



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 02:55 PM UTC

PDB ID : 9D48 / pdb_00009d48
EMDB ID : EMD-46553
Title : Atomic model of Ketoacyl Reductase domain and 4 helical bundle of *Candida albicans* Fatty Acid Synthase (FAS) in complex with Palmitoyl-CoA (in vivo binding)
Authors : Hasan, N.S.M.; Keszei, F.A.A.; Mazhab-Jafari, M.T.
Deposited on : 2024-08-12
Resolution : 2.66 Å (reported)
Based on initial model : 6U5V

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

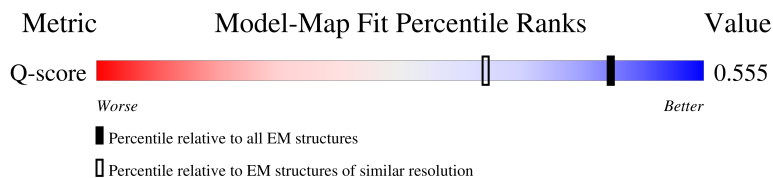
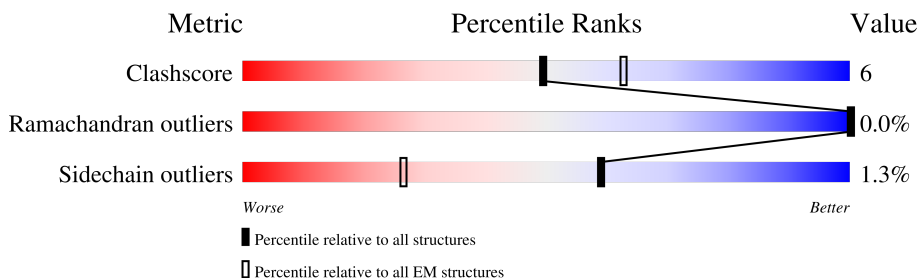
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.66 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	9119 (2.16 - 3.16)

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	2037	<div> <div>18%</div> <div>89%</div> <div>11%</div> </div>
1	E	2037	<div> <div>19%</div> <div>89%</div> <div>11%</div> </div>
1	I	2037	<div> <div>19%</div> <div>89%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	2037	
1	Q	2037	
1	W	2037	
2	B	1885	
2	F	1885	
2	G	1885	
2	N	1885	
2	R	1885	
2	X	1885	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 163304 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.

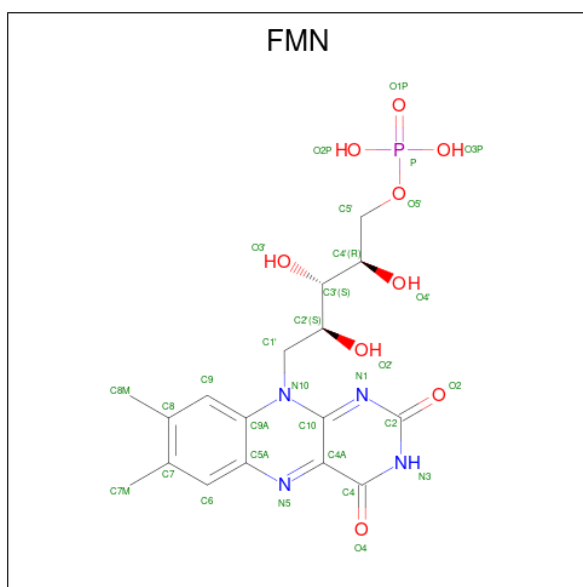
- Molecule 1 is a protein called Fatty acid synthase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2031	Total	C	N	O	S	0	0
			15784	10146	2631	2955	52		
1	E	2031	Total	C	N	O	S	0	0
			15784	10146	2631	2955	52		
1	I	2031	Total	C	N	O	S	0	0
			15784	10146	2631	2955	52		
1	M	2031	Total	C	N	O	S	0	0
			15784	10146	2631	2955	52		
1	Q	2031	Total	C	N	O	S	0	0
			15784	10146	2631	2955	52		
1	W	2031	Total	C	N	O	S	0	0
			15784	10146	2631	2955	52		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1421	Total	C	N	O	S	0	0
			11066	7037	1866	2117	46		
2	F	1421	Total	C	N	O	S	0	0
			11066	7037	1866	2117	46		
2	G	1421	Total	C	N	O	S	0	0
			11066	7037	1866	2117	46		
2	N	1421	Total	C	N	O	S	0	0
			11066	7037	1866	2117	46		
2	R	1421	Total	C	N	O	S	0	0
			11066	7037	1866	2117	46		
2	X	1421	Total	C	N	O	S	0	0
			11066	7037	1866	2117	46		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	I	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	M	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	Q	1	Total	C	N	O	P	0
			31	17	4	9	1	
3	W	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	80	Total	O	0
			80	80	
4	B	250	Total	O	0
			250	250	
4	E	84	Total	O	0
			84	84	
4	F	256	Total	O	0
			256	256	
4	G	266	Total	O	0
			266	266	
4	I	74	Total	O	0
			74	74	

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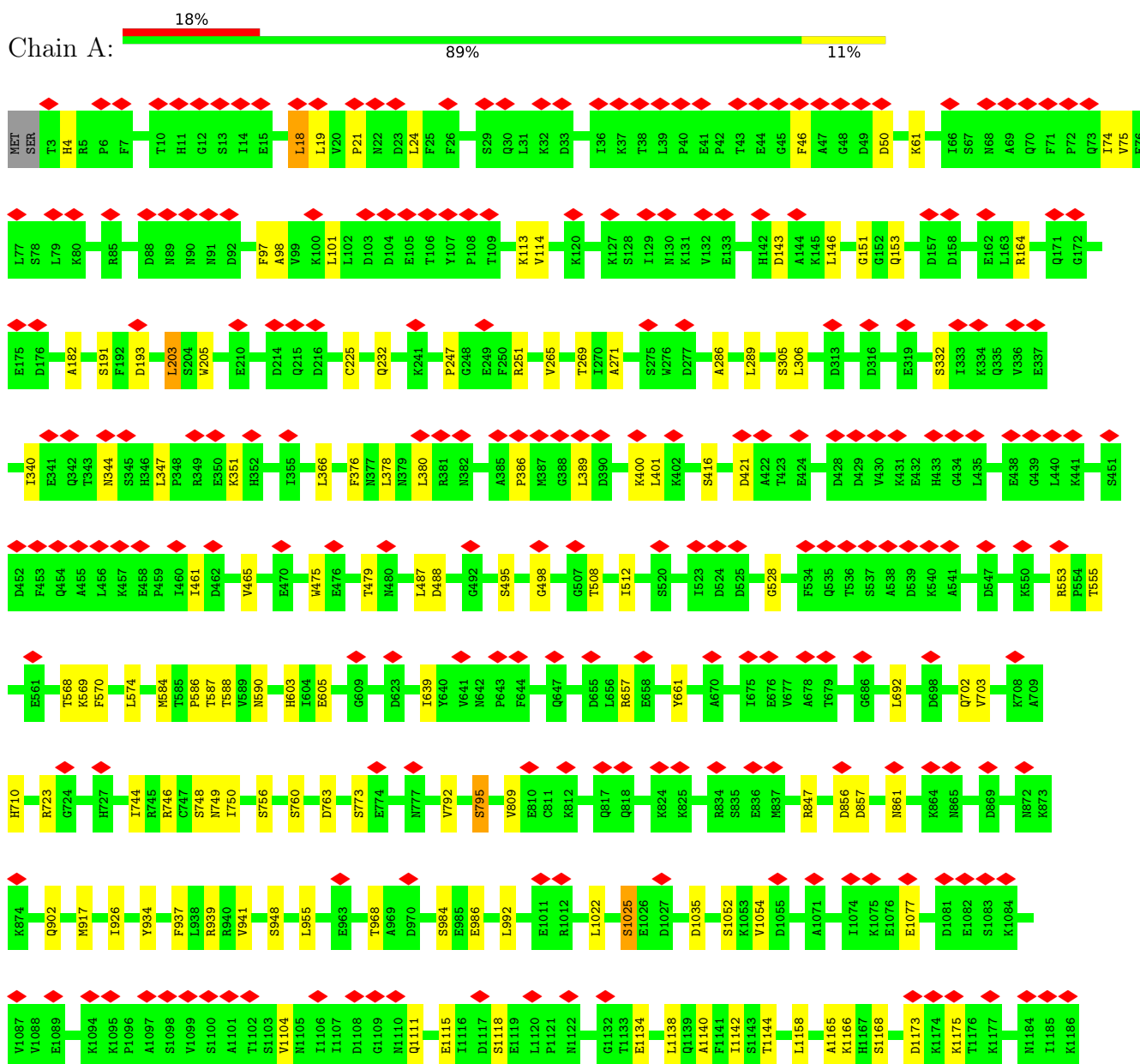
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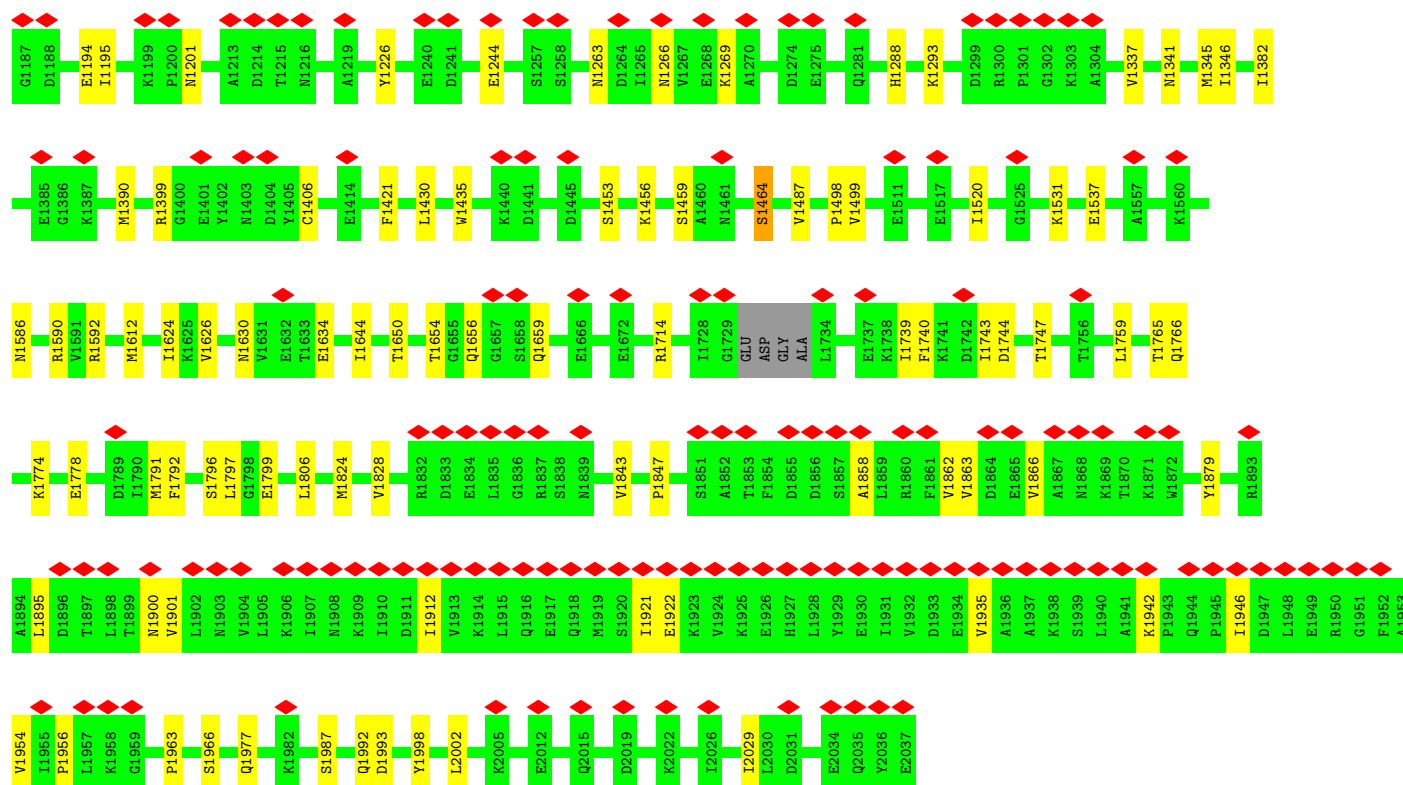
Mol	Chain	Residues	Atoms		AltConf
4	M	73	Total 73	O 73	0
4	N	263	Total 263	O 263	0
4	Q	84	Total 84	O 84	0
4	R	247	Total 247	O 247	0
4	W	86	Total 86	O 86	0
4	X	255	Total 255	O 255	0

3 Residue-property plots

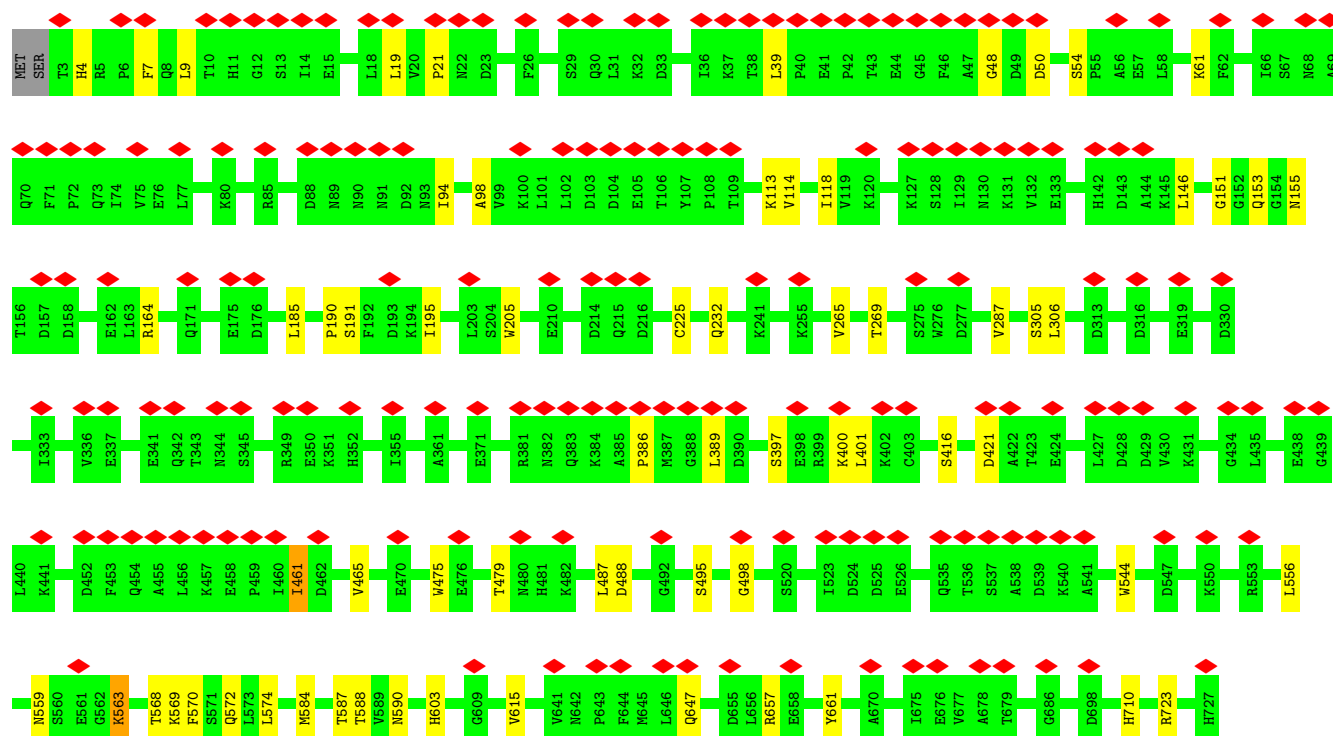
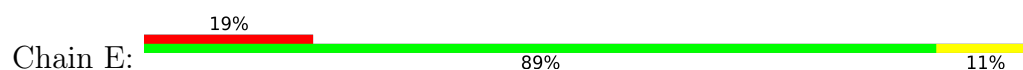
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

