



wwPDB EM Validation Summary Report ⓘ

Aug 24, 2026 – 11:09 pm BST

PDB ID : 9QTS / pdb_00009qts
EMDB ID : EMD-53361
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:

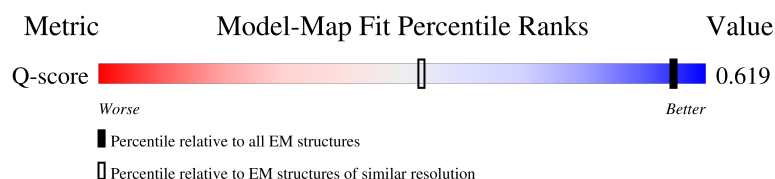
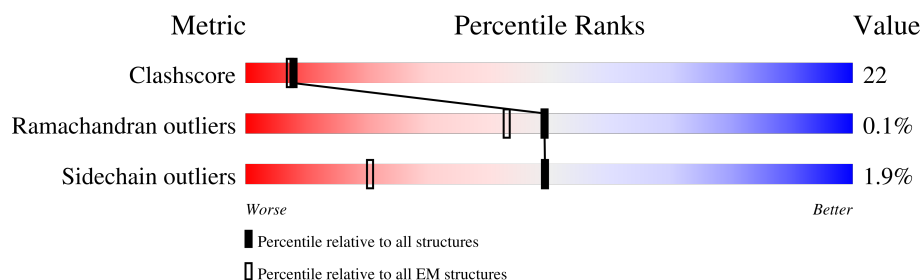
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 2.10 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.



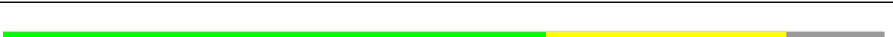
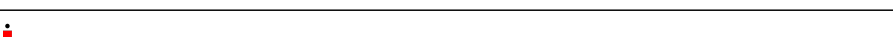
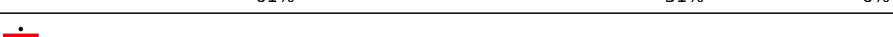
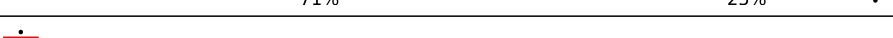
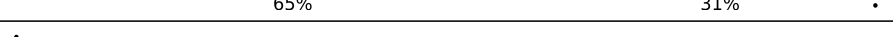
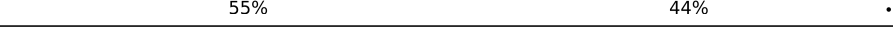
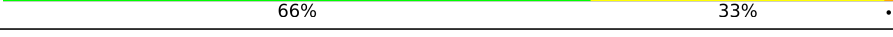
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	2317 (1.60 - 2.60)

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	
1	B	240	
1	C	240	
2	D	108	

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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	
8	i	68	
9	m	316	
9	n	316	
9	o	316	
9	p	316	
9	q	316	
9	r	316	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 45424 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	225	Total	C	N	O	S	0	0
			1660	1043	296	312	9		
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	104	Total	C	N	O	S	0	0
			807	517	130	157	3		
2	E	103	Total	C	N	O	S	0	0
			803	515	129	156	3		
2	F	104	Total	C	N	O	S	0	0
			807	517	130	157	3		

- 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	68	Total	C	N	O	S	0	0
			499	324	85	87	3		
6	Q	68	Total	C	N	O	S	0	0
			499	324	85	87	3		
6	R	68	Total	C	N	O	S	0	0
			499	324	85	87	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		

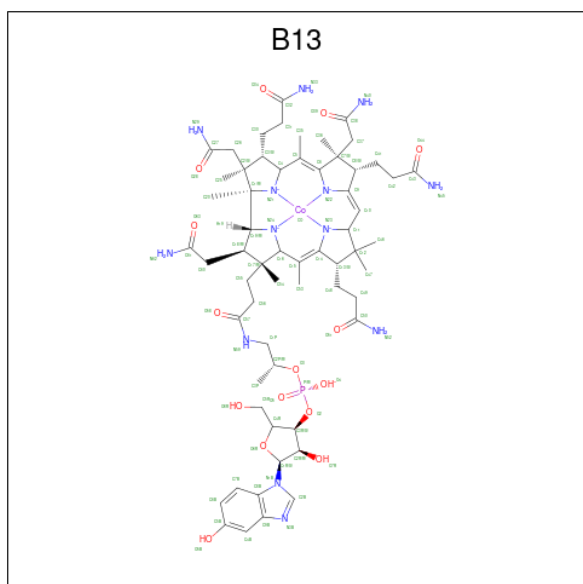
- Molecule 8 is a protein called Conserved protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	53	Total	C	N	O	S	0	0
			413	253	74	83	3		

- Molecule 9 is a protein called Tetrahydromethanopterin S-methyltransferase subunit H.

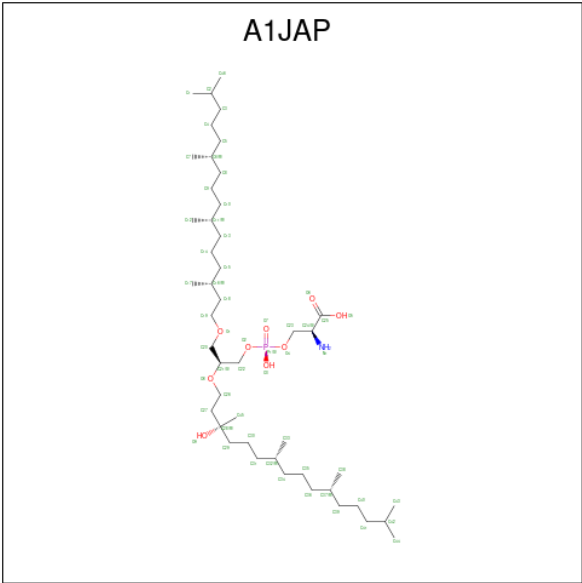
Mol	Chain	Residues	Atoms					AltConf	Trace
9	m	316	Total	C	N	O	S	0	0
			2396	1527	395	464	10		
9	n	316	Total	C	N	O	S	0	0
			2396	1527	395	464	10		
9	o	316	Total	C	N	O	S	0	0
			2396	1527	395	464	10		
9	p	316	Total	C	N	O	S	0	0
			2396	1527	395	464	10		
9	q	316	Total	C	N	O	S	0	0
			2396	1527	395	464	10		
9	r	316	Total	C	N	O	S	0	0
			2396	1527	395	464	10		

- Molecule 10 is 5-HYDROXYBENZIMIDAZOLYLCOB(III)AMIDE (CCD ID: B13) (formula: $C_{60}H_{88}CoN_{13}O_{15}P$) (labeled as "Ligand of Interest" by depositor).



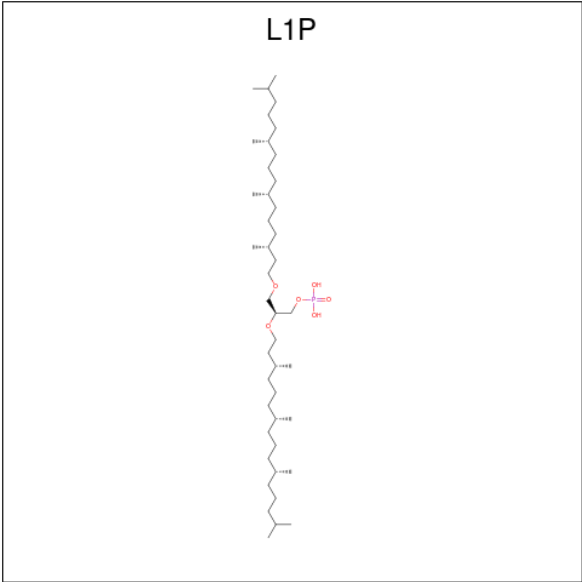
Mol	Chain	Residues	Atoms						AltConf
10	A	1	Total	C	Co	N	O	P	0
			90	60	1	13	15	1	

- Molecule 11 is 2-Hydroxy-archaetidylinositol (CCD ID: A1JAP) (formula: C₄₆H₉₄NO₉P) (labeled as "Ligand of Interest" by depositor).



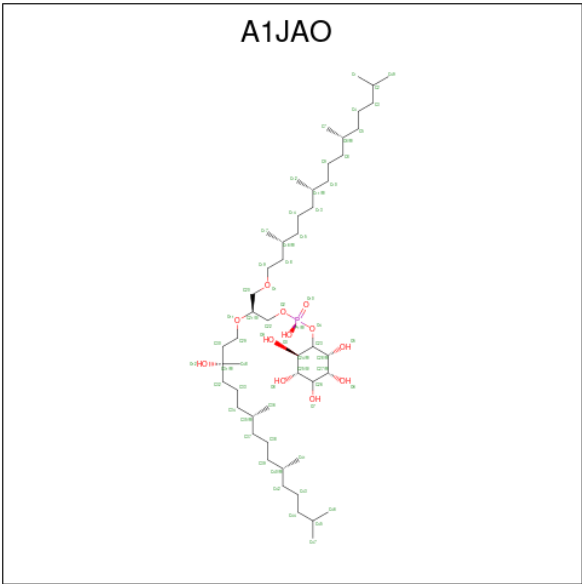
Mol	Chain	Residues	Atoms						AltConf
11	A	1	Total 150	C 46	H 93	N 1	O 9	P 1	0
11	M	1	Total 150	C 46	H 93	N 1	O 9	P 1	0
11	N	1	Total 150	C 46	H 93	N 1	O 9	P 1	0
11	S	1	Total 150	C 46	H 93	N 1	O 9	P 1	0
11	T	1	Total 150	C 46	H 93	N 1	O 9	P 1	0
11	U	1	Total 150	C 46	H 93	N 1	O 9	P 1	0

- Molecule 12 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
12	D	1	Total	C	H	O	P	0
			137	43	87	6	1	
12	G	1	Total	C	H	O	P	0
			137	43	87	6	1	
12	I	1	Total	C	H	O	P	0
			137	43	87	6	1	

- Molecule 13 is Archaeetidylinositol (CCD ID: A1JAO) (formula: C₄₉H₉₉O₁₂P) (labeled as "Ligand of Interest" by depositor).

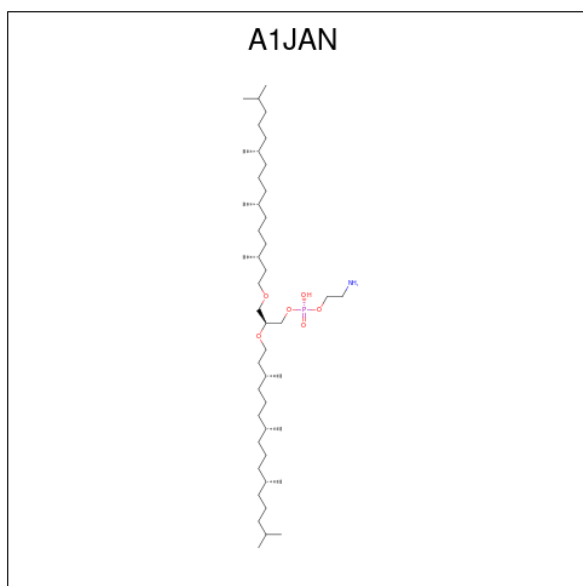


Mol	Chain	Residues	Atoms					AltConf
13	F	1	Total	C	H	O	P	0
			160	49	98	12	1	
13	G	1	Total	C	H	O	P	0
			160	49	98	12	1	
13	H	1	Total	C	H	O	P	0
			160	49	98	12	1	

- Molecule 14 is SODIUM ION (CCD ID: NA) (formula: Na) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 15 is Archaeidylethanolamine (CCD ID: A1JAN) (formula: C₄₅H₉₄NO₆P) (labeled as "Ligand of Interest" by depositor).



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

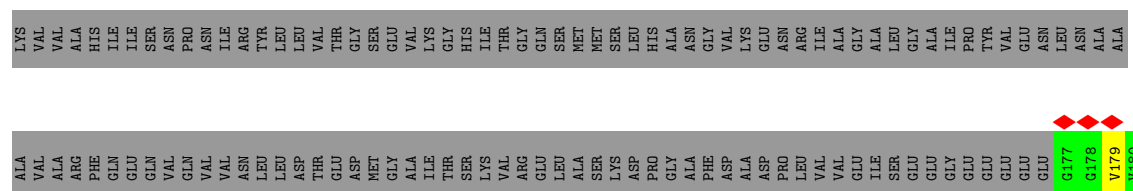
- Molecule 16 is water.

Mol	Chain	Residues	Atoms		AltConf
16	A	57	Total 57	O 57	0
16	B	38	Total 38	O 38	0
16	C	44	Total 44	O 44	0
16	D	96	Total 96	O 96	0
16	E	84	Total 84	O 84	0
16	F	107	Total 107	O 107	0
16	G	229	Total 229	O 229	0
16	H	230	Total 230	O 230	0
16	I	261	Total 261	O 261	0
16	J	173	Total 173	O 173	0
16	K	177	Total 177	O 177	0
16	L	206	Total 206	O 206	0
16	M	180	Total 180	O 180	0
16	N	188	Total 188	O 188	0
16	O	164	Total 164	O 164	0
16	P	67	Total 67	O 67	0
16	Q	49	Total 49	O 49	0
16	R	52	Total 52	O 52	0
16	S	63	Total 63	O 63	0
16	T	75	Total 75	O 75	0
16	U	67	Total 67	O 67	0

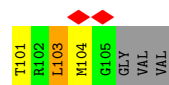
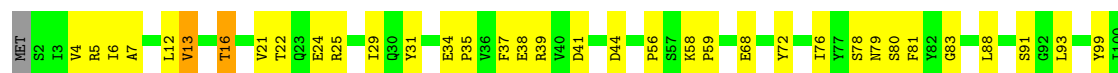
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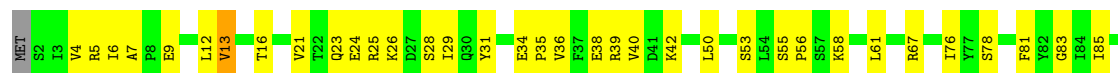
Mol	Chain	Residues	Atoms		AltConf
16	i	34	Total	O	0
			34	34	



• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B



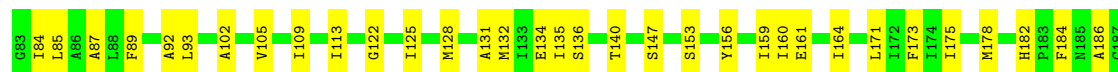
• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B

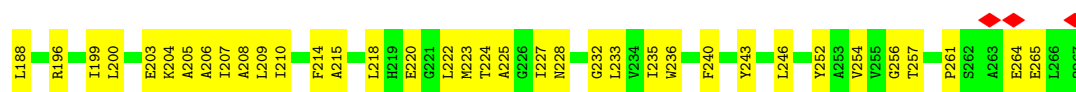


• Molecule 2: Tetrahydromethanopterin S-methyltransferase subunit B



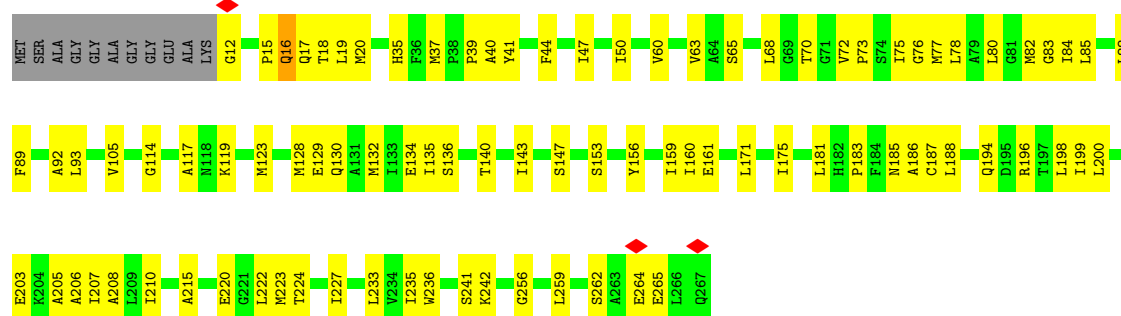
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C





