Full wwPDB EM Validation Report ⓘ

Jun 7, 2025 – 01:05 PM EDT

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

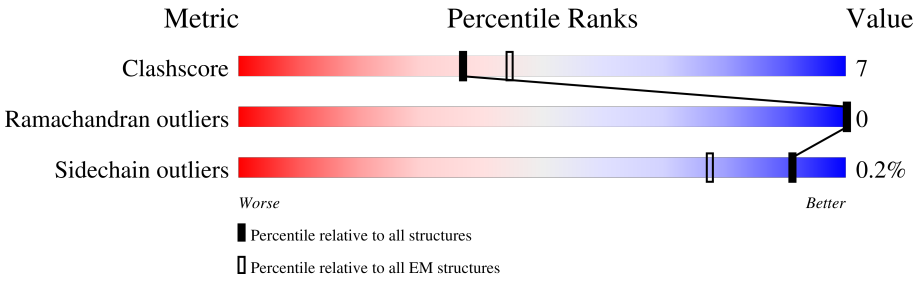
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.70 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	4301	28% 6% 67%
2	B	276	57% 8% 34%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13783 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 279 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4023	GLY	-	expression tag	UNP A0A0K3AWP8
A	4024	SER	-	expression tag	UNP A0A0K3AWP8
A	4025	GLY	-	expression tag	UNP A0A0K3AWP8
A	4026	VAL	-	expression tag	UNP A0A0K3AWP8
A	4027	SER	-	expression tag	UNP A0A0K3AWP8
A	4028	LYS	-	expression tag	UNP A0A0K3AWP8
A	4029	GLY	-	expression tag	UNP A0A0K3AWP8
A	4030	GLU	-	expression tag	UNP A0A0K3AWP8
A	4031	GLU	-	expression tag	UNP A0A0K3AWP8
A	4032	LEU	-	expression tag	UNP A0A0K3AWP8
A	4033	PHE	-	expression tag	UNP A0A0K3AWP8
A	4034	THR	-	expression tag	UNP A0A0K3AWP8
A	4035	GLY	-	expression tag	UNP A0A0K3AWP8
A	4036	VAL	-	expression tag	UNP A0A0K3AWP8
A	4037	VAL	-	expression tag	UNP A0A0K3AWP8
A	4038	PRO	-	expression tag	UNP A0A0K3AWP8
A	4039	ILE	-	expression tag	UNP A0A0K3AWP8
A	4040	LEU	-	expression tag	UNP A0A0K3AWP8
A	4041	VAL	-	expression tag	UNP A0A0K3AWP8
A	4042	GLU	-	expression tag	UNP A0A0K3AWP8
A	4043	LEU	-	expression tag	UNP A0A0K3AWP8
A	4044	ASP	-	expression tag	UNP A0A0K3AWP8
A	4045	GLY	-	expression tag	UNP A0A0K3AWP8
A	4046	ASP	-	expression tag	UNP A0A0K3AWP8
A	4047	VAL	-	expression tag	UNP A0A0K3AWP8
A	4048	ASN	-	expression tag	UNP A0A0K3AWP8
A	4049	GLY	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4050	HIS	-	expression tag	UNP A0A0K3AWP8
A	4051	LYS	-	expression tag	UNP A0A0K3AWP8
A	4052	PHE	-	expression tag	UNP A0A0K3AWP8
A	4053	SER	-	expression tag	UNP A0A0K3AWP8
A	4054	VAL	-	expression tag	UNP A0A0K3AWP8
A	4055	SER	-	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	GLU	-	expression tag	UNP A0A0K3AWP8
A	4060	GLY	-	expression tag	UNP A0A0K3AWP8
A	4061	ASP	-	expression tag	UNP A0A0K3AWP8
A	4062	ALA	-	expression tag	UNP A0A0K3AWP8
A	4063	THR	-	expression tag	UNP A0A0K3AWP8
A	4064	TYR	-	expression tag	UNP A0A0K3AWP8
A	4065	GLY	-	expression tag	UNP A0A0K3AWP8
A	4066	LYS	-	expression tag	UNP A0A0K3AWP8
A	4067	LEU	-	expression tag	UNP A0A0K3AWP8
A	4068	THR	-	expression tag	UNP A0A0K3AWP8
A	4069	LEU	-	expression tag	UNP A0A0K3AWP8
A	4070	LYS	-	expression tag	UNP A0A0K3AWP8
A	4071	LEU	-	expression tag	UNP A0A0K3AWP8
A	4072	ILE	-	expression tag	UNP A0A0K3AWP8
A	4073	CYS	-	expression tag	UNP A0A0K3AWP8
A	4074	THR	-	expression tag	UNP A0A0K3AWP8
A	4075	THR	-	expression tag	UNP A0A0K3AWP8
A	4076	GLY	-	expression tag	UNP A0A0K3AWP8
A	4077	LYS	-	expression tag	UNP A0A0K3AWP8
A	4078	LEU	-	expression tag	UNP A0A0K3AWP8
A	4079	PRO	-	expression tag	UNP A0A0K3AWP8
A	4080	VAL	-	expression tag	UNP A0A0K3AWP8
A	4081	PRO	-	expression tag	UNP A0A0K3AWP8
A	4082	TRP	-	expression tag	UNP A0A0K3AWP8
A	4083	PRO	-	expression tag	UNP A0A0K3AWP8
A	4084	THR	-	expression tag	UNP A0A0K3AWP8
A	4085	LEU	-	expression tag	UNP A0A0K3AWP8
A	4086	VAL	-	expression tag	UNP A0A0K3AWP8
A	4087	THR	-	expression tag	UNP A0A0K3AWP8
A	4088	THR	-	expression tag	UNP A0A0K3AWP8
A	4089	LEU	-	expression tag	UNP A0A0K3AWP8
A	4090	GLY	-	expression tag	UNP A0A0K3AWP8
A	4091	TYR	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4092	GLY	-	expression tag	UNP A0A0K3AWP8
A	4093	LEU	-	expression tag	UNP A0A0K3AWP8
A	4094	MET	-	expression tag	UNP A0A0K3AWP8
A	4095	CYS	-	expression tag	UNP A0A0K3AWP8
A	4096	PHE	-	expression tag	UNP A0A0K3AWP8
A	4097	ALA	-	expression tag	UNP A0A0K3AWP8
A	4098	ARG	-	expression tag	UNP A0A0K3AWP8
A	4099	TYR	-	expression tag	UNP A0A0K3AWP8
A	4100	PRO	-	expression tag	UNP A0A0K3AWP8
A	4101	ASP	-	expression tag	UNP A0A0K3AWP8
A	4102	HIS	-	expression tag	UNP A0A0K3AWP8
A	4103	MET	-	expression tag	UNP A0A0K3AWP8
A	4104	LYS	-	expression tag	UNP A0A0K3AWP8
A	4105	GLN	-	expression tag	UNP A0A0K3AWP8
A	4106	HIS	-	expression tag	UNP A0A0K3AWP8
A	4107	ASP	-	expression tag	UNP A0A0K3AWP8
A	4108	PHE	-	expression tag	UNP A0A0K3AWP8
A	4109	PHE	-	expression tag	UNP A0A0K3AWP8
A	4110	LYS	-	expression tag	UNP A0A0K3AWP8
A	4111	SER	-	expression tag	UNP A0A0K3AWP8
A	4112	ALA	-	expression tag	UNP A0A0K3AWP8
A	4113	MET	-	expression tag	UNP A0A0K3AWP8
A	4114	PRO	-	expression tag	UNP A0A0K3AWP8
A	4115	GLU	-	expression tag	UNP A0A0K3AWP8
A	4116	GLY	-	expression tag	UNP A0A0K3AWP8
A	4117	TYR	-	expression tag	UNP A0A0K3AWP8
A	4118	VAL	-	expression tag	UNP A0A0K3AWP8
A	4119	GLN	-	expression tag	UNP A0A0K3AWP8
A	4120	GLU	-	expression tag	UNP A0A0K3AWP8
A	4121	ARG	-	expression tag	UNP A0A0K3AWP8
A	4122	THR	-	expression tag	UNP A0A0K3AWP8
A	4123	ILE	-	expression tag	UNP A0A0K3AWP8
A	4124	PHE	-	expression tag	UNP A0A0K3AWP8
A	4125	PHE	-	expression tag	UNP A0A0K3AWP8
A	4126	LYS	-	expression tag	UNP A0A0K3AWP8
A	4127	ASP	-	expression tag	UNP A0A0K3AWP8
A	4128	ASP	-	expression tag	UNP A0A0K3AWP8
A	4129	GLY	-	expression tag	UNP A0A0K3AWP8
A	4130	ASN	-	expression tag	UNP A0A0K3AWP8
A	4131	TYR	-	expression tag	UNP A0A0K3AWP8
A	4132	LYS	-	expression tag	UNP A0A0K3AWP8
A	4133	THR	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4134	ARG	-	expression tag	UNP A0A0K3AWP8
A	4135	ALA	-	expression tag	UNP A0A0K3AWP8
A	4136	GLU	-	expression tag	UNP A0A0K3AWP8
A	4137	VAL	-	expression tag	UNP A0A0K3AWP8
A	4138	LYS	-	expression tag	UNP A0A0K3AWP8
A	4139	PHE	-	expression tag	UNP A0A0K3AWP8
A	4140	GLU	-	expression tag	UNP A0A0K3AWP8
A	4141	GLY	-	expression tag	UNP A0A0K3AWP8
A	4142	ASP	-	expression tag	UNP A0A0K3AWP8
A	4143	THR	-	expression tag	UNP A0A0K3AWP8
A	4144	LEU	-	expression tag	UNP A0A0K3AWP8
A	4145	VAL	-	expression tag	UNP A0A0K3AWP8
A	4146	ASN	-	expression tag	UNP A0A0K3AWP8
A	4147	ARG	-	expression tag	UNP A0A0K3AWP8
A	4148	ILE	-	expression tag	UNP A0A0K3AWP8
A	4149	GLU	-	expression tag	UNP A0A0K3AWP8
A	4150	LEU	-	expression tag	UNP A0A0K3AWP8
A	4151	LYS	-	expression tag	UNP A0A0K3AWP8
A	4152	GLY	-	expression tag	UNP A0A0K3AWP8
A	4153	ILE	-	expression tag	UNP A0A0K3AWP8
A	4154	ASP	-	expression tag	UNP A0A0K3AWP8
A	4155	PHE	-	expression tag	UNP A0A0K3AWP8
A	4156	LYS	-	expression tag	UNP A0A0K3AWP8
A	4157	GLU	-	expression tag	UNP A0A0K3AWP8
A	4158	ASP	-	expression tag	UNP A0A0K3AWP8
A	4159	GLY	-	expression tag	UNP A0A0K3AWP8
A	4160	ASN	-	expression tag	UNP A0A0K3AWP8
A	4161	ILE	-	expression tag	UNP A0A0K3AWP8
A	4162	LEU	-	expression tag	UNP A0A0K3AWP8
A	4163	GLY	-	expression tag	UNP A0A0K3AWP8
A	4164	HIS	-	expression tag	UNP A0A0K3AWP8
A	4165	LYS	-	expression tag	UNP A0A0K3AWP8
A	4166	LEU	-	expression tag	UNP A0A0K3AWP8
A	4167	GLU	-	expression tag	UNP A0A0K3AWP8
A	4168	TYR	-	expression tag	UNP A0A0K3AWP8
A	4169	ASN	-	expression tag	UNP A0A0K3AWP8
A	4170	TYR	-	expression tag	UNP A0A0K3AWP8
A	4171	ASN	-	expression tag	UNP A0A0K3AWP8
A	4172	SER	-	expression tag	UNP A0A0K3AWP8
A	4173	HIS	-	expression tag	UNP A0A0K3AWP8
A	4174	ASN	-	expression tag	UNP A0A0K3AWP8
A	4175	VAL	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4176	TYR	-	expression tag	UNP A0A0K3AWP8
A	4177	ILE	-	expression tag	UNP A0A0K3AWP8
A	4178	THR	-	expression tag	UNP A0A0K3AWP8
A	4179	ALA	-	expression tag	UNP A0A0K3AWP8
A	4180	ASP	-	expression tag	UNP A0A0K3AWP8
A	4181	LYS	-	expression tag	UNP A0A0K3AWP8
A	4182	GLN	-	expression tag	UNP A0A0K3AWP8
A	4183	LYS	-	expression tag	UNP A0A0K3AWP8
A	4184	ASN	-	expression tag	UNP A0A0K3AWP8
A	4185	GLY	-	expression tag	UNP A0A0K3AWP8
A	4186	ILE	-	expression tag	UNP A0A0K3AWP8
A	4187	LYS	-	expression tag	UNP A0A0K3AWP8
A	4188	ALA	-	expression tag	UNP A0A0K3AWP8
A	4189	ASN	-	expression tag	UNP A0A0K3AWP8
A	4190	PHE	-	expression tag	UNP A0A0K3AWP8
A	4191	LYS	-	expression tag	UNP A0A0K3AWP8
A	4192	ILE	-	expression tag	UNP A0A0K3AWP8
A	4193	ARG	-	expression tag	UNP A0A0K3AWP8
A	4194	HIS	-	expression tag	UNP A0A0K3AWP8
A	4195	ASN	-	expression tag	UNP A0A0K3AWP8
A	4196	ILE	-	expression tag	UNP A0A0K3AWP8
A	4197	GLU	-	expression tag	UNP A0A0K3AWP8
A	4198	ASP	-	expression tag	UNP A0A0K3AWP8
A	4199	GLY	-	expression tag	UNP A0A0K3AWP8
A	4200	GLY	-	expression tag	UNP A0A0K3AWP8
A	4201	VAL	-	expression tag	UNP A0A0K3AWP8
A	4202	GLN	-	expression tag	UNP A0A0K3AWP8
A	4203	LEU	-	expression tag	UNP A0A0K3AWP8
A	4204	ALA	-	expression tag	UNP A0A0K3AWP8
A	4205	ASP	-	expression tag	UNP A0A0K3AWP8
A	4206	HIS	-	expression tag	UNP A0A0K3AWP8
A	4207	TYR	-	expression tag	UNP A0A0K3AWP8
A	4208	GLN	-	expression tag	UNP A0A0K3AWP8
A	4209	GLN	-	expression tag	UNP A0A0K3AWP8
A	4210	ASN	-	expression tag	UNP A0A0K3AWP8
A	4211	THR	-	expression tag	UNP A0A0K3AWP8
A	4212	PRO	-	expression tag	UNP A0A0K3AWP8
A	4213	ILE	-	expression tag	UNP A0A0K3AWP8
A	4214	GLY	-	expression tag	UNP A0A0K3AWP8
A	4215	ASP	-	expression tag	UNP A0A0K3AWP8
A	4216	GLY	-	expression tag	UNP A0A0K3AWP8
A	4217	PRO	-	expression tag	UNP A0A0K3AWP8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	4218	VAL	-	expression tag	UNP A0A0K3AWP8
A	4219	LEU	-	expression tag	UNP A0A0K3AWP8
A	4220	LEU	-	expression tag	UNP A0A0K3AWP8
A	4221	PRO	-	expression tag	UNP A0A0K3AWP8
A	4222	ASP	-	expression tag	UNP A0A0K3AWP8
A	4223	ASN	-	expression tag	UNP A0A0K3AWP8
A	4224	HIS	-	expression tag	UNP A0A0K3AWP8
A	4225	TYR	-	expression tag	UNP A0A0K3AWP8
A	4226	LEU	-	expression tag	UNP A0A0K3AWP8
A	4227	SER	-	expression tag	UNP A0A0K3AWP8
A	4228	TYR	-	expression tag	UNP A0A0K3AWP8
A	4229	GLN	-	expression tag	UNP A0A0K3AWP8
A	4230	SER	-	expression tag	UNP A0A0K3AWP8
A	4231	LYS	-	expression tag	UNP A0A0K3AWP8
A	4232	LEU	-	expression tag	UNP A0A0K3AWP8
A	4233	SER	-	expression tag	UNP A0A0K3AWP8
A	4234	LYS	-	expression tag	UNP A0A0K3AWP8
A	4235	ASP	-	expression tag	UNP A0A0K3AWP8
A	4236	PRO	-	expression tag	UNP A0A0K3AWP8
A	4237	ASN	-	expression tag	UNP A0A0K3AWP8
A	4238	GLU	-	expression tag	UNP A0A0K3AWP8
A	4239	LYS	-	expression tag	UNP A0A0K3AWP8
A	4240	ARG	-	expression tag	UNP A0A0K3AWP8
A	4241	ASP	-	expression tag	UNP A0A0K3AWP8
A	4242	HIS	-	expression tag	UNP A0A0K3AWP8
A	4243	MET	-	expression tag	UNP A0A0K3AWP8
A	4244	VAL	-	expression tag	UNP A0A0K3AWP8
A	4245	LEU	-	expression tag	UNP A0A0K3AWP8
A	4246	LEU	-	expression tag	UNP A0A0K3AWP8
A	4247	GLU	-	expression tag	UNP A0A0K3AWP8
A	4248	PHE	-	expression tag	UNP A0A0K3AWP8
A	4249	VAL	-	expression tag	UNP A0A0K3AWP8
A	4250	THR	-	expression tag	UNP A0A0K3AWP8
A	4251	ALA	-	expression tag	UNP A0A0K3AWP8
A	4252	ALA	-	expression tag	UNP A0A0K3AWP8
A	4253	GLY	-	expression tag	UNP A0A0K3AWP8
A	4254	ILE	-	expression tag	UNP A0A0K3AWP8
A	4255	THR	-	expression tag	UNP A0A0K3AWP8
A	4256	LEU	-	expression tag	UNP A0A0K3AWP8
A	4257	GLY	-	expression tag	UNP A0A0K3AWP8
A	4258	MET	-	expression tag	UNP A0A0K3AWP8
A	4259	ASP	-	expression tag	UNP A0A0K3AWP8

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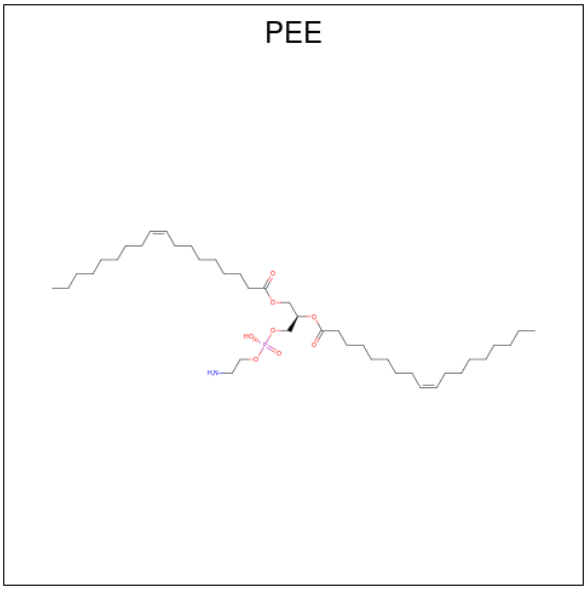
Chain	Residue	Modelled	Actual	Comment	Reference
A	4260	GLU	-	expression tag	UNP A0A0K3AWP8
A	4261	LEU	-	expression tag	UNP A0A0K3AWP8
A	4262	TYR	-	expression tag	UNP A0A0K3AWP8
A	4263	LYS	-	expression tag	UNP A0A0K3AWP8
A	4264	GLY	-	expression tag	UNP A0A0K3AWP8
A	4265	SER	-	expression tag	UNP A0A0K3AWP8
A	4266	GLY	-	expression tag	UNP A0A0K3AWP8
A	4267	LEU	-	expression tag	UNP A0A0K3AWP8
A	4268	GLU	-	expression tag	UNP A0A0K3AWP8
A	4269	VAL	-	expression tag	UNP A0A0K3AWP8
A	4270	LEU	-	expression tag	UNP A0A0K3AWP8
A	4271	PHE	-	expression tag	UNP A0A0K3AWP8
A	4272	GLN	-	expression tag	UNP A0A0K3AWP8
A	4273	GLY	-	expression tag	UNP A0A0K3AWP8
A	4274	PRO	-	expression tag	UNP A0A0K3AWP8
A	4275	ALA	-	expression tag	UNP A0A0K3AWP8
A	4276	ASN	-	expression tag	UNP A0A0K3AWP8
A	4277	SER	-	expression tag	UNP A0A0K3AWP8
A	4278	GLY	-	expression tag	UNP A0A0K3AWP8
A	4279	VAL	-	expression tag	UNP A0A0K3AWP8
A	4280	ASP	-	expression tag	UNP A0A0K3AWP8
A	4281	TYR	-	expression tag	UNP A0A0K3AWP8
A	4282	LYS	-	expression tag	UNP A0A0K3AWP8
A	4283	ASP	-	expression tag	UNP A0A0K3AWP8
A	4284	HIS	-	expression tag	UNP A0A0K3AWP8
A	4285	ASP	-	expression tag	UNP A0A0K3AWP8
A	4286	GLY	-	expression tag	UNP A0A0K3AWP8
A	4287	ASP	-	expression tag	UNP A0A0K3AWP8
A	4288	TYR	-	expression tag	UNP A0A0K3AWP8
A	4289	LYS	-	expression tag	UNP A0A0K3AWP8
A	4290	ASP	-	expression tag	UNP A0A0K3AWP8
A	4291	HIS	-	expression tag	UNP A0A0K3AWP8
A	4292	ASP	-	expression tag	UNP A0A0K3AWP8
A	4293	ILE	-	expression tag	UNP A0A0K3AWP8
A	4294	ASP	-	expression tag	UNP A0A0K3AWP8
A	4295	TYR	-	expression tag	UNP A0A0K3AWP8
A	4296	LYS	-	expression tag	UNP A0A0K3AWP8
A	4297	ASP	-	expression tag	UNP A0A0K3AWP8
A	4298	ASP	-	expression tag	UNP A0A0K3AWP8
A	4299	ASP	-	expression tag	UNP A0A0K3AWP8
A	4300	ASP	-	expression tag	UNP A0A0K3AWP8
A	4301	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 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			50	40	1	8	1	
3	A	1	Total	C	N	O	P	0
			35	25	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			37	27	1	8	1	
3	A	1	Total	C	N	O	P	0
			29	19	1	8	1	
3	A	1	Total	C	N	O	P	0
			30	20	1	8	1	
3	A	1	Total	C	N	O	P	0
			36	26	1	8	1	
3	A	1	Total	C	N	O	P	0
			39	29	1	8	1	

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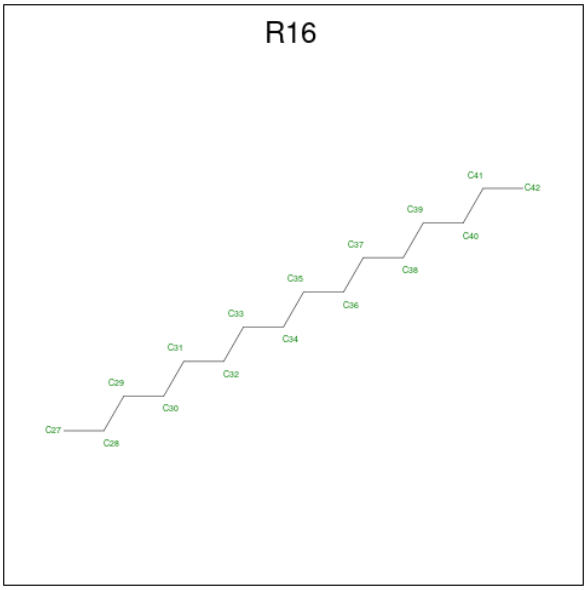
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			34	24	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			51	41	1	8	1	
3	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
3	A	1	Total	C	N	O	P	0
			44	34	1	8	1	
3	A	1	Total	C	N	O	P	0
			31	21	1	8	1	
3	A	1	Total	C	N	O	P	0
			45	35	1	8	1	
3	A	1	Total	C	N	O	P	0
			28	18	1	8	1	
3	A	1	Total	C	N	O	P	0
			27	17	1	8	1	

- Molecule 4 is HEXADECANE (CCD ID: R16) (formula: $C_{16}H_{34}$).



Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	C	0
			10	10	
4	A	1	Total	C	0
			16	16	

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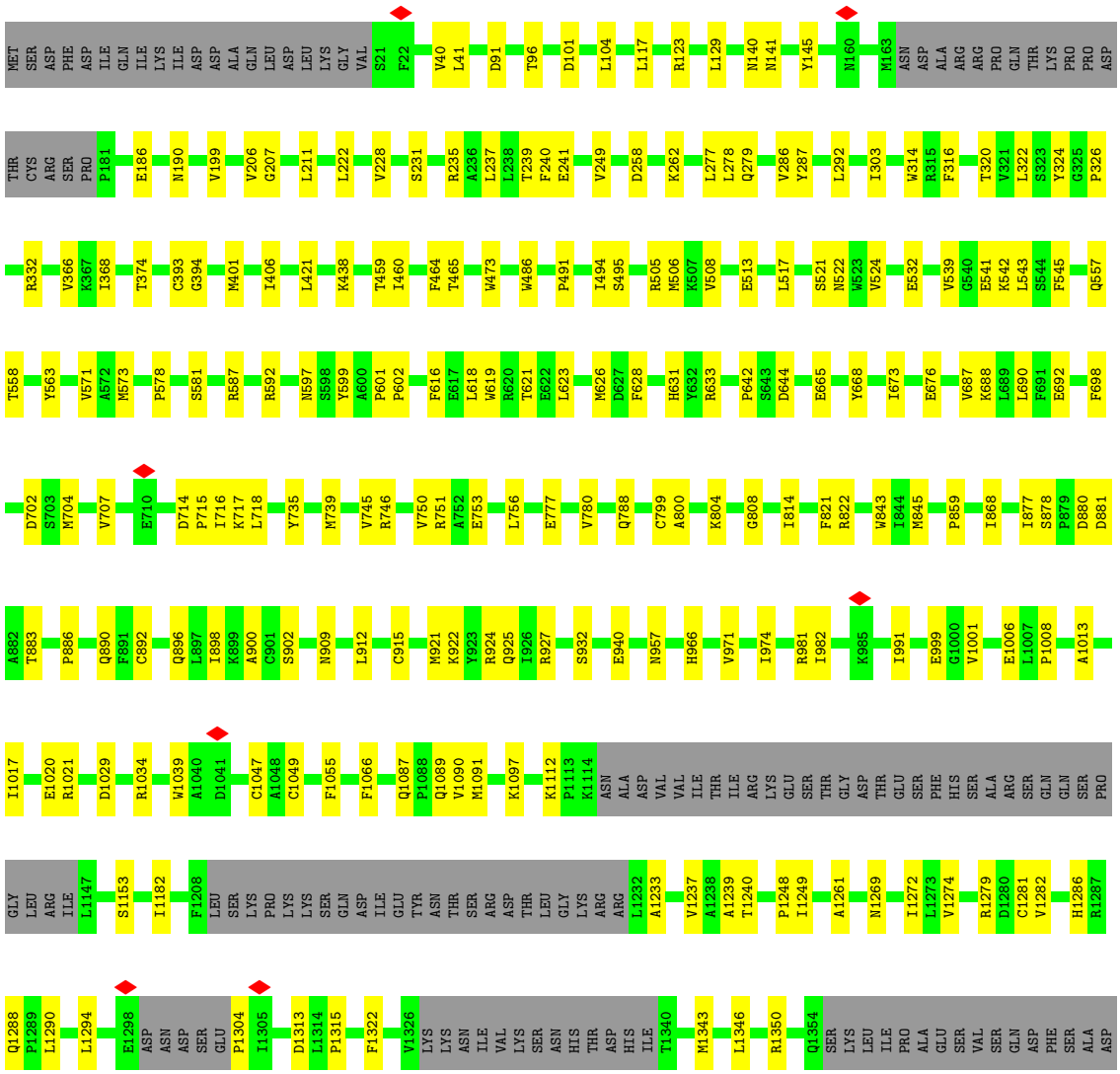
Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C 16 16	0
4	A	1	Total C 16 16	0
4	A	1	Total C 16 16	0
4	A	1	Total C 16 16	0
4	A	1	Total C 13 13	0
4	A	1	Total C 11 11	0
4	A	1	Total C 16 16	0
4	A	1	Total C 10 10	0
4	A	1	Total C 13 13	0
4	A	1	Total C 12 12	0

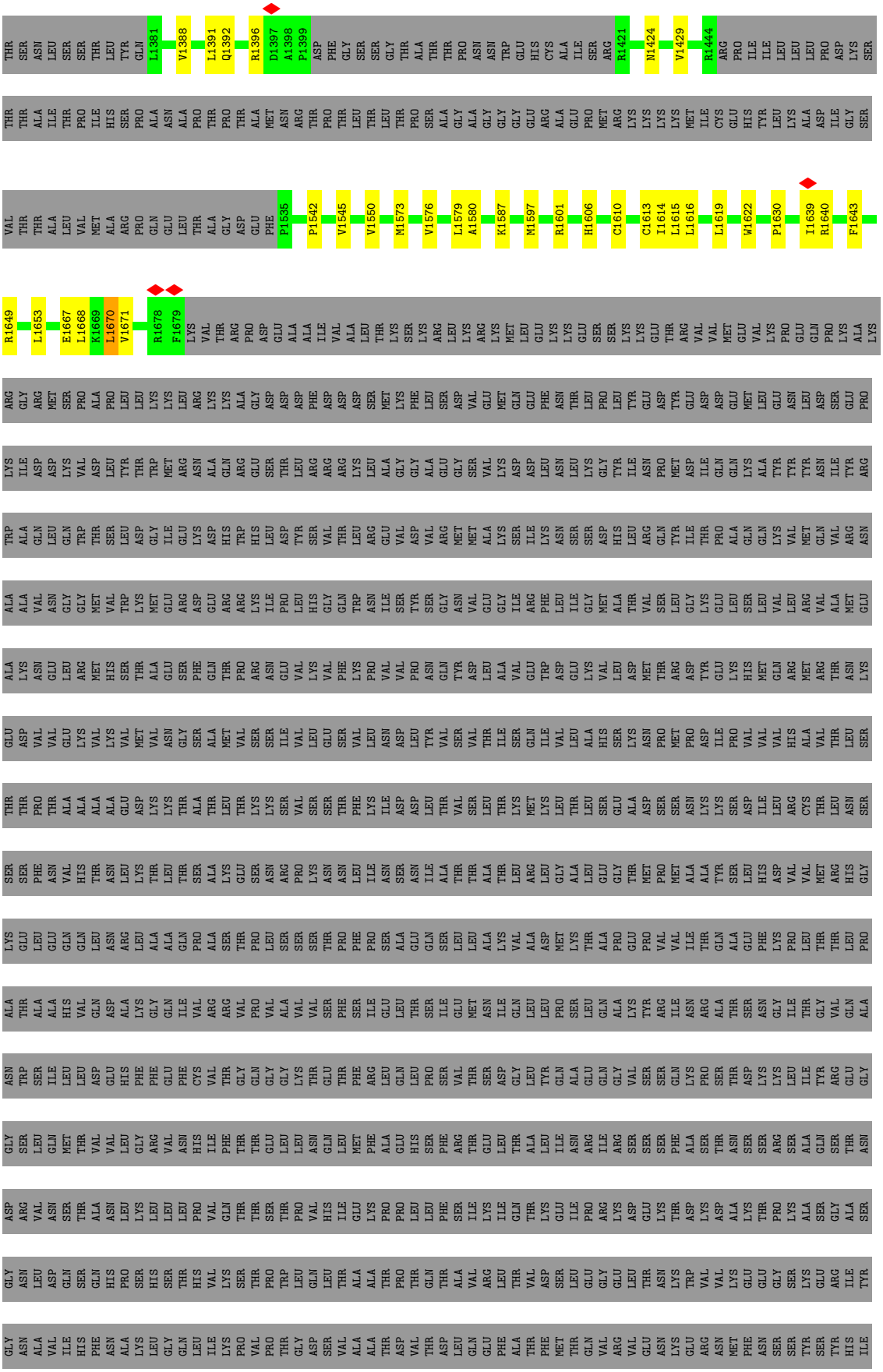
3 Residue-property plots (i)

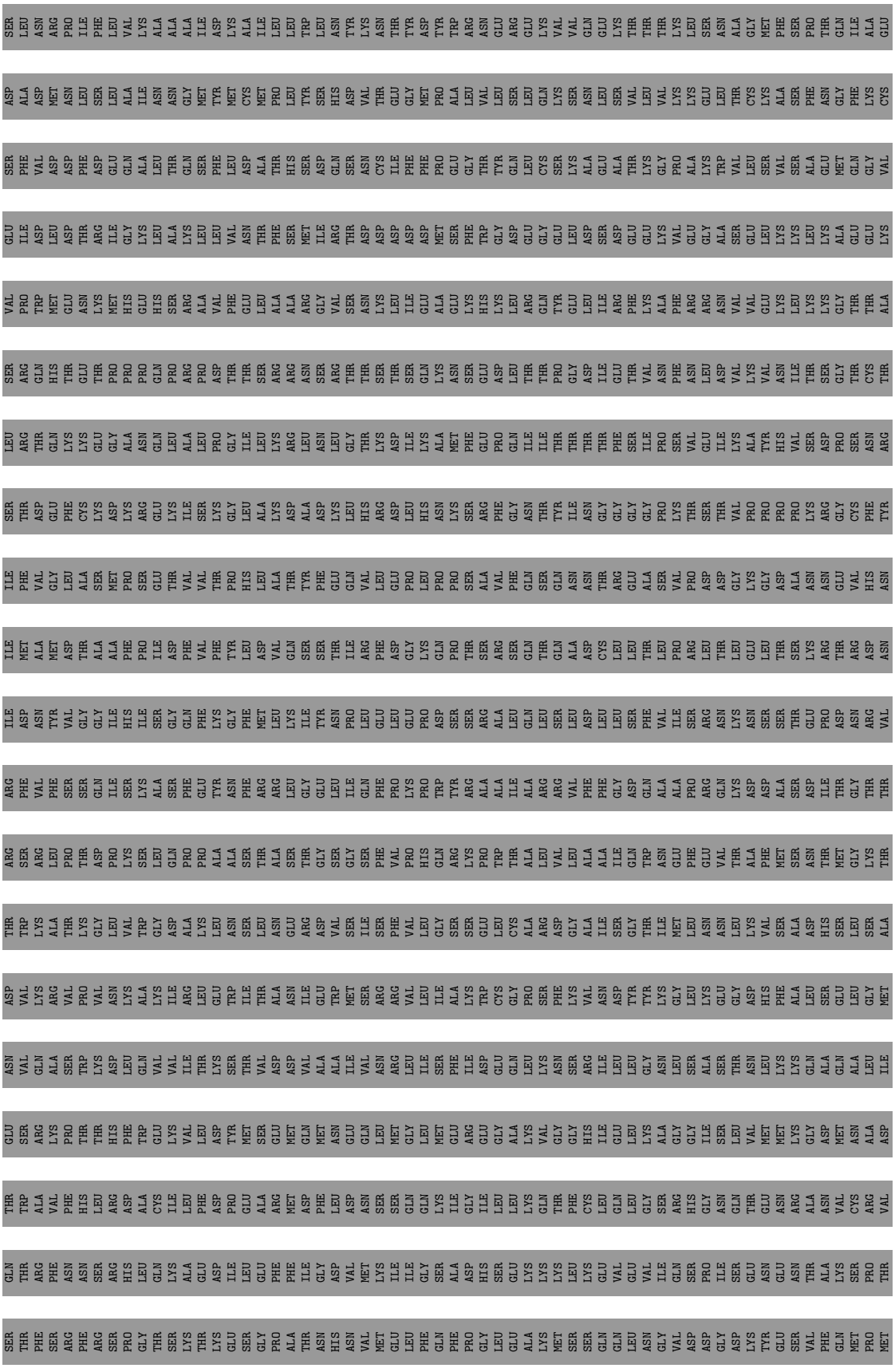
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

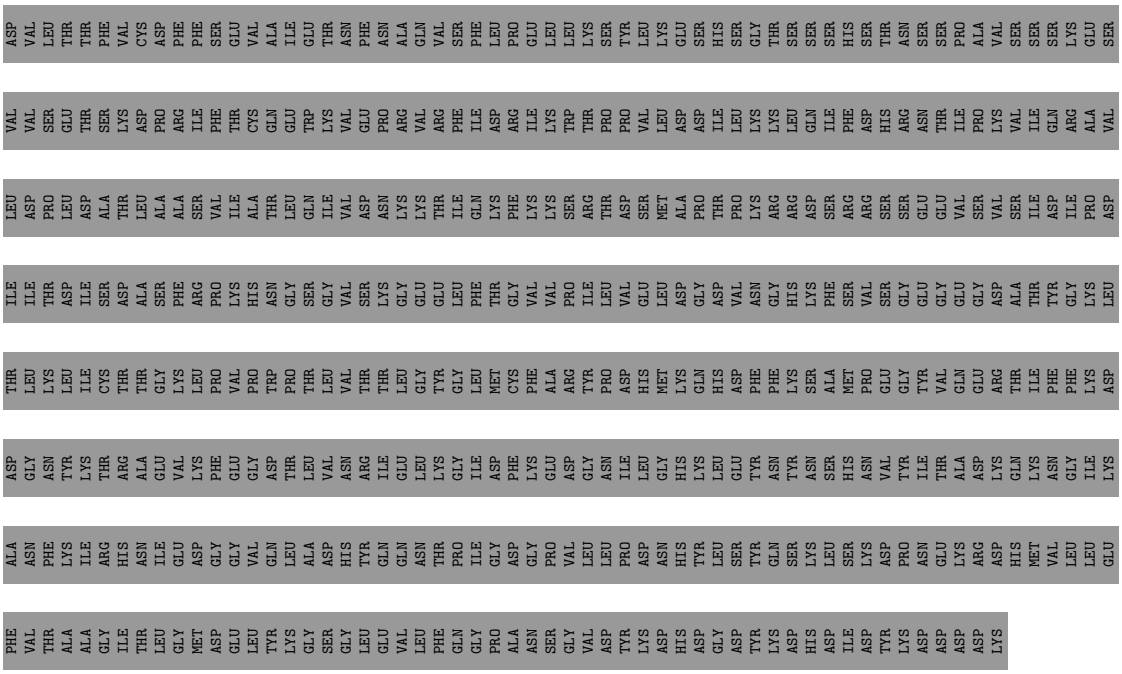
• Molecule 1: Bridge-like lipid transfer protein family member 1 C-terminal domain-containing protein

Chain A:



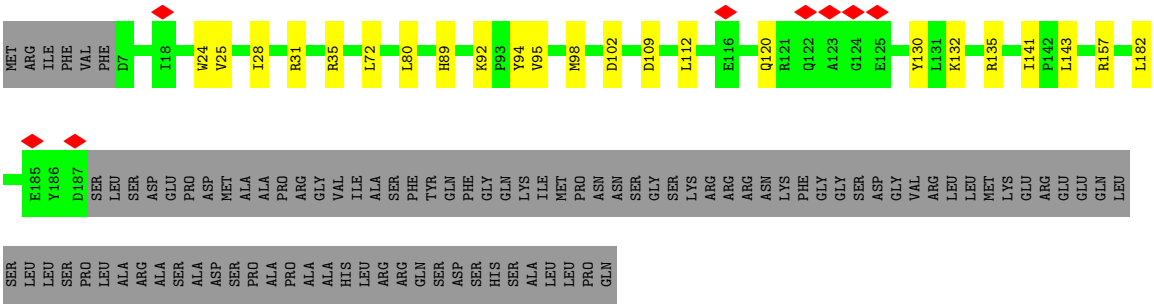

L1381
V1388
L1391
Q1392
R1396
D1397
A1398
P1399
R1421
N1424
V1429
R1444
P1535
P1542
V1545
V1550
M1573
V1576
L1579
A1580
K1587
M1597
R1601
H1606
C1610
C1613
I1614
L1615
L1616
L1619
W1622
P1630
I1639
R1640
F1643
R1649
L1653
E1667
L1668
K1669
L1670
V1671
R1678
F1679





• Molecule 2: Defect at low temperature protein 1

Chain B:



4 Experimental information (i)

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 ($e^-/Å^2$)	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: R16, PEE

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	0.19	0/11702	0.32	0/15874
2	B	0.10	0/1502	0.25	0/2028
All	All	0.18	0/13204	0.31	0/17902