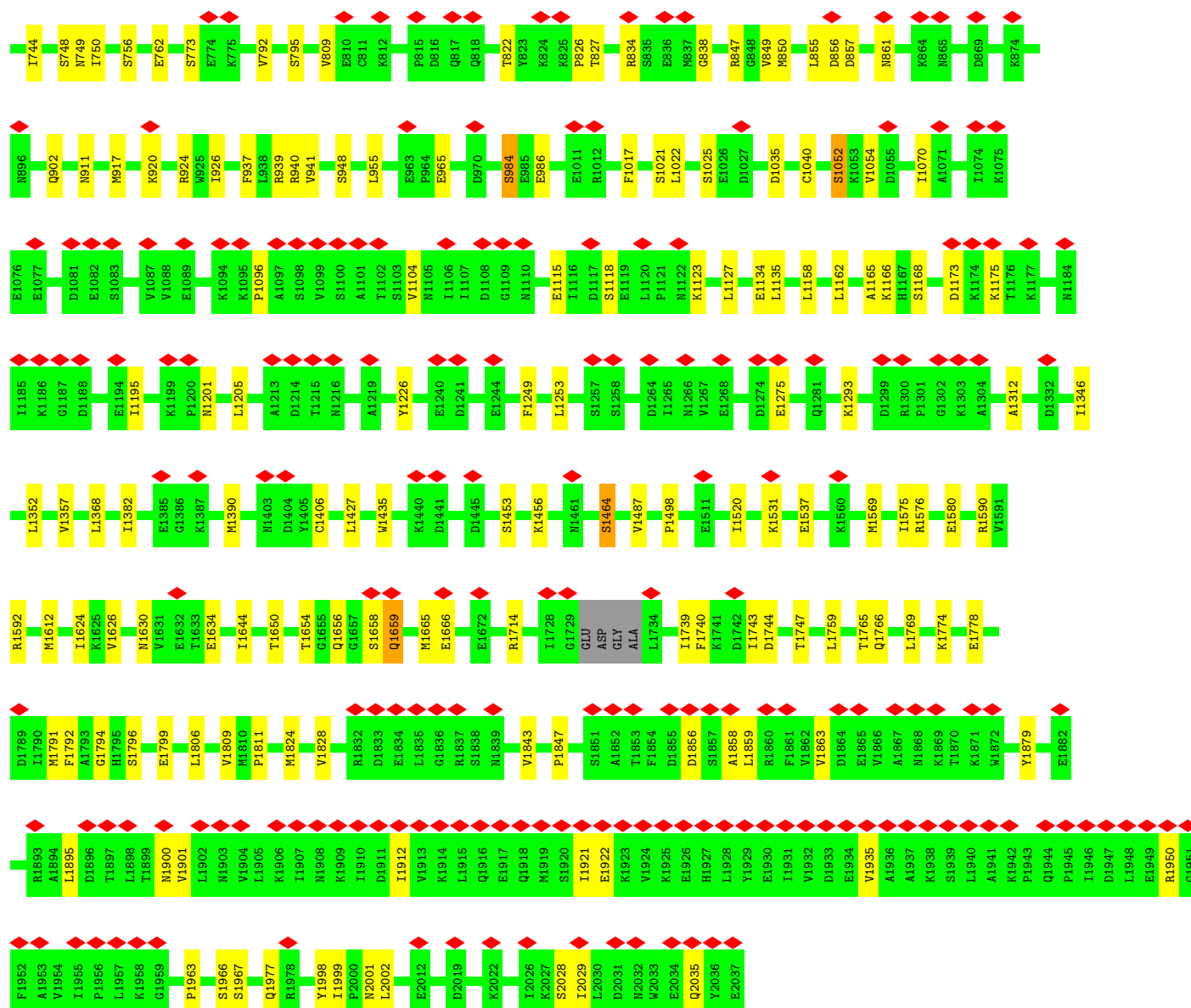
• Molecule 1: Fatty acid synthase subunit beta



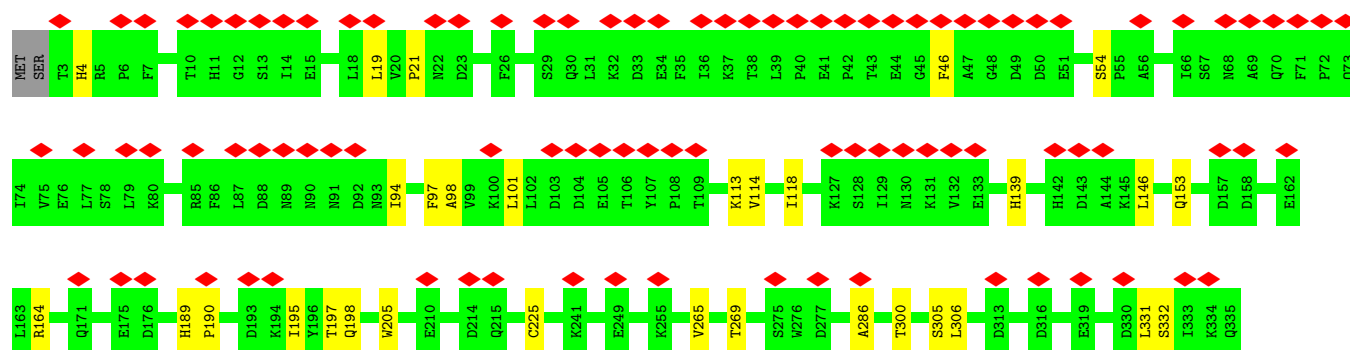
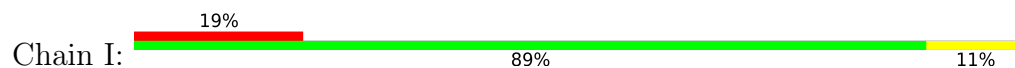


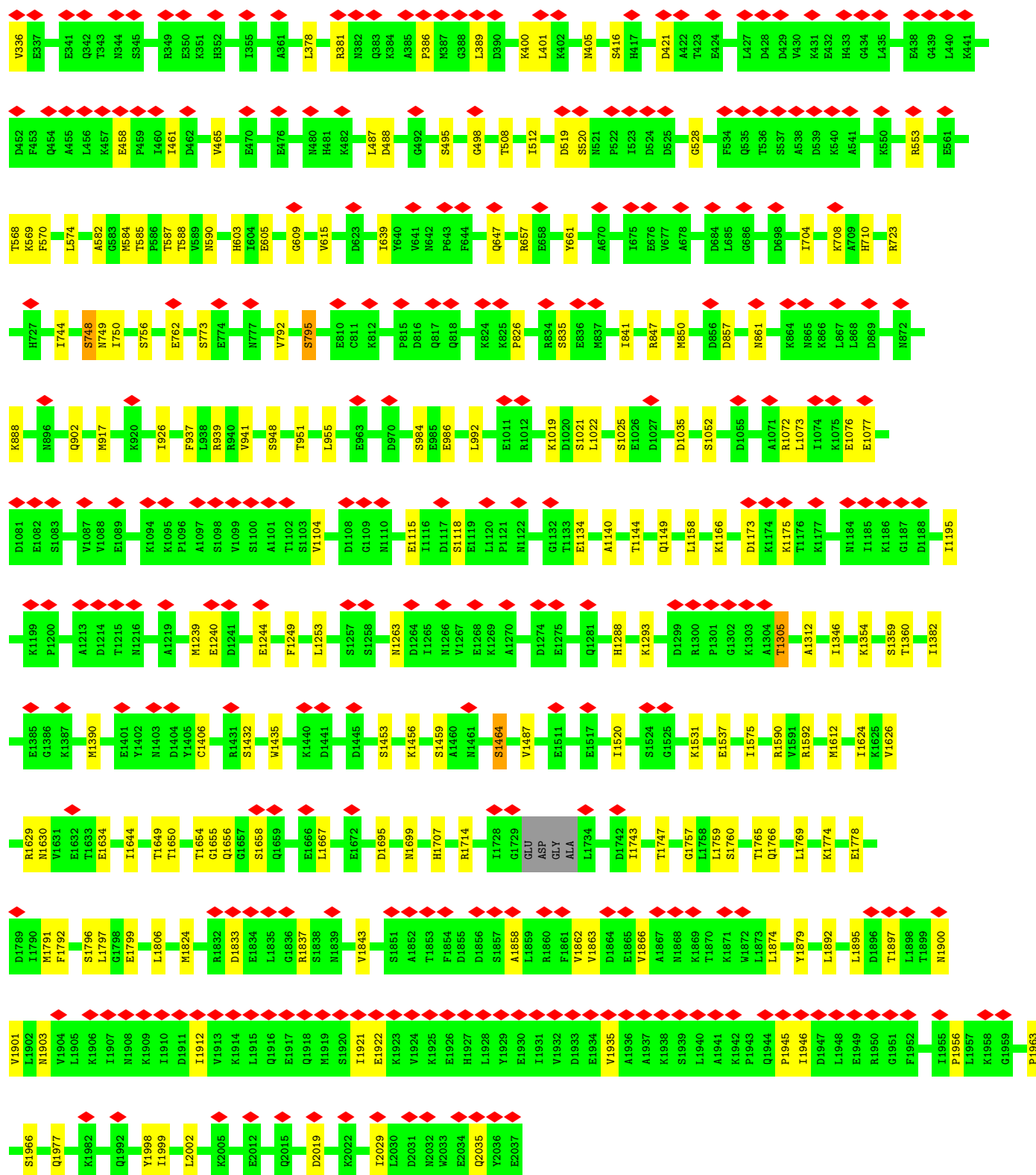
• Molecule 1: Fatty acid synthase subunit beta





• Molecule 1: Fatty acid synthase subunit beta

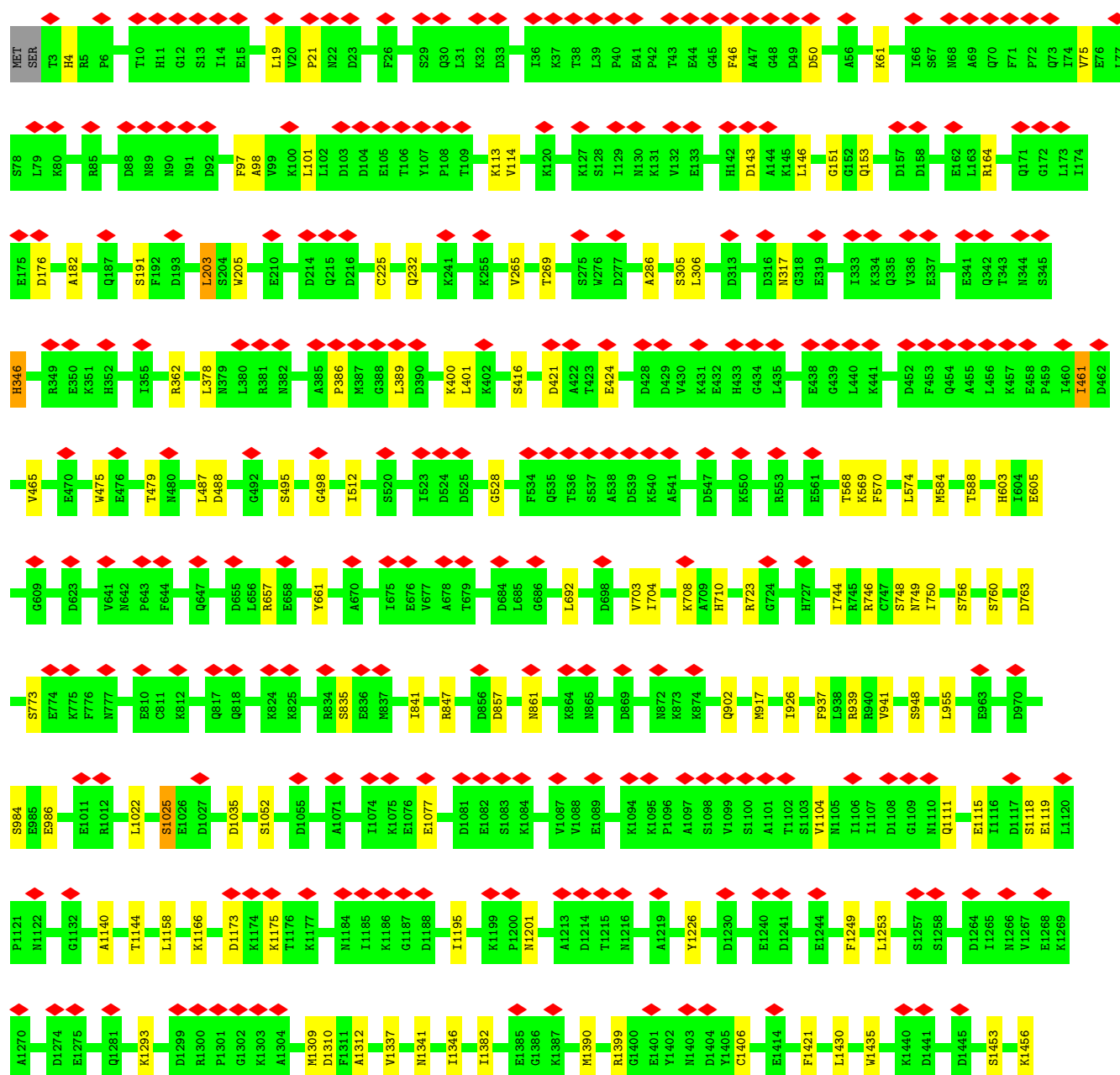
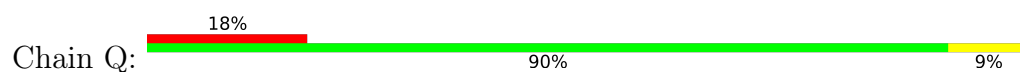


