



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:50 AM UTC

PDB ID : 6QL5 / pdb_00006ql5
EMDB ID : EMD-4577
Title : Structure of fatty acid synthase complex with bound gamma subunit from *Saccharomyces cerevisiae* at 2.8 angstrom
Authors : Singh, K.; Graf, B.; Linden, A.; Sautner, V.; Urlaub, H.; Tittmann, K.; Stark, H.; Chari, A.
Deposited on : 2019-01-31
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

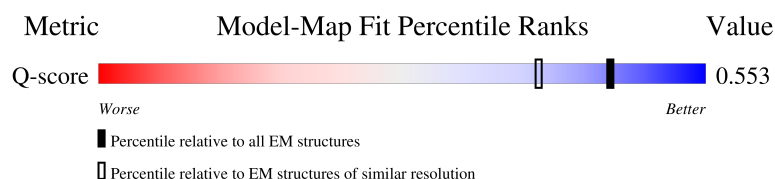
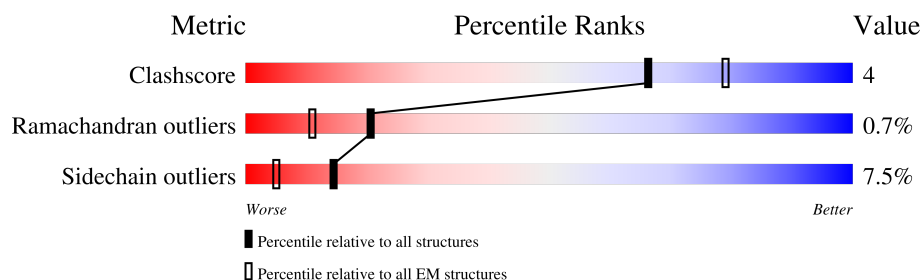
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	1887	 77% 13% • 7%
1	B	1887	 77% 13% • 7%
1	C	1887	 77% 13% • 7%
1	D	1887	 77% 13% • 7%

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Mol	Chain	Length	Quality of chain
1	E	1887	 5% 77% 14% 7%
1	F	1887	 5% 78% 13% 7%
2	G	2040	 85% 13%
2	H	2040	 85% 13%
2	I	2040	 85% 13%
2	J	2040	 85% 13%
2	K	2040	 85% 13%
2	L	2040	 85% 13%
3	M	148	 61% 11% 24%
3	N	148	 61% 11% 24%
3	O	148	 61% 11% 24%
3	P	148	 61% 11% 24%
3	Q	148	 61% 11% 24%
3	R	148	 61% 11% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 183444 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 Fatty acid synthase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	B	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	C	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	D	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	E	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		
1	F	1752	Total	C	N	O	S	0	0
			13625	8627	2300	2647	51		

- Molecule 2 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	H	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	I	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	J	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	K	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		
2	L	2036	Total	C	N	O	S	0	0
			16018	10265	2663	3034	56		

- Molecule 3 is a protein called Translation machinery-associated protein 17.

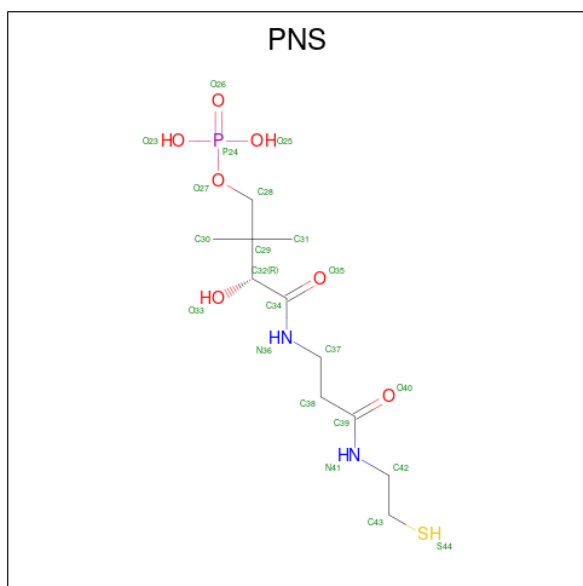
Mol	Chain	Residues	Atoms					AltConf	Trace
3	M	112	Total	C	N	O	S	0	0
			879	542	155	179	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	O	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	P	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	Q	112	Total	C	N	O	S	0	0
			879	542	155	179	3		
3	R	112	Total	C	N	O	S	0	0
			879	542	155	179	3		

- Molecule 4 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).

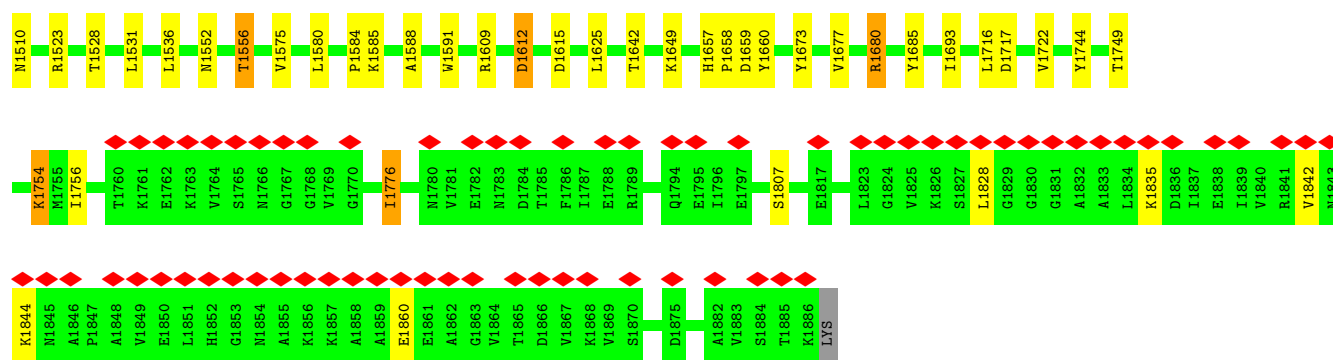


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	B	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	C	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	D	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	E	1	Total	C	N	O	P	S
			21	11	2	6	1	1
4	F	1	Total	C	N	O	P	S
			21	11	2	6	1	1

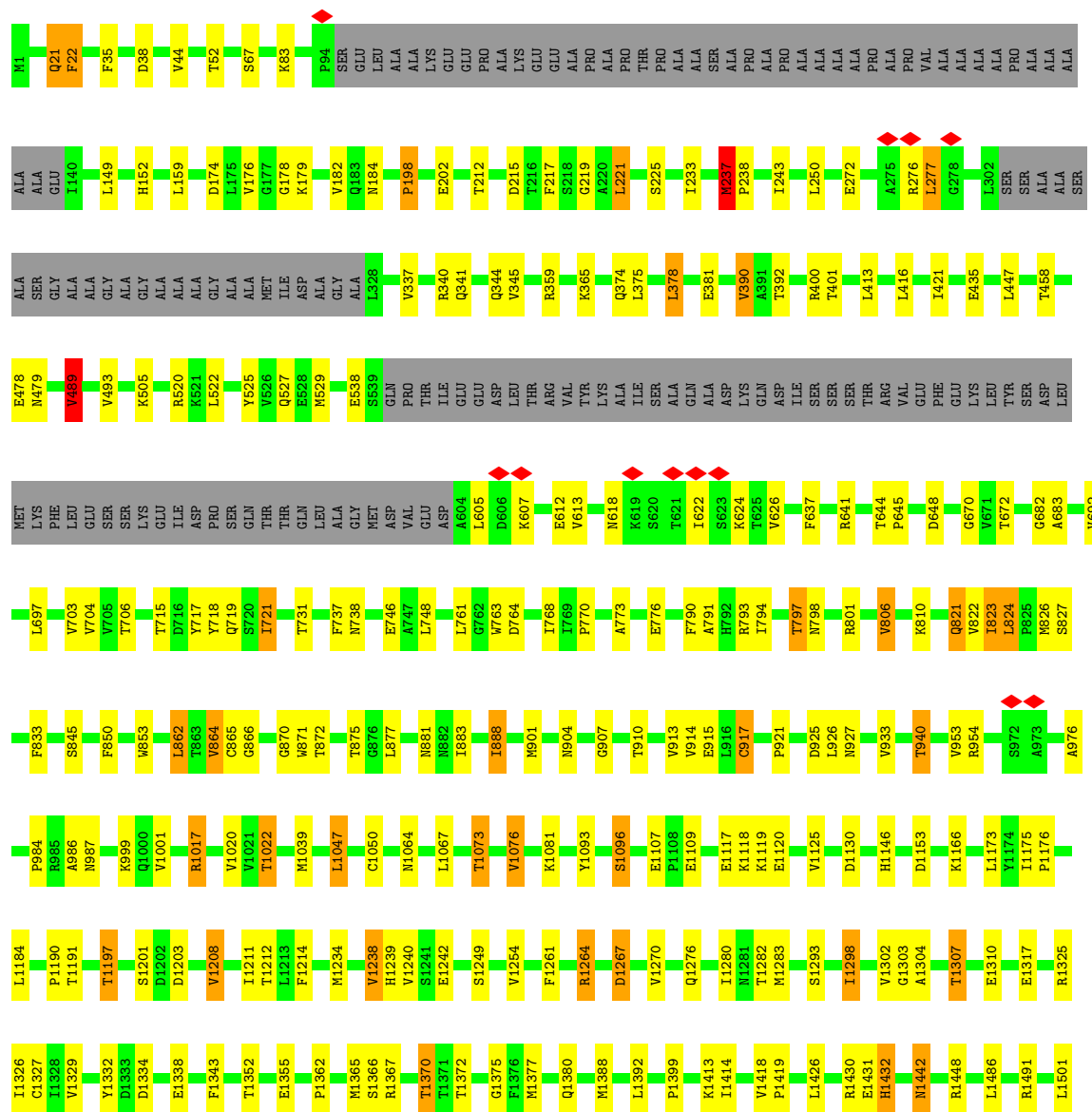
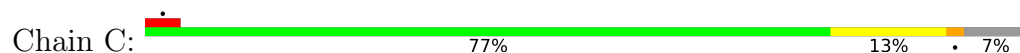
-
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The ring atoms are labeled: N1, N5, N10 for the nitrogen atoms and C2, C4A, C5A, C6, C7, C8, C9 for the carbon atoms. The structure is substituted with a ribityl chain at the N10 position. The ribityl chain consists of a ribitol backbone with a phosphate group at the end. The ribitol backbone is shown with stereochemistry: the hydroxyl group at C2' is on a wedge, and the hydroxyl group at C3' is on a dash. The phosphate group is represented as a phosphorus atom (P) double-bonded to one oxygen (O1P) and single-bonded to three others (O2P, O3P, O4P). The ribitol chain is also labeled with C1', C2'(S), C3'(S), C4'(R), and C5'.

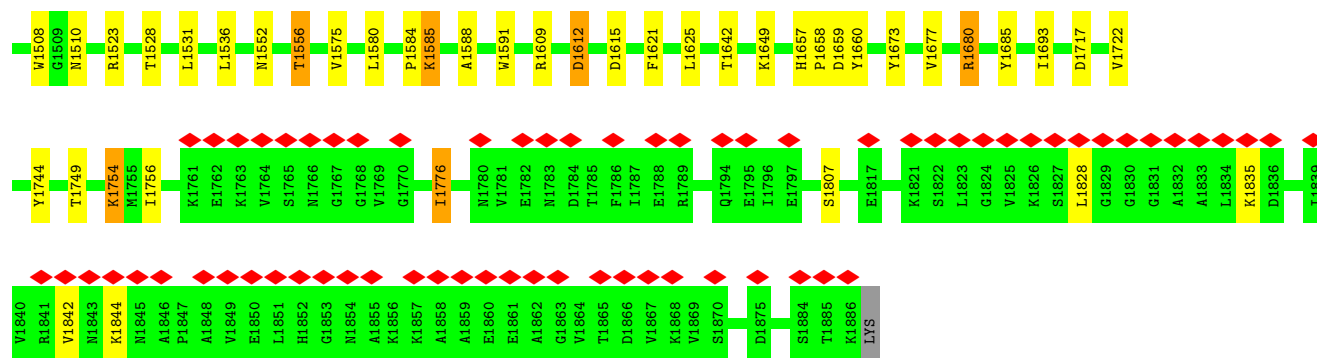
Mol	Chain	Residues	Atoms					AltConf
5	G	1	Total 31	C 17	N 4	O 9	P 1	0
5	H	1	Total 31	C 17	N 4	O 9	P 1	0
5	I	1	Total 31	C 17	N 4	O 9	P 1	0
5	J	1	Total 31	C 17	N 4	O 9	P 1	0
5	K	1	Total 31	C 17	N 4	O 9	P 1	0
5	L	1	Total 31	C 17	N 4	O 9	P 1	0



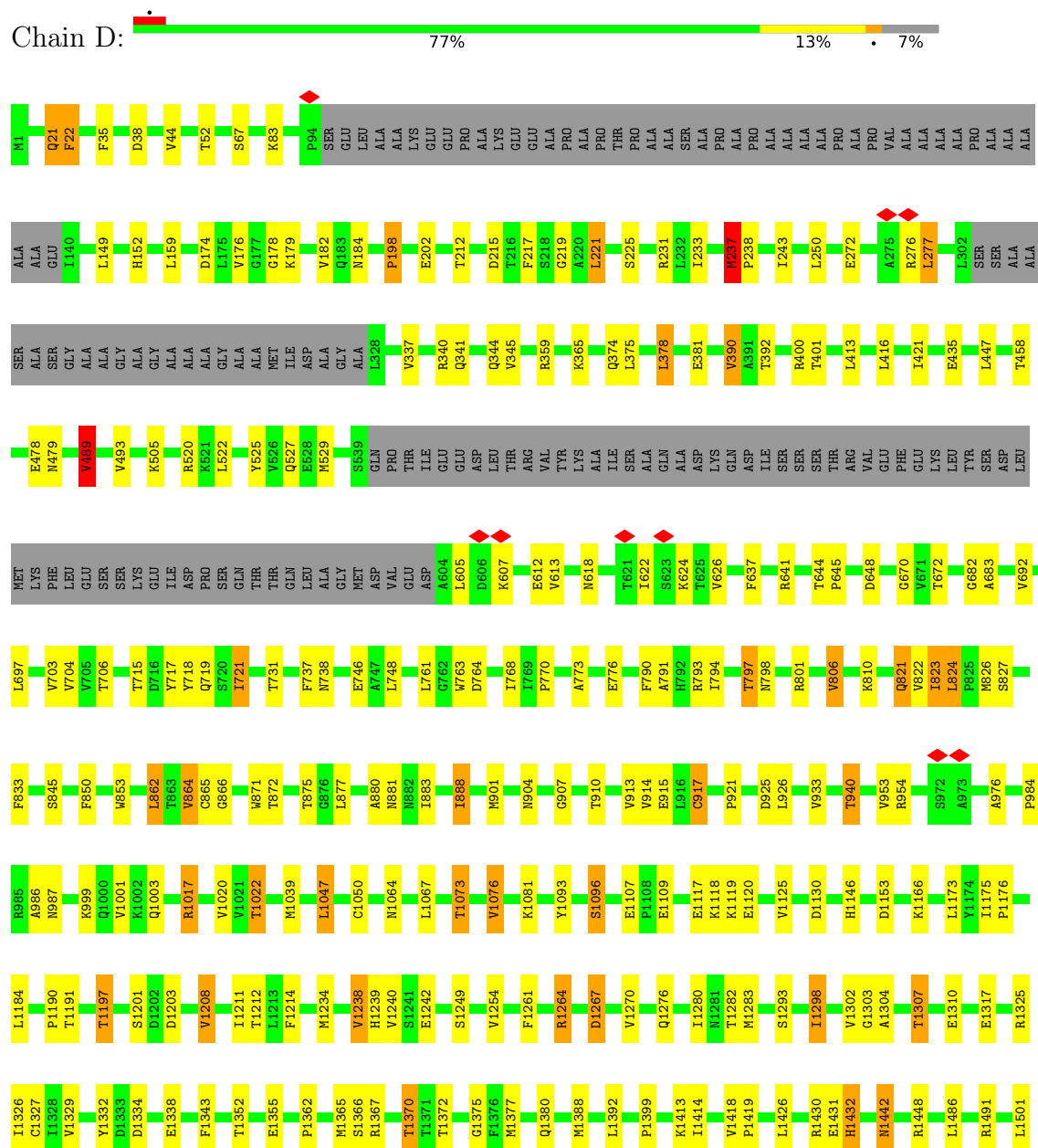


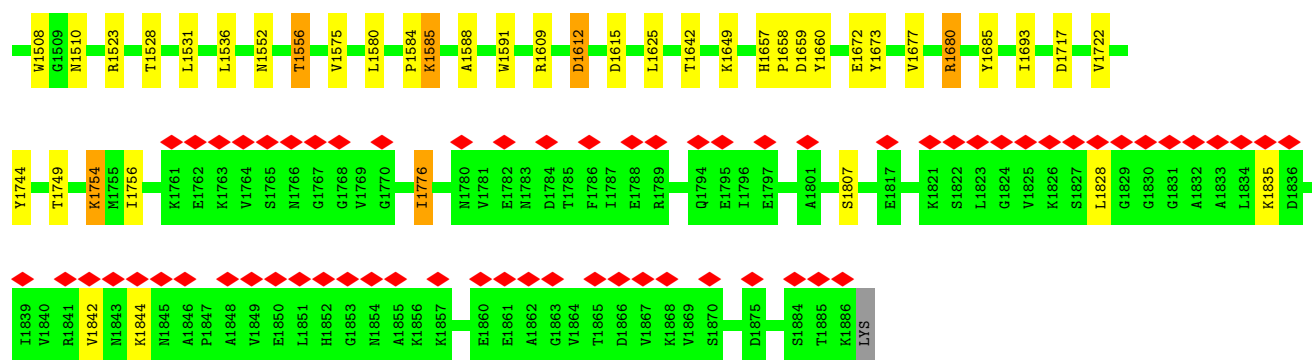
• Molecule 1: Fatty acid synthase subunit alpha