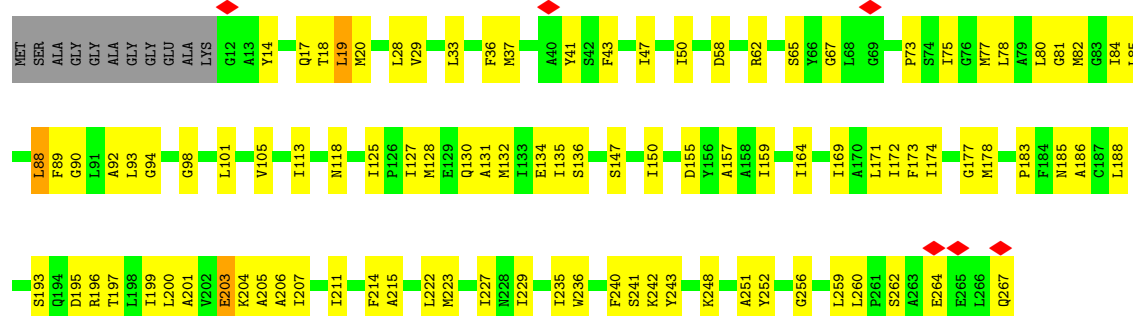
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

Chain H: 62% 33%



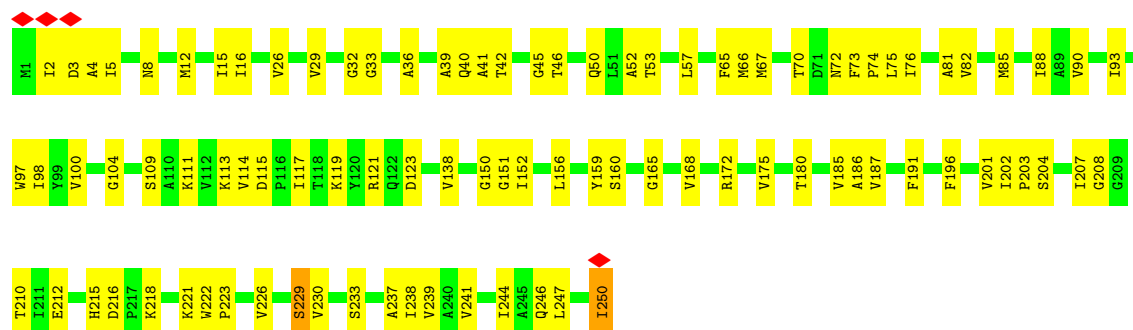
• Molecule 3: Tetrahydromethanopterin S-methyltransferase subunit C

Chain I: 59% 36%



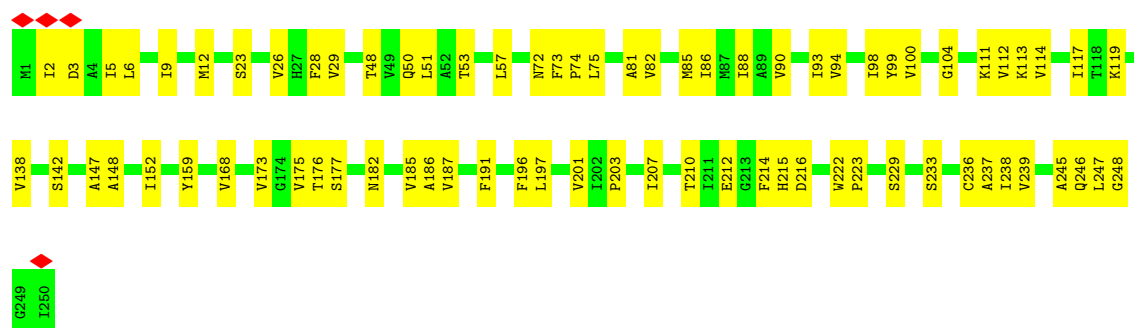
• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

Chain J: 62% 37%

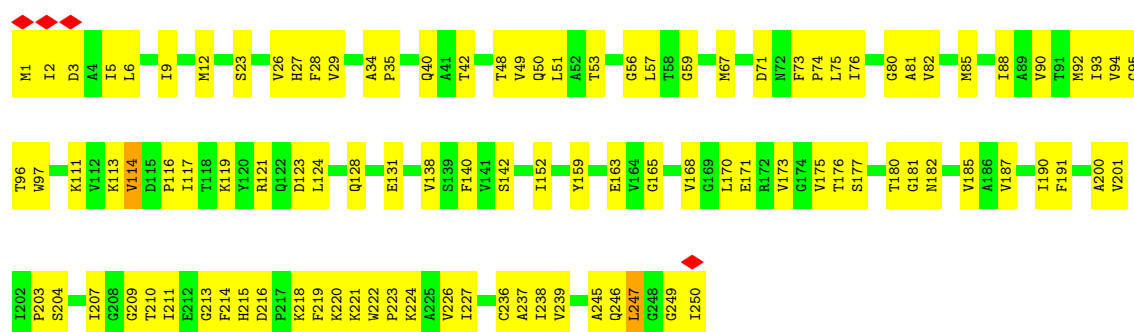


• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D

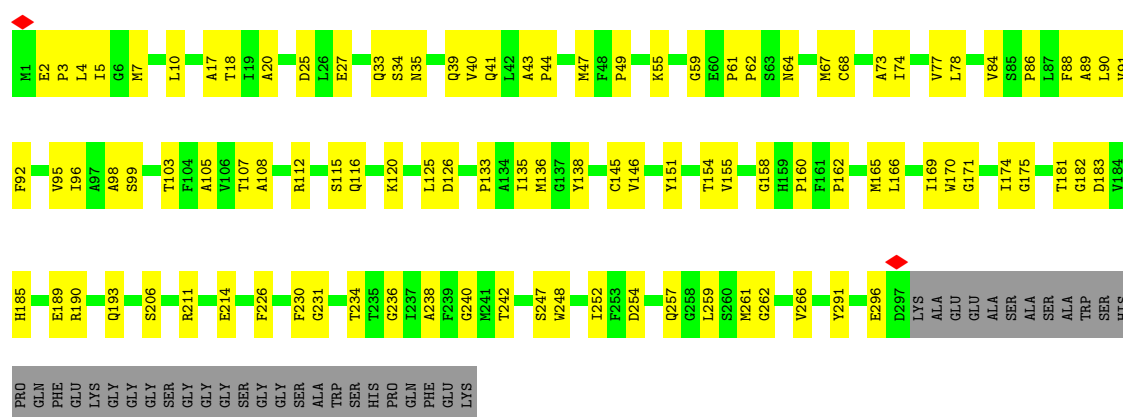
Chain K: 70% 30%



• Molecule 4: Tetrahydromethanopterin S-methyltransferase subunit D



• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E



• Molecule 5: Tetrahydromethanopterin S-methyltransferase subunit E





- Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



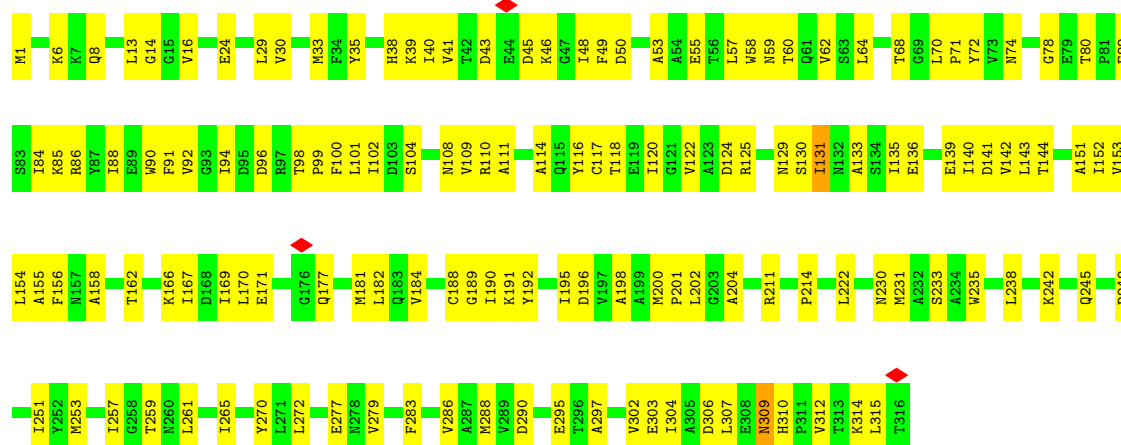
- Molecule 7: Tetrahydromethanopterin S-methyltransferase subunit G



- Molecule 8: Conserved protein

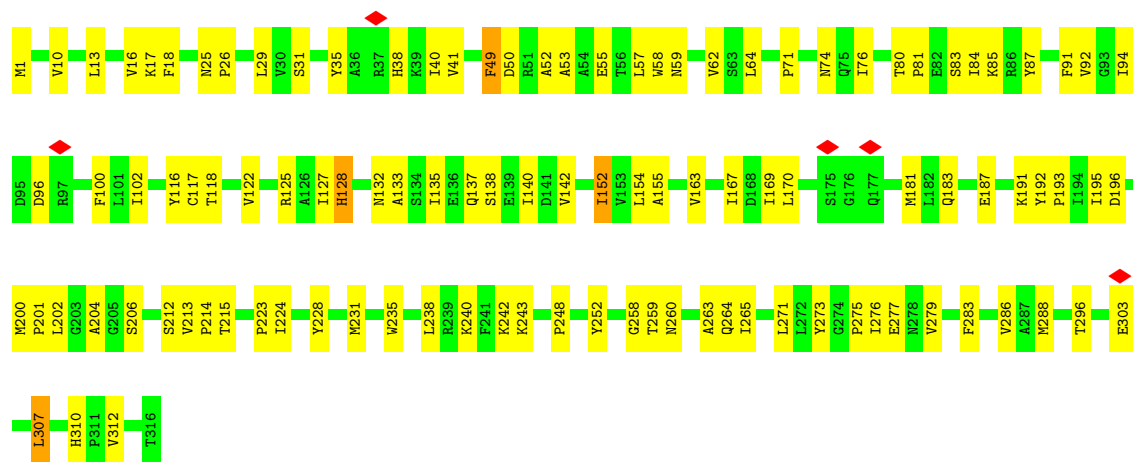


- Molecule 9: Tetrahydromethanopterin S-methyltransferase subunit H



- Molecule 9: Tetrahydromethanopterin S-methyltransferase subunit H

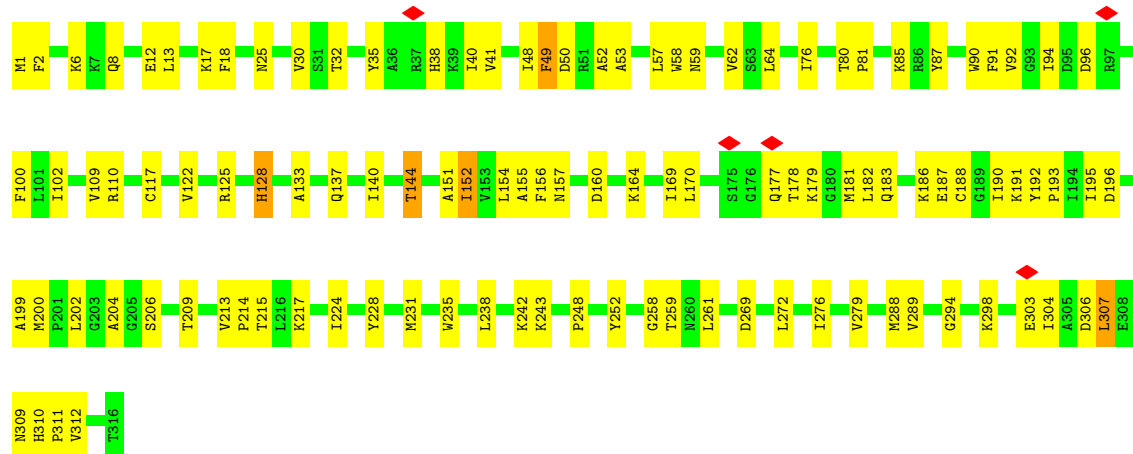




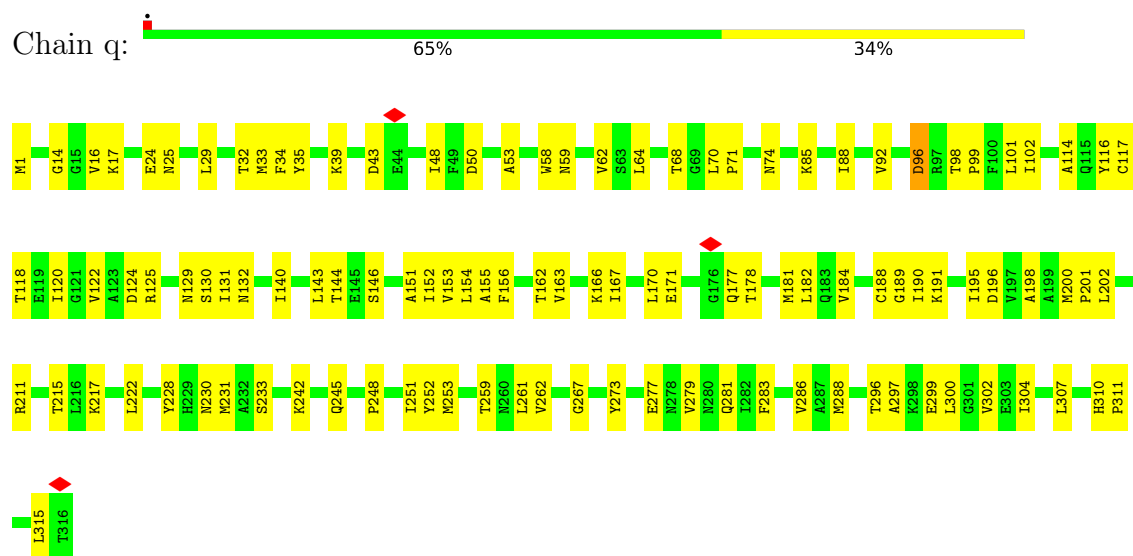
• Molecule 9: Tetrahydromethanopterin S-methyltransferase subunit H