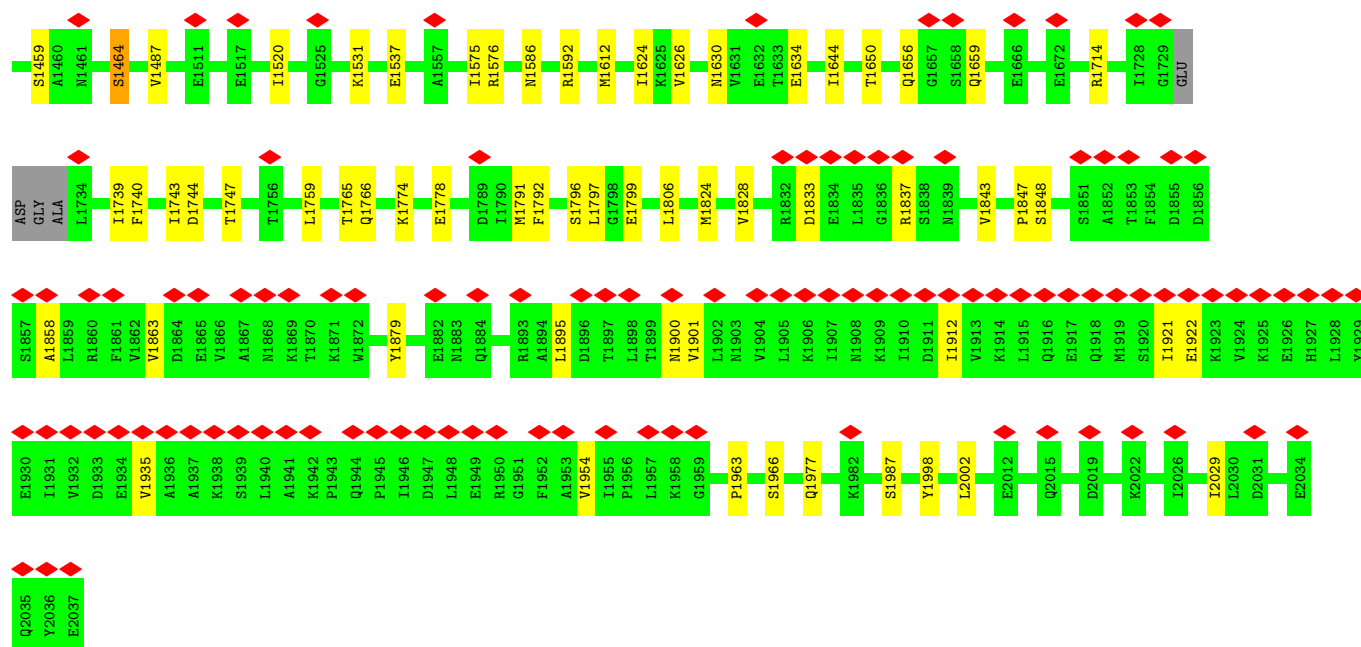


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R1629	N1630	V1631	E1632	T1633	E1634	I1644	T1649	T1650	Q1656	G1657	S1658	Q1659	E1666	E1672	H1707	R1714	I1728	G1729	GLU	ASP	GLY	ALA	L1734	D1742	I1743	D1744	T1747	G1757	L1758	L1759	S1760	T1765	Q1766	K1774	E1778	D1789	I1790	M1791	F1792	G1793	H1794	H1795	S1796	L1797	D1798	T1799	F1792	N1900	V1901	L1902	N1903	V1904	L1905	K1906	I1907	N1908	K1909																																				
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K874	D885	K888	N896	Q902	M917	K920	I926	F937	L938	R939	R940	V941	S948	L955	E963	D970	S984	E985	E986	L992	E1011	R1012	K1019	D1020	S1021	L1022	S1025	E1026	D1027	D1035	S1052	K1053	V1054	D1055	A1071	R1072	L1073	I1074	K1075	K874	D885	K888	N896	Q902	M917	K920	I926	F937	L938	R939	R940	V941	S948	L955	E963	D970	S984	E985	E986	L992	E1011	R1012	K1019	D1020	S1021	L1022	S1025	E1026	D1027	D1035	S1052	K1053	V1054	D1055	A1071	R1072	L1073	I1074	K1075														
R723	H727	I744	S748	N749	I750	S756	E762	S773	E774	N777	V809	E810	C811	K812	P815	D816	Q817	Q818	Y823	K824	K825	P826	R834	S835	E836	M837	T841	R847	M850	D856	D857	N861	K864	N865	K866	L867	L868	D869	N872	K873	R723	H727	I744	S748	N749	I750	S756	E762	S773	E774	N777	V809	E810	C811	K812	P815	D816	Q817	Q818	Y823	K824	K825	P826	R834	S835	E836	M837	T841	R847	M850	D856	D857	N861	K864	N865	K866	L867	L868	D869	N872	K873												
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V336	E337	E341	Q342	T343	N344	S345	R349	E350	K351	H352	I355	A361	L378	R381	N382	Q383	K384	A385	P386	M387	G388	L389	D390	P395	K400	L401	K402	N405	S416	H417	D421	A422	T423	E424	L427	D428	D429	V430	K431	L432	S433	I434	E438	G439	L440	V336	E337	E341	Q342	T343	N344	S345	R349	E350	K351	H352	I355	A361	L378	R381	N382	Q383	K384	A385	P386	M387	G388	L389	D390	P395	K400	L401	K402	N405	S416	H417	D421	A422	T423	E424	L427	D428	D429	V430	K431	L432	S433	I434	E438	G439	L440		
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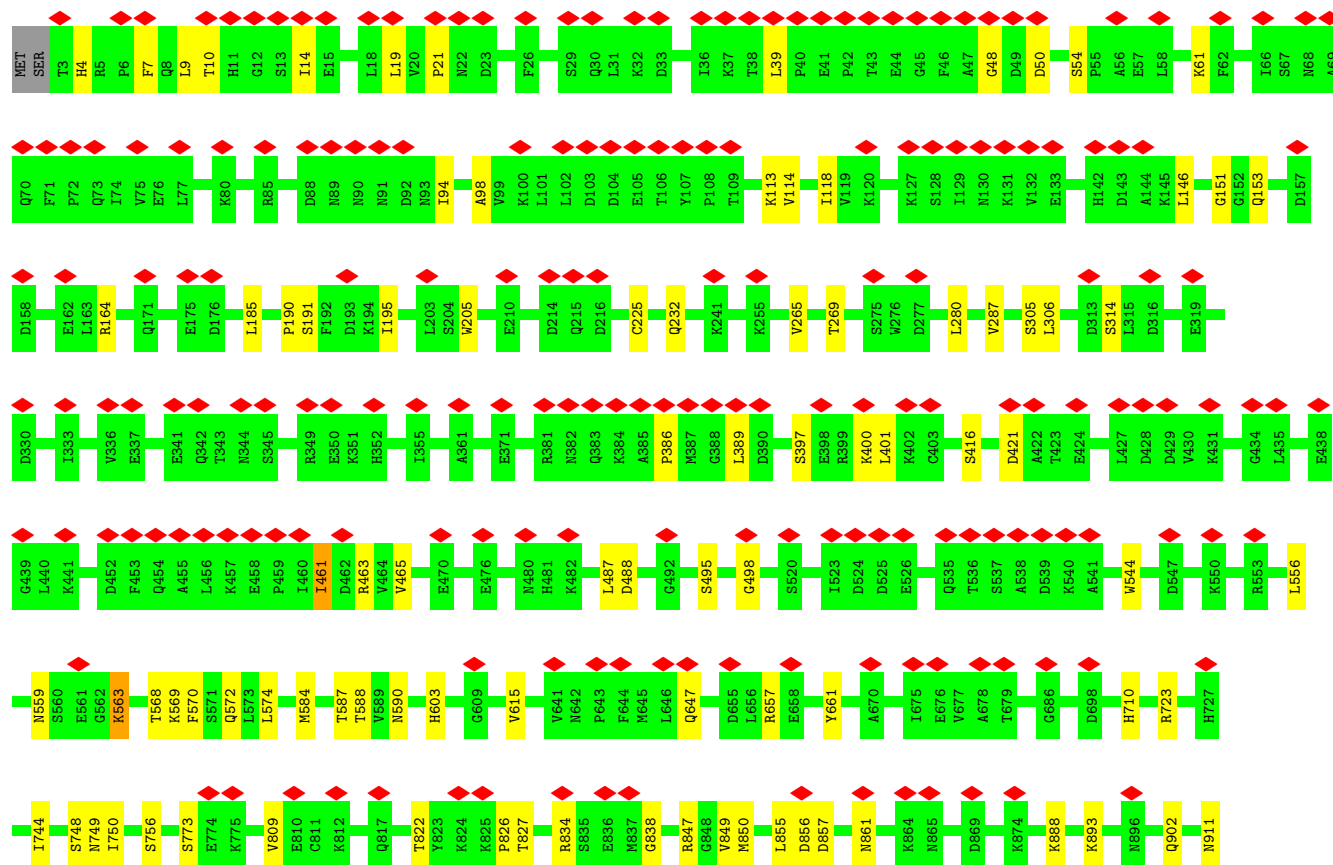
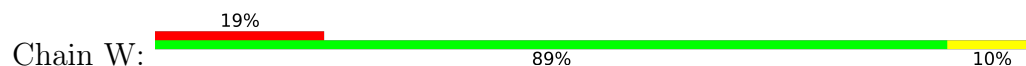


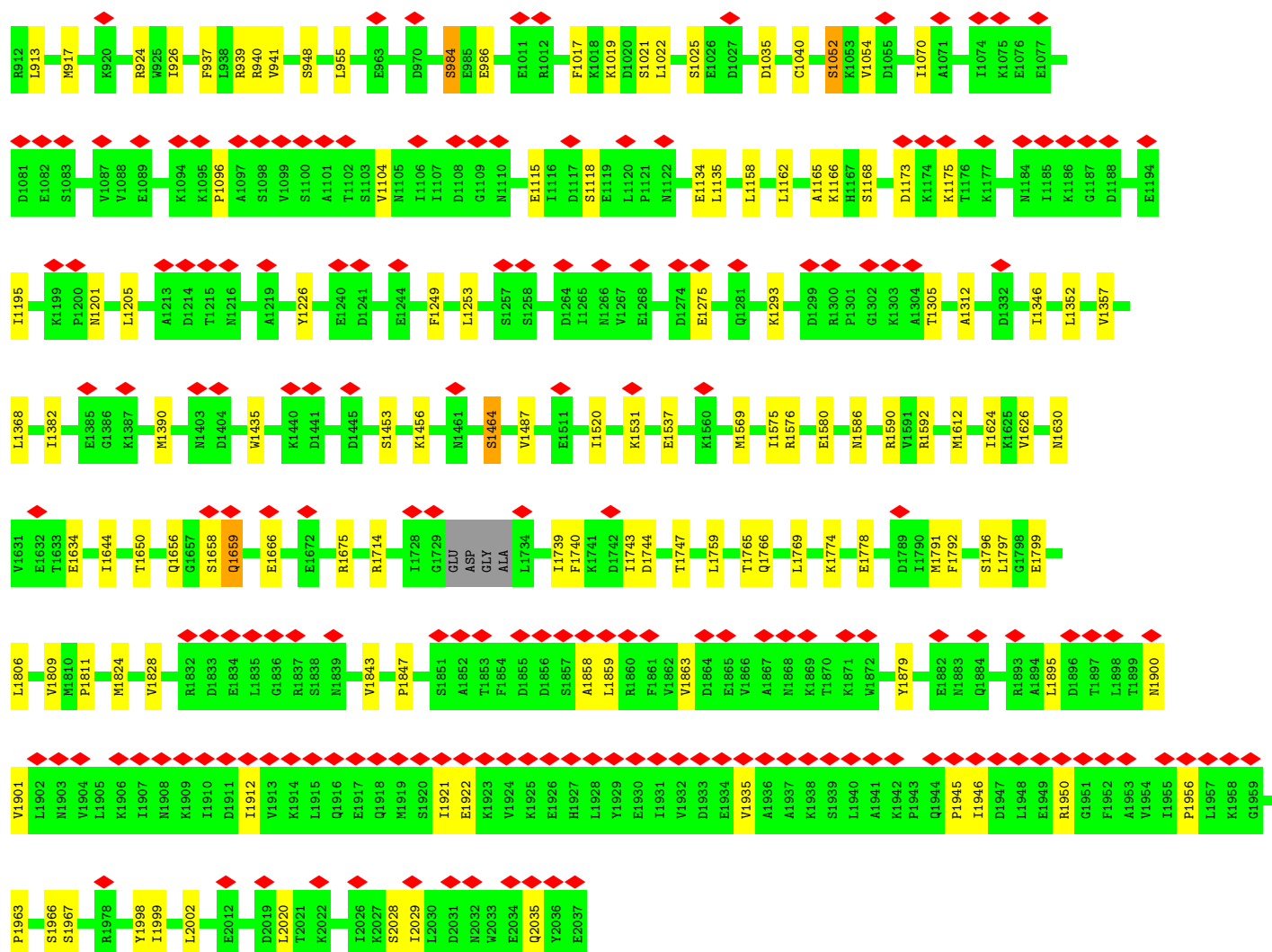
• Molecule 1: Fatty acid synthase subunit beta





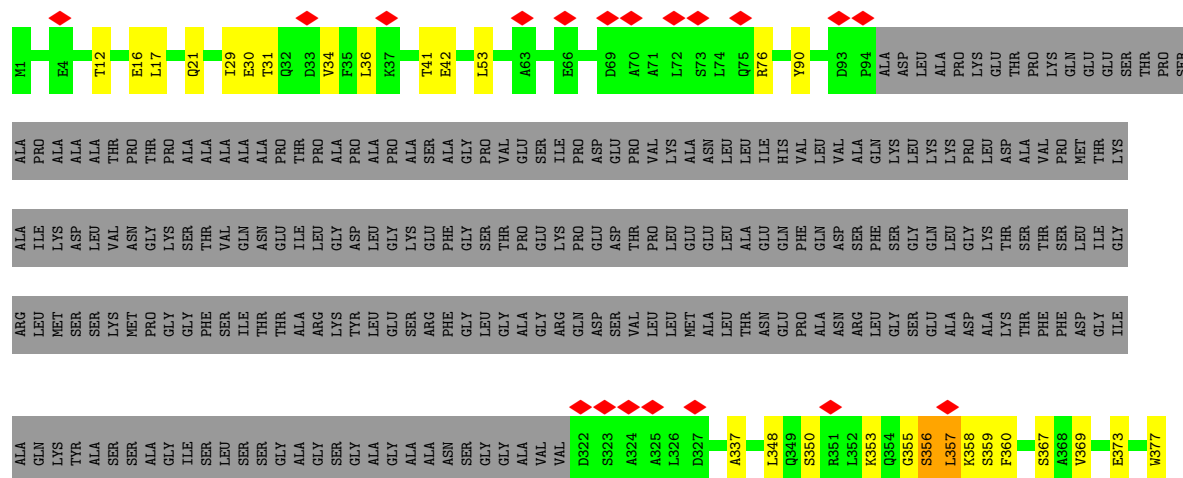
• Molecule 1: Fatty acid synthase subunit beta

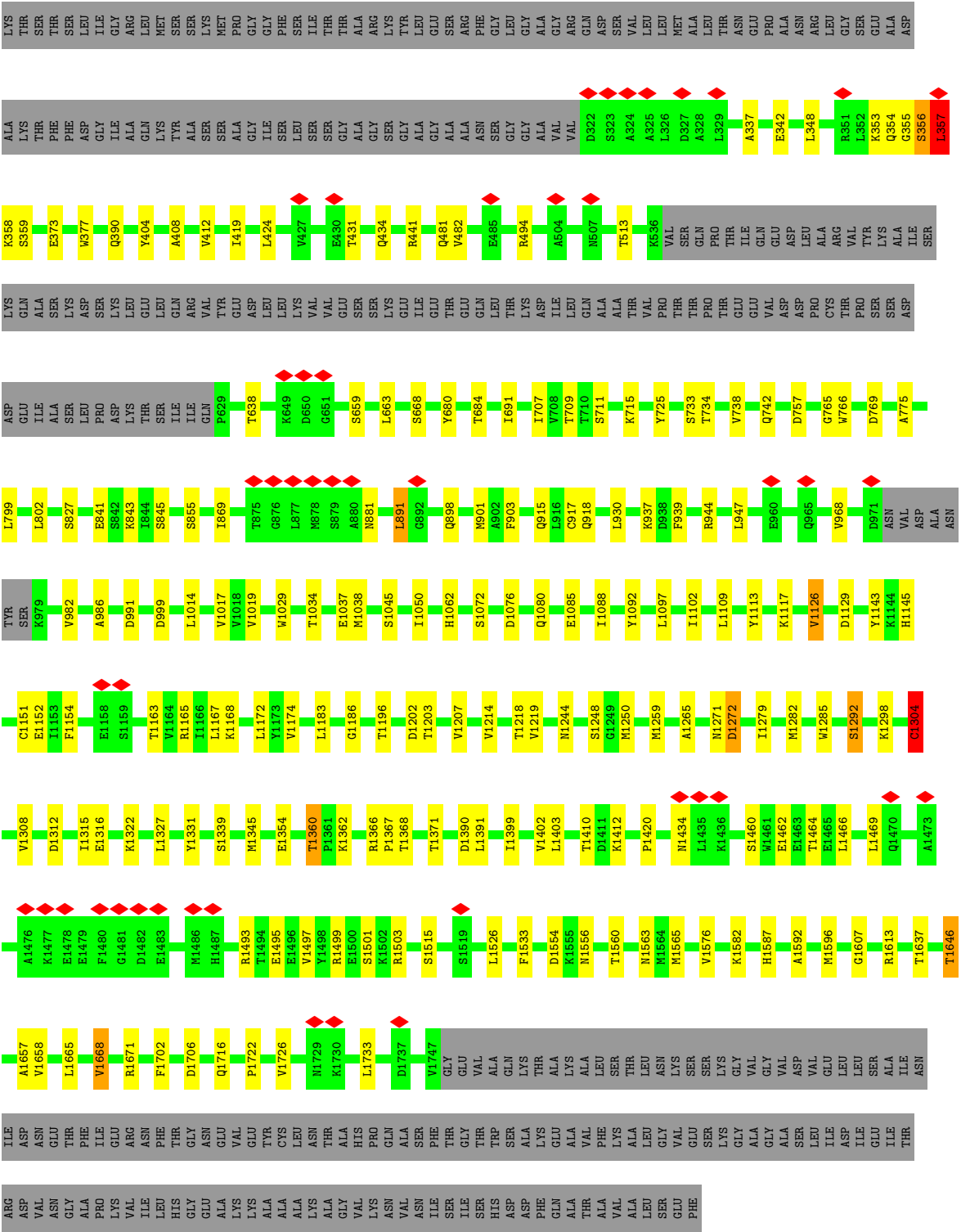




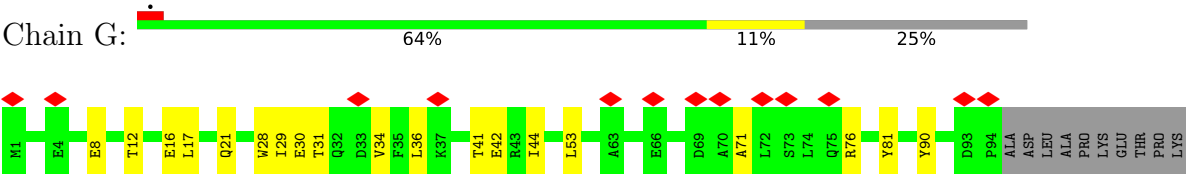
● Molecule 2: Fatty acid synthase subunit alpha