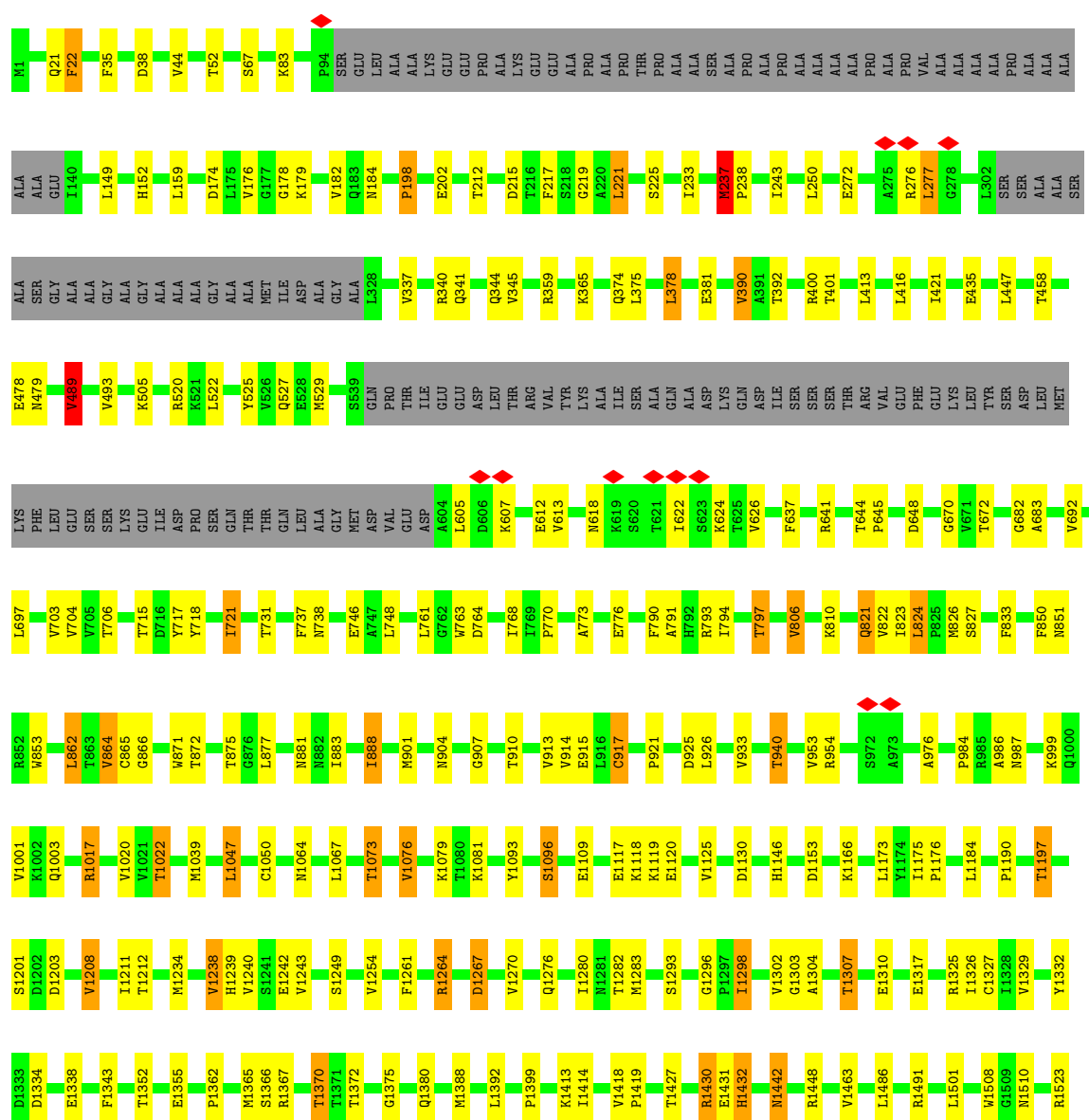
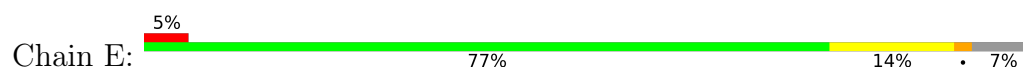


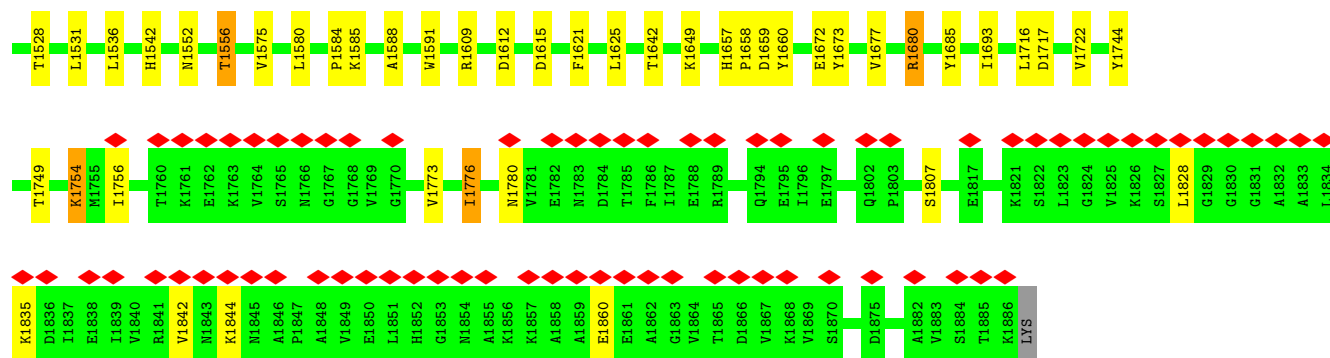
- Molecule 1: Fatty acid synthase subunit alpha





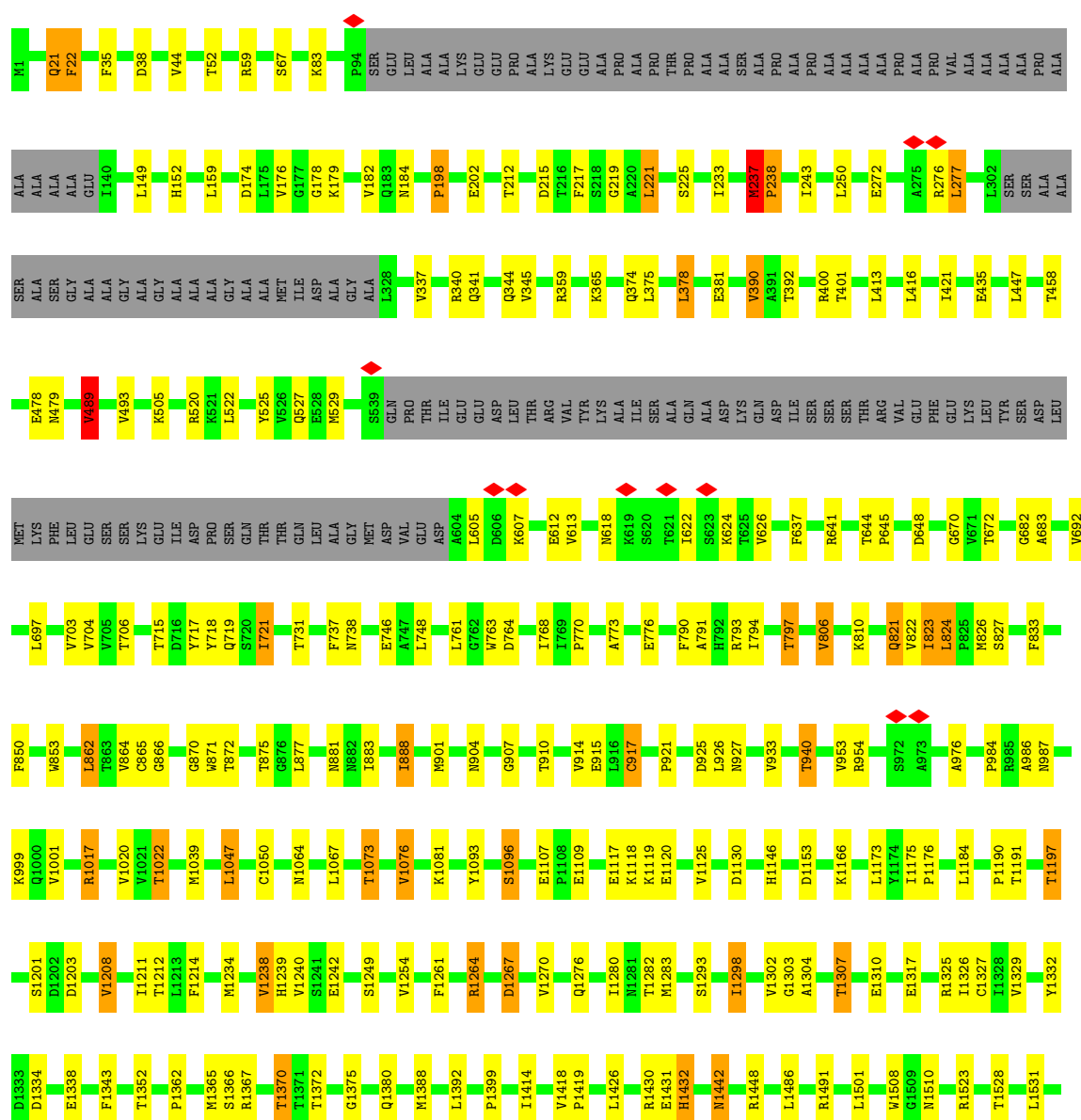
● Molecule 1: Fatty acid synthase subunit alpha



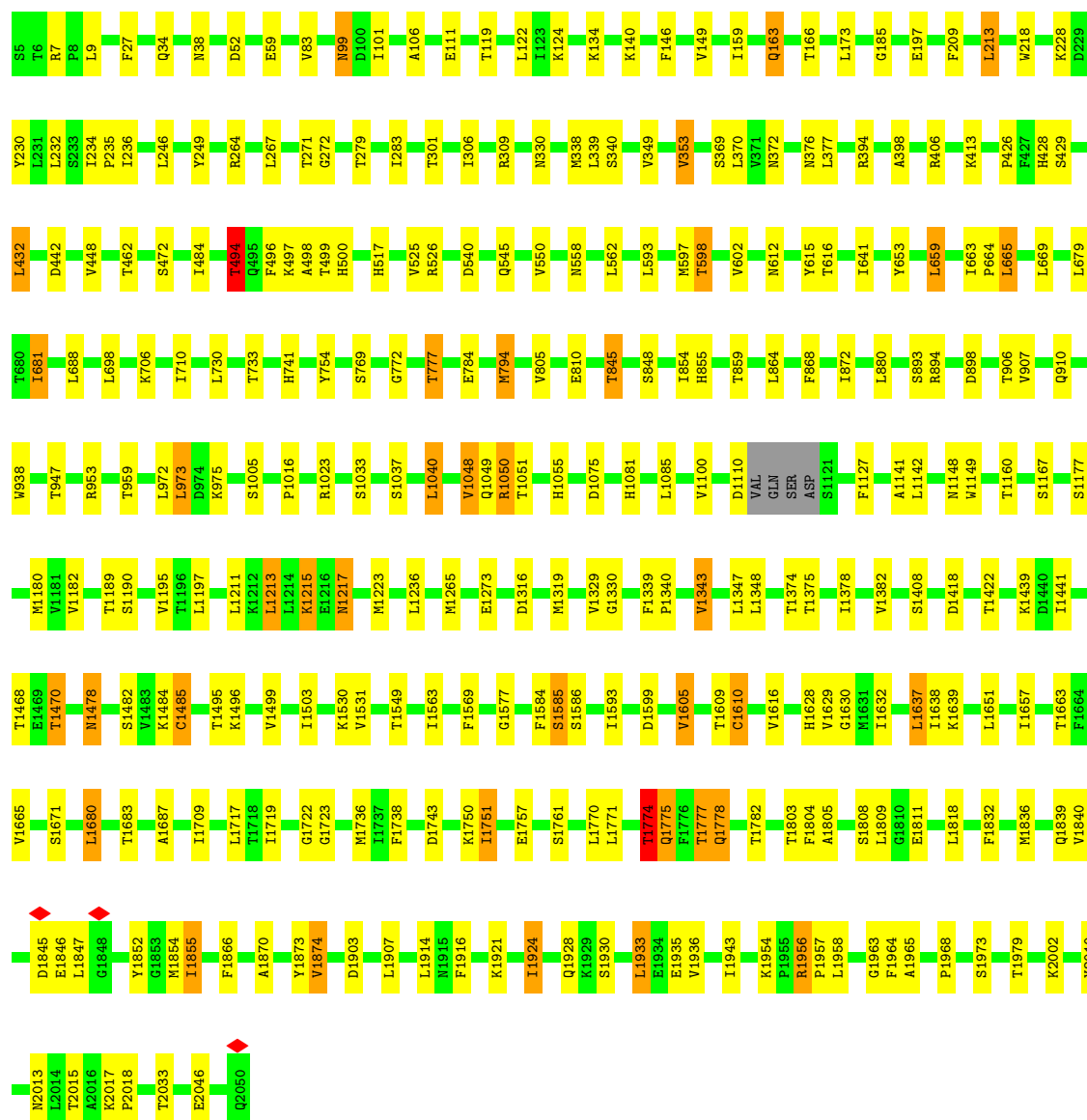


● Molecule 1: Fatty acid synthase subunit alpha

Chain F: 78% 13% 7%

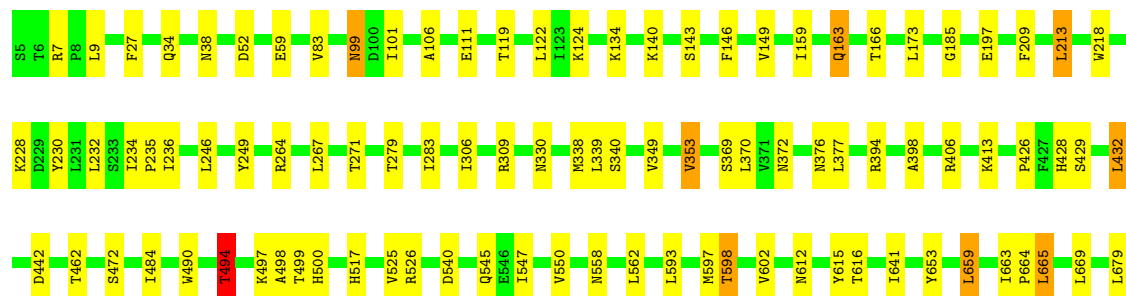


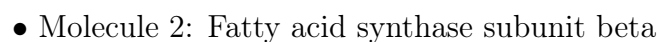
Chain H:  85% 13% .



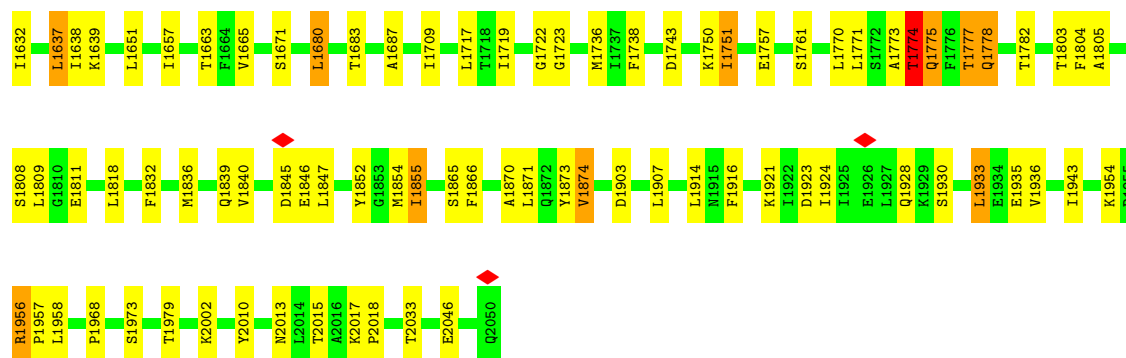
• Molecule 2: Fatty acid synthase subunit beta

Chain I:  85% 13% .



