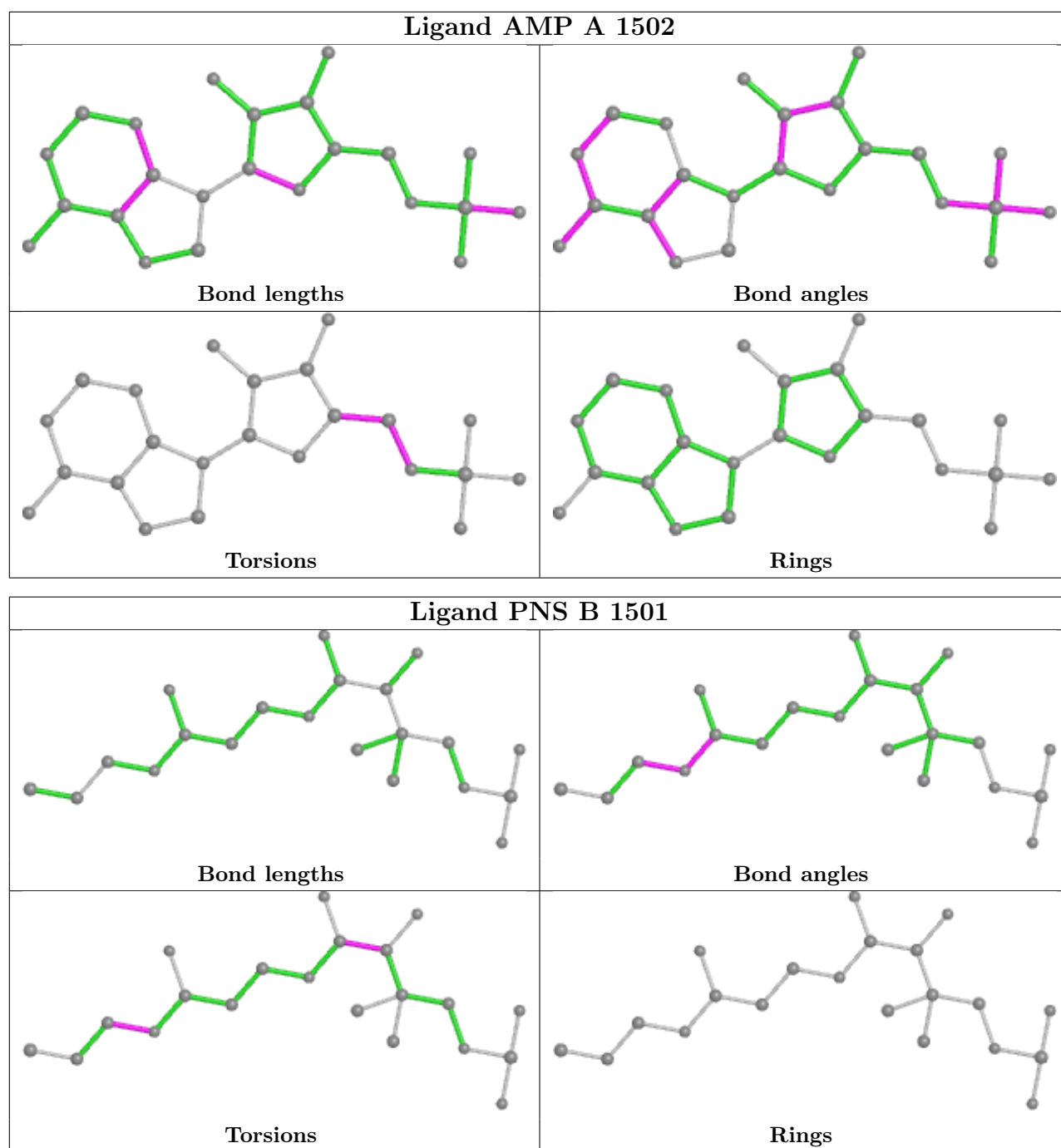
Mol	Chain	Res	Type	Atoms
2	A	1501	PNS	O27-C28-C29-C32
2	B	1501	PNS	C43-C42-N41-C39
3	A	1502	AMP	O4'-C4'-C5'-O5'
3	B	1502	AMP	O4'-C4'-C5'-O5'
3	B	1502	AMP	C3'-C4'-C5'-O5'
3	A	1502	AMP	C3'-C4'-C5'-O5'
2	B	1501	PNS	O33-C32-C34-O35
2	A	1501	PNS	O27-C28-C29-C30
2	A	1501	PNS	O27-C28-C29-C31
3	A	1502	AMP	C4'-C5'-O5'-P
2	B	1501	PNS	C29-C32-C34-N36
3	B	1502	AMP	C4'-C5'-O5'-P
2	A	1501	PNS	O33-C32-C34-O35
2	B	1501	PNS	C29-C32-C34-O35

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

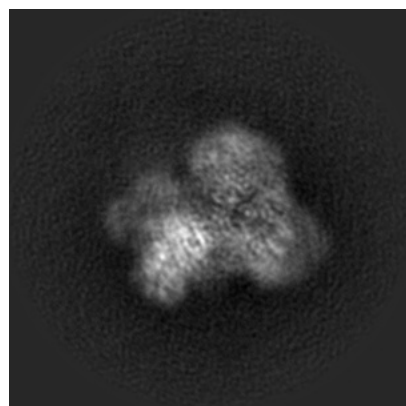
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31200. These allow visual inspection of the internal detail of the map and identification of artifacts.