Chain B: 64% 11% 25%





● Molecule 2: Fatty acid synthase subunit alpha







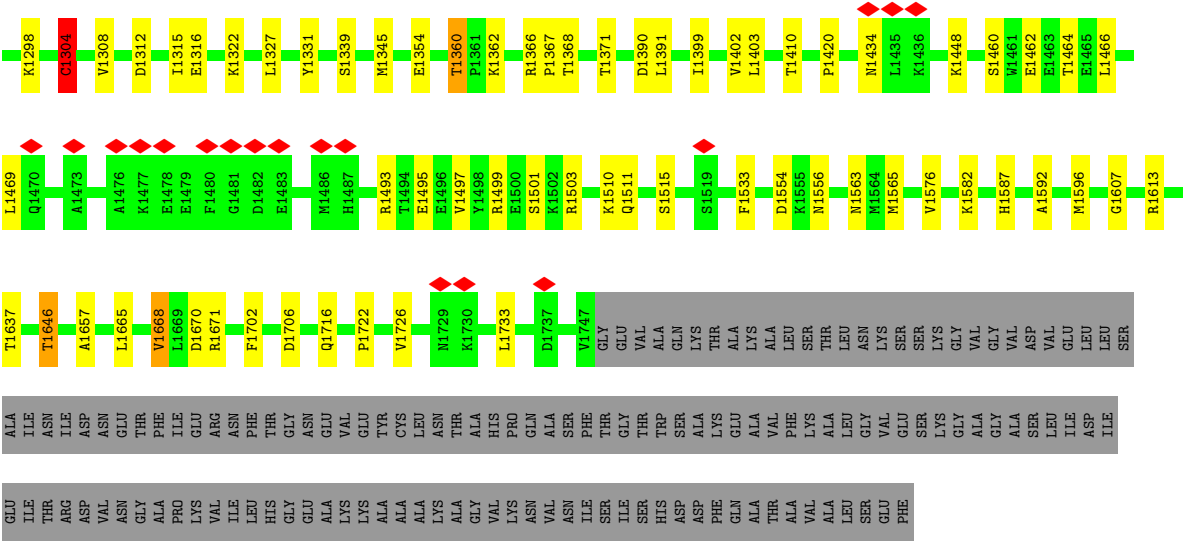
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GLU	ALA	LYS	ALA	ALA	ALA	ALA	LYS	ALA	GLY	ALA	VAL	LYS	ASN	VAL	ILE	SER	THR	ILE	SER	ASP	PHE	GLN	ALA	THR	VAL	ALA	ALA	LEU	GLY	SER	VAL	GLU	SER	LYS	ALA	GLY	ALA	SER	LEU	ILE	ASP	ALA	ALA	PRO	LYS	VAL	ILE	LEU	THR	HIS	ASP	VAL	ASN	GLY	ALA	ALA	PRO	LYS	VAL	ILE	LEU	THR	HIS	GLY

● Molecule 2: Fatty acid synthase subunit alpha

Chain R:  66% 9% 25%

L1475	A1476	K1477	E1478	E1479	F1480	G1481	D1482	E1483	M1486	H1487	K1491	E1492	T1493	T1494	E1495	E1496	Y1497	R1499	E1500	S1501	A1502	R1503	S1506	S1515	S1519	F1533	T1536	V1551	D1554	K1555	N1556	T1560	N1563	M1564	M1565	V1576	K1582	H1587	P1588	K1589	M1596	R1613																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
S1292	K1298	G1302	A1303	C1304	A1305	T1306	D1312	T1315	E1316	K1322	L1327	D1332	S1339	Y1497	Y1498	R1499	F1500	S1501	A1502	T1360	E1363	T1368	R1372	M1387	D1390	L1391	T1399	V1402	L1403	T1406	N1434	L1435	K1436	E1462	L1466	L1469	A1473	E1474																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
M1038	I1050	H1062	S1072	D1076	Q1080	E1085	I1088	Y1092	E1108	K1117	D1129	F1133	Y1143	K1144	H1145	C1151	E1152	I1153	F1154	E1157	E1158	S1159	T1163	L1167	K1168	V1174	R1195	E1201	T1218	S1248	A1265	I1279	W1285																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
S855	S860	W871	T875	G876	L877	M878	S879	A880	N881	G892	T910	V914	Q915	L916	C917	Q918	L930	K937	R944	L947	E960	Q965	D971	ASN	VAL	ASP	ALA	ASN	TYR	SER	K979	V982	A986	D999	D1013	N1016	V1017	V1018	V1019	T1021																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
ALA	SER	LEU	PRO	ASP	LYS	THR	ILE	ILE	GLN	P629	S636	K649	D650	G651	S659	L663	S668	Y680	L696	K705	V706	I707	A726	D747	D757	K760	G765	W766	D769	A776	W798	D816	S827	E841	S842	K843	I844	S845																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
SER	LYS	ASP	SER	LYS	LEU	GLU	GLN	ARG	VAL	TYR	GLU	LEU	LYS	VAL	GLU	SER	SER	THR	GLN	LEU	THR	LYS	ILE	THR	GLN	ALA	PRO	THR	GLU	GLU	VAL	ASP	ASP	PRO	CYS	THR	PRO	SER	SER	ASP	GLU	ILE																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
PHE	PHE	ASP	GLY	ILE	GLN	LYS	TYR	SER	SER	SER	C435	I436	M439	K440	R441	T445	E459	E485	D486	P487	V488	R494	K499	T500	A504	N507	S323	A324	A325	L326	D327	A337	L348	Q349	S350	R351	L352	K353	Q354	S355	S356	L357	K358	S359	V369	E373																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
THR	SER	LEU	THR	GLY	ARG	LEU	LYS	MET	ASN	PRO	GLY	GLY	PHE	SER	ILE	THR	ARG	LYS	TYR	LEU	GLY	GLY	PHE	GLY	LEU	ALA	GLN	ASN	VAL	LEU	MET	ALA	GLU	LEU	THR	ASN	GLU	PRO	ALA	ASN	ARG	LEU	GLY	SER	GLY	GLN	ALA	LYS	PRO	GLY	ASP	ALA	THR	SER																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
GLU	SER	THR	PRO	SER	ALA	PRO	THR	PRO	THR	THR	THR	THR	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	252339	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 ($e^-/\text{\AA}^2$)	51.2	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.754	Depositor
Minimum map value	-4.459	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.273	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	333.72, 333.72, 333.72	wwPDB
Map dimensions	324, 324, 324	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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

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	0.18	0/16153	0.39	1/21953 (0.0%)
1	E	0.21	1/16153 (0.0%)	0.42	3/21953 (0.0%)
1	I	0.20	2/16153 (0.0%)	0.42	4/21953 (0.0%)
1	M	0.20	2/16153 (0.0%)	0.42	4/21953 (0.0%)
1	Q	0.17	0/16153	0.38	0/21953
1	W	0.17	0/16153	0.39	1/21953 (0.0%)
2	B	0.20	0/11293	0.40	0/15287
2	F	0.20	0/11293	0.40	1/15287 (0.0%)
2	G	0.20	0/11293	0.40	1/15287 (0.0%)
2	N	0.20	0/11293	0.40	1/15287 (0.0%)
2	R	0.20	0/11293	0.41	1/15287 (0.0%)
2	X	0.20	0/11293	0.40	1/15287 (0.0%)
All	All	0.19	5/164676 (0.0%)	0.40	18/223440 (0.0%)

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	E	0	1
1	I	0	1
1	M	0	1
1	W	0	1
2	B	0	1
2	F	0	1
2	G	0	1
2	N	0	1
2	R	0	1
2	X	0	1
All	All	0	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	190	PRO	CG-CD	-12.46	1.08	1.50
1	M	190	PRO	CG-CD	-9.61	1.18	1.50
1	I	190	PRO	CG-CD	-9.55	1.18	1.50
1	M	190	PRO	CB-CG	-7.15	1.13	1.49
1	I	190	PRO	CB-CG	-7.06	1.14	1.49

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	190	PRO	N-CD-CG	-20.86	71.92	103.20
1	M	190	PRO	N-CD-CG	-17.69	76.66	103.20
1	I	190	PRO	N-CD-CG	-17.08	77.57	103.20
1	E	190	PRO	CA-CB-CG	-13.66	78.54	104.50
1	M	190	PRO	CA-CB-CG	-12.93	79.94	104.50

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	356	SER	Peptide
1	E	1950	ARG	Sidechain
2	F	356	SER	Peptide
2	G	356	SER	Peptide
1	I	381	ARG	Sidechain

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	15784	0	15632	144	0
1	E	15784	0	15632	155	0
1	I	15784	0	15632	159	0
1	M	15784	0	15632	153	0
1	Q	15784	0	15632	128	0
1	W	15784	0	15632	163	0
2	B	11066	0	10904	195	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	11066	0	10904	188	0
2	G	11066	0	10904	184	0
2	N	11066	0	10904	176	0
2	R	11066	0	10904	158	0
2	X	11066	0	10904	187	0
3	A	31	0	19	2	0
3	E	31	0	19	0	0
3	I	31	0	19	1	0
3	M	31	0	19	1	0
3	Q	31	0	19	0	0
3	W	31	0	19	0	0
4	A	80	0	0	24	0
4	B	250	0	0	83	0
4	E	84	0	0	48	0
4	F	256	0	0	67	0
4	G	266	0	0	65	0
4	I	74	0	0	51	0
4	M	73	0	0	46	0
4	N	263	0	0	63	0
4	Q	84	0	0	24	0
4	R	247	0	0	56	0
4	W	86	0	0	54	0
4	X	255	0	0	70	0
All	All	163304	0	159330	1813	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1813 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:G:424:LEU:HD12	4:G:2144:HOH:O	1.31	1.26
1:W:1666:GLU:HB2	4:W:2264:HOH:O	1.40	1.20
1:E:1666:GLU:HB2	4:E:2264:HOH:O	1.41	1.18
2:N:1626:GLU:HB3	4:N:2154:HOH:O	1.45	1.17
2:N:1735:PHE:HZ	4:N:2091:HOH:O	1.28	1.16

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	2027/2037 (100%)	1976 (98%)	51 (2%)	0	100	100
1	E	2027/2037 (100%)	1976 (98%)	51 (2%)	0	100	100
1	I	2027/2037 (100%)	1976 (98%)	51 (2%)	0	100	100
1	M	2027/2037 (100%)	1975 (97%)	52 (3%)	0	100	100
1	Q	2027/2037 (100%)	1975 (97%)	52 (3%)	0	100	100
1	W	2027/2037 (100%)	1975 (97%)	52 (3%)	0	100	100
2	B	1413/1885 (75%)	1378 (98%)	34 (2%)	1 (0%)	48	66
2	F	1413/1885 (75%)	1375 (97%)	37 (3%)	1 (0%)	48	66
2	G	1413/1885 (75%)	1373 (97%)	39 (3%)	1 (0%)	48	66
2	N	1413/1885 (75%)	1376 (97%)	36 (2%)	1 (0%)	48	66
2	R	1413/1885 (75%)	1377 (98%)	35 (2%)	1 (0%)	48	66
2	X	1413/1885 (75%)	1375 (97%)	37 (3%)	1 (0%)	48	66
All	All	20640/23532 (88%)	20107 (97%)	527 (3%)	6 (0%)	100	100

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1304	CYS
2	X	1304	CYS
2	R	1589	LYS
2	B	1589	LYS
2	G	1589	LYS

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	1713/1784 (96%)	1691 (99%)	22 (1%)	61	77
1	E	1713/1784 (96%)	1690 (99%)	23 (1%)	61	77
1	I	1713/1784 (96%)	1689 (99%)	24 (1%)	59	76
1	M	1713/1784 (96%)	1694 (99%)	19 (1%)	65	80
1	Q	1713/1784 (96%)	1694 (99%)	19 (1%)	65	80
1	W	1713/1784 (96%)	1691 (99%)	22 (1%)	61	77
2	B	1173/1580 (74%)	1157 (99%)	16 (1%)	59	76
2	F	1173/1580 (74%)	1152 (98%)	21 (2%)	51	72
2	G	1173/1580 (74%)	1163 (99%)	10 (1%)	70	82
2	N	1173/1580 (74%)	1160 (99%)	13 (1%)	65	80
2	R	1173/1580 (74%)	1158 (99%)	15 (1%)	61	77
2	X	1173/1580 (74%)	1147 (98%)	26 (2%)	45	67
All	All	17316/20184 (86%)	17086 (99%)	230 (1%)	59	77

5 of 230 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	2035	GLN
2	X	1292	SER
2	N	1183	LEU
2	X	1250	MET
1	W	1659	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 137 such sidechains are listed below:

Mol	Chain	Res	Type
2	R	1287	ASN
1	W	30	GLN
1	W	1883	ASN
2	F	1270	GLN
2	F	1119	GLN

5.3.3 RNA ⓘ

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](#)

6 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
3	FMN	M	2101	-	33,33,33	1.06	2 (6%)	48,50,50	1.37	7 (14%)
3	FMN	W	2101	-	33,33,33	1.06	2 (6%)	48,50,50	1.41	10 (20%)
3	FMN	A	2101	-	33,33,33	1.03	2 (6%)	48,50,50	1.37	7 (14%)
3	FMN	Q	2101	-	33,33,33	1.06	2 (6%)	48,50,50	1.39	7 (14%)
3	FMN	I	2101	-	33,33,33	1.05	2 (6%)	48,50,50	1.38	7 (14%)
3	FMN	E	2101	-	33,33,33	1.06	2 (6%)	48,50,50	1.37	8 (16%)

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
3	FMN	M	2101	-	-	6/18/18/18	0/3/3/3
3	FMN	W	2101	-	-	3/18/18/18	0/3/3/3
3	FMN	A	2101	-	-	2/18/18/18	0/3/3/3
3	FMN	Q	2101	-	-	7/18/18/18	0/3/3/3
3	FMN	I	2101	-	-	6/18/18/18	0/3/3/3
3	FMN	E	2101	-	-	6/18/18/18	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Q	2101	FMN	C4A-N5	3.39	1.38	1.30
3	E	2101	FMN	C4A-N5	3.37	1.38	1.30
3	M	2101	FMN	C4A-N5	3.34	1.38	1.30
3	I	2101	FMN	C4A-N5	3.32	1.37	1.30
3	W	2101	FMN	C4A-N5	3.28	1.37	1.30

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	2101	FMN	C4-N3-C2	-3.88	118.75	125.64
3	I	2101	FMN	C4-N3-C2	-3.84	118.82	125.64
3	M	2101	FMN	C4-N3-C2	-3.83	118.84	125.64
3	W	2101	FMN	C4-N3-C2	-3.72	119.04	125.64
3	A	2101	FMN	C4-N3-C2	-3.69	119.09	125.64

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2101	FMN	C5'-O5'-P-O1P
3	E	2101	FMN	C5'-O5'-P-O1P
3	E	2101	FMN	C5'-O5'-P-O2P
3	I	2101	FMN	C5'-O5'-P-O1P
3	I	2101	FMN	C5'-O5'-P-O2P

