



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 07:11 AM UTC

PDB ID : 9QTQ / pdb_00009qtq
EMDB ID : EMD-53359
Title : Structure of the energy converting methyltransferase (Mtr) of Methanosarcina mazei in complex with a novel protein binder
Authors : Reif-Trauttmansdorff, T.; Herdering, E.; Bohn, S.; Pascoa, T.C.; Kumar, A.; Zimmer, E.; Schmitz, R.A.; Schuller, J.M.
Deposited on : 2025-04-09
Resolution : 2.10 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

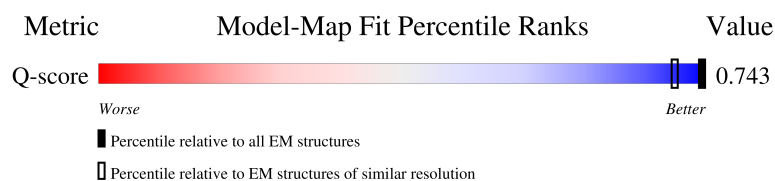
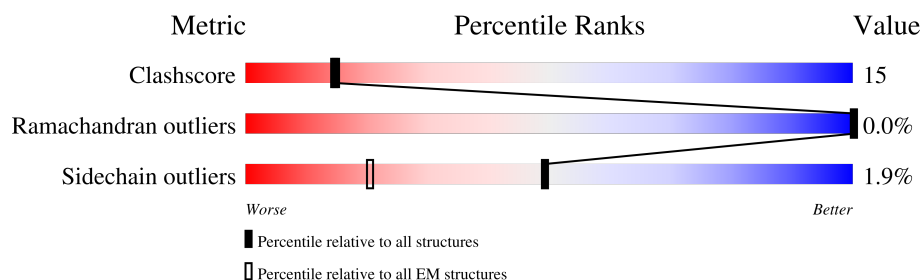
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.10 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.



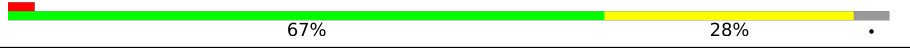
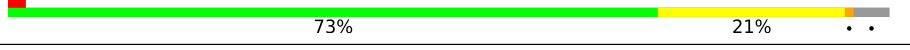
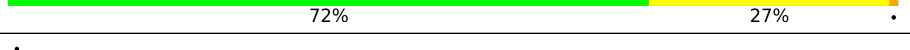
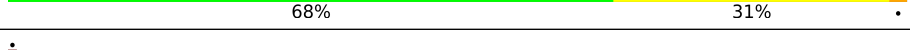
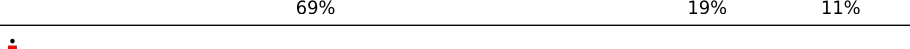
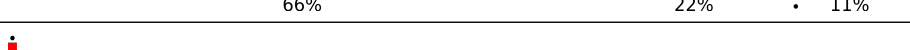
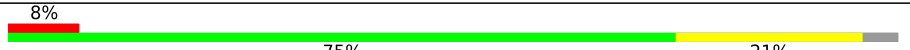
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	240	19% 8% 74%
1	B	240	20% 6% 74%
1	C	240	21% 5% 73%
2	D	108	52% 19% 28%

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Mol	Chain	Length	Quality of chain
2	E	108	
2	F	108	
3	G	267	
3	H	267	
3	I	267	
4	J	250	
4	K	250	
4	L	250	
5	M	334	
5	N	334	
5	O	334	
6	P	72	
6	Q	72	
6	R	72	
7	S	72	
7	T	72	
7	U	72	

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 28650 atoms, of which 1392 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 Tetrahydromethanopterin S-methyltransferase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	63	Total	C	N	O	S	0	0
			465	295	87	80	3		
1	B	63	Total	C	N	O	S	0	0
			465	295	87	80	3		
1	C	64	Total	C	N	O	S	0	0
			469	297	88	81	3		

- Molecule 2 is a protein called Tetrahydromethanopterin S-methyltransferase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	78	Total	C	N	O	S	0	0
			606	395	95	114	2		
2	E	77	Total	C	N	O	S	0	0
			602	393	94	113	2		
2	F	78	Total	C	N	O	S	0	0
			606	395	95	114	2		

- Molecule 3 is a protein called Tetrahydromethanopterin S-methyltransferase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	256	Total	C	N	O	S	0	0
			1830	1206	290	322	12		
3	H	256	Total	C	N	O	S	0	0
			1830	1206	290	322	12		
3	I	256	Total	C	N	O	S	0	0
			1830	1206	290	322	12		

- Molecule 4 is a protein called Tetrahydromethanopterin S-methyltransferase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	250	Total	C	N	O	S	0	0
			1778	1166	284	318	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	250	Total	C	N	O	S	0	0
			1778	1166	284	318	10		
4	L	250	Total	C	N	O	S	0	0
			1778	1166	284	318	10		

- Molecule 5 is a protein called Tetrahydromethanopterin S-methyltransferase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	297	Total	C	N	O	S	0	0
			2237	1453	363	405	16		
5	N	297	Total	C	N	O	S	0	0
			2237	1453	363	405	16		
5	O	297	Total	C	N	O	S	0	0
			2237	1453	363	405	16		

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	305	SER	-	expression tag	UNP P80651
M	306	ALA	-	expression tag	UNP P80651
M	307	TRP	-	expression tag	UNP P80651
M	308	SER	-	expression tag	UNP P80651
M	309	HIS	-	expression tag	UNP P80651
M	310	PRO	-	expression tag	UNP P80651
M	311	GLN	-	expression tag	UNP P80651
M	312	PHE	-	expression tag	UNP P80651
M	313	GLU	-	expression tag	UNP P80651
M	314	LYS	-	expression tag	UNP P80651
M	315	GLY	-	expression tag	UNP P80651
M	316	GLY	-	expression tag	UNP P80651
M	317	GLY	-	expression tag	UNP P80651
M	318	SER	-	expression tag	UNP P80651
M	319	GLY	-	expression tag	UNP P80651
M	320	GLY	-	expression tag	UNP P80651
M	321	GLY	-	expression tag	UNP P80651
M	322	SER	-	expression tag	UNP P80651
M	323	GLY	-	expression tag	UNP P80651
M	324	GLY	-	expression tag	UNP P80651
M	325	SER	-	expression tag	UNP P80651
M	326	ALA	-	expression tag	UNP P80651
M	327	TRP	-	expression tag	UNP P80651
M	328	SER	-	expression tag	UNP P80651

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Chain	Residue	Modelled	Actual	Comment	Reference
M	329	HIS	-	expression tag	UNP P80651
M	330	PRO	-	expression tag	UNP P80651
M	331	GLN	-	expression tag	UNP P80651
M	332	PHE	-	expression tag	UNP P80651
M	333	GLU	-	expression tag	UNP P80651
M	334	LYS	-	expression tag	UNP P80651
N	305	SER	-	expression tag	UNP P80651
N	306	ALA	-	expression tag	UNP P80651
N	307	TRP	-	expression tag	UNP P80651
N	308	SER	-	expression tag	UNP P80651
N	309	HIS	-	expression tag	UNP P80651
N	310	PRO	-	expression tag	UNP P80651
N	311	GLN	-	expression tag	UNP P80651
N	312	PHE	-	expression tag	UNP P80651
N	313	GLU	-	expression tag	UNP P80651
N	314	LYS	-	expression tag	UNP P80651
N	315	GLY	-	expression tag	UNP P80651
N	316	GLY	-	expression tag	UNP P80651
N	317	GLY	-	expression tag	UNP P80651
N	318	SER	-	expression tag	UNP P80651
N	319	GLY	-	expression tag	UNP P80651
N	320	GLY	-	expression tag	UNP P80651
N	321	GLY	-	expression tag	UNP P80651
N	322	SER	-	expression tag	UNP P80651
N	323	GLY	-	expression tag	UNP P80651
N	324	GLY	-	expression tag	UNP P80651
N	325	SER	-	expression tag	UNP P80651
N	326	ALA	-	expression tag	UNP P80651
N	327	TRP	-	expression tag	UNP P80651
N	328	SER	-	expression tag	UNP P80651
N	329	HIS	-	expression tag	UNP P80651
N	330	PRO	-	expression tag	UNP P80651
N	331	GLN	-	expression tag	UNP P80651
N	332	PHE	-	expression tag	UNP P80651
N	333	GLU	-	expression tag	UNP P80651
N	334	LYS	-	expression tag	UNP P80651
O	305	SER	-	expression tag	UNP P80651
O	306	ALA	-	expression tag	UNP P80651
O	307	TRP	-	expression tag	UNP P80651
O	308	SER	-	expression tag	UNP P80651
O	309	HIS	-	expression tag	UNP P80651
O	310	PRO	-	expression tag	UNP P80651

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Chain	Residue	Modelled	Actual	Comment	Reference
O	311	GLN	-	expression tag	UNP P80651
O	312	PHE	-	expression tag	UNP P80651
O	313	GLU	-	expression tag	UNP P80651
O	314	LYS	-	expression tag	UNP P80651
O	315	GLY	-	expression tag	UNP P80651
O	316	GLY	-	expression tag	UNP P80651
O	317	GLY	-	expression tag	UNP P80651
O	318	SER	-	expression tag	UNP P80651
O	319	GLY	-	expression tag	UNP P80651
O	320	GLY	-	expression tag	UNP P80651
O	321	GLY	-	expression tag	UNP P80651
O	322	SER	-	expression tag	UNP P80651
O	323	GLY	-	expression tag	UNP P80651
O	324	GLY	-	expression tag	UNP P80651
O	325	SER	-	expression tag	UNP P80651
O	326	ALA	-	expression tag	UNP P80651
O	327	TRP	-	expression tag	UNP P80651
O	328	SER	-	expression tag	UNP P80651
O	329	HIS	-	expression tag	UNP P80651
O	330	PRO	-	expression tag	UNP P80651
O	331	GLN	-	expression tag	UNP P80651
O	332	PHE	-	expression tag	UNP P80651
O	333	GLU	-	expression tag	UNP P80651
O	334	LYS	-	expression tag	UNP P80651

- Molecule 6 is a protein called Tetrahydromethanopterin S-methyltransferase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	64	Total	C	N	O	S	0	0
			467	305	78	81	3		
6	Q	64	Total	C	N	O	S	0	0
			467	305	78	81	3		
6	R	64	Total	C	N	O	S	0	0
			467	305	78	81	3		

- Molecule 7 is a protein called Tetrahydromethanopterin S-methyltransferase subunit G.

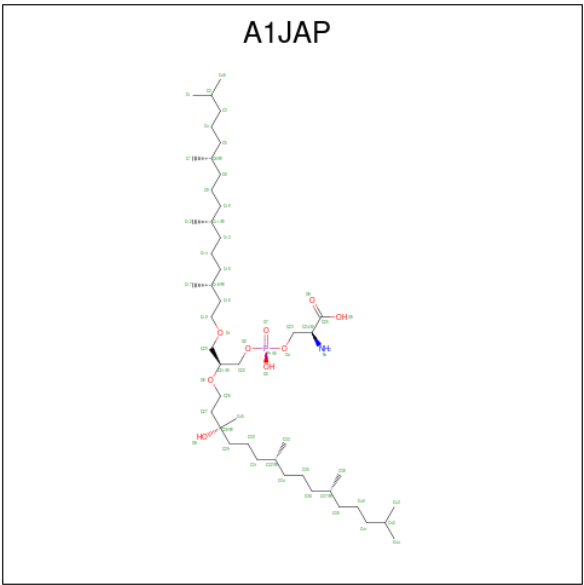
Mol	Chain	Residues	Atoms					AltConf	Trace
7	S	69	Total	C	N	O	S	0	0
			543	354	88	98	3		
7	T	69	Total	C	N	O	S	0	0
			543	354	88	98	3		

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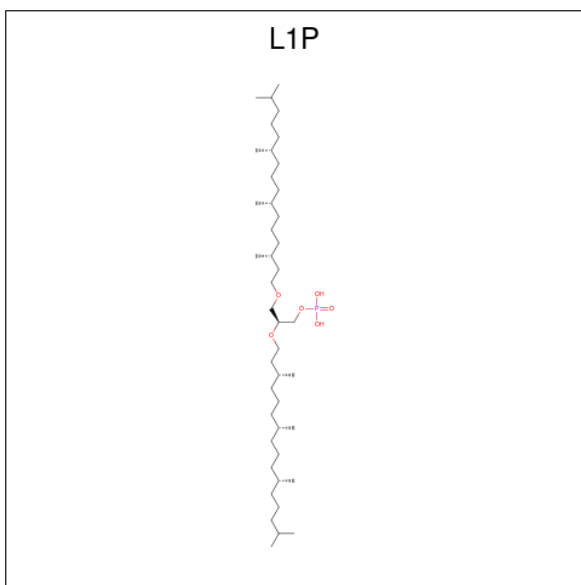
Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	69	Total	C	N	O	S	0	0
			543	354	88	98	3		

- Molecule 8 is 2-Hydroxy-archaetidylinositol (CCD ID: A1JAP) (formula: C₄₆H₉₄NO₉P) (labeled as "Ligand of Interest" by depositor).



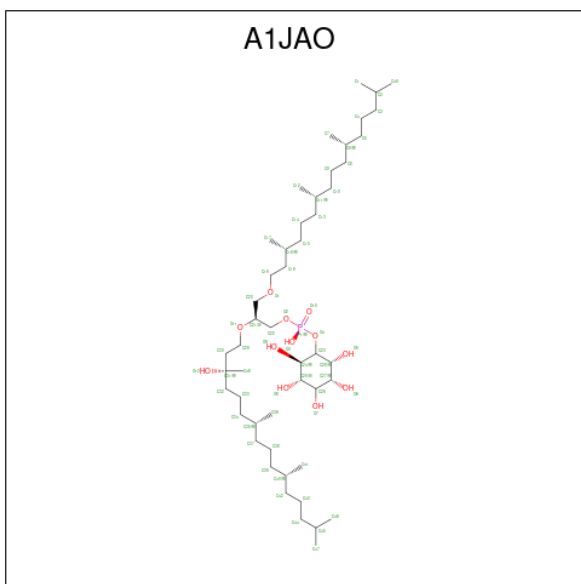
Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	C	H	N	O	P	0
			150	46	93	1	9	1	
8	M	1	Total	C	H	N	O	P	0
			150	46	93	1	9	1	
8	N	1	Total	C	H	N	O	P	0
			150	46	93	1	9	1	
8	S	1	Total	C	H	N	O	P	0
			150	46	93	1	9	1	
8	T	1	Total	C	H	N	O	P	0
			150	46	93	1	9	1	
8	U	1	Total	C	H	N	O	P	0
			150	46	93	1	9	1	

- Molecule 9 is 3-PHOSPHORYL-[1,2-DI-PHYTANYL]GLYCEROL (CCD ID: L1P) (formula: C₄₃H₈₉O₆P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	D	1	Total	C	H	O	P	0
			137	43	87	6	1	
9	F	1	Total	C	H	O	P	0
			137	43	87	6	1	
9	G	1	Total	C	H	O	P	0
			137	43	87	6	1	

- Molecule 10 is Archaeetidylinositol (CCD ID: A1JAO) (formula: $C_{49}H_{99}O_{12}P$) (labeled as "Ligand of Interest" by depositor).