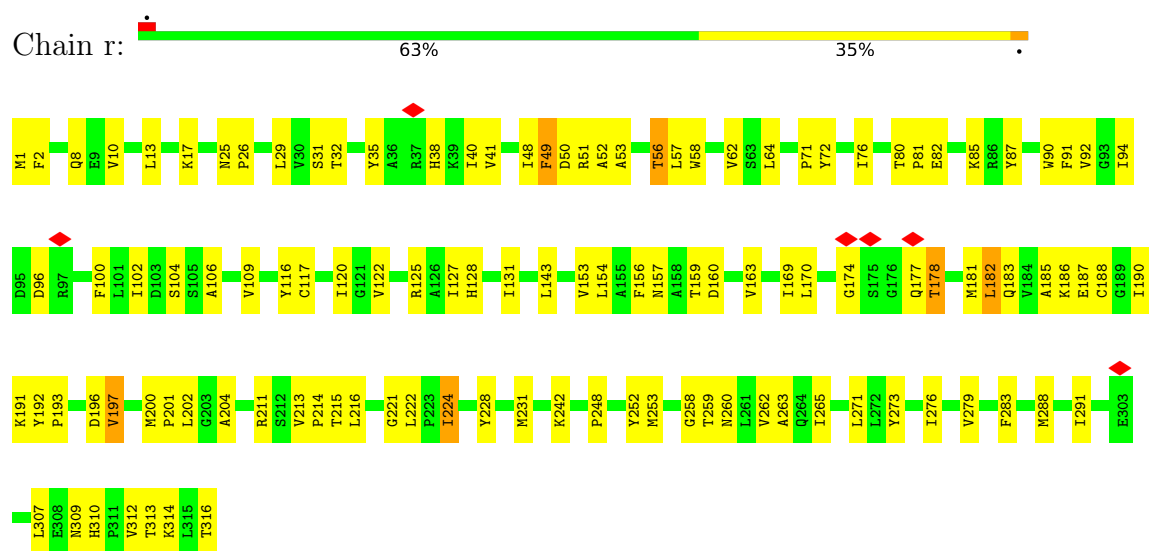
• Molecule 9: Tetrahydromethanopterin S-methyltransferase subunit H



● Molecule 9: Tetrahydromethanopterin S-methyltransferase subunit H



● Molecule 9: Tetrahydromethanopterin S-methyltransferase subunit H



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	150000	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	0.544	Depositor
Minimum map value	0.122	Depositor
Average map value	0.160	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.2	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1JAO, L1P, A1JAP, B13, 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	0.10	0/1682	0.26	0/2273
1	B	0.14	0/468	0.28	0/625
1	C	0.11	0/472	0.25	0/630
2	D	0.13	0/821	0.28	0/1116
2	E	0.12	0/817	0.24	0/1111
2	F	0.12	0/821	0.28	0/1116
3	G	0.10	0/1864	0.24	0/2536
3	H	0.12	0/1864	0.27	0/2536
3	I	0.10	0/1864	0.23	0/2536
4	J	0.11	0/1813	0.25	0/2475
4	K	0.10	0/1813	0.26	0/2475
4	L	0.11	0/1813	0.26	0/2475
5	M	0.11	0/2294	0.24	0/3121
5	N	0.10	0/2294	0.24	0/3121
5	O	0.10	0/2294	0.24	0/3121
6	P	0.11	0/506	0.25	0/684
6	Q	0.11	0/506	0.28	0/684
6	R	0.11	0/506	0.28	0/684
7	S	0.11	0/551	0.20	0/737
7	T	0.12	0/551	0.21	0/737
7	U	0.12	0/551	0.21	0/737
8	i	0.08	0/417	0.18	0/563
9	m	0.11	0/2444	0.24	0/3318
9	n	0.11	0/2444	0.24	0/3318
9	o	0.12	0/2444	0.23	0/3318
9	p	0.12	0/2444	0.26	0/3318
9	q	0.11	0/2444	0.22	0/3318
9	r	0.11	0/2444	0.23	0/3318
All	All	0.11	0/41246	0.25	0/56001

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	1660	0	1718	102	0
1	B	465	0	510	28	0
1	C	469	0	513	27	0
2	D	807	0	817	50	0
2	E	803	0	814	41	0
2	F	807	0	817	35	0
3	G	1830	0	1918	104	0
3	H	1830	0	1918	91	0
3	I	1830	0	1918	92	0
4	J	1778	0	1862	91	0
4	K	1778	0	1862	89	0
4	L	1778	0	1862	98	0
5	M	2237	0	2234	92	0
5	N	2237	0	2234	97	0
5	O	2237	0	2234	105	0
6	P	499	0	531	25	0
6	Q	499	0	531	25	0
6	R	499	0	531	38	0
7	S	543	0	562	26	0
7	T	543	0	562	28	0
7	U	543	0	562	24	0
8	i	413	0	398	31	0
9	m	2396	0	2396	140	0
9	n	2396	0	2396	109	0
9	o	2396	0	2396	112	0
9	p	2396	0	2396	118	0
9	q	2396	0	2396	100	0
9	r	2396	0	2396	124	0
10	A	90	0	81	10	0
11	A	57	93	0	1	0
11	M	57	93	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	N	57	93	0	0	0
11	S	57	93	0	0	0
11	T	57	93	0	2	0
11	U	57	93	0	1	0
12	D	50	87	87	9	0
12	G	50	87	87	7	0
12	I	50	87	87	6	0
13	F	62	98	0	3	0
13	G	62	98	0	0	0
13	H	62	98	0	0	0
14	M	1	0	0	0	0
14	N	1	0	0	0	0
14	O	1	0	0	0	0
15	N	53	93	0	2	0
15	O	53	93	0	0	0
15	T	53	93	0	3	0
16	A	57	0	0	6	0
16	B	38	0	0	4	0
16	C	44	0	0	2	0
16	D	96	0	0	10	0
16	E	84	0	0	5	0
16	F	107	0	0	8	0
16	G	229	0	0	27	0
16	H	230	0	0	15	0
16	I	261	0	0	29	0
16	J	173	0	0	20	0
16	K	177	0	0	22	0
16	L	206	0	0	27	0
16	M	180	0	0	10	0
16	N	188	0	0	17	0
16	O	164	0	0	20	0
16	P	67	0	0	7	0
16	Q	49	0	0	1	0
16	R	52	0	0	6	0
16	S	63	0	0	12	0
16	T	75	0	0	13	0
16	U	67	0	0	4	0
16	i	34	0	0	11	0
All	All	44032	1392	41626	1799	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 22.

The worst 5 of 1799 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)
9:p:133:ALA:HA	9:p:181:MET:HE3	1.33	1.10
2:F:16:THR:HG21	9:r:215:THR:HA	1.33	1.10
2:E:34:GLU:HG3	2:E:35:PRO:HD3	1.33	1.07
3:H:16:GLN:HG3	3:H:20:MET:HE3	1.32	1.06
9:r:92:VAL:HG21	9:r:122:VAL:HG21	1.35	1.04

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	221/240 (92%)	213 (96%)	8 (4%)	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	102/108 (94%)	97 (95%)	5 (5%)	0	100	100
2	E	101/108 (94%)	95 (94%)	6 (6%)	0	100	100
2	F	102/108 (94%)	96 (94%)	6 (6%)	0	100	100
3	G	254/267 (95%)	249 (98%)	5 (2%)	0	100	100
3	H	254/267 (95%)	245 (96%)	9 (4%)	0	100	100
3	I	254/267 (95%)	251 (99%)	3 (1%)	0	100	100
4	J	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
4	K	248/250 (99%)	241 (97%)	7 (3%)	0	100	100
4	L	248/250 (99%)	242 (98%)	6 (2%)	0	100	100
5	M	295/334 (88%)	293 (99%)	2 (1%)	0	100	100
5	N	295/334 (88%)	291 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	O	295/334 (88%)	292 (99%)	3 (1%)	0	100	100
6	P	66/72 (92%)	63 (96%)	3 (4%)	0	100	100
6	Q	66/72 (92%)	64 (97%)	2 (3%)	0	100	100
6	R	66/72 (92%)	62 (94%)	4 (6%)	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
8	i	51/68 (75%)	51 (100%)	0	0	100	100
9	m	314/316 (99%)	304 (97%)	10 (3%)	0	100	100
9	n	314/316 (99%)	299 (95%)	14 (4%)	1 (0%)	36	36
9	o	314/316 (99%)	305 (97%)	9 (3%)	0	100	100
9	p	314/316 (99%)	296 (94%)	17 (5%)	1 (0%)	36	36
9	q	314/316 (99%)	302 (96%)	12 (4%)	0	100	100
9	r	314/316 (99%)	298 (95%)	15 (5%)	1 (0%)	36	36
All	All	5374/5993 (90%)	5215 (97%)	156 (3%)	3 (0%)	49	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	n	49	PHE
9	p	49	PHE
9	r	49	PHE

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	177/190 (93%)	174 (98%)	3 (2%)	53	62
1	B	49/190 (26%)	48 (98%)	1 (2%)	48	56
1	C	49/190 (26%)	49 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	91/94 (97%)	87 (96%)	4 (4%)	25	26
2	E	91/94 (97%)	87 (96%)	4 (4%)	25	26
2	F	91/94 (97%)	87 (96%)	4 (4%)	25	26
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%)	182 (98%)	3 (2%)	55	64
4	K	185/185 (100%)	185 (100%)	0	100	100
4	L	185/185 (100%)	182 (98%)	3 (2%)	55	64
5	M	237/261 (91%)	236 (100%)	1 (0%)	84	89
5	N	237/261 (91%)	236 (100%)	1 (0%)	84	89
5	O	237/261 (91%)	234 (99%)	3 (1%)	61	69
6	P	51/54 (94%)	50 (98%)	1 (2%)	48	56
6	Q	51/54 (94%)	49 (96%)	2 (4%)	28	31
6	R	51/54 (94%)	49 (96%)	2 (4%)	28	31
7	S	58/60 (97%)	58 (100%)	0	100	100
7	T	58/60 (97%)	57 (98%)	1 (2%)	53	62
7	U	58/60 (97%)	57 (98%)	1 (2%)	53	62
8	i	44/57 (77%)	43 (98%)	1 (2%)	44	51
9	m	255/255 (100%)	251 (98%)	4 (2%)	55	64
9	n	255/255 (100%)	248 (97%)	7 (3%)	39	45
9	o	255/255 (100%)	249 (98%)	6 (2%)	43	49
9	p	255/255 (100%)	248 (97%)	7 (3%)	39	45
9	q	255/255 (100%)	250 (98%)	5 (2%)	48	56
9	r	255/255 (100%)	248 (97%)	7 (3%)	39	45
All	All	4255/4671 (91%)	4175 (98%)	80 (2%)	49	58

5 of 80 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	o	132	ASN
9	q	177	GLN
9	o	178	THR

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Mol	Chain	Res	Type
9	p	164	LYS
9	r	159	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
9	o	132	ASN
9	q	177	GLN
9	o	229	HIS
9	p	183	GLN
9	r	128	HIS

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 19 ligands modelled in this entry, 3 are monoatomic - leaving 16 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	$\# Z > 2$
11	A1JAP	T	102	-	53,56,56	0.39	0	61,71,71	0.50	0
11	A1JAP	U	101	-	53,56,56	0.40	0	61,71,71	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	A1JAP	M	402	-	53,56,56	0.39	0	61,71,71	0.47	0
13	A1JAO	F	201	-	60,62,62	0.29	0	74,82,82	1.02	3 (4%)
15	A1JAN	N	402	-	52,52,52	0.31	0	59,63,63	0.36	0
11	A1JAP	S	101	-	53,56,56	0.40	0	61,71,71	0.55	0
13	A1JAO	G	302	-	60,62,62	0.30	0	74,82,82	0.41	0
15	A1JAN	O	402	-	52,52,52	0.31	0	59,63,63	0.45	0
12	L1P	I	301	-	49,49,49	0.29	0	57,60,60	0.37	0
12	L1P	G	301	-	49,49,49	0.29	0	57,60,60	0.36	0
12	L1P	D	201	-	49,49,49	0.28	0	57,60,60	0.39	0
15	A1JAN	T	101	-	52,52,52	0.30	0	59,63,63	0.44	0
11	A1JAP	N	403	-	53,56,56	0.40	0	61,71,71	0.47	0
13	A1JAO	H	301	-	60,62,62	0.30	0	74,82,82	0.44	0
11	A1JAP	A	302	-	53,56,56	0.39	0	61,71,71	0.47	0
10	B13	A	301	1	81,100,100	2.06	18 (22%)	108,164,164	1.93	24 (22%)

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
11	A1JAP	T	102	-	-	14/67/67/67	-
11	A1JAP	U	101	-	-	17/67/67/67	-
11	A1JAP	M	402	-	-	11/67/67/67	-
13	A1JAO	F	201	-	-	8/62/86/86	0/1/1/1
15	A1JAN	N	402	-	-	16/60/60/60	-
11	A1JAP	S	101	-	-	12/67/67/67	-
13	A1JAO	G	302	-	-	10/62/86/86	0/1/1/1
15	A1JAN	O	402	-	-	22/60/60/60	-
12	L1P	I	301	-	-	16/55/55/55	-
12	L1P	G	301	-	-	17/55/55/55	-
12	L1P	D	201	-	-	21/55/55/55	-
15	A1JAN	T	101	-	-	14/60/60/60	-
11	A1JAP	N	403	-	-	14/67/67/67	-
13	A1JAO	H	301	-	-	7/62/86/86	0/1/1/1
11	A1JAP	A	302	-	-	16/67/67/67	-
10	B13	A	301	1	-	21/56/223/223	0/3/11/11

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	301	B13	C5R-C4R	-8.94	1.21	1.51
10	A	301	B13	O5B-C5B	6.13	1.51	1.37
10	A	301	B13	C11-C10	-5.77	1.36	1.50
10	A	301	B13	C6-N22	5.26	1.41	1.35
10	A	301	B13	C20-C1	3.75	1.61	1.52

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	301	B13	O6R-C4R-C5R	7.09	124.53	109.21
13	F	201	A1JAO	C28-C23-C24	6.30	119.94	110.85
10	A	301	B13	C8B-N1B-C1R	5.91	135.45	125.39
10	A	301	B13	O7R-C2R-C3R	4.83	124.89	111.17
10	A	301	B13	O6R-C1R-N1B	4.81	117.54	108.06

There are no chirality outliers.

5 of 236 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	301	B13	N59-C1P-C2P-O3
10	A	301	B13	N59-C1P-C2P-C3P
10	A	301	B13	C54-C17-C55-C56
10	A	301	B13	C18-C17-C55-C56
10	A	301	B13	C16-C17-C55-C56

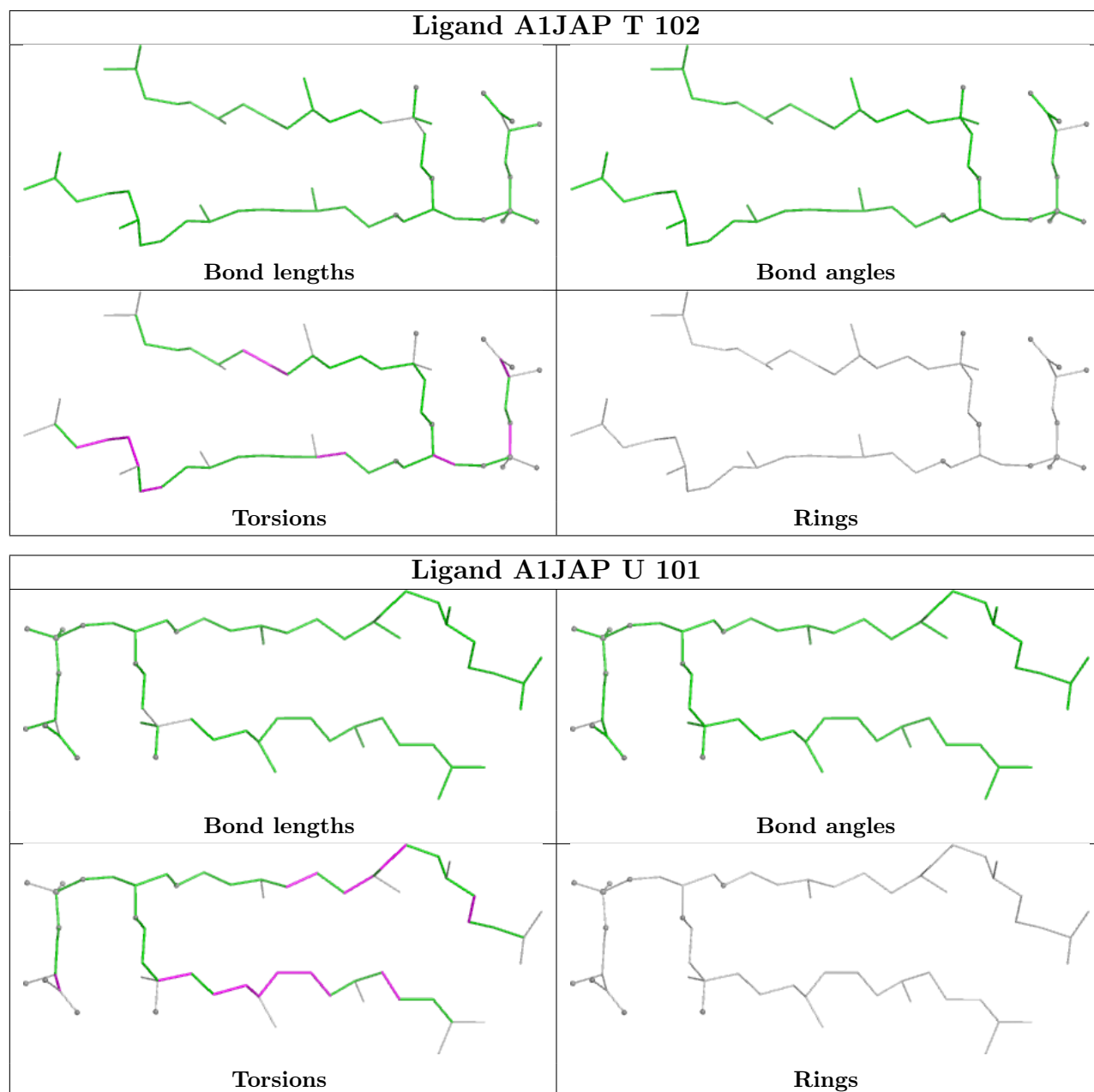
There are no ring outliers.