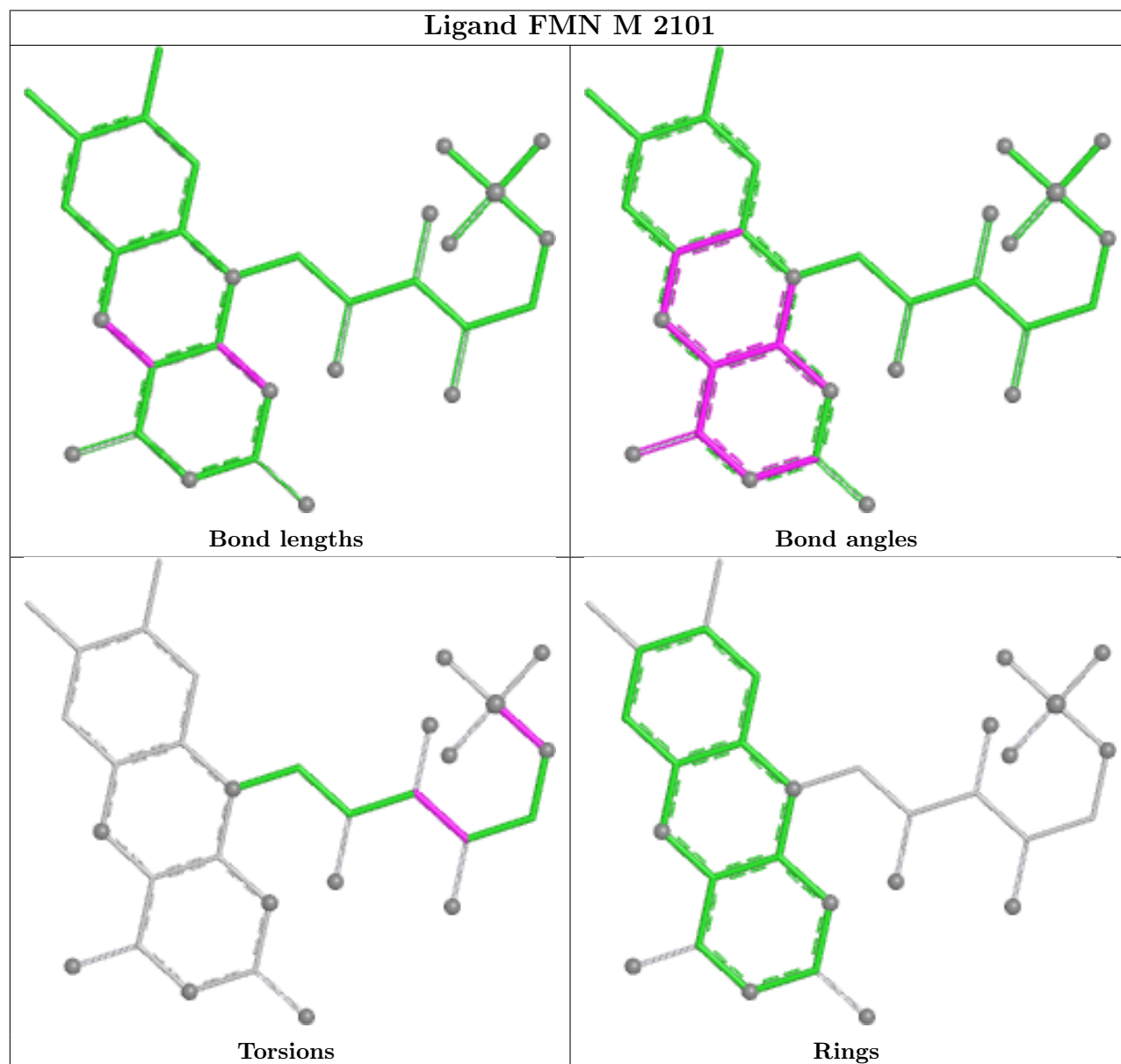
There are no ring outliers.

3 monomers are involved in 4 short contacts:

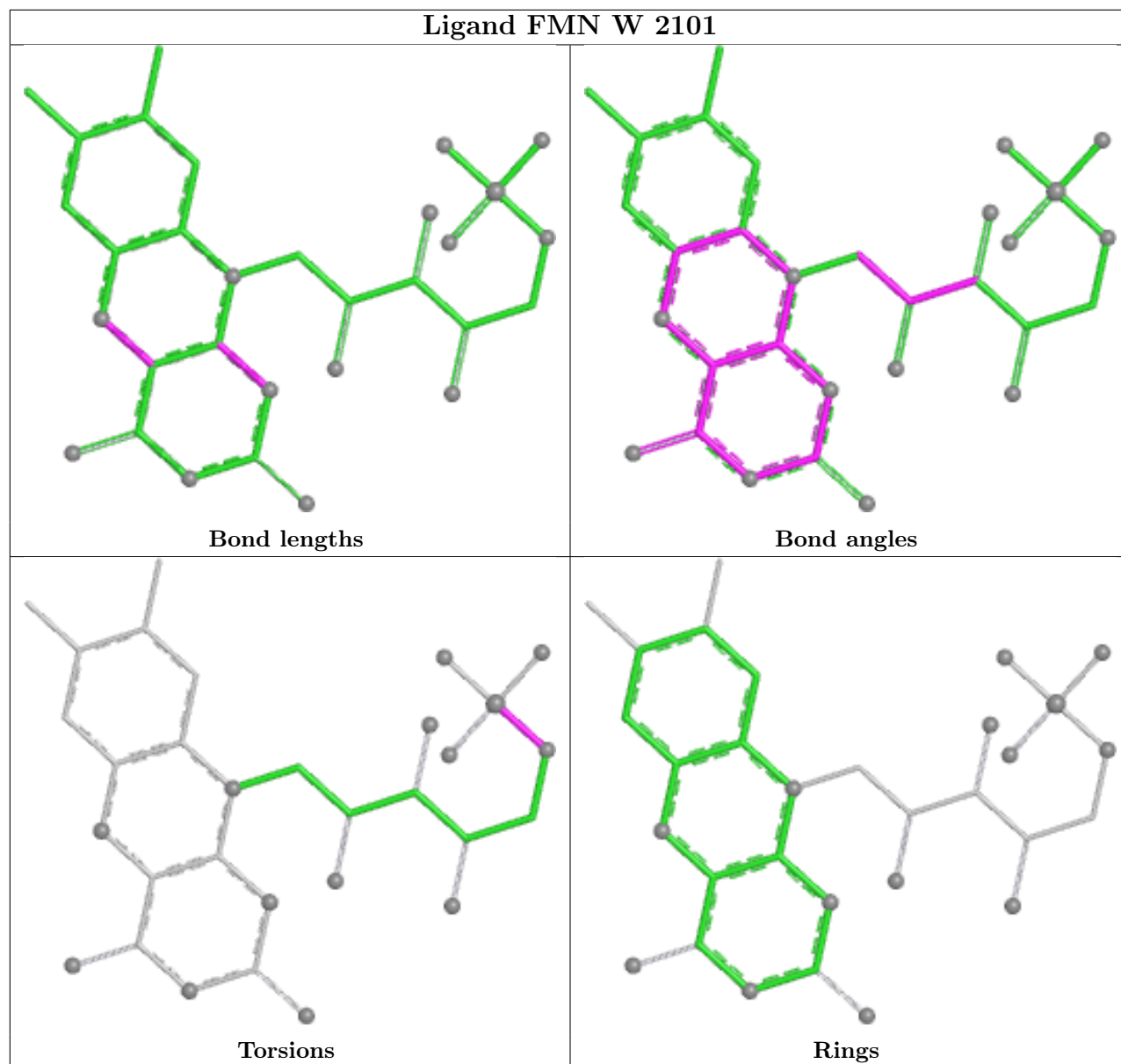
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	2101	FMN	1	0
3	A	2101	FMN	2	0
3	I	2101	FMN	1	0

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

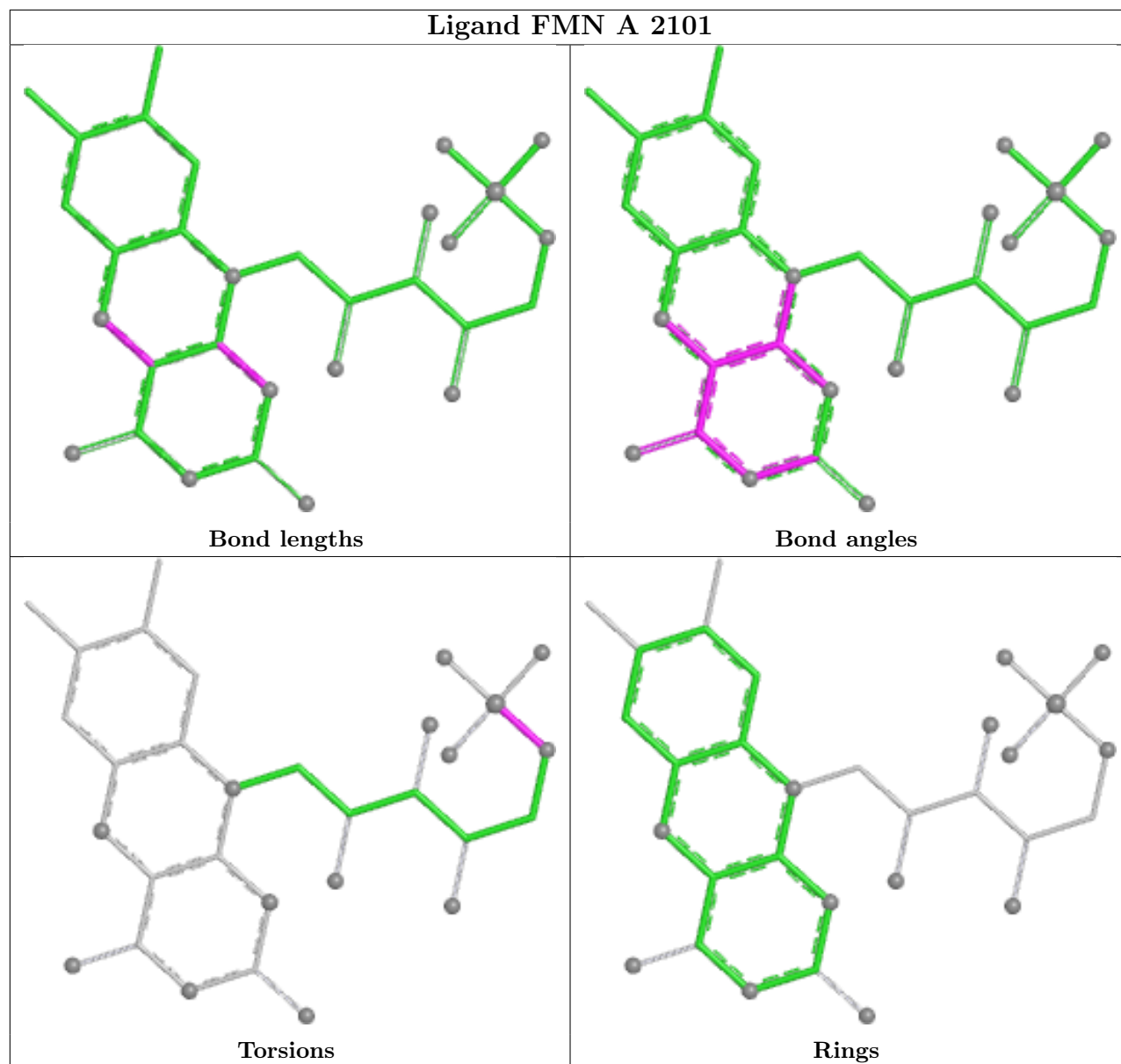
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