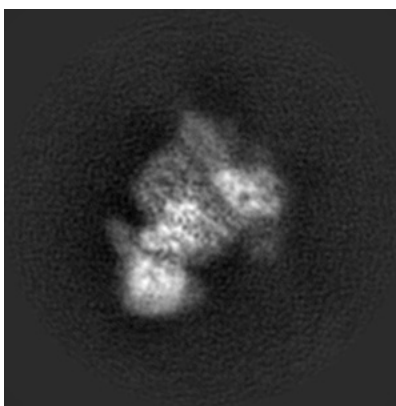
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

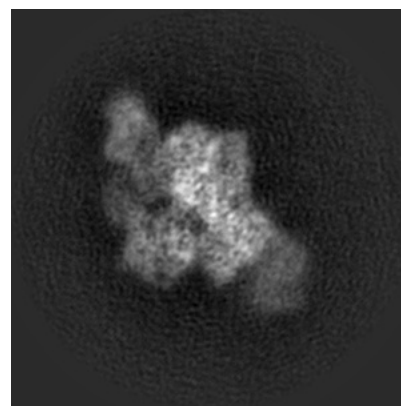
6.1.1 Primary map



X

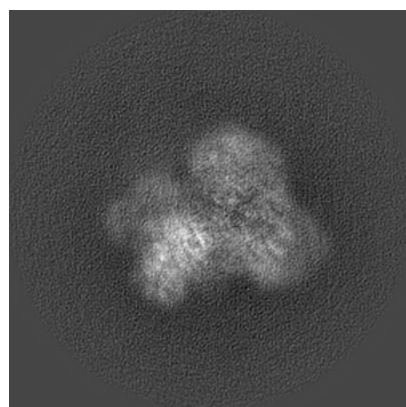


Y

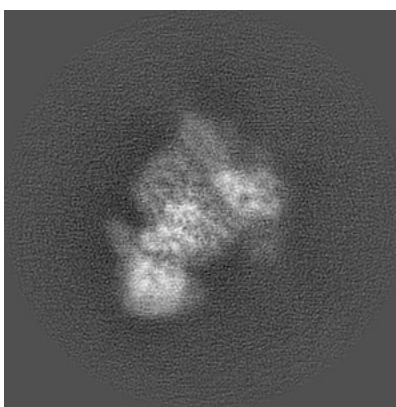


Z

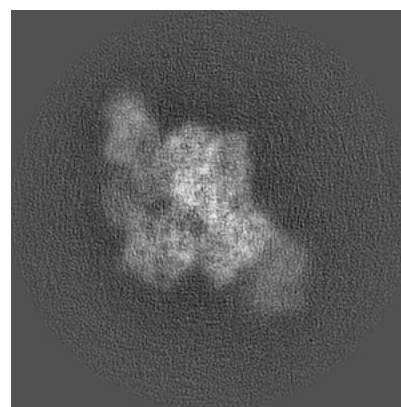
6.1.2 Raw map



X



Y

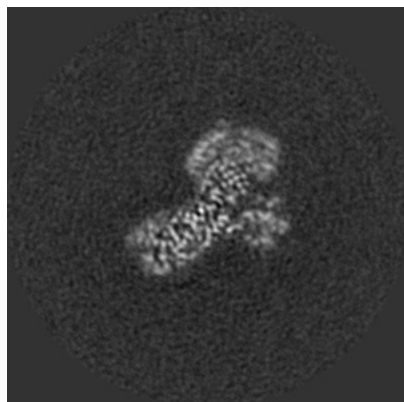


Z

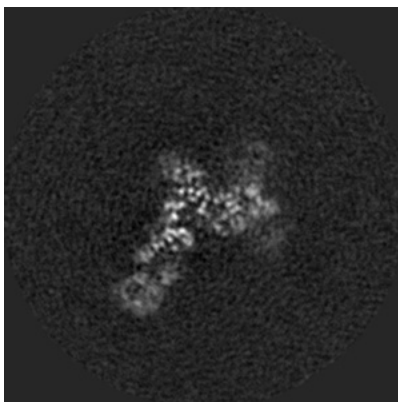
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