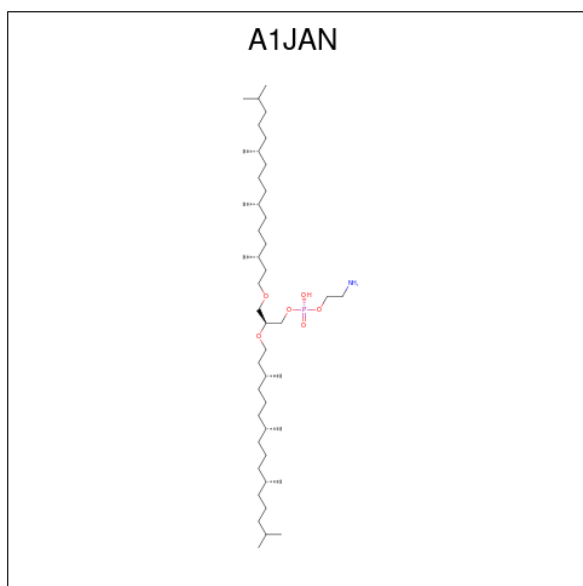


Mol	Chain	Residues	Atoms					AltConf
10	F	1	Total	C	H	O	P	0
			160	49	98	12	1	
10	G	1	Total	C	H	O	P	0
			160	49	98	12	1	
10	H	1	Total	C	H	O	P	0
			160	49	98	12	1	

- Molecule 11 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
11	M	1	Total	Na	0
			1	1	
11	N	1	Total	Na	0
			1	1	
11	O	1	Total	Na	0
			1	1	

- Molecule 12 is Archaeidylethanolamine (CCD ID: A1JAN) (formula: C₄₅H₉₄NO₆P) (labeled as "Ligand of Interest" by depositor).

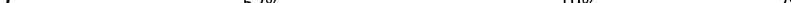


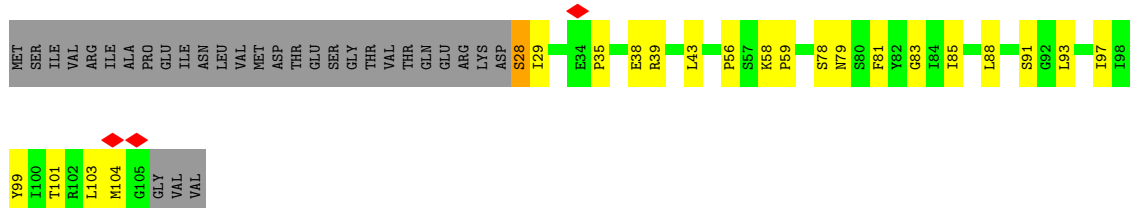
Mol	Chain	Residues	Atoms					AltConf	
12	M	1	Total 146	C 45	H 93	N 1	O 6	P 1	0
12	N	1	Total 146	C 45	H 93	N 1	O 6	P 1	0
12	O	1	Total 146	C 45	H 93	N 1	O 6	P 1	0

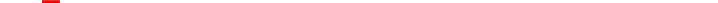
- Molecule 13 is water.

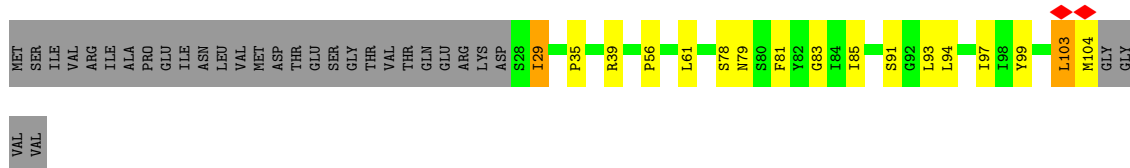
Mol	Chain	Residues	Atoms		AltConf
13	A	50	Total 50	O 50	0
13	B	42	Total 42	O 42	0
13	C	39	Total 39	O 39	0
13	D	93	Total 93	O 93	0
13	E	82	Total 82	O 82	0
13	F	119	Total 119	O 119	0
13	G	242	Total 242	O 242	0
13	H	232	Total 232	O 232	0
13	I	243	Total 243	O 243	0
13	J	183	Total 183	O 183	0
13	K	175	Total 175	O 175	0
13	L	204	Total 204	O 204	0
13	M	193	Total 193	O 193	0
13	N	191	Total 191	O 191	0
13	O	179	Total 179	O 179	0
13	P	62	Total 62	O 62	0
13	Q	49	Total 49	O 49	0
13	R	48	Total 48	O 48	0
13	S	64	Total 64	O 64	0
13	T	73	Total 73	O 73	0
13	U	77	Total 77	O 77	0

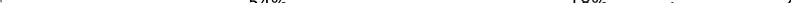


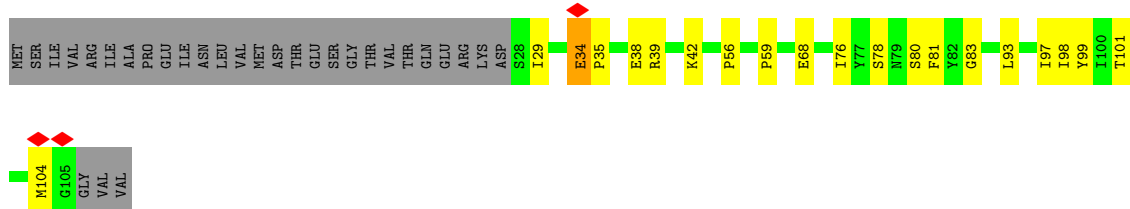
Chain D: 

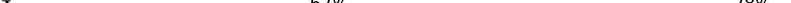


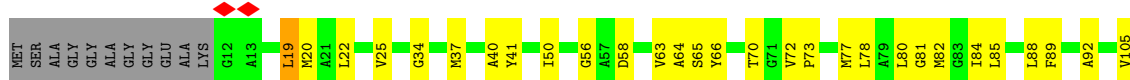
Chain E: 

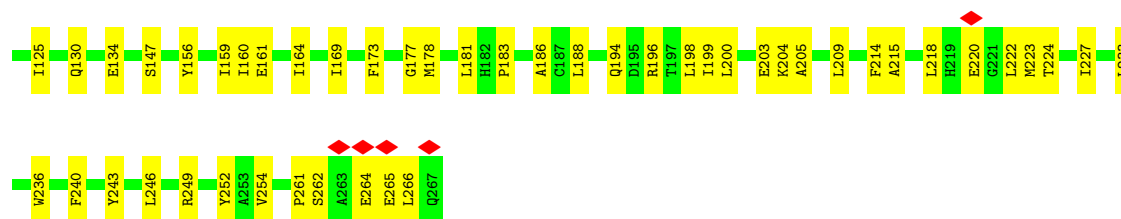


Chain F:  54% 18% 28%



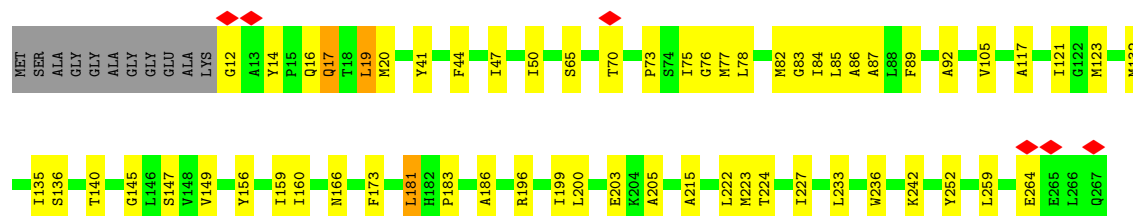
Chain G:  67% 28%





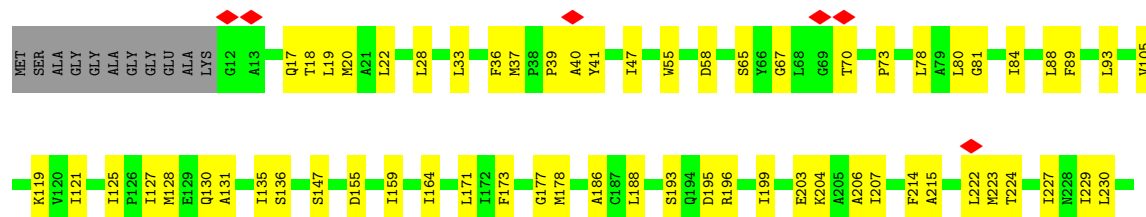
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

Chain H: 73% 21%



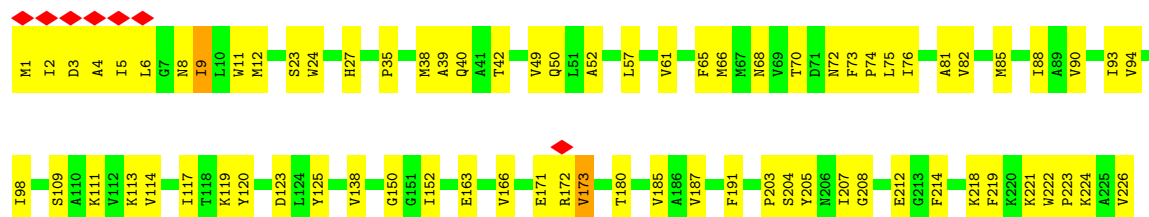
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

Chain I: 68% 28%



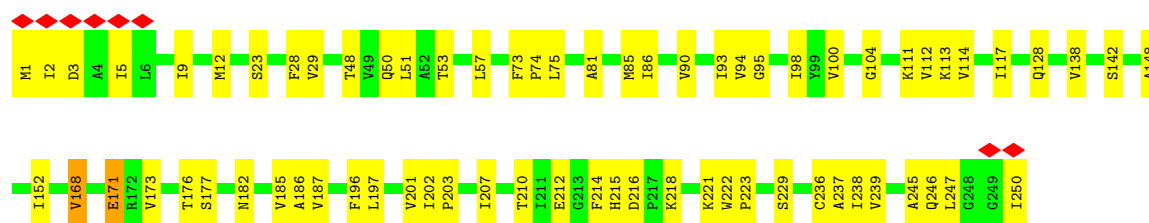
• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain J: 66% 33%



• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain K:  72% 27% .



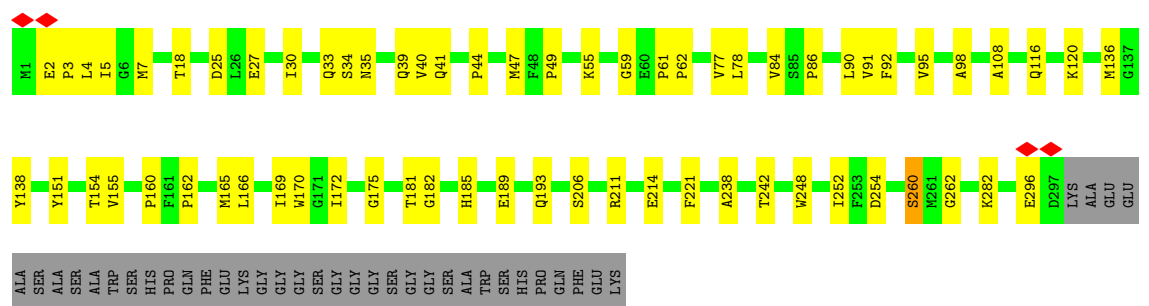
• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain L:  68% 31% .



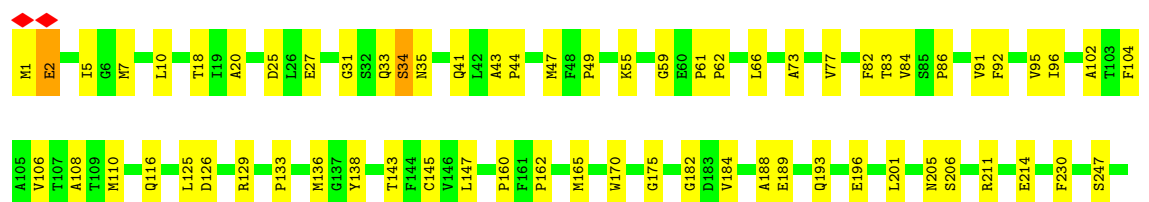
• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

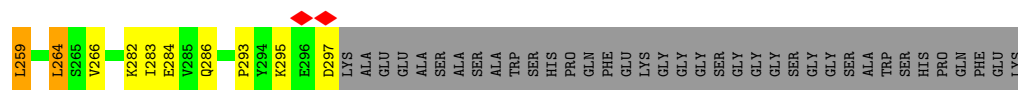
Chain M:  69% 19% 11%



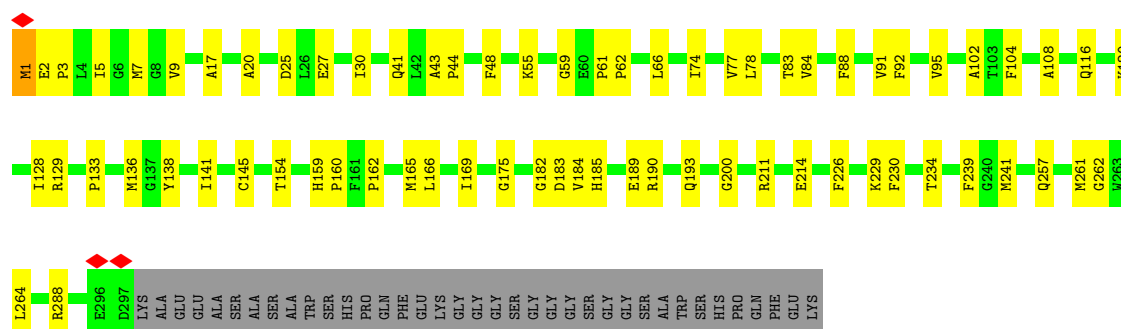
• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E

Chain N:  66% 22% 11%

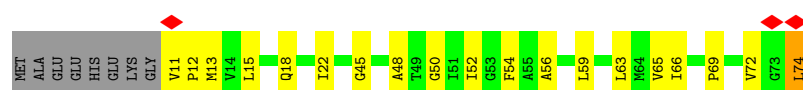




- Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E



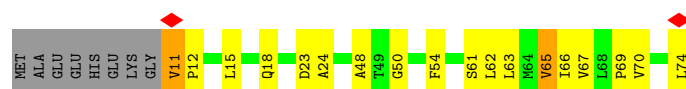
- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