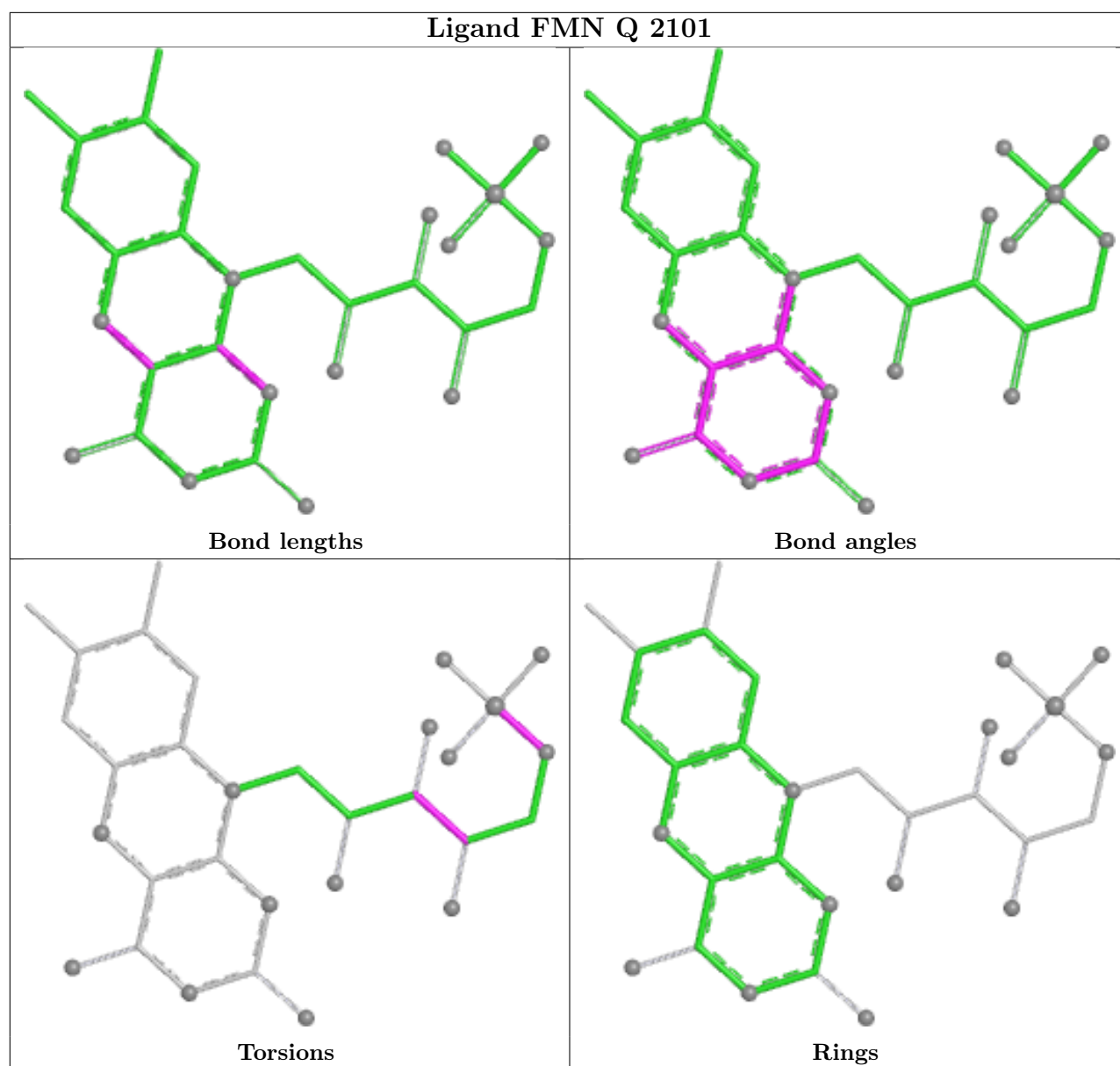


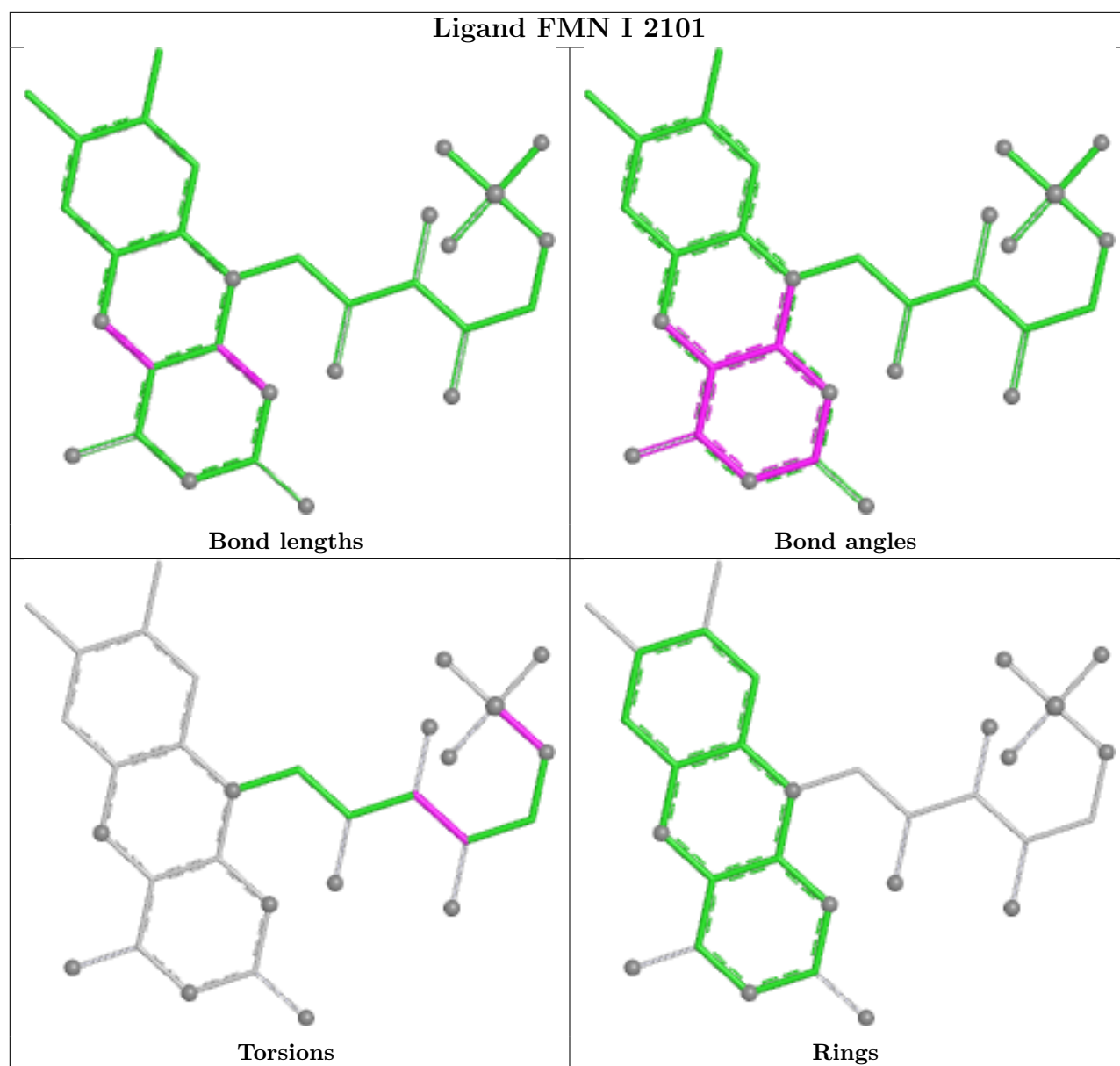
Ligand FMN W 2101

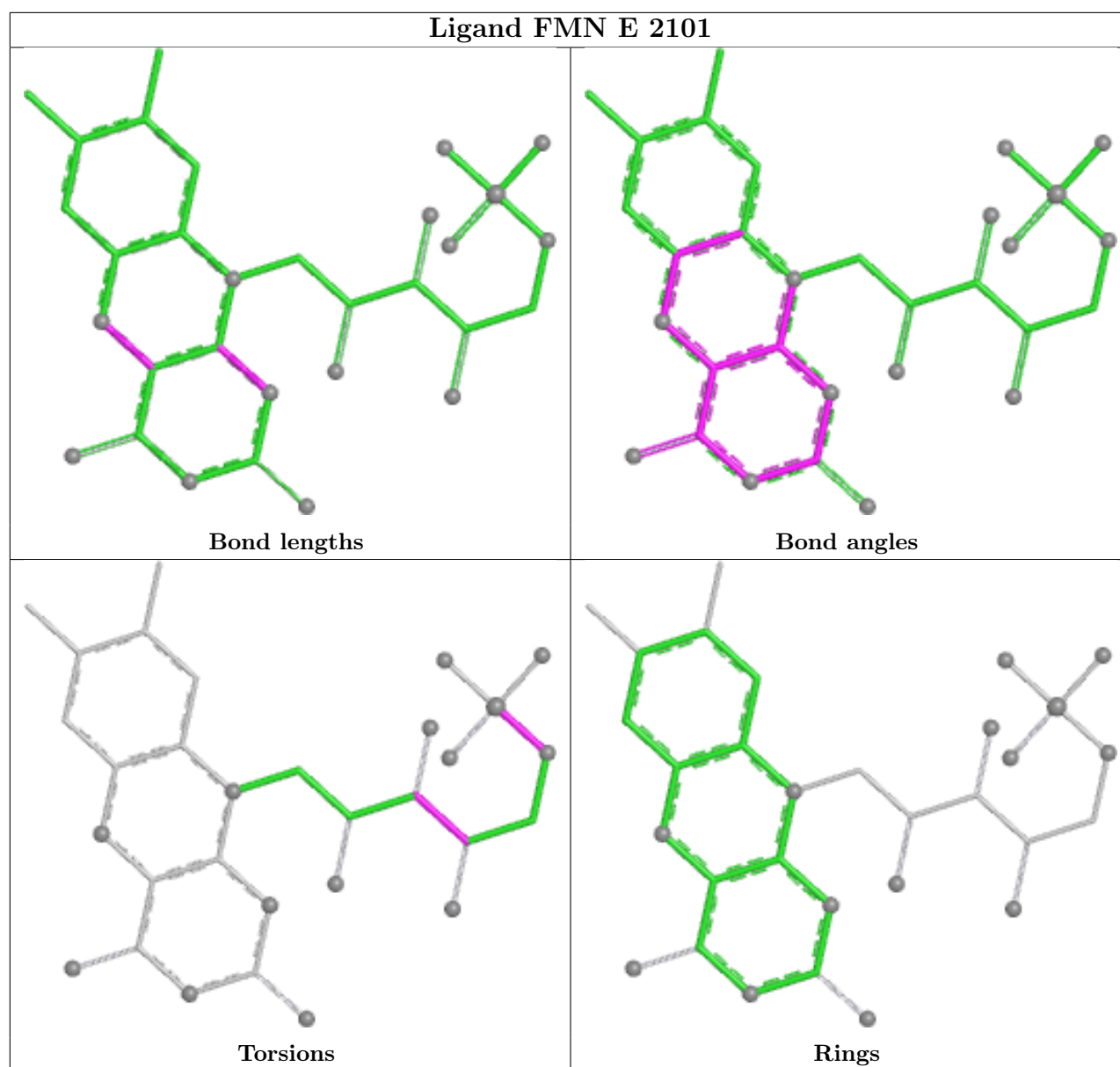


Ligand FMN A 2101









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.

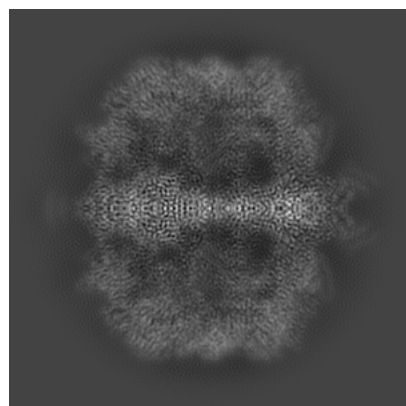
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-46553. These allow visual inspection of the internal detail of the map and identification of artifacts.

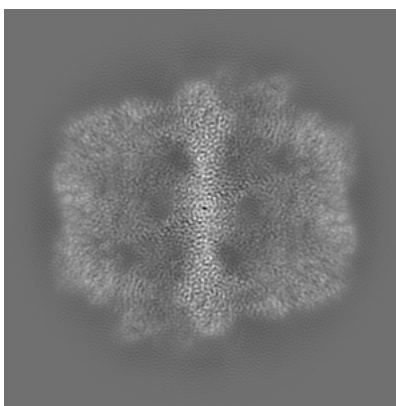
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

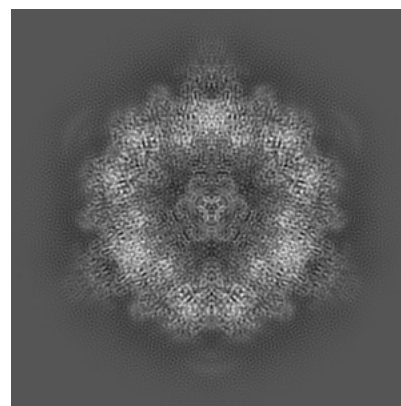
6.1.1 Primary map



X

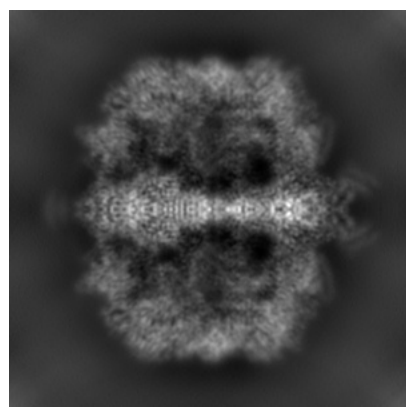


Y

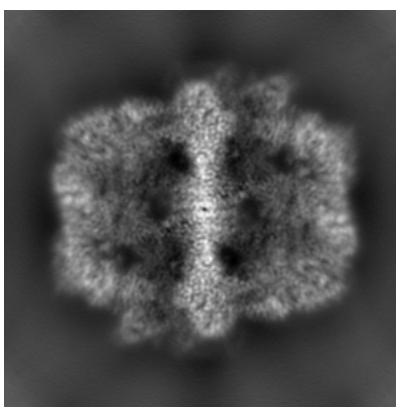


Z

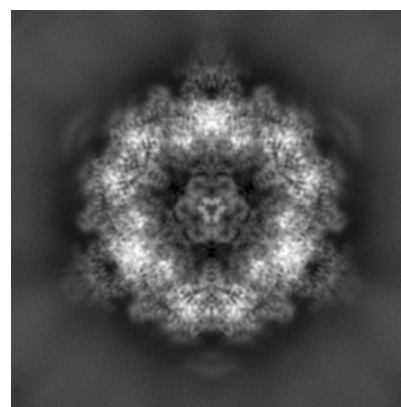
6.1.2 Raw map



X



Y

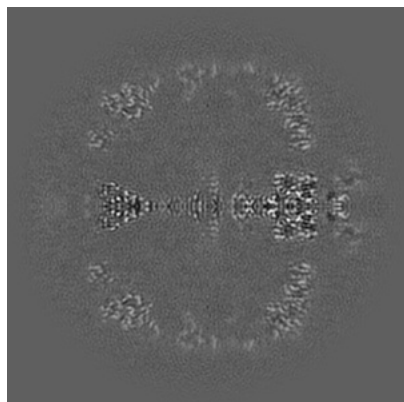


Z

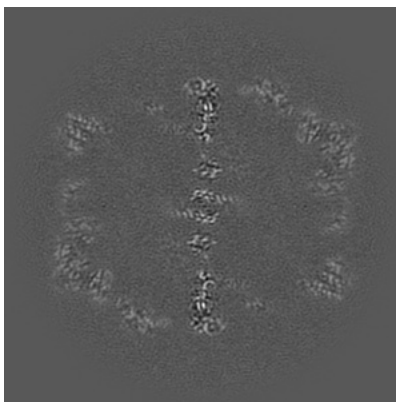
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

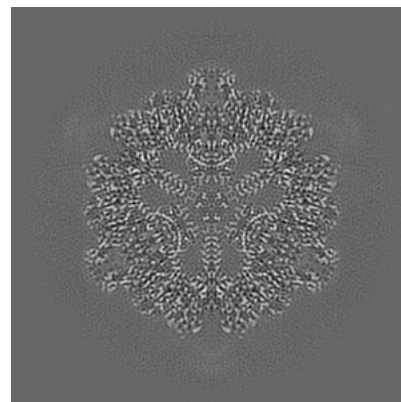
6.2.1 Primary map



X Index: 162

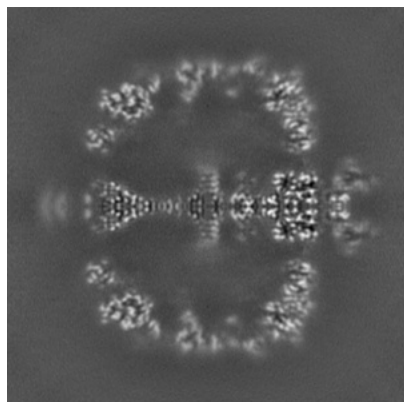


Y Index: 162

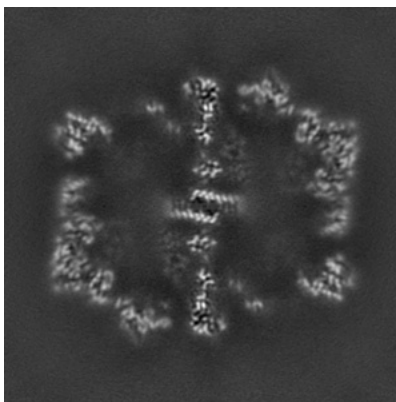


Z Index: 162

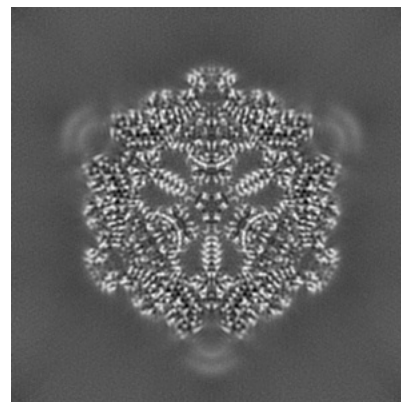
6.2.2 Raw map



X Index: 162



Y Index: 162

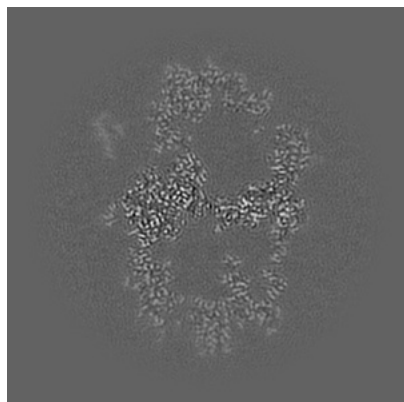


Z Index: 162

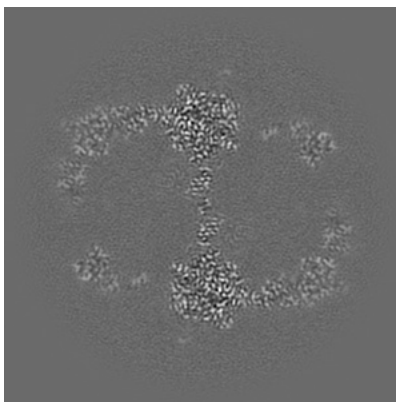
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

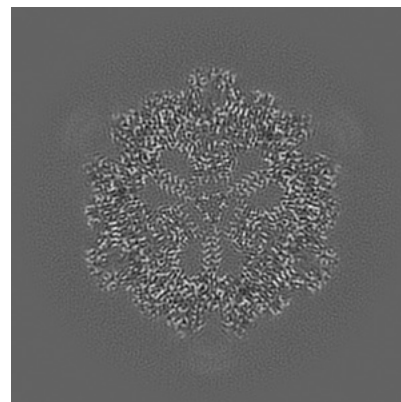
6.3.1 Primary map



X Index: 99

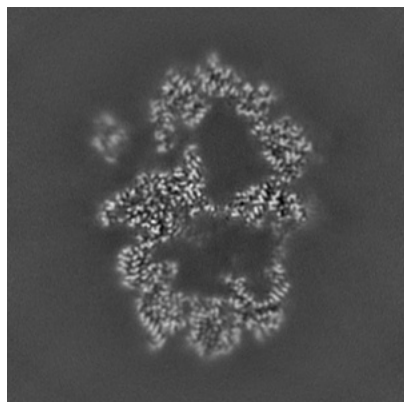


Y Index: 134

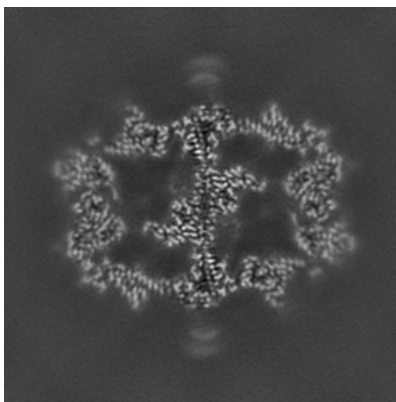


Z Index: 163

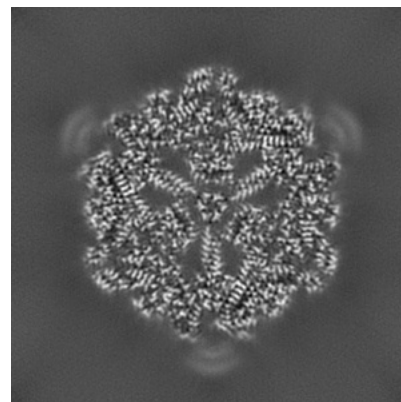
6.3.2 Raw map



X Index: 104



Y Index: 219

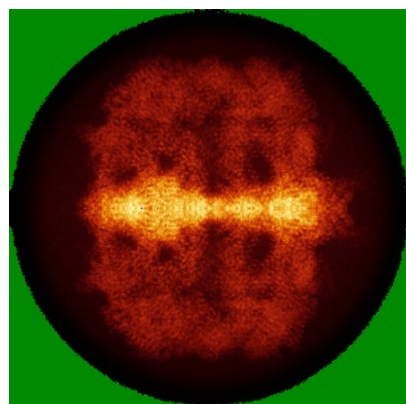


Z Index: 160

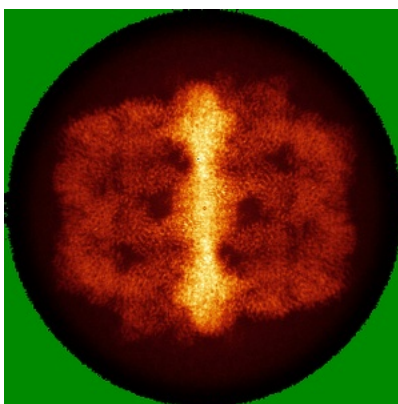
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

