



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:49 PM UTC

PDB ID : 9CAP / pdb_00009cap
EMDB ID : EMD-45399
Title : Structure of the LPD-3 complex
Authors : Clark, S.A.; Vanni, S.; Kang, Y.
Deposited on : 2024-06-17
Resolution : 2.70 Å(reported)

This is a wwPDB EM Validation Summary 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

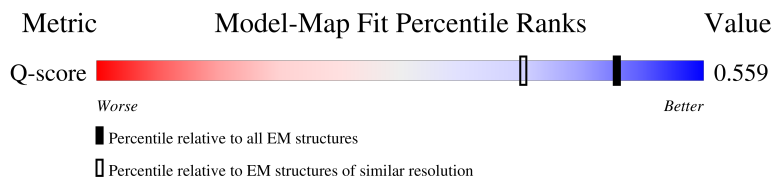
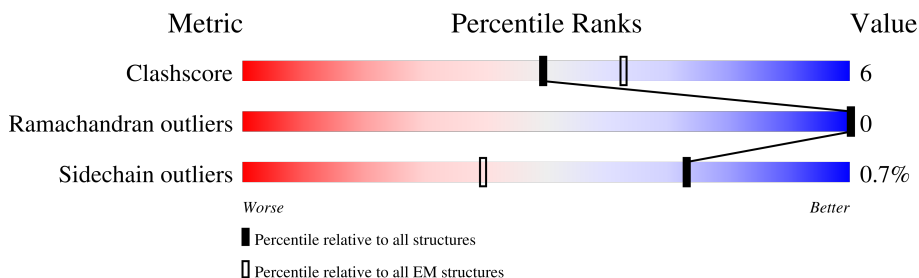
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY




The reported resolution of this entry is 2.70 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	10327 (2.20 - 3.20)

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	4299	 28% 5% 67%
2	B	276	 59% 6% 34%
3	C	143	 69% 13% 18%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14705 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bridge-like lipid transfer protein family member 1 C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1432	Total	C	N	O	S	0	0
			11425	7345	1923	2089	68		

There are 281 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PHE	deletion	UNP A0A0K3AWP8
A	?	-	GLN	deletion	UNP A0A0K3AWP8
A	4021	GLY	-	expression tag	UNP A0A0K3AWP8
A	4022	SER	-	expression tag	UNP A0A0K3AWP8
A	4023	GLY	-	expression tag	UNP A0A0K3AWP8
A	4024	VAL	-	expression tag	UNP A0A0K3AWP8
A	4025	SER	-	expression tag	UNP A0A0K3AWP8
A	4026	LYS	-	expression tag	UNP A0A0K3AWP8
A	4027	GLY	-	expression tag	UNP A0A0K3AWP8
A	4028	GLU	-	expression tag	UNP A0A0K3AWP8
A	4029	GLU	-	expression tag	UNP A0A0K3AWP8
A	4030	LEU	-	expression tag	UNP A0A0K3AWP8
A	4031	PHE	-	expression tag	UNP A0A0K3AWP8
A	4032	THR	-	expression tag	UNP A0A0K3AWP8
A	4033	GLY	-	expression tag	UNP A0A0K3AWP8
A	4034	VAL	-	expression tag	UNP A0A0K3AWP8
A	4035	VAL	-	expression tag	UNP A0A0K3AWP8
A	4036	PRO	-	expression tag	UNP A0A0K3AWP8
A	4037	ILE	-	expression tag	UNP A0A0K3AWP8
A	4038	LEU	-	expression tag	UNP A0A0K3AWP8
A	4039	VAL	-	expression tag	UNP A0A0K3AWP8
A	4040	GLU	-	expression tag	UNP A0A0K3AWP8
A	4041	LEU	-	expression tag	UNP A0A0K3AWP8
A	4042	ASP	-	expression tag	UNP A0A0K3AWP8
A	4043	GLY	-	expression tag	UNP A0A0K3AWP8
A	4044	ASP	-	expression tag	UNP A0A0K3AWP8
A	4045	VAL	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4046	ASN	-	expression tag	UNP A0A0K3AWP8
A	4047	GLY	-	expression tag	UNP A0A0K3AWP8
A	4048	HIS	-	expression tag	UNP A0A0K3AWP8
A	4049	LYS	-	expression tag	UNP A0A0K3AWP8
A	4050	PHE	-	expression tag	UNP A0A0K3AWP8
A	4051	SER	-	expression tag	UNP A0A0K3AWP8
A	4052	VAL	-	expression tag	UNP A0A0K3AWP8
A	4053	SER	-	expression tag	UNP A0A0K3AWP8
A	4054	GLY	-	expression tag	UNP A0A0K3AWP8
A	4055	GLU	-	expression tag	UNP A0A0K3AWP8
A	4056	GLY	-	expression tag	UNP A0A0K3AWP8
A	4057	GLU	-	expression tag	UNP A0A0K3AWP8
A	4058	GLY	-	expression tag	UNP A0A0K3AWP8
A	4059	ASP	-	expression tag	UNP A0A0K3AWP8
A	4060	ALA	-	expression tag	UNP A0A0K3AWP8
A	4061	THR	-	expression tag	UNP A0A0K3AWP8
A	4062	TYR	-	expression tag	UNP A0A0K3AWP8
A	4063	GLY	-	expression tag	UNP A0A0K3AWP8
A	4064	LYS	-	expression tag	UNP A0A0K3AWP8
A	4065	LEU	-	expression tag	UNP A0A0K3AWP8
A	4066	THR	-	expression tag	UNP A0A0K3AWP8
A	4067	LEU	-	expression tag	UNP A0A0K3AWP8
A	4068	LYS	-	expression tag	UNP A0A0K3AWP8
A	4069	LEU	-	expression tag	UNP A0A0K3AWP8
A	4070	ILE	-	expression tag	UNP A0A0K3AWP8
A	4071	CYS	-	expression tag	UNP A0A0K3AWP8
A	4072	THR	-	expression tag	UNP A0A0K3AWP8
A	4073	THR	-	expression tag	UNP A0A0K3AWP8
A	4074	GLY	-	expression tag	UNP A0A0K3AWP8
A	4075	LYS	-	expression tag	UNP A0A0K3AWP8
A	4076	LEU	-	expression tag	UNP A0A0K3AWP8
A	4077	PRO	-	expression tag	UNP A0A0K3AWP8
A	4078	VAL	-	expression tag	UNP A0A0K3AWP8
A	4079	PRO	-	expression tag	UNP A0A0K3AWP8
A	4080	TRP	-	expression tag	UNP A0A0K3AWP8
A	4081	PRO	-	expression tag	UNP A0A0K3AWP8
A	4082	THR	-	expression tag	UNP A0A0K3AWP8
A	4083	LEU	-	expression tag	UNP A0A0K3AWP8
A	4084	VAL	-	expression tag	UNP A0A0K3AWP8
A	4085	THR	-	expression tag	UNP A0A0K3AWP8
A	4086	THR	-	expression tag	UNP A0A0K3AWP8
A	4087	LEU	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4088	GLY	-	expression tag	UNP A0A0K3AWP8
A	4089	TYR	-	expression tag	UNP A0A0K3AWP8
A	4090	GLY	-	expression tag	UNP A0A0K3AWP8
A	4091	LEU	-	expression tag	UNP A0A0K3AWP8
A	4092	MET	-	expression tag	UNP A0A0K3AWP8
A	4093	CYS	-	expression tag	UNP A0A0K3AWP8
A	4094	PHE	-	expression tag	UNP A0A0K3AWP8
A	4095	ALA	-	expression tag	UNP A0A0K3AWP8
A	4096	ARG	-	expression tag	UNP A0A0K3AWP8
A	4097	TYR	-	expression tag	UNP A0A0K3AWP8
A	4098	PRO	-	expression tag	UNP A0A0K3AWP8
A	4099	ASP	-	expression tag	UNP A0A0K3AWP8
A	4100	HIS	-	expression tag	UNP A0A0K3AWP8
A	4101	MET	-	expression tag	UNP A0A0K3AWP8
A	4102	LYS	-	expression tag	UNP A0A0K3AWP8
A	4103	GLN	-	expression tag	UNP A0A0K3AWP8
A	4104	HIS	-	expression tag	UNP A0A0K3AWP8
A	4105	ASP	-	expression tag	UNP A0A0K3AWP8
A	4106	PHE	-	expression tag	UNP A0A0K3AWP8
A	4107	PHE	-	expression tag	UNP A0A0K3AWP8
A	4108	LYS	-	expression tag	UNP A0A0K3AWP8
A	4109	SER	-	expression tag	UNP A0A0K3AWP8
A	4110	ALA	-	expression tag	UNP A0A0K3AWP8
A	4111	MET	-	expression tag	UNP A0A0K3AWP8
A	4112	PRO	-	expression tag	UNP A0A0K3AWP8
A	4113	GLU	-	expression tag	UNP A0A0K3AWP8
A	4114	GLY	-	expression tag	UNP A0A0K3AWP8
A	4115	TYR	-	expression tag	UNP A0A0K3AWP8
A	4116	VAL	-	expression tag	UNP A0A0K3AWP8
A	4117	GLN	-	expression tag	UNP A0A0K3AWP8
A	4118	GLU	-	expression tag	UNP A0A0K3AWP8
A	4119	ARG	-	expression tag	UNP A0A0K3AWP8
A	4120	THR	-	expression tag	UNP A0A0K3AWP8
A	4121	ILE	-	expression tag	UNP A0A0K3AWP8
A	4122	PHE	-	expression tag	UNP A0A0K3AWP8
A	4123	PHE	-	expression tag	UNP A0A0K3AWP8
A	4124	LYS	-	expression tag	UNP A0A0K3AWP8
A	4125	ASP	-	expression tag	UNP A0A0K3AWP8
A	4126	ASP	-	expression tag	UNP A0A0K3AWP8
A	4127	GLY	-	expression tag	UNP A0A0K3AWP8
A	4128	ASN	-	expression tag	UNP A0A0K3AWP8
A	4129	TYR	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4130	LYS	-	expression tag	UNP A0A0K3AWP8
A	4131	THR	-	expression tag	UNP A0A0K3AWP8
A	4132	ARG	-	expression tag	UNP A0A0K3AWP8
A	4133	ALA	-	expression tag	UNP A0A0K3AWP8
A	4134	GLU	-	expression tag	UNP A0A0K3AWP8
A	4135	VAL	-	expression tag	UNP A0A0K3AWP8
A	4136	LYS	-	expression tag	UNP A0A0K3AWP8
A	4137	PHE	-	expression tag	UNP A0A0K3AWP8
A	4138	GLU	-	expression tag	UNP A0A0K3AWP8
A	4139	GLY	-	expression tag	UNP A0A0K3AWP8
A	4140	ASP	-	expression tag	UNP A0A0K3AWP8
A	4141	THR	-	expression tag	UNP A0A0K3AWP8
A	4142	LEU	-	expression tag	UNP A0A0K3AWP8
A	4143	VAL	-	expression tag	UNP A0A0K3AWP8
A	4144	ASN	-	expression tag	UNP A0A0K3AWP8
A	4145	ARG	-	expression tag	UNP A0A0K3AWP8
A	4146	ILE	-	expression tag	UNP A0A0K3AWP8
A	4147	GLU	-	expression tag	UNP A0A0K3AWP8
A	4148	LEU	-	expression tag	UNP A0A0K3AWP8
A	4149	LYS	-	expression tag	UNP A0A0K3AWP8
A	4150	GLY	-	expression tag	UNP A0A0K3AWP8
A	4151	ILE	-	expression tag	UNP A0A0K3AWP8
A	4152	ASP	-	expression tag	UNP A0A0K3AWP8
A	4153	PHE	-	expression tag	UNP A0A0K3AWP8
A	4154	LYS	-	expression tag	UNP A0A0K3AWP8
A	4155	GLU	-	expression tag	UNP A0A0K3AWP8
A	4156	ASP	-	expression tag	UNP A0A0K3AWP8
A	4157	GLY	-	expression tag	UNP A0A0K3AWP8
A	4158	ASN	-	expression tag	UNP A0A0K3AWP8
A	4159	ILE	-	expression tag	UNP A0A0K3AWP8
A	4160	LEU	-	expression tag	UNP A0A0K3AWP8
A	4161	GLY	-	expression tag	UNP A0A0K3AWP8
A	4162	HIS	-	expression tag	UNP A0A0K3AWP8
A	4163	LYS	-	expression tag	UNP A0A0K3AWP8
A	4164	LEU	-	expression tag	UNP A0A0K3AWP8
A	4165	GLU	-	expression tag	UNP A0A0K3AWP8
A	4166	TYR	-	expression tag	UNP A0A0K3AWP8
A	4167	ASN	-	expression tag	UNP A0A0K3AWP8
A	4168	TYR	-	expression tag	UNP A0A0K3AWP8
A	4169	ASN	-	expression tag	UNP A0A0K3AWP8
A	4170	SER	-	expression tag	UNP A0A0K3AWP8
A	4171	HIS	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4172	ASN	-	expression tag	UNP A0A0K3AWP8
A	4173	VAL	-	expression tag	UNP A0A0K3AWP8
A	4174	TYR	-	expression tag	UNP A0A0K3AWP8
A	4175	ILE	-	expression tag	UNP A0A0K3AWP8
A	4176	THR	-	expression tag	UNP A0A0K3AWP8
A	4177	ALA	-	expression tag	UNP A0A0K3AWP8
A	4178	ASP	-	expression tag	UNP A0A0K3AWP8
A	4179	LYS	-	expression tag	UNP A0A0K3AWP8
A	4180	GLN	-	expression tag	UNP A0A0K3AWP8
A	4181	LYS	-	expression tag	UNP A0A0K3AWP8
A	4182	ASN	-	expression tag	UNP A0A0K3AWP8
A	4183	GLY	-	expression tag	UNP A0A0K3AWP8
A	4184	ILE	-	expression tag	UNP A0A0K3AWP8
A	4185	LYS	-	expression tag	UNP A0A0K3AWP8
A	4186	ALA	-	expression tag	UNP A0A0K3AWP8
A	4187	ASN	-	expression tag	UNP A0A0K3AWP8
A	4188	PHE	-	expression tag	UNP A0A0K3AWP8
A	4189	LYS	-	expression tag	UNP A0A0K3AWP8
A	4190	ILE	-	expression tag	UNP A0A0K3AWP8
A	4191	ARG	-	expression tag	UNP A0A0K3AWP8
A	4192	HIS	-	expression tag	UNP A0A0K3AWP8
A	4193	ASN	-	expression tag	UNP A0A0K3AWP8
A	4194	ILE	-	expression tag	UNP A0A0K3AWP8
A	4195	GLU	-	expression tag	UNP A0A0K3AWP8
A	4196	ASP	-	expression tag	UNP A0A0K3AWP8
A	4197	GLY	-	expression tag	UNP A0A0K3AWP8
A	4198	GLY	-	expression tag	UNP A0A0K3AWP8
A	4199	VAL	-	expression tag	UNP A0A0K3AWP8
A	4200	GLN	-	expression tag	UNP A0A0K3AWP8
A	4201	LEU	-	expression tag	UNP A0A0K3AWP8
A	4202	ALA	-	expression tag	UNP A0A0K3AWP8
A	4203	ASP	-	expression tag	UNP A0A0K3AWP8
A	4204	HIS	-	expression tag	UNP A0A0K3AWP8
A	4205	TYR	-	expression tag	UNP A0A0K3AWP8
A	4206	GLN	-	expression tag	UNP A0A0K3AWP8
A	4207	GLN	-	expression tag	UNP A0A0K3AWP8
A	4208	ASN	-	expression tag	UNP A0A0K3AWP8
A	4209	THR	-	expression tag	UNP A0A0K3AWP8
A	4210	PRO	-	expression tag	UNP A0A0K3AWP8
A	4211	ILE	-	expression tag	UNP A0A0K3AWP8
A	4212	GLY	-	expression tag	UNP A0A0K3AWP8
A	4213	ASP	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4214	GLY	-	expression tag	UNP A0A0K3AWP8
A	4215	PRO	-	expression tag	UNP A0A0K3AWP8
A	4216	VAL	-	expression tag	UNP A0A0K3AWP8
A	4217	LEU	-	expression tag	UNP A0A0K3AWP8
A	4218	LEU	-	expression tag	UNP A0A0K3AWP8
A	4219	PRO	-	expression tag	UNP A0A0K3AWP8
A	4220	ASP	-	expression tag	UNP A0A0K3AWP8
A	4221	ASN	-	expression tag	UNP A0A0K3AWP8
A	4222	HIS	-	expression tag	UNP A0A0K3AWP8
A	4223	TYR	-	expression tag	UNP A0A0K3AWP8
A	4224	LEU	-	expression tag	UNP A0A0K3AWP8
A	4225	SER	-	expression tag	UNP A0A0K3AWP8
A	4226	TYR	-	expression tag	UNP A0A0K3AWP8
A	4227	GLN	-	expression tag	UNP A0A0K3AWP8
A	4228	SER	-	expression tag	UNP A0A0K3AWP8
A	4229	LYS	-	expression tag	UNP A0A0K3AWP8
A	4230	LEU	-	expression tag	UNP A0A0K3AWP8
A	4231	SER	-	expression tag	UNP A0A0K3AWP8
A	4232	LYS	-	expression tag	UNP A0A0K3AWP8
A	4233	ASP	-	expression tag	UNP A0A0K3AWP8
A	4234	PRO	-	expression tag	UNP A0A0K3AWP8
A	4235	ASN	-	expression tag	UNP A0A0K3AWP8
A	4236	GLU	-	expression tag	UNP A0A0K3AWP8
A	4237	LYS	-	expression tag	UNP A0A0K3AWP8
A	4238	ARG	-	expression tag	UNP A0A0K3AWP8
A	4239	ASP	-	expression tag	UNP A0A0K3AWP8
A	4240	HIS	-	expression tag	UNP A0A0K3AWP8
A	4241	MET	-	expression tag	UNP A0A0K3AWP8
A	4242	VAL	-	expression tag	UNP A0A0K3AWP8
A	4243	LEU	-	expression tag	UNP A0A0K3AWP8
A	4244	LEU	-	expression tag	UNP A0A0K3AWP8
A	4245	GLU	-	expression tag	UNP A0A0K3AWP8
A	4246	PHE	-	expression tag	UNP A0A0K3AWP8
A	4247	VAL	-	expression tag	UNP A0A0K3AWP8
A	4248	THR	-	expression tag	UNP A0A0K3AWP8
A	4249	ALA	-	expression tag	UNP A0A0K3AWP8
A	4250	ALA	-	expression tag	UNP A0A0K3AWP8
A	4251	GLY	-	expression tag	UNP A0A0K3AWP8
A	4252	ILE	-	expression tag	UNP A0A0K3AWP8
A	4253	THR	-	expression tag	UNP A0A0K3AWP8
A	4254	LEU	-	expression tag	UNP A0A0K3AWP8
A	4255	GLY	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4256	MET	-	expression tag	UNP A0A0K3AWP8
A	4257	ASP	-	expression tag	UNP A0A0K3AWP8
A	4258	GLU	-	expression tag	UNP A0A0K3AWP8
A	4259	LEU	-	expression tag	UNP A0A0K3AWP8
A	4260	TYR	-	expression tag	UNP A0A0K3AWP8
A	4261	LYS	-	expression tag	UNP A0A0K3AWP8
A	4262	GLY	-	expression tag	UNP A0A0K3AWP8
A	4263	SER	-	expression tag	UNP A0A0K3AWP8
A	4264	GLY	-	expression tag	UNP A0A0K3AWP8
A	4265	LEU	-	expression tag	UNP A0A0K3AWP8
A	4266	GLU	-	expression tag	UNP A0A0K3AWP8
A	4267	VAL	-	expression tag	UNP A0A0K3AWP8
A	4268	LEU	-	expression tag	UNP A0A0K3AWP8
A	4269	PHE	-	expression tag	UNP A0A0K3AWP8
A	4270	GLN	-	expression tag	UNP A0A0K3AWP8
A	4271	GLY	-	expression tag	UNP A0A0K3AWP8
A	4272	PRO	-	expression tag	UNP A0A0K3AWP8
A	4273	ALA	-	expression tag	UNP A0A0K3AWP8
A	4274	ASN	-	expression tag	UNP A0A0K3AWP8
A	4275	SER	-	expression tag	UNP A0A0K3AWP8
A	4276	GLY	-	expression tag	UNP A0A0K3AWP8
A	4277	VAL	-	expression tag	UNP A0A0K3AWP8
A	4278	ASP	-	expression tag	UNP A0A0K3AWP8
A	4279	TYR	-	expression tag	UNP A0A0K3AWP8
A	4280	LYS	-	expression tag	UNP A0A0K3AWP8
A	4281	ASP	-	expression tag	UNP A0A0K3AWP8
A	4282	HIS	-	expression tag	UNP A0A0K3AWP8
A	4283	ASP	-	expression tag	UNP A0A0K3AWP8
A	4284	GLY	-	expression tag	UNP A0A0K3AWP8
A	4285	ASP	-	expression tag	UNP A0A0K3AWP8
A	4286	TYR	-	expression tag	UNP A0A0K3AWP8
A	4287	LYS	-	expression tag	UNP A0A0K3AWP8
A	4288	ASP	-	expression tag	UNP A0A0K3AWP8
A	4289	HIS	-	expression tag	UNP A0A0K3AWP8
A	4290	ASP	-	expression tag	UNP A0A0K3AWP8
A	4291	ILE	-	expression tag	UNP A0A0K3AWP8
A	4292	ASP	-	expression tag	UNP A0A0K3AWP8
A	4293	TYR	-	expression tag	UNP A0A0K3AWP8
A	4294	LYS	-	expression tag	UNP A0A0K3AWP8
A	4295	ASP	-	expression tag	UNP A0A0K3AWP8
A	4296	ASP	-	expression tag	UNP A0A0K3AWP8
A	4297	ASP	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4298	ASP	-	expression tag	UNP A0A0K3AWP8
A	4299	LYS	-	expression tag	UNP A0A0K3AWP8