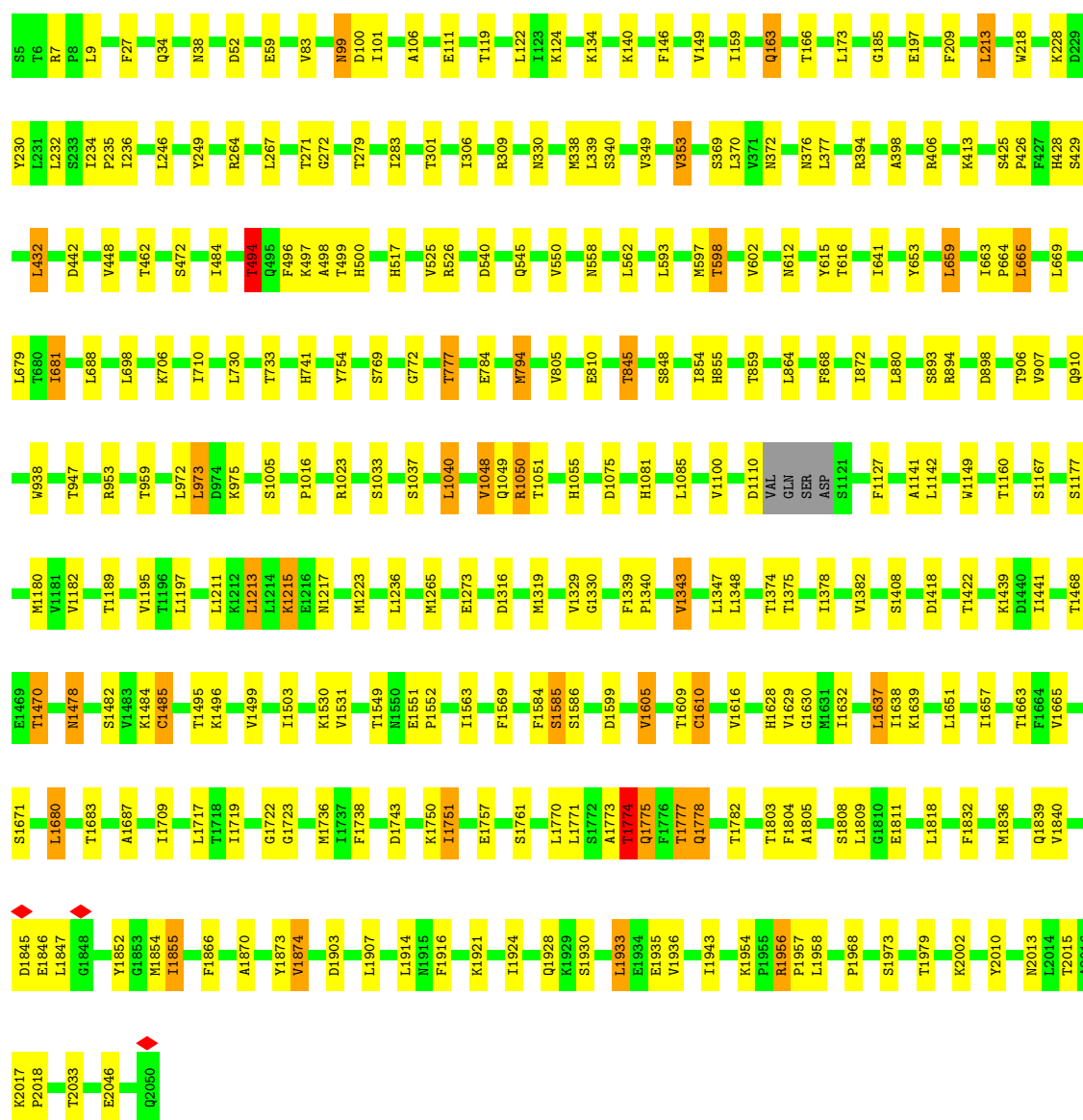


D1418		R894	L865	H428	W218	S5
T1422	M1148	D898	L669	S429	K228	T6
K1439	T1160	T906	L679	L432	D229	P8
T1441	S1187	V907	T680	D442	T230	L9
	S1177	Q910	L681	V448	L231	F27
T1468		W938	L688		S233	F28
F1469	M1180		E689	T462	T234	L29
T1470	V1181	T947	V690	S472	P235	Q34
	V1182		E693		L236	
M1478	T1189	R953	L698	T484	L246	W38
S1482	S1190	T959	K706	T492	Y249	D52
K1484	V1195	L972	T710	Q495	R264	E59
C1485	L1197	L973	T719	F496	L267	W83
T1495	L1211	K975	L730	K497	T271	N99
K1496	K1212		T733	T499	D100	D100
V1499	L1213	S1005	H741	H517	T279	I101
I1503	K1215	P1016	Y754	V525	I283	A106
K1530	E1216	R1023	T769	R526	T301	E111
V1531	N1217	S1033	S769	D540	T306	T119
	M1223		G772	Q545	R309	L122
T1549	L1236	S1037	T777	E546	N330	I123
M1550		L1040	E784	I547	N338	K124
P1551	M1265	V1043	W794	V550	L339	K134
P1552	E1273	Q1049	R794	N558	S340	K140
	D1316	R1050	V805	L562	V349	S143
F1569	M1319	T1051	E810	L593	V353	F146
G1577	V1329	H1055	T845	M597	S369	V149
F1584	G1330	D1075	S948	T598	L370	I159
S1585	F1339	H1081	L854	V602	N372	Q163
S1586	P1340	L1085	H855	N612	R376	T166
I1593	V1343	V1100	T859	T615	L377	T166
D1599	L1347	D1110	L864	T616	R394	L173
V1605	T1348	VAL			A398	G185
T1609	T1374	GLN				
C1610	T1375	SER				
		ASP	F668	Y653	R406	E197
V1616		S1121	L872	L659	K413	F209
H1628	T1378	F1127	L880	T663		
V1629	V1382	A1141		R644		
G1630	S1408	L1142	S502	T463		
F1633						



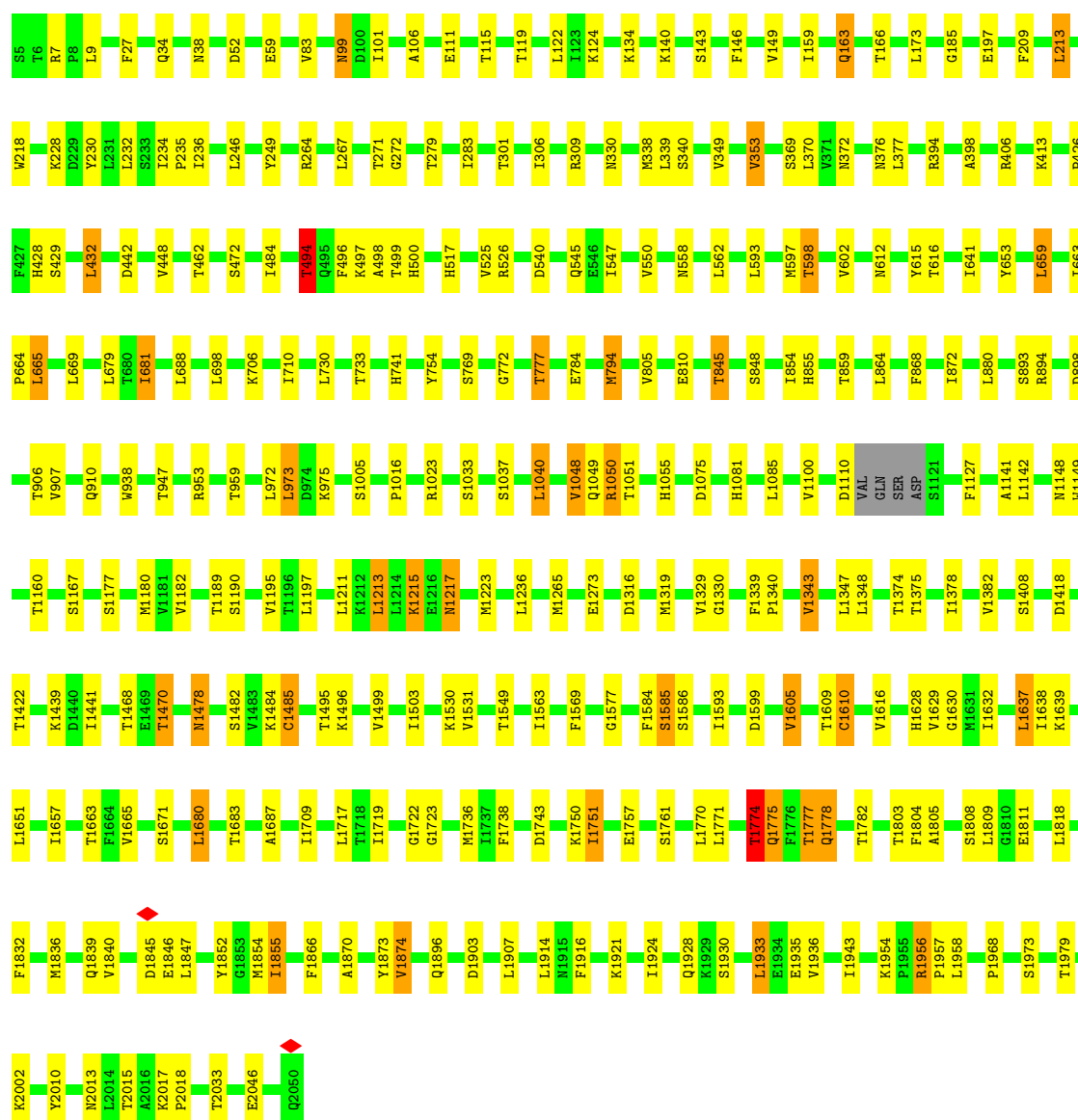
• Molecule 2: Fatty acid synthase subunit beta

Chain K: 85% 13% .



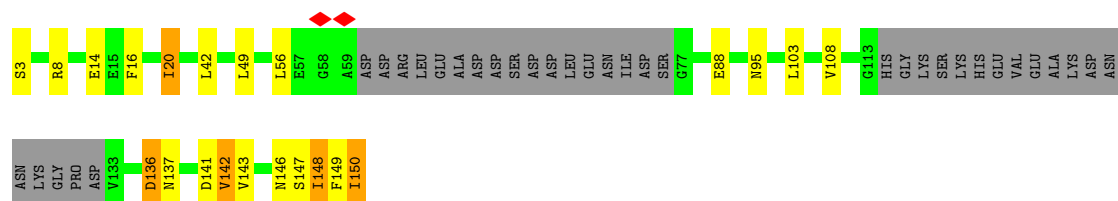
• Molecule 2: Fatty acid synthase subunit beta

Chain L:  85% 13% .



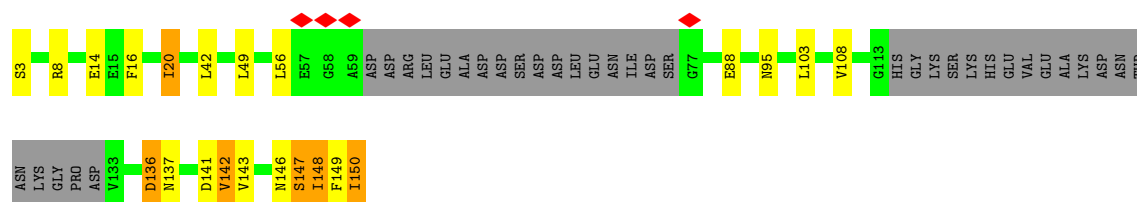
• Molecule 3: Translation machinery-associated protein 17

Chain M:  61% 11% 24% .

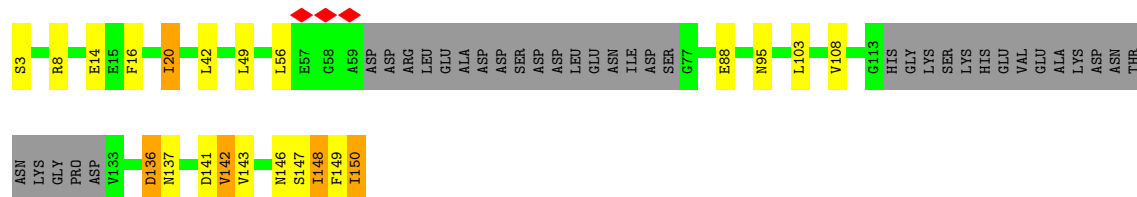


• Molecule 3: Translation machinery-associated protein 17

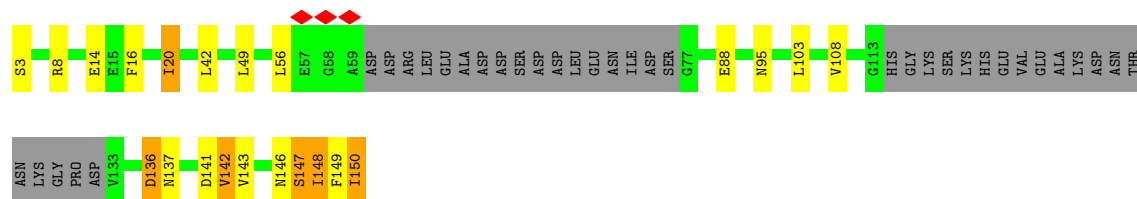
Chain N:  61% 11% 24% .



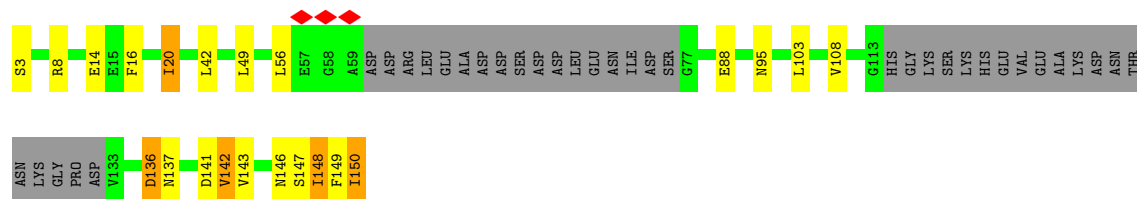
• Molecule 3: Translation machinery-associated protein 17



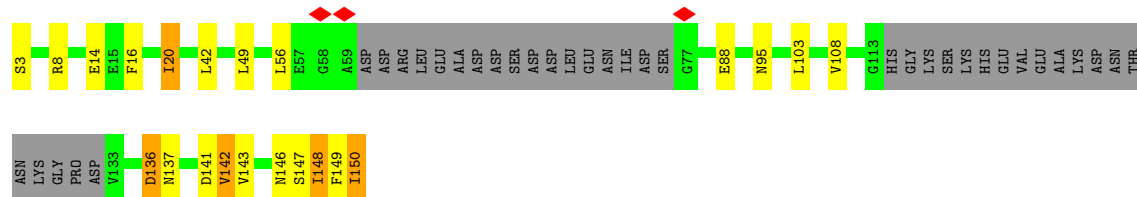
• Molecule 3: Translation machinery-associated protein 17



• Molecule 3: Translation machinery-associated protein 17



• Molecule 3: Translation machinery-associated protein 17



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	110597	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	132000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.142	Depositor
Minimum map value	-0.058	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.13	6/13878 (0.0%)	1.59	50/18755 (0.3%)
1	B	1.13	4/13878 (0.0%)	1.59	51/18755 (0.3%)
1	C	1.13	4/13878 (0.0%)	1.59	47/18755 (0.3%)
1	D	1.13	4/13878 (0.0%)	1.59	49/18755 (0.3%)
1	E	1.13	5/13878 (0.0%)	1.59	54/18755 (0.3%)
1	F	1.13	5/13878 (0.0%)	1.59	45/18755 (0.2%)
2	G	1.03	1/16383 (0.0%)	1.50	16/22229 (0.1%)
2	H	1.03	1/16383 (0.0%)	1.49	17/22229 (0.1%)
2	I	1.03	1/16383 (0.0%)	1.50	16/22229 (0.1%)
2	J	1.03	1/16383 (0.0%)	1.50	18/22229 (0.1%)
2	K	1.03	1/16383 (0.0%)	1.50	15/22229 (0.1%)
2	L	1.03	1/16383 (0.0%)	1.50	16/22229 (0.1%)
3	M	1.10	0/885	1.73	0/1189
3	N	1.11	0/885	1.72	0/1189
3	O	1.10	0/885	1.73	0/1189
3	P	1.10	0/885	1.73	0/1189
3	Q	1.11	0/885	1.73	0/1189
3	R	1.10	0/885	1.73	0/1189
All	All	1.08	34/186876 (0.0%)	1.55	394/253038 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
2	G	0	6
2	H	0	6
2	I	0	6
2	J	0	6
2	K	0	6
2	L	0	6
All	All	0	42

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1399	PRO	C-O	-6.00	1.16	1.23
1	F	1399	PRO	C-O	-5.97	1.16	1.23
1	C	1399	PRO	C-O	-5.93	1.16	1.23
1	E	1399	PRO	C-O	-5.90	1.16	1.23
1	D	1399	PRO	C-O	-5.90	1.16	1.23

The worst 5 of 394 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	494	THR	CB-CA-C	7.95	121.66	111.40
2	G	494	THR	CB-CA-C	7.95	121.65	111.40
2	K	494	THR	CB-CA-C	7.92	121.62	111.40
2	I	494	THR	CB-CA-C	7.91	121.61	111.40
2	J	494	THR	CB-CA-C	7.89	121.58	111.40

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	MET	Peptide
1	B	237	MET	Peptide
1	C	237	MET	Peptide
1	D	237	MET	Peptide
1	E	237	MET	Peptide

5.2 Too-close contacts [i](#)

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	13625	0	13615	123	0
1	B	13625	0	13615	127	0
1	C	13625	0	13615	130	0
1	D	13625	0	13615	131	0
1	E	13625	0	13615	123	0
1	F	13625	0	13615	125	0
2	G	16018	0	15993	124	0
2	H	16018	0	15993	119	0
2	I	16018	0	15993	120	0
2	J	16018	0	15993	120	0
2	K	16018	0	15993	118	0
2	L	16018	0	15993	120	0
3	M	879	0	871	19	0
3	N	879	0	871	20	0
3	O	879	0	871	19	0
3	P	879	0	871	19	0
3	Q	879	0	871	18	0
3	R	879	0	871	20	0
4	A	21	0	21	3	0
4	B	21	0	21	4	0
4	C	21	0	21	3	0
4	D	21	0	21	3	0
4	E	21	0	21	3	0
4	F	21	0	21	3	0
5	G	31	0	19	2	0
5	H	31	0	19	2	0
5	I	31	0	19	2	0
5	J	31	0	19	2	0
5	K	31	0	19	2	0
5	L	31	0	19	2	0
All	All	183444	0	183114	1446	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 4.