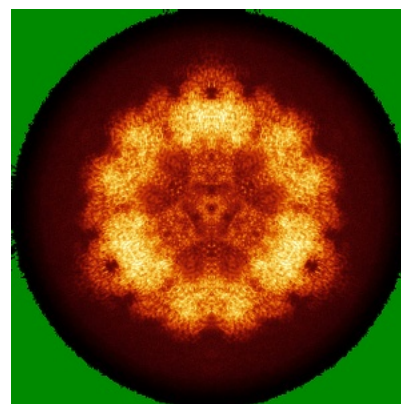
6.4.1 Primary map



X

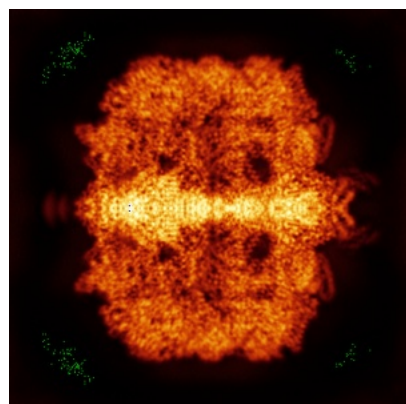


Y

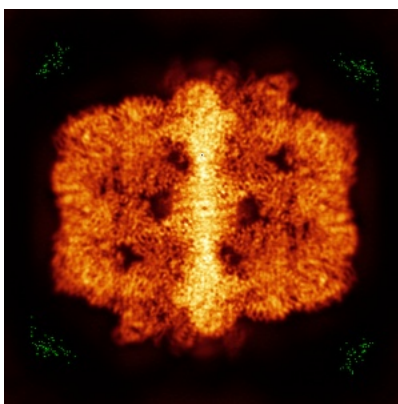


Z

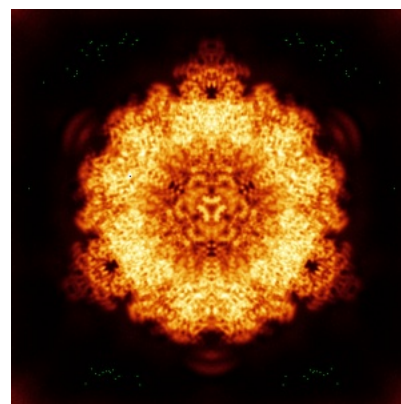
6.4.2 Raw map



X



Y

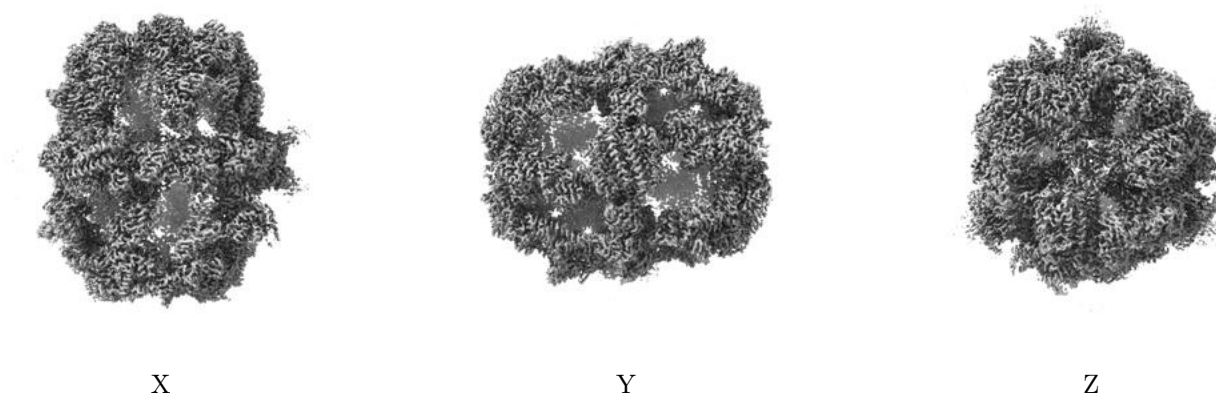


Z

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.

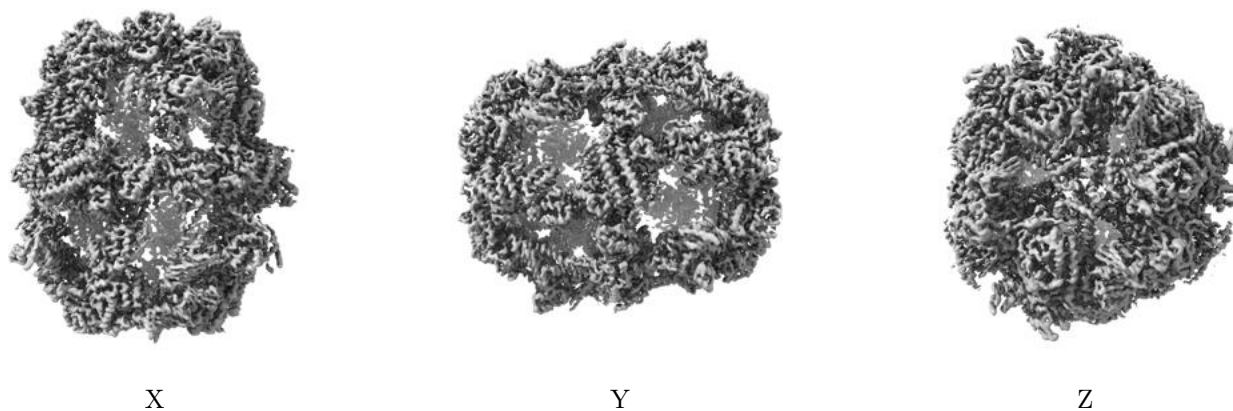
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.7. 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.

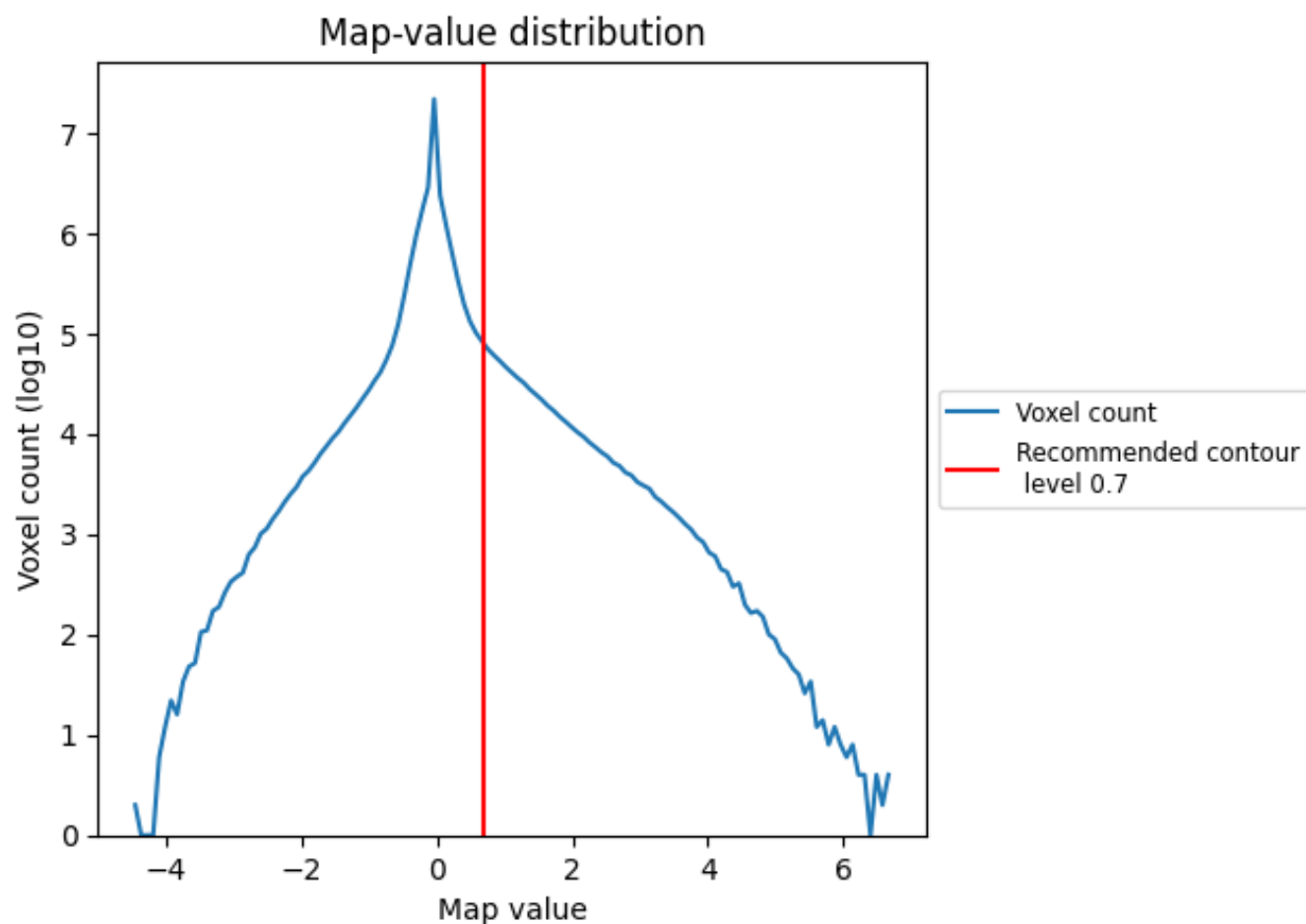
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

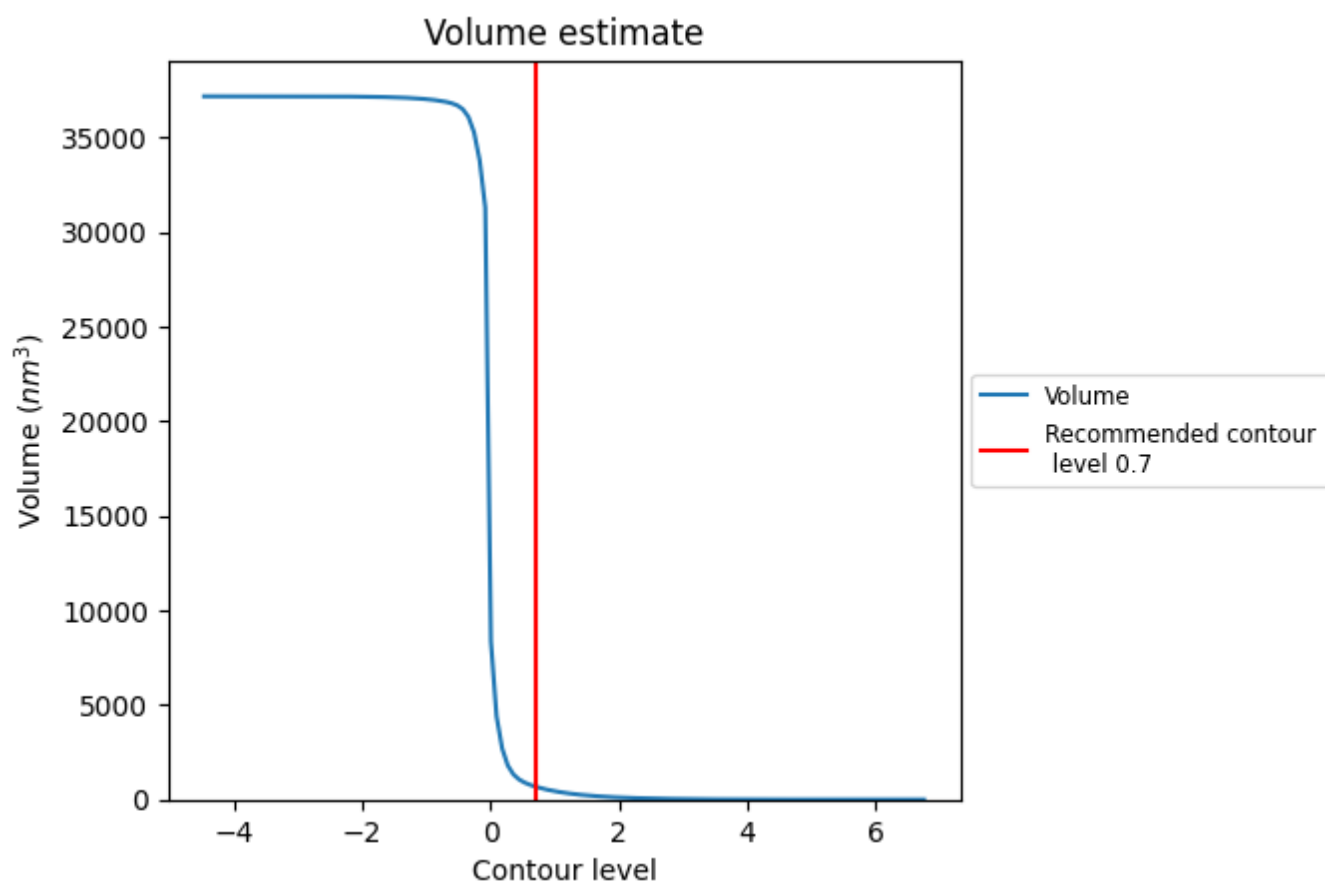
This section contains the results of statistical analysis of the map.

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.

