



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:22 AM UTC

PDB ID : 8XLH / pdb_00008xlh
EMDB ID : EMD-38448
Title : Structure of chimeric RyR-I4657M/G4819E
Authors : Lin, L.; Wang, C.; Wang, W.; Jiang, H.; Yuchi, Z.
Deposited on : 2023-12-26
Resolution : 3.62 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:

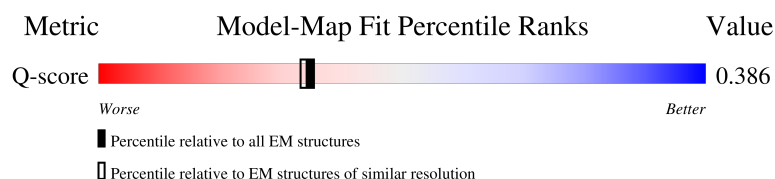
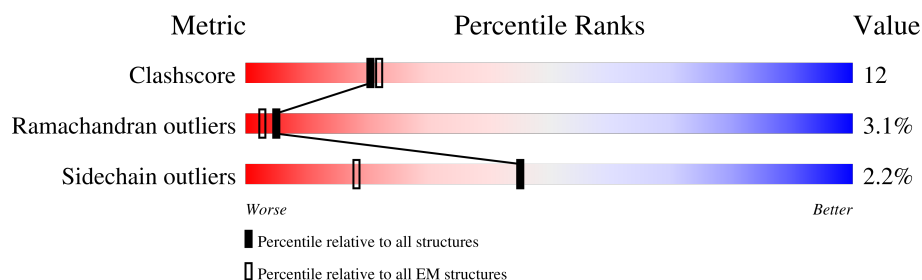
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

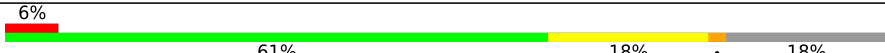
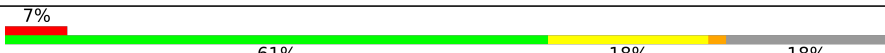
The reported resolution of this entry is 3.62 Å.

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.



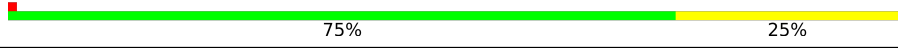
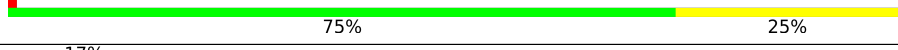
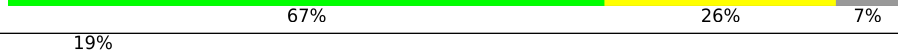
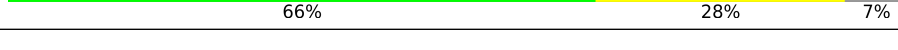
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11773 (3.12 - 4.12)

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	5037	
1	B	5037	
1	C	5037	
1	D	5037	

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Mol	Chain	Length	Quality of chain
2	E	107	 77%23%
2	F	107	 75%25%
2	G	107	 75%25%
2	H	107	 75%25%
3	I	149	 17%67%26%7%
3	J	149	 17%66%27%7%
3	K	149	 17%67%26%7%
3	L	149	 19%66%28%7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 124364 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4135	Total 29207	C 18536	N 5163	O 5346	S 162	0	0
1	D	4135	Total 29207	C 18536	N 5163	O 5346	S 162	0	0
1	C	4135	Total 29207	C 18536	N 5163	O 5346	S 162	0	0
1	B	4135	Total 29207	C 18536	N 5163	O 5346	S 162	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4563	LYS	ARG	engineered mutation	UNP P11716
A	4564	TYR	PHE	engineered mutation	UNP P11716
A	4657	MET	CYS	engineered mutation	UNP P11716
A	4792	SER	LEU	engineered mutation	UNP P11716
A	4819	GLU	GLY	engineered mutation	UNP P11716
D	4563	LYS	ARG	engineered mutation	UNP P11716
D	4564	TYR	PHE	engineered mutation	UNP P11716
D	4657	MET	CYS	engineered mutation	UNP P11716
D	4792	SER	LEU	engineered mutation	UNP P11716
D	4819	GLU	GLY	engineered mutation	UNP P11716
C	4563	LYS	ARG	engineered mutation	UNP P11716
C	4564	TYR	PHE	engineered mutation	UNP P11716
C	4657	MET	CYS	engineered mutation	UNP P11716
C	4792	SER	LEU	engineered mutation	UNP P11716
C	4819	GLU	GLY	engineered mutation	UNP P11716
B	4563	LYS	ARG	engineered mutation	UNP P11716
B	4564	TYR	PHE	engineered mutation	UNP P11716
B	4657	MET	CYS	engineered mutation	UNP P11716
B	4792	SER	LEU	engineered mutation	UNP P11716
B	4819	GLU	GLY	engineered mutation	UNP P11716