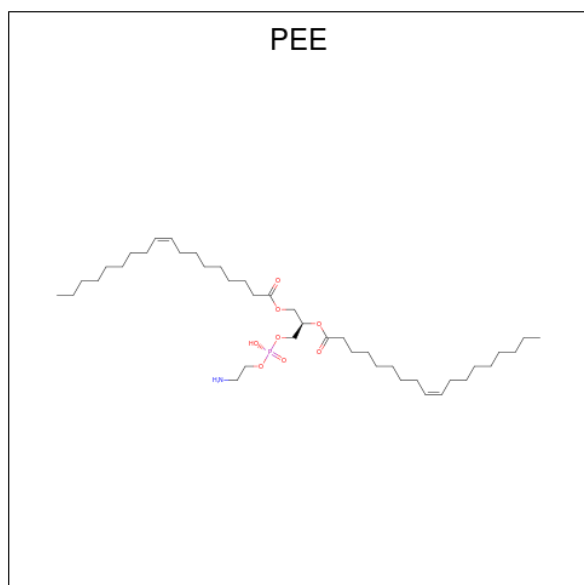
- Molecule 2 is a protein called Defect at low temperature protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	181	Total	C	N	O	S	0	0
			1479	935	276	262	6		

- Molecule 3 is a protein called Vesicle transport protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	117	Total	C	N	O	S	0	0
			922	626	137	149	10		

- Molecule 4 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



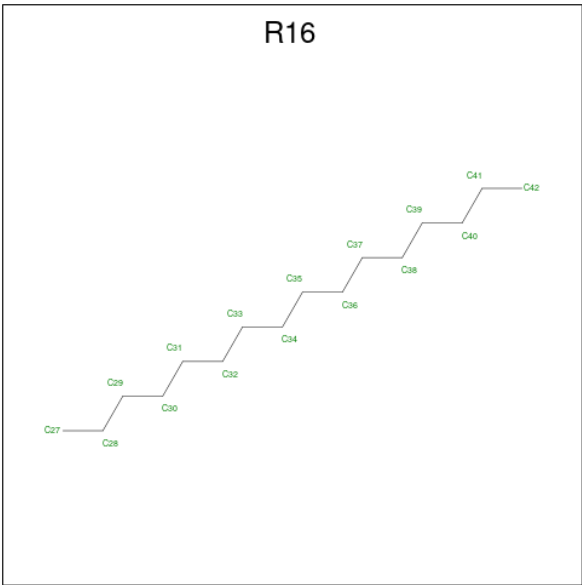
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
4	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	

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Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
4	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
4	A	1	Total	C	N	O	P	0
			30	20	1	8	1	
4	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
4	A	1	Total	C	N	O	P	0
			39	29	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
4	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
4	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
4	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
4	A	1	Total	C	N	O	P	0
			28	18	1	8	1	
4	A	1	Total	C	N	O	P	0
			27	17	1	8	1	
4	C	1	Total	C	N	O	P	0
			34	24	1	8	1	

- Molecule 5 is HEXADECANE (CCD ID: R16) (formula: C₁₆H₃₄).



Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			10	10	
5	A	1	Total	C	0
			16	16	
5	A	1	Total	C	0
			16	16	
5	A	1	Total	C	0
			16	16	
5	A	1	Total	C	0
			16	16	
5	A	1	Total	C	0
			13	13	
5	A	1	Total	C	0
			11	11	
5	A	1	Total	C	0
			16	16	
5	A	1	Total	C	0
			10	10	
5	C	1	Total	C	0
			13	13	
5	C	1	Total	C	0
			12	12	

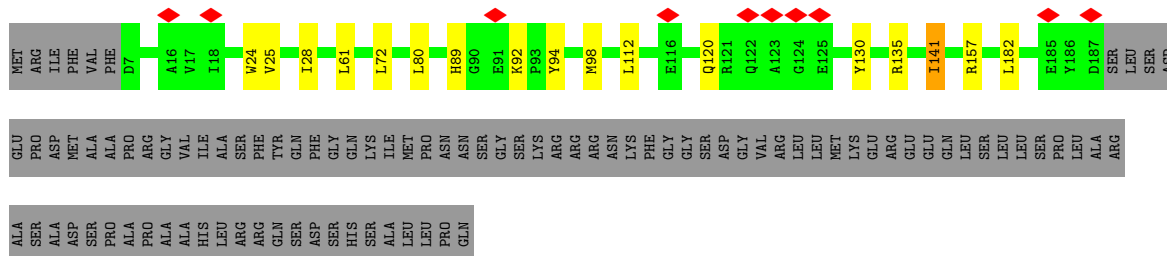




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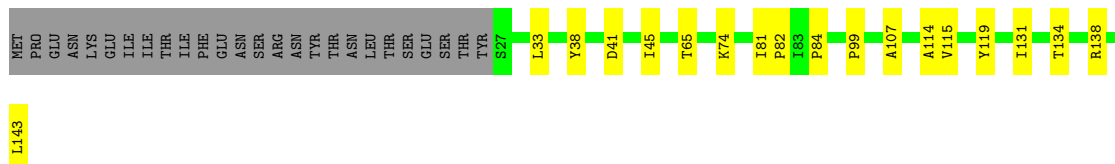
- Molecule 2: Defect at low temperature protein 1

Chain B:  59% 6% 34%



- Molecule 3: Vesicle transport protein

Chain C:  69% 13% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	285377	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.712	Depositor
Minimum map value	-0.310	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	595.72797, 595.72797, 595.72797	wwPDB
Map dimensions	756, 756, 756	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.7879999, 0.7879999, 0.7879999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEE, R16

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	0.16	0/11702	0.26	0/15874
2	B	0.11	0/1502	0.21	0/2028
3	C	0.12	0/949	0.26	0/1293
All	All	0.15	0/14153	0.26	0/19195

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	11425	0	11342	131	0
2	B	1479	0	1531	11	0
3	C	922	0	969	12	0
4	A	680	0	960	40	0
4	C	34	0	42	0	0
5	A	140	0	288	10	0
5	C	25	0	48	0	0
All	All	14705	0	15180	171	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 6.