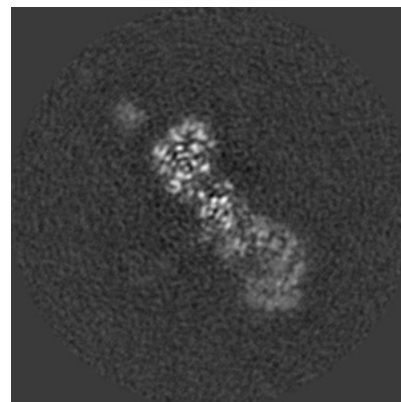
6.2.1 Primary map



X Index: 125

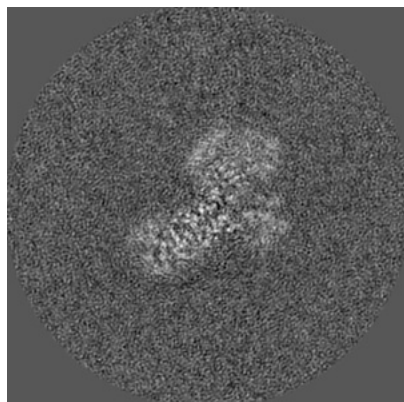


Y Index: 125

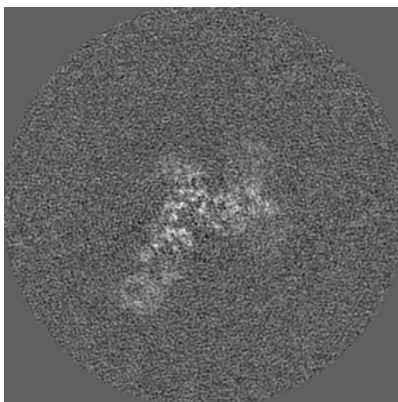


Z Index: 125

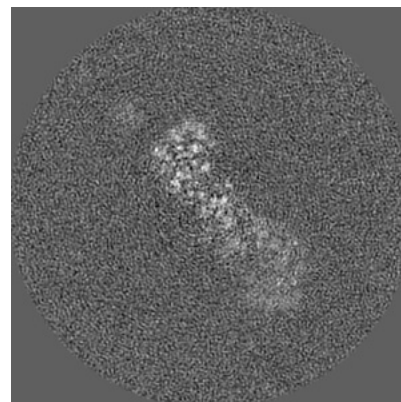
6.2.2 Raw map



X Index: 125



Y Index: 125



Z Index: 125

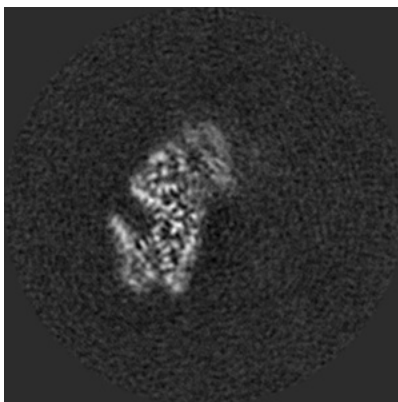
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