The worst 5 of 1446 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)
2:H:1811:GLU:OE2	2:H:2010:TYR:OH	1.80	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:1811:GLU:OE2	2:L:2010:TYR:OH	1.80	1.00
2:K:1811:GLU:OE2	2:K:2010:TYR:OH	1.80	0.99
2:G:1811:GLU:OE2	2:G:2010:TYR:OH	1.80	0.99
2:I:1811:GLU:OE2	2:I:2010:TYR:OH	1.80	0.99

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	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	18	47
1	B	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	18	47
1	C	1744/1887 (92%)	1612 (92%)	119 (7%)	13 (1%)	18	47
1	D	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	18	47
1	E	1744/1887 (92%)	1612 (92%)	120 (7%)	12 (1%)	18	47
1	F	1744/1887 (92%)	1613 (92%)	119 (7%)	12 (1%)	18	47
2	G	2032/2040 (100%)	1843 (91%)	177 (9%)	12 (1%)	21	51
2	H	2032/2040 (100%)	1843 (91%)	176 (9%)	13 (1%)	21	51
2	I	2032/2040 (100%)	1844 (91%)	174 (9%)	14 (1%)	18	47
2	J	2032/2040 (100%)	1842 (91%)	178 (9%)	12 (1%)	21	51
2	K	2032/2040 (100%)	1844 (91%)	176 (9%)	12 (1%)	21	51
2	L	2032/2040 (100%)	1844 (91%)	176 (9%)	12 (1%)	21	51
3	M	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
3	N	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
3	O	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
3	P	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
3	R	106/148 (72%)	99 (93%)	5 (5%)	2 (2%)	6	22
All	All	23292/24450 (95%)	21327 (92%)	1805 (8%)	160 (1%)	20	47

5 of 160 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1130	ASP
1	B	1130	ASP
1	C	1130	ASP
1	D	1130	ASP
1	E	1130	ASP

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	1476/1566 (94%)	1367 (93%)	109 (7%)	13	37
1	B	1476/1566 (94%)	1365 (92%)	111 (8%)	12	37
1	C	1476/1566 (94%)	1365 (92%)	111 (8%)	12	37
1	D	1476/1566 (94%)	1365 (92%)	111 (8%)	12	37
1	E	1476/1566 (94%)	1364 (92%)	112 (8%)	12	36
1	F	1476/1566 (94%)	1366 (92%)	110 (8%)	12	37
2	G	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	H	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	I	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	J	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	K	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
2	L	1775/1779 (100%)	1646 (93%)	129 (7%)	13	38
3	M	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	N	97/129 (75%)	84 (87%)	13 (13%)	4	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	O	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	P	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	Q	97/129 (75%)	84 (87%)	13 (13%)	4	13
3	R	97/129 (75%)	84 (87%)	13 (13%)	4	13
All	All	20088/20844 (96%)	18572 (92%)	1516 (8%)	14	37

5 of 1516 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	119	THR
2	J	1605	VAL
2	I	659	LEU
2	I	111	GLU
2	I	1930	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 542 such sidechains are listed below:

Mol	Chain	Res	Type
2	L	211	GLN
2	L	747	HIS
2	L	165	ASN
3	N	146	ASN
1	F	1271	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FMN	J	2101	-	33,33,33	1.59	8 (24%)	48,50,50	1.82	15 (31%)
4	PNS	D	1901	1	14,20,21	0.87	0	18,26,29	1.50	3 (16%)
4	PNS	F	1901	1	14,20,21	0.87	0	18,26,29	1.50	3 (16%)
5	FMN	G	2101	-	33,33,33	1.56	8 (24%)	48,50,50	1.84	15 (31%)
5	FMN	I	2101	-	33,33,33	1.58	7 (21%)	48,50,50	1.80	15 (31%)
4	PNS	C	1901	1	14,20,21	0.88	0	18,26,29	1.51	3 (16%)
4	PNS	B	1901	1	14,20,21	0.85	0	18,26,29	1.49	2 (11%)
4	PNS	A	1901	1	14,20,21	0.87	0	18,26,29	1.51	3 (16%)
5	FMN	L	2101	-	33,33,33	1.58	8 (24%)	48,50,50	1.82	15 (31%)
4	PNS	E	1901	1	14,20,21	0.88	0	18,26,29	1.50	3 (16%)
5	FMN	H	2101	-	33,33,33	1.57	8 (24%)	48,50,50	1.82	15 (31%)
5	FMN	K	2101	-	33,33,33	1.55	8 (24%)	48,50,50	1.83	15 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FMN	J	2101	-	-	6/18/18/18	0/3/3/3
4	PNS	D	1901	1	-	7/24/26/27	-
4	PNS	F	1901	1	-	6/24/26/27	-
5	FMN	G	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	I	2101	-	-	6/18/18/18	0/3/3/3
4	PNS	C	1901	1	-	6/24/26/27	-
4	PNS	B	1901	1	-	7/24/26/27	-
4	PNS	A	1901	1	-	6/24/26/27	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FMN	L	2101	-	-	6/18/18/18	0/3/3/3
4	PNS	E	1901	1	-	6/24/26/27	-
5	FMN	H	2101	-	-	6/18/18/18	0/3/3/3
5	FMN	K	2101	-	-	6/18/18/18	0/3/3/3

The worst 5 of 47 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2101	FMN	C9A-C5A	4.04	1.47	1.41
5	G	2101	FMN	C9A-C5A	4.03	1.47	1.41
5	I	2101	FMN	C9A-C5A	4.01	1.47	1.41
5	H	2101	FMN	C9A-C5A	3.96	1.47	1.41
5	L	2101	FMN	C9A-C5A	3.94	1.47	1.41

The worst 5 of 107 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	2101	FMN	O3P-P-O5'	-4.36	95.31	106.67
5	H	2101	FMN	O3P-P-O5'	-4.28	95.51	106.67
5	J	2101	FMN	O3P-P-O5'	-4.22	95.67	106.67
5	L	2101	FMN	O3P-P-O5'	-4.20	95.70	106.67
5	K	2101	FMN	O3P-P-O5'	-4.08	96.03	106.67

There are no chirality outliers.

5 of 74 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1901	PNS	O27-C28-C29-C32
4	A	1901	PNS	N36-C37-C38-C39
4	A	1901	PNS	N41-C42-C43-S44
4	B	1901	PNS	O27-C28-C29-C32
4	B	1901	PNS	N36-C37-C38-C39

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	2101	FMN	2	0
4	D	1901	PNS	3	0
4	F	1901	PNS	3	0

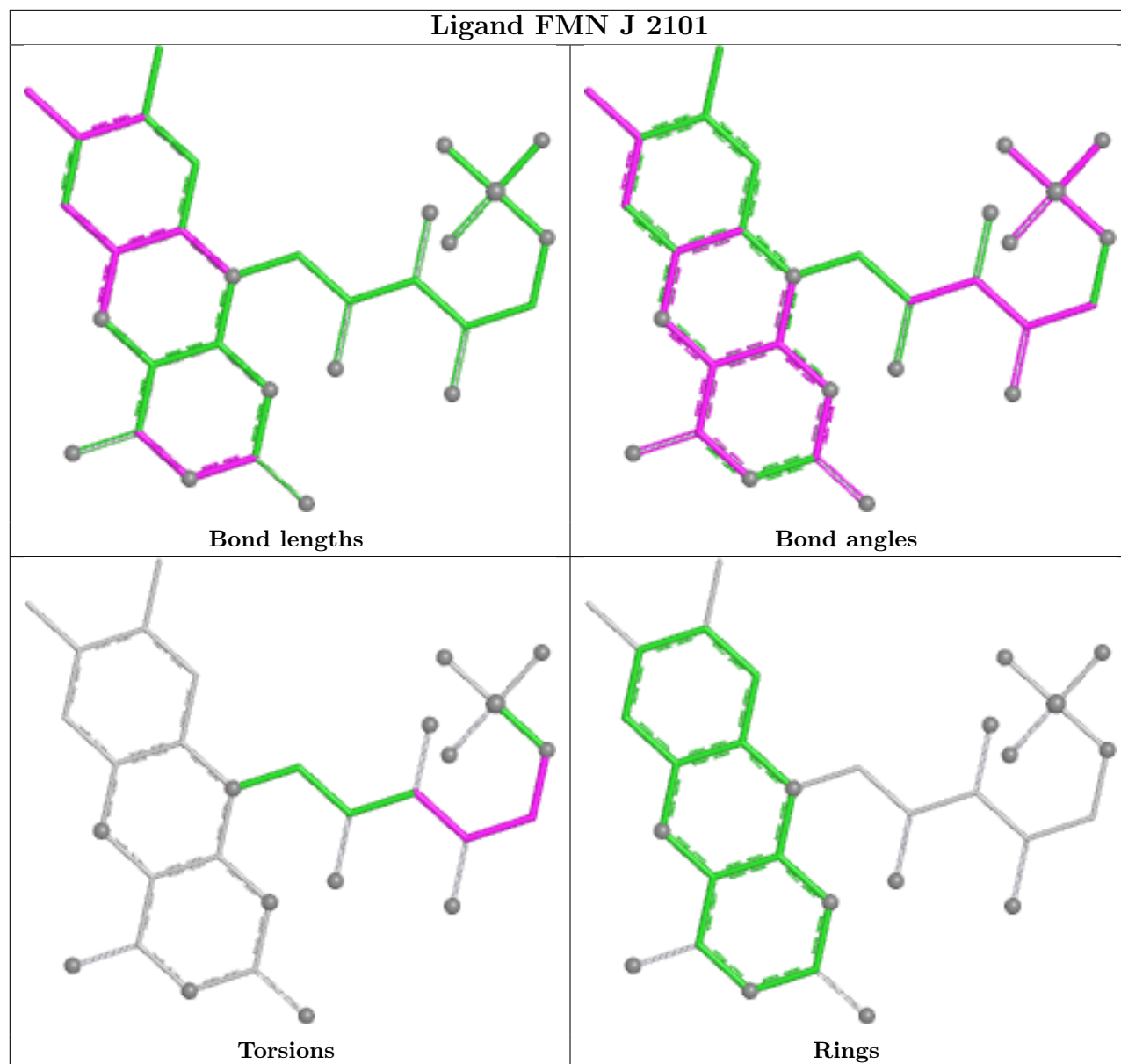
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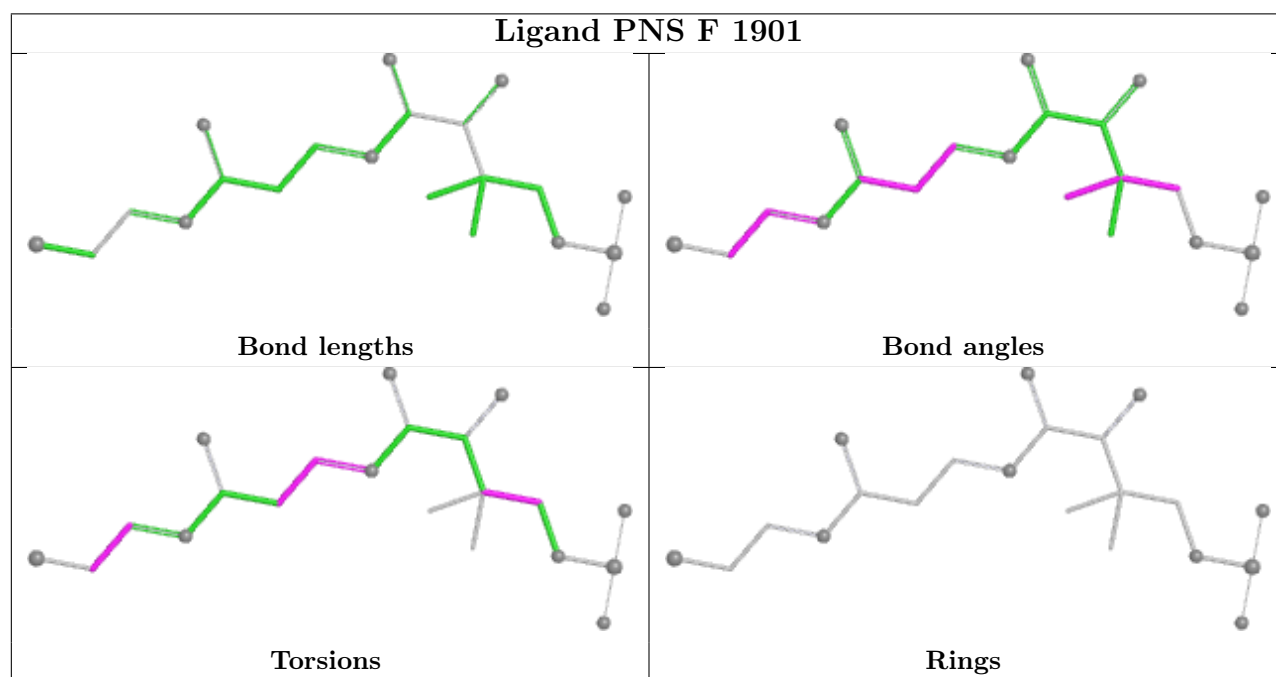
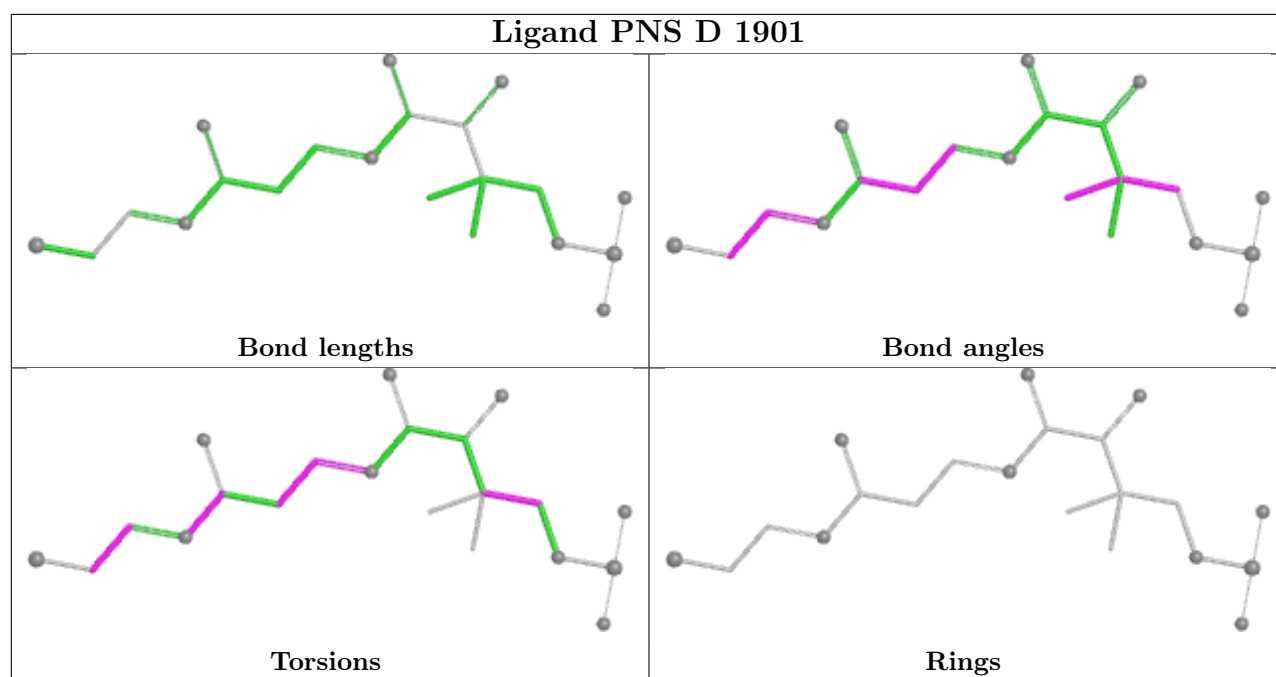
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	2101	FMN	2	0
5	I	2101	FMN	2	0
4	C	1901	PNS	3	0
4	B	1901	PNS	4	0
4	A	1901	PNS	3	0
5	L	2101	FMN	2	0
4	E	1901	PNS	3	0
5	H	2101	FMN	2	0
5	K	2101	FMN	2	0