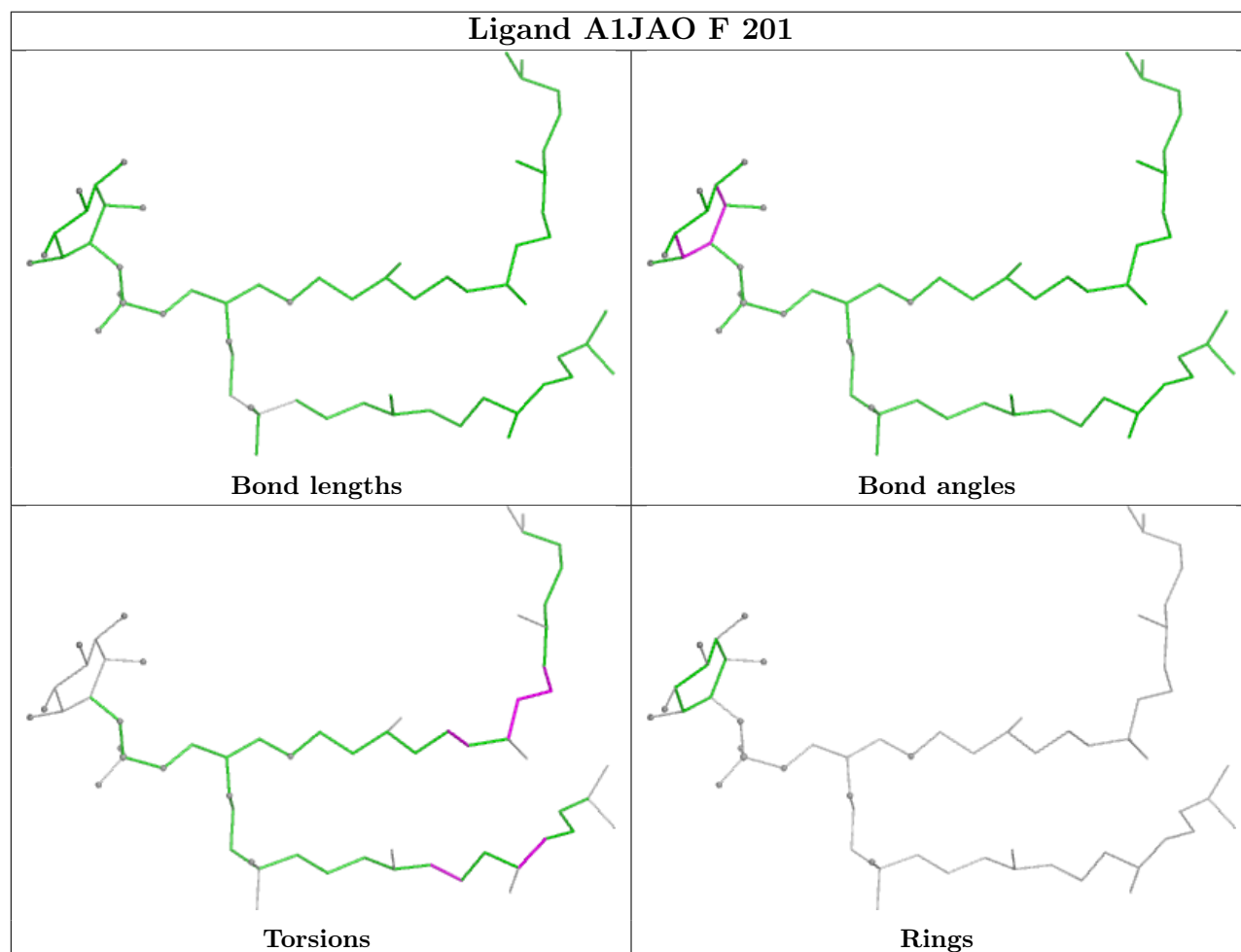
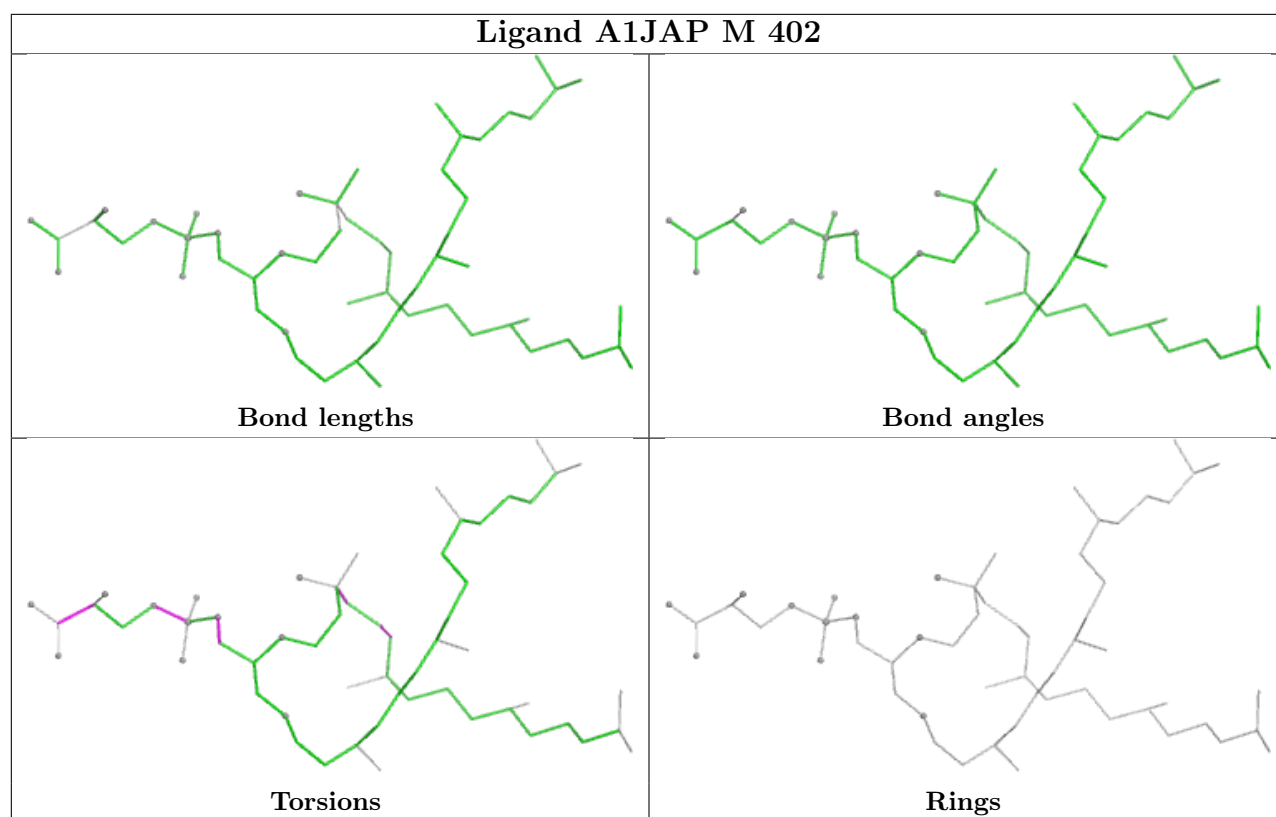
10 monomers are involved in 44 short contacts:

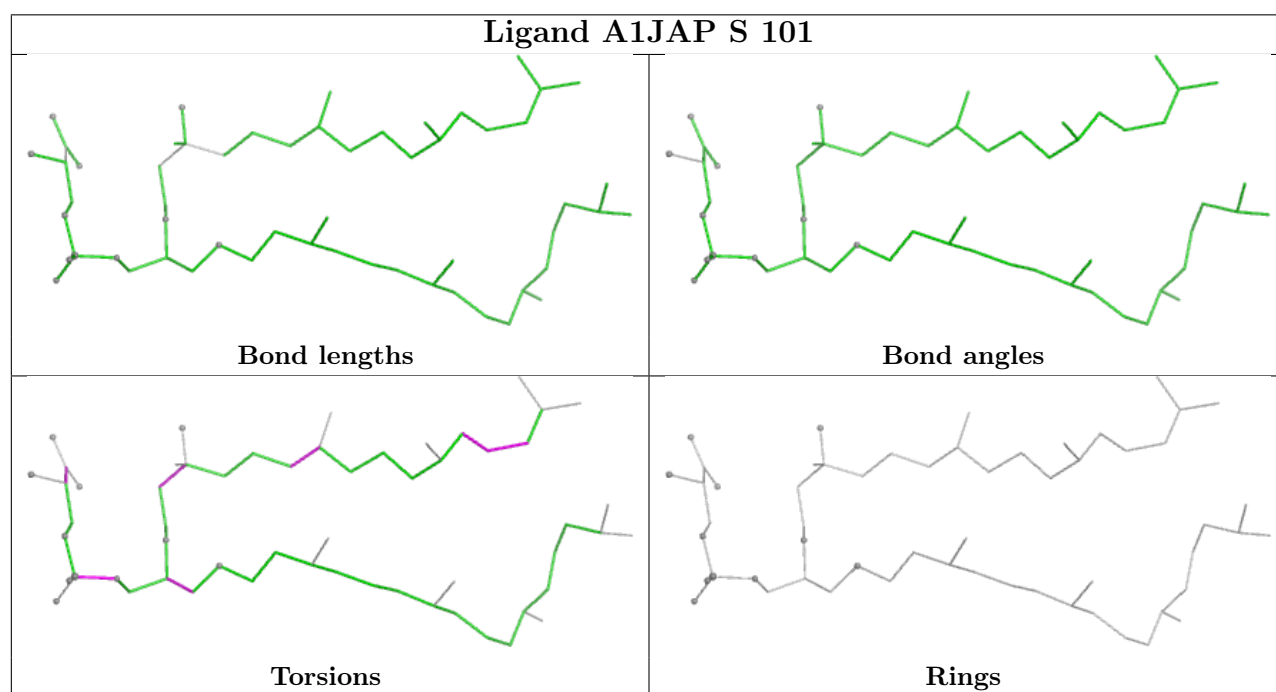
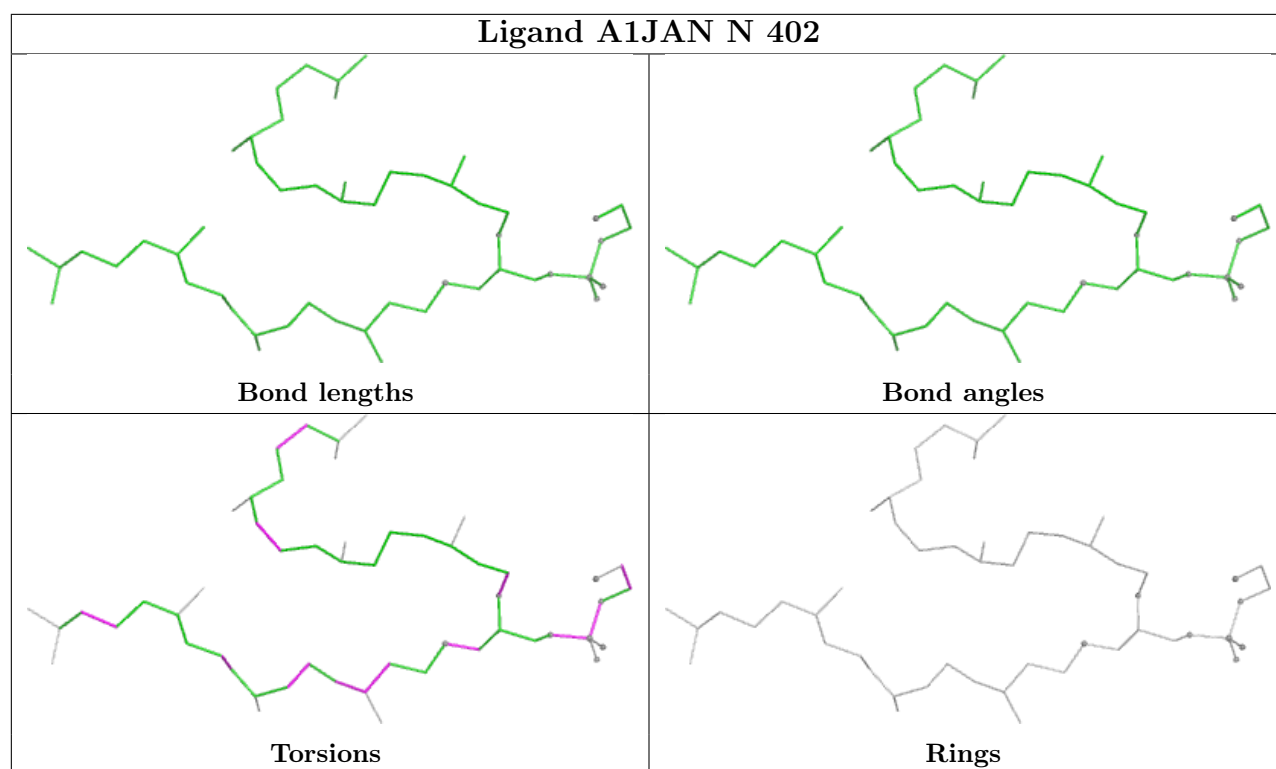
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	102	A1JAP	2	0
11	U	101	A1JAP	1	0
13	F	201	A1JAO	3	0
15	N	402	A1JAN	2	0
12	I	301	L1P	6	0
12	G	301	L1P	7	0
12	D	201	L1P	9	0
15	T	101	A1JAN	3	0
11	A	302	A1JAP	1	0
10	A	301	B13	10	0