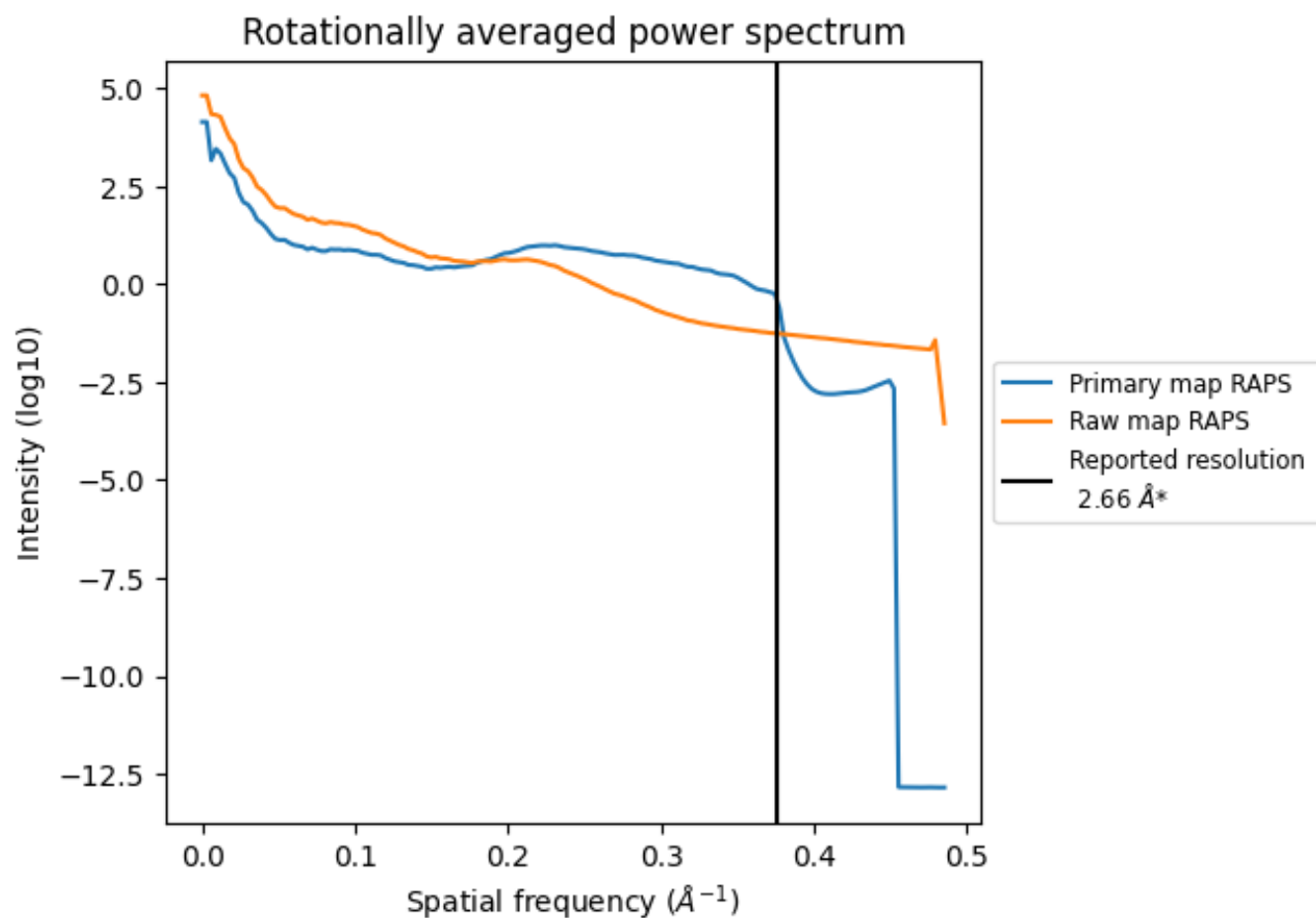
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 686 nm³; this corresponds to an approximate mass of 620 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 ⓘ

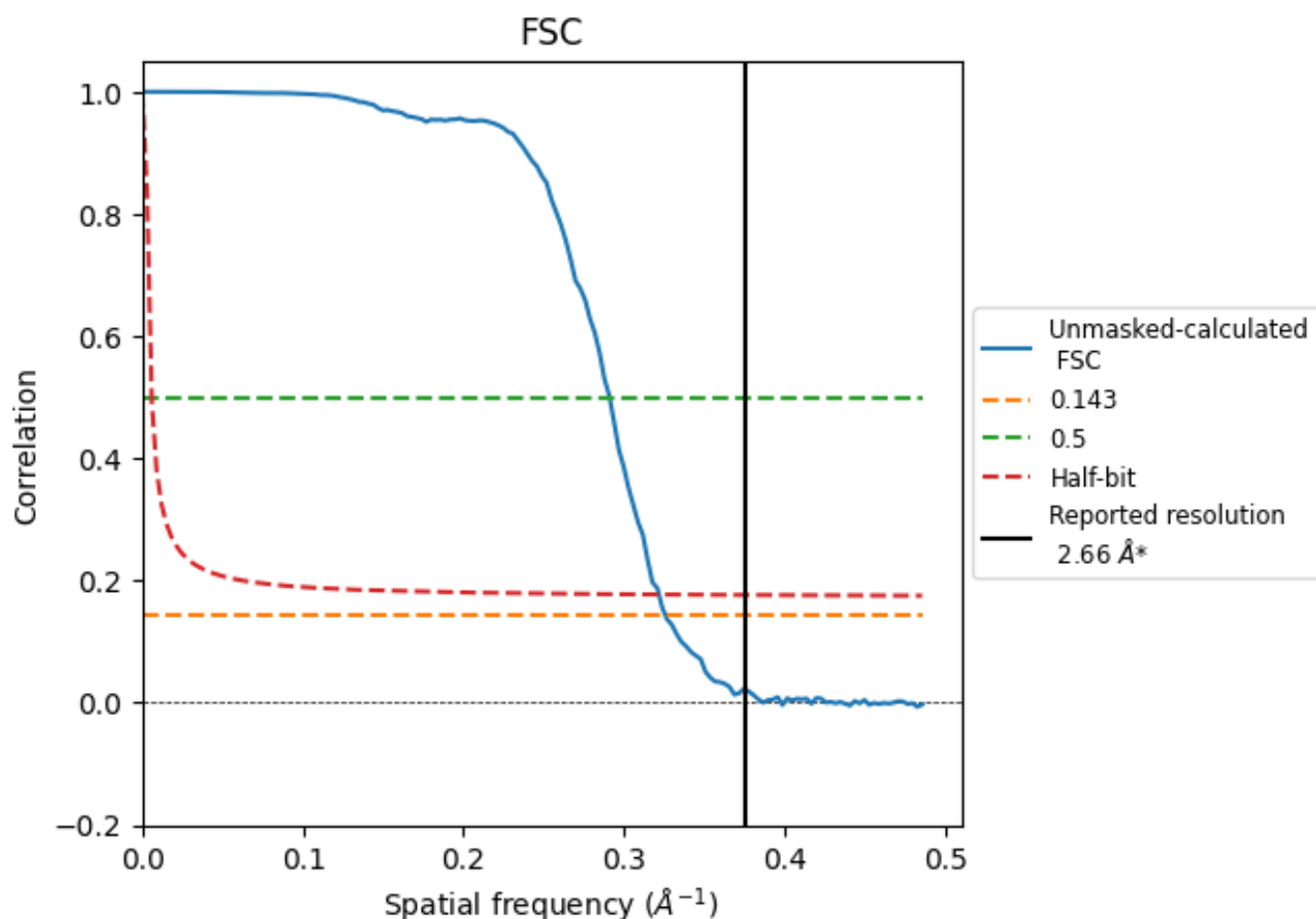


*Reported resolution corresponds to spatial frequency of 0.376 \AA^{-1}

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 0.376 Å⁻¹

8.2 Resolution estimates [i](#)

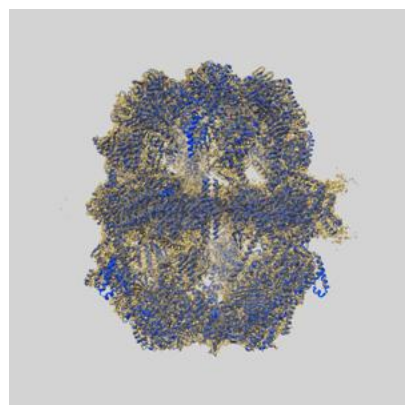
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.07	3.44	3.11

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.07 differs from the reported value 2.66 by more than 10 %

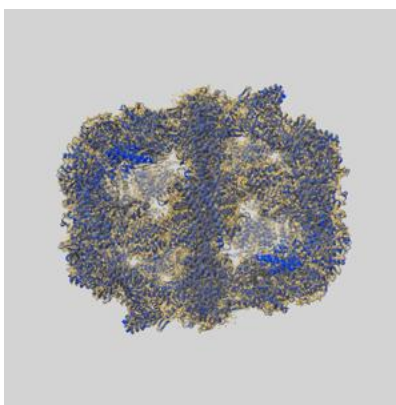
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-46553 and PDB model 9D48. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

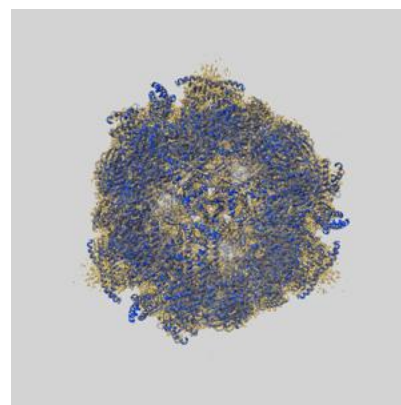
9.1 Map-model overlay [i](#)



X



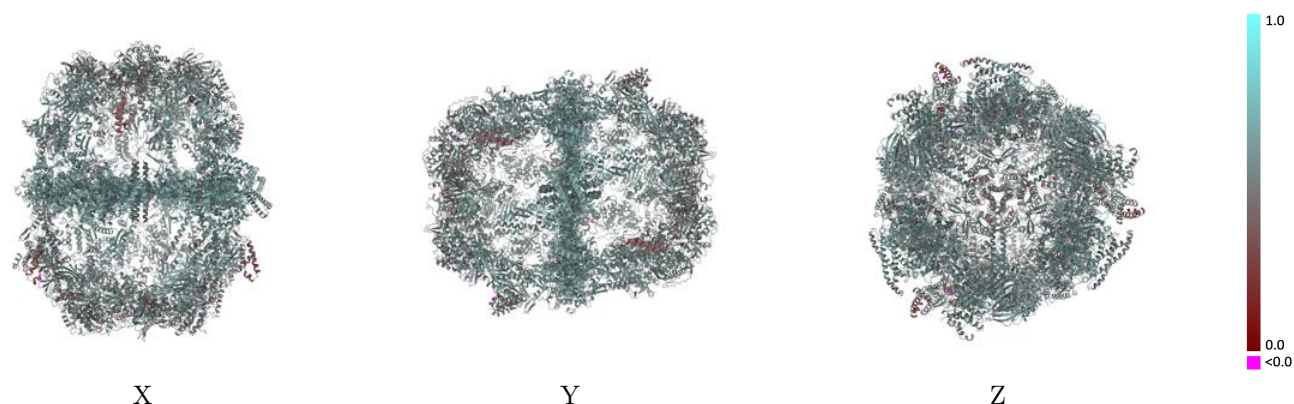
Y



Z

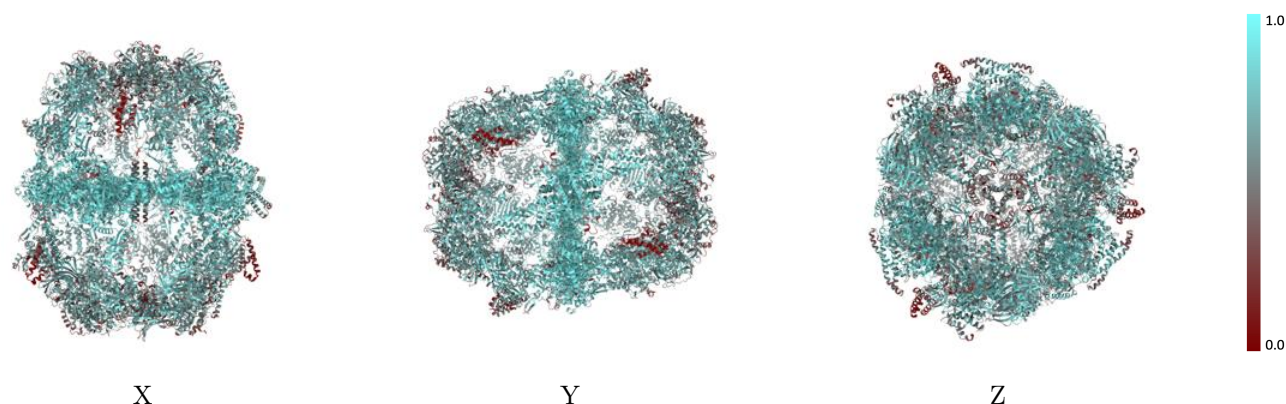
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



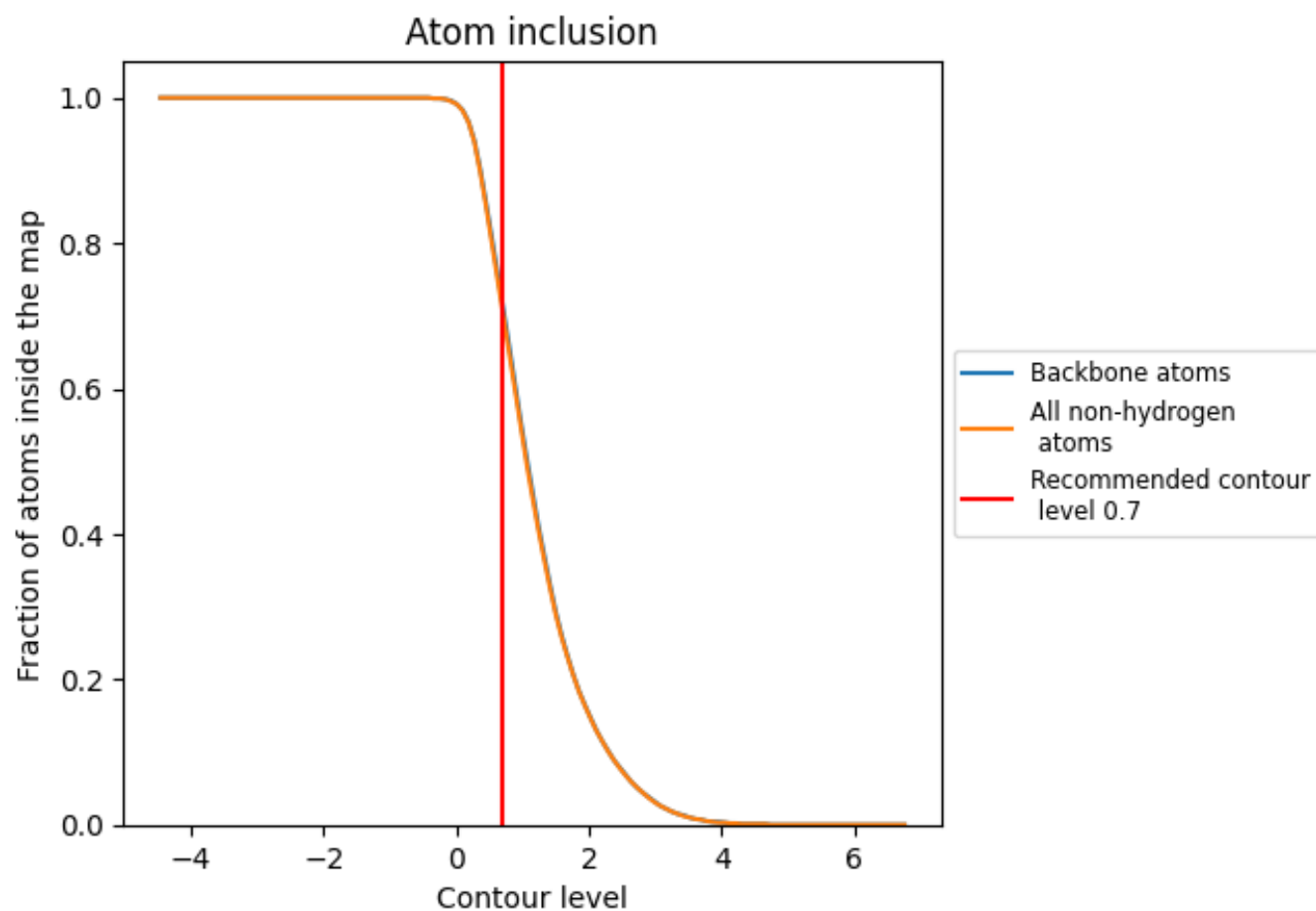
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 70% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7040	<div></div> 0.5550
A	<div></div> 0.6260	<div></div> 0.5300
B	<div></div> 0.8260	<div></div> 0.5910
E	<div></div> 0.6240	<div></div> 0.5290
F	<div></div> 0.8250	<div></div> 0.5910
G	<div></div> 0.8260	<div></div> 0.5920
I	<div></div> 0.6230	<div></div> 0.5290
M	<div></div> 0.6230	<div></div> 0.5290
N	<div></div> 0.8270	<div></div> 0.5920
Q	<div></div> 0.6250	<div></div> 0.5290
R	<div></div> 0.8240	<div></div> 0.5910
W	<div></div> 0.6240	<div></div> 0.5300
X	<div></div> 0.8250	<div></div> 0.5910

1.0

0.0

<0.0