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	165	0
2	B	1479	0	1531	18	0
3	A	714	0	982	46	0
4	A	165	0	336	11	0
All	All	13783	0	14191	207	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (207) 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	0.78
3:A:4403:PEE:H55	3:A:4403:PEE:H28	1.69	0.74
3:A:4401:PEE:H61	3:A:4421:PEE:H53	1.71	0.71
1:A:1288:GLN:NE2	1:A:1610:CYS:SG	2.64	0.71
3:A:4404:PEE:H63	3:A:4410:PEE:H56	1.75	0.69
1:A:1668:LEU:HD11	1:A:1670:LEU:HD23	1.73	0.69
1:A:1281:CYS:SG	1:A:1286:HIS:ND1	2.65	0.69
1:A:714:ASP:HB3	1:A:717:LYS:HG2	1.74	0.68
2:B:89:HIS:HA	2:B:92:LYS:HD2	1.77	0.67
1:A:845:MET:HE1	3:A:4401:PEE:H48	1.77	0.67
1:A:1639:ILE:HG23	1:A:1640:ARG:HG3	1.77	0.66
1:A:1614:ILE:HG21	1:A:1667:GLU:OE2	1.96	0.66
1:A:1274:VAL:HG13	1:A:1616:LEU:HD22	1.80	0.63
1:A:368:ILE:HD13	3:A:4413:PEE:H44	1.81	0.63
1:A:991:ILE:HD11	1:A:1249:ILE:HD13	1.81	0.62
1:A:859:PRO:HG3	1:A:1261:ALA:HA	1.81	0.62
1:A:631:HIS:HB2	1:A:668:TYR:HB3	1.79	0.62
1:A:924:ARG:H	1:A:957:ASN:HD21	1.48	0.62
1:A:1396:ARG:NH1	1:A:1424:ASN:O	2.34	0.60
1:A:303:ILE:HG23	1:A:406:ILE:HD11	1.81	0.60
1:A:921:MET:HE1	1:A:1020:GLU:HB3	1.84	0.59
1:A:822:ARG:NH2	1:A:1089:GLN:O	2.36	0.59
3:A:4405:PEE:H53	4:A:4407:R16:H362	1.85	0.59
3:A:4411:PEE:H48	3:A:4413:PEE:H33	1.85	0.59
1:A:459:THR:HG23	1:A:505:ARG:HH12	1.68	0.59
1:A:1248:PRO:HB3	1:A:1550:VAL:HG21	1.83	0.59
1:A:1290:LEU:HD13	1:A:1670:LEU:HD21	1.83	0.59
1:A:557:GLN:HG3	1:A:558:THR:HG22	1.86	0.58
1:A:735:TYR:O	3:A:4425:PEE:N	2.36	0.58
1:A:101:ASP:OD2	2:B:35:ARG:NH1	2.37	0.58
1:A:925:GLN:HE22	1:A:927:ARG:HG2	1.69	0.58
4:A:4406:R16:H273	3:A:4420:PEE:H1	1.84	0.58
1:A:117:LEU:HB2	1:A:190:ASN:HB2	1.85	0.58
3:A:4404:PEE:H25	3:A:4423:PEE:H55	1.86	0.57
1:A:626:MET:HE1	3:A:4403:PEE:H59	1.86	0.57
1:A:687:VAL:HG13	4:A:4406:R16:H312	1.87	0.56
1:A:900:ALA:HB1	1:A:912:LEU:HD13	1.87	0.56
1:A:1008:PRO:HG3	1:A:1304:PRO:HG3	1.86	0.56
1:A:896:GLN:OE1	1:A:902:SER:N	2.32	0.55
2:B:80:LEU:HD23	2:B:98:MET:HG2	1.88	0.55
1:A:366:VAL:HB	1:A:401:MET:HB3	1.88	0.55
1:A:883:THR:HA	1:A:1601:ARG:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:ASN:O	1:A:522:ASN:OD1	2.25	0.55
1:A:673:ILE:HD11	3:A:4419:PEE:H22	1.89	0.55
1:A:751:ARG:NH2	1:A:753:GLU:OE2	2.40	0.55
1:A:892:CYS:SG	1:A:915:CYS:HB2	2.46	0.55
1:A:1013:ALA:HB1	1:A:1017:ILE:HG21	1.89	0.54
1:A:573:MET:HB2	3:A:4419:PEE:H78	1.88	0.54
1:A:123:ARG:NH2	1:A:228:VAL:O	2.37	0.54
1:A:1240:THR:O	1:A:1350:ARG:NH1	2.41	0.54
1:A:644:ASP:OD1	1:A:644:ASP:N	2.41	0.54
1:A:821:PHE:HE1	1:A:845:MET:HE3	1.73	0.54
1:A:746:ARG:NH1	1:A:777:GLU:OE2	2.35	0.54
1:A:541:GLU:HG2	1:A:542:LYS:HG3	1.89	0.53
1:A:745:VAL:HG11	3:A:4419:PEE:H62	1.90	0.53
1:A:1237:VAL:HG12	1:A:1313:ASP:HB2	1.90	0.53
1:A:1322:PHE:HD1	1:A:1343:MET:HB3	1.74	0.53
1:A:506:MET:HB3	1:A:545:PHE:HB3	1.91	0.52
1:A:40:VAL:HG11	2:B:24:TRP:CE2	2.44	0.52
1:A:326:PRO:HB3	1:A:486:TRP:HA	1.91	0.52
1:A:578:PRO:HB2	1:A:581:SER:HB3	1.90	0.52
1:A:716:ILE:HD13	1:A:912:LEU:HD12	1.92	0.52
1:A:1055:PHE:O	1:A:1087:GLN:NE2	2.42	0.52
1:A:563:TYR:HB2	1:A:628:PHE:HB2	1.92	0.52
1:A:690:LEU:HD21	3:A:4419:PEE:H67	1.92	0.52
1:A:597:ASN:O	1:A:751:ARG:NH2	2.43	0.52
1:A:800:ALA:HB3	1:A:814:ILE:HB	1.92	0.52
4:A:4406:R16:H291	3:A:4420:PEE:H22	1.92	0.51
3:A:4419:PEE:H63	3:A:4420:PEE:H27	1.92	0.51
1:A:971:VAL:HB	1:A:1001:VAL:HB	1.92	0.51
1:A:1239:ALA:HB3	1:A:1315:PRO:HB3	1.93	0.51
1:A:199:VAL:HB	1:A:222:LEU:HB3	1.93	0.51
1:A:513:GLU:HG3	1:A:539:VAL:HG12	1.93	0.51
1:A:508:VAL:HB	1:A:543:LEU:HB3	1.93	0.51
1:A:892:CYS:SG	1:A:898:ILE:HD13	2.51	0.51
1:A:521:SER:HB3	1:A:886:PRO:HD3	1.92	0.51
1:A:878:SER:HB3	1:A:881:ASP:HB3	1.93	0.50
1:A:1029:ASP:HB3	1:A:1039:TRP:CH2	2.46	0.50
1:A:1047:CYS:SG	1:A:1049:CYS:N	2.70	0.50
2:B:135:ARG:HG3	2:B:141:ILE:HG13	1.92	0.50
1:A:587:ARG:HD3	1:A:616:PHE:CG	2.46	0.50
3:A:4403:PEE:H12	3:A:4419:PEE:H9	1.94	0.50
3:A:4419:PEE:H61	3:A:4419:PEE:H29	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4401:PEE:H57	3:A:4420:PEE:H53	1.93	0.49
1:A:982:ILE:HD13	1:A:1153:SER:HB2	1.93	0.49
1:A:140:ASN:OD1	1:A:141:ASN:N	2.45	0.48
1:A:698:PHE:CZ	3:A:4419:PEE:H23	2.48	0.48
1:A:880:ASP:OD1	1:A:1286:HIS:NE2	2.47	0.48
3:A:4419:PEE:H76	3:A:4419:PEE:H38	1.95	0.48
3:A:4421:PEE:H22	3:A:4421:PEE:H28	1.73	0.48
1:A:316:PHE:HB3	1:A:320:THR:HG21	1.95	0.48
1:A:145:TYR:HD1	2:B:72:LEU:HD22	1.77	0.48
1:A:517:LEU:HD23	1:A:524:VAL:HG12	1.96	0.48
1:A:909:ASN:ND2	1:A:909:ASN:O	2.47	0.48
1:A:1580:ALA:HA	1:A:1622:TRP:CD1	2.47	0.48
1:A:1090:VAL:HG12	1:A:1091:MET:HG2	1.95	0.48
1:A:394:GLY:N	1:A:421:LEU:O	2.47	0.48
1:A:788:GLN:HB3	1:A:1034:ARG:NH1	2.28	0.48
1:A:532:GLU:O	1:A:1597:MET:HG3	2.14	0.47
1:A:633:ARG:NH1	1:A:665:GLU:OE1	2.43	0.47
1:A:532:GLU:HB3	1:A:578:PRO:HB3	1.96	0.47
1:A:940:GLU:O	1:A:981:ARG:NH2	2.31	0.47
1:A:494:ILE:HG22	2:B:157:ARG:HG3	1.97	0.47
1:A:1346:LEU:HD13	1:A:1388:VAL:HG22	1.95	0.47
1:A:890:GLN:HB3	1:A:898:ILE:HG12	1.96	0.47
3:A:4405:PEE:H62	3:A:4421:PEE:H30	1.96	0.47
4:A:4415:R16:H401	4:A:4415:R16:H372	1.74	0.47
1:A:522:ASN:OD1	1:A:704:MET:HA	2.15	0.47
1:A:1576:VAL:HG12	1:A:1619:LEU:HD22	1.96	0.47
1:A:999:GLU:O	1:A:1240:THR:N	2.45	0.47
1:A:599:TYR:CZ	1:A:1112:LYS:HG2	2.49	0.46
1:A:799:CYS:SG	1:A:1182:ILE:HG23	2.55	0.46
1:A:877:ILE:HD13	4:A:4407:R16:H282	1.97	0.46
1:A:1392:GLN:HB3	1:A:1429:VAL:HG23	1.97	0.46
1:A:91:ASP:OD2	1:A:96:THR:OG1	2.28	0.46
1:A:258:ASP:OD1	1:A:258:ASP:N	2.47	0.46
1:A:324:TYR:HB2	3:A:4412:PEE:H45	1.96	0.46
1:A:1616:LEU:HD23	1:A:1619:LEU:HD12	1.96	0.46
1:A:1579:LEU:HB3	1:A:1622:TRP:CZ2	2.51	0.46
3:A:4419:PEE:C39	3:A:4420:PEE:H27	2.45	0.46
1:A:573:MET:HB3	1:A:619:TRP:HB3	1.96	0.46
1:A:1670:LEU:HA	1:A:1670:LEU:HD22	1.70	0.46
2:B:120:GLN:HG2	2:B:130:TYR:CG	2.51	0.46
1:A:464:PHE:HB2	1:A:508:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLU:HG2	1:A:286:VAL:HG22	1.97	0.45
1:A:104:LEU:HD13	1:A:129:LEU:HD13	1.98	0.45
1:A:235:ARG:NH1	1:A:292:LEU:O	2.50	0.45
1:A:240:PHE:HB3	1:A:287:TYR:HB3	1.98	0.45
1:A:707:VAL:HG11	1:A:1597:MET:SD	2.55	0.45
1:A:1668:LEU:CD1	1:A:1670:LEU:HD23	2.43	0.45
1:A:924:ARG:H	1:A:957:ASN:ND2	2.12	0.45
1:A:206:VAL:HG11	4:A:4414:R16:H342	1.98	0.45
1:A:117:LEU:HB3	1:A:186:GLU:HG3	1.99	0.45
1:A:1029:ASP:HB3	1:A:1039:TRP:HH2	1.81	0.45
2:B:112:LEU:HD21	2:B:182:LEU:HD23	1.99	0.45
1:A:1269:ASN:O	1:A:1272:ILE:HG22	2.17	0.44
2:B:132:LYS:HE2	2:B:143:LEU:HD11	1.98	0.44
1:A:1006:GLU:HB3	1:A:1233:ALA:HB3	2.00	0.44
1:A:1097:LYS:HE3	1:A:1097:LYS:HB2	1.85	0.44
1:A:1294:LEU:HG	1:A:1671:VAL:HG11	1.99	0.44
1:A:592:ARG:NH1	1:A:1630:PRO:HD3	2.32	0.44
1:A:715:PRO:HB2	1:A:900:ALA:HB2	1.99	0.44
1:A:750:VAL:HG11	3:A:4420:PEE:H39	2.00	0.44
1:A:207:GLY:HA2	1:A:211:LEU:HD12	2.00	0.44
1:A:739:MET:HE1	3:A:4403:PEE:H7	2.00	0.43
1:A:922:LYS:O	1:A:1021:ARG:NH1	2.51	0.43
1:A:1614:ILE:HD12	1:A:1668:LEU:HD23	1.99	0.43
4:A:4409:R16:H331	4:A:4409:R16:H381	1.99	0.43
1:A:715:PRO:HA	1:A:718:LEU:HB3	2.00	0.43
2:B:80:LEU:N	2:B:102:ASP:OD2	2.51	0.43
1:A:314:TRP:CH2	3:A:4404:PEE:H71	2.53	0.43
2:B:31:ARG:O	2:B:35:ARG:HG3	2.19	0.43
3:A:4413:PEE:H31	3:A:4413:PEE:H25	1.81	0.43
1:A:249:VAL:HB	1:A:277:LEU:O	2.19	0.43
1:A:1542:PRO:HA	1:A:1545:VAL:HG22	2.00	0.42
1:A:927:ARG:HB3	1:A:1066:PHE:CZ	2.54	0.42
1:A:1610:CYS:HB3	1:A:1613:CYS:HB2	1.48	0.42
2:B:135:ARG:HA	2:B:141:ILE:HD11	2.01	0.42
1:A:491:PRO:HG3	1:A:642:PRO:HD3	2.01	0.42
1:A:279:GLN:O	1:A:320:THR:HA	2.20	0.42
1:A:1573:MET:HG3	1:A:1653:LEU:HD11	2.00	0.42
1:A:688:LYS:O	1:A:692:GLU:HG2	2.19	0.42
2:B:25:VAL:HA	2:B:28:ILE:HG22	2.02	0.42
2:B:92:LYS:HD3	2:B:94:TYR:OH	2.19	0.42
1:A:231:SER:HB2	1:A:237:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:NH1	3:A:4413:PEE:O5	2.52	0.42
1:A:401:MET:SD	3:A:4413:PEE:H24	2.59	0.42
1:A:460:ILE:HD13	3:A:4422:PEE:H28	2.01	0.42
1:A:780:VAL:HG21	3:A:4420:PEE:H23	2.02	0.42
3:A:4412:PEE:H49	3:A:4413:PEE:H23	2.01	0.42
1:A:506:MET:HE3	1:A:508:VAL:HG23	2.02	0.41
1:A:616:PHE:CE2	1:A:618:LEU:HB3	2.56	0.41
1:A:262:LYS:HE3	1:A:262:LYS:HB3	1.87	0.41
1:A:506:MET:HB2	3:A:4425:PEE:H73	2.00	0.41
3:A:4402:PEE:H57	3:A:4402:PEE:H50	1.97	0.41
3:A:4404:PEE:H58	3:A:4410:PEE:H52	2.01	0.41
1:A:249:VAL:HG11	3:A:4412:PEE:H33	2.03	0.41
1:A:1643:PHE:O	1:A:1649:ARG:HD3	2.21	0.41
1:A:1667:GLU:H	1:A:1667:GLU:HG3	1.60	0.41
3:A:4404:PEE:H30	3:A:4404:PEE:H23	1.85	0.41
4:A:4406:R16:H273	3:A:4420:PEE:H13	2.03	0.41
1:A:278:LEU:HD13	1:A:322:LEU:HD13	2.01	0.41
1:A:756:LEU:HD23	1:A:868:ILE:HG13	2.03	0.41
1:A:804:LYS:HE3	1:A:808:GLY:HA2	2.02	0.41
1:A:619:TRP:CD1	3:A:4419:PEE:H82	2.56	0.41
1:A:1343:MET:HG3	1:A:1391:LEU:HB2	2.02	0.41
3:A:4403:PEE:H57	3:A:4403:PEE:H50	1.69	0.41
2:B:89:HIS:HB3	2:B:95:VAL:HG22	2.03	0.41
1:A:843:TRP:HD1	1:A:924:ARG:HG3	1.86	0.41
3:A:4419:PEE:H36	3:A:4419:PEE:H30	1.56	0.41
1:A:239:THR:HG22	1:A:241:GLU:HG3	2.03	0.41
1:A:974:ILE:O	1:A:974:ILE:HG13	2.21	0.41
1:A:1294:LEU:HD13	1:A:1606:HIS:CE1	2.56	0.41
3:A:4412:PEE:H25	3:A:4413:PEE:H54	2.03	0.41
1:A:374:THR:HB	1:A:393:CYS:SG	2.61	0.40
1:A:473:TRP:CD1	1:A:702:ASP:HB3	2.57	0.40
1:A:966:HIS:NE2	1:A:1006:GLU:HG3	2.36	0.40
1:A:571:VAL:HB	1:A:621:THR:HG23	2.04	0.40
1:A:1587:LYS:HE2	1:A:1587:LYS:HB3	1.98	0.40
1:A:601:PRO:HA	1:A:602:PRO:HD3	1.99	0.40
1:A:623:LEU:HB3	1:A:676:GLU:HB2	2.02	0.40
4:A:4414:R16:H381	4:A:4414:R16:H351	1.91	0.40
1:A:438:LYS:HG2	1:A:465:THR:O	2.21	0.40
1:A:495:SER:HA	2:B:80:LEU:HD11	2.02	0.40
1:A:1279:ARG:HA	1:A:1282:VAL:HG22	2.04	0.40
3:A:4405:PEE:H59	4:A:4407:R16:H381	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:ASP:OD1	2:B:109:ASP:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1414/4301 (33%)	1380 (98%)	34 (2%)	0	100	100
2	B	179/276 (65%)	173 (97%)	6 (3%)	0	100	100
All	All	1593/4577 (35%)	1553 (98%)	40 (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	1265/3803 (33%)	1262 (100%)	3 (0%)	92	98
2	B	164/243 (68%)	164 (100%)	0	100	100
All	All	1429/4046 (35%)	1426 (100%)	3 (0%)	91	98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	932	SER
1	A	1615	LEU
1	A	1670	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	468	ASN
1	A	559	GLN
1	A	740	ASN
1	A	863	HIS
1	A	995	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	$\#\|Z\| > 2$
4	R16	A	4409	-	15,15,15	0.28	0	14,14,14	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	PEE	A	4405	-	36,36,50	1.41	5 (13%)	39,41,55	1.35	4 (10%)
3	PEE	A	4412	-	35,35,50	1.35	4 (11%)	38,40,55	1.16	2 (5%)
3	PEE	A	4425	-	44,44,50	1.30	5 (11%)	47,49,55	1.18	3 (6%)
3	PEE	A	4418	-	33,33,50	1.44	5 (15%)	36,38,55	1.36	3 (8%)
3	PEE	A	4403	-	50,50,50	1.24	5 (10%)	53,55,55	1.21	3 (5%)
4	R16	A	4408	-	15,15,15	0.29	0	14,14,14	0.88	0
3	PEE	A	4402	-	34,34,50	1.41	5 (14%)	37,39,55	1.13	2 (5%)
4	R16	A	4424	-	15,15,15	0.27	0	14,14,14	0.88	0
4	R16	A	4428	-	12,12,15	0.29	0	11,11,14	0.85	0
4	R16	A	4415	-	15,15,15	0.29	0	14,14,14	0.86	0
3	PEE	A	4401	-	49,49,50	1.24	5 (10%)	52,54,55	1.19	3 (5%)
3	PEE	A	4419	-	50,50,50	1.24	5 (10%)	53,55,55	1.18	3 (5%)
4	R16	A	4416	-	12,12,15	0.29	0	11,11,14	0.84	0
3	PEE	A	4422	-	43,43,50	1.30	5 (11%)	46,48,55	1.24	4 (8%)
4	R16	A	4426	-	9,9,15	0.30	0	8,8,14	0.78	0
3	PEE	A	4404	-	50,50,50	1.23	5 (10%)	53,55,55	1.18	3 (5%)
3	PEE	A	4427	-	27,27,50	1.53	5 (18%)	30,32,55	1.24	2 (6%)
3	PEE	A	4410	-	28,28,50	1.51	5 (17%)	31,33,55	1.20	2 (6%)
4	R16	A	4417	-	10,10,15	0.30	0	9,9,14	0.82	0
3	PEE	A	4420	-	50,50,50	1.24	5 (10%)	53,55,55	1.17	3 (5%)
4	R16	A	4430	-	11,11,15	0.28	0	10,10,14	0.86	0
3	PEE	A	4423	-	30,30,50	1.47	5 (16%)	33,35,55	1.16	2 (6%)
3	PEE	A	4421	-	44,44,50	1.30	5 (11%)	47,49,55	1.21	3 (6%)
3	PEE	A	4413	-	38,38,50	1.33	5 (13%)	41,43,55	1.11	2 (4%)
4	R16	A	4406	-	9,9,15	0.27	0	8,8,14	0.85	0
3	PEE	A	4429	-	26,26,50	1.55	5 (19%)	29,31,55	1.29	3 (10%)
4	R16	A	4407	-	15,15,15	0.28	0	14,14,14	0.86	0
3	PEE	A	4411	-	29,29,50	1.49	4 (13%)	32,34,55	1.22	2 (6%)
4	R16	A	4414	-	15,15,15	0.27	0	14,14,14	0.87	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
4	R16	A	4409	-	-	6/13/13/13	-
3	PEE	A	4405	-	-	18/40/40/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEE	A	4412	-	-	21/39/39/54	-
3	PEE	A	4425	-	-	30/48/48/54	-
3	PEE	A	4418	-	-	19/37/37/54	-
3	PEE	A	4403	-	-	28/54/54/54	-
4	R16	A	4408	-	-	2/13/13/13	-
3	PEE	A	4402	-	-	16/38/38/54	-
4	R16	A	4424	-	-	6/13/13/13	-
4	R16	A	4428	-	-	1/10/10/13	-
4	R16	A	4415	-	-	4/13/13/13	-
3	PEE	A	4401	-	-	27/53/53/54	-
3	PEE	A	4419	-	-	31/54/54/54	-
4	R16	A	4416	-	-	2/10/10/13	-
3	PEE	A	4422	-	-	25/47/47/54	-
4	R16	A	4426	-	-	1/7/7/13	-
3	PEE	A	4404	-	-	29/54/54/54	-
3	PEE	A	4427	-	-	17/31/31/54	-
3	PEE	A	4410	-	-	11/32/32/54	-
4	R16	A	4417	-	-	0/8/8/13	-
3	PEE	A	4420	-	-	35/54/54/54	-
4	R16	A	4430	-	-	3/9/9/13	-
3	PEE	A	4423	-	-	16/34/34/54	-
3	PEE	A	4421	-	-	24/48/48/54	-
3	PEE	A	4413	-	-	18/42/42/54	-
4	R16	A	4406	-	-	3/7/7/13	-
3	PEE	A	4429	-	-	17/30/30/54	-
4	R16	A	4407	-	-	4/13/13/13	-
3	PEE	A	4411	-	-	14/33/33/54	-
4	R16	A	4414	-	-	4/13/13/13	-