The worst 5 of 171 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:40:VAL:HG13	1:A:41:LEU:HG	1.65	0.79
5:A:4306:R16:H291	4:A:4319:PEE:H22	1.77	0.67
4:A:4305:PEE:H50	4:A:4320:PEE:H19	1.77	0.67
1:A:1090:VAL:HG12	1:A:1091:MET:HG2	1.77	0.66
1:A:714:ASP:HB3	1:A:717:LYS:HG2	1.78	0.65

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	1414/4299 (33%)	1383 (98%)	31 (2%)	0	100	100
2	B	179/276 (65%)	177 (99%)	2 (1%)	0	100	100
3	C	115/143 (80%)	112 (97%)	3 (3%)	0	100	100
All	All	1708/4718 (36%)	1672 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	1265/3801 (33%)	1257 (99%)	8 (1%)	78	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	164/243 (68%)	162 (99%)	2 (1%)	63	84
3	C	102/128 (80%)	101 (99%)	1 (1%)	68	86
All	All	1531/4172 (37%)	1520 (99%)	11 (1%)	73	90

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1637	LEU
2	B	61	LEU
3	C	33	LEU
2	B	141	ILE
1	A	952	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	468	ASN
1	A	559	GLN
1	A	866	HIS
1	A	863	HIS
1	A	160	ASN

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](#)

30 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$
5	R16	C	202	-	12,12,15	0.23	0	11,11,14	0.21	0
4	PEE	A	4320	-	44,44,50	0.94	2 (4%)	47,49,55	0.70	1 (2%)
4	PEE	A	4312	-	35,35,50	0.84	1 (2%)	38,40,55	0.63	0
4	PEE	A	4327	-	26,26,50	0.68	0	29,31,55	0.55	0
4	PEE	A	4326	-	27,27,50	0.65	0	30,32,55	0.61	1 (3%)
4	PEE	A	4311	-	29,29,50	0.62	0	32,34,55	0.56	0
4	PEE	A	4313	-	38,38,50	0.82	1 (2%)	41,43,55	0.63	0
4	PEE	A	4322	-	30,30,50	0.62	0	33,35,55	0.51	0
5	R16	A	4317	-	10,10,15	0.23	0	9,9,14	0.19	0
4	PEE	A	4301	-	49,49,50	0.90	2 (4%)	52,54,55	0.61	0
4	PEE	A	4305	-	36,36,50	0.94	2 (5%)	39,41,55	0.87	3 (7%)
5	R16	A	4307	-	15,15,15	0.22	0	14,14,14	0.19	0
4	PEE	A	4303	-	50,50,50	0.90	2 (4%)	53,55,55	0.62	0
5	R16	A	4306	-	9,9,15	0.21	0	8,8,14	0.24	0
4	PEE	A	4319	-	50,50,50	0.89	2 (4%)	53,55,55	0.62	0
4	PEE	A	4302	-	34,34,50	0.81	1 (2%)	37,39,55	0.73	1 (2%)
5	R16	A	4314	-	15,15,15	0.21	0	14,14,14	0.21	0
4	PEE	A	4304	-	50,50,50	0.89	2 (4%)	53,55,55	0.62	0
5	R16	A	4315	-	15,15,15	0.22	0	14,14,14	0.22	0
5	R16	C	203	-	11,11,15	0.23	0	10,10,14	0.19	0
4	PEE	A	4324	-	44,44,50	0.95	2 (4%)	47,49,55	0.67	1 (2%)
5	R16	A	4323	-	15,15,15	0.21	0	14,14,14	0.24	0
4	PEE	C	201	-	33,33,50	0.88	1 (3%)	36,38,55	0.70	1 (2%)
5	R16	A	4316	-	12,12,15	0.21	0	11,11,14	0.24	0
5	R16	A	4309	-	15,15,15	0.22	0	14,14,14	0.19	0
5	R16	A	4308	-	15,15,15	0.23	0	14,14,14	0.20	0
5	R16	A	4325	-	9,9,15	0.24	0	8,8,14	0.18	0
4	PEE	A	4321	-	43,43,50	0.92	2 (4%)	46,48,55	0.70	1 (2%)
4	PEE	A	4310	-	28,28,50	0.65	0	31,33,55	0.56	0
4	PEE	A	4318	-	50,50,50	0.90	2 (4%)	53,55,55	0.61	0

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
5	R16	C	202	-	-	0/10/10/13	-
4	PEE	A	4320	-	-	16/48/48/54	-
4	PEE	A	4312	-	-	8/39/39/54	-
4	PEE	A	4327	-	-	8/30/30/54	-
4	PEE	A	4326	-	-	12/31/31/54	-
4	PEE	A	4311	-	-	11/33/33/54	-
4	PEE	A	4313	-	-	18/42/42/54	-
4	PEE	A	4322	-	-	16/34/34/54	-
5	R16	A	4317	-	-	0/8/8/13	-
4	PEE	A	4301	-	-	16/53/53/54	-
4	PEE	A	4305	-	-	17/40/40/54	-
5	R16	A	4307	-	-	5/13/13/13	-
4	PEE	A	4303	-	-	22/54/54/54	-
5	R16	A	4306	-	-	2/7/7/13	-
4	PEE	A	4319	-	-	25/54/54/54	-
4	PEE	A	4302	-	-	18/38/38/54	-
5	R16	A	4314	-	-	4/13/13/13	-
4	PEE	A	4304	-	-	21/54/54/54	-
5	R16	A	4315	-	-	3/13/13/13	-
5	R16	C	203	-	-	1/9/9/13	-
4	PEE	A	4324	-	-	12/48/48/54	-
5	R16	A	4323	-	-	4/13/13/13	-
4	PEE	C	201	-	-	10/37/37/54	-
5	R16	A	4316	-	-	3/10/10/13	-
5	R16	A	4309	-	-	6/13/13/13	-
5	R16	A	4308	-	-	1/13/13/13	-
5	R16	A	4325	-	-	0/7/7/13	-
4	PEE	A	4321	-	-	15/47/47/54	-
4	PEE	A	4310	-	-	6/32/32/54	-
4	PEE	A	4318	-	-	23/54/54/54	-

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	4303	PEE	C18-C19	3.74	1.53	1.31
4	A	4318	PEE	C39-C38	3.73	1.52	1.31
4	C	201	PEE	C39-C38	3.71	1.52	1.31
4	A	4321	PEE	C18-C19	3.70	1.52	1.31
4	A	4324	PEE	C18-C19	3.70	1.52	1.31

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	PEE	C40-C39-C38	-2.35	112.31	126.42
4	A	4302	PEE	C17-C18-C19	-2.31	112.99	130.48
4	A	4305	PEE	C17-C18-C19	-2.24	113.49	130.48
4	A	4320	PEE	C20-C19-C18	-2.24	112.93	126.42
4	A	4324	PEE	C20-C19-C18	-2.23	113.03	126.42

There are no chirality outliers.

5 of 303 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4301	PEE	C11-C10-O2-C2
4	A	4301	PEE	O4-C10-O2-C2
4	A	4301	PEE	C1-O3P-P-O2P
4	A	4302	PEE	C1-O3P-P-O1P
4	A	4302	PEE	C1-O3P-P-O4P

There are no ring outliers.

19 monomers are involved in 44 short contacts:

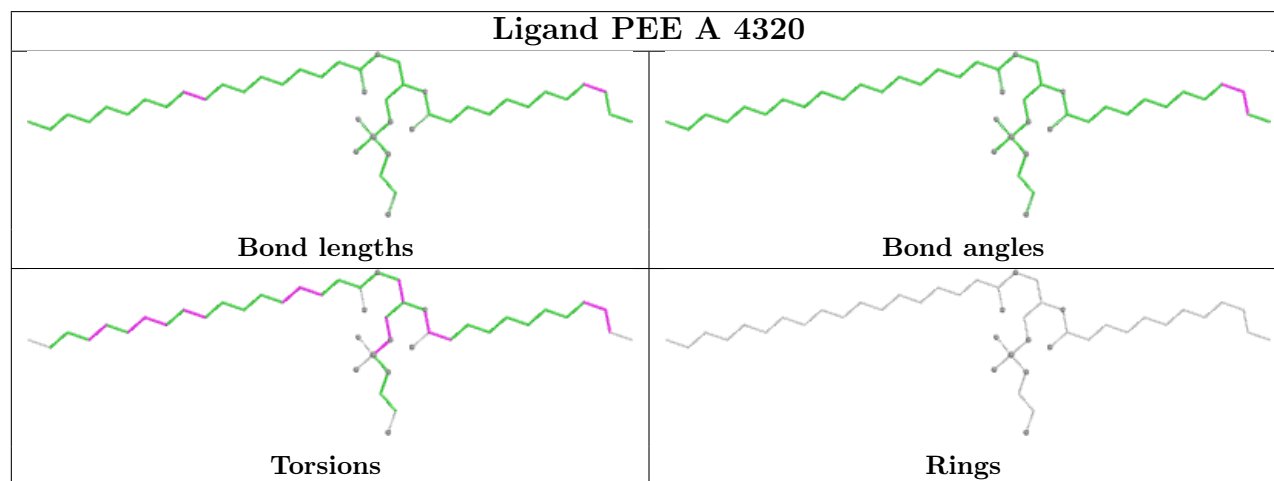
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4320	PEE	6	0
4	A	4312	PEE	3	0
4	A	4327	PEE	3	0
4	A	4311	PEE	1	0
4	A	4313	PEE	1	0
4	A	4301	PEE	5	0
4	A	4305	PEE	5	0
5	A	4307	R16	4	0
4	A	4303	PEE	1	0
5	A	4306	R16	4	0
4	A	4319	PEE	11	0
4	A	4302	PEE	2	0
5	A	4314	R16	1	0