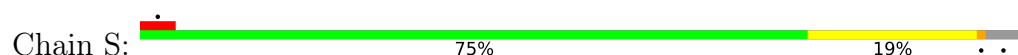
- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



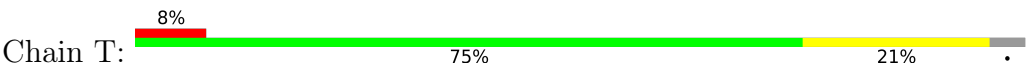
- Molecule 6: Tetrahydromethanopterin S-methyltransferase subunit F



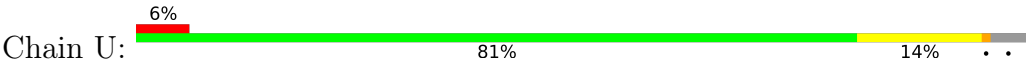
- Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



- Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



● Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136531	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.540	Depositor
Minimum map value	-0.261	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	417.6, 417.6, 417.6	wwPDB
Map dimensions	576, 576, 576	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.725, 0.725, 0.725	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1JAO, L1P, A1JAP, A1JAN, NA

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	0.20	0/468	0.37	0/625
1	B	0.18	0/468	0.35	0/625
1	C	0.19	0/472	0.36	0/630
2	D	0.17	0/619	0.28	0/842
2	E	0.16	0/615	0.29	0/837
2	F	0.18	0/619	0.28	0/842
3	G	0.15	0/1864	0.30	0/2536
3	H	0.15	0/1864	0.31	0/2536
3	I	0.14	0/1864	0.29	0/2536
4	J	0.15	0/1813	0.30	0/2475
4	K	0.14	0/1813	0.30	0/2475
4	L	0.15	0/1813	0.29	0/2475
5	M	0.15	0/2294	0.30	0/3121
5	N	0.15	0/2294	0.29	0/3121
5	O	0.16	0/2294	0.30	0/3121
6	P	0.16	0/473	0.31	0/641
6	Q	0.16	0/473	0.35	0/641
6	R	0.15	0/473	0.31	0/641
7	S	0.15	0/551	0.24	0/737
7	T	0.16	0/551	0.23	0/737
7	U	0.16	0/551	0.24	0/737
All	All	0.15	0/24246	0.30	0/32931

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	465	0	510	25	0
1	B	465	0	510	17	0
1	C	469	0	513	17	0
2	D	606	0	612	27	0
2	E	602	0	609	21	0
2	F	606	0	612	20	0
3	G	1830	0	1918	74	0
3	H	1830	0	1918	62	0
3	I	1830	0	1918	68	0
4	J	1778	0	1862	83	0
4	K	1778	0	1862	70	0
4	L	1778	0	1862	74	0
5	M	2237	0	2234	63	0
5	N	2237	0	2234	78	0
5	O	2237	0	2234	75	0
6	P	467	0	502	21	0
6	Q	467	0	502	21	0
6	R	467	0	502	20	0
7	S	543	0	562	17	0
7	T	543	0	562	16	0
7	U	543	0	562	14	0
8	A	57	93	0	1	0
8	M	57	93	0	0	0
8	N	57	93	0	0	0
8	S	57	93	0	0	0
8	T	57	93	0	0	0
8	U	57	93	0	1	0
9	D	50	87	87	11	0
9	F	50	87	87	6	0
9	G	50	87	87	10	0
10	F	62	98	0	4	0
10	G	62	98	0	0	0
10	H	62	98	0	0	0
11	M	1	0	0	0	0
11	N	1	0	0	0	0
11	O	1	0	0	0	0
12	M	53	93	0	3	0

Continued on next page...

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	N	53	93	0	2	0
12	O	53	93	0	0	0
13	A	50	0	0	4	0
13	B	42	0	0	2	0
13	C	39	0	0	0	0
13	D	93	0	0	8	0
13	E	82	0	0	3	0
13	F	119	0	0	6	0
13	G	242	0	0	24	0
13	H	232	0	0	10	0
13	I	243	0	0	21	0
13	J	183	0	0	23	0
13	K	175	0	0	18	0
13	L	204	0	0	25	0
13	M	193	0	0	13	0
13	N	191	0	0	20	0
13	O	179	0	0	17	0
13	P	62	0	0	5	0
13	Q	49	0	0	3	0
13	R	48	0	0	5	0
13	S	64	0	0	7	0
13	T	73	0	0	11	0
13	U	77	0	0	3	0
All	All	27258	1392	24861	747	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 15.

The worst 5 of 747 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)
4:J:5:ILE:HG23	4:J:12:MET:HE1	1.38	1.06
3:G:41:TYR:CE1	3:G:227:ILE:HD12	2.02	0.94
3:G:41:TYR:HE1	3:G:227:ILE:HD12	1.29	0.93
4:K:214:PHE:O	4:K:215:HIS:ND1	2.06	0.89
4:L:214:PHE:O	4:L:215:HIS:ND1	2.06	0.89

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	61/240 (25%)	59 (97%)	2 (3%)	0	100	100
1	B	61/240 (25%)	61 (100%)	0	0	100	100
1	C	62/240 (26%)	62 (100%)	0	0	100	100
2	D	76/108 (70%)	76 (100%)	0	0	100	100
2	E	75/108 (69%)	75 (100%)	0	0	100	100
2	F	76/108 (70%)	75 (99%)	1 (1%)	0	100	100
3	G	254/267 (95%)	249 (98%)	5 (2%)	0	100	100
3	H	254/267 (95%)	251 (99%)	3 (1%)	0	100	100
3	I	254/267 (95%)	248 (98%)	6 (2%)	0	100	100
4	J	248/250 (99%)	237 (96%)	11 (4%)	0	100	100
4	K	248/250 (99%)	239 (96%)	9 (4%)	0	100	100
4	L	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
5	M	295/334 (88%)	290 (98%)	5 (2%)	0	100	100
5	N	295/334 (88%)	288 (98%)	6 (2%)	1 (0%)	36	36
5	O	295/334 (88%)	291 (99%)	4 (1%)	0	100	100
6	P	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
6	Q	62/72 (86%)	60 (97%)	2 (3%)	0	100	100
6	R	62/72 (86%)	61 (98%)	1 (2%)	0	100	100
7	S	67/72 (93%)	67 (100%)	0	0	100	100
7	T	67/72 (93%)	67 (100%)	0	0	100	100
7	U	67/72 (93%)	67 (100%)	0	0	100	100
All	All	3189/4029 (79%)	3125 (98%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	N	34	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	49/190 (26%)	49 (100%)	0	100	100
1	B	49/190 (26%)	49 (100%)	0	100	100
1	C	49/190 (26%)	48 (98%)	1 (2%)	48	56
2	D	67/94 (71%)	65 (97%)	2 (3%)	36	41
2	E	67/94 (71%)	64 (96%)	3 (4%)	24	25
2	F	67/94 (71%)	64 (96%)	3 (4%)	24	25
3	G	180/184 (98%)	178 (99%)	2 (1%)	65	74
3	H	180/184 (98%)	177 (98%)	3 (2%)	53	62
3	I	180/184 (98%)	176 (98%)	4 (2%)	45	53
4	J	185/185 (100%)	180 (97%)	5 (3%)	39	45
4	K	185/185 (100%)	182 (98%)	3 (2%)	55	64
4	L	185/185 (100%)	179 (97%)	6 (3%)	34	38
5	M	237/261 (91%)	235 (99%)	2 (1%)	73	81
5	N	237/261 (91%)	232 (98%)	5 (2%)	47	54
5	O	237/261 (91%)	235 (99%)	2 (1%)	73	81
6	P	48/54 (89%)	47 (98%)	1 (2%)	47	54
6	Q	48/54 (89%)	47 (98%)	1 (2%)	47	54
6	R	48/54 (89%)	46 (96%)	2 (4%)	26	28
7	S	58/60 (97%)	57 (98%)	1 (2%)	53	62
7	T	58/60 (97%)	58 (100%)	0	100	100
7	U	58/60 (97%)	56 (97%)	2 (3%)	32	35
All	All	2472/3084 (80%)	2424 (98%)	48 (2%)	49	58

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	L	226	VAL
5	N	84	VAL
4	L	229	SER
5	M	40	VAL
5	N	259	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
7	S	24	GLN
6	P	40	GLN
4	L	40	GLN
5	O	185	HIS
4	K	50	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 3 are monoatomic - leaving 15 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	L1P	F	201	-	49,49,49	0.28	0	56,60,60	0.38	0
8	A1JAP	S	101	-	53,56,56	0.41	0	59,71,71	0.53	1 (1%)
10	A1JAO	G	302	-	60,62,62	0.30	0	73,82,82	0.41	0
12	A1JAN	N	402	-	52,52,52	0.30	0	59,63,63	0.37	0
9	L1P	G	301	-	49,49,49	0.29	0	56,60,60	0.37	0
9	L1P	D	201	-	49,49,49	0.27	0	56,60,60	0.40	0
8	A1JAP	N	403	-	53,56,56	0.40	0	59,71,71	0.45	0
8	A1JAP	U	101	-	53,56,56	0.41	0	59,71,71	0.50	0
8	A1JAP	A	301	-	53,56,56	0.40	0	59,71,71	0.39	0
12	A1JAN	O	402	-	52,52,52	0.31	0	59,63,63	0.46	0
12	A1JAN	M	402	-	52,52,52	0.31	0	59,63,63	0.46	0
10	A1JAO	F	202	-	60,62,62	0.30	0	73,82,82	1.08	3 (4%)
8	A1JAP	T	101	-	53,56,56	0.40	0	59,71,71	0.84	1 (1%)
10	A1JAO	H	301	-	60,62,62	0.30	0	73,82,82	0.46	0
8	A1JAP	M	403	-	53,56,56	0.39	0	59,71,71	0.46	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	L1P	F	201	-	-	16/55/55/55	-
8	A1JAP	S	101	-	-	9/67/67/67	-
10	A1JAO	G	302	-	-	10/62/86/86	0/1/1/1
12	A1JAN	N	402	-	-	16/60/60/60	-
9	L1P	G	301	-	-	16/55/55/55	-
9	L1P	D	201	-	-	19/55/55/55	-
8	A1JAP	N	403	-	-	13/67/67/67	-
8	A1JAP	U	101	-	-	17/67/67/67	-
8	A1JAP	A	301	-	-	18/67/67/67	-
12	A1JAN	O	402	-	-	24/60/60/60	-
12	A1JAN	M	402	-	-	14/60/60/60	-
10	A1JAO	F	202	-	-	7/62/86/86	0/1/1/1
8	A1JAP	T	101	-	-	17/67/67/67	-
10	A1JAO	H	301	-	-	7/62/86/86	0/1/1/1
8	A1JAP	M	403	-	-	9/67/67/67	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	F	202	A1JAO	C28-C23-C24	6.63	120.06	110.86
8	T	101	A1JAP	C4-C3-C2	5.45	140.25	115.94
10	F	202	A1JAO	C27-C28-C23	3.30	117.17	109.68
10	F	202	A1JAO	C25-C24-C23	3.16	116.86	109.68
8	S	101	A1JAP	O8-C26-C27	2.22	113.12	108.81

There are no chirality outliers.

5 of 212 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	301	A1JAP	O4-C23-C24-N1
8	A	301	A1JAP	N1-C24-C25-O6
8	A	301	A1JAP	C23-O4-P1-O2
8	A	301	A1JAP	C23-O4-P1-O3
8	M	403	A1JAP	N1-C24-C25-O6

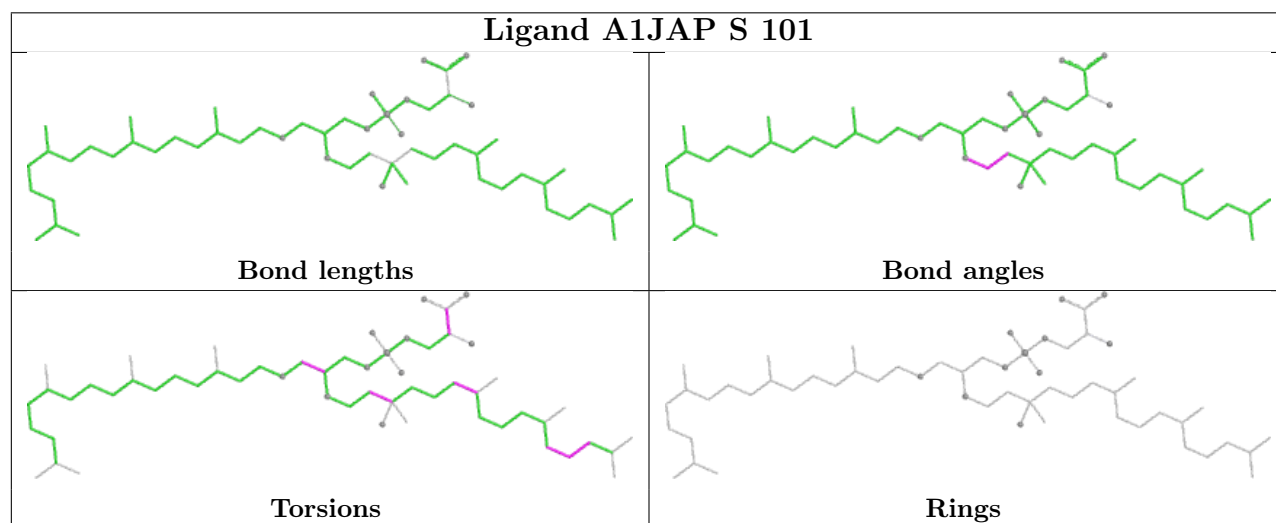
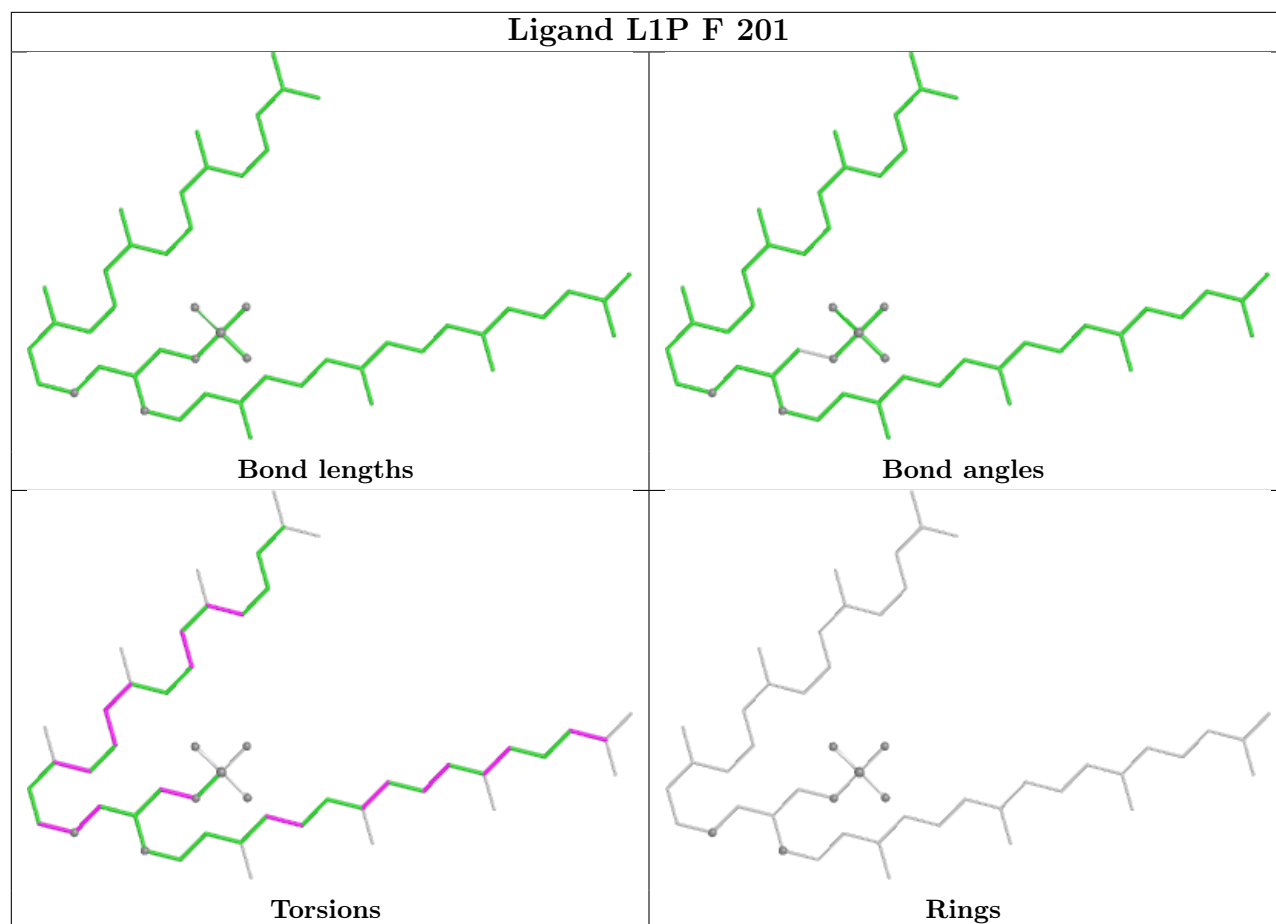
There are no ring outliers.