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4413	PEE	O3-C30	4.02	1.45	1.33
3	A	4422	PEE	O3-C30	4.01	1.45	1.33
3	A	4412	PEE	O3-C30	4.01	1.45	1.33
3	A	4419	PEE	O3-C30	4.01	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4401	PEE	O3-C30	4.00	1.45	1.33
3	A	4418	PEE	O3-C30	4.00	1.45	1.33
3	A	4405	PEE	O3-C30	4.00	1.45	1.33
3	A	4402	PEE	O3-C30	4.00	1.45	1.33
3	A	4421	PEE	O3-C30	3.98	1.45	1.33
3	A	4423	PEE	O3-C30	3.98	1.44	1.33
3	A	4425	PEE	O3-C30	3.98	1.44	1.33
3	A	4410	PEE	O3-C30	3.97	1.44	1.33
3	A	4429	PEE	O3-C30	3.96	1.44	1.33
3	A	4411	PEE	O3-C30	3.96	1.44	1.33
3	A	4427	PEE	O3-C30	3.96	1.44	1.33
3	A	4420	PEE	O3-C30	3.96	1.44	1.33
3	A	4404	PEE	O3-C30	3.95	1.44	1.33
3	A	4403	PEE	O3-C30	3.93	1.44	1.33
3	A	4405	PEE	O2-C10	3.16	1.43	1.34
3	A	4411	PEE	O2-C10	3.12	1.43	1.34
3	A	4419	PEE	O2-C10	3.11	1.43	1.34
3	A	4402	PEE	O2-C10	3.11	1.43	1.34
3	A	4420	PEE	O2-C10	3.10	1.43	1.34
3	A	4412	PEE	O2-C10	3.10	1.43	1.34
3	A	4422	PEE	O2-C10	3.09	1.43	1.34
3	A	4404	PEE	O2-C10	3.09	1.43	1.34
3	A	4427	PEE	O2-C10	3.09	1.43	1.34
3	A	4413	PEE	O2-C10	3.08	1.43	1.34
3	A	4425	PEE	O2-C10	3.07	1.42	1.34
3	A	4421	PEE	O2-C10	3.06	1.42	1.34
3	A	4410	PEE	O2-C10	3.06	1.42	1.34
3	A	4423	PEE	O2-C10	3.05	1.42	1.34
3	A	4418	PEE	O2-C10	3.03	1.42	1.34
3	A	4403	PEE	O2-C10	3.03	1.42	1.34
3	A	4401	PEE	O2-C10	3.00	1.42	1.34
3	A	4429	PEE	O2-C10	2.94	1.42	1.34
3	A	4429	PEE	O2-C2	-2.85	1.39	1.46
3	A	4419	PEE	O2-C2	-2.80	1.40	1.46
3	A	4413	PEE	O2-C2	-2.80	1.40	1.46
3	A	4421	PEE	O2-C2	-2.78	1.40	1.46
3	A	4402	PEE	O2-C2	-2.78	1.40	1.46
3	A	4410	PEE	O2-C2	-2.77	1.40	1.46
3	A	4418	PEE	O2-C2	-2.77	1.40	1.46
3	A	4427	PEE	O2-C2	-2.75	1.40	1.46
3	A	4420	PEE	O2-C2	-2.75	1.40	1.46
3	A	4403	PEE	O2-C2	-2.75	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	4401	PEE	O2-C2	-2.74	1.40	1.46
3	A	4422	PEE	O2-C2	-2.74	1.40	1.46
3	A	4425	PEE	O2-C2	-2.74	1.40	1.46
3	A	4423	PEE	O2-C2	-2.73	1.40	1.46
3	A	4412	PEE	O2-C2	-2.73	1.40	1.46
3	A	4411	PEE	O2-C2	-2.73	1.40	1.46
3	A	4404	PEE	O2-C2	-2.71	1.40	1.46
3	A	4405	PEE	O2-C2	-2.62	1.40	1.46
3	A	4403	PEE	C31-C30	2.24	1.57	1.50
3	A	4404	PEE	C31-C30	2.23	1.57	1.50
3	A	4427	PEE	C31-C30	2.23	1.57	1.50
3	A	4418	PEE	C31-C30	2.22	1.57	1.50
3	A	4413	PEE	C31-C30	2.22	1.57	1.50
3	A	4405	PEE	C31-C30	2.21	1.57	1.50
3	A	4419	PEE	C31-C30	2.21	1.57	1.50
3	A	4429	PEE	C31-C30	2.21	1.57	1.50
3	A	4401	PEE	C31-C30	2.20	1.57	1.50
3	A	4410	PEE	C31-C30	2.20	1.57	1.50
3	A	4422	PEE	C31-C30	2.19	1.57	1.50
3	A	4423	PEE	C31-C30	2.19	1.57	1.50
3	A	4420	PEE	C31-C30	2.18	1.57	1.50
3	A	4425	PEE	C31-C30	2.16	1.57	1.50
3	A	4402	PEE	C31-C30	2.16	1.57	1.50
3	A	4421	PEE	C31-C30	2.15	1.56	1.50
3	A	4411	PEE	C31-C30	2.15	1.56	1.50
3	A	4420	PEE	P-O4P	2.09	1.67	1.59
3	A	4419	PEE	P-O4P	2.09	1.67	1.59
3	A	4422	PEE	P-O4P	2.07	1.67	1.59
3	A	4412	PEE	P-O4P	2.06	1.67	1.59
3	A	4403	PEE	P-O4P	2.06	1.67	1.59
3	A	4405	PEE	P-O4P	2.06	1.67	1.59
3	A	4418	PEE	P-O4P	2.05	1.67	1.59
3	A	4423	PEE	P-O4P	2.05	1.67	1.59
3	A	4401	PEE	P-O4P	2.05	1.67	1.59
3	A	4410	PEE	P-O4P	2.04	1.67	1.59
3	A	4421	PEE	P-O4P	2.03	1.67	1.59
3	A	4402	PEE	P-O4P	2.03	1.67	1.59
3	A	4425	PEE	P-O4P	2.03	1.67	1.59
3	A	4404	PEE	P-O4P	2.03	1.67	1.59
3	A	4429	PEE	P-O4P	2.02	1.67	1.59
3	A	4413	PEE	P-O4P	2.02	1.67	1.59
3	A	4427	PEE	P-O4P	2.01	1.67	1.59

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4418	PEE	C40-C39-C38	4.36	152.66	126.42
3	A	4405	PEE	O2-C10-C11	4.32	120.83	111.48
3	A	4429	PEE	O2-C10-C11	4.30	120.78	111.48
3	A	4403	PEE	O2-C10-C11	4.20	120.56	111.48
3	A	4411	PEE	O2-C10-C11	4.19	120.55	111.48
3	A	4427	PEE	O2-C10-C11	4.13	120.41	111.48
3	A	4410	PEE	O2-C10-C11	4.04	120.22	111.48
3	A	4420	PEE	O2-C10-C11	4.03	120.20	111.48
3	A	4412	PEE	O2-C10-C11	4.03	120.20	111.48
3	A	4422	PEE	O2-C10-C11	3.98	120.10	111.48
3	A	4413	PEE	O2-C10-C11	3.93	119.98	111.48
3	A	4423	PEE	O2-C10-C11	3.92	119.95	111.48
3	A	4401	PEE	O2-C10-C11	3.91	119.95	111.48
3	A	4419	PEE	O2-C10-C11	3.91	119.94	111.48
3	A	4404	PEE	O2-C10-C11	3.88	119.88	111.48
3	A	4421	PEE	C40-C39-C38	3.86	153.74	124.83
3	A	4418	PEE	O2-C10-C11	3.83	119.77	111.48
3	A	4419	PEE	C40-C39-C38	3.77	153.05	124.83
3	A	4404	PEE	C40-C39-C38	3.76	153.01	124.83
3	A	4402	PEE	O2-C10-C11	3.75	119.60	111.48
3	A	4420	PEE	C40-C39-C38	3.74	152.86	124.83
3	A	4421	PEE	O2-C10-C11	3.71	119.50	111.48
3	A	4425	PEE	C40-C39-C38	3.71	152.59	124.83
3	A	4403	PEE	C40-C39-C38	3.63	152.01	124.83
3	A	4401	PEE	C40-C39-C38	3.58	151.66	124.83
3	A	4425	PEE	O2-C10-C11	3.56	119.19	111.48
3	A	4422	PEE	C40-C39-C38	3.40	153.00	126.43
3	A	4405	PEE	C40-C39-C38	3.37	152.80	126.43
3	A	4412	PEE	O3-C30-C31	2.98	120.21	111.15
3	A	4427	PEE	O3-C30-C31	2.80	120.37	111.83
3	A	4411	PEE	O3-C30-C31	2.77	120.27	111.83
3	A	4429	PEE	O3-C30-C31	2.74	120.20	111.83
3	A	4402	PEE	O3-C30-C31	2.74	120.19	111.83
3	A	4405	PEE	O3-C30-C31	2.73	120.16	111.83
3	A	4419	PEE	O3-C30-C31	2.73	120.16	111.83
3	A	4422	PEE	O3-C30-C31	2.73	120.16	111.83
3	A	4404	PEE	O3-C30-C31	2.69	120.04	111.83
3	A	4403	PEE	O3-C30-C31	2.69	120.03	111.83
3	A	4401	PEE	O3-C30-C31	2.67	119.98	111.83
3	A	4418	PEE	O3-C30-C31	2.67	119.97	111.83
3	A	4410	PEE	O3-C30-C31	2.65	119.90	111.83
3	A	4413	PEE	O3-C30-C31	2.63	119.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4423	PEE	O3-C30-C31	2.63	119.84	111.83
3	A	4421	PEE	O3-C30-C31	2.61	119.79	111.83
3	A	4425	PEE	O3-C30-C31	2.59	119.73	111.83
3	A	4420	PEE	O3-C30-C31	2.46	119.34	111.83
3	A	4405	PEE	C37-C38-C39	-2.37	112.54	130.48
3	A	4422	PEE	C37-C38-C39	-2.34	112.73	130.48
3	A	4429	PEE	C2-O2-C10	-2.27	112.36	117.80

There are no chirality outliers.

All (432) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	4401	PEE	O4-C10-O2-C2
3	A	4401	PEE	C4-O4P-P-O3P
3	A	4401	PEE	C4-O4P-P-O1P
3	A	4402	PEE	C11-C10-O2-C2
3	A	4402	PEE	C4-O4P-P-O3P
3	A	4403	PEE	C11-C10-O2-C2
3	A	4403	PEE	C4-O4P-P-O3P
3	A	4403	PEE	C4-O4P-P-O1P
3	A	4403	PEE	O4P-C4-C5-N
3	A	4404	PEE	O2-C2-C3-O3
3	A	4404	PEE	C4-O4P-P-O3P
3	A	4404	PEE	C4-O4P-P-O1P
3	A	4404	PEE	O4P-C4-C5-N
3	A	4405	PEE	C11-C10-O2-C2
3	A	4405	PEE	O4-C10-O2-C2
3	A	4405	PEE	C4-O4P-P-O3P
3	A	4405	PEE	C4-O4P-P-O2P
3	A	4405	PEE	C4-O4P-P-O1P
3	A	4410	PEE	C11-C10-O2-C2
3	A	4411	PEE	C11-C10-O2-C2
3	A	4411	PEE	O4-C10-O2-C2
3	A	4411	PEE	C1-O3P-P-O1P
3	A	4411	PEE	O4P-C4-C5-N
3	A	4412	PEE	C1-O3P-P-O1P
3	A	4413	PEE	C11-C10-O2-C2
3	A	4413	PEE	O4P-C4-C5-N
3	A	4418	PEE	C11-C10-O2-C2
3	A	4418	PEE	O3P-C1-C2-O2
3	A	4418	PEE	O2-C2-C3-O3
3	A	4418	PEE	C1-O3P-P-O2P

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Mol	Chain	Res	Type	Atoms
3	A	4418	PEE	C1-O3P-P-O1P
3	A	4418	PEE	C1-O3P-P-O4P
3	A	4418	PEE	O4P-C4-C5-N
3	A	4419	PEE	O2-C2-C3-O3
3	A	4419	PEE	C1-O3P-P-O2P
3	A	4419	PEE	C1-O3P-P-O1P
3	A	4419	PEE	C1-O3P-P-O4P
3	A	4419	PEE	C4-O4P-P-O3P
3	A	4419	PEE	C4-O4P-P-O2P
3	A	4419	PEE	C4-O4P-P-O1P
3	A	4420	PEE	O4-C10-O2-C2
3	A	4420	PEE	O3P-C1-C2-O2
3	A	4420	PEE	C1-O3P-P-O1P
3	A	4420	PEE	C1-O3P-P-O4P
3	A	4420	PEE	C4-O4P-P-O1P
3	A	4420	PEE	O4P-C4-C5-N
3	A	4421	PEE	C11-C10-O2-C2
3	A	4421	PEE	C1-O3P-P-O2P
3	A	4421	PEE	C1-O3P-P-O4P
3	A	4421	PEE	O4P-C4-C5-N
3	A	4422	PEE	C11-C10-O2-C2
3	A	4422	PEE	O4-C10-O2-C2
3	A	4422	PEE	C4-O4P-P-O3P
3	A	4422	PEE	C4-O4P-P-O2P
3	A	4422	PEE	C4-O4P-P-O1P
3	A	4423	PEE	C4-O4P-P-O3P
3	A	4423	PEE	C4-O4P-P-O1P
3	A	4423	PEE	O4P-C4-C5-N
3	A	4425	PEE	C4-O4P-P-O3P
3	A	4425	PEE	C4-O4P-P-O2P
3	A	4427	PEE	C11-C10-O2-C2
3	A	4427	PEE	C4-O4P-P-O3P
3	A	4427	PEE	C4-O4P-P-O2P
3	A	4427	PEE	O4P-C4-C5-N
3	A	4429	PEE	C1-O3P-P-O1P
3	A	4429	PEE	C1-O3P-P-O4P
3	A	4429	PEE	C4-O4P-P-O3P
3	A	4429	PEE	C4-O4P-P-O2P
3	A	4429	PEE	C4-O4P-P-O1P
3	A	4429	PEE	O4P-C4-C5-N
3	A	4405	PEE	O5-C30-O3-C3
3	A	4405	PEE	C31-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
3	A	4402	PEE	O4-C10-O2-C2
3	A	4403	PEE	O4-C10-O2-C2
3	A	4410	PEE	O4-C10-O2-C2
3	A	4413	PEE	O4-C10-O2-C2
3	A	4418	PEE	O4-C10-O2-C2
3	A	4421	PEE	O4-C10-O2-C2
3	A	4427	PEE	O4-C10-O2-C2
3	A	4401	PEE	C11-C10-O2-C2
3	A	4420	PEE	C11-C10-O2-C2
3	A	4425	PEE	C31-C30-O3-C3
3	A	4425	PEE	O5-C30-O3-C3
3	A	4422	PEE	C30-C31-C32-C33
3	A	4429	PEE	O2-C2-C3-O3
3	A	4411	PEE	C10-C11-C12-C13
3	A	4421	PEE	C30-C31-C32-C33
3	A	4401	PEE	C10-C11-C12-C13
3	A	4403	PEE	C10-C11-C12-C13
3	A	4413	PEE	C10-C11-C12-C13
3	A	4419	PEE	C10-C11-C12-C13
3	A	4423	PEE	C10-C11-C12-C13
3	A	4403	PEE	C30-C31-C32-C33
3	A	4403	PEE	C32-C33-C34-C35
3	A	4425	PEE	C42-C43-C44-C45
3	A	4411	PEE	C30-C31-C32-C33
3	A	4423	PEE	C11-C10-O2-C2
3	A	4423	PEE	O4-C10-O2-C2
3	A	4427	PEE	C31-C30-O3-C3
3	A	4422	PEE	C31-C30-O3-C3
3	A	4412	PEE	C10-C11-C12-C13
3	A	4403	PEE	C20-C21-C22-C23
3	A	4405	PEE	C12-C13-C14-C15
4	A	4414	R16	C36-C37-C38-C39
3	A	4402	PEE	C34-C35-C36-C37
3	A	4403	PEE	C13-C14-C15-C16
3	A	4425	PEE	C31-C32-C33-C34
3	A	4405	PEE	C11-C12-C13-C14
3	A	4419	PEE	C31-C32-C33-C34
4	A	4409	R16	C36-C37-C38-C39
3	A	4410	PEE	C30-C31-C32-C33
3	A	4420	PEE	C10-C11-C12-C13
3	A	4425	PEE	C30-C31-C32-C33
3	A	4421	PEE	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
3	A	4420	PEE	C32-C33-C34-C35
3	A	4425	PEE	C34-C35-C36-C37
3	A	4419	PEE	C43-C44-C45-C46
3	A	4429	PEE	C11-C12-C13-C14
4	A	4408	R16	C37-C38-C39-C40
4	A	4414	R16	C32-C33-C34-C35
3	A	4401	PEE	C21-C22-C23-C24
3	A	4403	PEE	C34-C35-C36-C37
3	A	4405	PEE	C31-C32-C33-C34
3	A	4421	PEE	C32-C33-C34-C35
4	A	4407	R16	C32-C33-C34-C35
3	A	4402	PEE	C13-C14-C15-C16
3	A	4412	PEE	C12-C13-C14-C15
3	A	4412	PEE	C22-C23-C24-C25
3	A	4419	PEE	C42-C43-C44-C45
3	A	4423	PEE	C31-C32-C33-C34
3	A	4402	PEE	C30-C31-C32-C33
3	A	4404	PEE	C30-C31-C32-C33
3	A	4404	PEE	C13-C14-C15-C16
3	A	4404	PEE	C40-C41-C42-C43
3	A	4420	PEE	C31-C32-C33-C34
3	A	4413	PEE	C14-C15-C16-C17
3	A	4419	PEE	C21-C22-C23-C24
3	A	4422	PEE	C14-C15-C16-C17
3	A	4420	PEE	C34-C35-C36-C37
3	A	4422	PEE	C31-C32-C33-C34
3	A	4420	PEE	C14-C15-C16-C17
3	A	4429	PEE	C31-C32-C33-C34
3	A	4422	PEE	O5-C30-O3-C3
3	A	4427	PEE	O5-C30-O3-C3
3	A	4418	PEE	C35-C36-C37-C38
3	A	4425	PEE	C35-C36-C37-C38
3	A	4404	PEE	C22-C23-C24-C25
3	A	4401	PEE	C22-C23-C24-C25
3	A	4404	PEE	C21-C22-C23-C24
3	A	4405	PEE	C34-C35-C36-C37
3	A	4404	PEE	C14-C15-C16-C17
3	A	4401	PEE	C14-C15-C16-C17
3	A	4404	PEE	C10-C11-C12-C13
3	A	4403	PEE	C21-C22-C23-C24
3	A	4405	PEE	C14-C15-C16-C17
3	A	4419	PEE	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
3	A	4425	PEE	C40-C41-C42-C43
3	A	4421	PEE	C18-C19-C20-C21
3	A	4425	PEE	C11-C10-O2-C2
3	A	4401	PEE	C32-C33-C34-C35
3	A	4422	PEE	C22-C23-C24-C25
3	A	4404	PEE	C15-C16-C17-C18
3	A	4412	PEE	C19-C20-C21-C22
3	A	4420	PEE	C35-C36-C37-C38
3	A	4402	PEE	C31-C32-C33-C34
3	A	4418	PEE	C33-C34-C35-C36
3	A	4425	PEE	C10-C11-C12-C13
3	A	4405	PEE	O3P-C1-C2-O2
3	A	4421	PEE	O3P-C1-C2-O2
4	A	4430	R16	C29-C30-C31-C32
3	A	4402	PEE	C32-C33-C34-C35
3	A	4412	PEE	O2-C2-C3-O3
3	A	4421	PEE	C15-C16-C17-C18
3	A	4423	PEE	O2-C2-C3-O3
3	A	4420	PEE	C13-C14-C15-C16
3	A	4404	PEE	C12-C13-C14-C15
3	A	4404	PEE	C16-C17-C18-C19
3	A	4401	PEE	C34-C35-C36-C37
3	A	4413	PEE	C23-C24-C25-C26
3	A	4425	PEE	O4-C10-O2-C2
3	A	4418	PEE	C31-C32-C33-C34
3	A	4418	PEE	C34-C35-C36-C37
3	A	4413	PEE	C32-C33-C34-C35
3	A	4403	PEE	C12-C13-C14-C15
3	A	4420	PEE	C41-C42-C43-C44
3	A	4404	PEE	C34-C35-C36-C37
4	A	4409	R16	C29-C30-C31-C32
3	A	4412	PEE	C15-C16-C17-C18
3	A	4420	PEE	C19-C20-C21-C22
3	A	4421	PEE	C35-C36-C37-C38
3	A	4403	PEE	C22-C23-C24-C25
3	A	4412	PEE	C21-C22-C23-C24
3	A	4420	PEE	O3P-C1-C2-C3
3	A	4402	PEE	C11-C12-C13-C14
3	A	4425	PEE	C32-C33-C34-C35
3	A	4429	PEE	C30-C31-C32-C33
3	A	4401	PEE	C42-C43-C44-C45
3	A	4421	PEE	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
3	A	4411	PEE	C31-C32-C33-C34
3	A	4418	PEE	C1-C2-C3-O3
3	A	4422	PEE	C1-C2-C3-O3
3	A	4425	PEE	C1-C2-C3-O3
3	A	4429	PEE	C1-C2-C3-O3
3	A	4404	PEE	C35-C36-C37-C38
3	A	4419	PEE	C39-C40-C41-C42
3	A	4410	PEE	C31-C32-C33-C34
3	A	4412	PEE	C14-C15-C16-C17
4	A	4409	R16	C34-C35-C36-C37
3	A	4403	PEE	C11-C12-C13-C14
3	A	4405	PEE	C3-C2-O2-C10
3	A	4419	PEE	C13-C14-C15-C16
3	A	4403	PEE	C19-C20-C21-C22
3	A	4419	PEE	C19-C20-C21-C22
3	A	4403	PEE	C43-C44-C45-C46
4	A	4424	R16	C33-C34-C35-C36
3	A	4403	PEE	O3P-C1-C2-O2
3	A	4422	PEE	O3P-C1-C2-O2
3	A	4427	PEE	O3P-C1-C2-O2
3	A	4425	PEE	C14-C15-C16-C17
4	A	4430	R16	C33-C34-C35-C36
3	A	4423	PEE	C35-C36-C37-C38
3	A	4404	PEE	C31-C32-C33-C34
3	A	4401	PEE	C44-C45-C46-C47
3	A	4425	PEE	C44-C45-C46-C47
3	A	4427	PEE	C13-C14-C15-C16
3	A	4418	PEE	C13-C14-C15-C16
3	A	4421	PEE	C44-C45-C46-C47
3	A	4411	PEE	C13-C14-C15-C16
3	A	4422	PEE	C34-C35-C36-C37
4	A	4409	R16	C31-C32-C33-C34
3	A	4412	PEE	C11-C10-O2-C2
3	A	4404	PEE	C44-C45-C46-C47
3	A	4413	PEE	C21-C22-C23-C24
3	A	4420	PEE	C33-C34-C35-C36
3	A	4410	PEE	C34-C35-C36-C37
3	A	4401	PEE	C38-C39-C40-C41
3	A	4404	PEE	C42-C43-C44-C45
3	A	4404	PEE	C23-C24-C25-C26
3	A	4413	PEE	C12-C13-C14-C15
3	A	4425	PEE	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
3	A	4403	PEE	C14-C15-C16-C17
4	A	4415	R16	C33-C34-C35-C36
3	A	4405	PEE	O3P-C1-C2-C3
3	A	4413	PEE	O3P-C1-C2-C3
3	A	4418	PEE	O3P-C1-C2-C3
3	A	4427	PEE	O3P-C1-C2-C3
3	A	4429	PEE	C11-C10-O2-C2
3	A	4423	PEE	C13-C14-C15-C16
3	A	4418	PEE	C32-C33-C34-C35
3	A	4420	PEE	C23-C24-C25-C26
4	A	4407	R16	C28-C29-C30-C31
3	A	4420	PEE	C40-C41-C42-C43
3	A	4420	PEE	C11-C12-C13-C14
3	A	4402	PEE	C15-C16-C17-C18
3	A	4420	PEE	C42-C43-C44-C45
3	A	4425	PEE	C43-C44-C45-C46
4	A	4415	R16	C34-C35-C36-C37
3	A	4401	PEE	C1-C2-C3-O3
3	A	4412	PEE	C1-C2-C3-O3
3	A	4413	PEE	C1-C2-C3-O3
3	A	4423	PEE	C1-C2-C3-O3
3	A	4427	PEE	C1-C2-C3-O3
3	A	4401	PEE	C23-C24-C25-C26
4	A	4407	R16	C34-C35-C36-C37
3	A	4412	PEE	O3P-C1-C2-O2
4	A	4407	R16	C29-C30-C31-C32
3	A	4421	PEE	C31-C30-O3-C3
3	A	4423	PEE	C34-C35-C36-C37
3	A	4420	PEE	C20-C21-C22-C23
3	A	4419	PEE	C38-C39-C40-C41
3	A	4405	PEE	C13-C14-C15-C16
3	A	4404	PEE	C31-C30-O3-C3
3	A	4420	PEE	C31-C30-O3-C3
4	A	4406	R16	C27-C28-C29-C30
3	A	4422	PEE	C20-C21-C22-C23
3	A	4421	PEE	O3P-C1-C2-C3
3	A	4422	PEE	O3P-C1-C2-C3
4	A	4409	R16	C33-C34-C35-C36
3	A	4420	PEE	C44-C45-C46-C47
3	A	4427	PEE	C30-C31-C32-C33
4	A	4416	R16	C30-C31-C32-C33
3	A	4421	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
3	A	4402	PEE	C10-C11-C12-C13
3	A	4403	PEE	C31-C32-C33-C34
3	A	4423	PEE	C32-C33-C34-C35
4	A	4424	R16	C30-C31-C32-C33
3	A	4405	PEE	C32-C33-C34-C35
3	A	4402	PEE	O3P-C1-C2-O2
3	A	4411	PEE	O3P-C1-C2-O2
3	A	4413	PEE	O3P-C1-C2-O2
3	A	4411	PEE	C34-C35-C36-C37
3	A	4404	PEE	C1-C2-C3-O3
3	A	4419	PEE	C1-C2-C3-O3
3	A	4420	PEE	O5-C30-O3-C3
3	A	4401	PEE	O2-C2-C3-O3
3	A	4422	PEE	C12-C13-C14-C15
4	A	4430	R16	C31-C32-C33-C34
3	A	4404	PEE	O5-C30-O3-C3
3	A	4429	PEE	C10-C11-C12-C13
3	A	4419	PEE	C40-C41-C42-C43
3	A	4425	PEE	C11-C12-C13-C14
3	A	4411	PEE	C2-C1-O3P-P
4	A	4409	R16	C35-C36-C37-C38
3	A	4412	PEE	O4-C10-O2-C2
3	A	4429	PEE	O4-C10-O2-C2
3	A	4403	PEE	C35-C36-C37-C38
3	A	4420	PEE	C30-C31-C32-C33
3	A	4427	PEE	C11-C12-C13-C14
3	A	4410	PEE	C31-C30-O3-C3
3	A	4420	PEE	C21-C22-C23-C24
3	A	4421	PEE	C13-C14-C15-C16
3	A	4403	PEE	C23-C24-C25-C26
3	A	4421	PEE	C36-C37-C38-C39
3	A	4402	PEE	O3P-C1-C2-C3
3	A	4403	PEE	O3P-C1-C2-C3
3	A	4419	PEE	O3P-C1-C2-C3
3	A	4425	PEE	C33-C34-C35-C36
4	A	4424	R16	C32-C33-C34-C35
3	A	4413	PEE	C31-C30-O3-C3
3	A	4402	PEE	O2-C10-C11-C12
3	A	4419	PEE	O3P-C1-C2-O2
3	A	4404	PEE	C32-C33-C34-C35
3	A	4423	PEE	C11-C12-C13-C14
3	A	4410	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
3	A	4413	PEE	O5-C30-O3-C3
3	A	4413	PEE	O2-C2-C3-O3
3	A	4422	PEE	O2-C2-C3-O3
3	A	4427	PEE	O2-C2-C3-O3
3	A	4410	PEE	C11-C12-C13-C14
3	A	4422	PEE	C13-C14-C15-C16
3	A	4401	PEE	C12-C13-C14-C15
3	A	4401	PEE	C1-O3P-P-O2P
3	A	4401	PEE	C1-O3P-P-O1P
3	A	4401	PEE	C1-O3P-P-O4P
3	A	4401	PEE	C4-O4P-P-O2P
3	A	4401	PEE	O4P-C4-C5-N
3	A	4402	PEE	C4-O4P-P-O1P
3	A	4410	PEE	C1-O3P-P-O1P
3	A	4410	PEE	C4-O4P-P-O1P
3	A	4411	PEE	C1-O3P-P-O2P
3	A	4411	PEE	C1-O3P-P-O4P
3	A	4412	PEE	C1-O3P-P-O2P
3	A	4412	PEE	C1-O3P-P-O4P
3	A	4412	PEE	C4-O4P-P-O1P
3	A	4412	PEE	O4P-C4-C5-N
3	A	4413	PEE	C4-O4P-P-O1P
3	A	4419	PEE	O4P-C4-C5-N
3	A	4420	PEE	C4-O4P-P-O3P
3	A	4420	PEE	C4-O4P-P-O2P
3	A	4421	PEE	C4-O4P-P-O1P
3	A	4422	PEE	C1-O3P-P-O1P
3	A	4422	PEE	O4P-C4-C5-N
3	A	4425	PEE	C1-O3P-P-O1P
3	A	4425	PEE	C4-O4P-P-O1P
3	A	4427	PEE	C4-O4P-P-O1P
4	A	4406	R16	C31-C32-C33-C34
3	A	4405	PEE	C2-C1-O3P-P
3	A	4403	PEE	C42-C43-C44-C45
4	A	4424	R16	C34-C35-C36-C37
3	A	4425	PEE	C3-C2-O2-C10
4	A	4408	R16	C32-C33-C34-C35
3	A	4425	PEE	C13-C14-C15-C16
3	A	4423	PEE	C30-C31-C32-C33
3	A	4419	PEE	C2-C1-O3P-P
3	A	4425	PEE	O2-C2-C3-O3
3	A	4418	PEE	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
3	A	4425	PEE	C18-C19-C20-C21
3	A	4401	PEE	C40-C41-C42-C43
3	A	4404	PEE	C19-C20-C21-C22
3	A	4422	PEE	C35-C36-C37-C38
3	A	4404	PEE	C11-C10-O2-C2
3	A	4419	PEE	C31-C30-O3-C3
3	A	4419	PEE	O5-C30-O3-C3
3	A	4425	PEE	C39-C40-C41-C42
3	A	4404	PEE	O4-C10-O2-C2
3	A	4412	PEE	C23-C24-C25-C26
3	A	4420	PEE	C36-C37-C38-C39
4	A	4416	R16	C29-C30-C31-C32
3	A	4420	PEE	C43-C44-C45-C46
4	A	4414	R16	C31-C32-C33-C34
3	A	4401	PEE	C3-C2-O2-C10
4	A	4428	R16	C31-C32-C33-C34
3	A	4419	PEE	C20-C21-C22-C23
3	A	4419	PEE	C35-C36-C37-C38
3	A	4425	PEE	C2-C1-O3P-P
4	A	4406	R16	C29-C30-C31-C32
4	A	4415	R16	C31-C32-C33-C34
4	A	4424	R16	C29-C30-C31-C32
4	A	4424	R16	C35-C36-C37-C38
4	A	4415	R16	C32-C33-C34-C35
3	A	4420	PEE	C1-C2-C3-O3
3	A	4403	PEE	C18-C19-C20-C21
3	A	4403	PEE	C24-C25-C26-C27
3	A	4411	PEE	O3P-C1-C2-C3
3	A	4412	PEE	O3P-C1-C2-C3
4	A	4414	R16	C33-C34-C35-C36
3	A	4404	PEE	C24-C25-C26-C27
3	A	4420	PEE	C38-C39-C40-C41
3	A	4425	PEE	C36-C37-C38-C39
3	A	4403	PEE	C38-C39-C40-C41
3	A	4429	PEE	C32-C33-C34-C35
3	A	4419	PEE	C12-C13-C14-C15
3	A	4422	PEE	C2-C1-O3P-P
3	A	4401	PEE	C18-C19-C20-C21
3	A	4403	PEE	C36-C37-C38-C39
3	A	4412	PEE	C18-C19-C20-C21
3	A	4429	PEE	O2-C10-C11-C12
4	A	4426	R16	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
3	A	4427	PEE	C32-C33-C34-C35
3	A	4410	PEE	O3P-C1-C2-O2
3	A	4421	PEE	C31-C32-C33-C34
3	A	4422	PEE	C24-C25-C26-C27
3	A	4401	PEE	O3-C30-C31-C32
3	A	4421	PEE	O2-C10-C11-C12
3	A	4419	PEE	C24-C25-C26-C27
3	A	4419	PEE	C11-C12-C13-C14
3	A	4422	PEE	C21-C22-C23-C24
3	A	4412	PEE	O3-C30-C31-C32
3	A	4418	PEE	O5-C30-O3-C3
3	A	4402	PEE	C33-C34-C35-C36
3	A	4423	PEE	O2-C10-C11-C12
3	A	4429	PEE	O4-C10-C11-C12
3	A	4421	PEE	C41-C42-C43-C44
3	A	4401	PEE	O5-C30-C31-C32
3	A	4427	PEE	C2-C1-O3P-P
3	A	4418	PEE	O3-C30-C31-C32
3	A	4420	PEE	C18-C19-C20-C21
3	A	4413	PEE	O2-C10-C11-C12
3	A	4404	PEE	C43-C44-C45-C46
3	A	4413	PEE	C18-C19-C20-C21
3	A	4419	PEE	O2-C10-C11-C12
3	A	4421	PEE	O4-C10-C11-C12