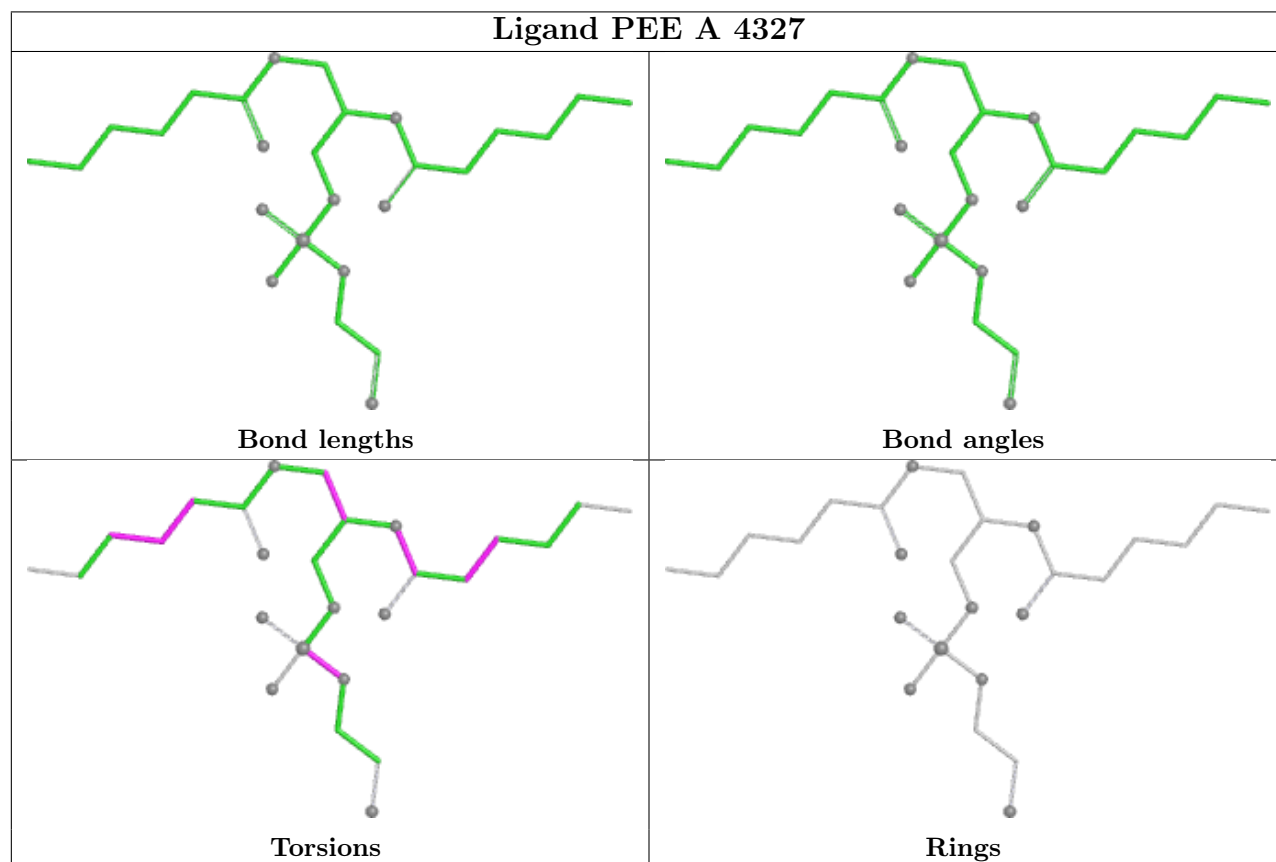
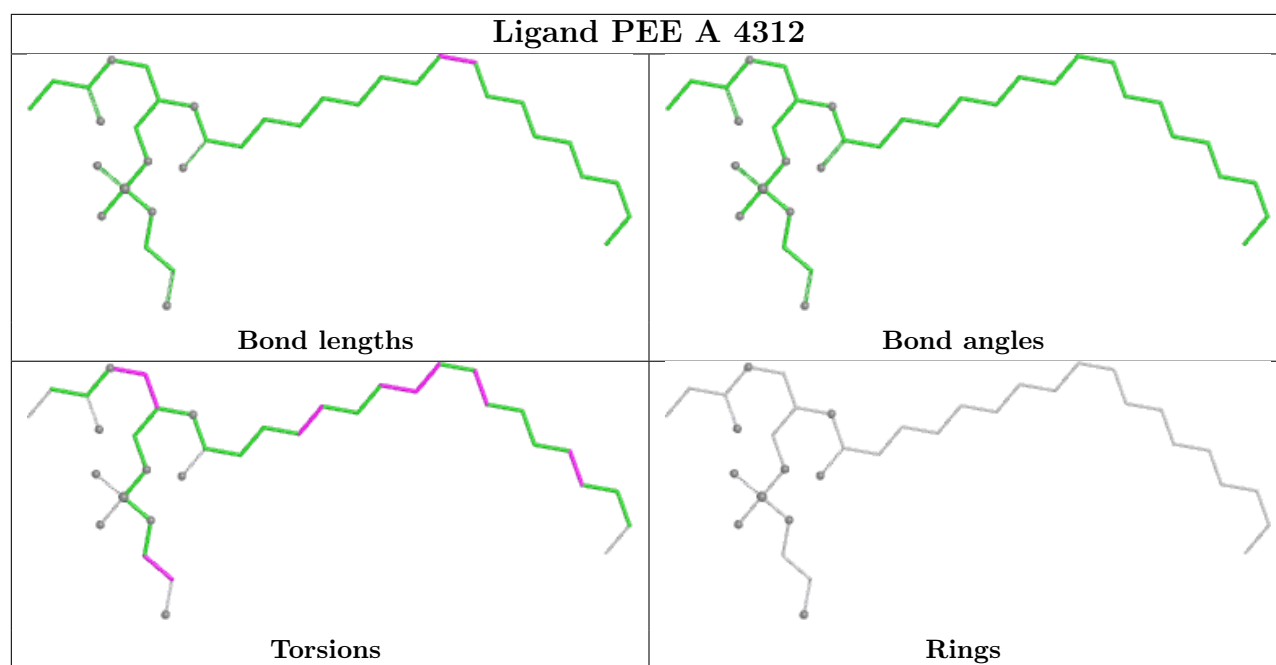
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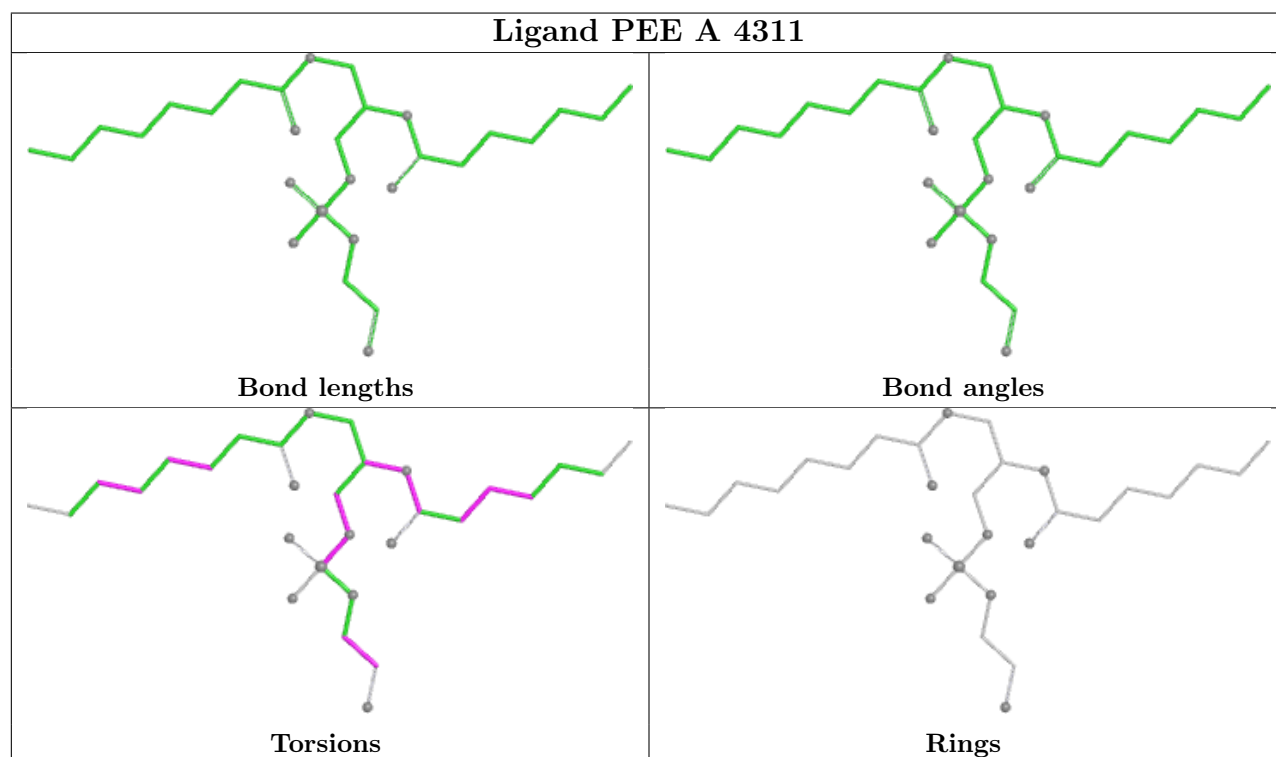
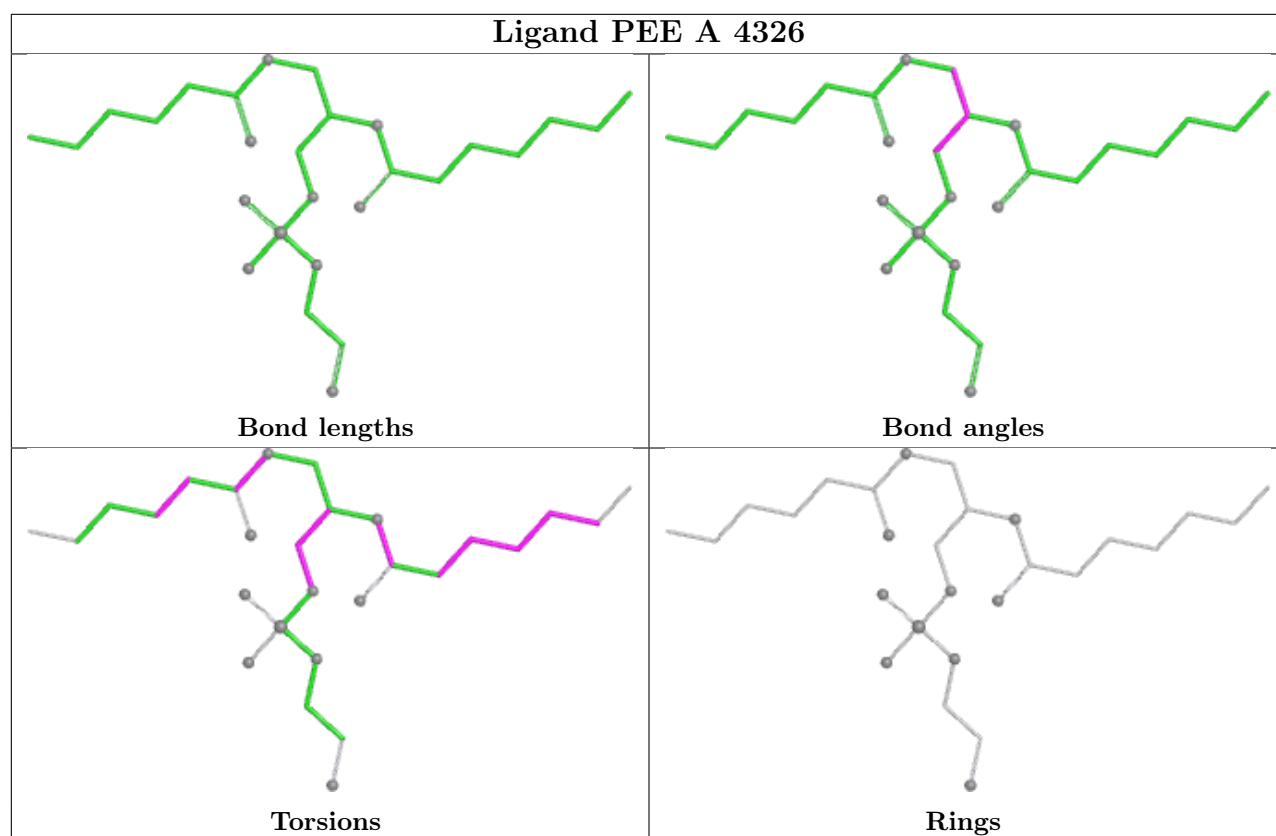
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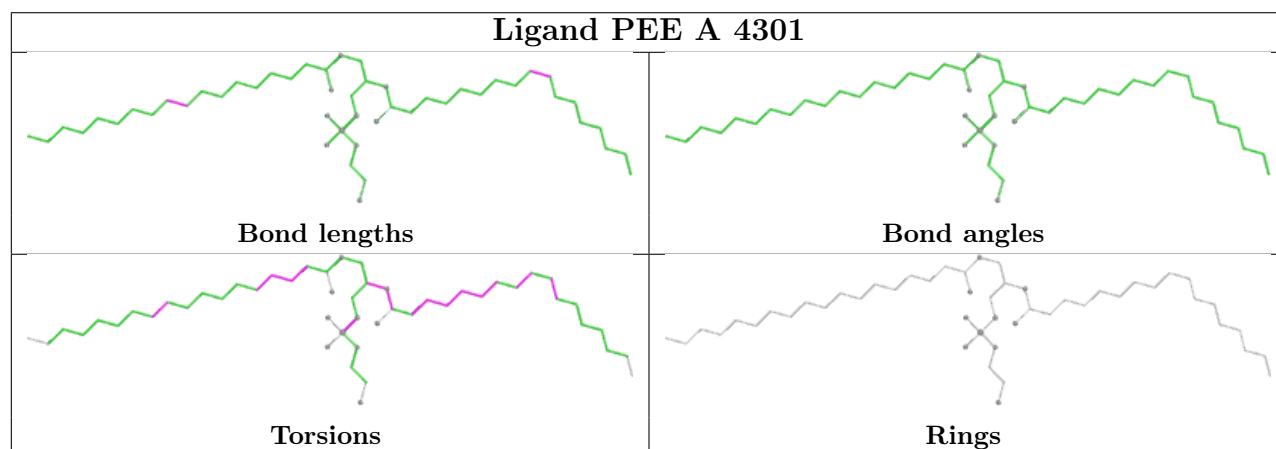
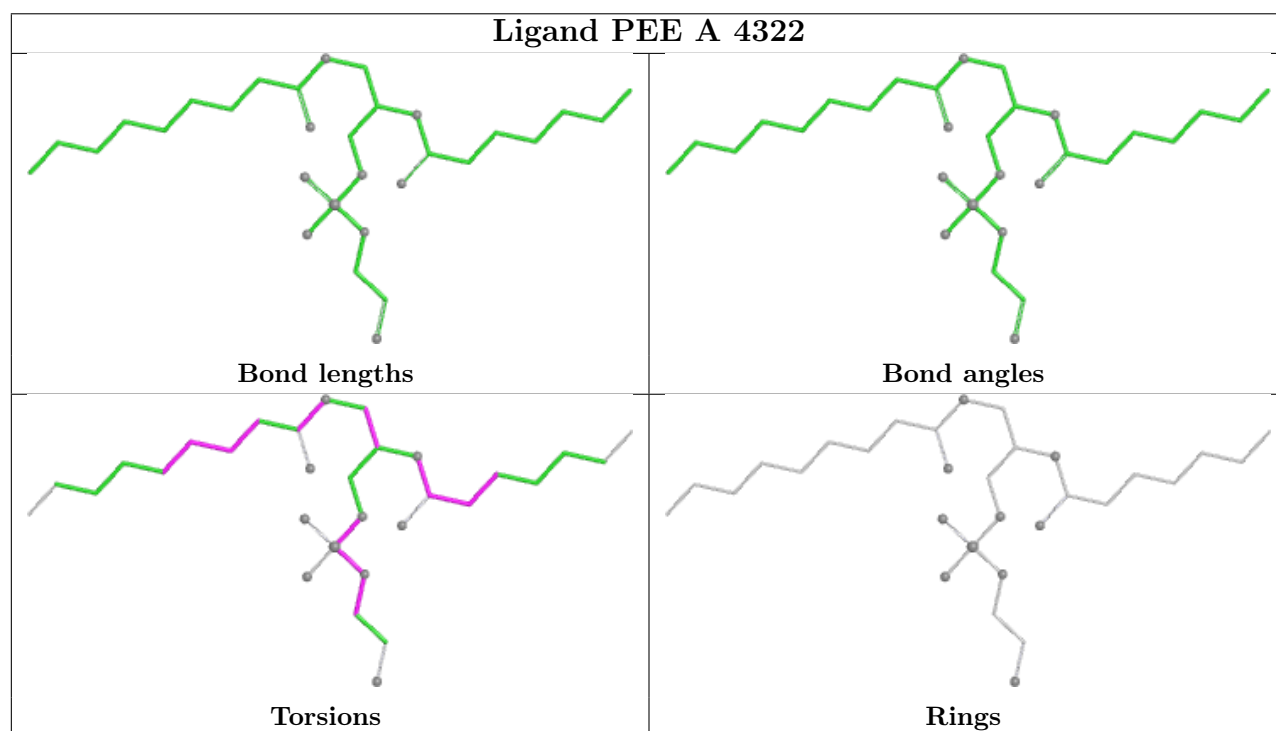
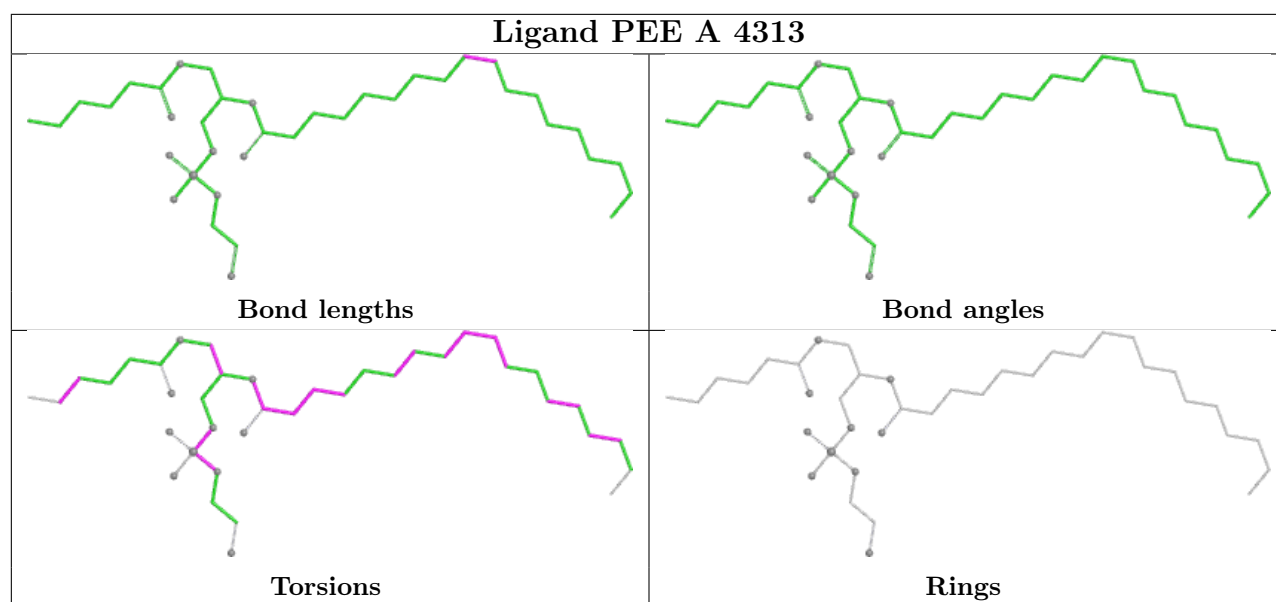
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4304	PEE	2	0
4	A	4324	PEE	1	0
5	A	4309	R16	1	0
5	A	4308	R16	1	0
4	A	4321	PEE	1	0
4	A	4318	PEE	7	0