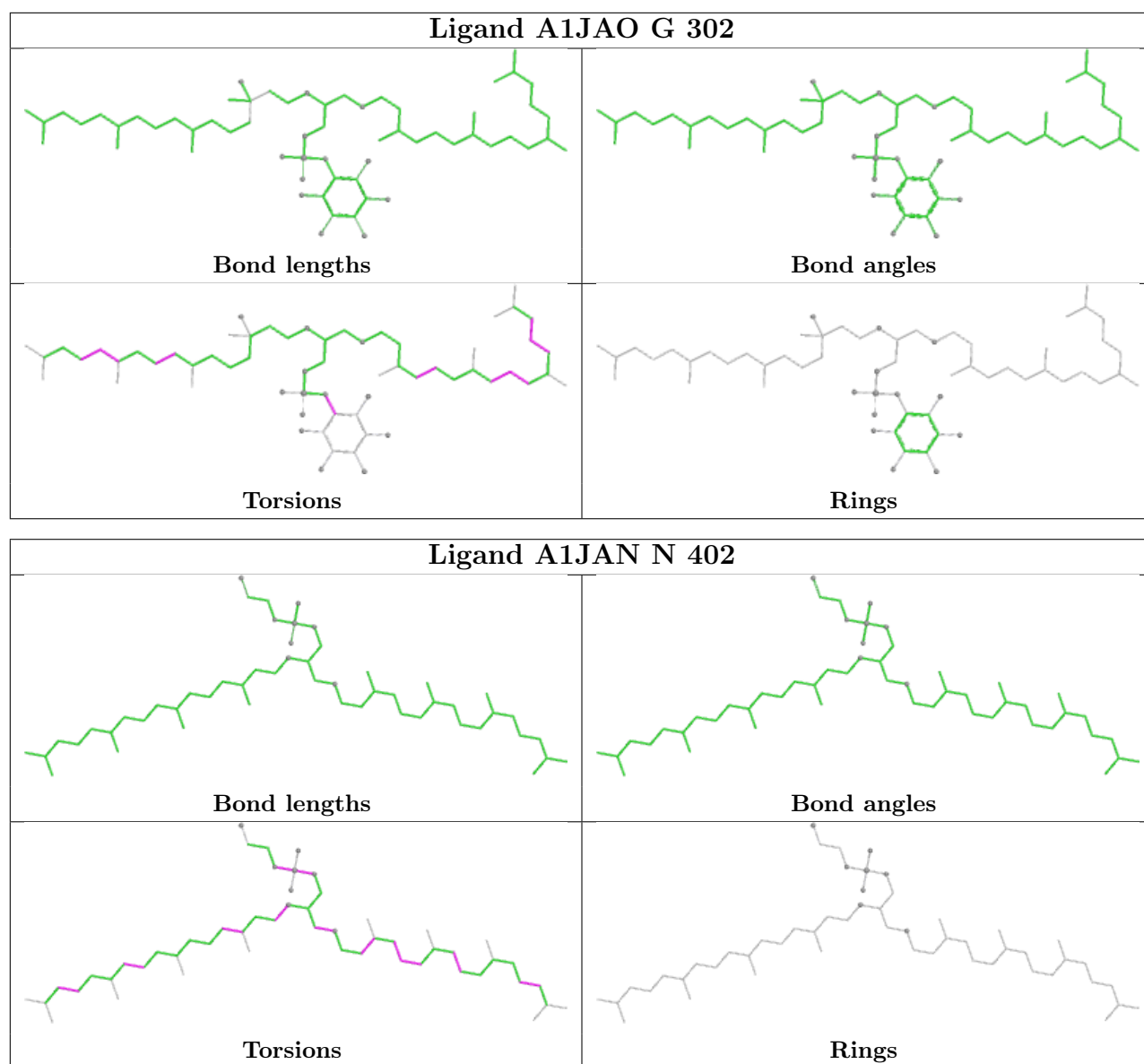
8 monomers are involved in 38 short contacts:

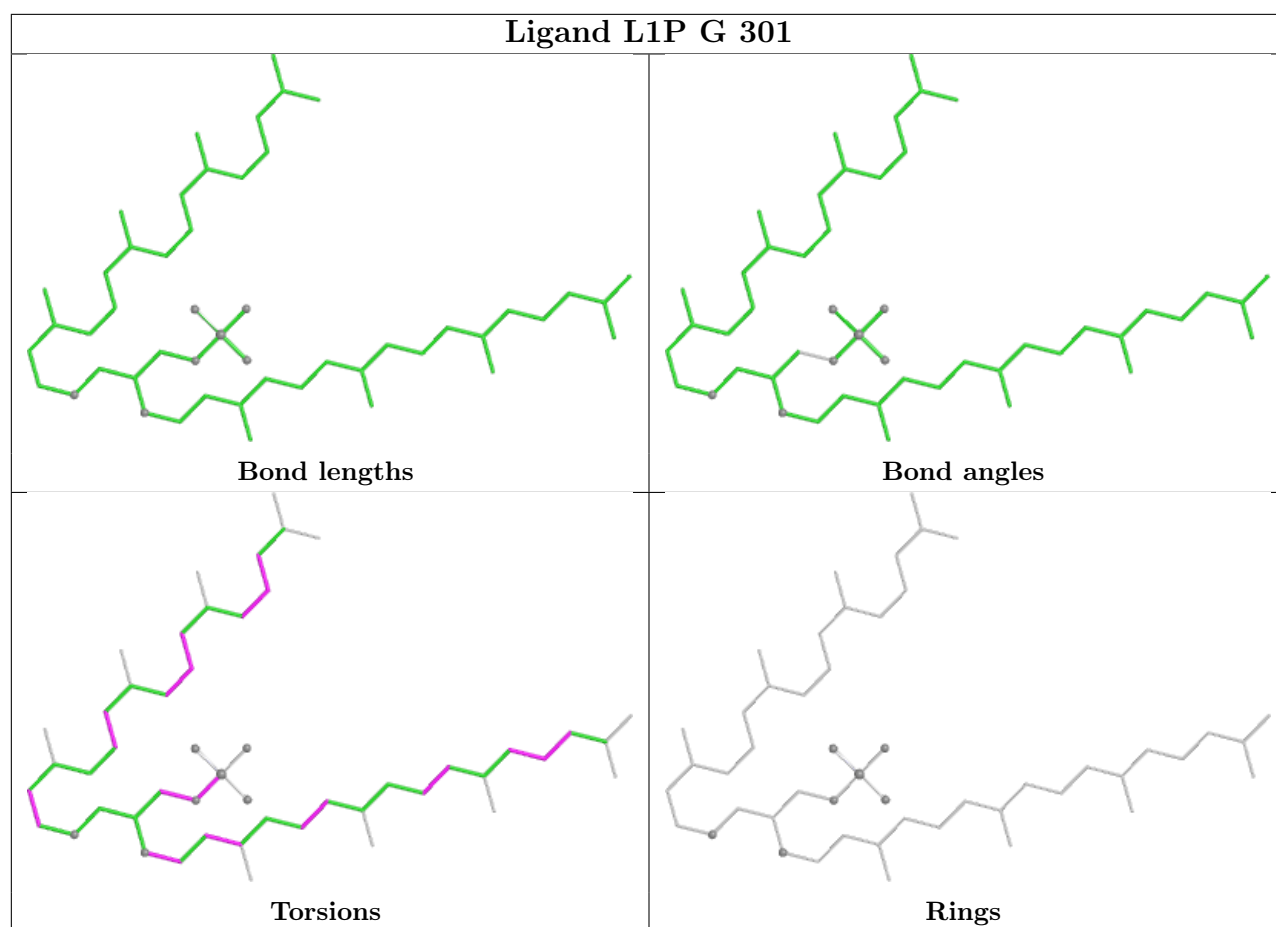
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	201	L1P	6	0
12	N	402	A1JAN	2	0
9	G	301	L1P	10	0
9	D	201	L1P	11	0
8	U	101	A1JAP	1	0
8	A	301	A1JAP	1	0
12	M	402	A1JAN	3	0
10	F	202	A1JAO	4	0

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

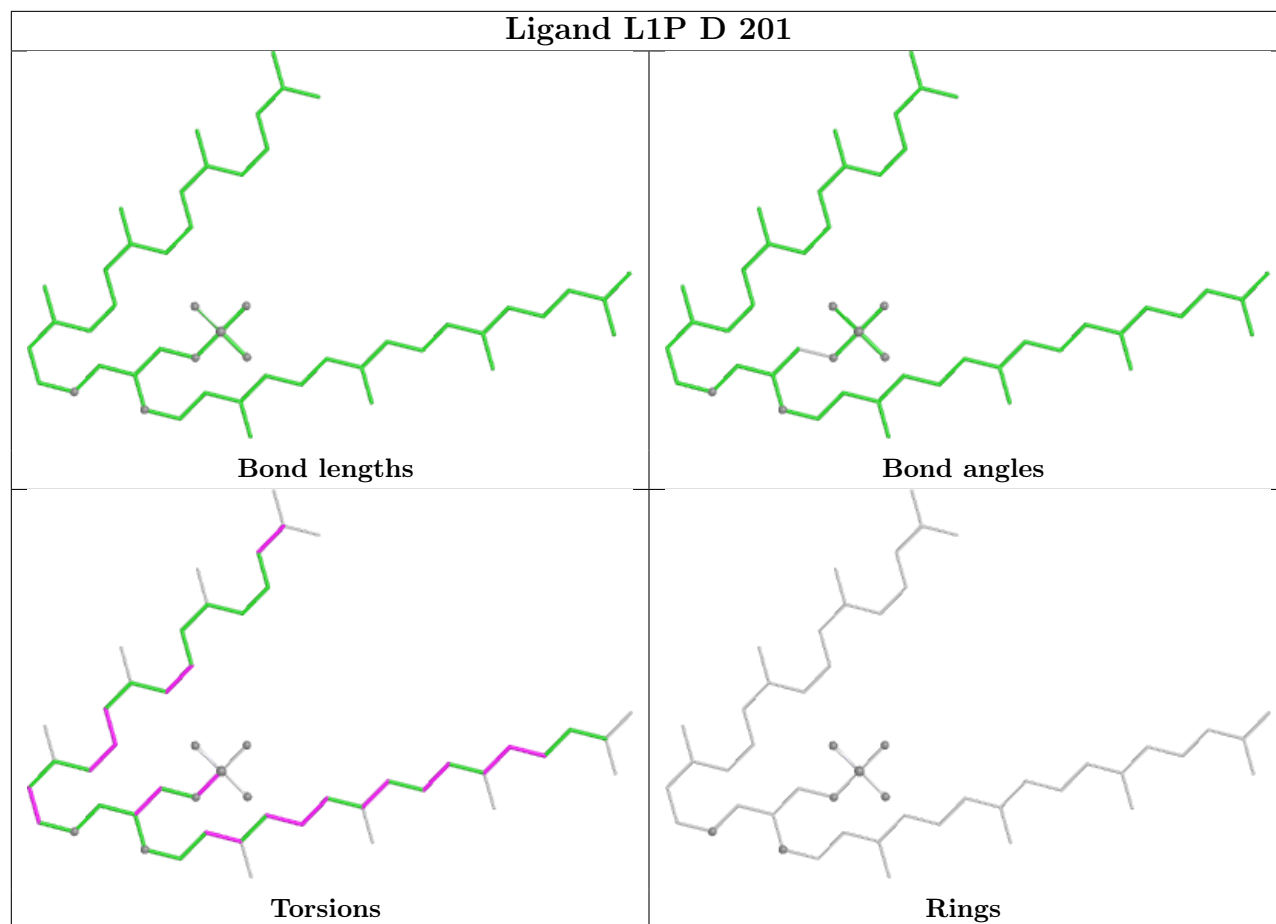
equivalents in the CSD to analyse the geometry.