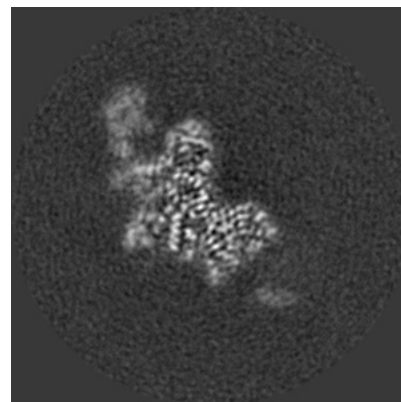
6.3.1 Primary map



X Index: 127

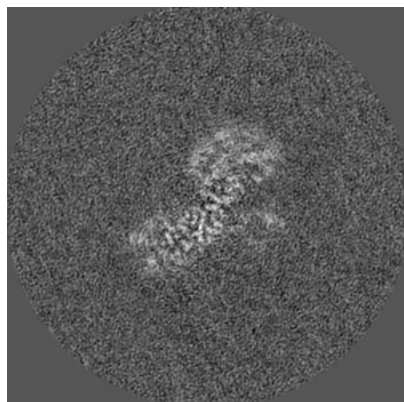


Y Index: 106

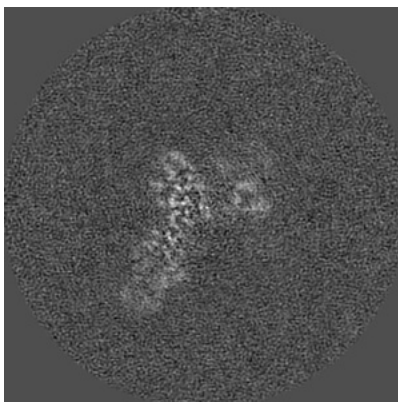


Z Index: 107

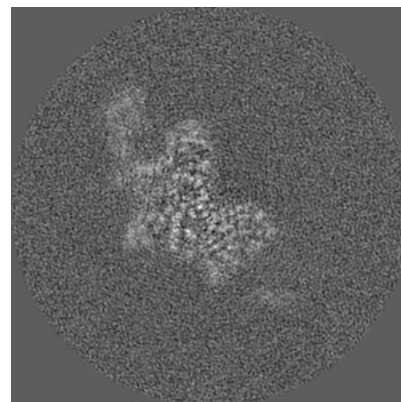
6.3.2 Raw map



X Index: 127



Y Index: 120

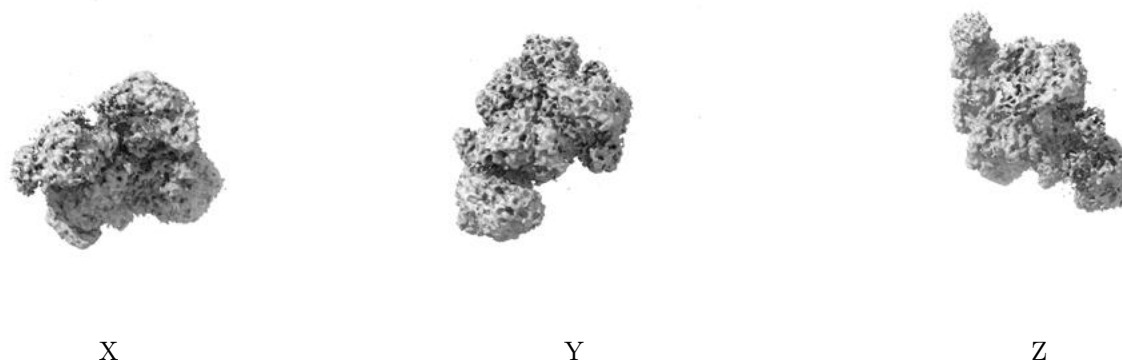


Z Index: 107

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

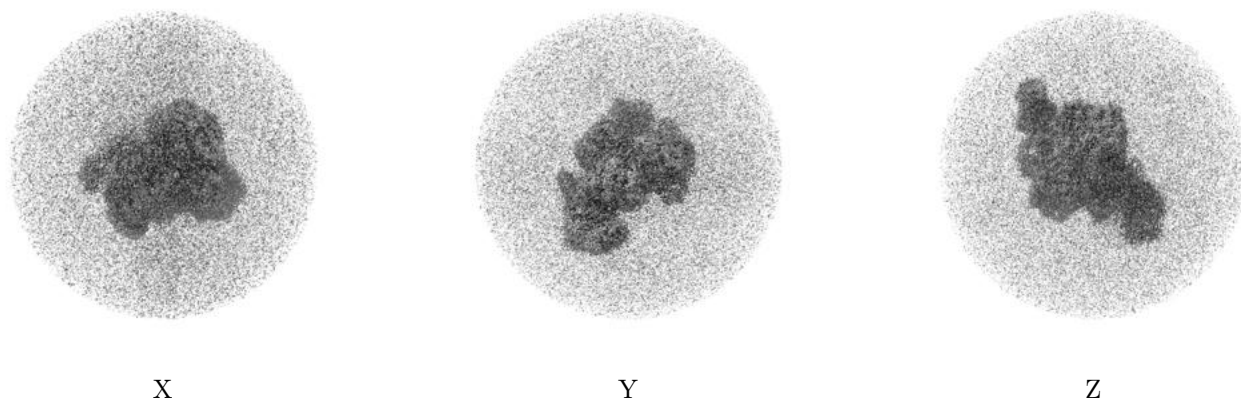
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

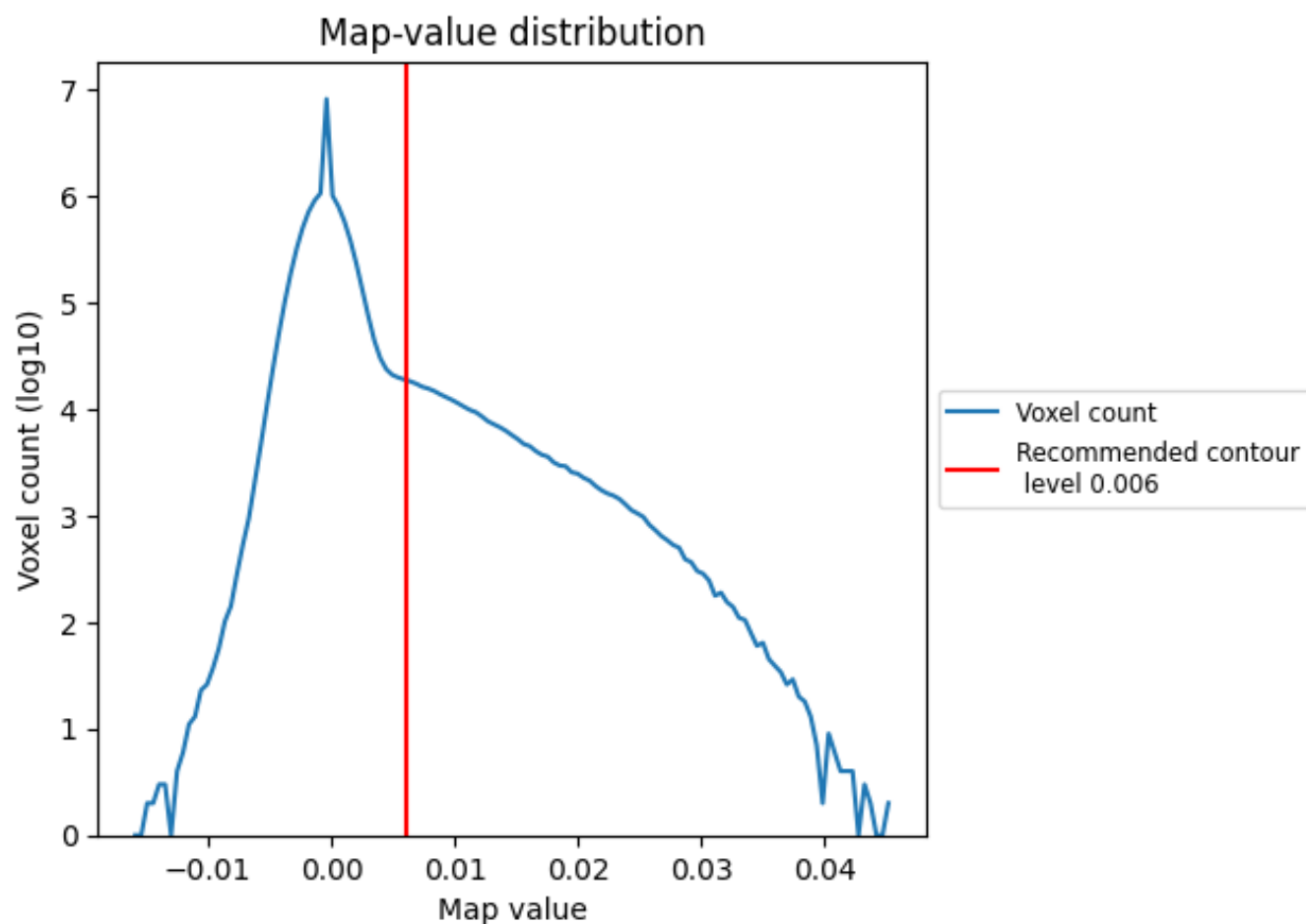
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