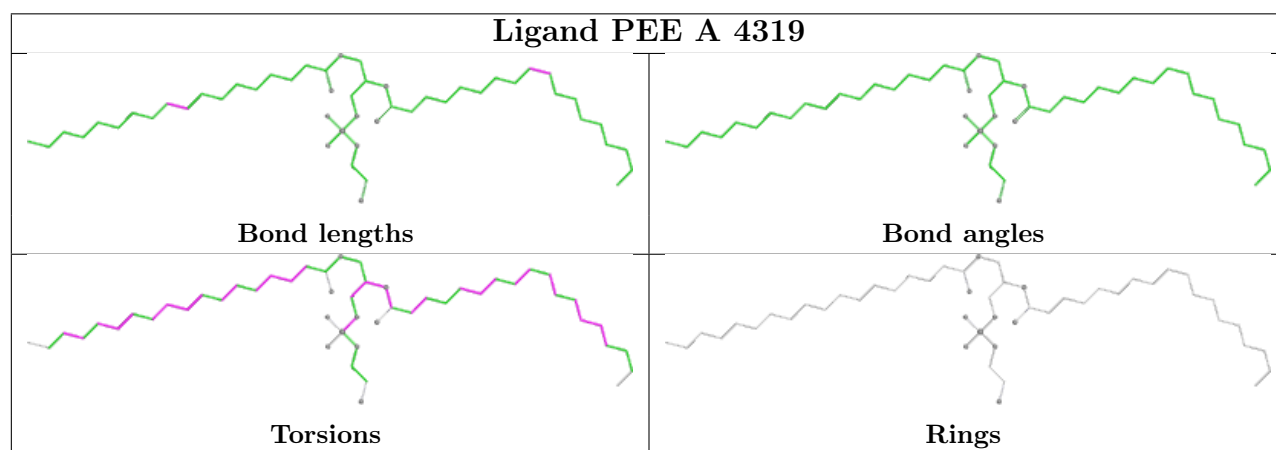
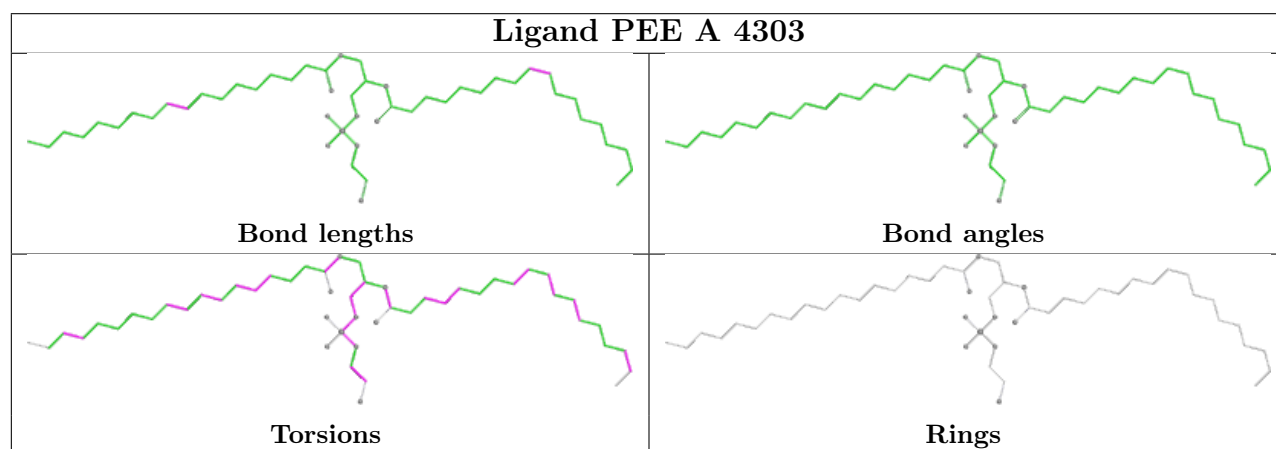
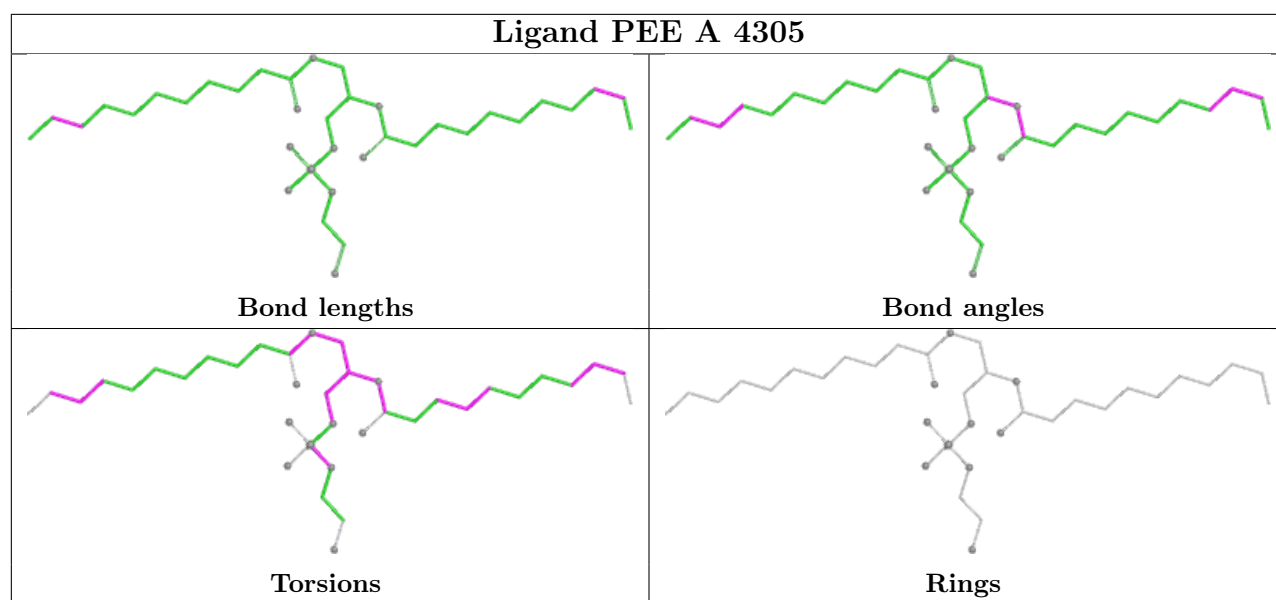
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