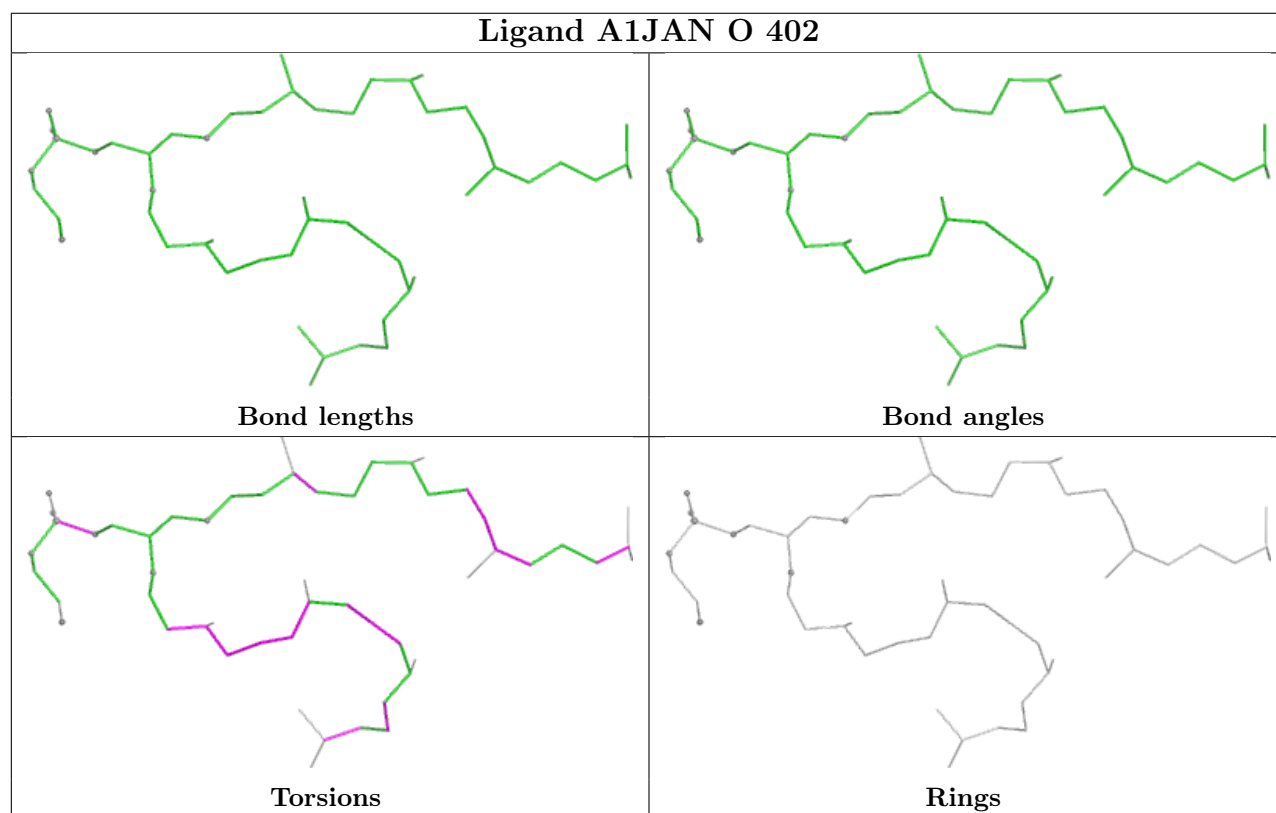
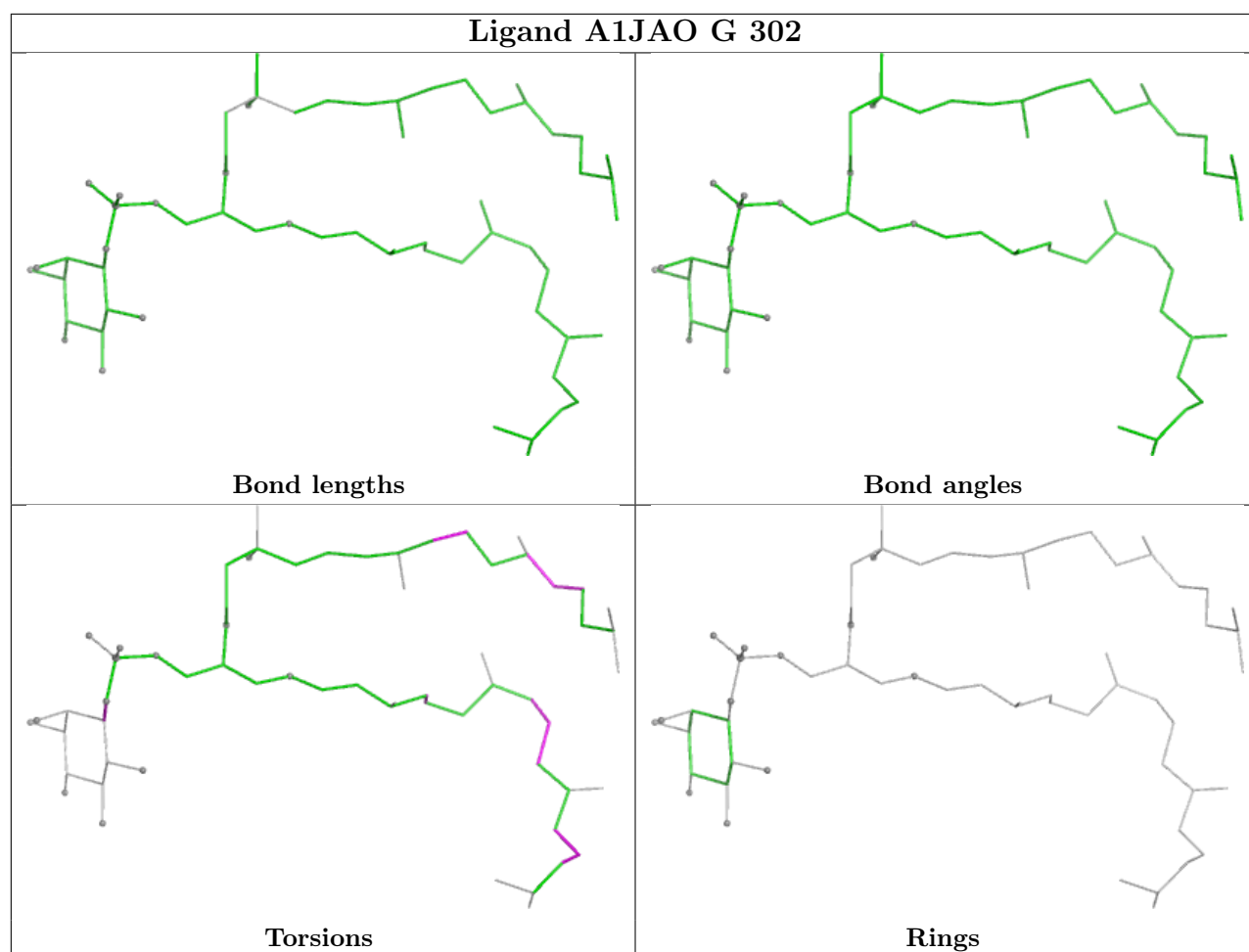
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

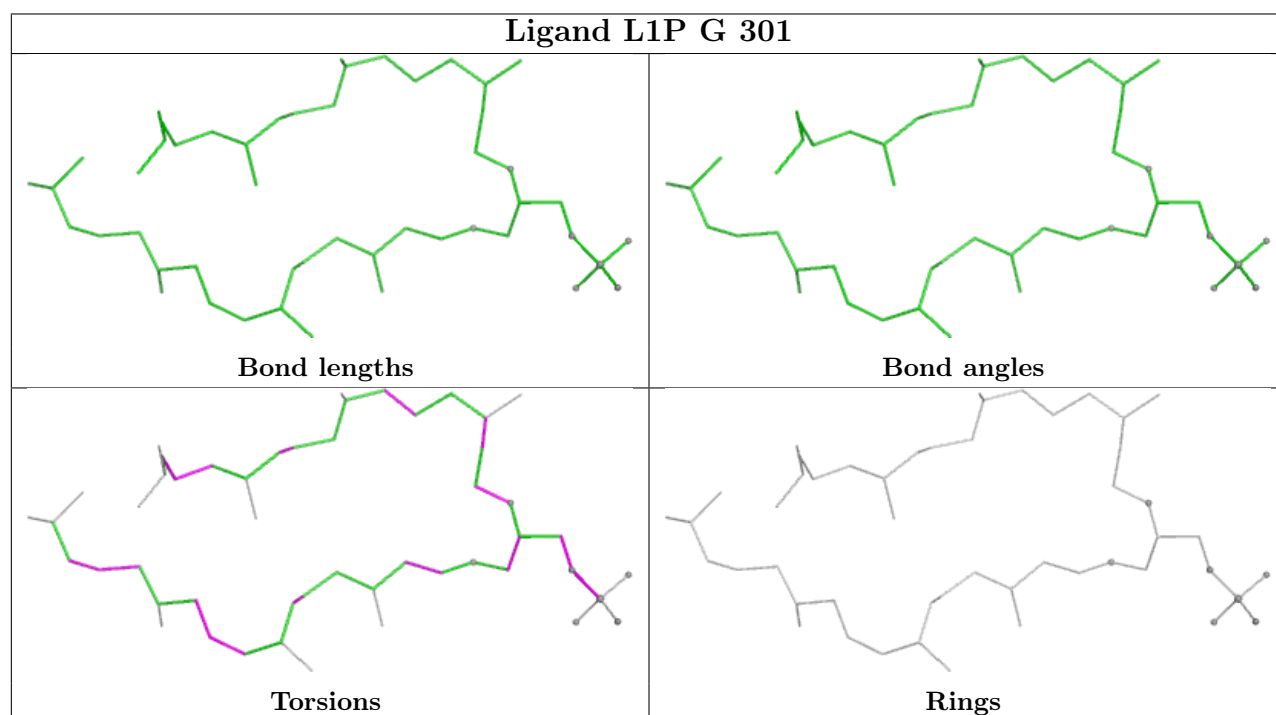
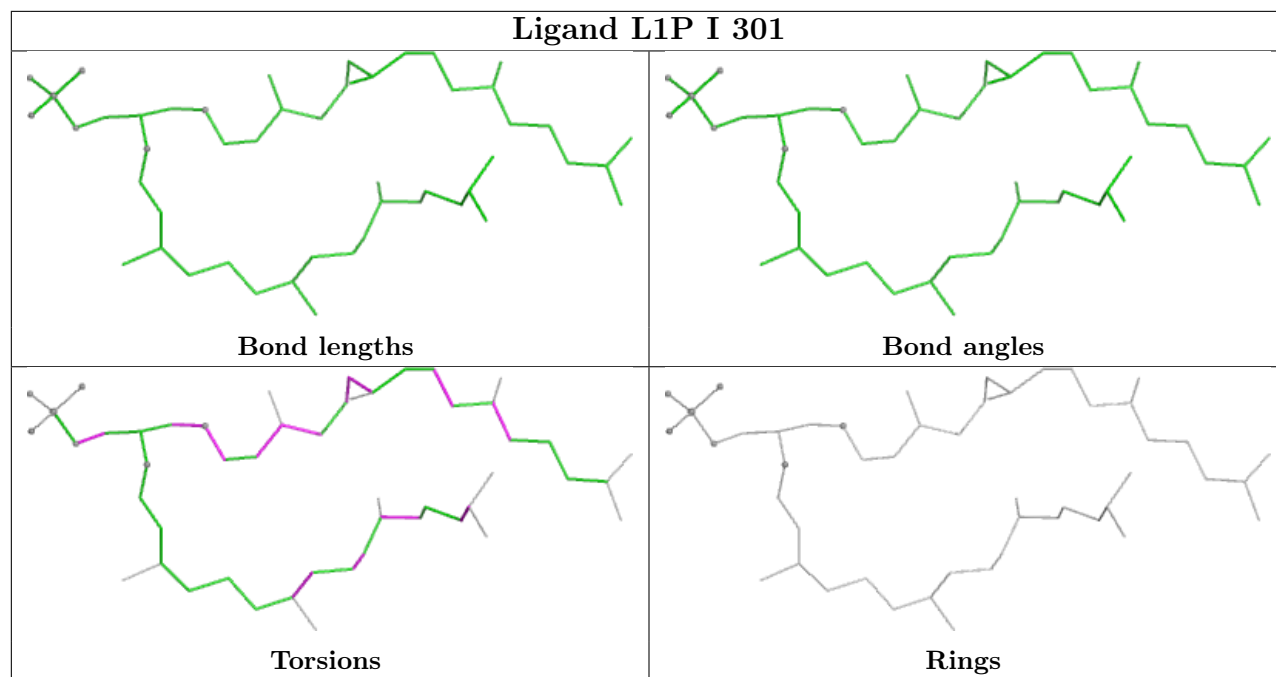
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