There are no ring outliers.

20 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	4409	R16	1	0
3	A	4405	PEE	3	0
3	A	4412	PEE	4	0
3	A	4425	PEE	2	0
3	A	4403	PEE	5	0
3	A	4402	PEE	1	0
4	A	4415	R16	1	0
3	A	4401	PEE	3	0
3	A	4419	PEE	12	0
3	A	4422	PEE	1	0
3	A	4404	PEE	5	0
3	A	4410	PEE	2	0
3	A	4420	PEE	8	0

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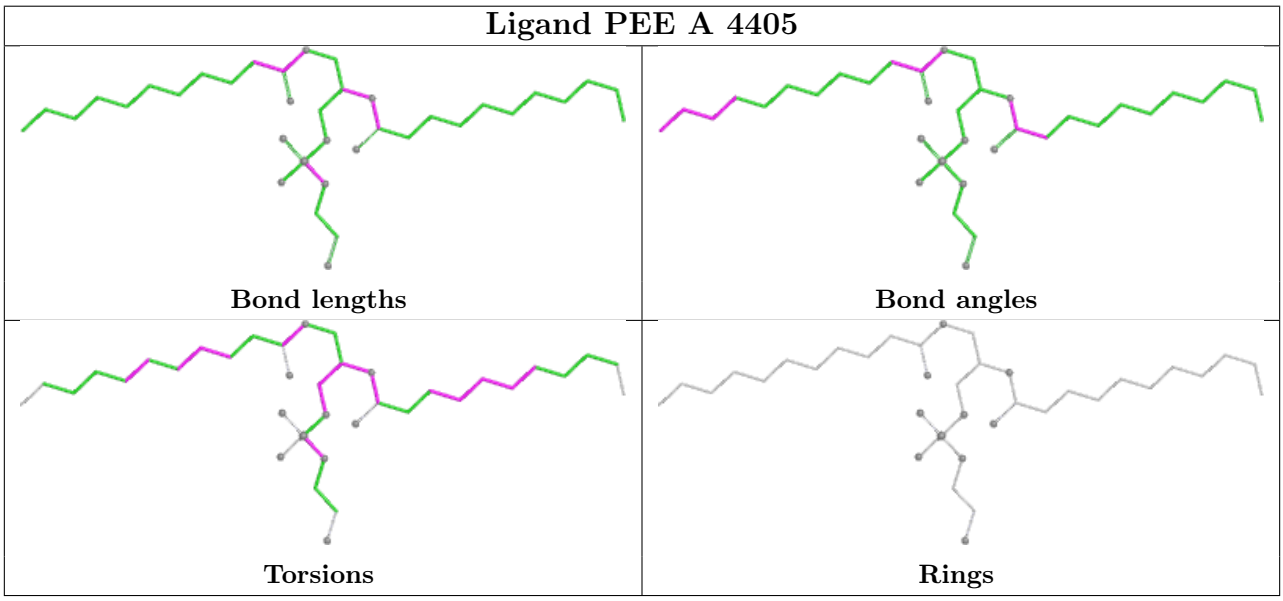
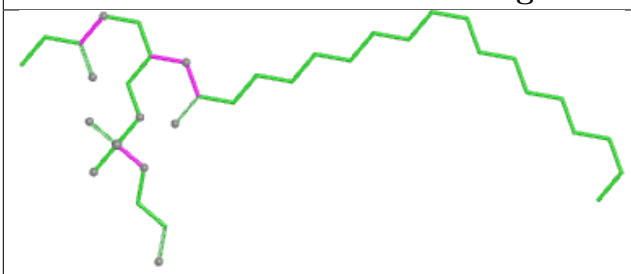
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4423	PEE	1	0
3	A	4421	PEE	3	0
3	A	4413	PEE	7	0
4	A	4406	R16	4	0
4	A	4407	R16	3	0
3	A	4411	PEE	1	0
4	A	4414	R16	2	0

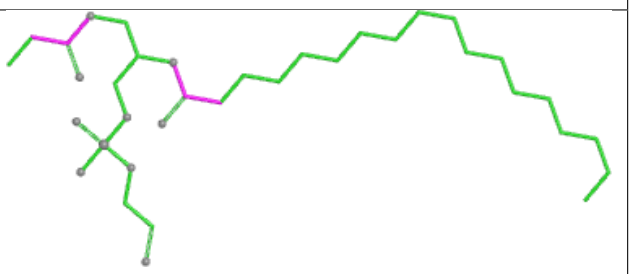
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