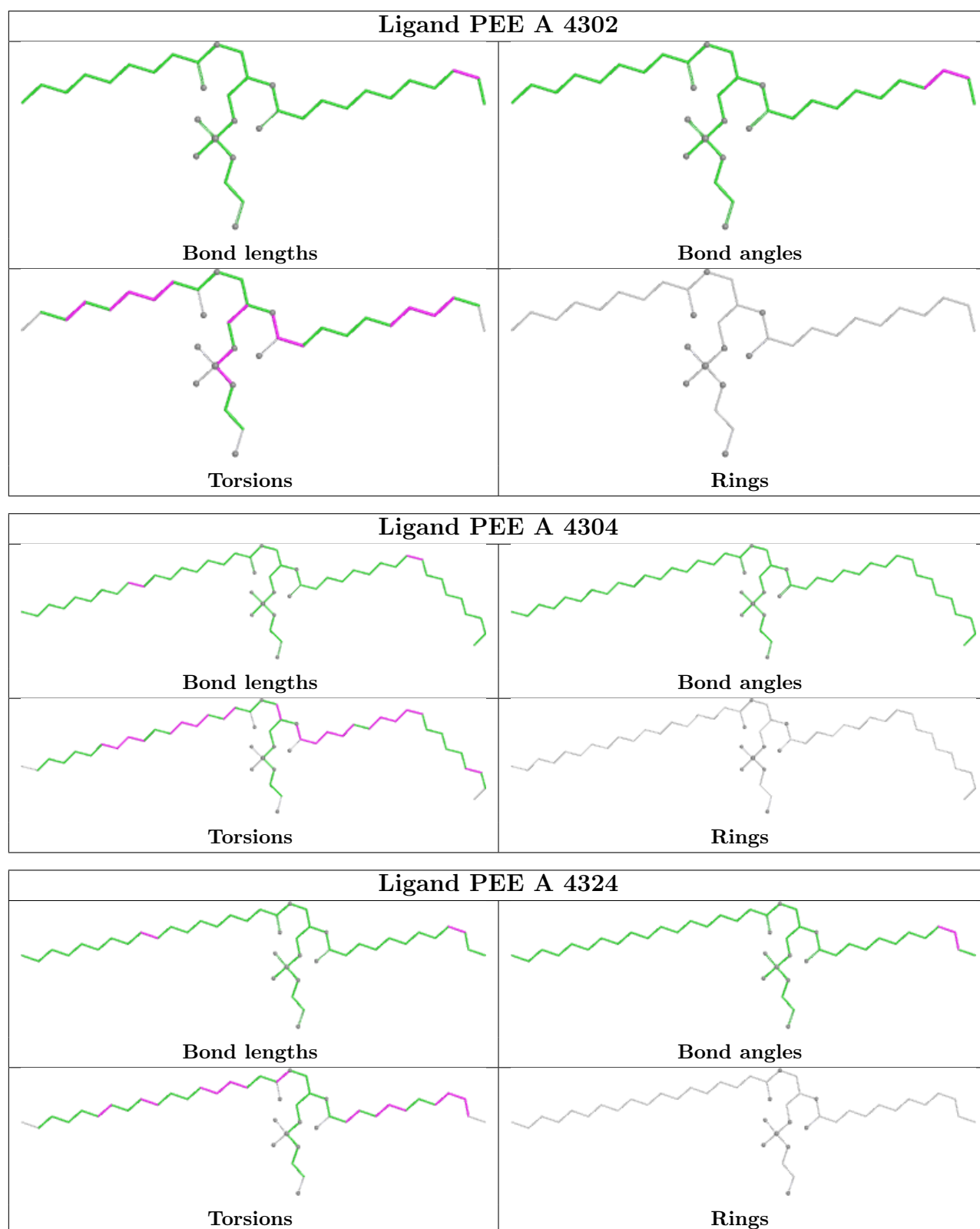


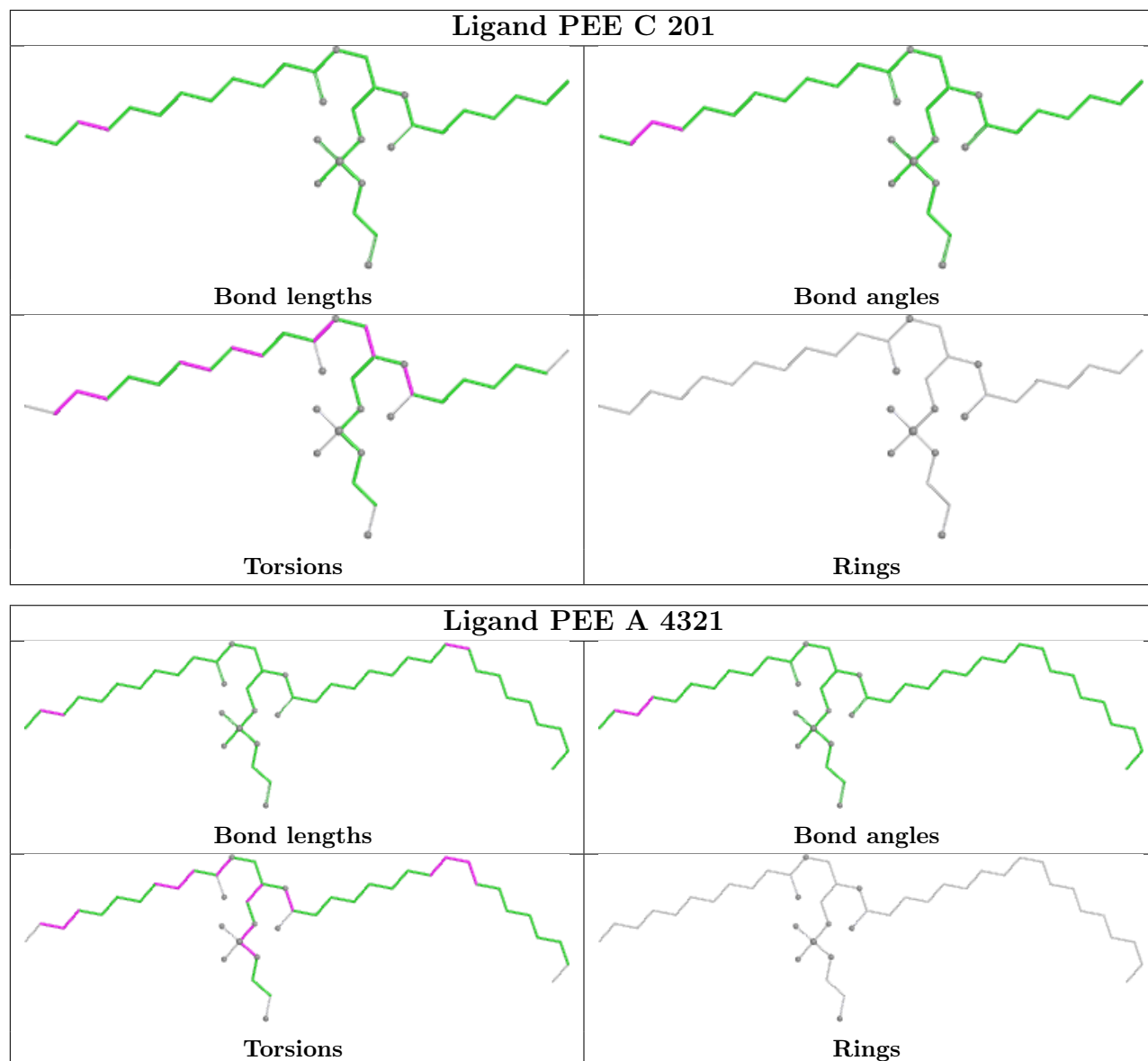


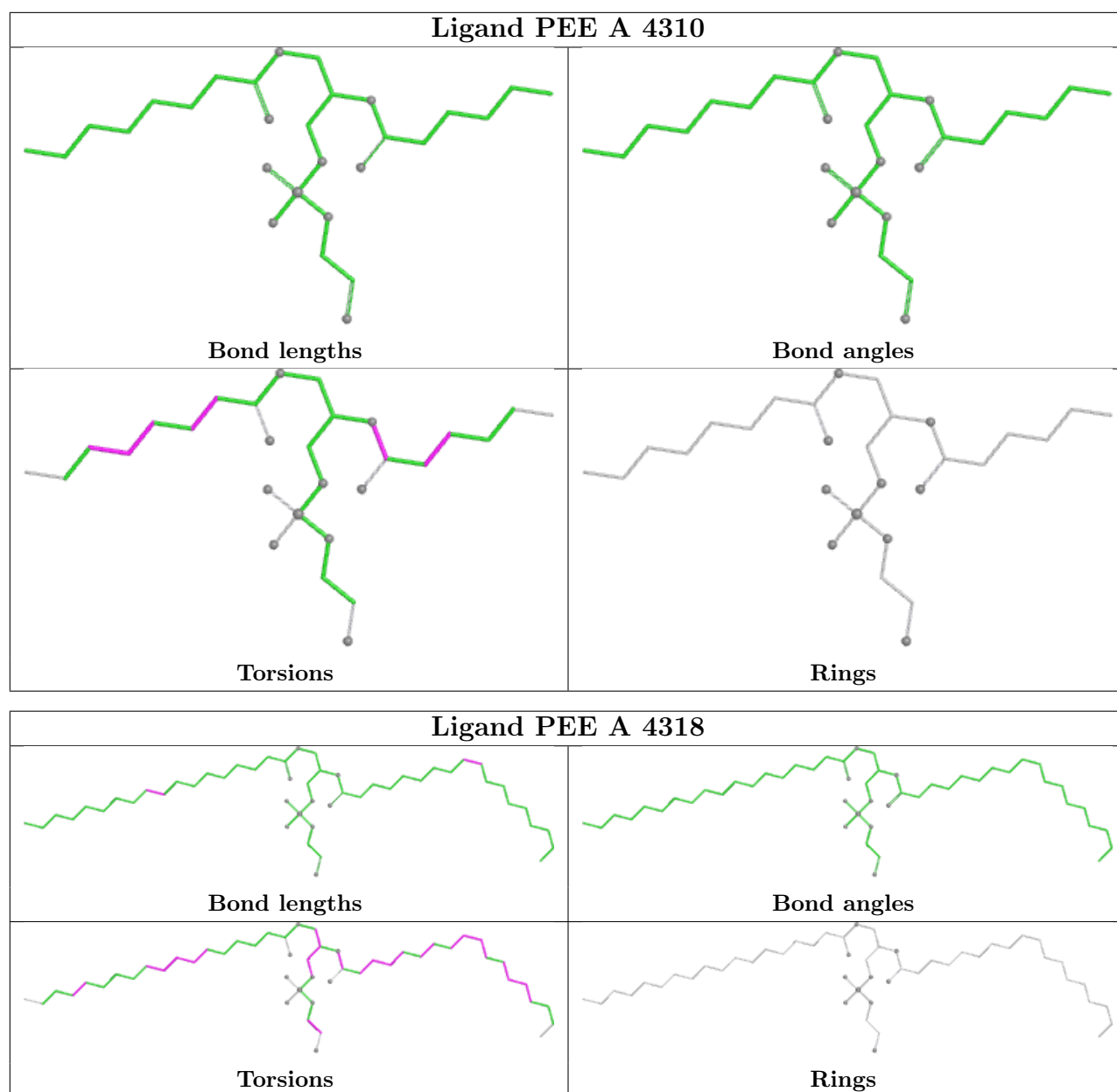












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

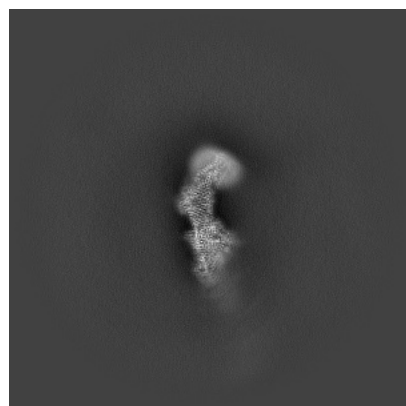
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45399. These allow visual inspection of the internal detail of the map and identification of artifacts.

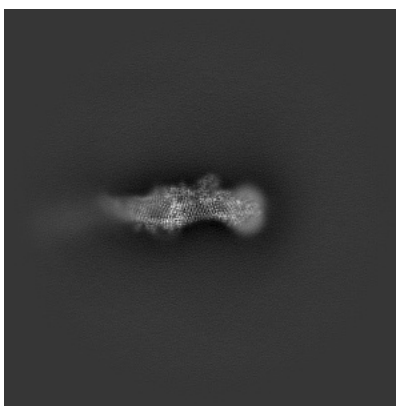
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

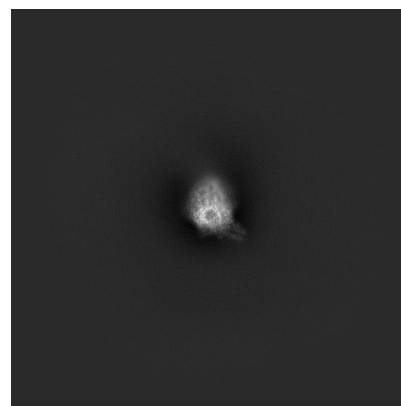
6.1.1 Primary map



X



Y

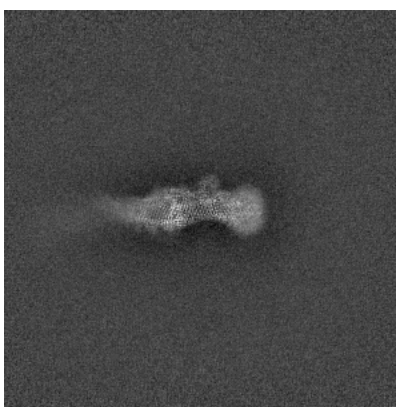


Z

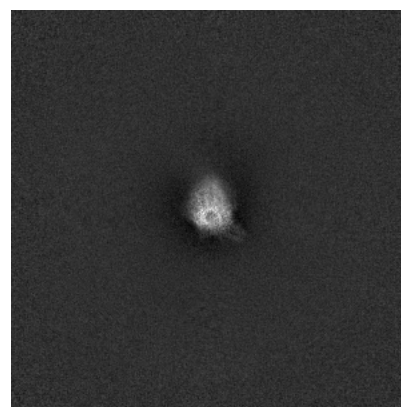
6.1.2 Raw map



X



Y



Z

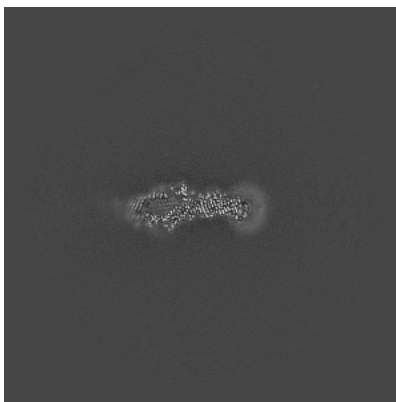
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

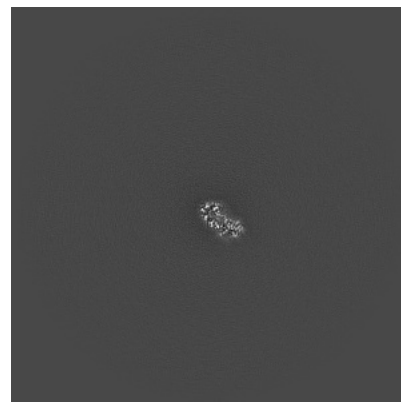
6.2.1 Primary map



X Index: 378



Y Index: 378

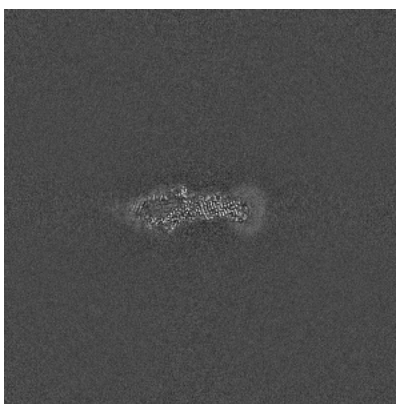


Z Index: 378

6.2.2 Raw map



X Index: 378



Y Index: 378

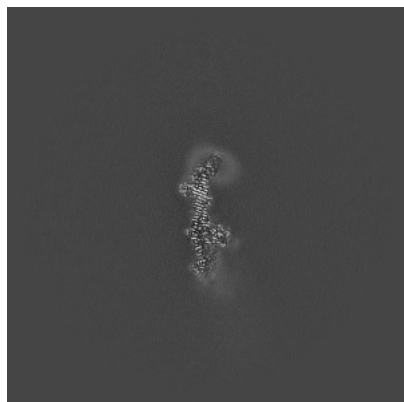


Z Index: 378

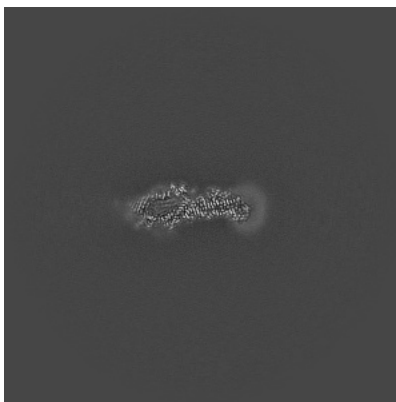
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

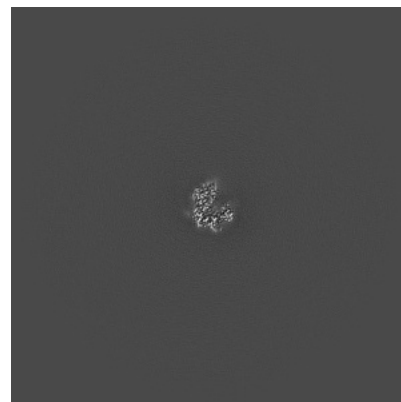
6.3.1 Primary map



X Index: 365

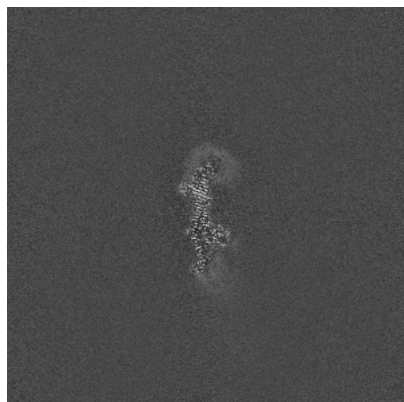


Y Index: 375

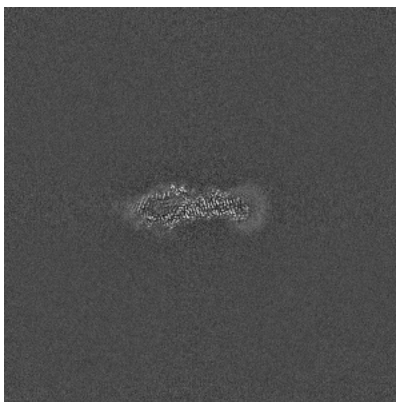


Z Index: 328

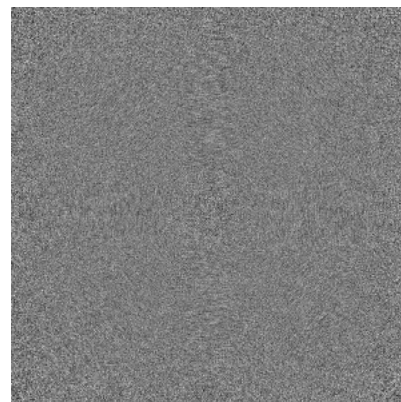
6.3.2 Raw map



X Index: 365



Y Index: 375



Z Index: 0

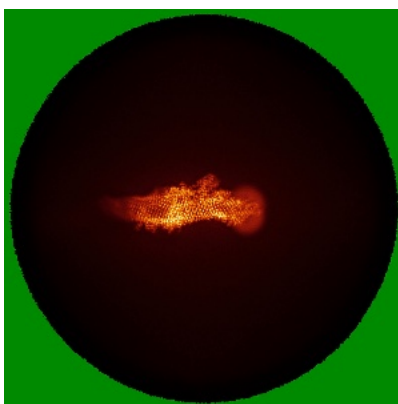
The images above show the largest variance slices of the map in three orthogonal directions.