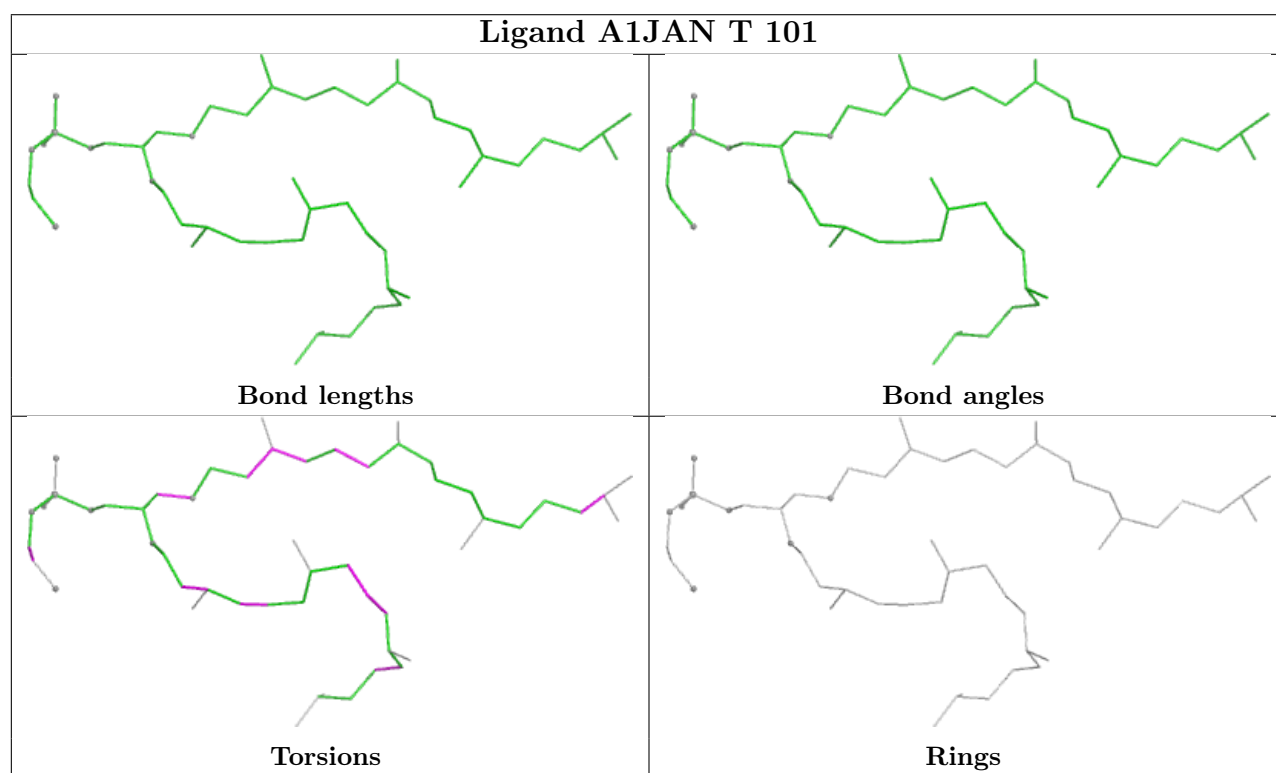
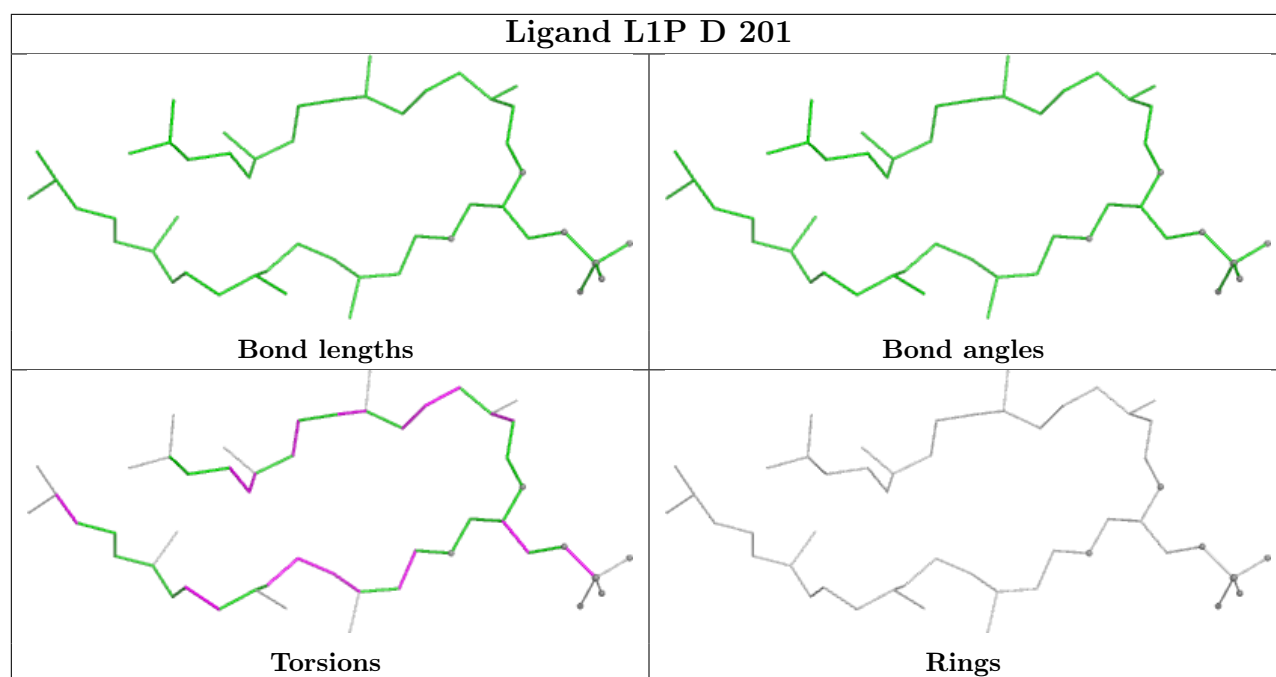


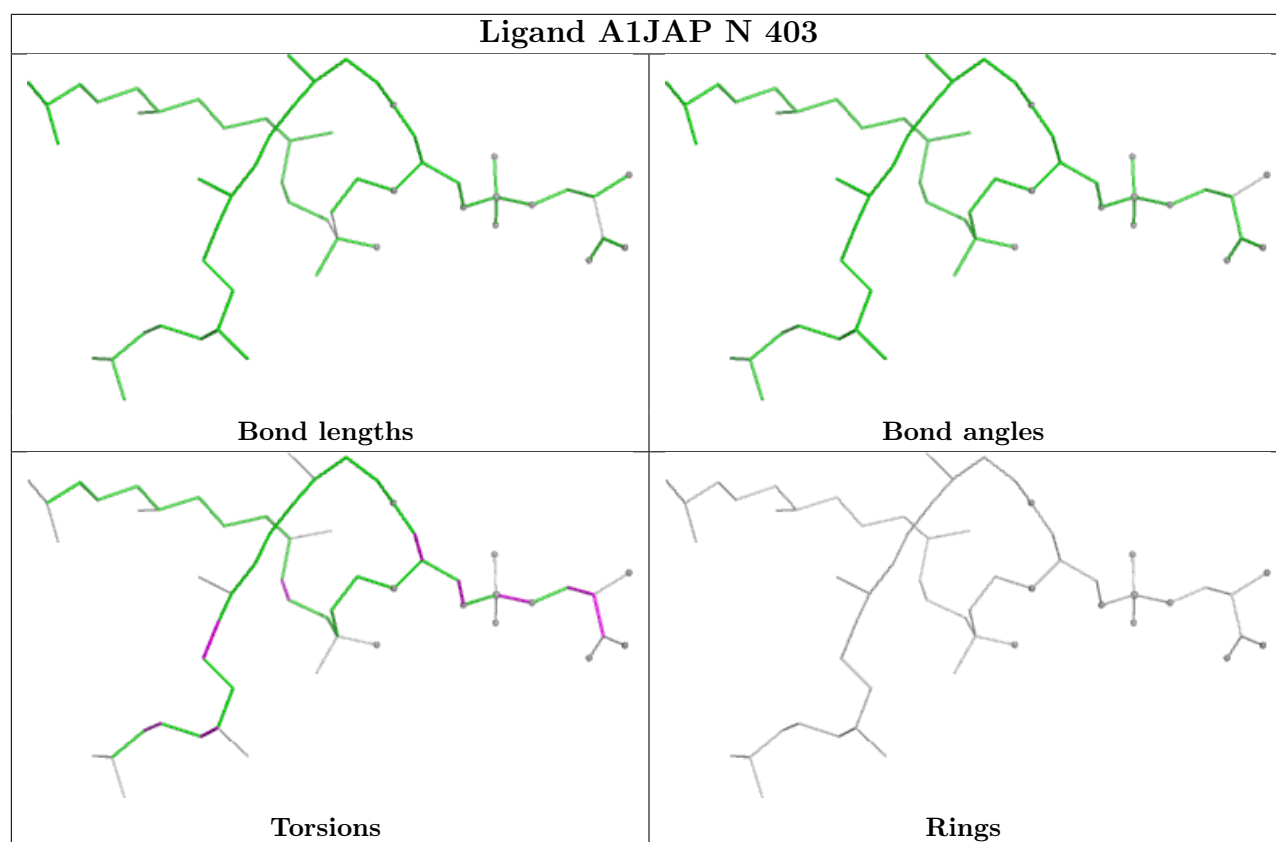


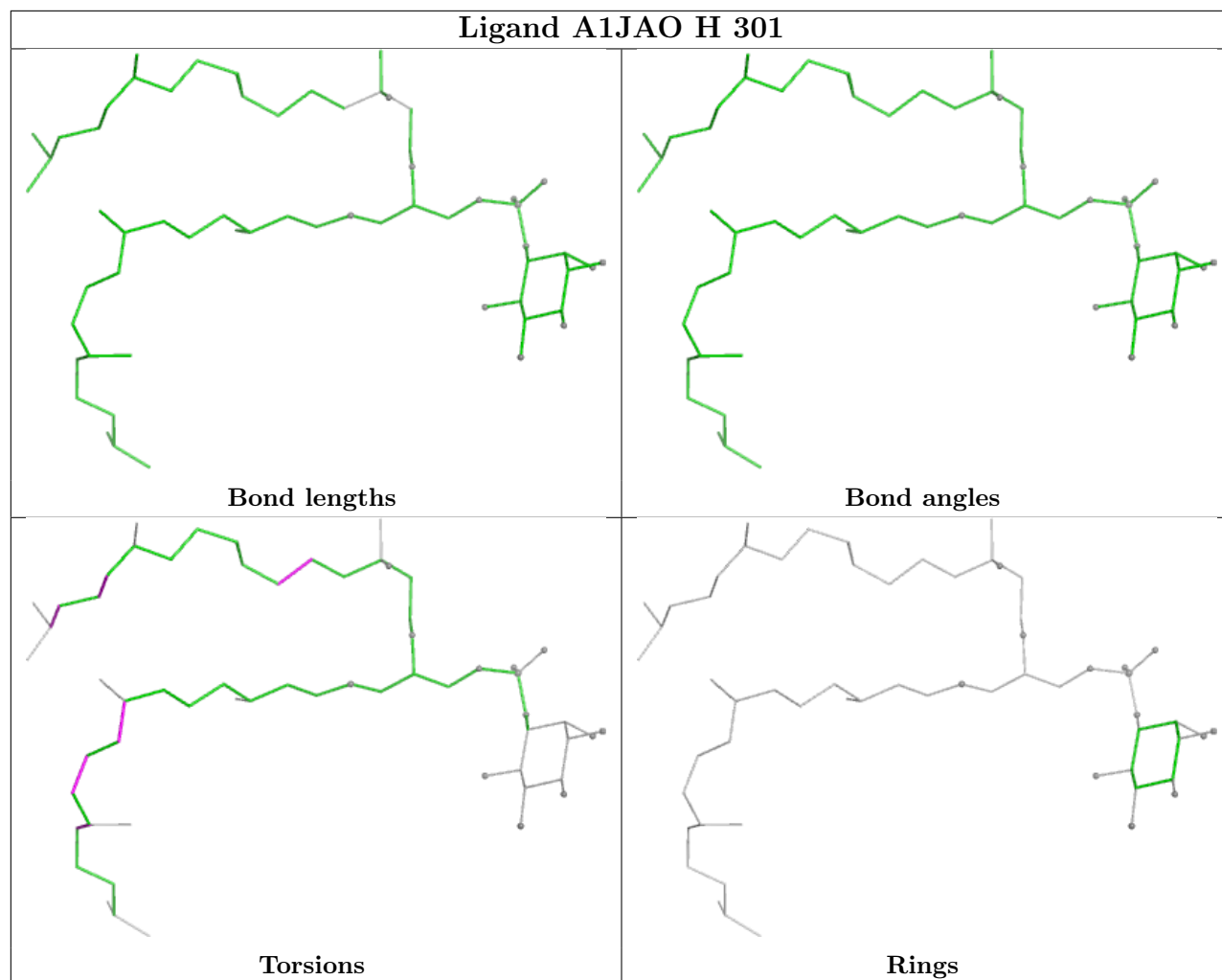


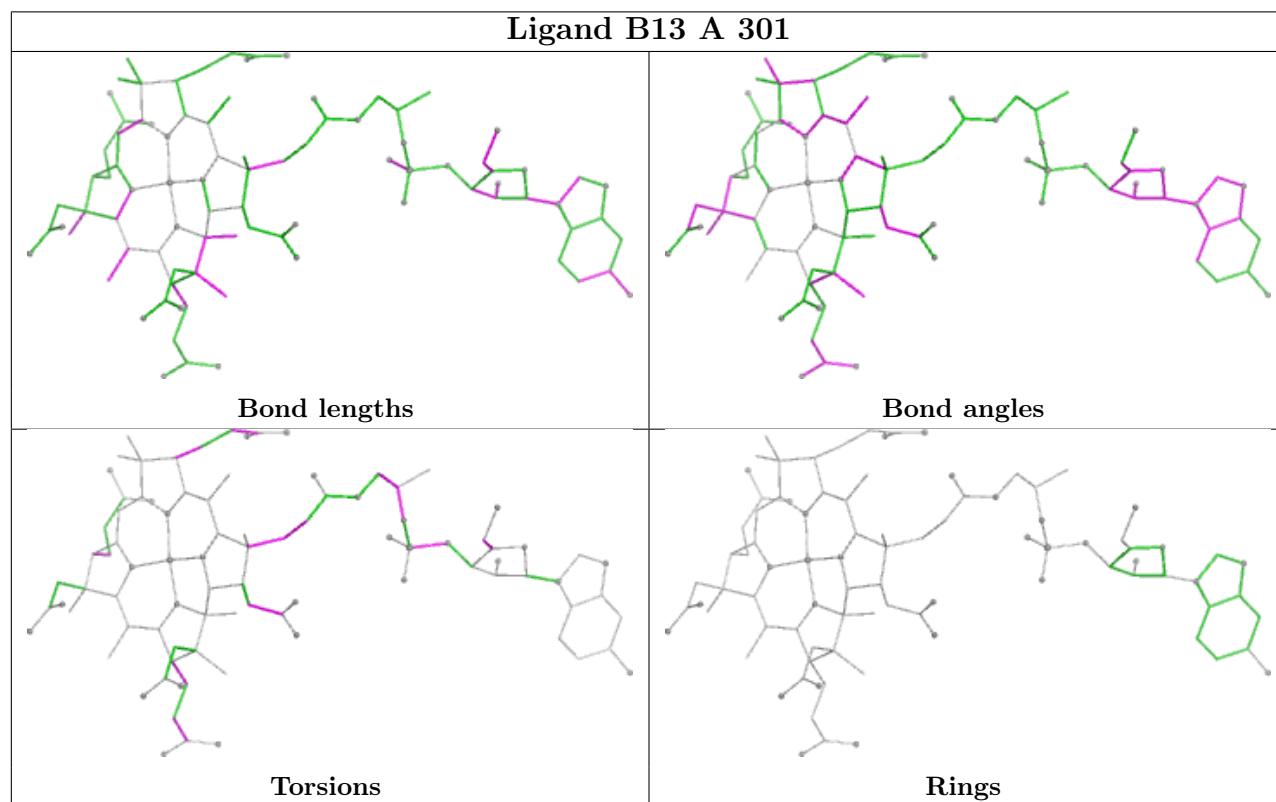
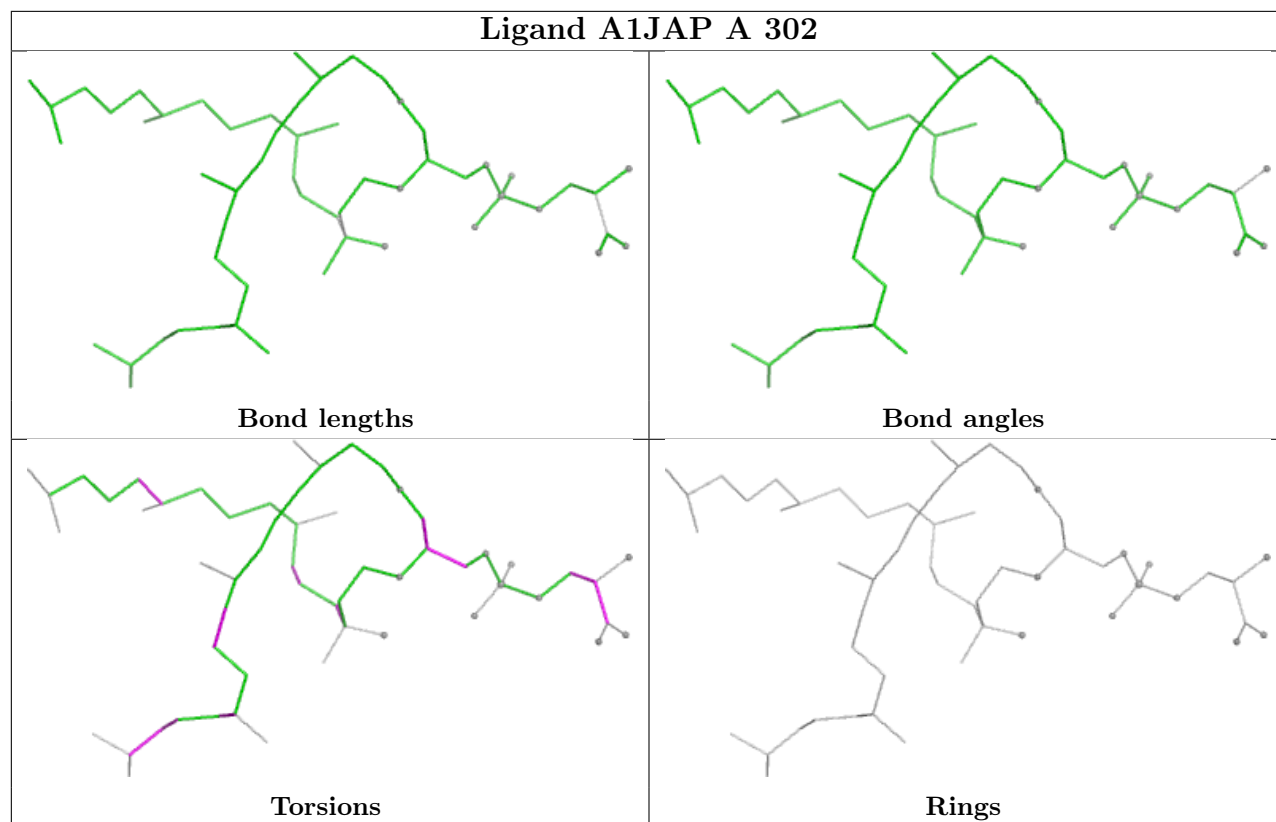












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53361. These allow visual inspection of the internal detail of the map and identification of artifacts.