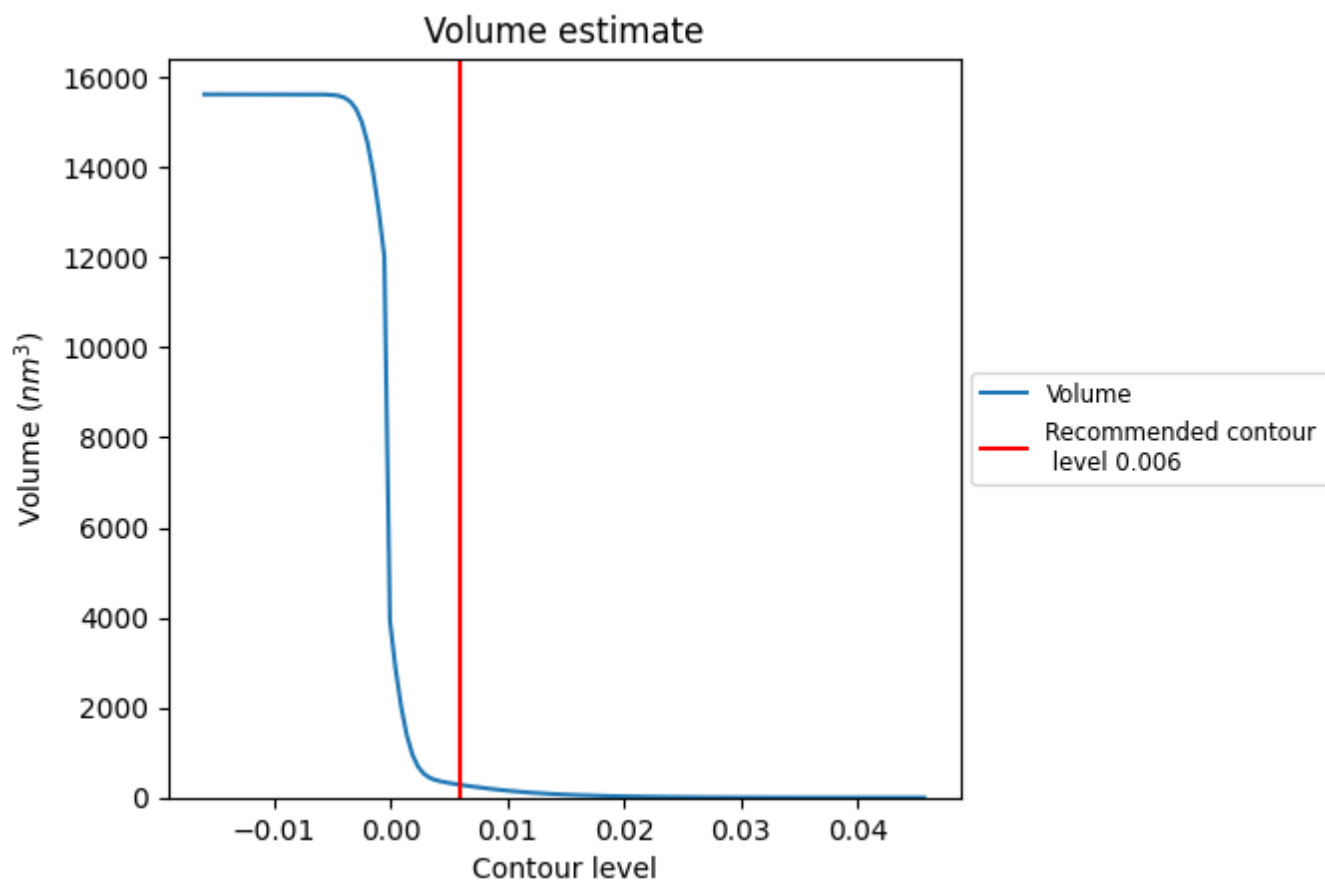
This section contains the results of statistical analysis of the map.

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.