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

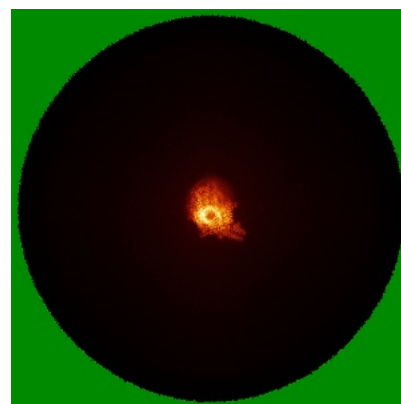
6.4.1 Primary map



X



Y

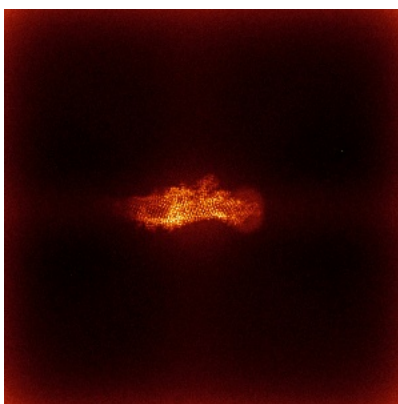


Z

6.4.2 Raw map



X



Y

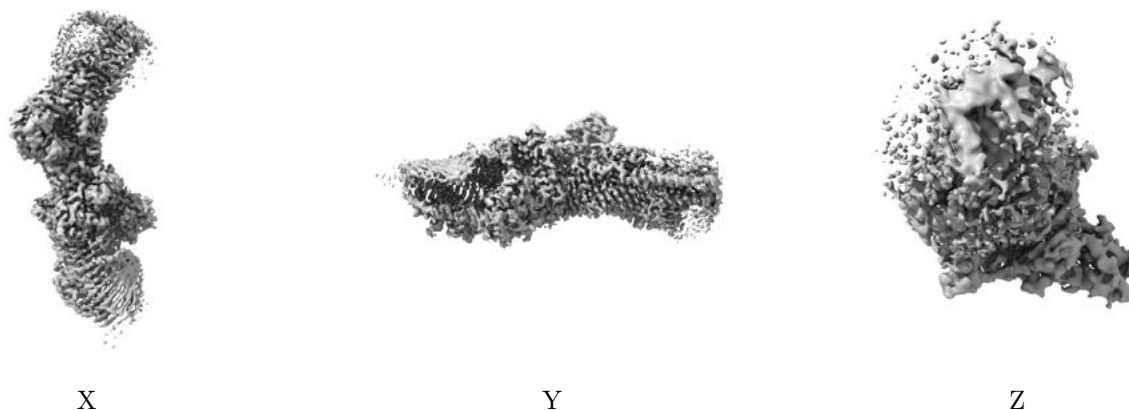


Z

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 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

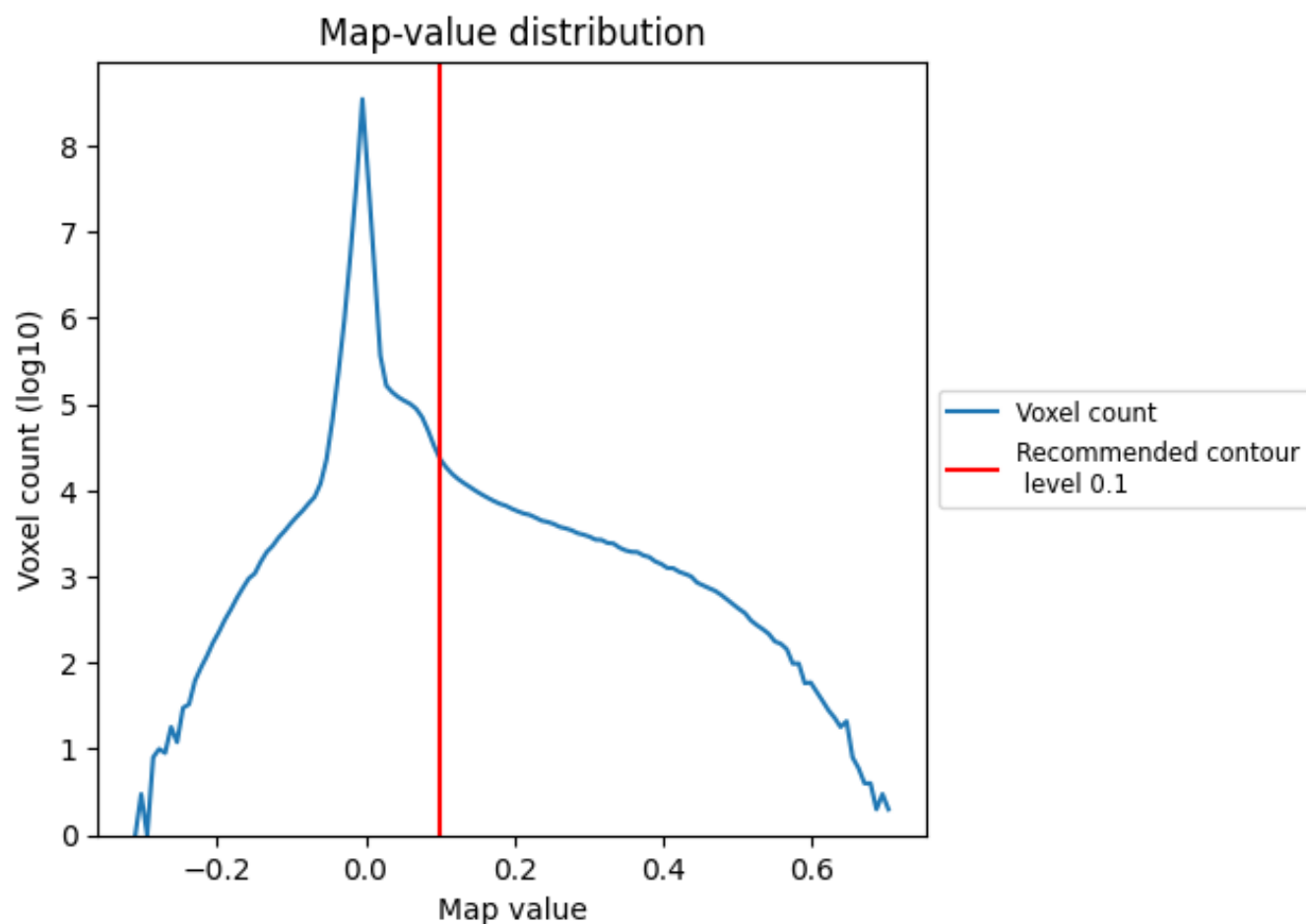
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

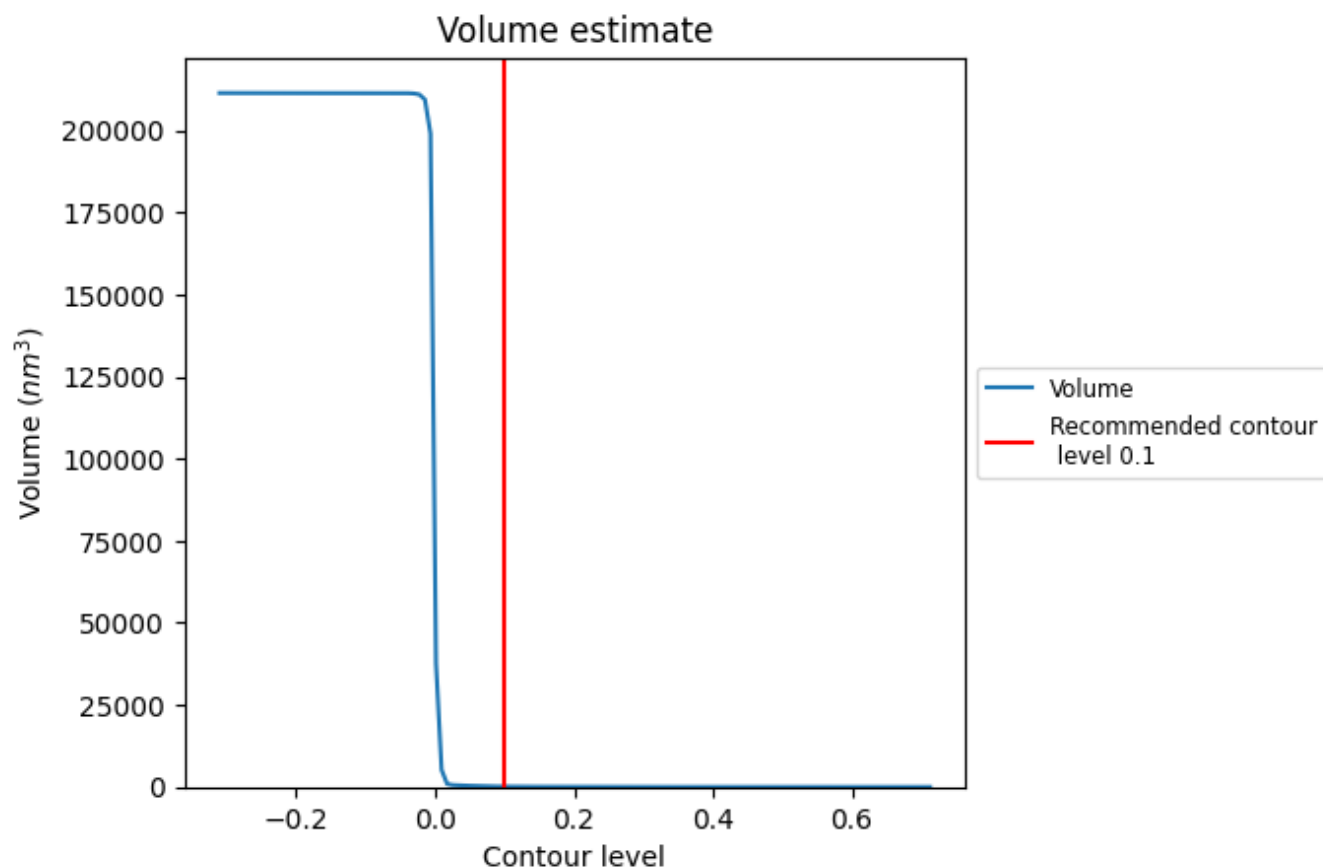
This section contains the results of statistical analysis of the map.

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.

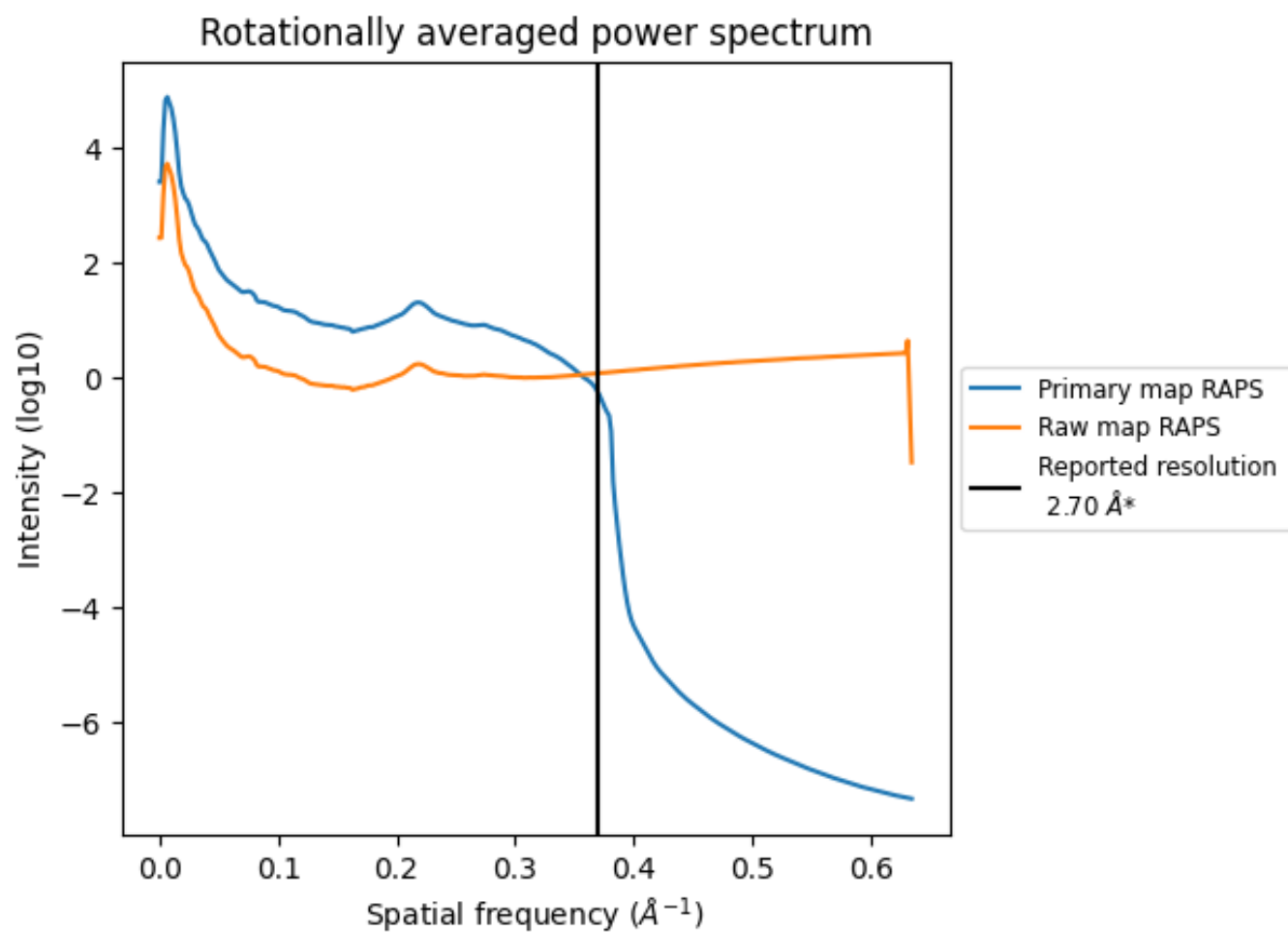
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm^3 ; this corresponds to an approximate mass of 107 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 ⓘ