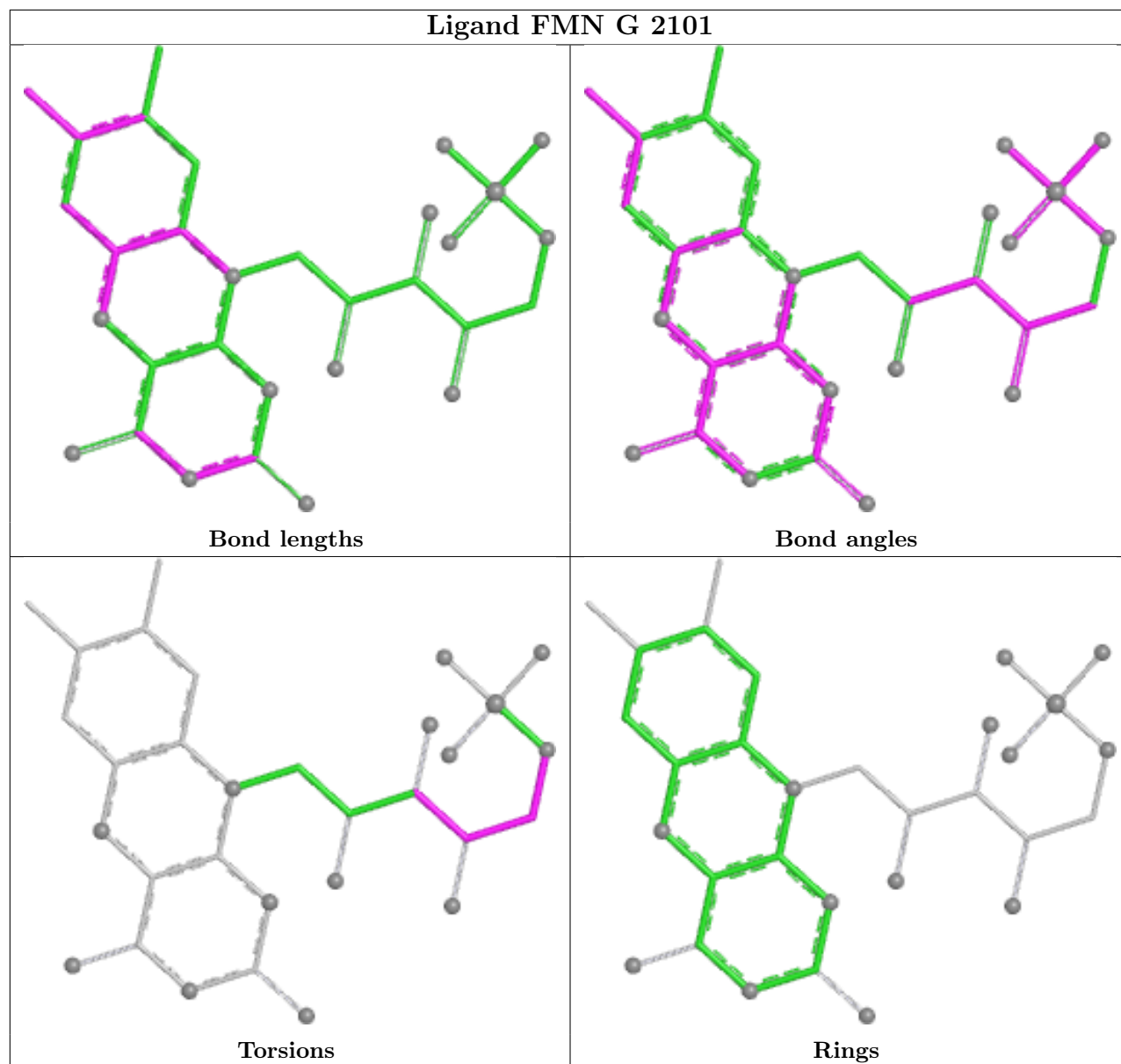
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

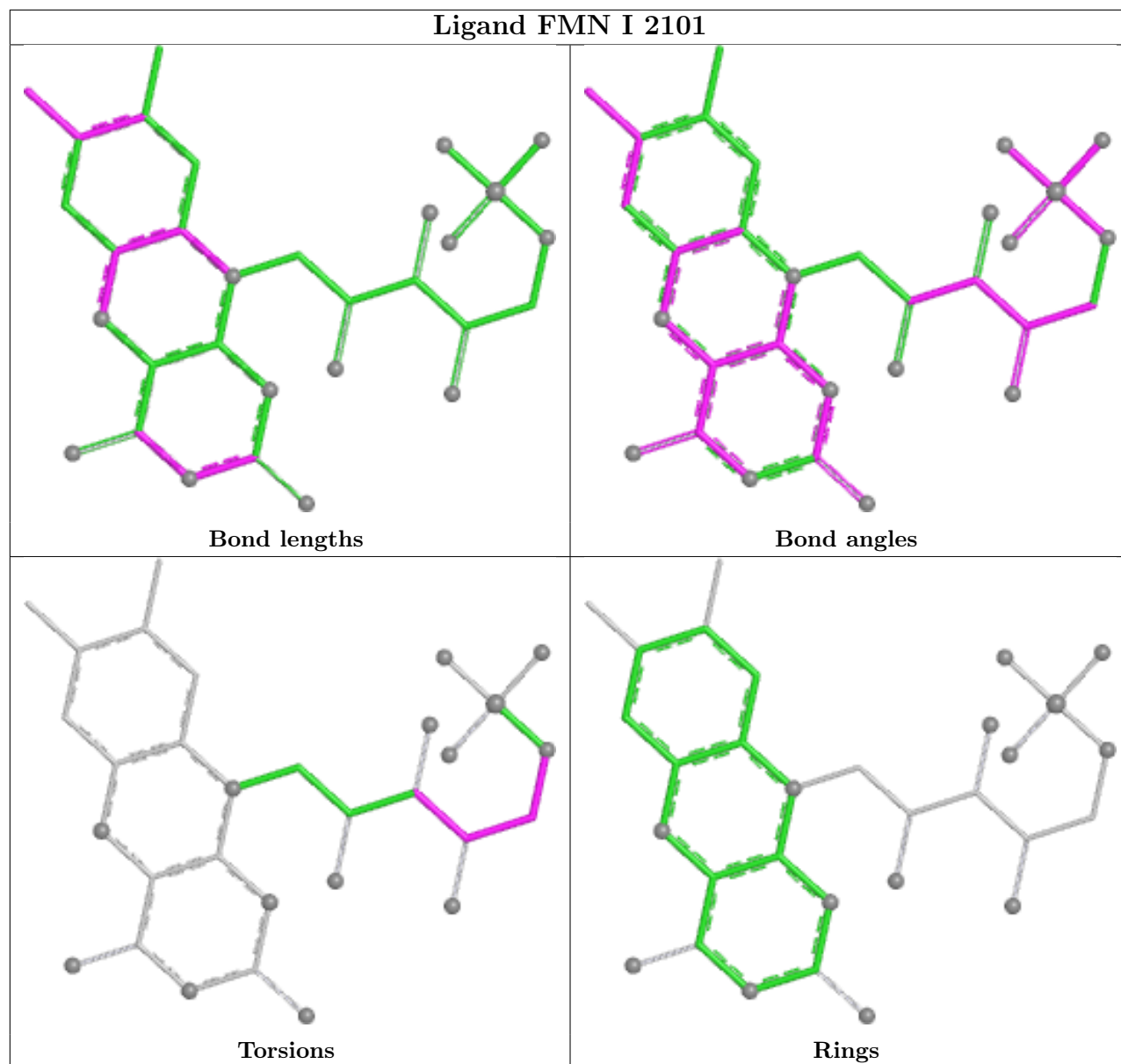
Ligand FMN J 2101

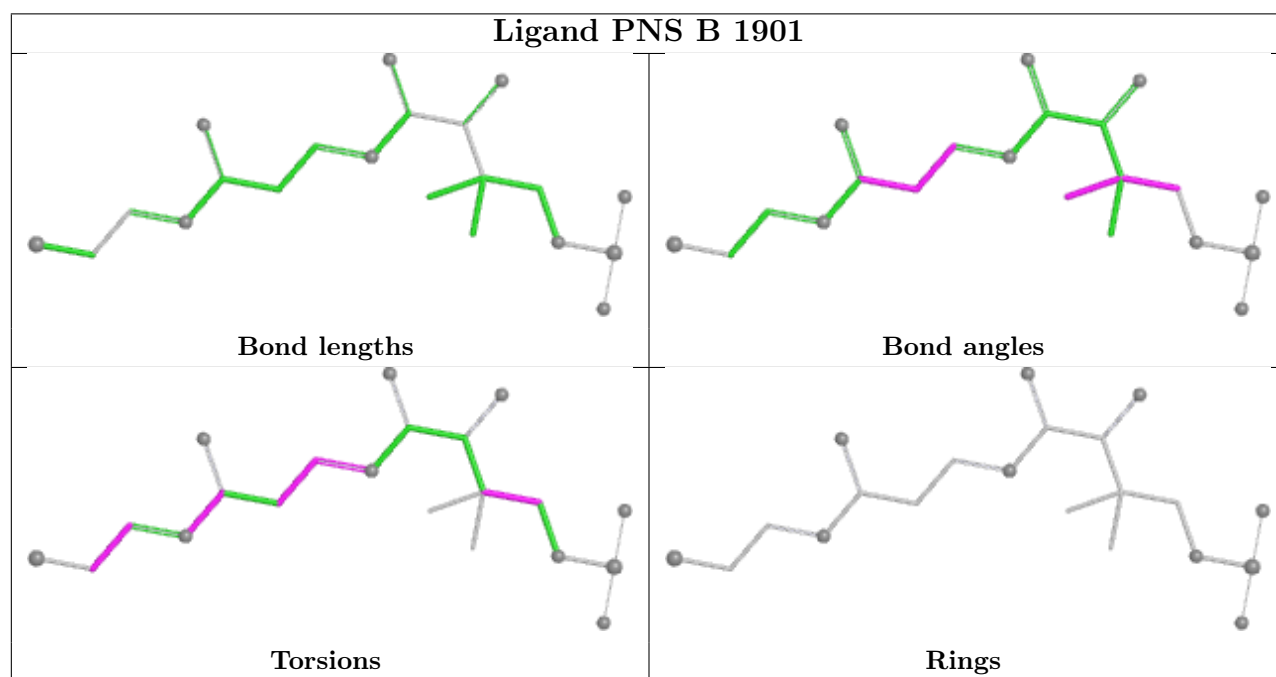
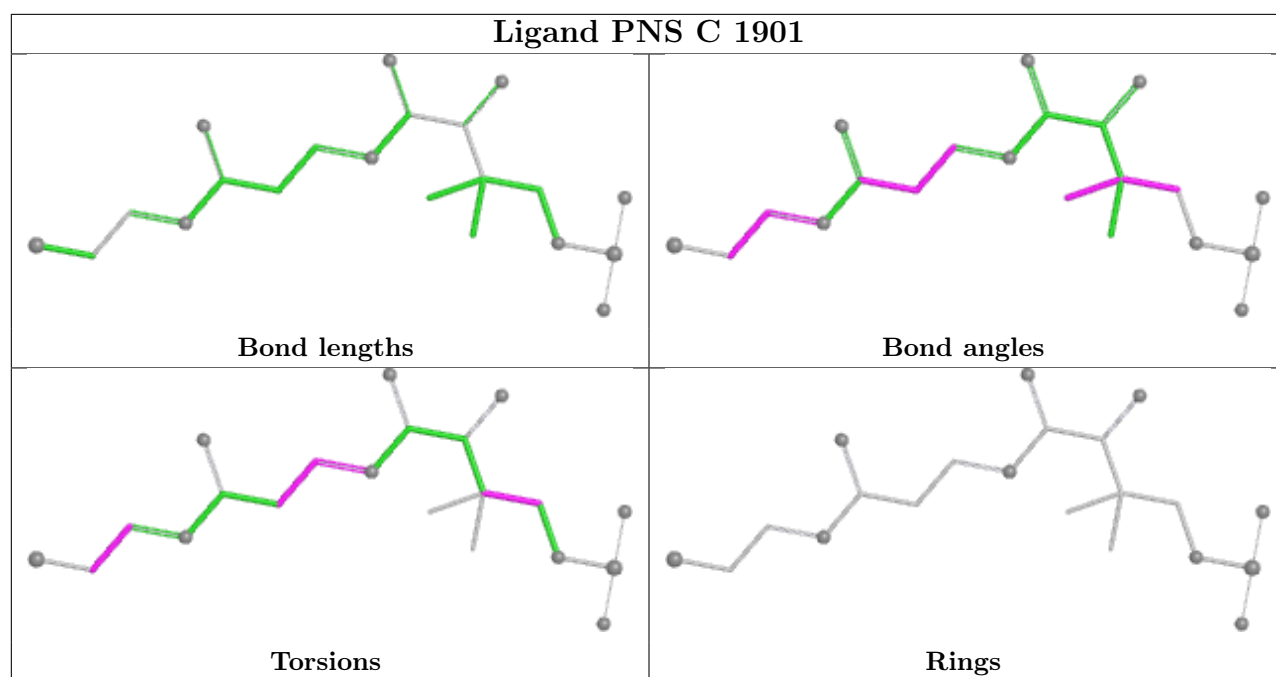