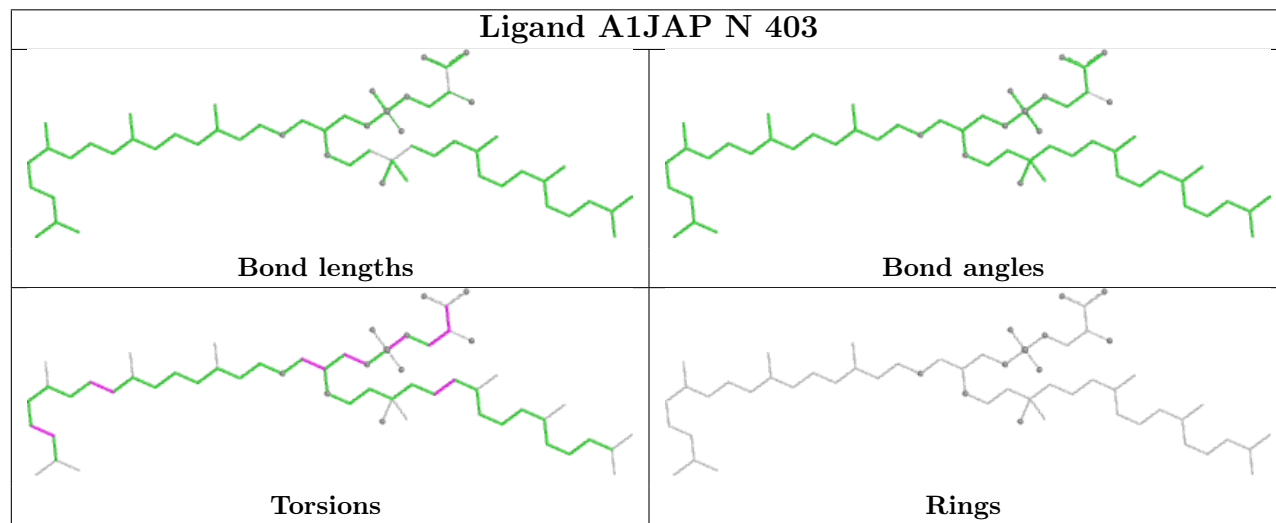


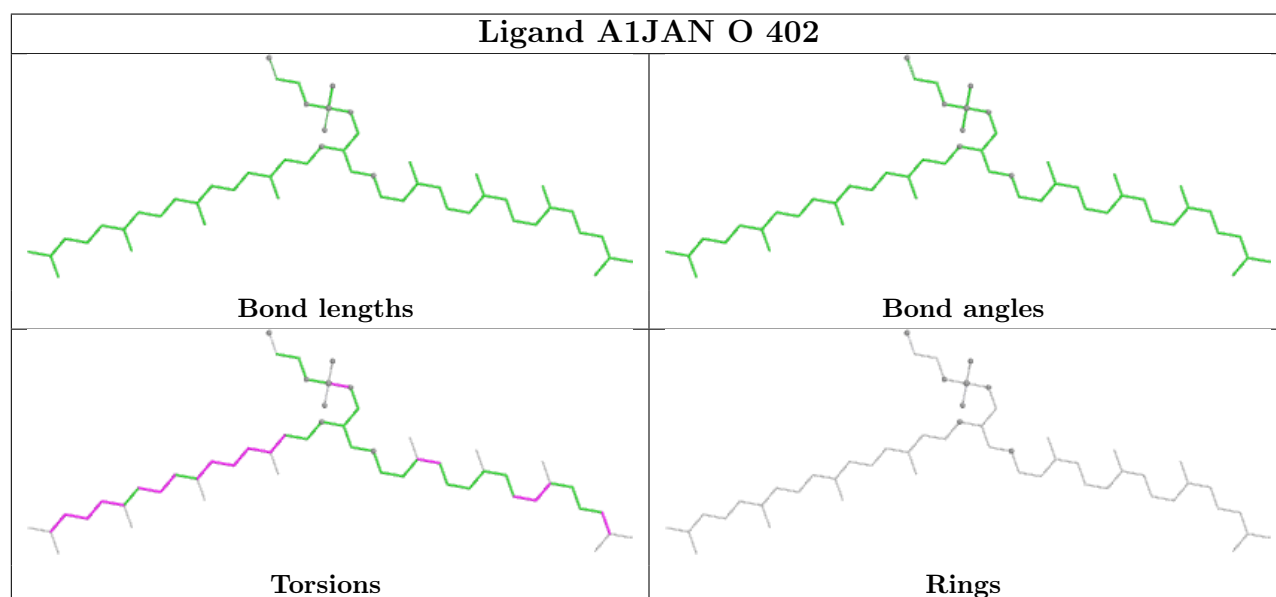
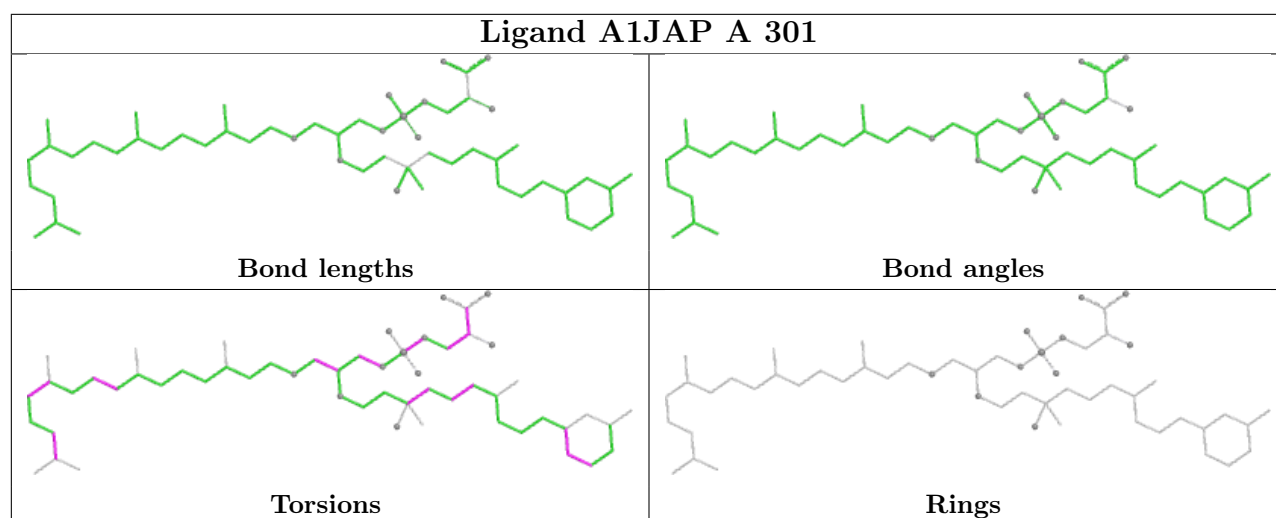
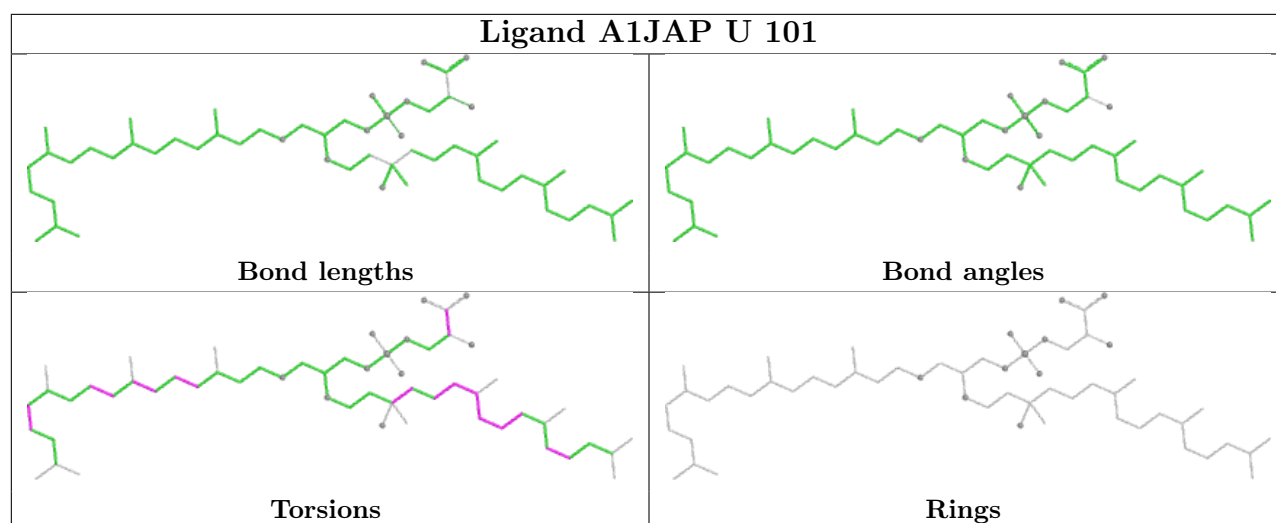


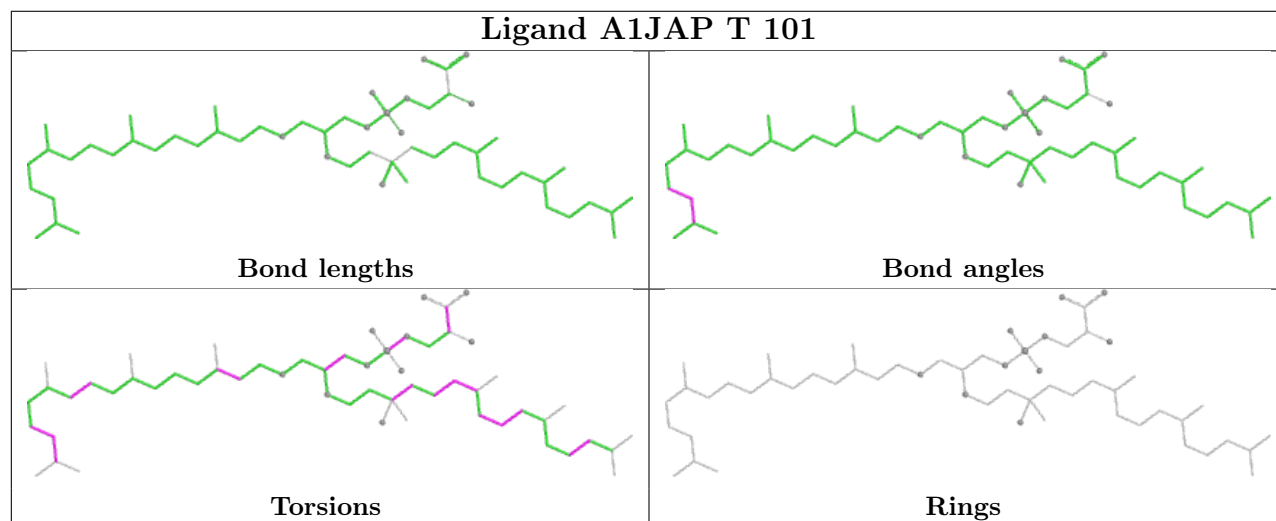
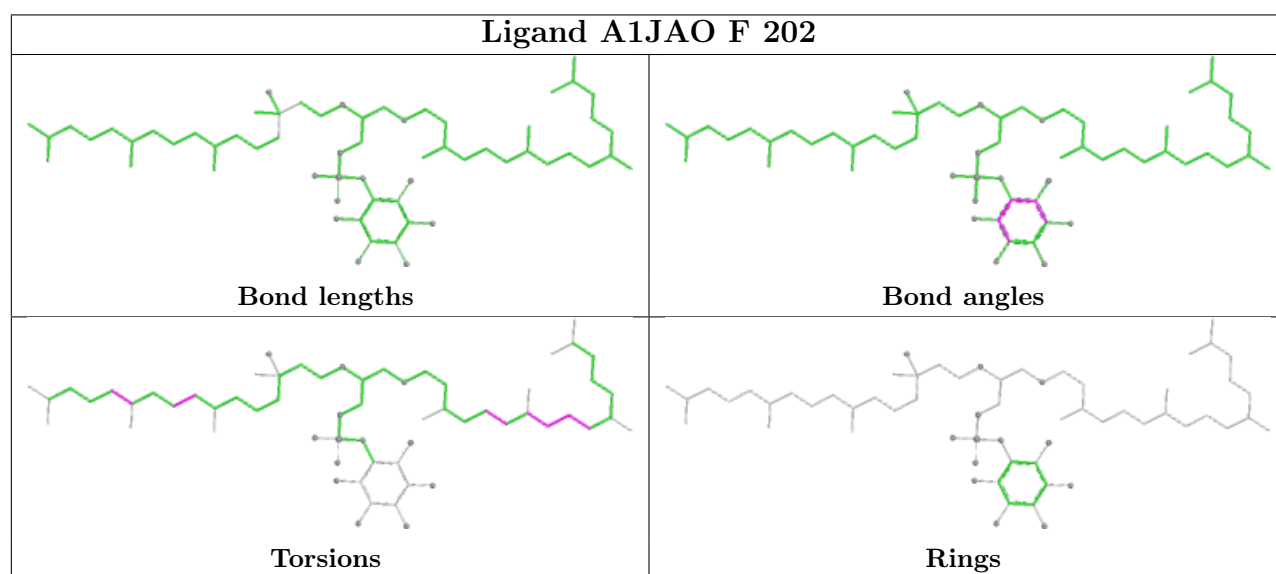
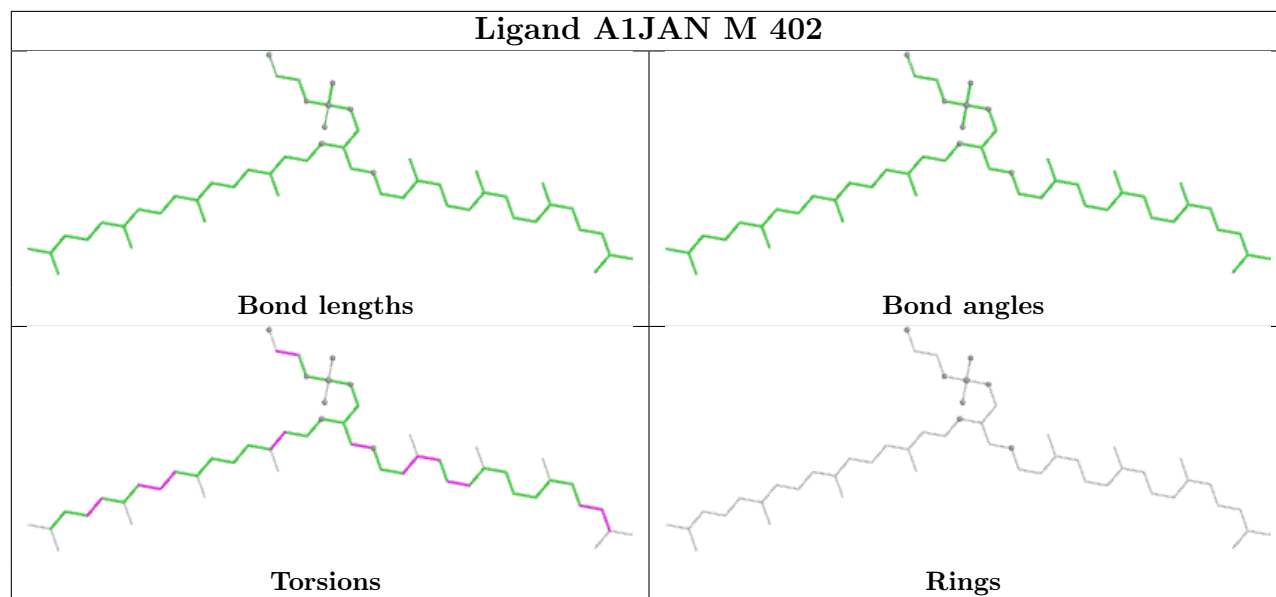
Ligand L1P D 201