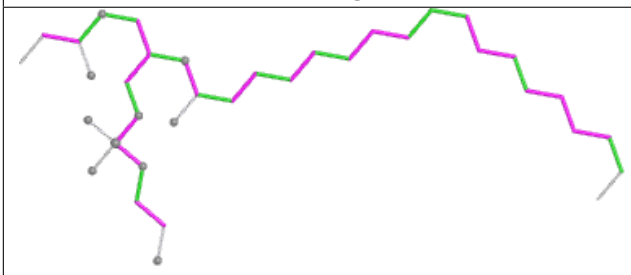
Ligand PEE A 4412



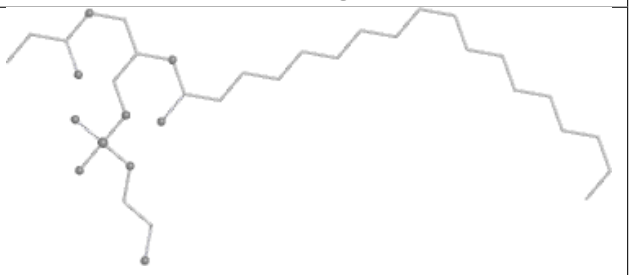
Bond lengths



Bond angles

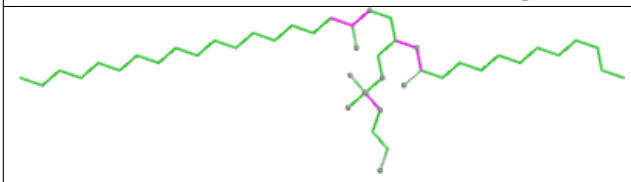


Torsions

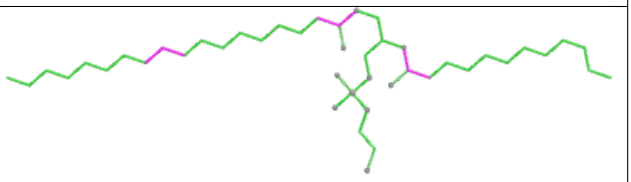


Rings

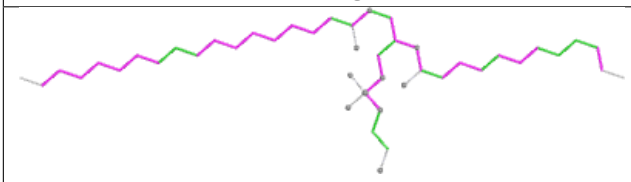
Ligand PEE A 4425



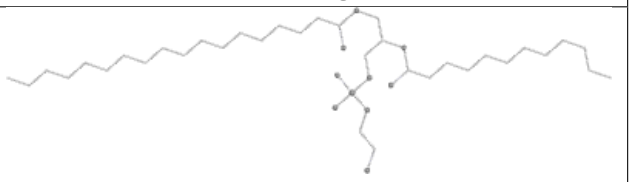
Bond lengths



Bond angles

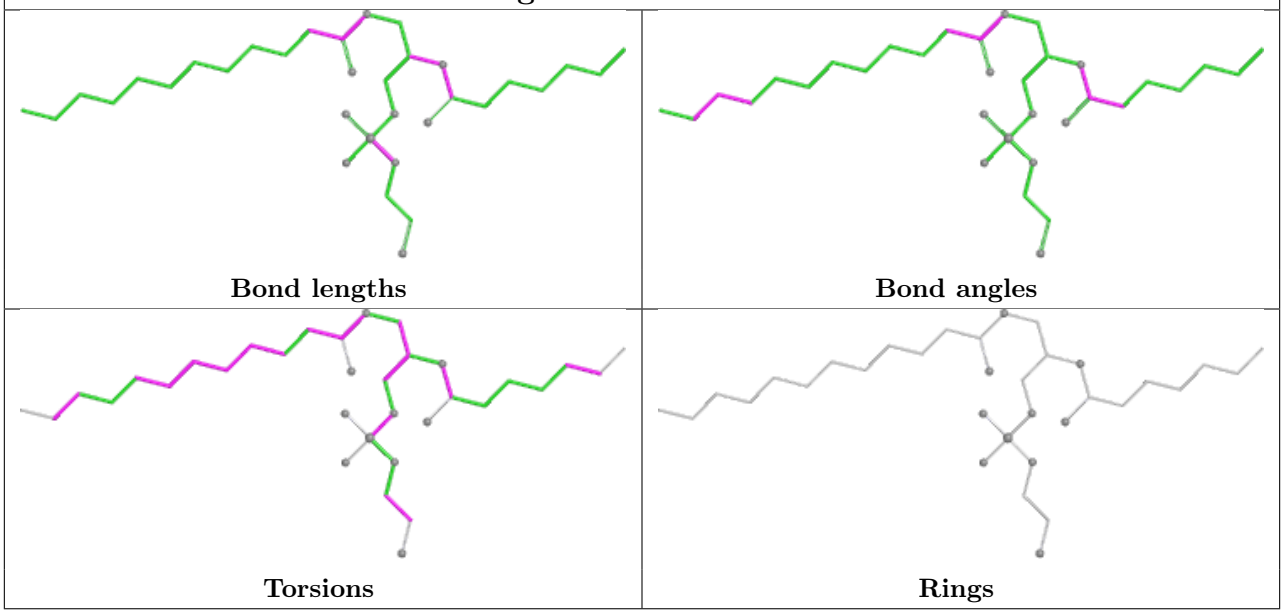


Torsions

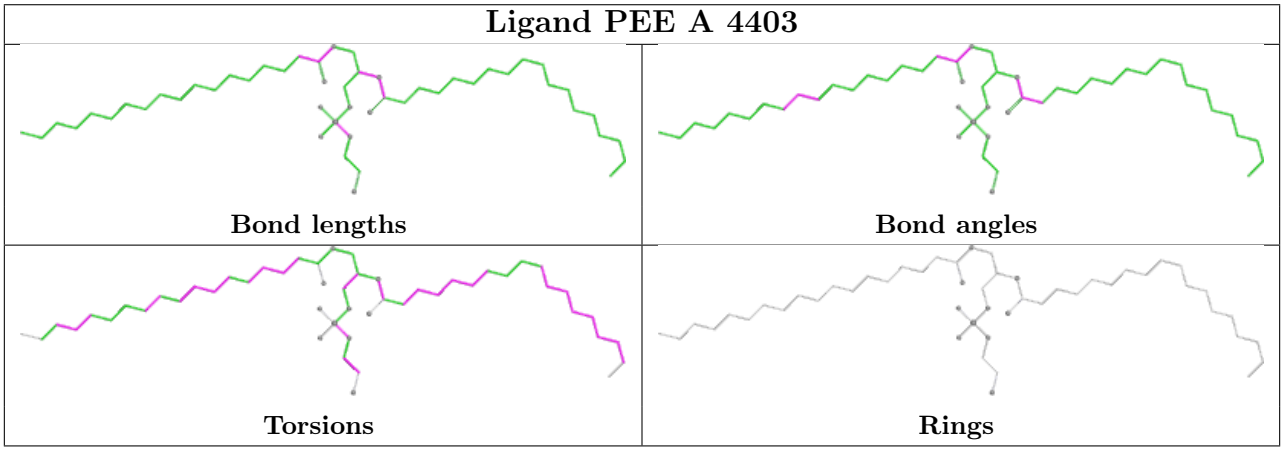


Rings

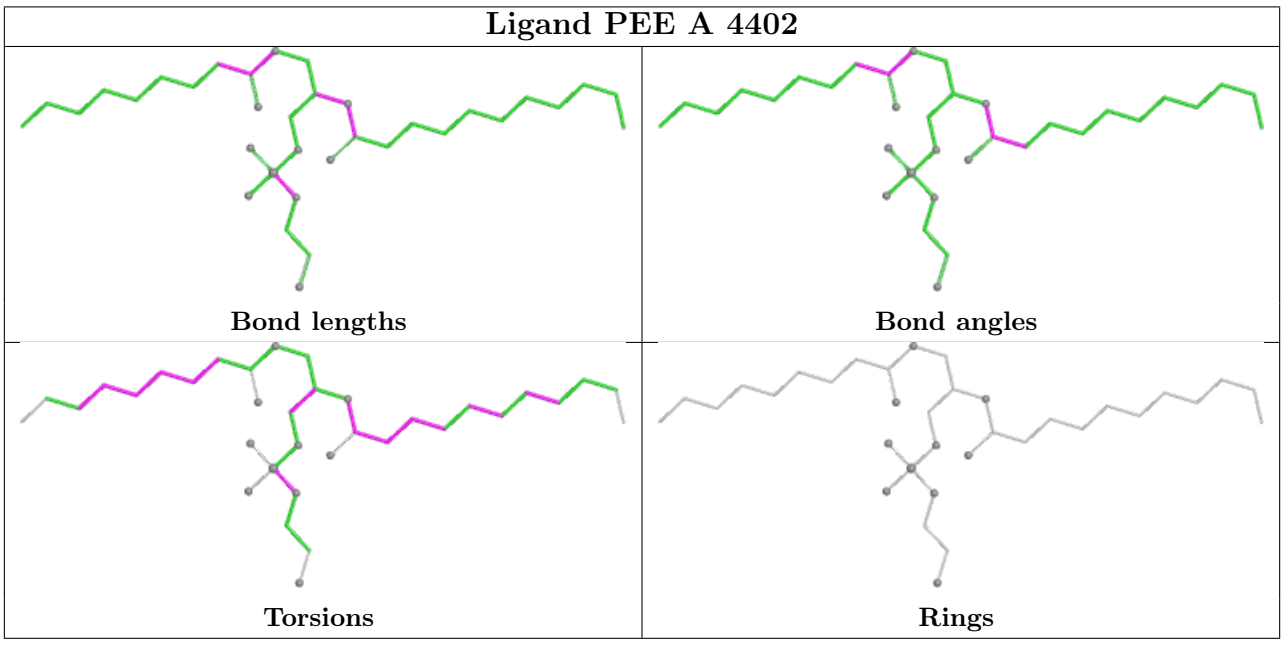
Ligand PEE A 4418



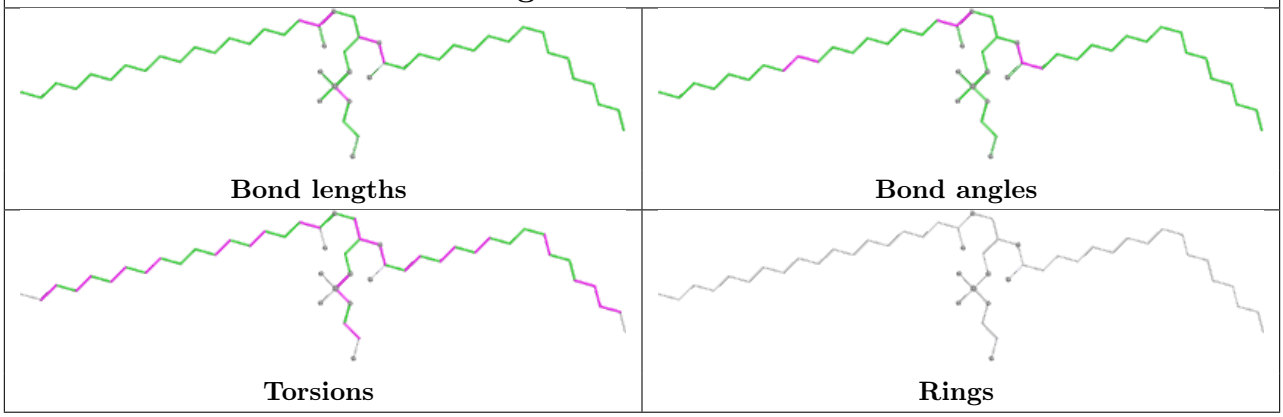
Ligand PEE A 4403



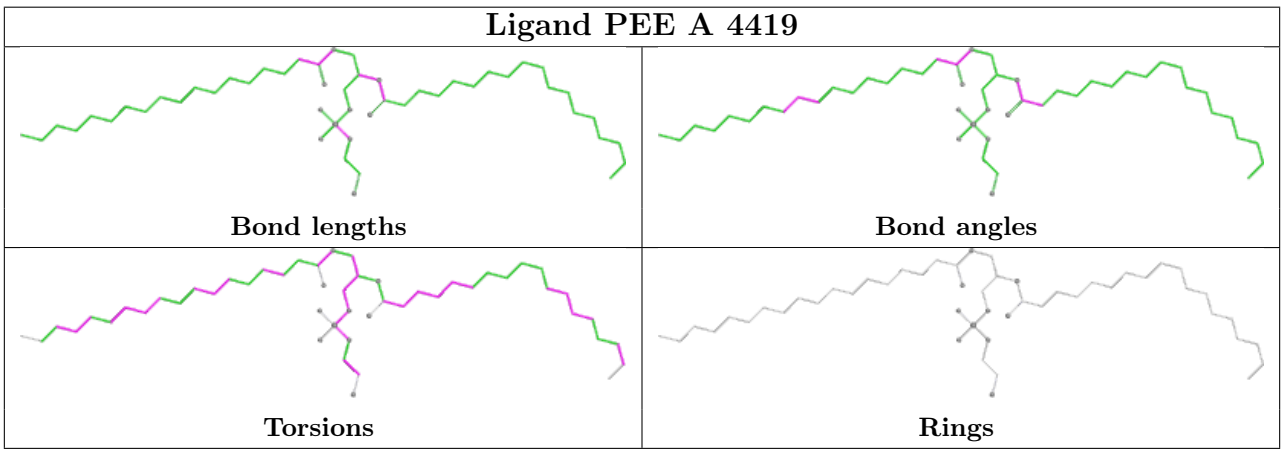
Ligand PEE A 4402



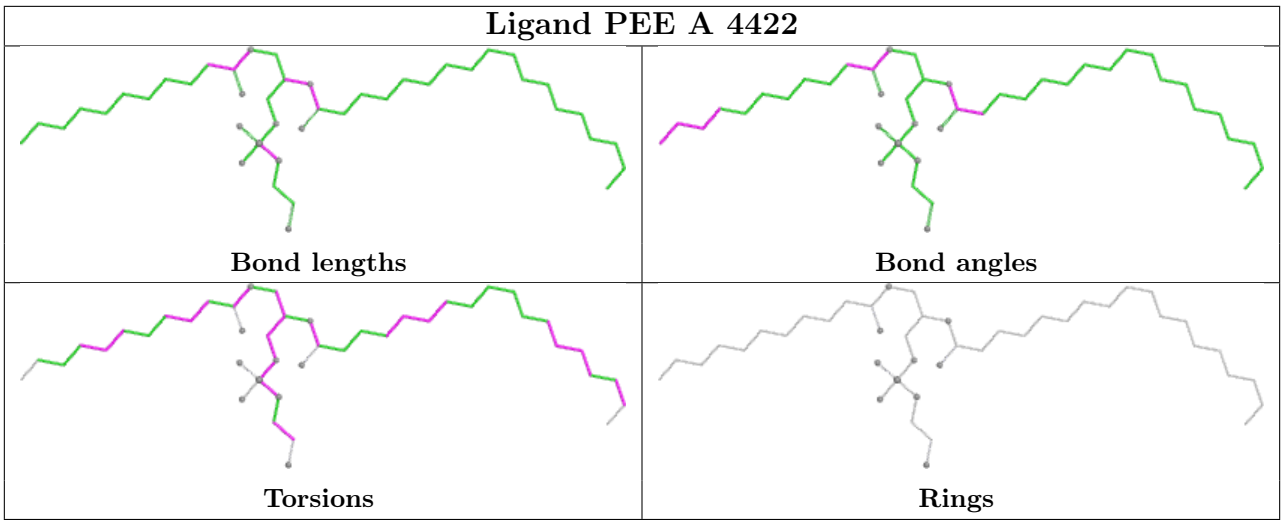
Ligand PEE A 4401



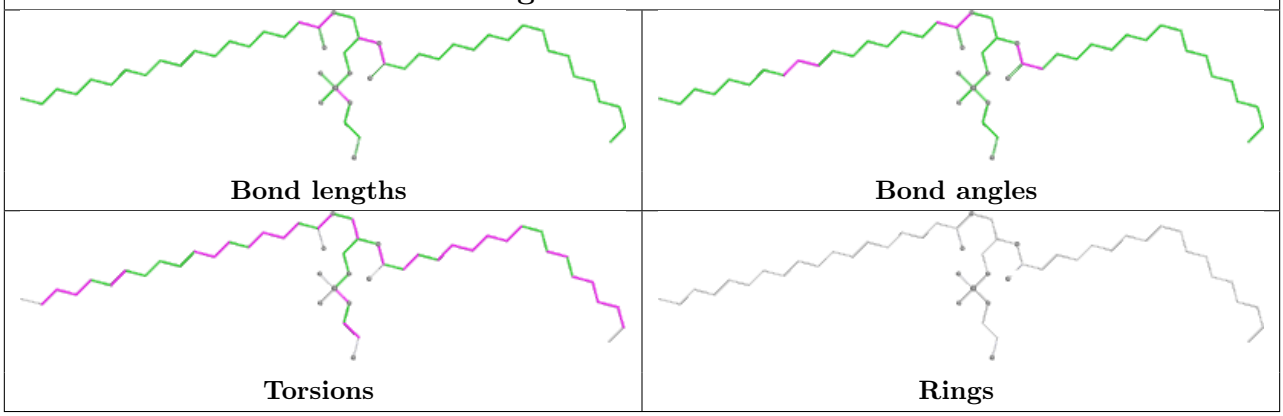
Ligand PEE A 4419



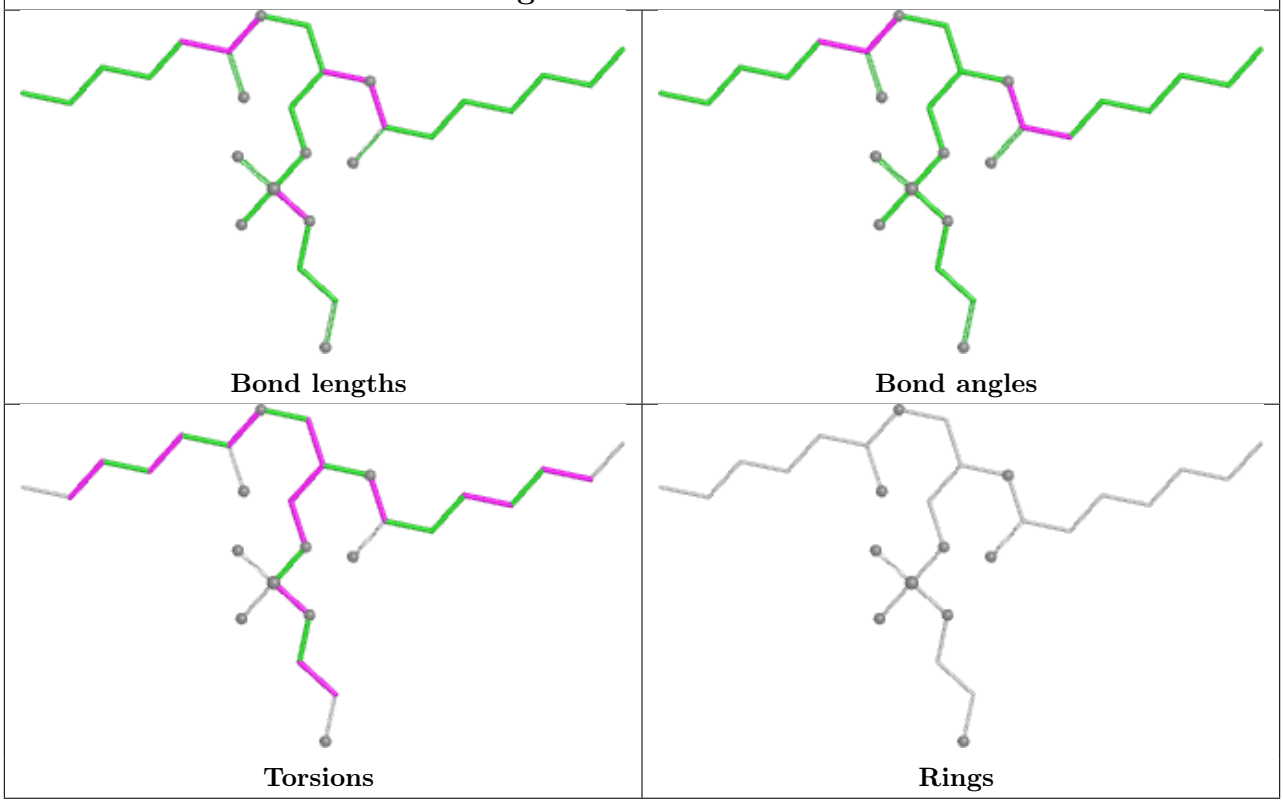
Ligand PEE A 4422



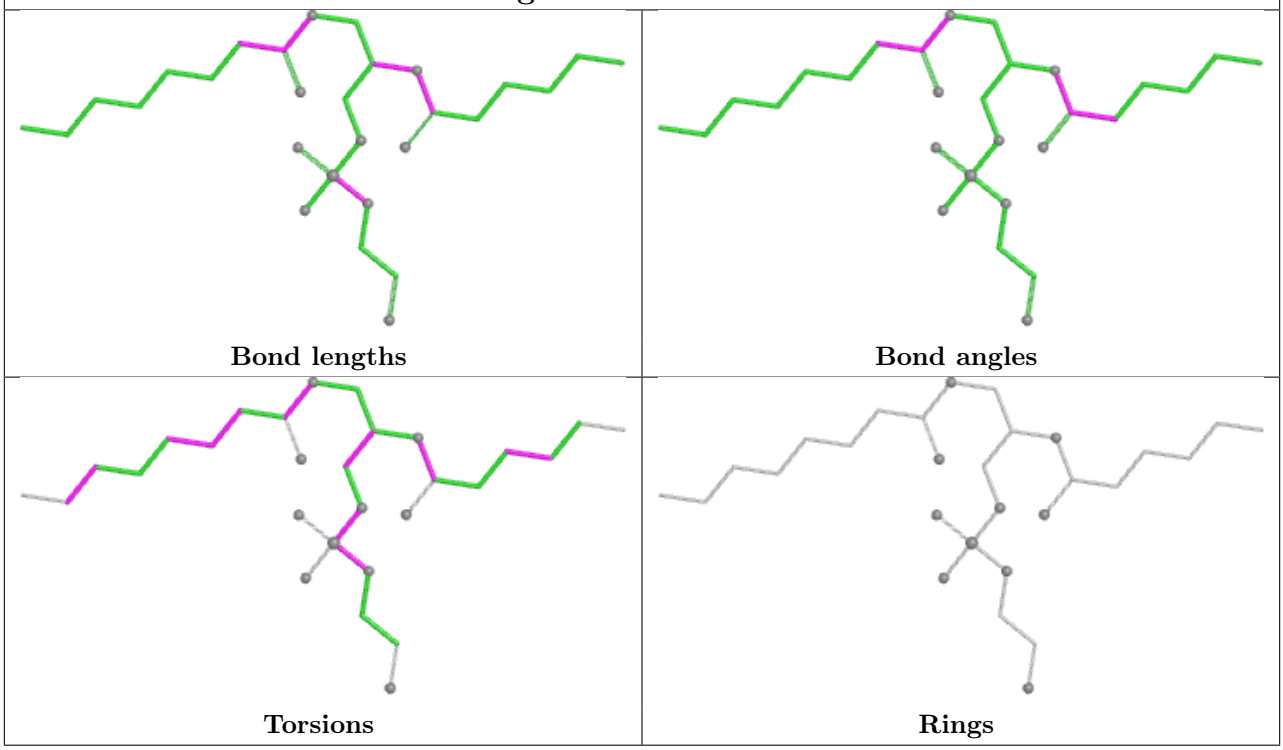
Ligand PEE A 4404



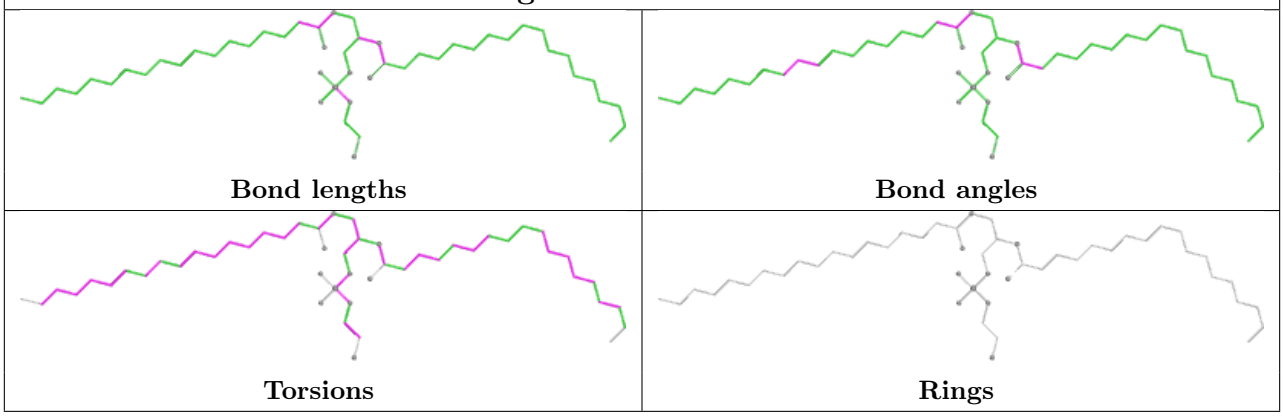
Ligand PEE A 4427



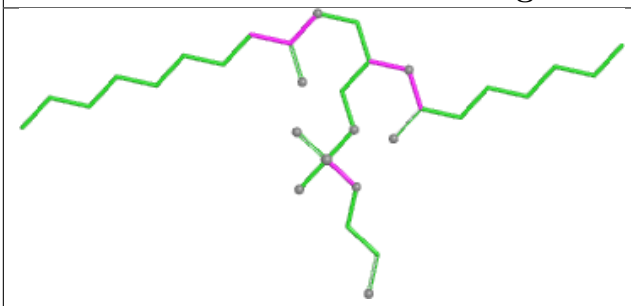
Ligand PEE A 4410



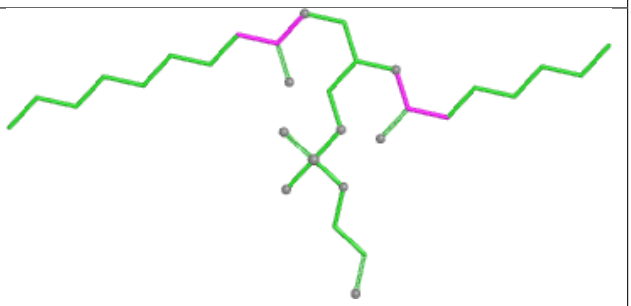
Ligand PEE A 4420



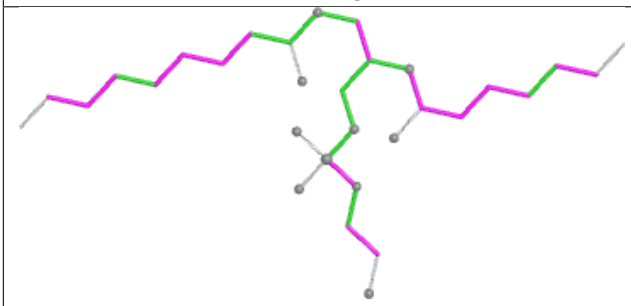
Ligand PEE A 4423



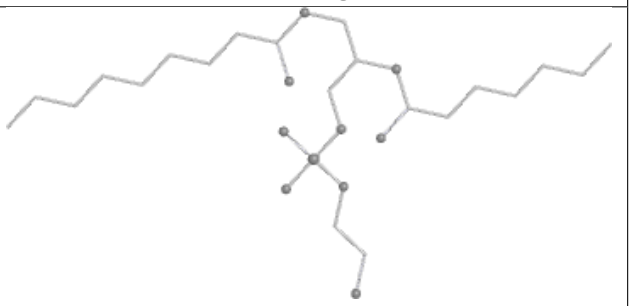
Bond lengths



Bond angles

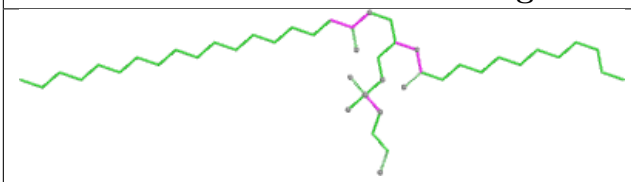


Torsions

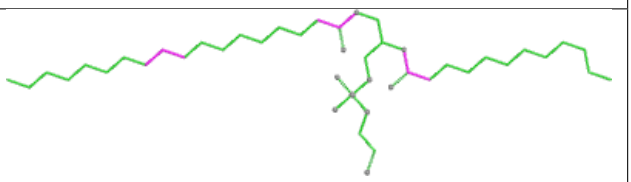


Rings

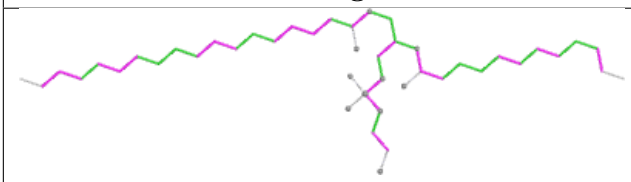
Ligand PEE A 4421



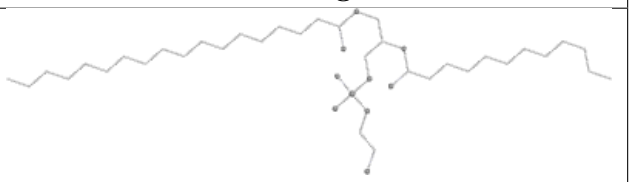
Bond lengths



Bond angles

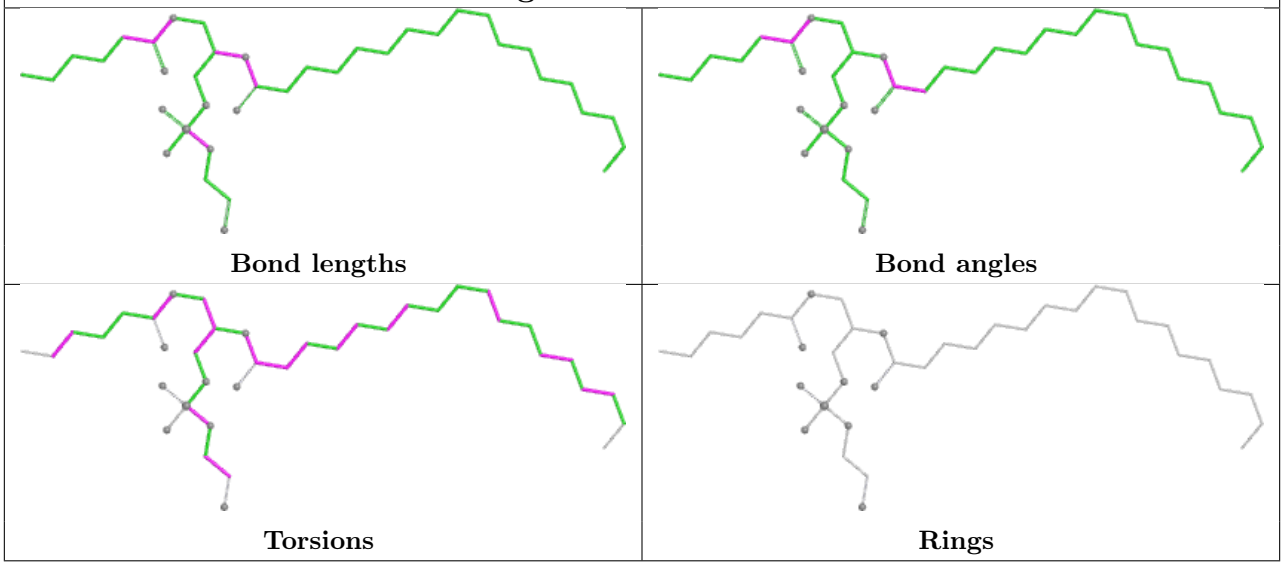


Torsions

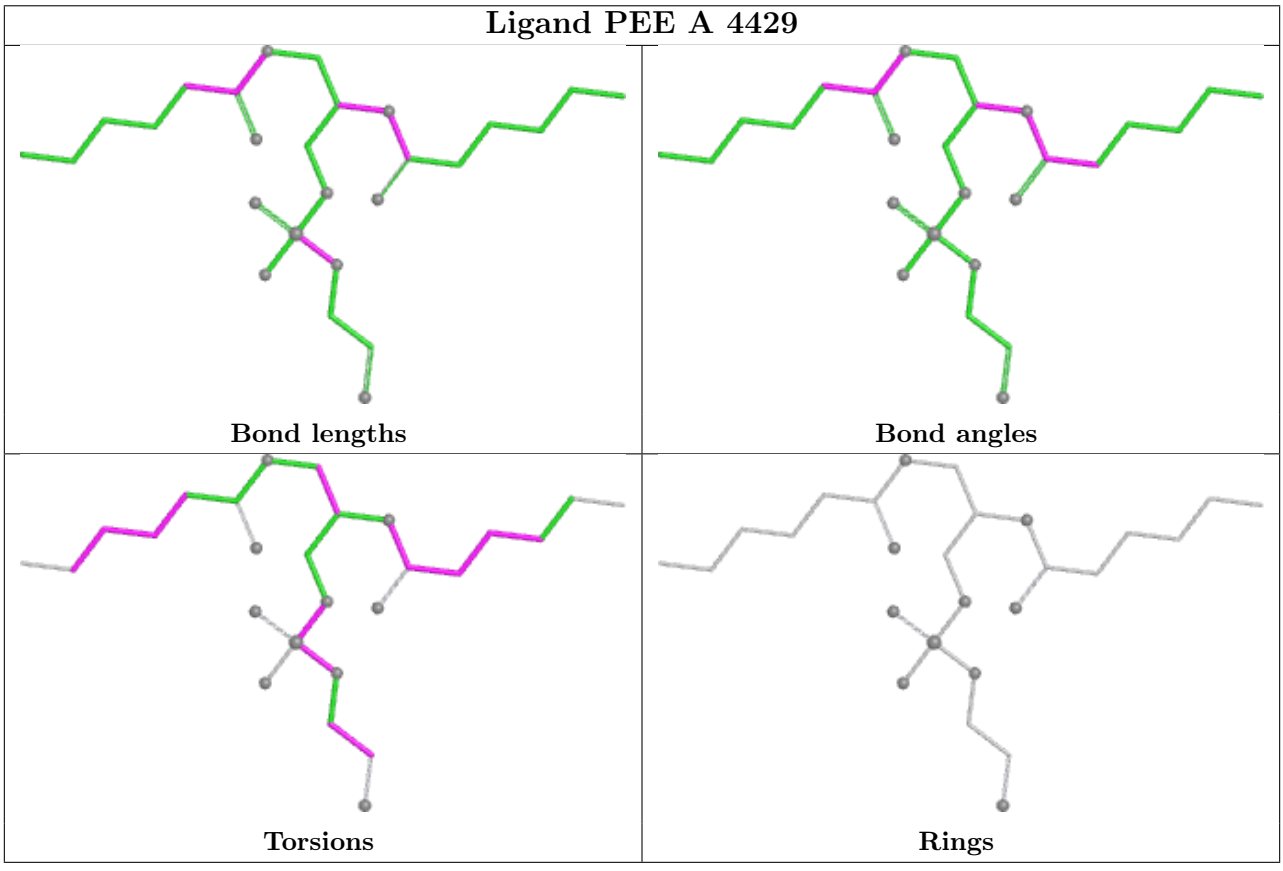


Rings

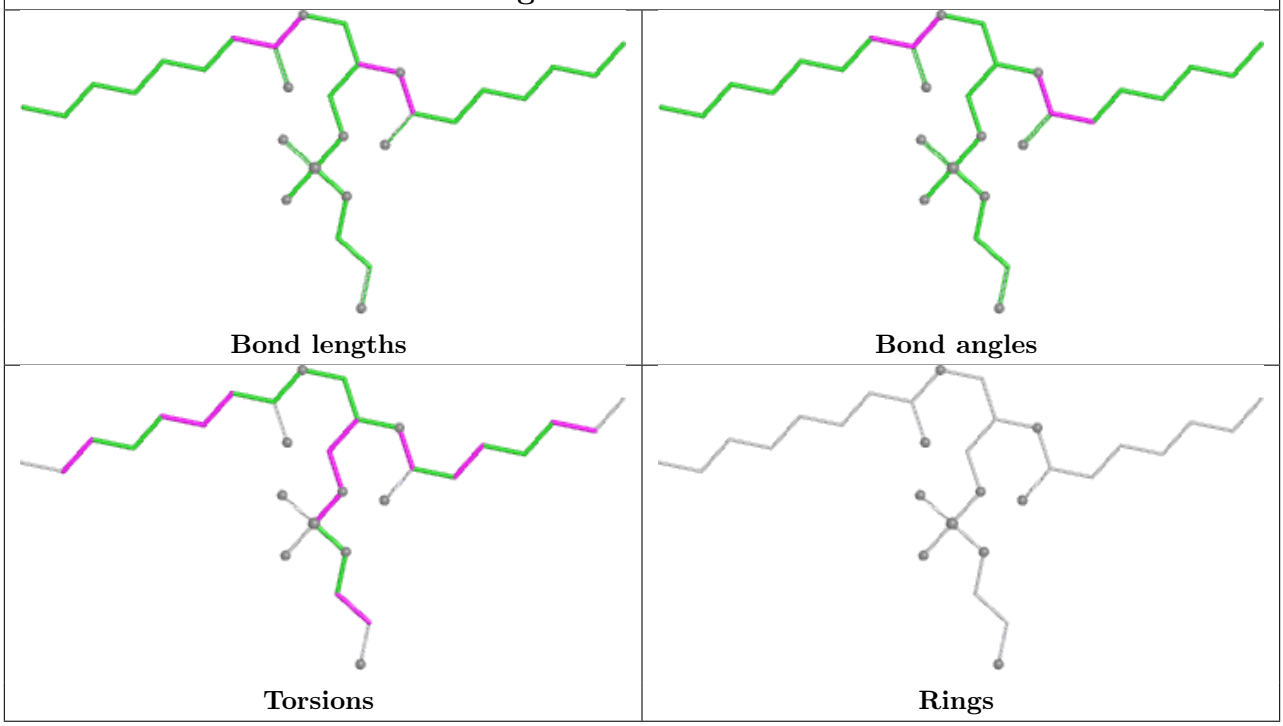
Ligand PEE A 4413



Ligand PEE A 4429



Ligand PEE A 4411



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.

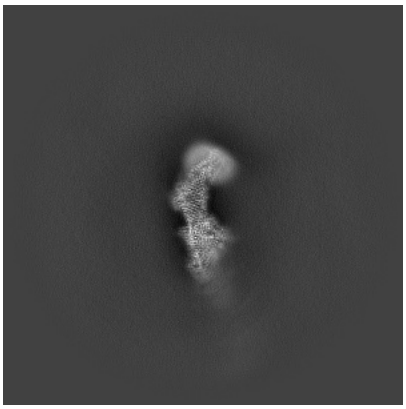