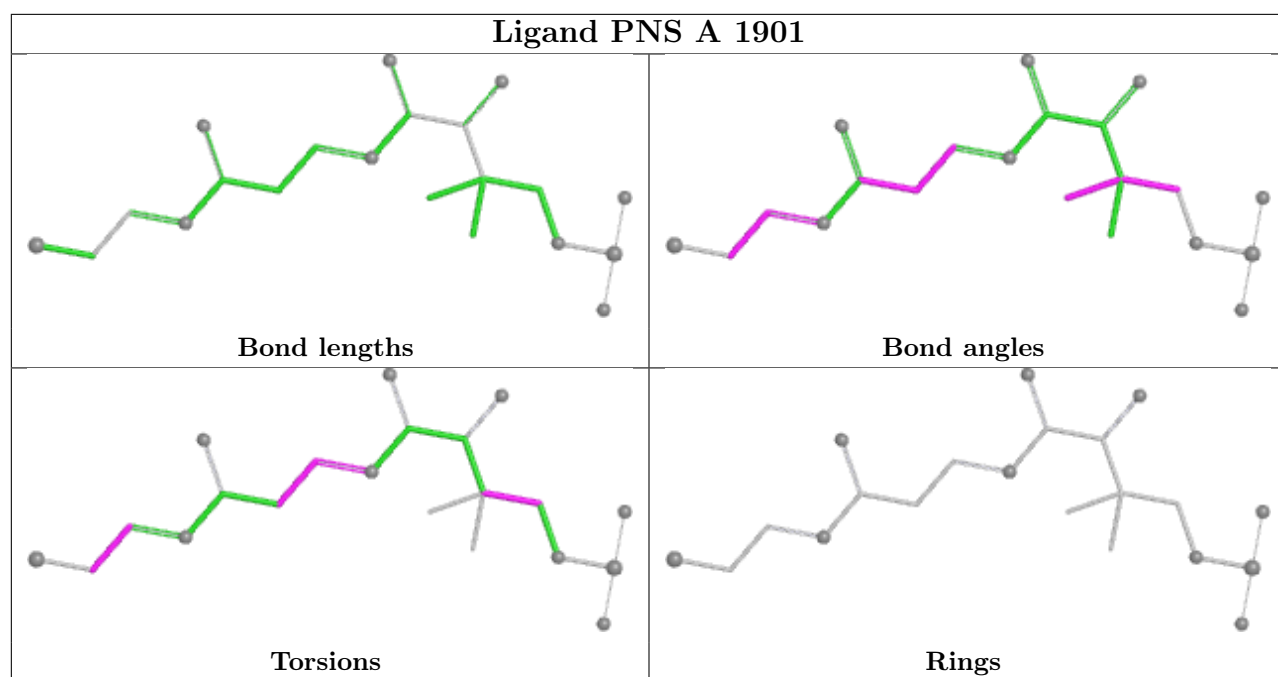


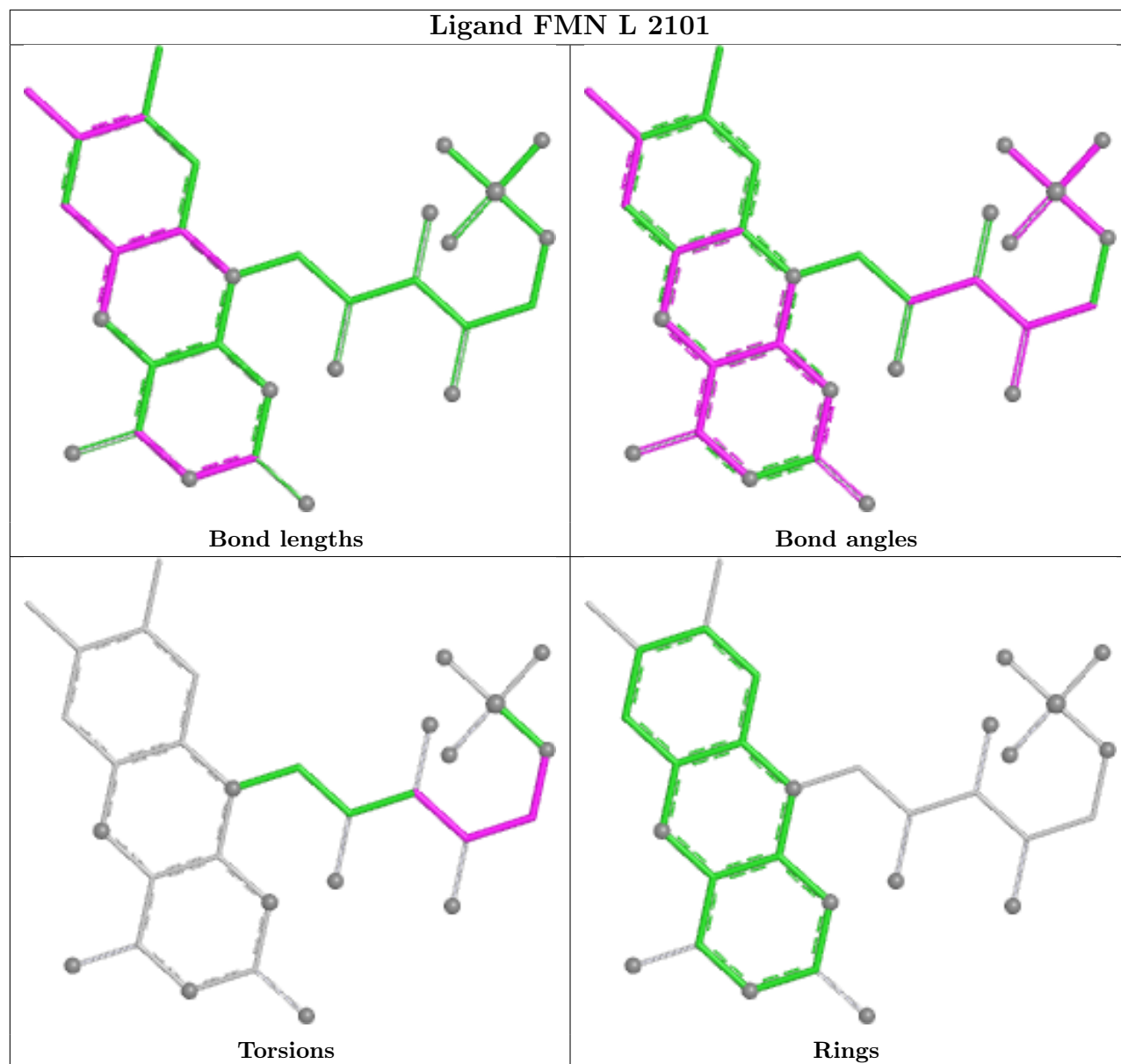
Ligand FMN G 2101

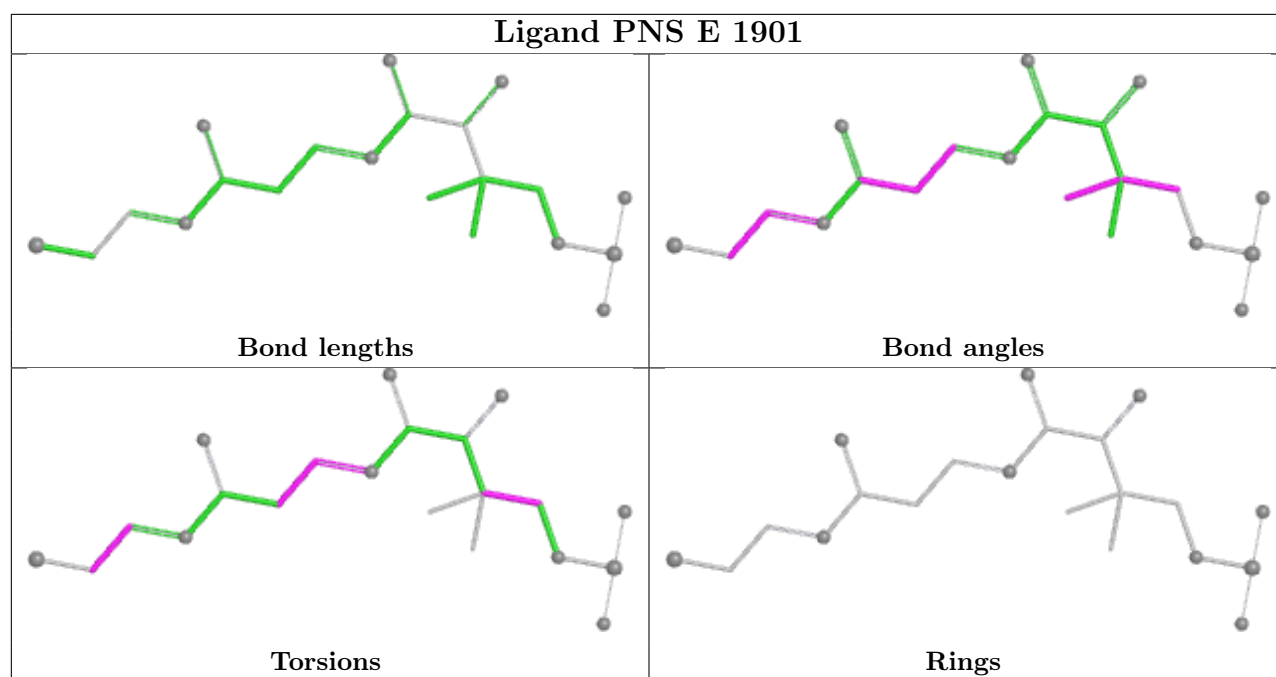




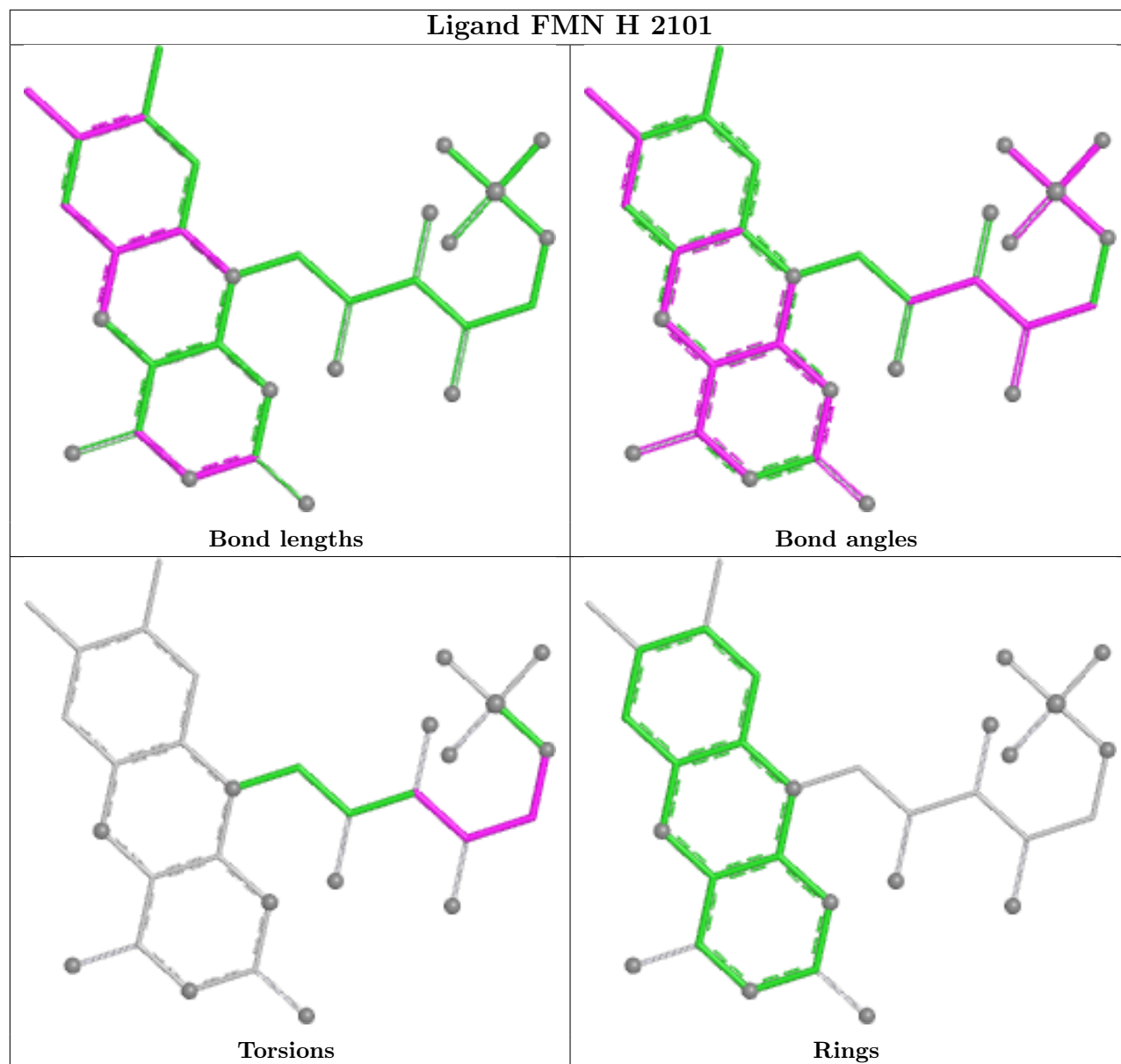


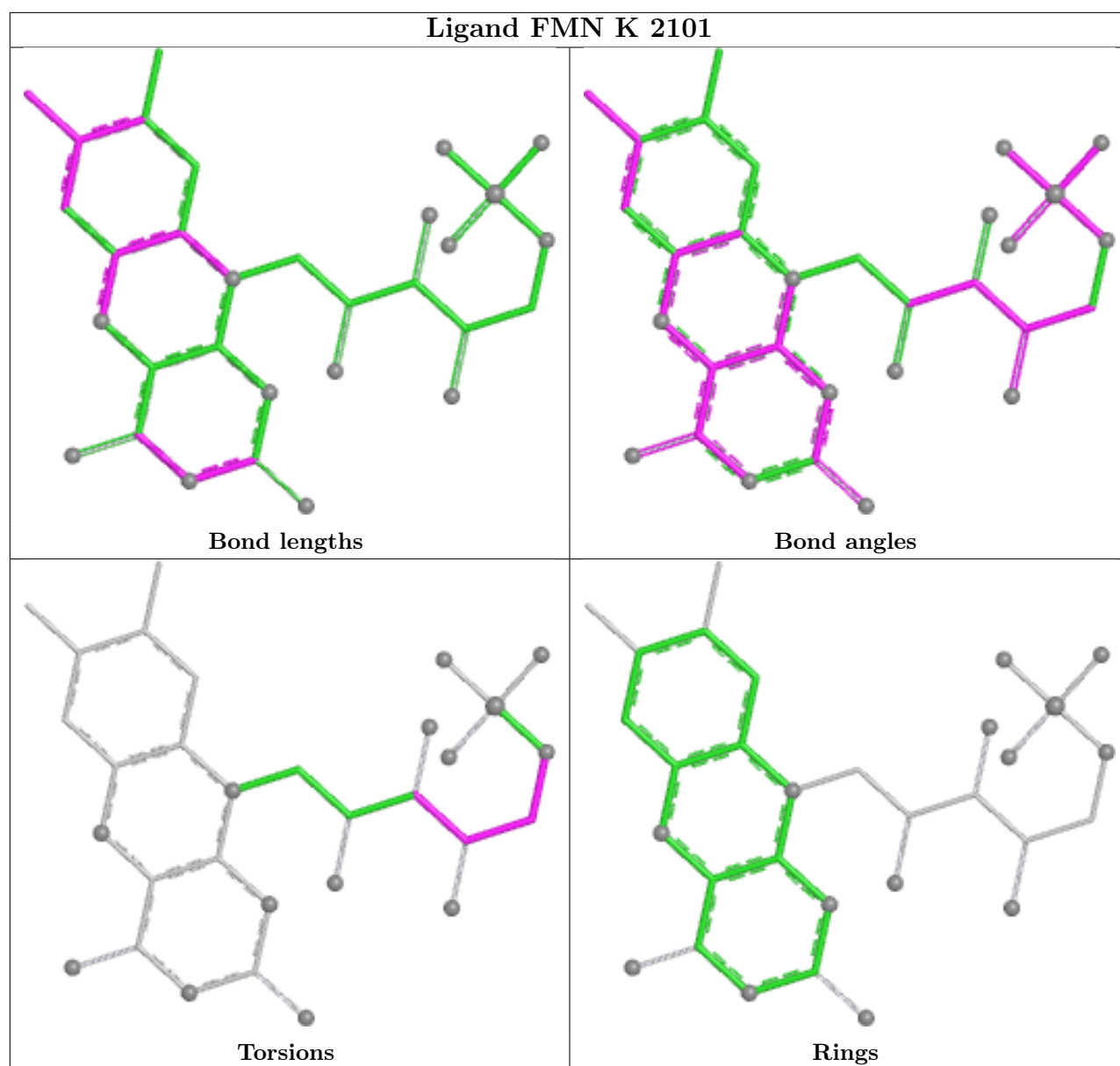






Ligand FMN H 2101





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.

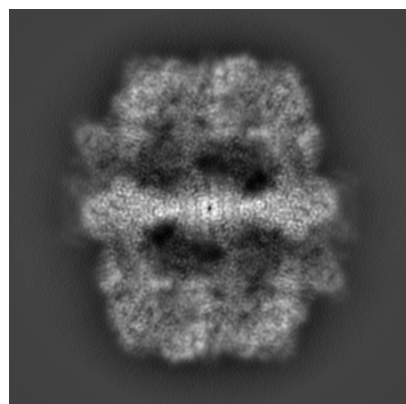
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4577. These allow visual inspection of the internal detail of the map and identification of artifacts.

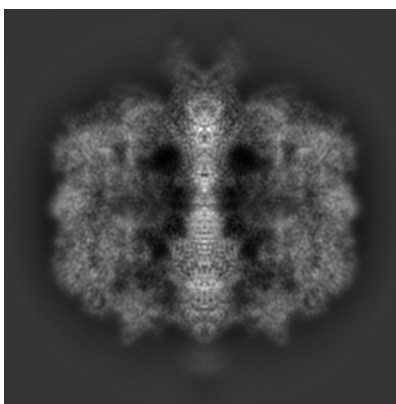
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

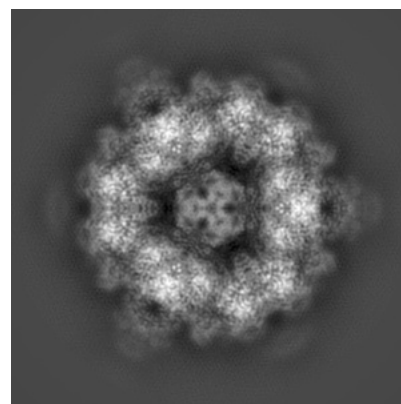
6.1.1 Primary map



X

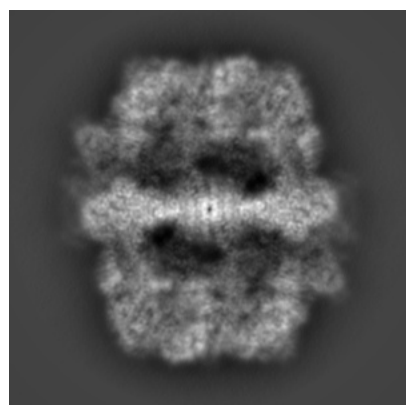


Y

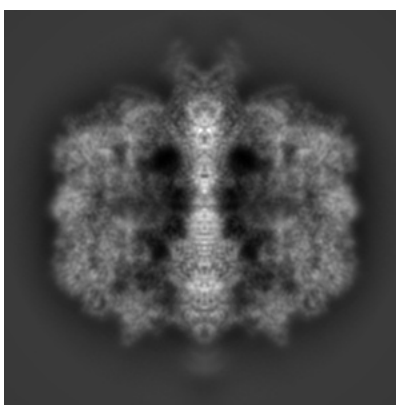


Z

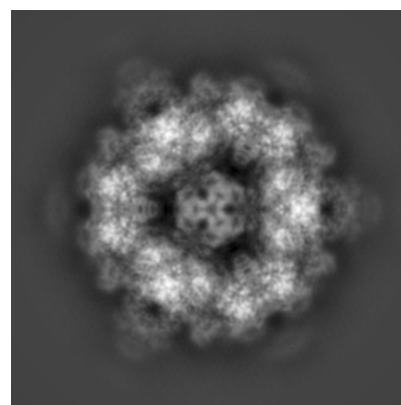
6.1.2 Raw map



X



Y

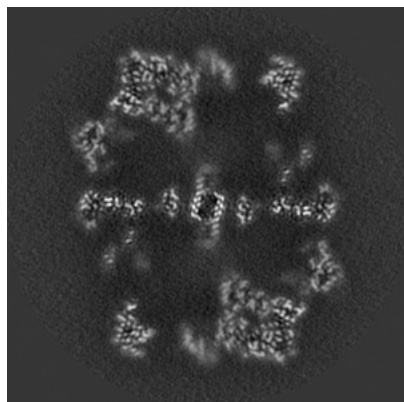


Z

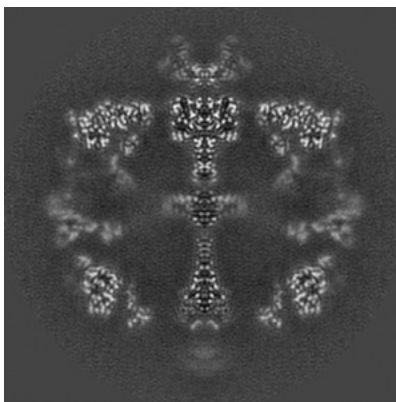
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

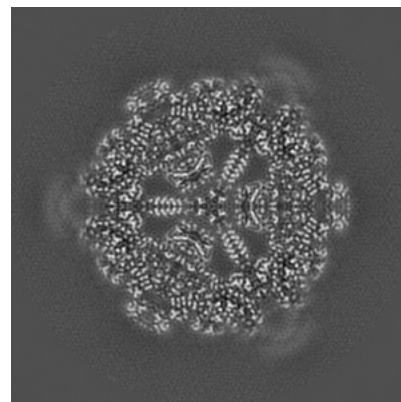
6.2.1 Primary map



X Index: 160

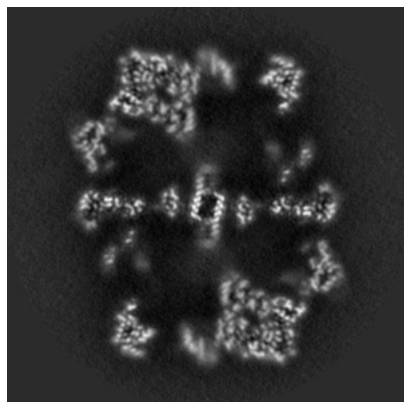


Y Index: 160

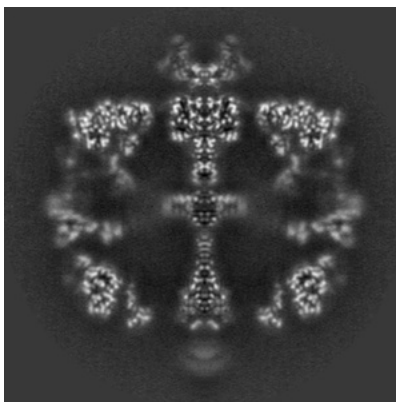


Z Index: 160

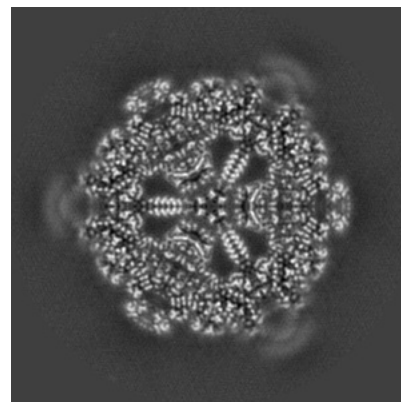
6.2.2 Raw map



X Index: 160



Y Index: 160

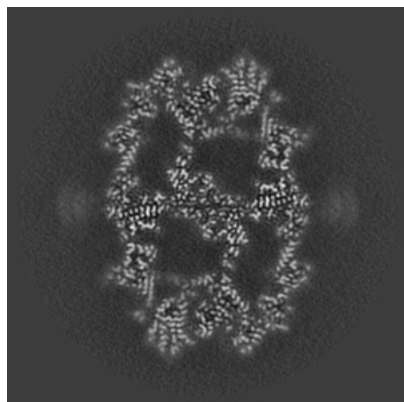


Z Index: 160

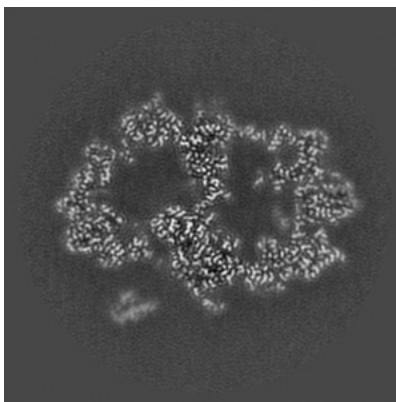
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