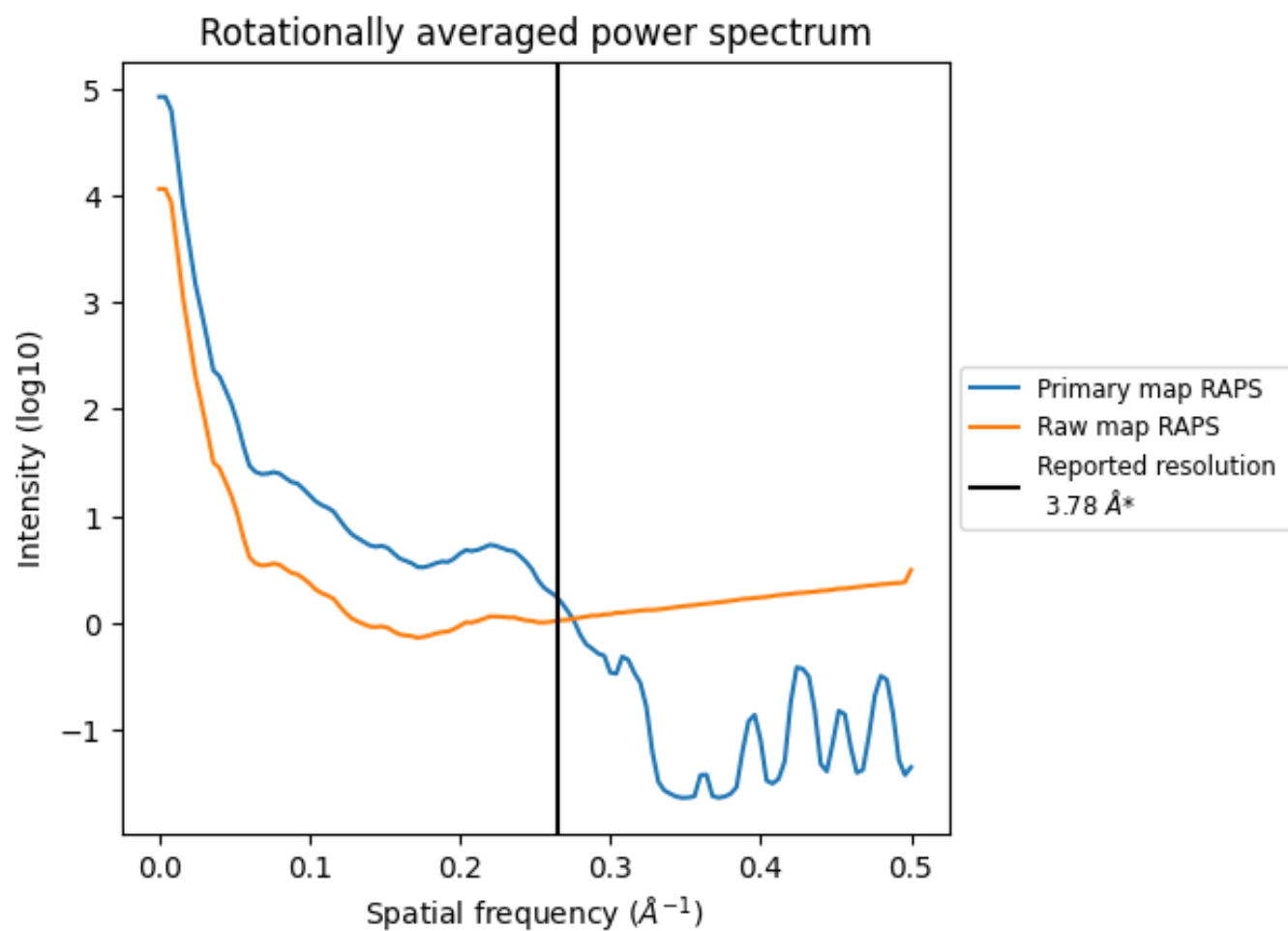
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 282 nm^3 ; this corresponds to an approximate mass of 255 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 ⓘ