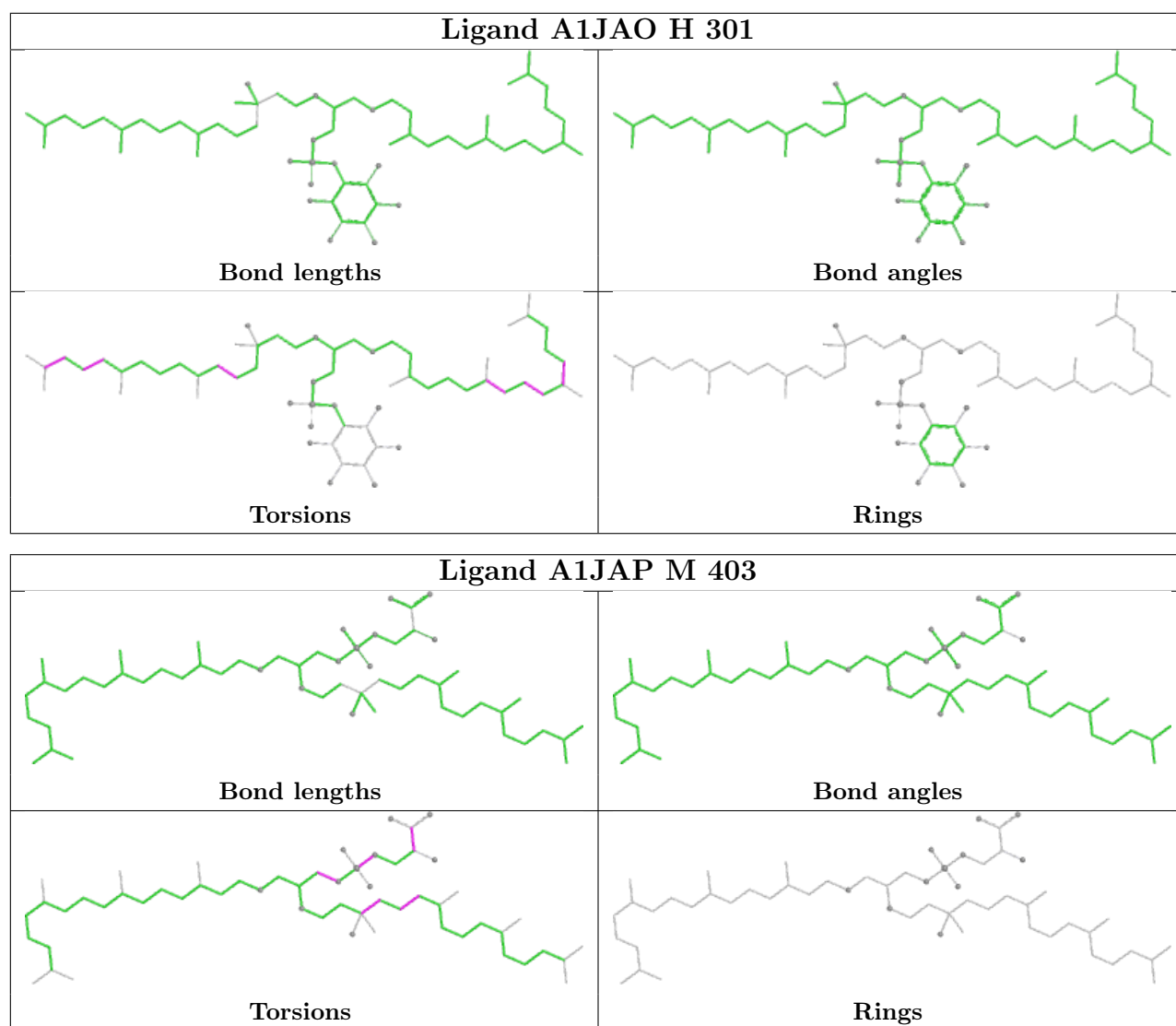


Ligand A1JAP N 403









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

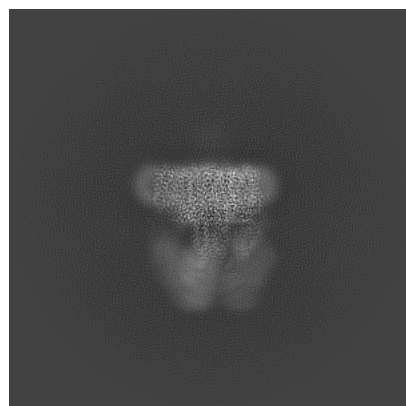
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53359. These allow visual inspection of the internal detail of the map and identification of artifacts.

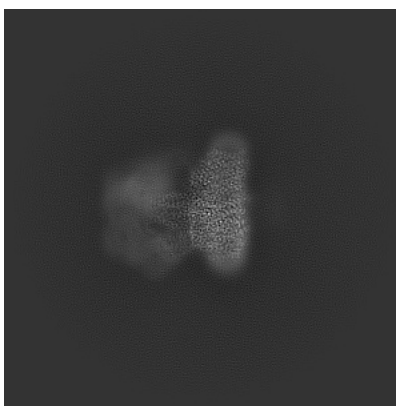
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

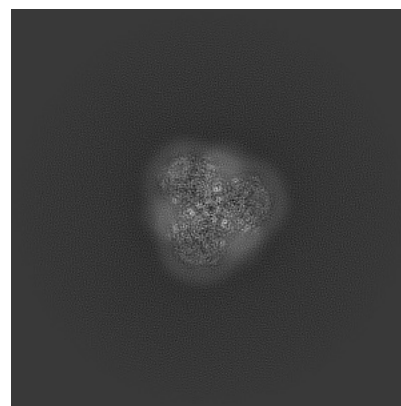
6.1.1 Primary map



X

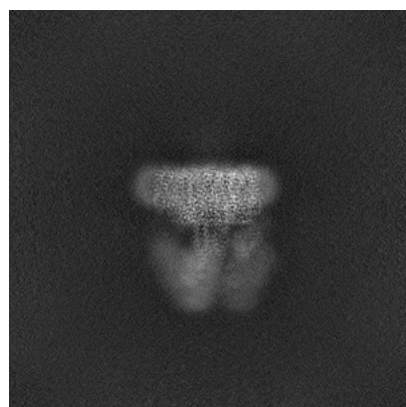


Y

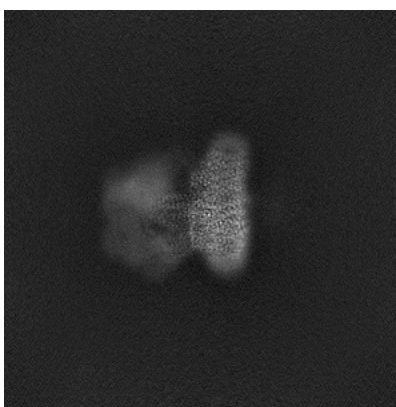


Z

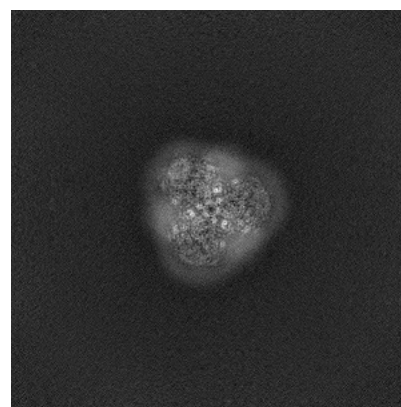
6.1.2 Raw map



X



Y

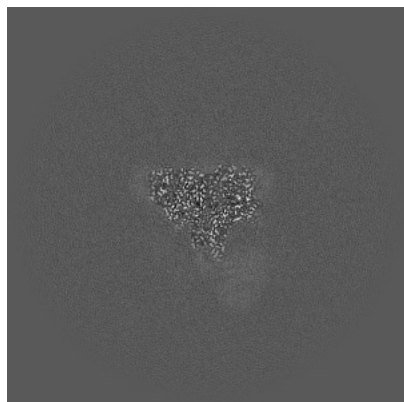


Z

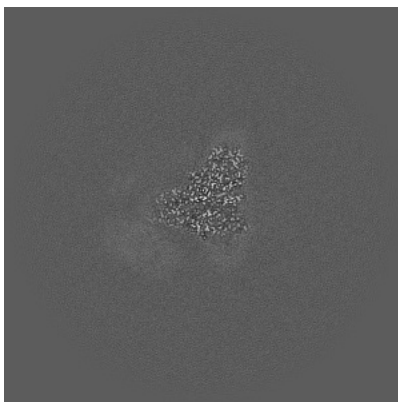
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

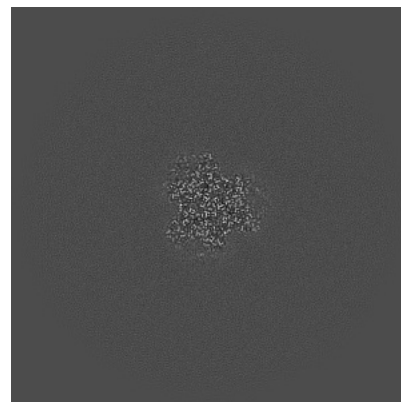
6.2.1 Primary map



X Index: 288

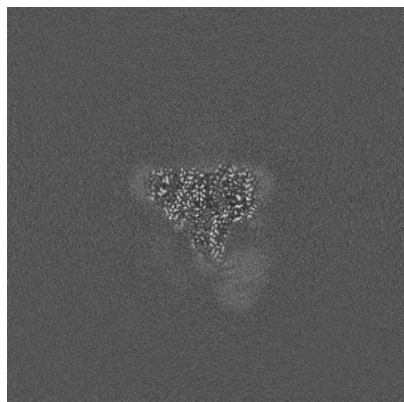


Y Index: 288

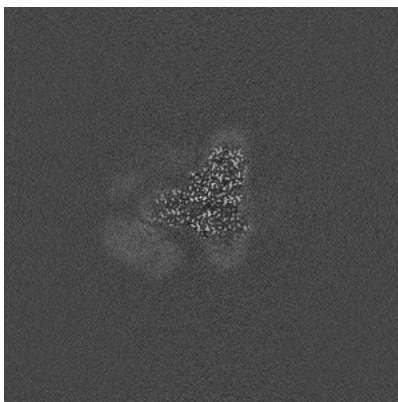


Z Index: 288

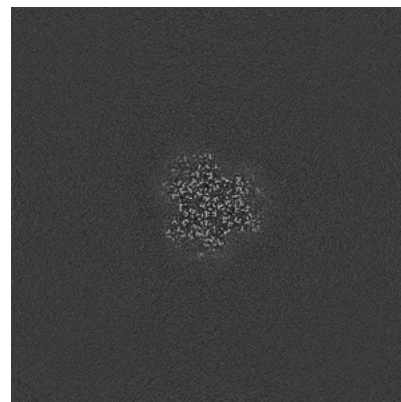
6.2.2 Raw map



X Index: 288



Y Index: 288

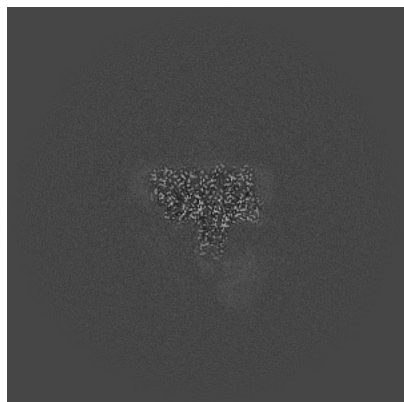


Z Index: 288

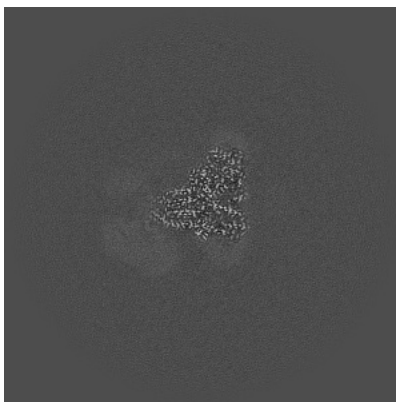
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

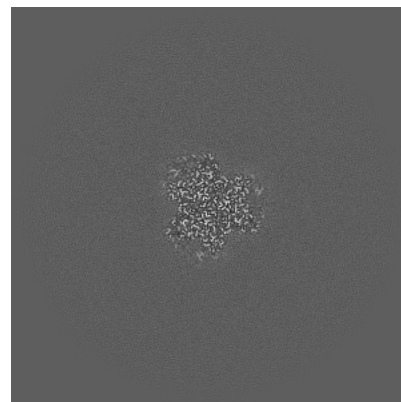
6.3.1 Primary map



X Index: 284

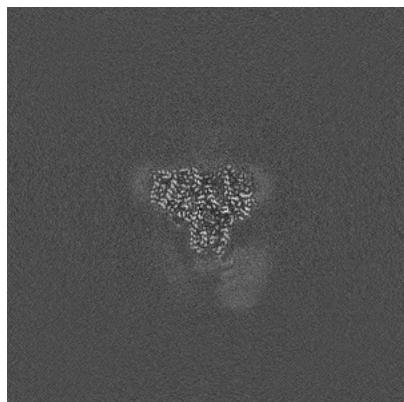


Y Index: 283

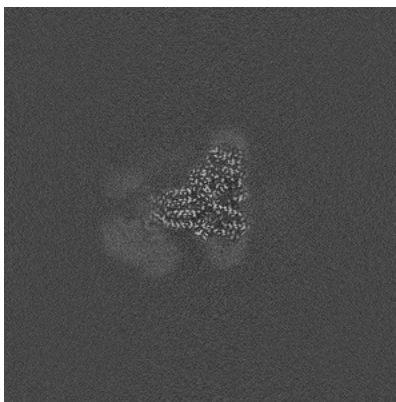


Z Index: 289

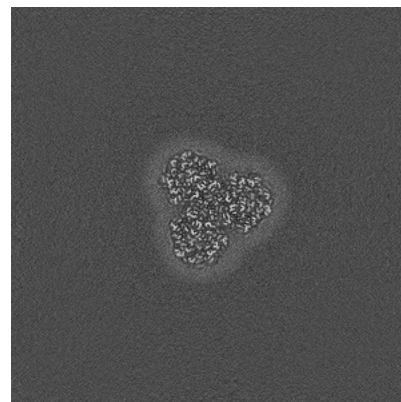
6.3.2 Raw map



X Index: 292



Y Index: 283

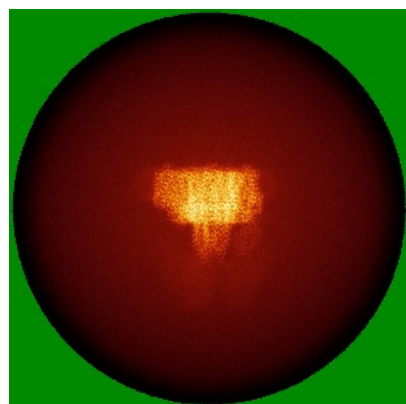


Z Index: 306

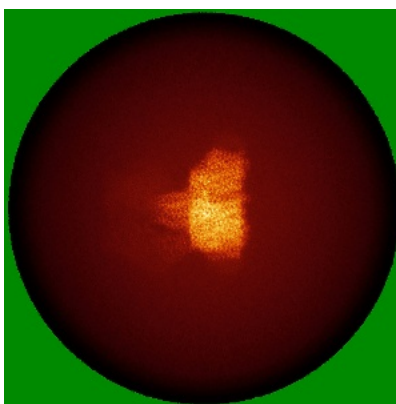
The images above show the largest variance slices of the map in three orthogonal directions.