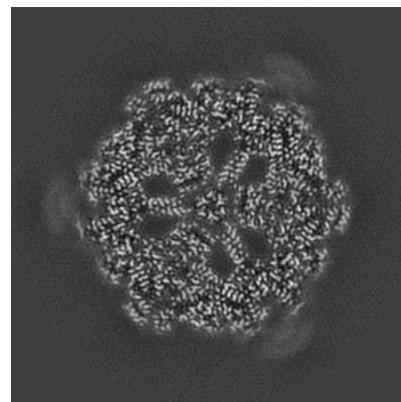
6.3.1 Primary map



X Index: 215

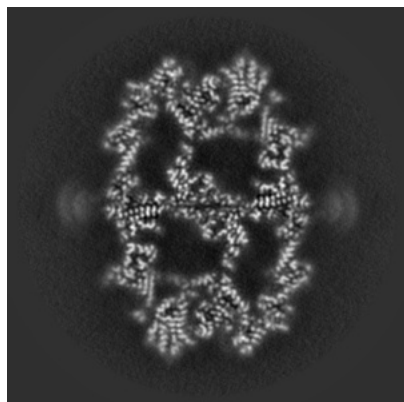


Y Index: 99

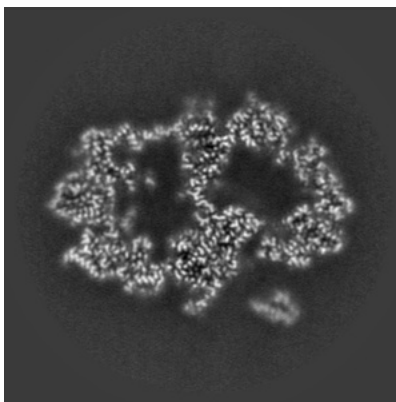


Z Index: 162

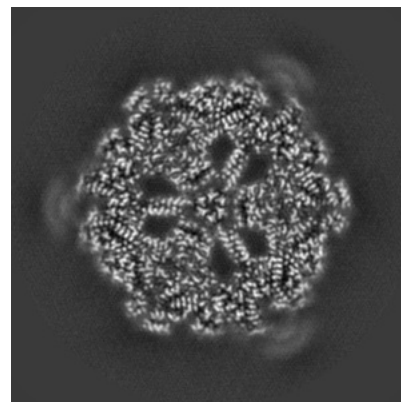
6.3.2 Raw map



X Index: 215



Y Index: 220

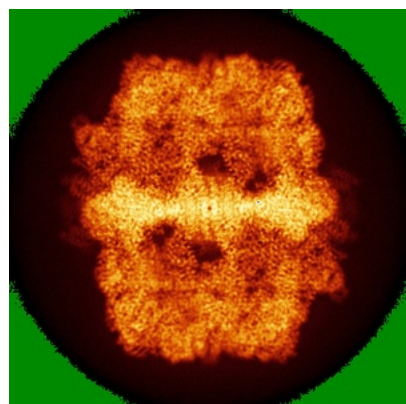


Z Index: 158

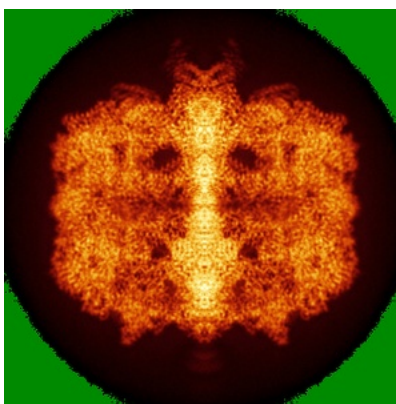
The images above show the largest variance slices of the map in three orthogonal directions.

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

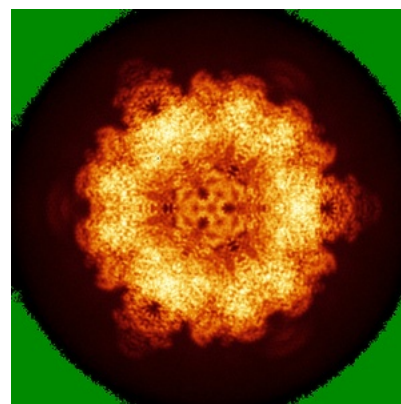
6.4.1 Primary map



X

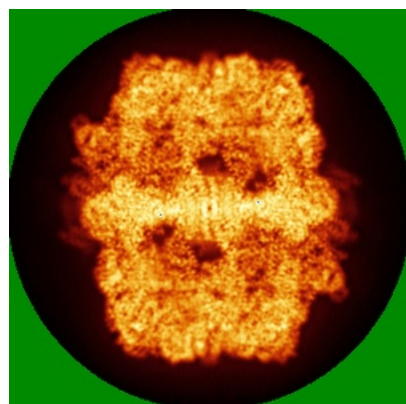


Y

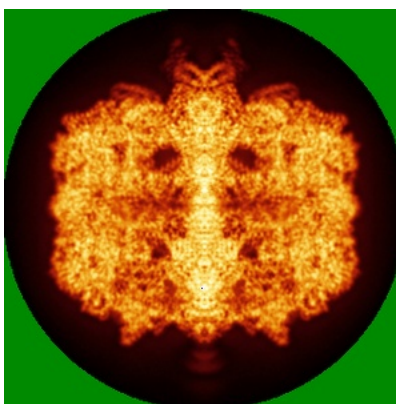


Z

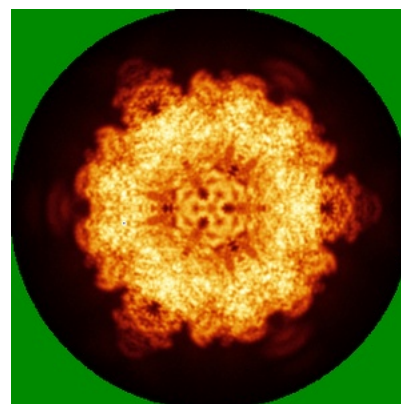
6.4.2 Raw map



X



Y

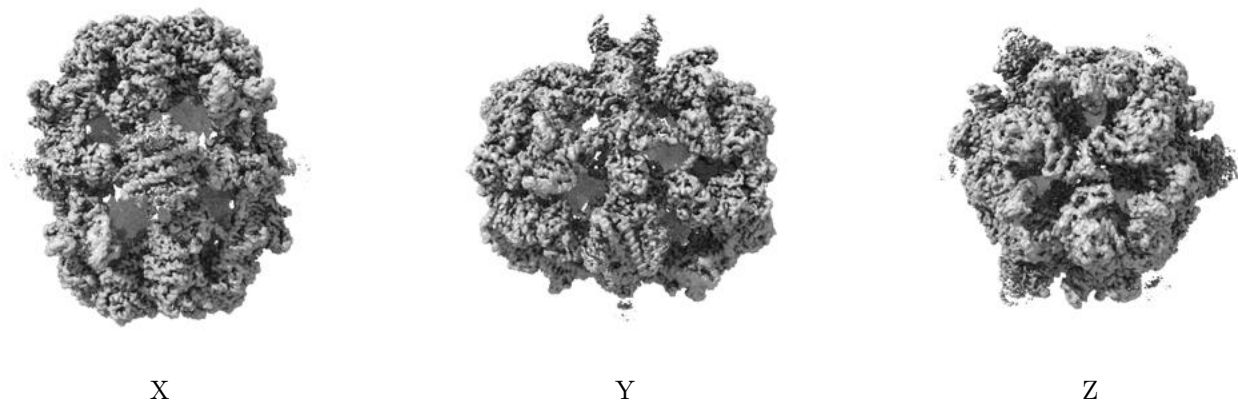


Z

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

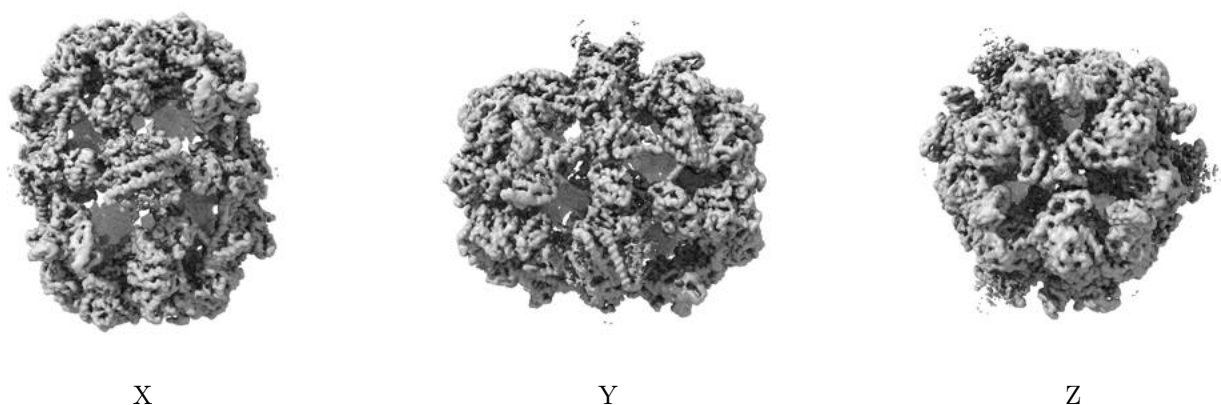
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. 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



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.

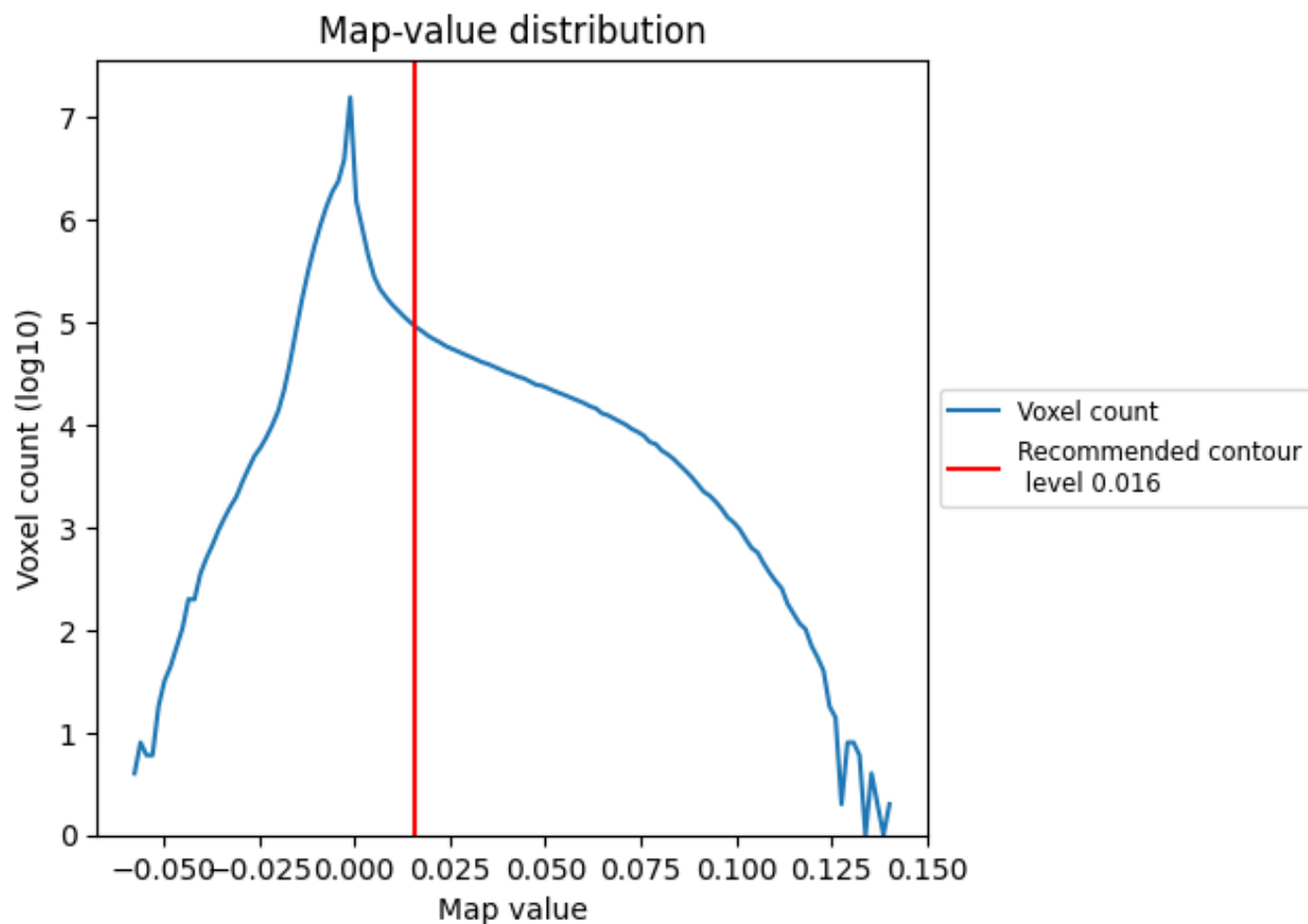
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

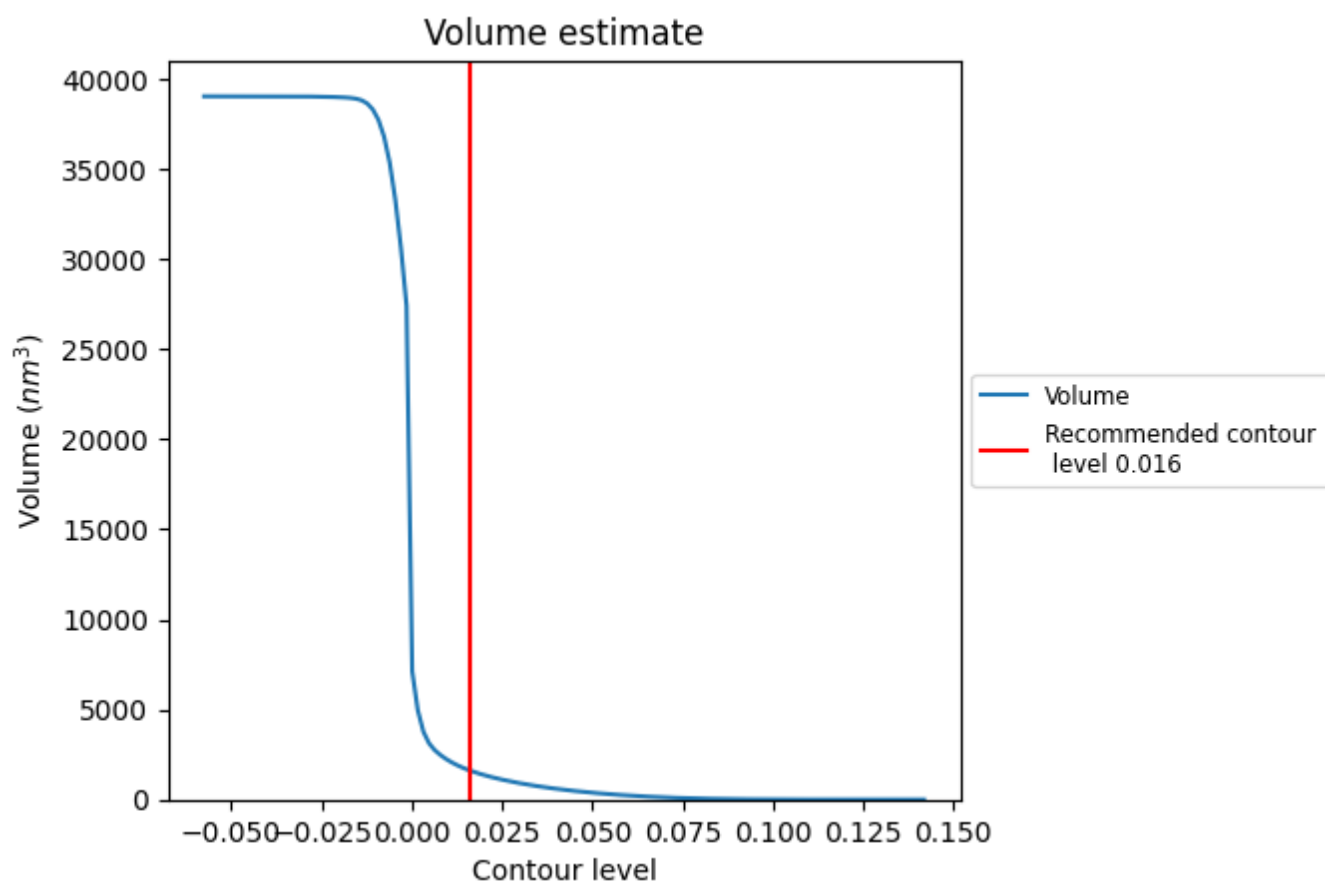
This section contains the results of statistical analysis of the map.