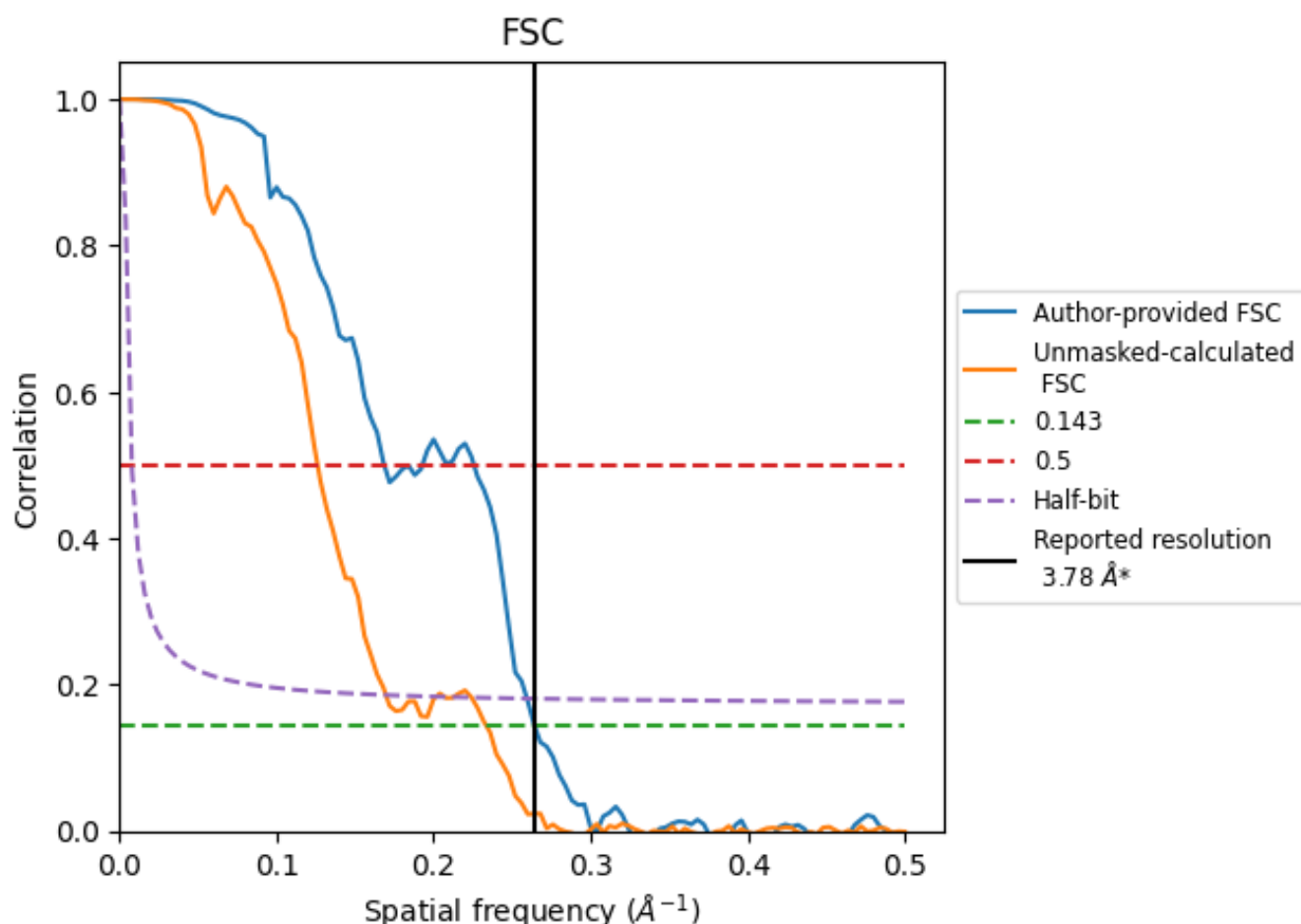


*Reported resolution corresponds to spatial frequency of 0.265 \AA^{-1}

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 0.265 Å⁻¹

8.2 Resolution estimates [i](#)

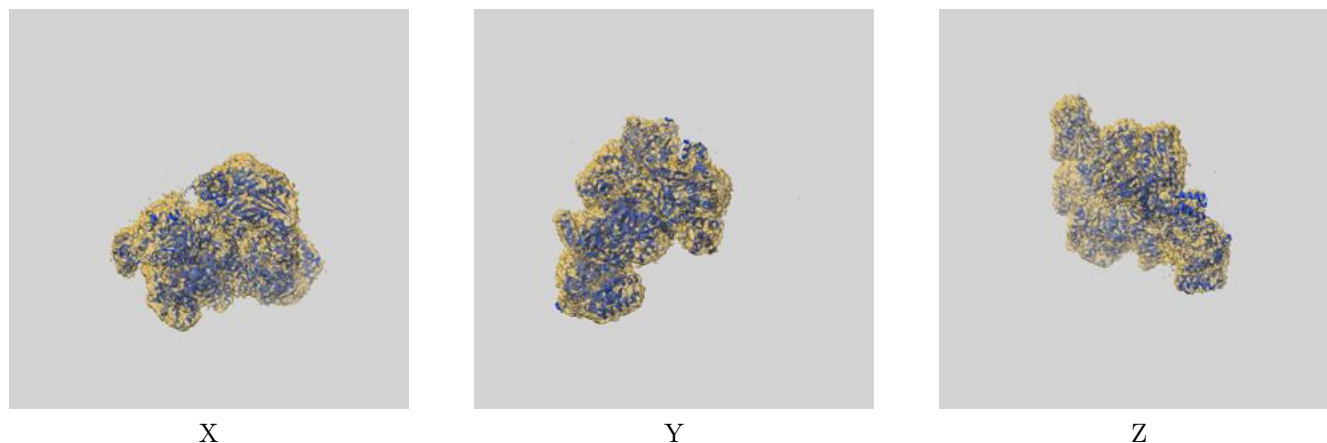
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.78	-	-
Author-provided FSC curve	3.78	5.93	3.86
Unmasked-calculated*	4.28	7.93	5.89

*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 4.28 differs from the reported value 3.78 by more than 10 %

9 Map-model fit [i](#)

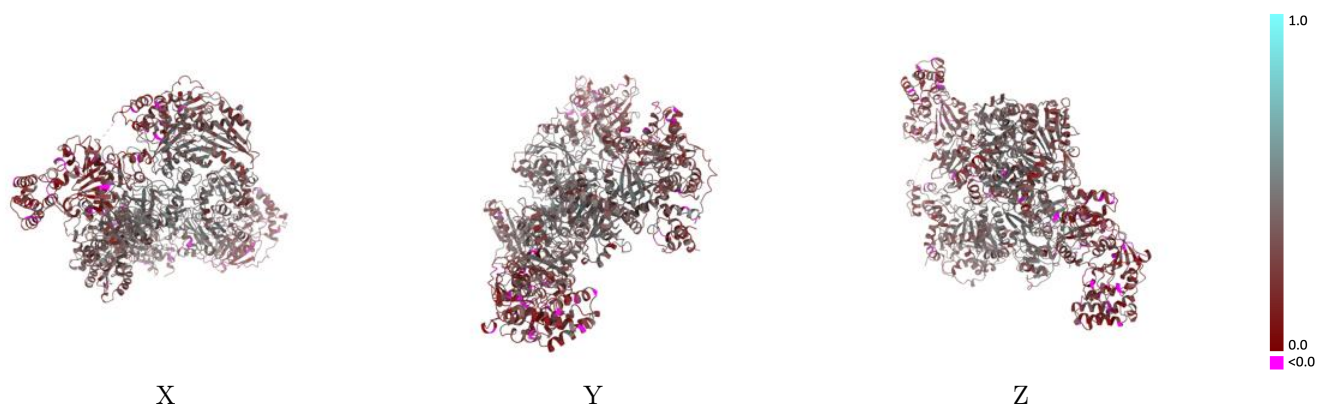
This section contains information regarding the fit between EMDB map EMD-31200 and PDB model 7EN2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