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

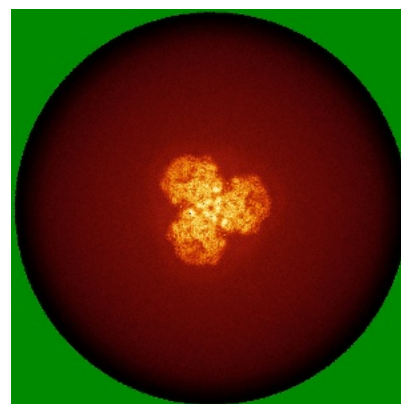
6.4.1 Primary map



X

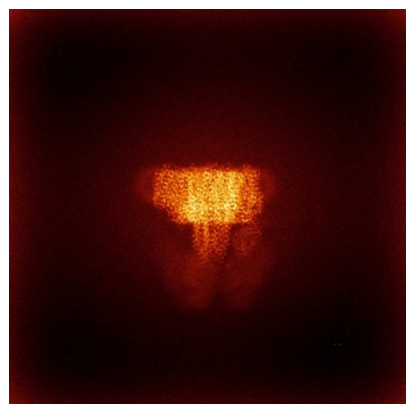


Y

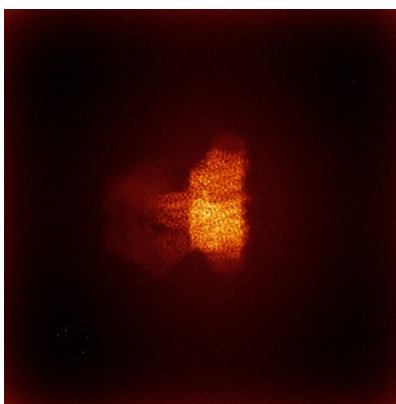


Z

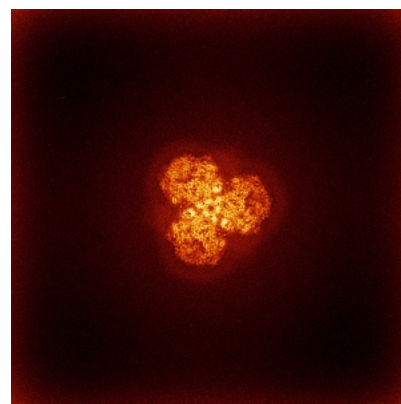
6.4.2 Raw map



X



Y



Z

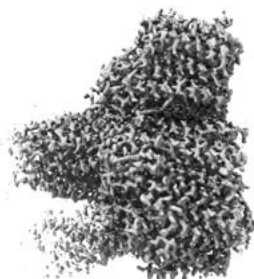
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

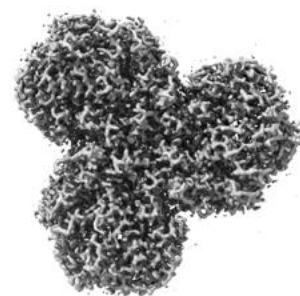
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

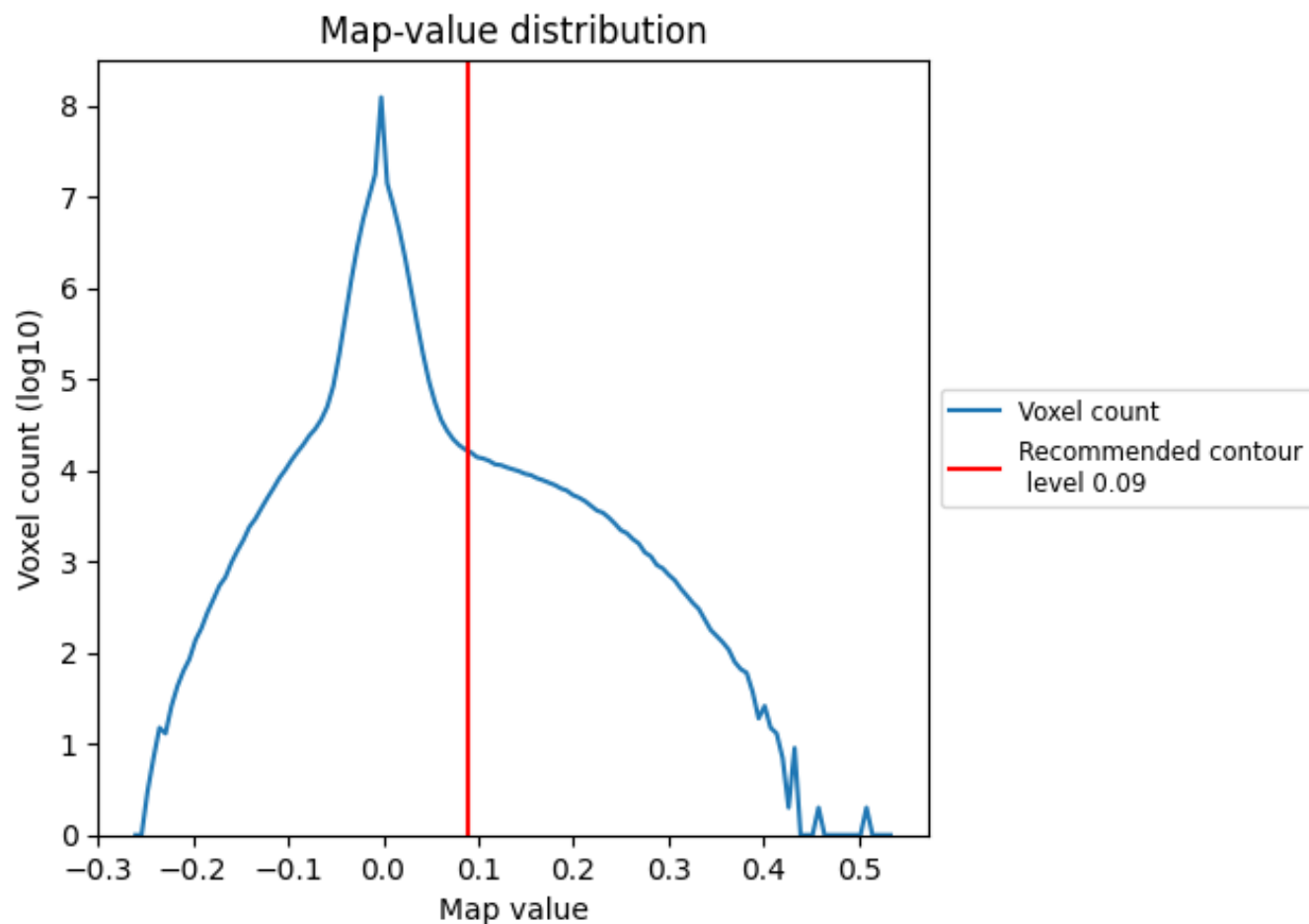
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

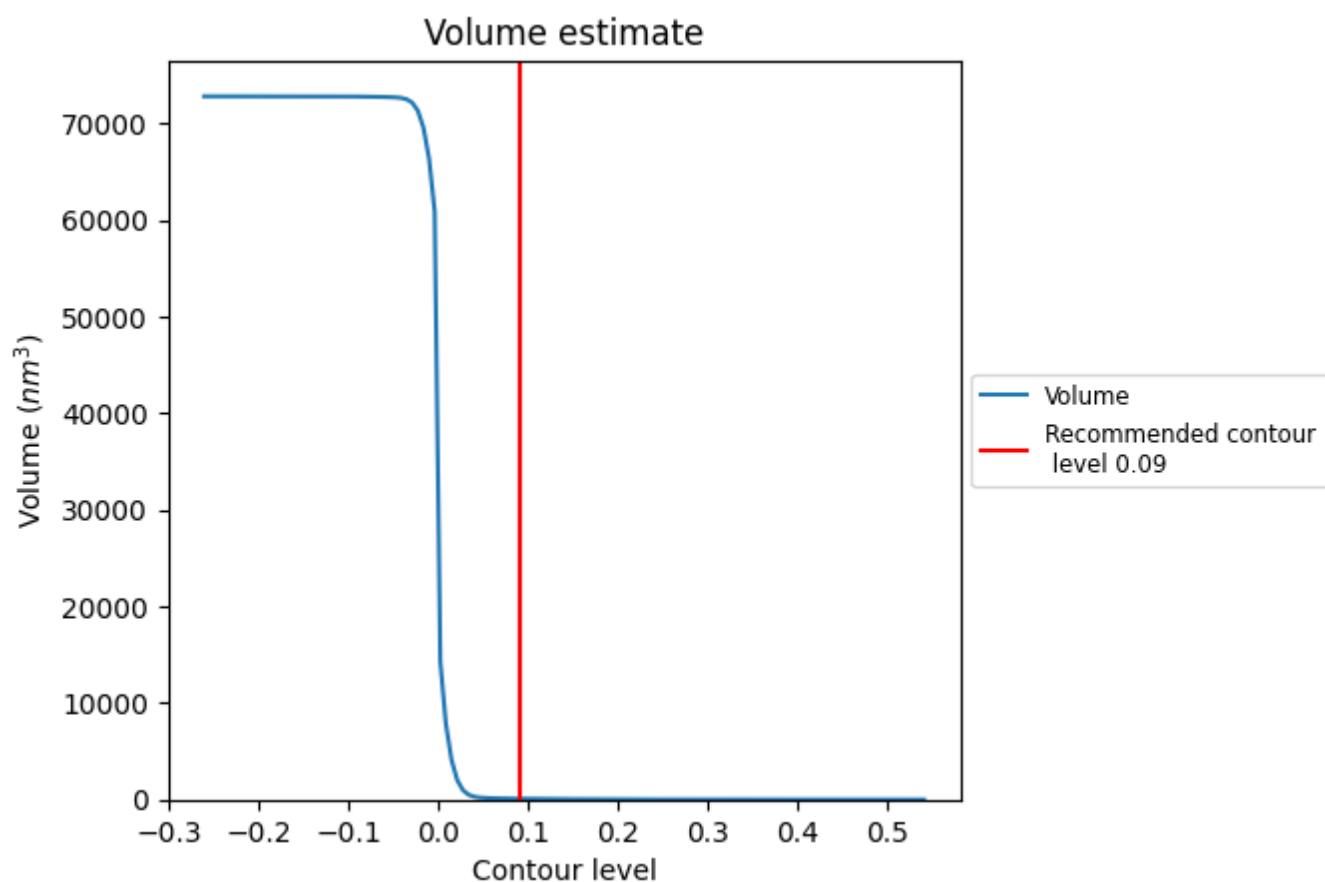
This section contains the results of statistical analysis of the map.

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.

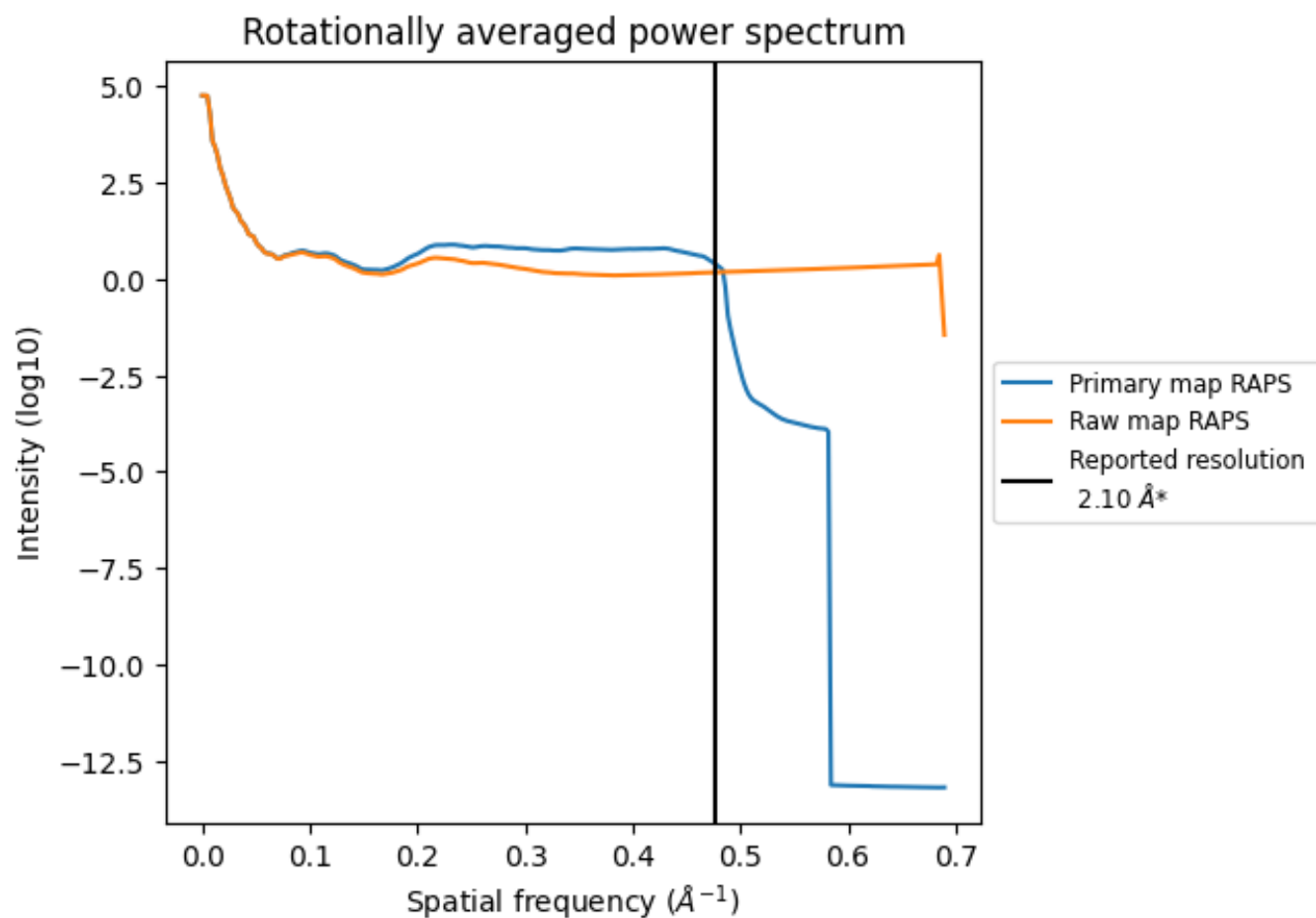
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 85 nm³; this corresponds to an approximate mass of 77 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 ⓘ