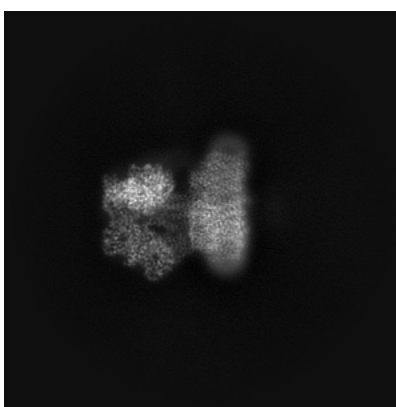
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

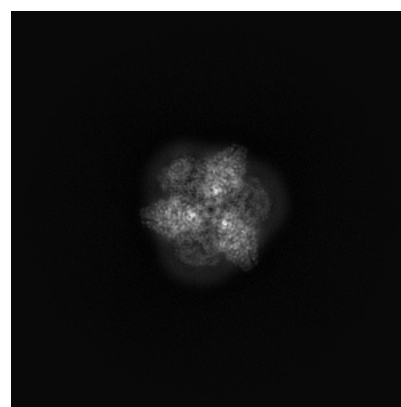
6.1.1 Primary map



X



Y

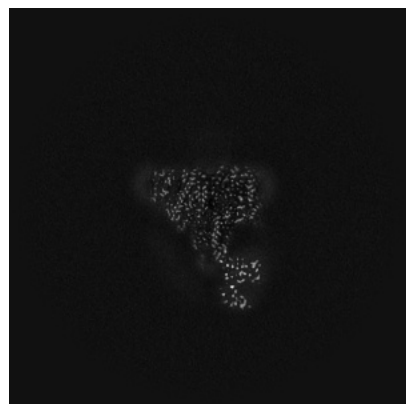


Z

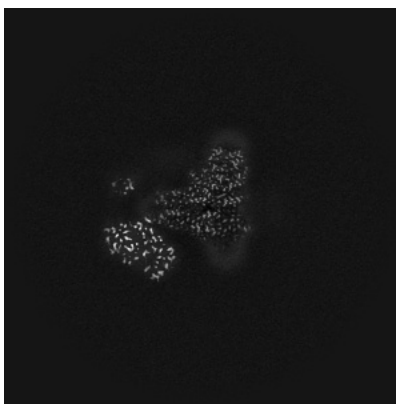
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

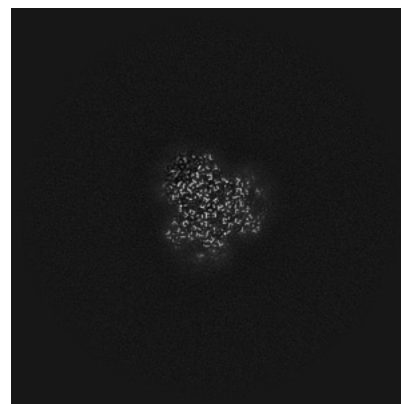
6.2.1 Primary map



X Index: 288



Y Index: 288

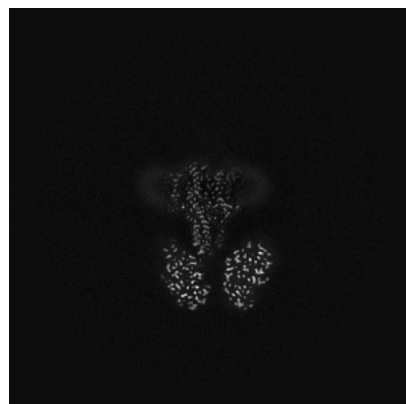


Z Index: 288

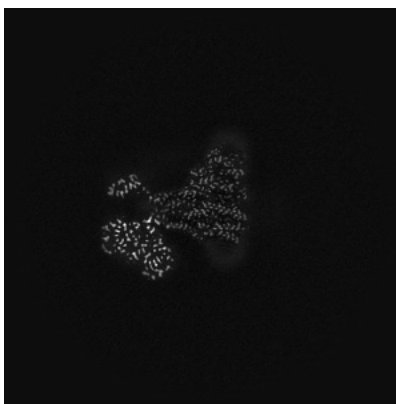
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

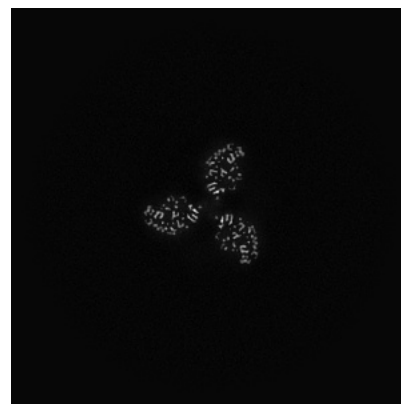
6.3.1 Primary map



X Index: 308



Y Index: 280

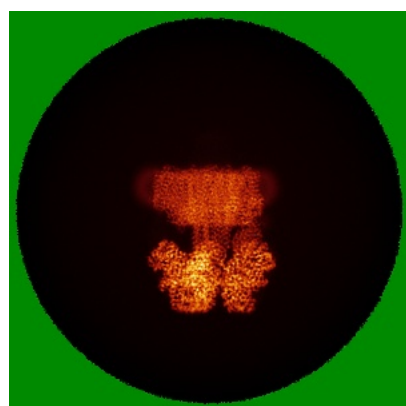


Z Index: 204

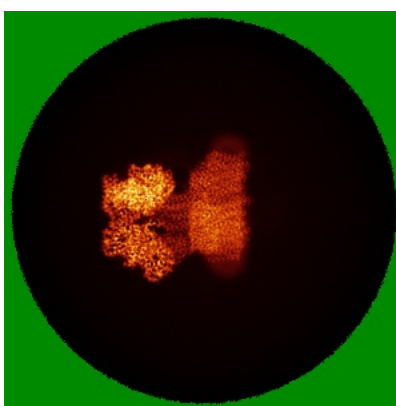
The images above show the largest variance slices of the map in three orthogonal directions.

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

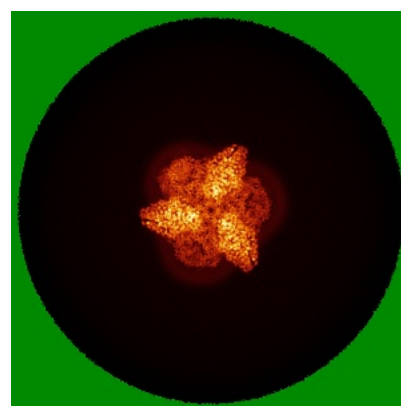
6.4.1 Primary map



X



Y

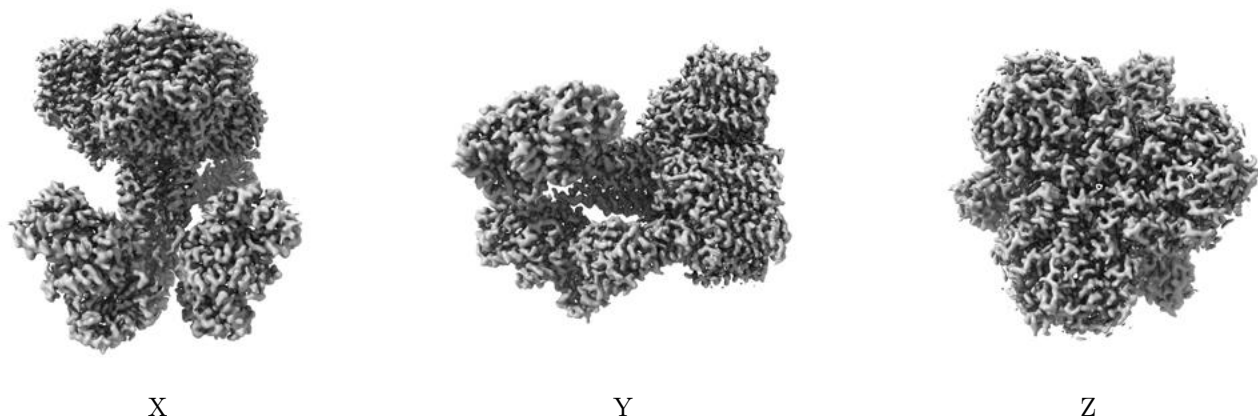


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

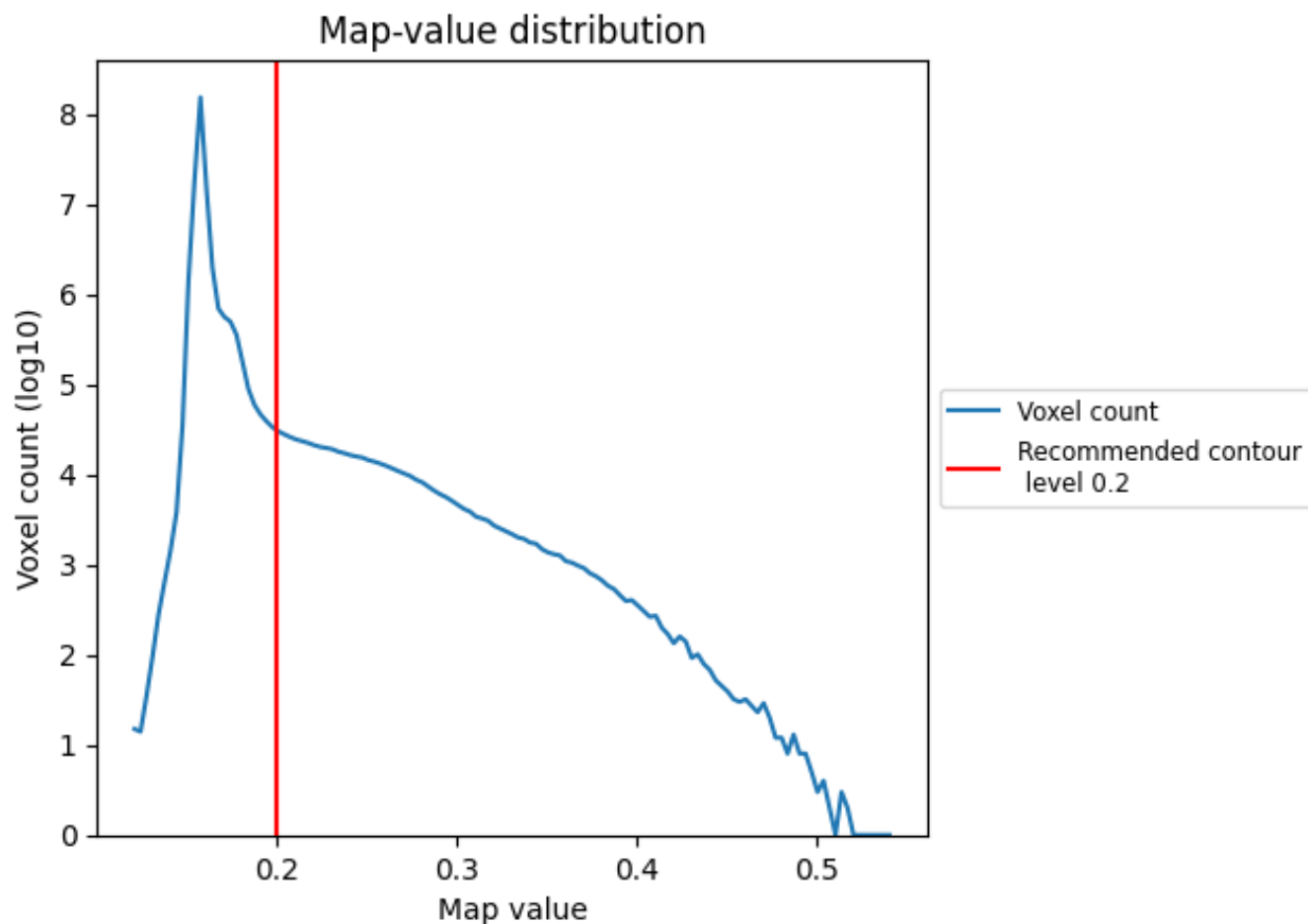
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

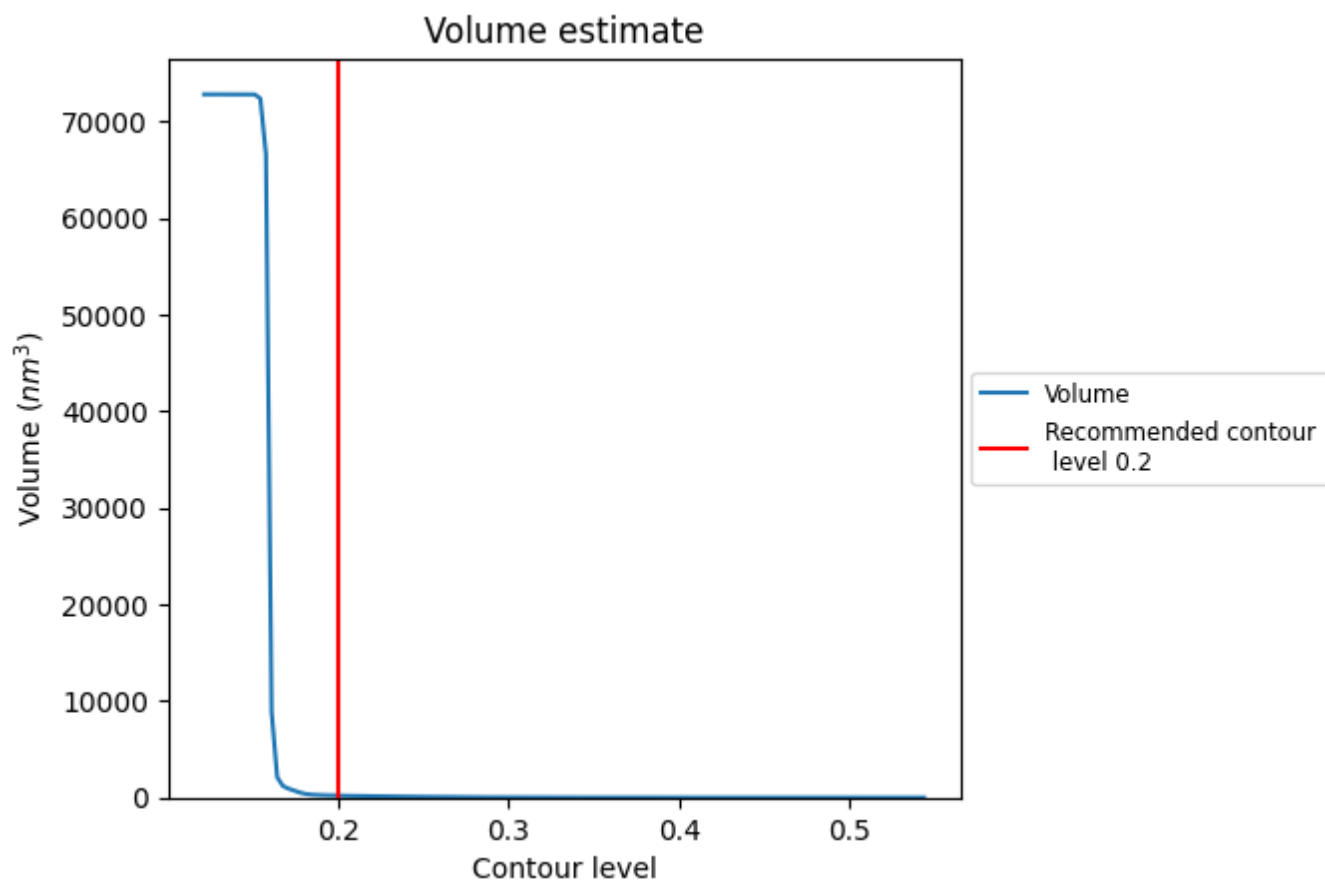
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