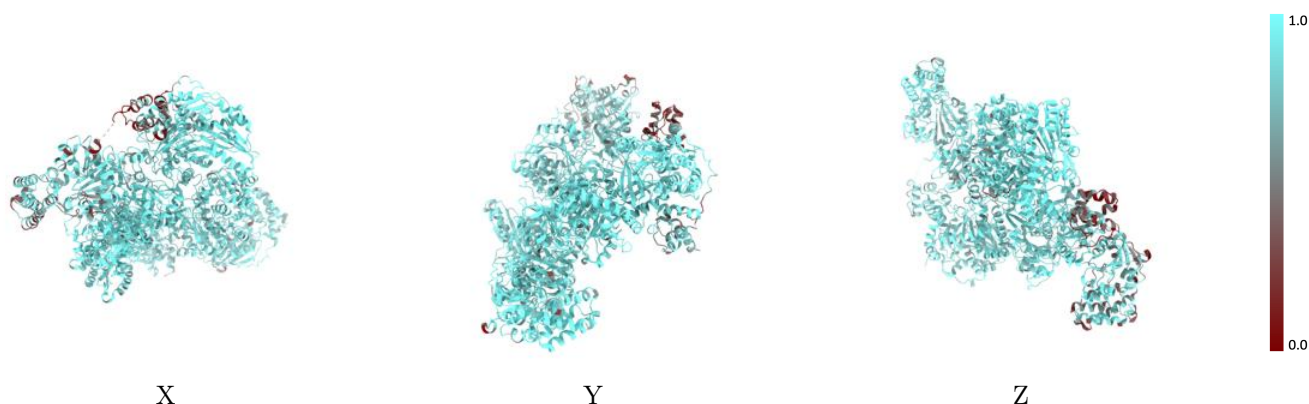
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



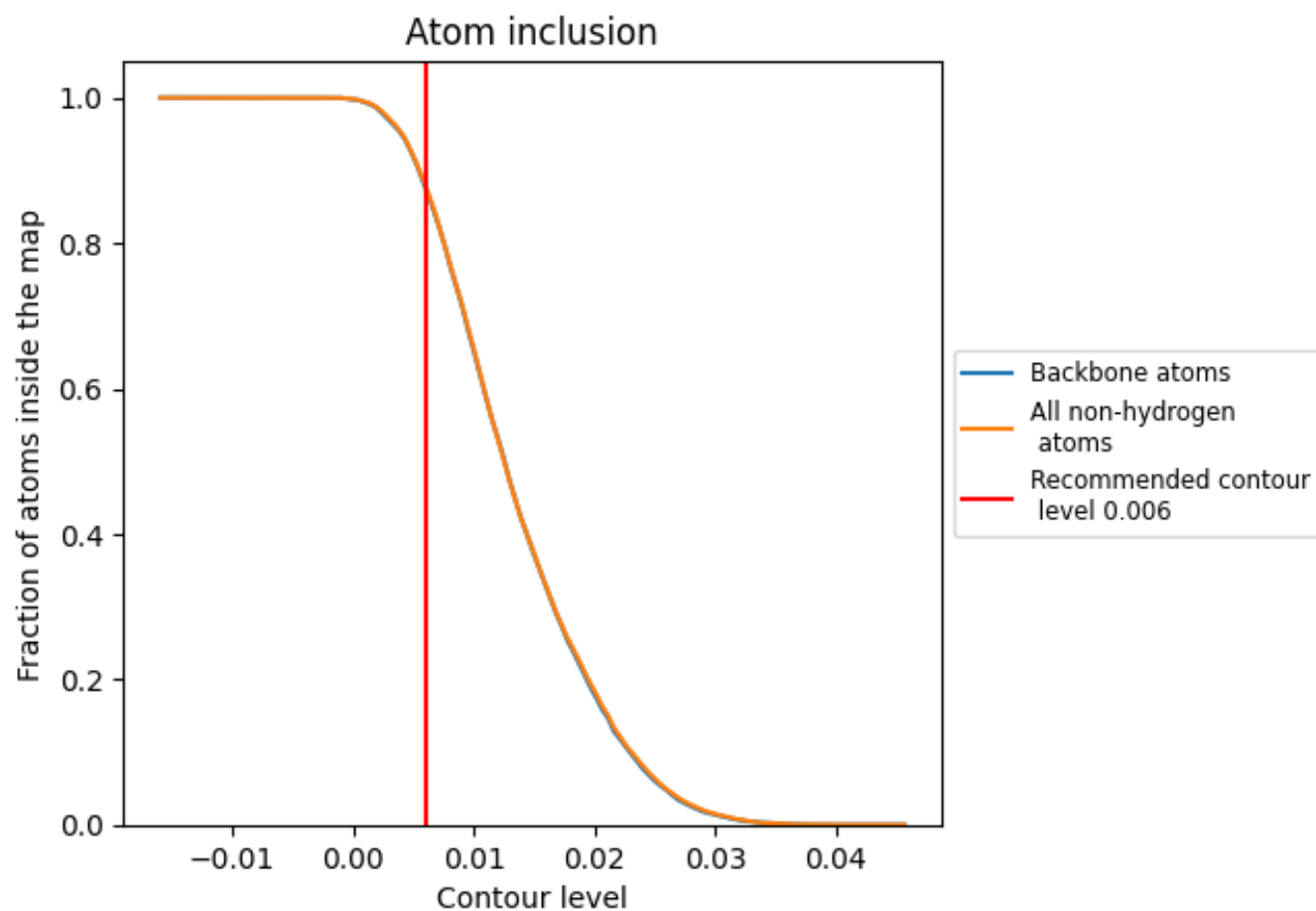
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.006).

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 88% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8796	<div></div> 0.3300
A	<div></div> 0.9259	<div></div> 0.3340
B	<div></div> 0.8552	<div></div> 0.3260