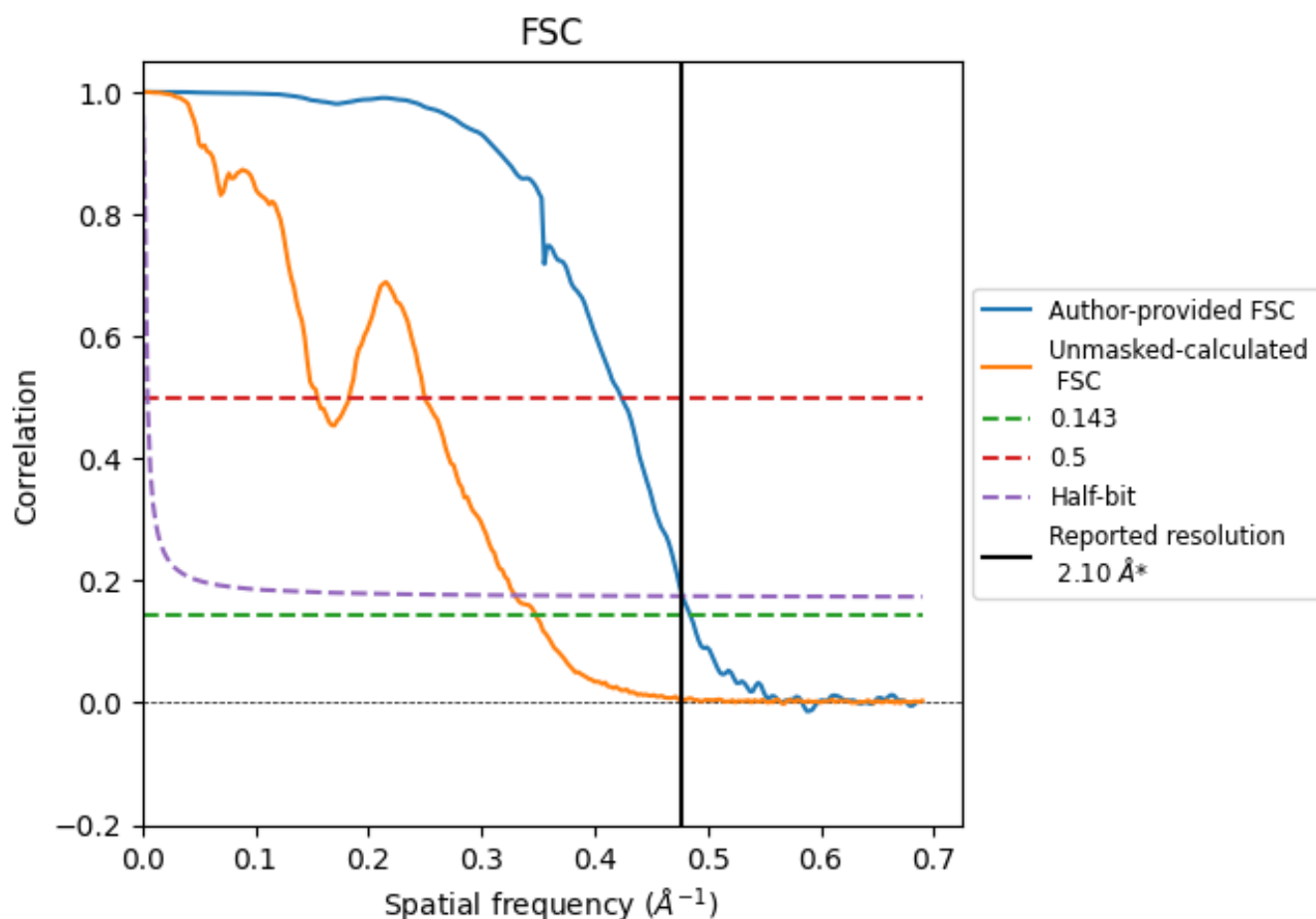


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

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 0.476 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

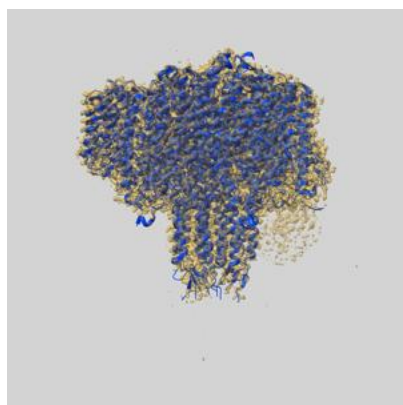
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.06	2.36	2.09
Unmasked-calculated*	2.87	6.46	3.03

*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 2.87 differs from the reported value 2.1 by more than 10 %

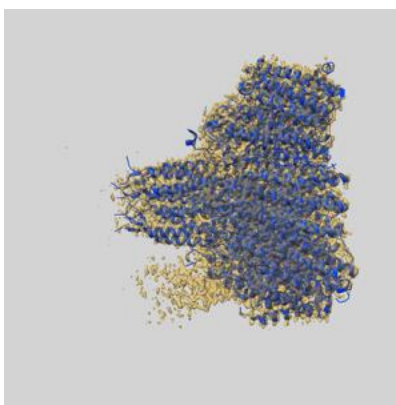
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53359 and PDB model 9QTQ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

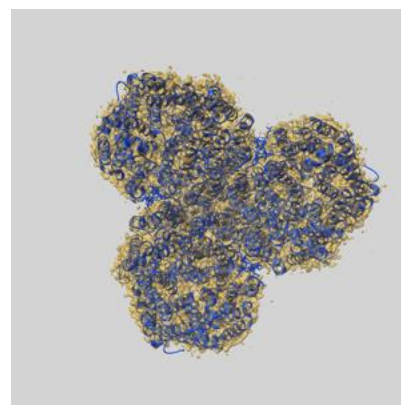
9.1 Map-model overlay [i](#)



X



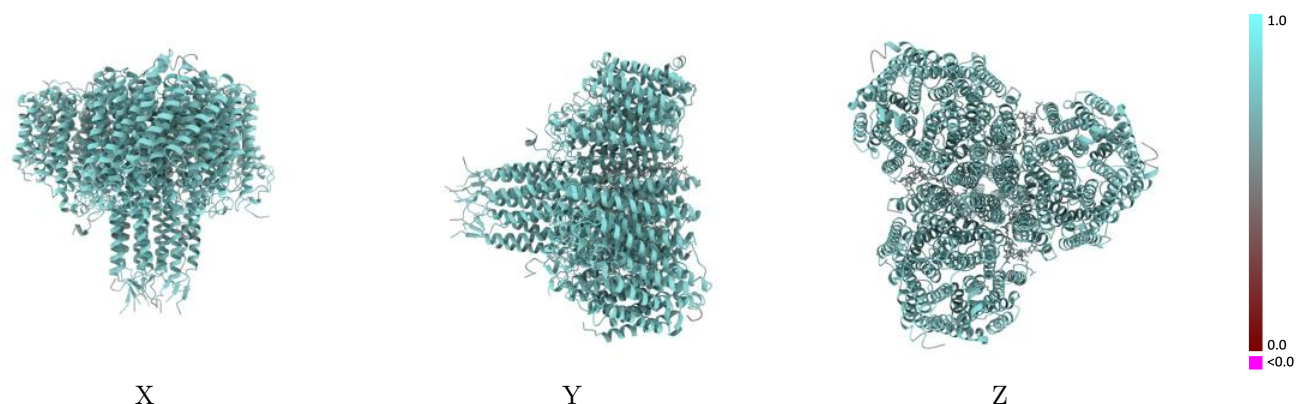
Y



Z

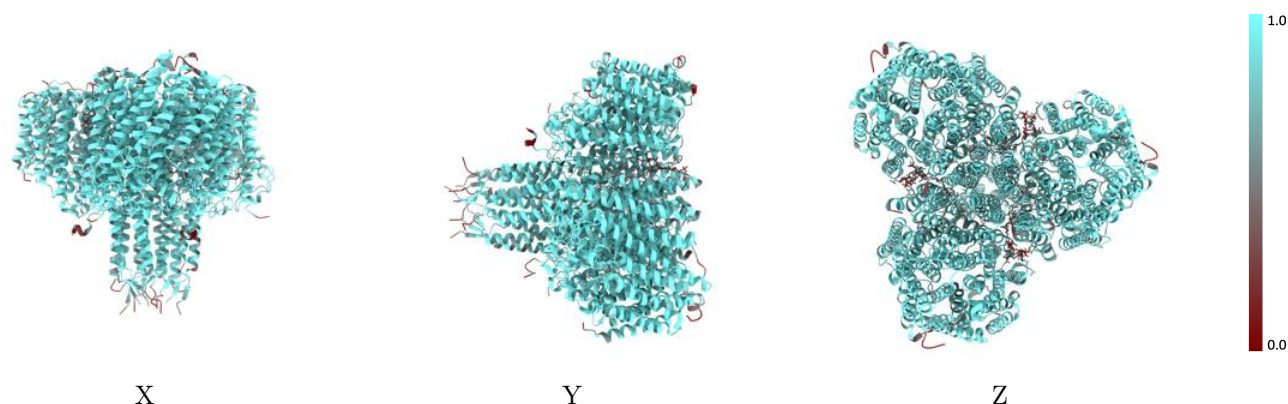
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



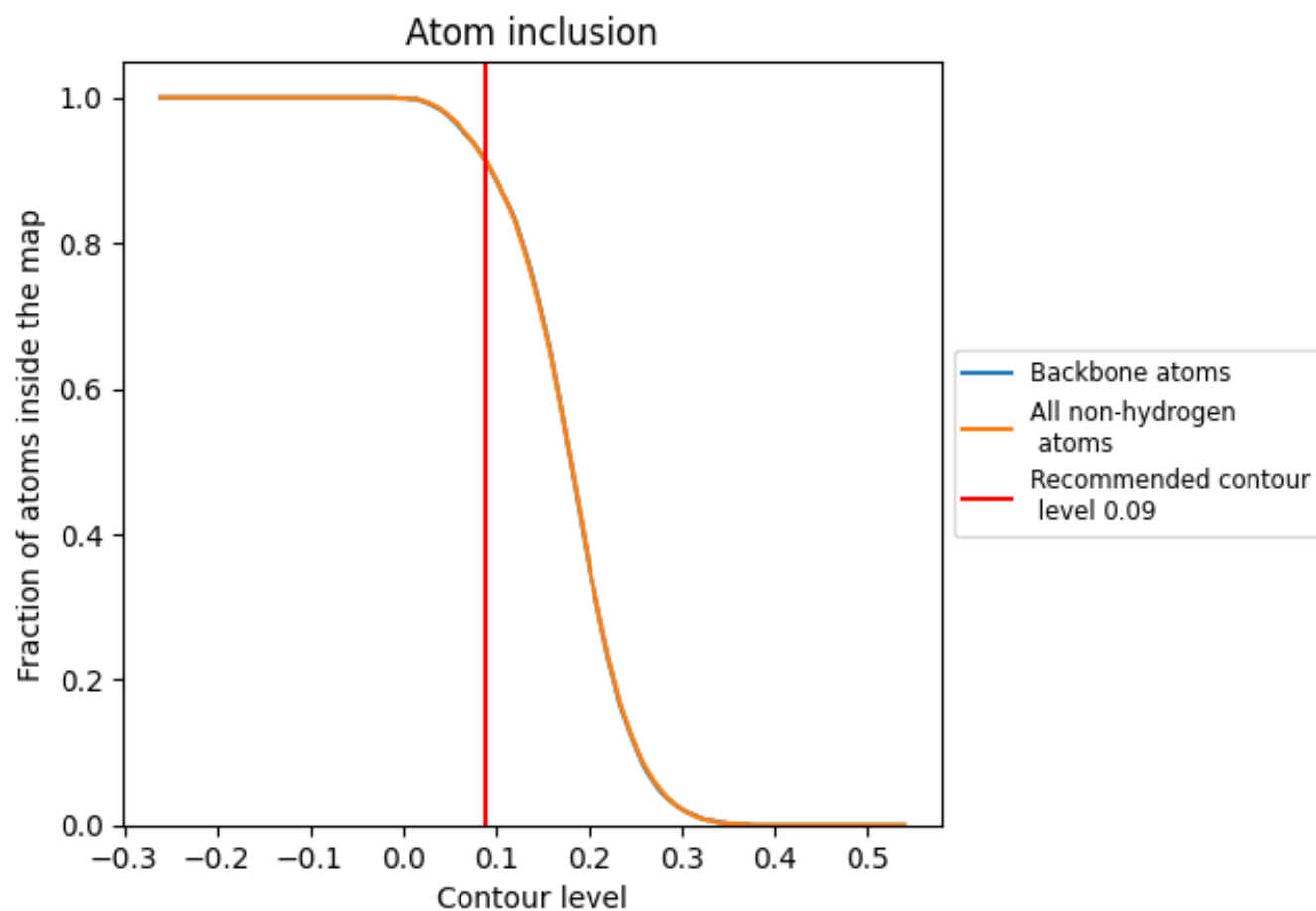
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9140	 0.7430
A	 0.9080	 0.7490
B	 0.9230	 0.7440
C	 0.9260	 0.7470
D	 0.8530	 0.7290
E	 0.9170	 0.7460
F	 0.8470	 0.7250
G	 0.8870	 0.7310
H	 0.8970	 0.7340
I	 0.9090	 0.7350
J	 0.9190	 0.7410
K	 0.9250	 0.7410
L	 0.9280	 0.7370
M	 0.9450	 0.7550
N	 0.9460	 0.7560
O	 0.9520	 0.7580
P	 0.9090	 0.7490
Q	 0.9110	 0.7460
R	 0.9000	 0.7510
S	 0.8430	 0.7300
T	 0.8310	 0.7340
U	 0.8400	 0.7290