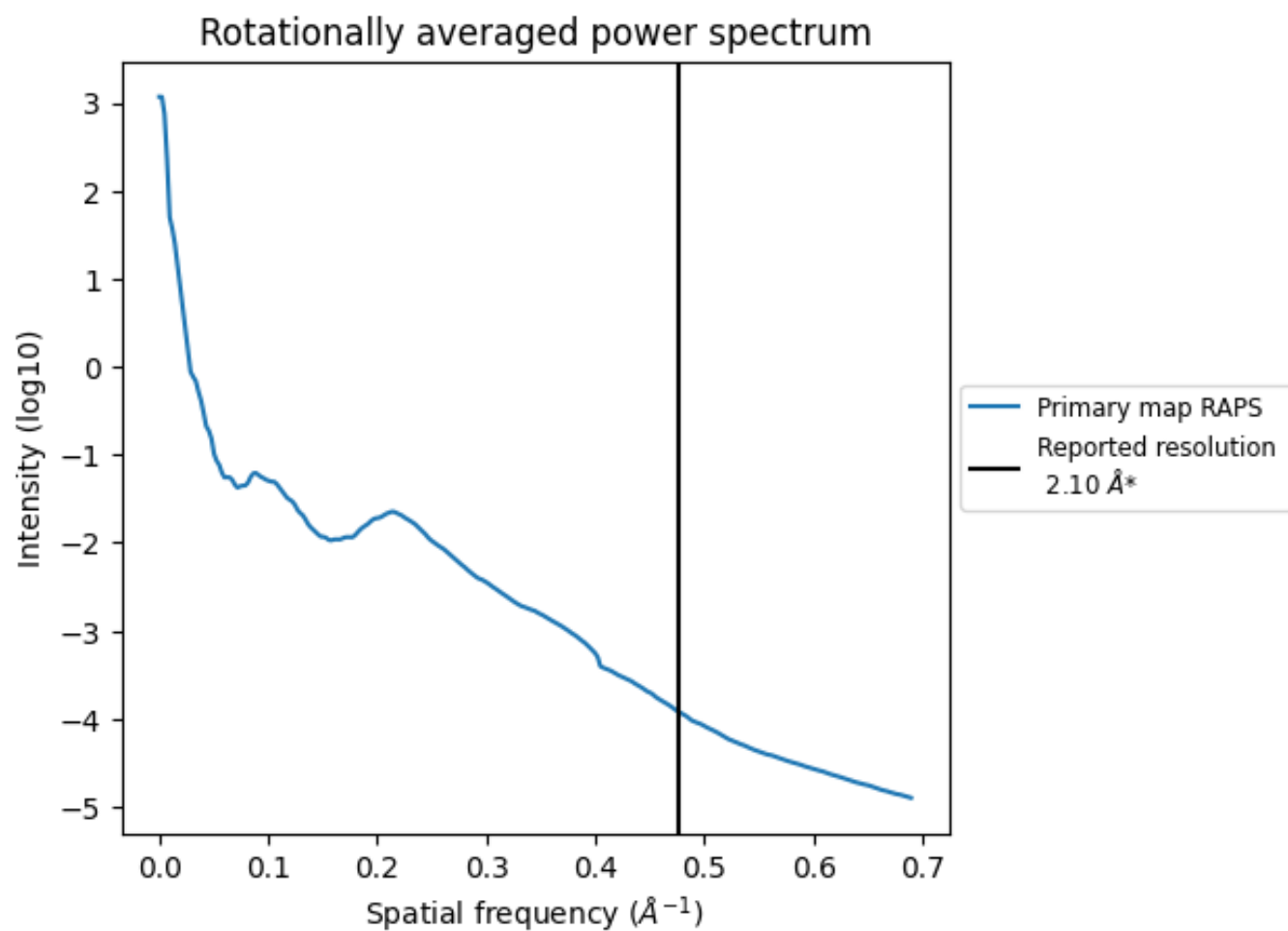
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 202 nm^3 ; this corresponds to an approximate mass of 183 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

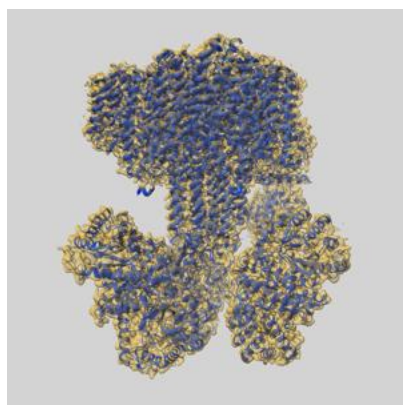
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

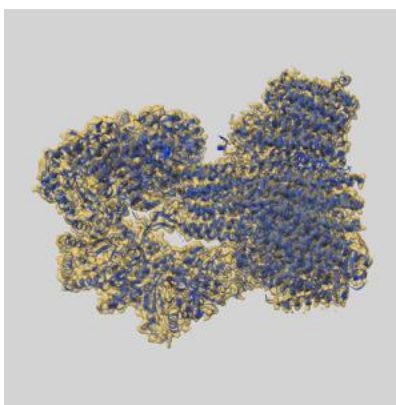
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53361 and PDB model 9QTS. Per-residue inclusion information can be found in section [3](#) on page [14](#).

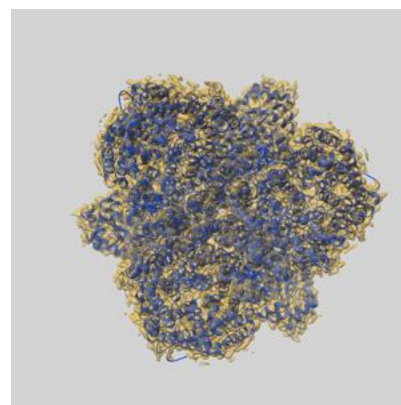
9.1 Map-model overlay [i](#)



X



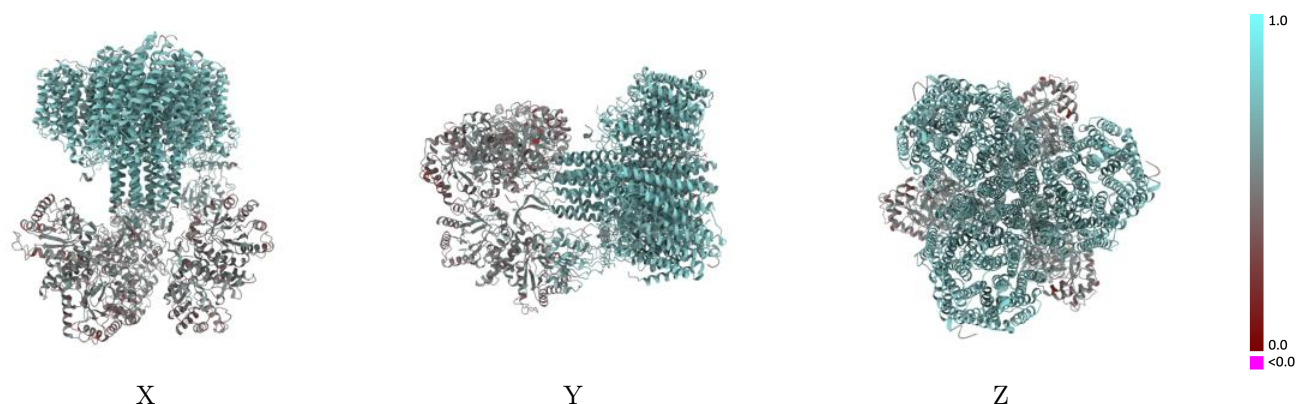
Y



Z

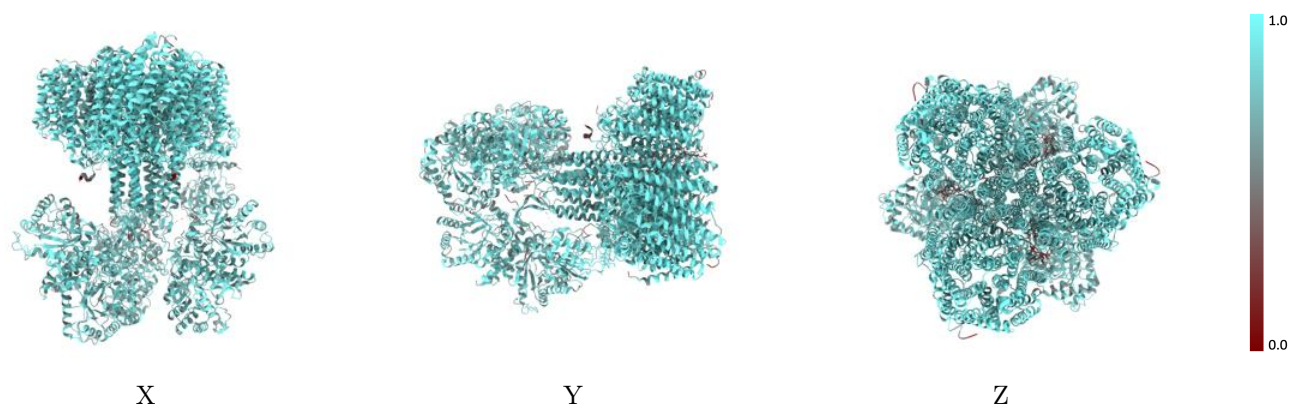
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



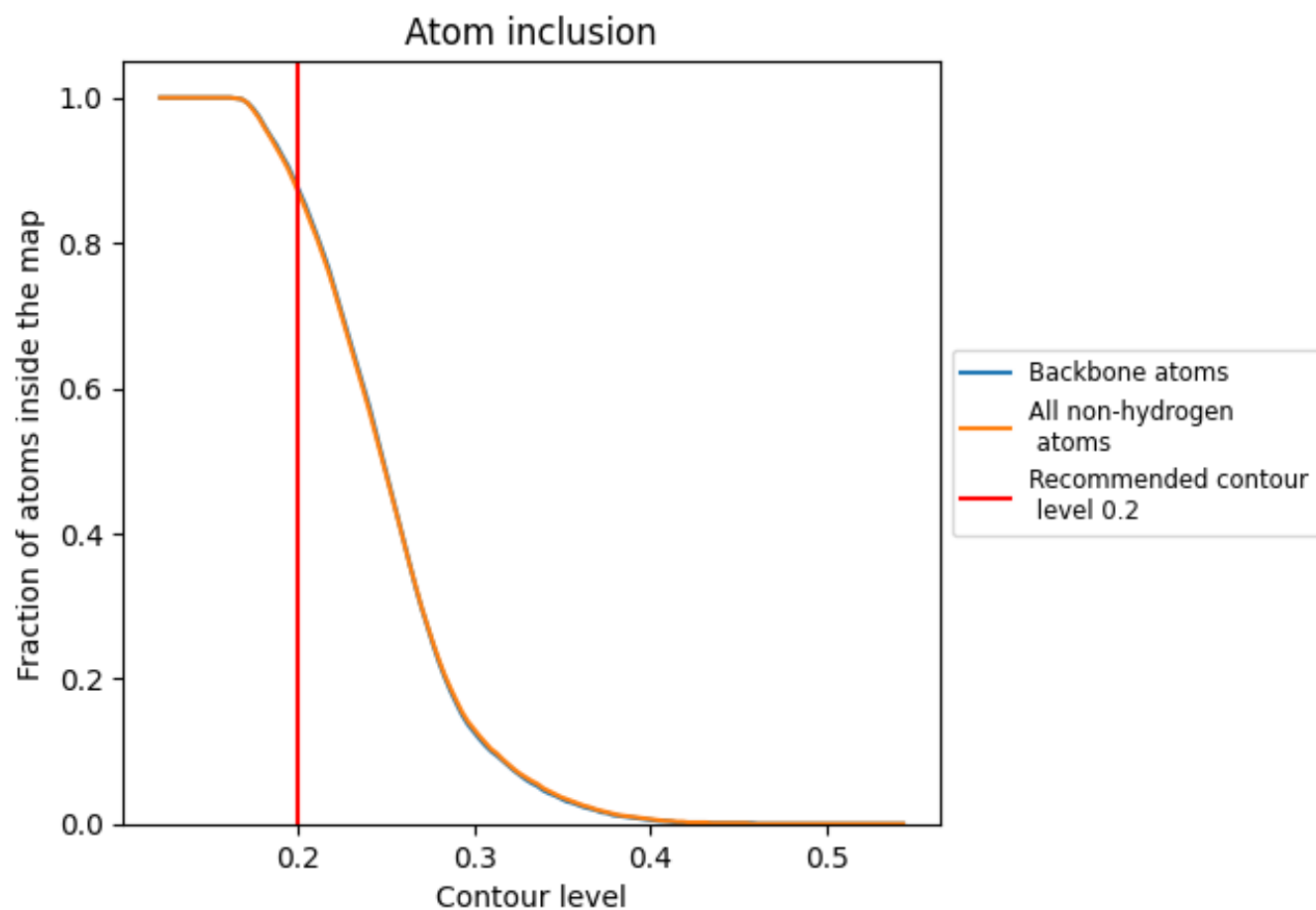
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 87% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.6190
A	 0.8580	 0.6360
B	 0.9210	 0.7160
C	 0.9240	 0.7170
D	 0.8490	 0.6360
E	 0.8960	 0.6510
F	 0.8820	 0.6540
G	 0.9060	 0.6880
H	 0.9090	 0.7010
I	 0.8970	 0.6960
J	 0.9310	 0.6930
K	 0.9350	 0.7060
L	 0.9340	 0.7040
M	 0.9570	 0.7300
N	 0.9490	 0.7290
O	 0.9540	 0.7190
P	 0.8900	 0.6750
Q	 0.8880	 0.6720
R	 0.8820	 0.6730
S	 0.8550	 0.6920
T	 0.8250	 0.6870
U	 0.8480	 0.6890
i	 0.8200	 0.6230
m	 0.8020	 0.4780
n	 0.7900	 0.4790
o	 0.8200	 0.4830
p	 0.8090	 0.4800
q	 0.8030	 0.4770
r	 0.7950	 0.4760