6 Map visualisation

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.

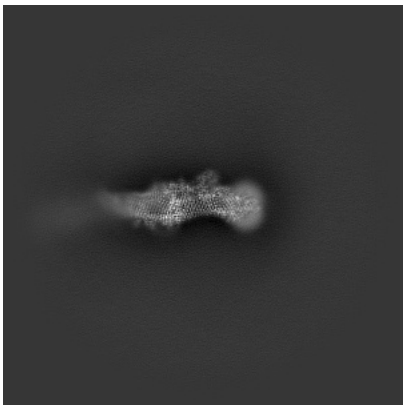
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

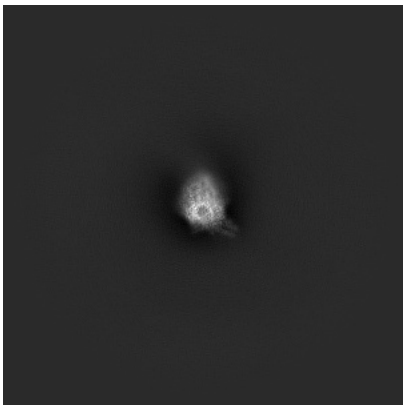
6.1.1 Primary map



X

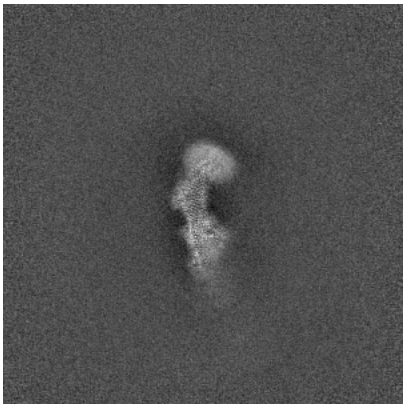


Y

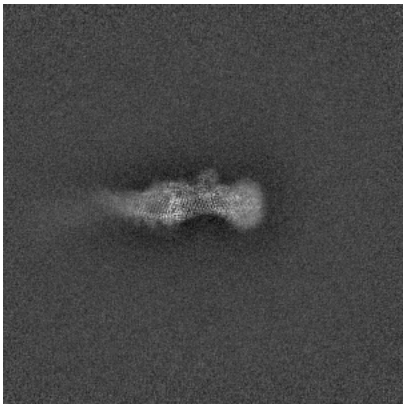


Z

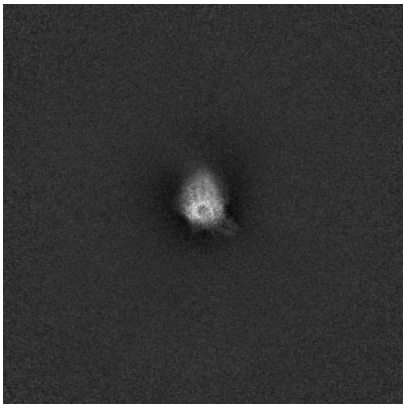
6.1.2 Raw map



X



Y

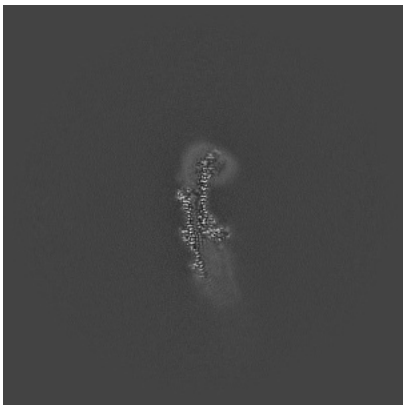


Z

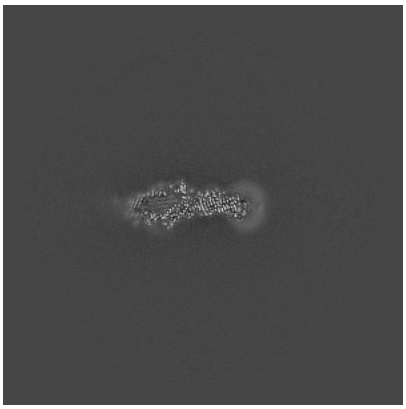
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

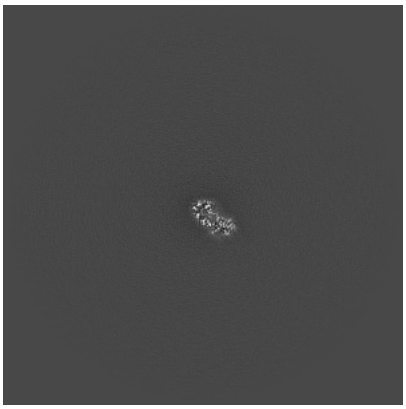
6.2.1 Primary map



X Index: 378

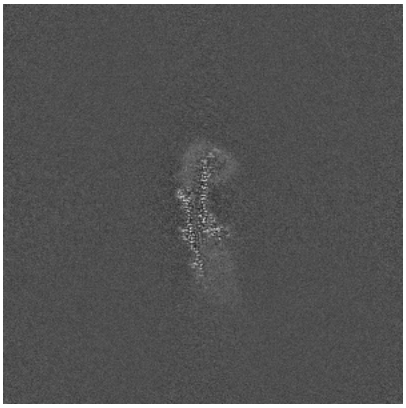


Y Index: 378

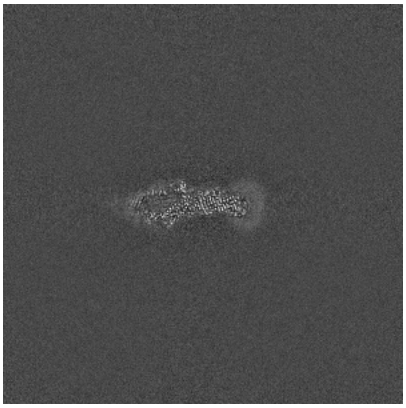


Z Index: 378

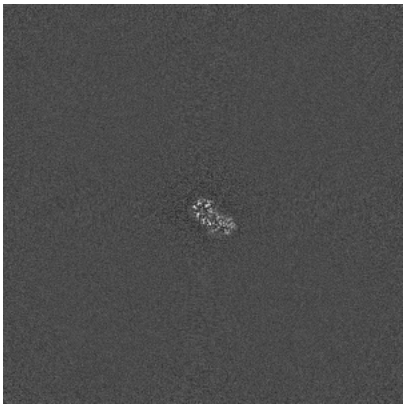
6.2.2 Raw map



X Index: 378



Y Index: 378

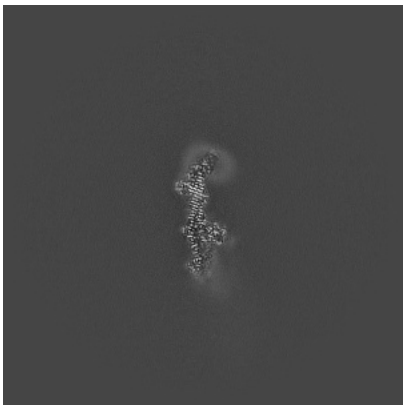


Z Index: 378

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

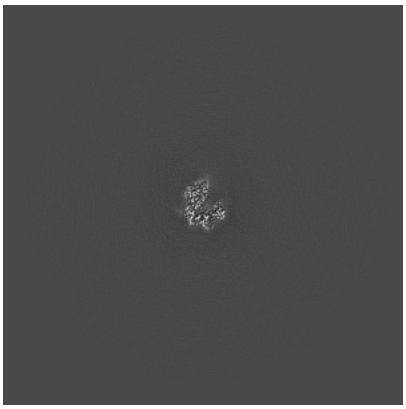
6.3 Largest variance slices (i)

6.3.1 Primary map



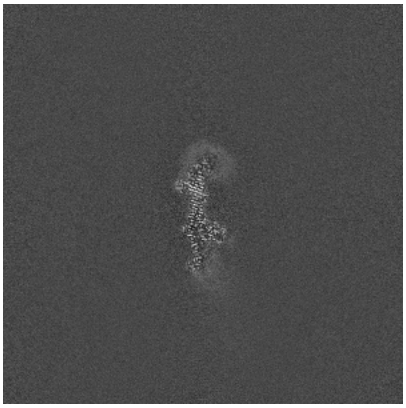
X Index: 365

Y Index: 375

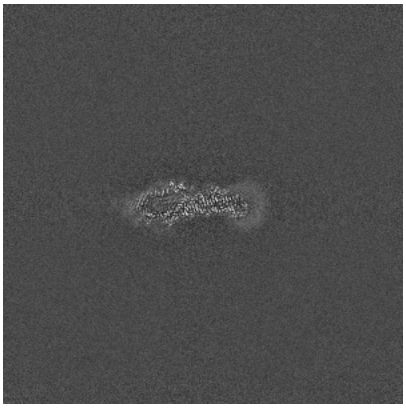


Z Index: 328

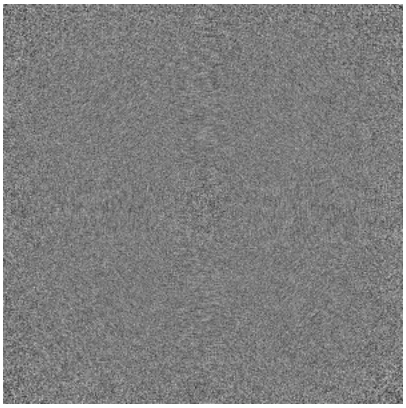
6.3.2 Raw map



X Index: 365



Y Index: 375



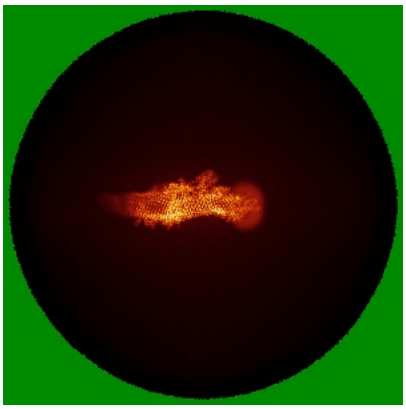
Z Index: 0

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

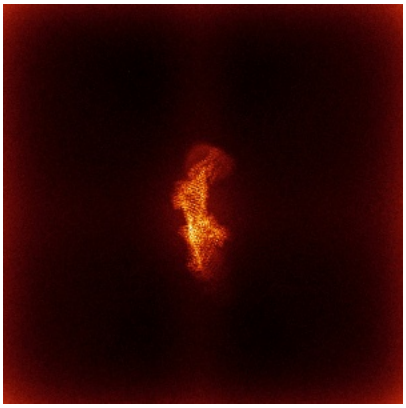
X



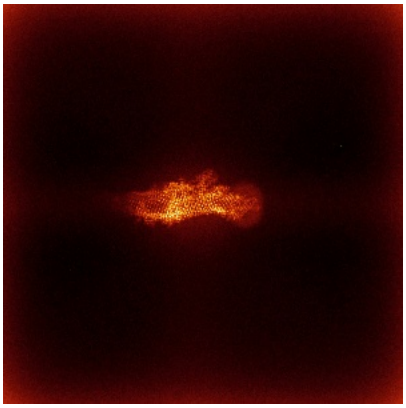
Y

Z

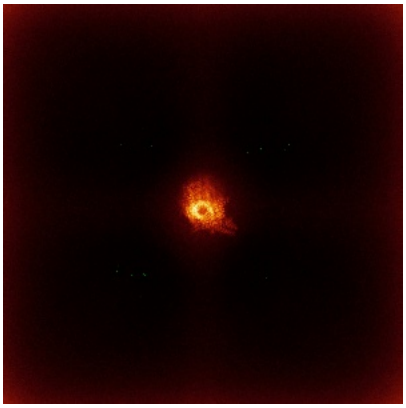
6.4.2 Raw map



X



Y

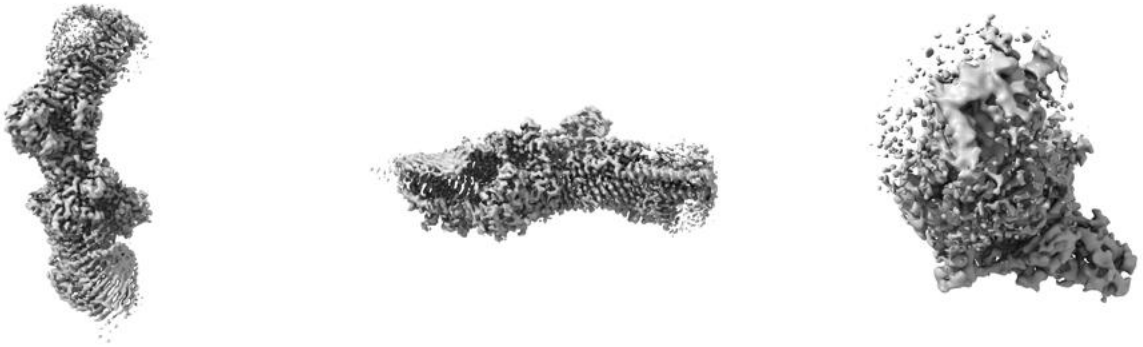


Z

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



X Y Z

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.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