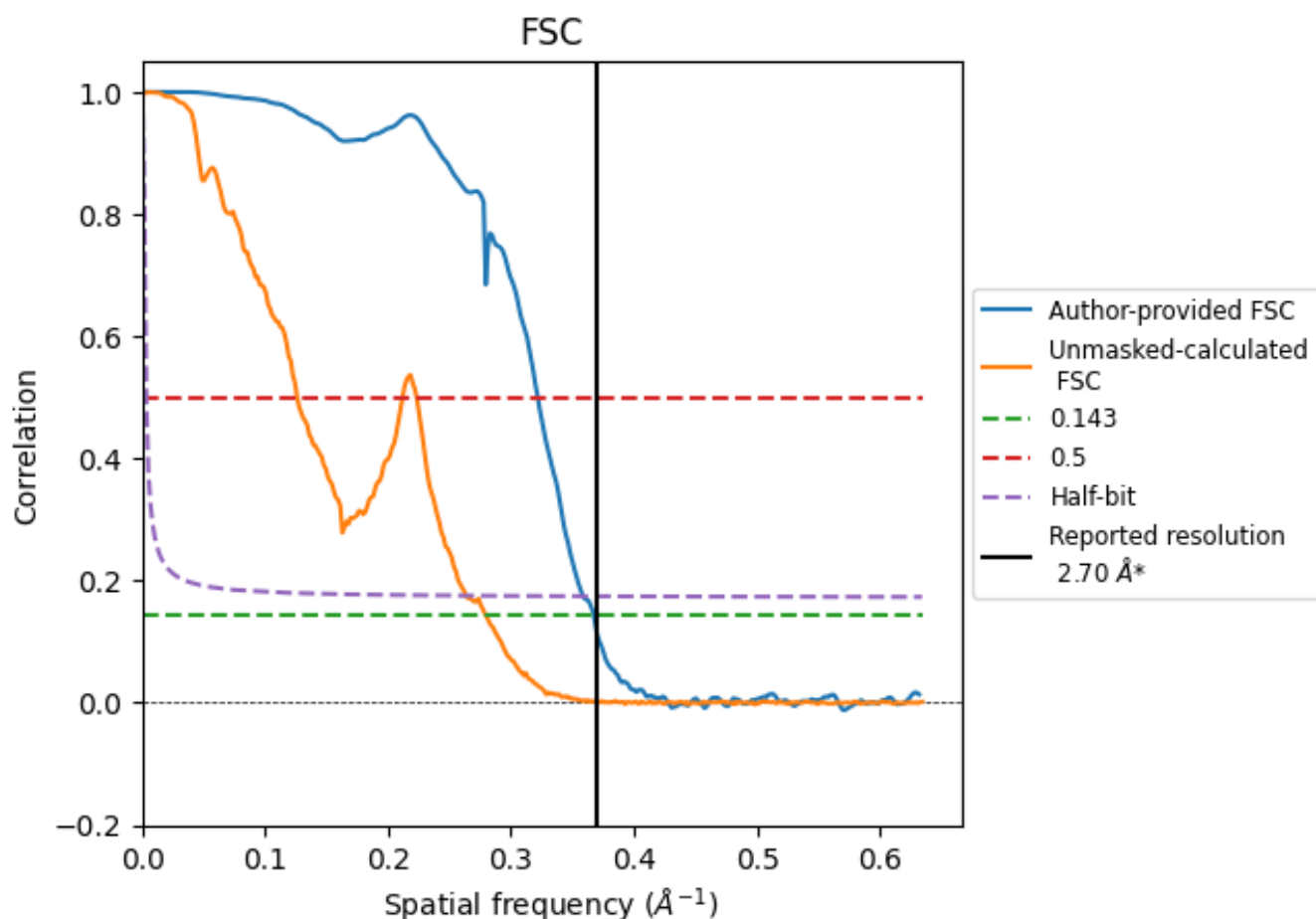


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

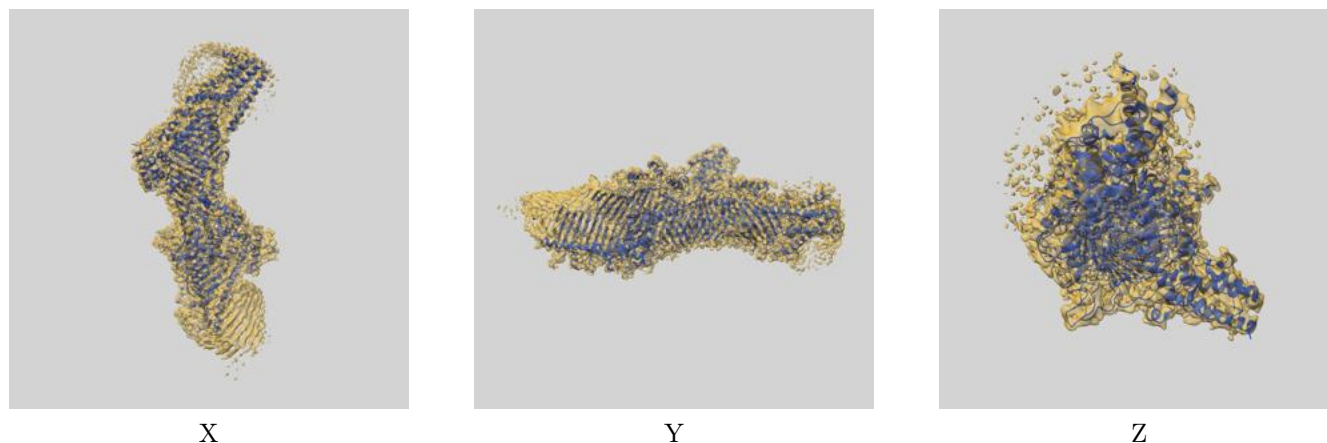
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.11	2.79
Unmasked-calculated*	3.58	7.93	3.80

*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 3.58 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

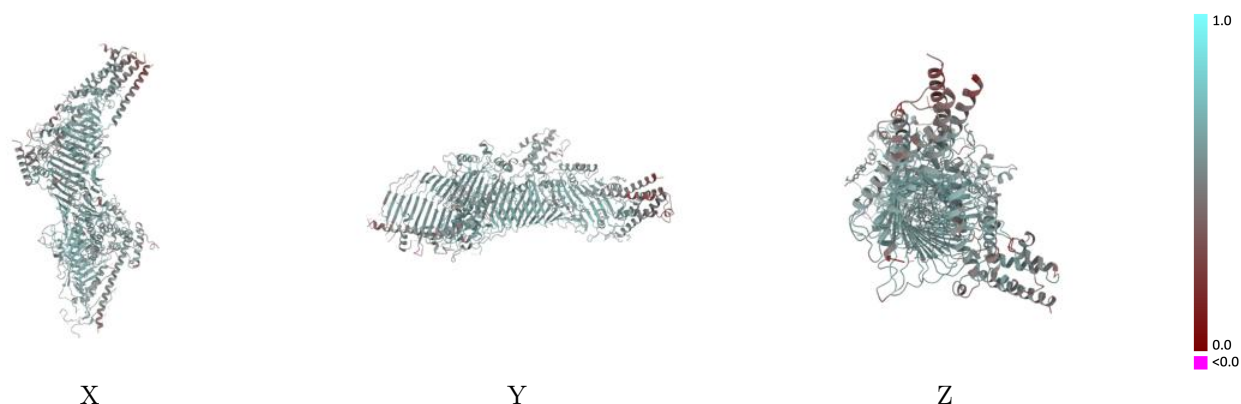
This section contains information regarding the fit between EMDB map EMD-45399 and PDB model 9CAP. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



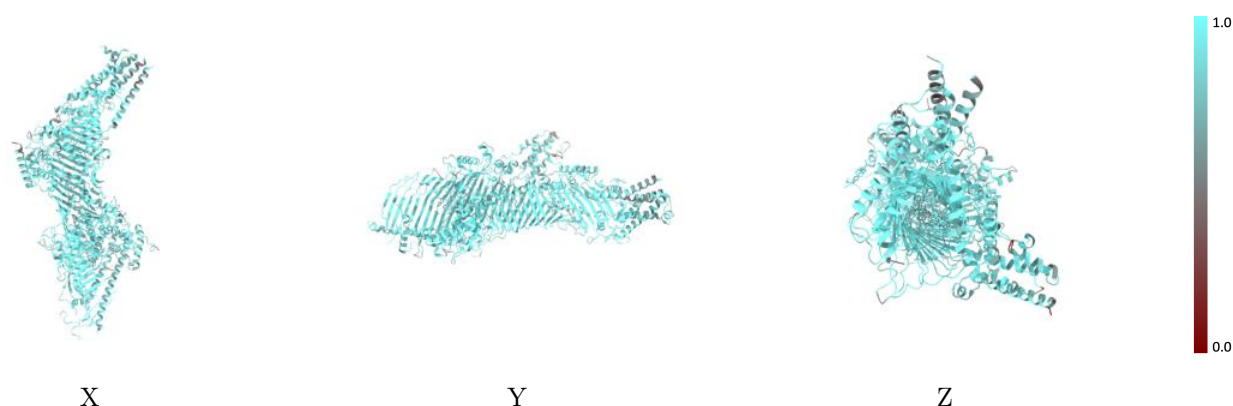
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



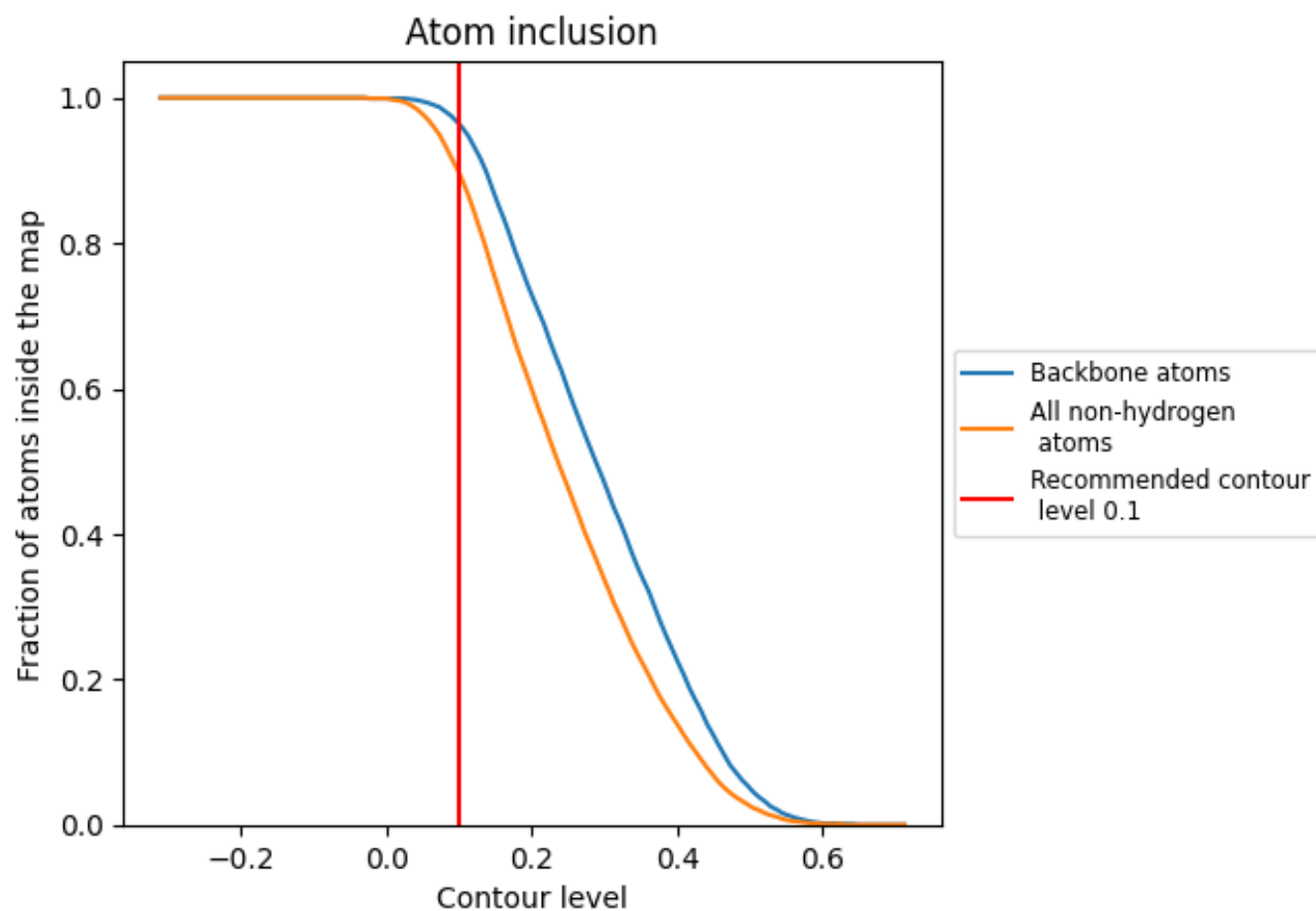
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 90% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8970	<div></div> 0.5590
A	<div></div> 0.9100	<div></div> 0.5710
B	<div></div> 0.8140	<div></div> 0.4970
C	<div></div> 0.8510	<div></div> 0.4990