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.

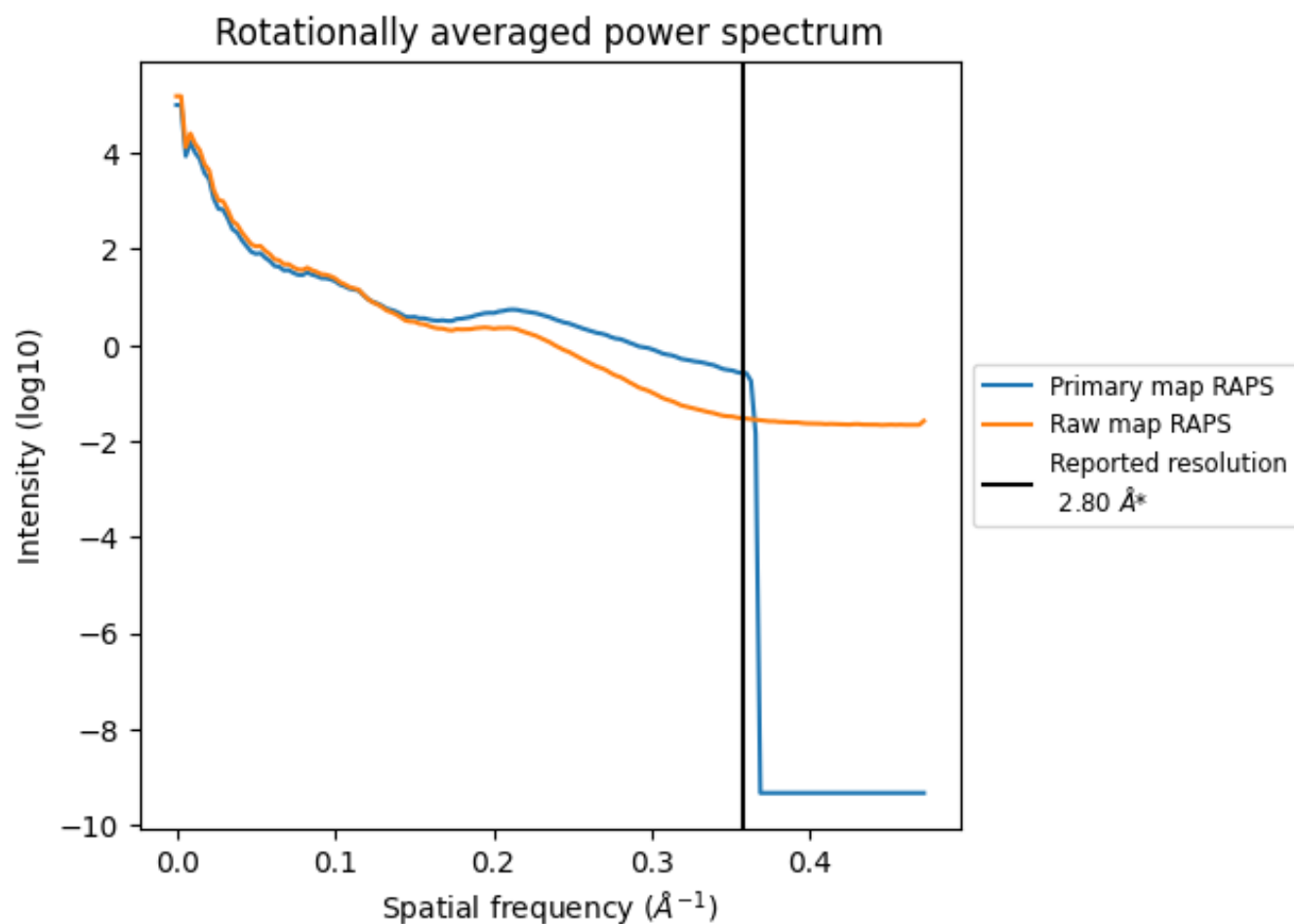
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1616 nm³; this corresponds to an approximate mass of 1460 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 ⓘ

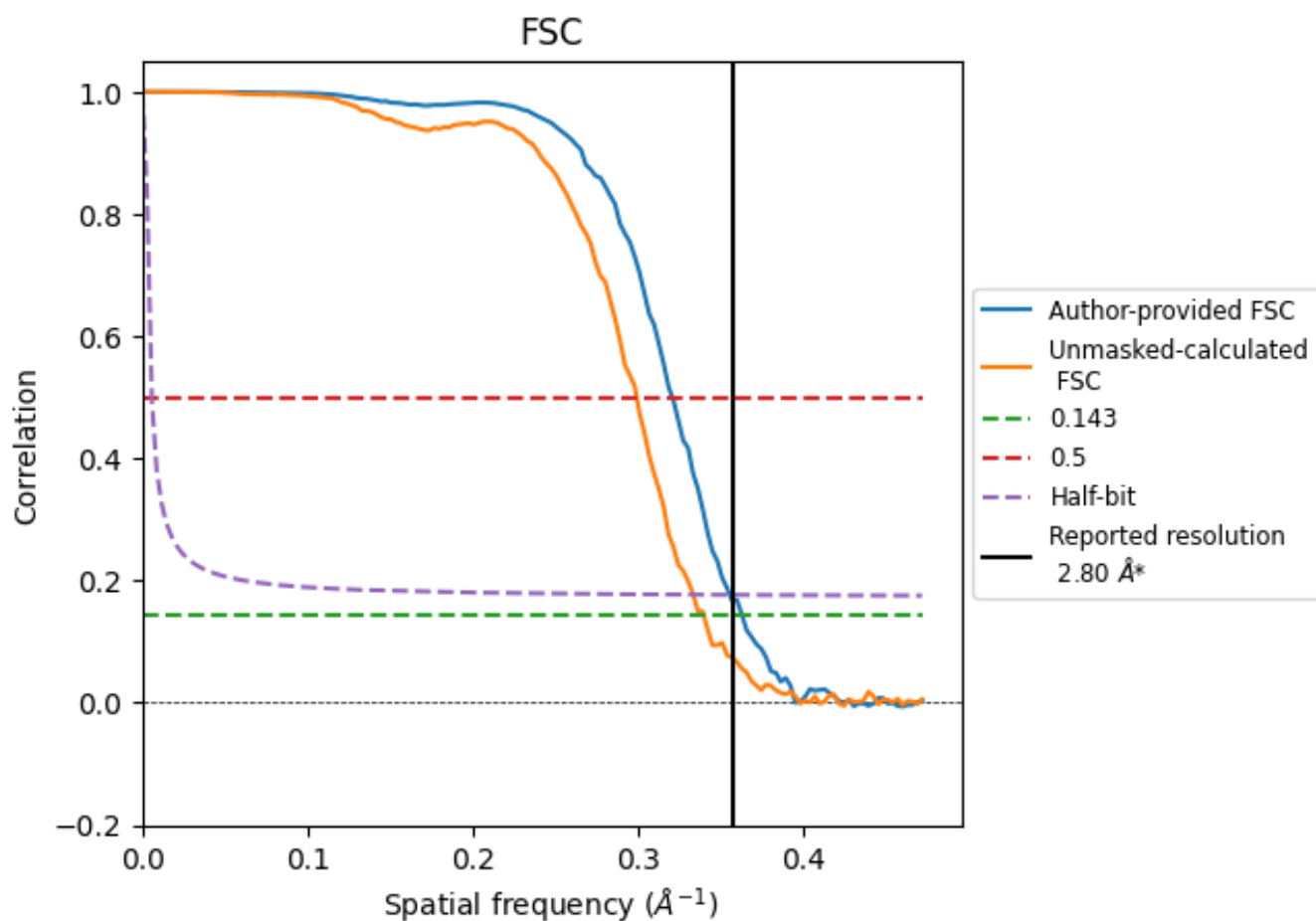


*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

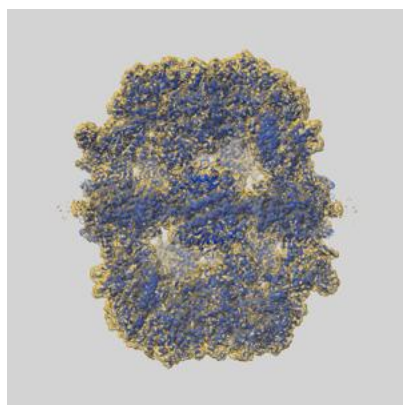
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.76	3.12	2.81
Unmasked-calculated*	2.94	3.34	3.00

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

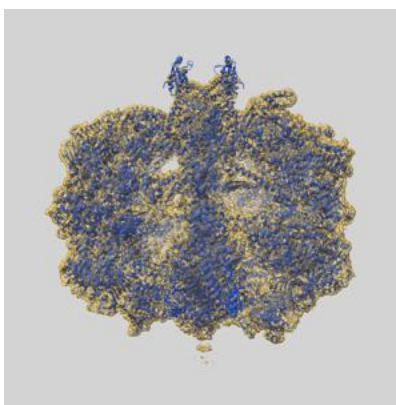
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4577 and PDB model 6QL5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

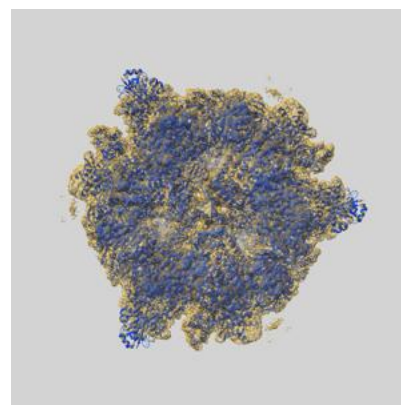
9.1 Map-model overlay [i](#)



X



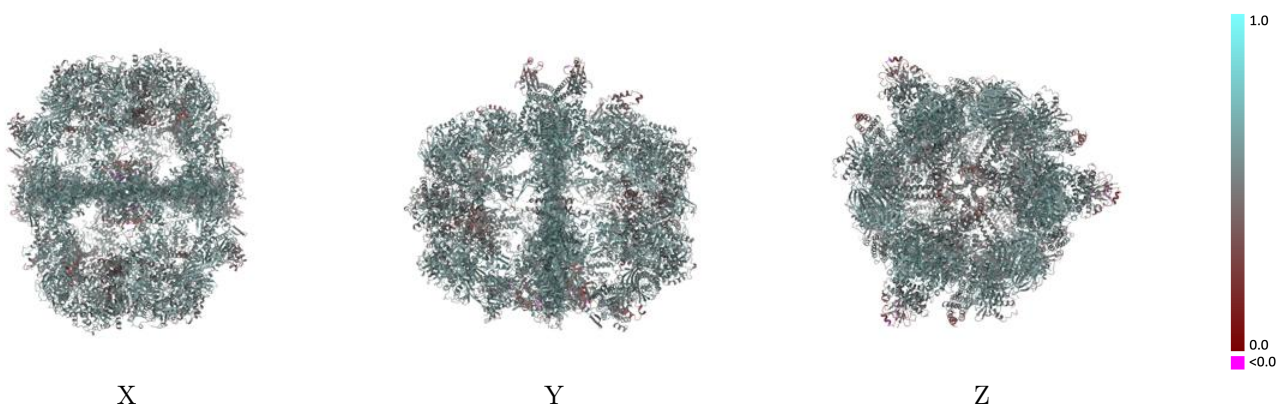
Y



Z

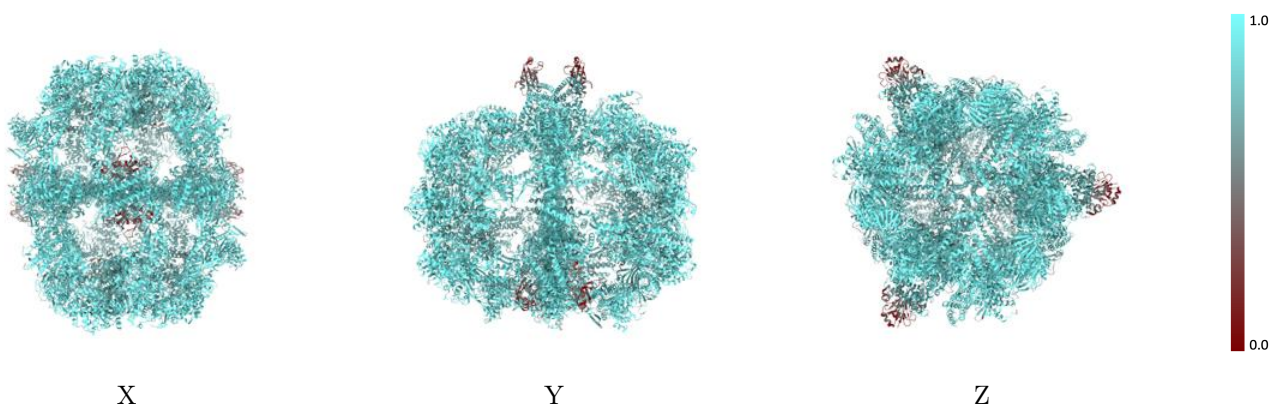
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



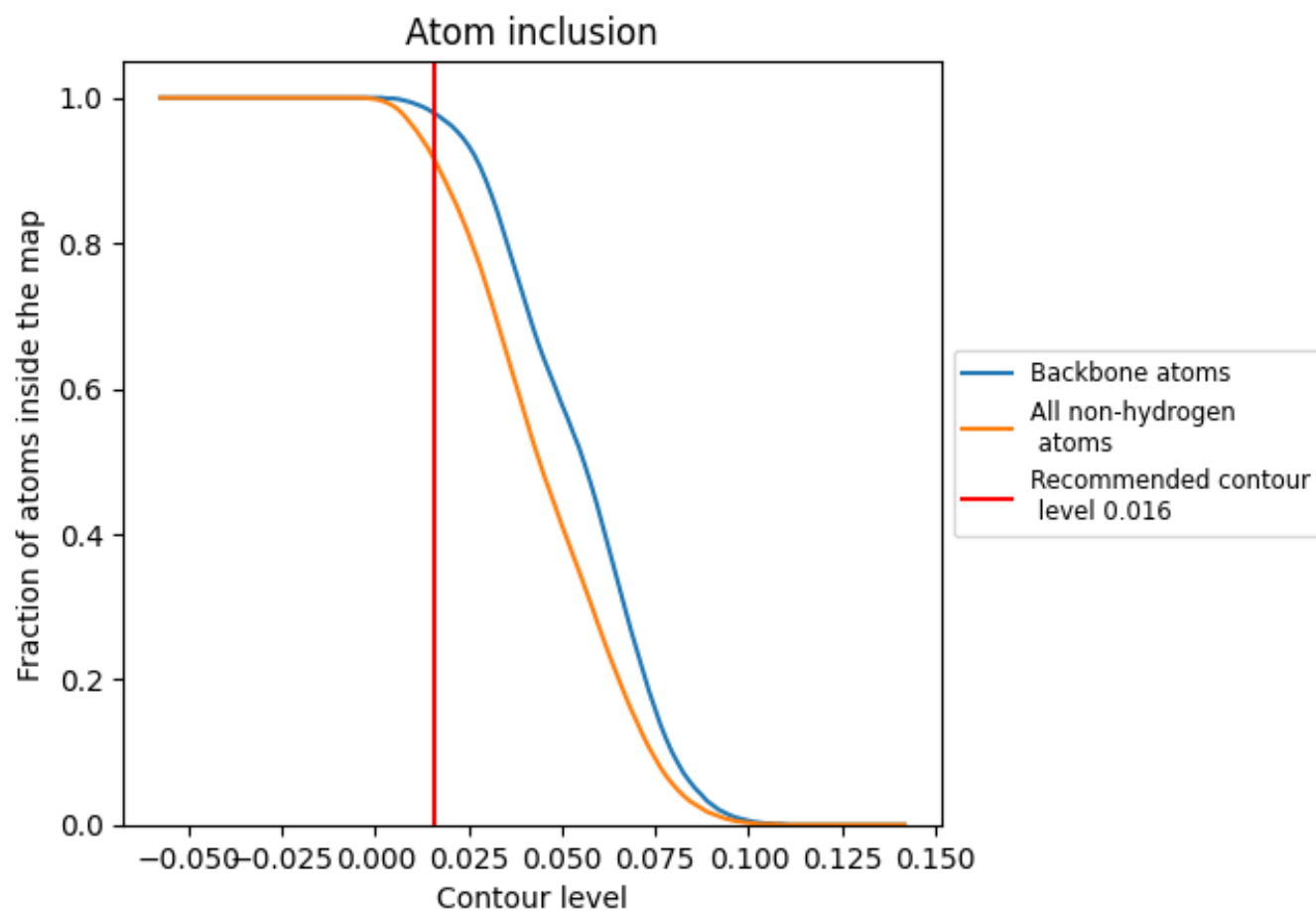
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.016).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9130	0.5530
A	0.8870	0.5610
B	0.8880	0.5610
C	0.8870	0.5620
D	0.8880	0.5620
E	0.8870	0.5620
F	0.8870	0.5610
G	0.9390	0.5490
H	0.9390	0.5490
I	0.9400	0.5480
J	0.9400	0.5490
K	0.9400	0.5490
L	0.9390	0.5490
M	0.8430	0.5150
N	0.8300	0.5160
O	0.8300	0.5140
P	0.8340	0.5140
Q	0.8330	0.5130
R	0.8360	0.5150

1.0

0.0

<0.0