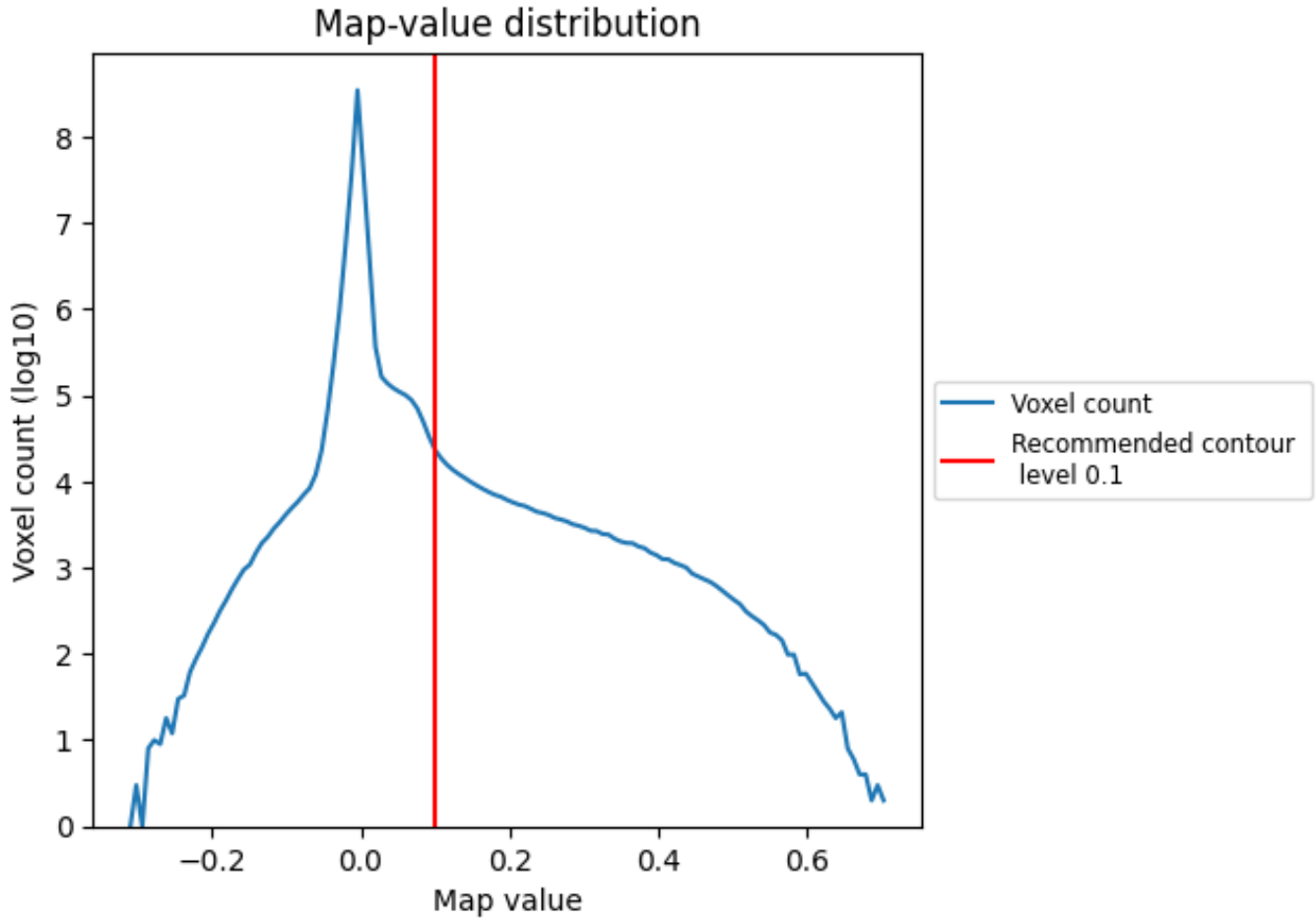
6.6 Mask visualisation (i)

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

7 Map analysis

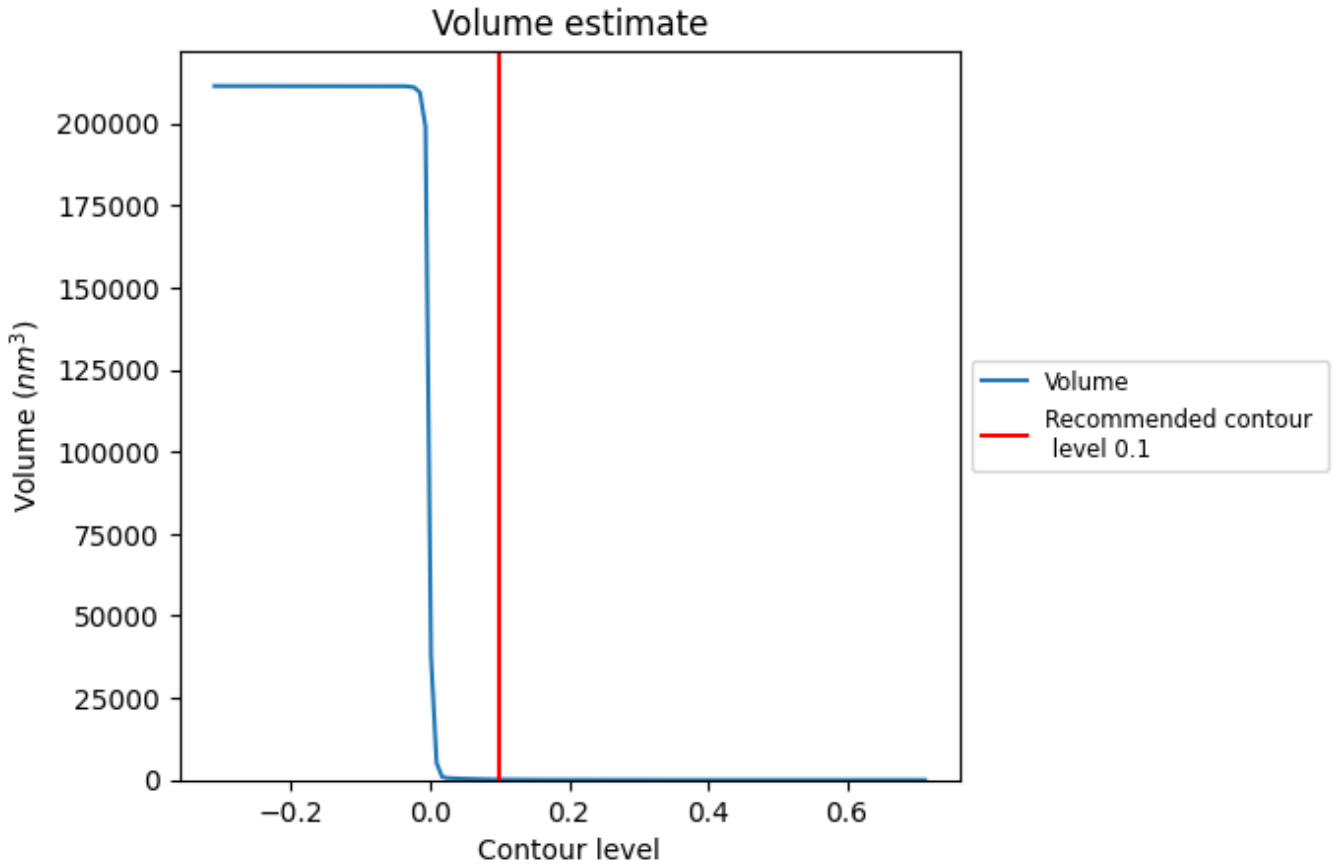
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

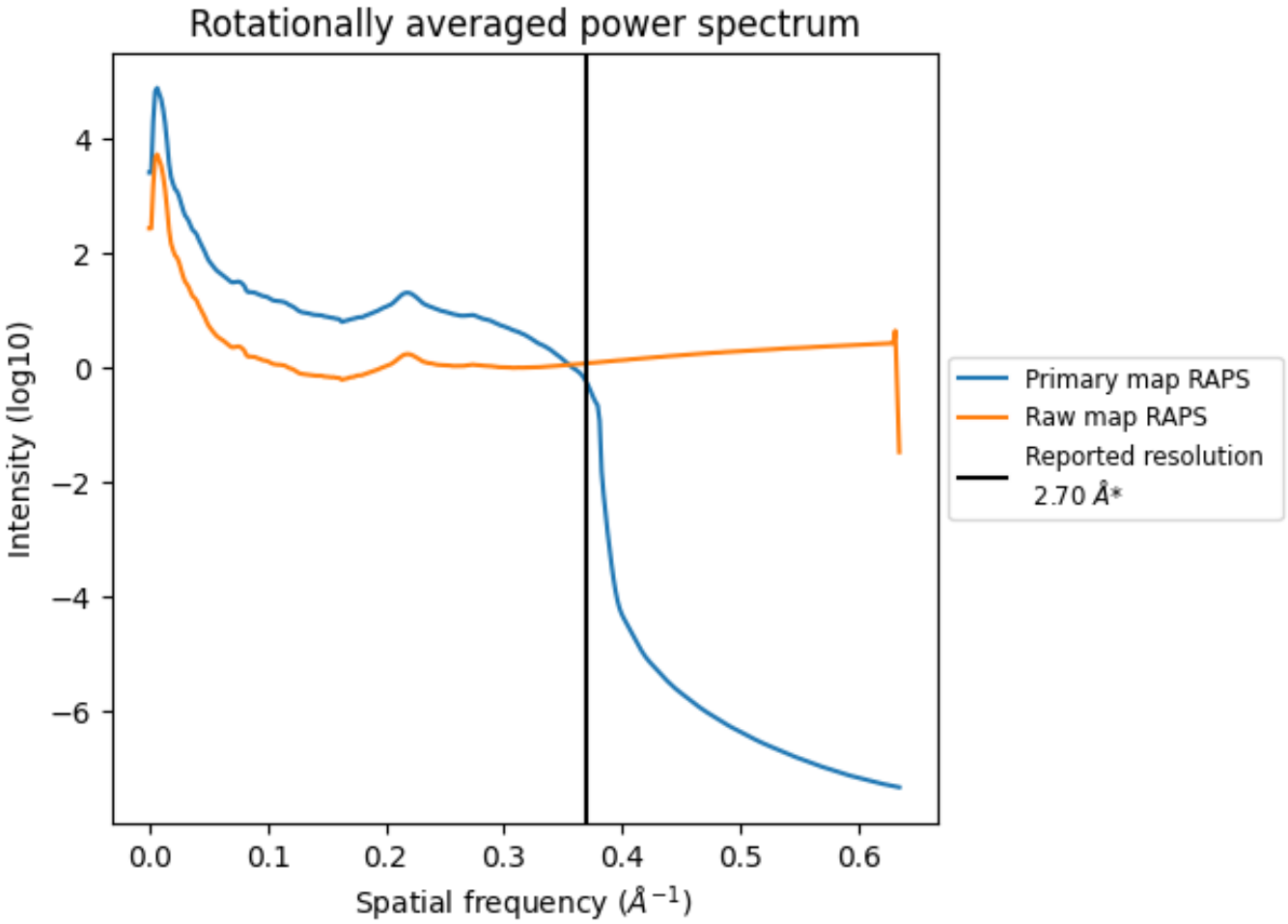
7.2 Volume estimate



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 (i)

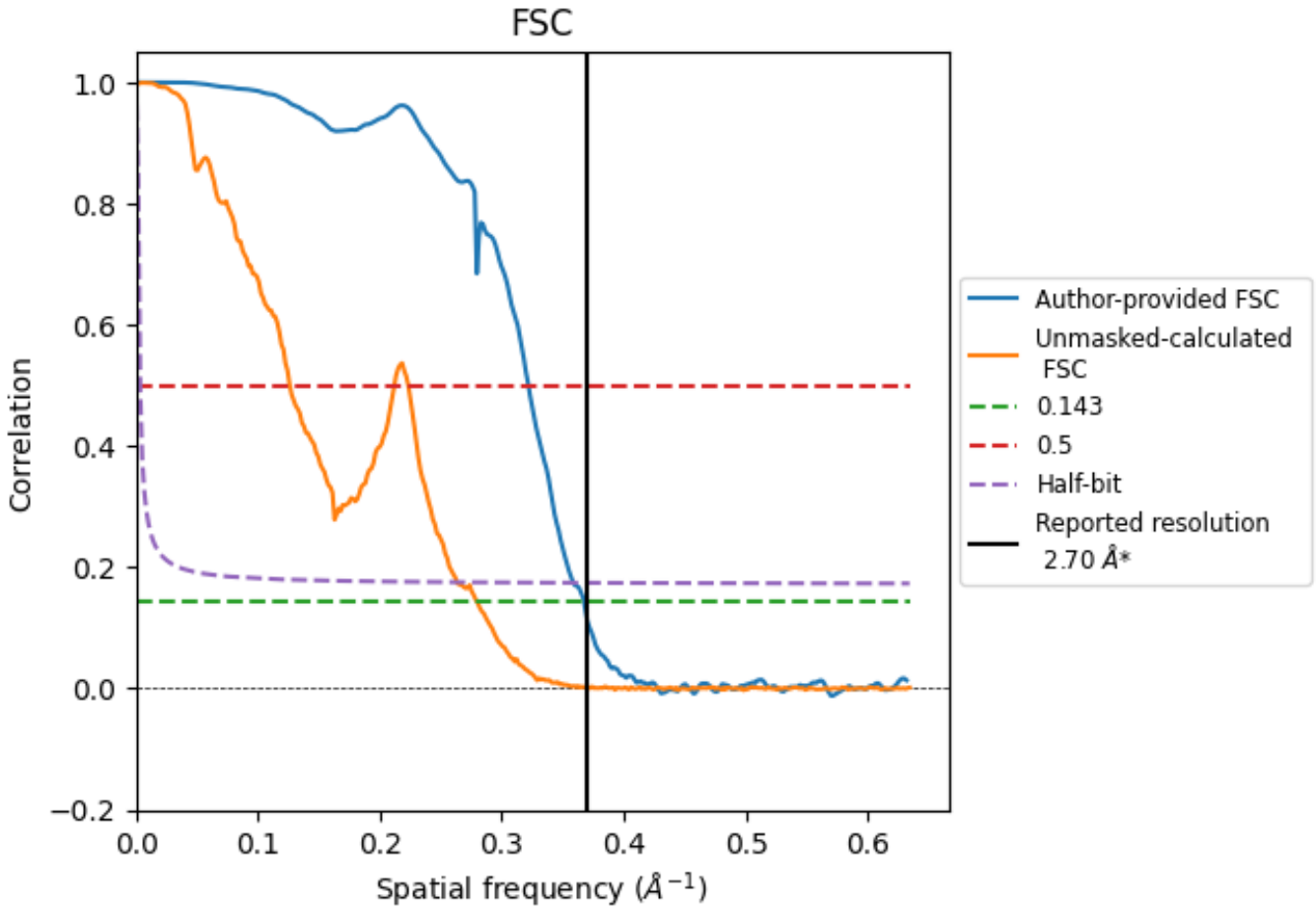


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

8.2 Resolution estimates (i)

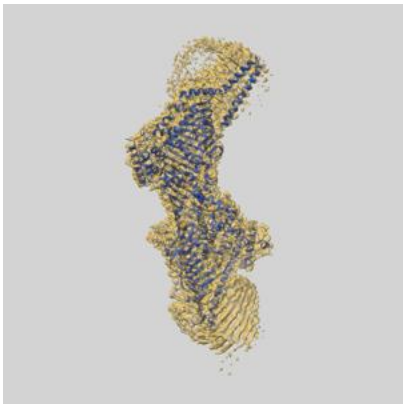
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.72	3.11	2.79
Unmasked-calculated*	3.58	7.93	3.80

*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 %

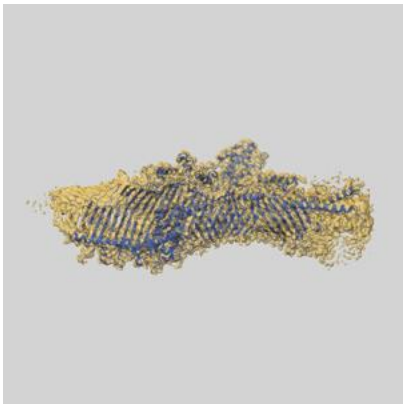
9 Map-model fit

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.

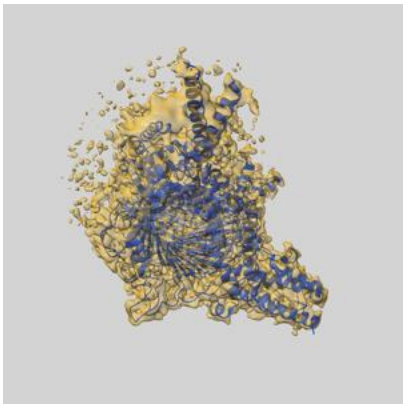
9.1 Map-model overlay



X



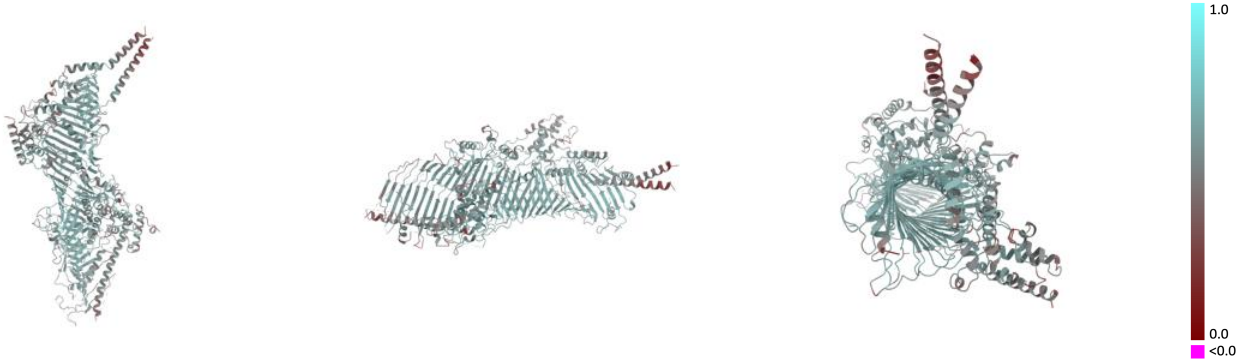
Y



Z

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)



X Y Z

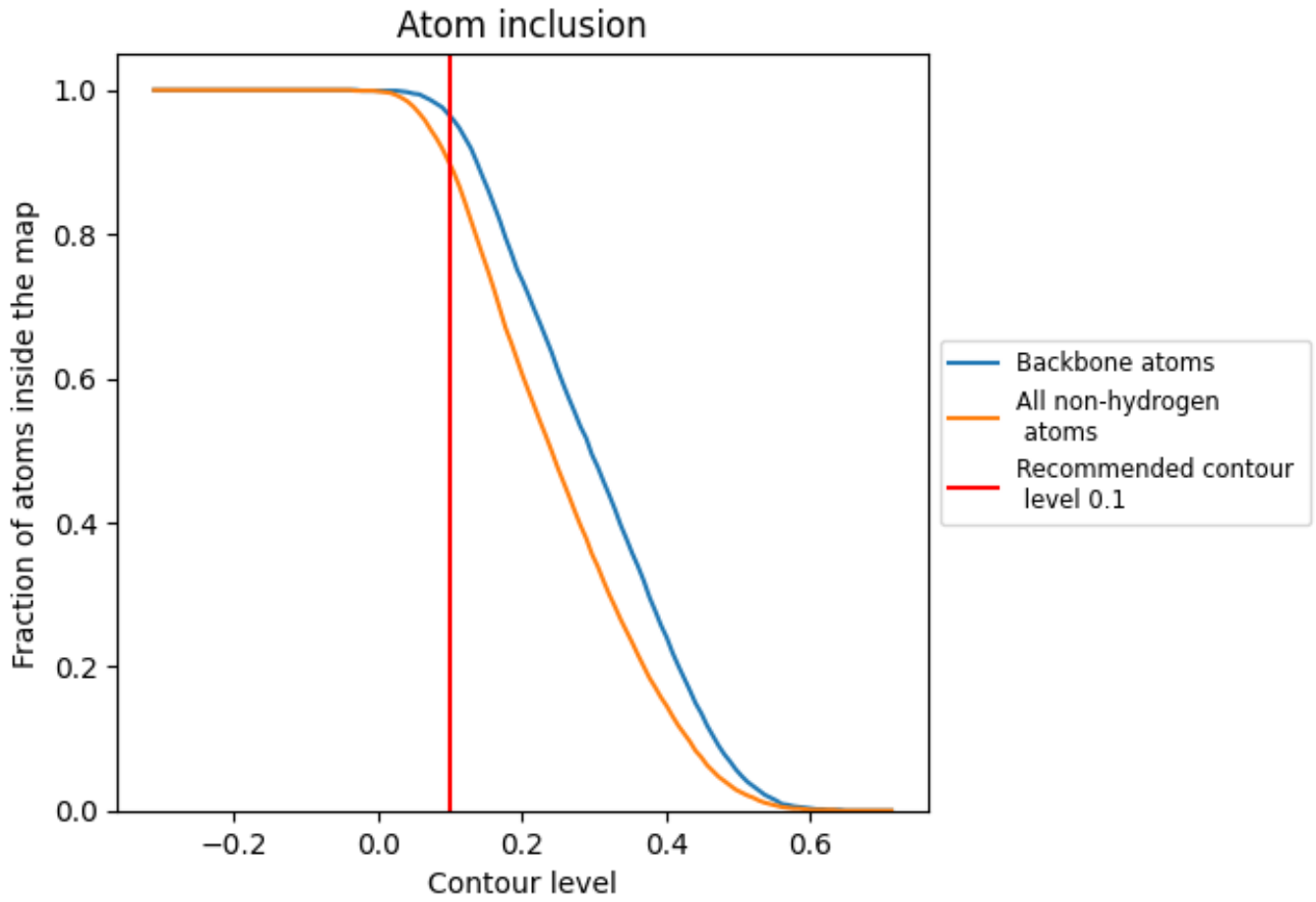
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X Y Z

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 (i)

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	0.8970	0.5590
A	0.9060	0.5670
B	0.8180	0.4940