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	G	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
2	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	139	Total	C	N	O	S	0	0
			1033	638	174	212	9		
3	L	139	Total	C	N	O	S	0	0
			1033	638	174	212	9		
3	K	139	Total	C	N	O	S	0	0
			1033	638	174	212	9		
3	J	139	Total	C	N	O	S	0	0
			1033	638	174	212	9		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23
K	32	ALA	GLU	engineered mutation	UNP P0DP23
K	68	ALA	GLU	engineered mutation	UNP P0DP23
K	105	ALA	GLU	engineered mutation	UNP P0DP23
K	141	ALA	GLU	engineered mutation	UNP P0DP23
J	32	ALA	GLU	engineered mutation	UNP P0DP23
J	68	ALA	GLU	engineered mutation	UNP P0DP23
J	105	ALA	GLU	engineered mutation	UNP P0DP23
J	141	ALA	GLU	engineered mutation	UNP P0DP23

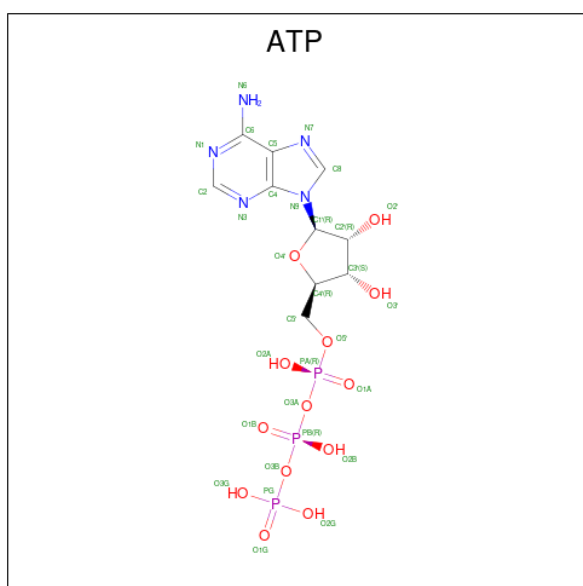
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	

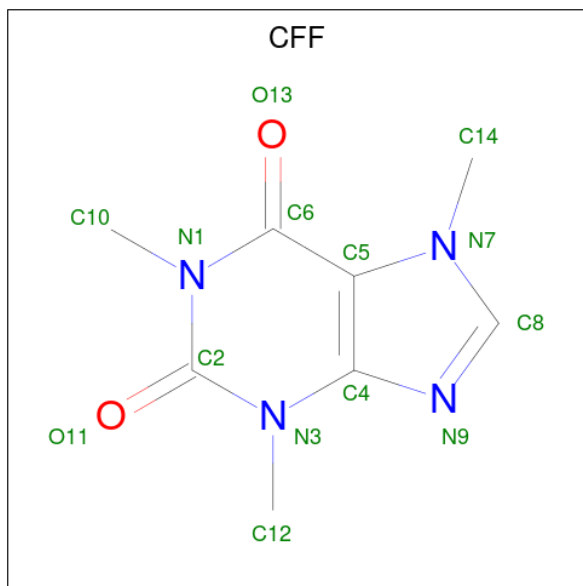
- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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Mol	Chain	Residues	Atoms					AltConf
6	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).

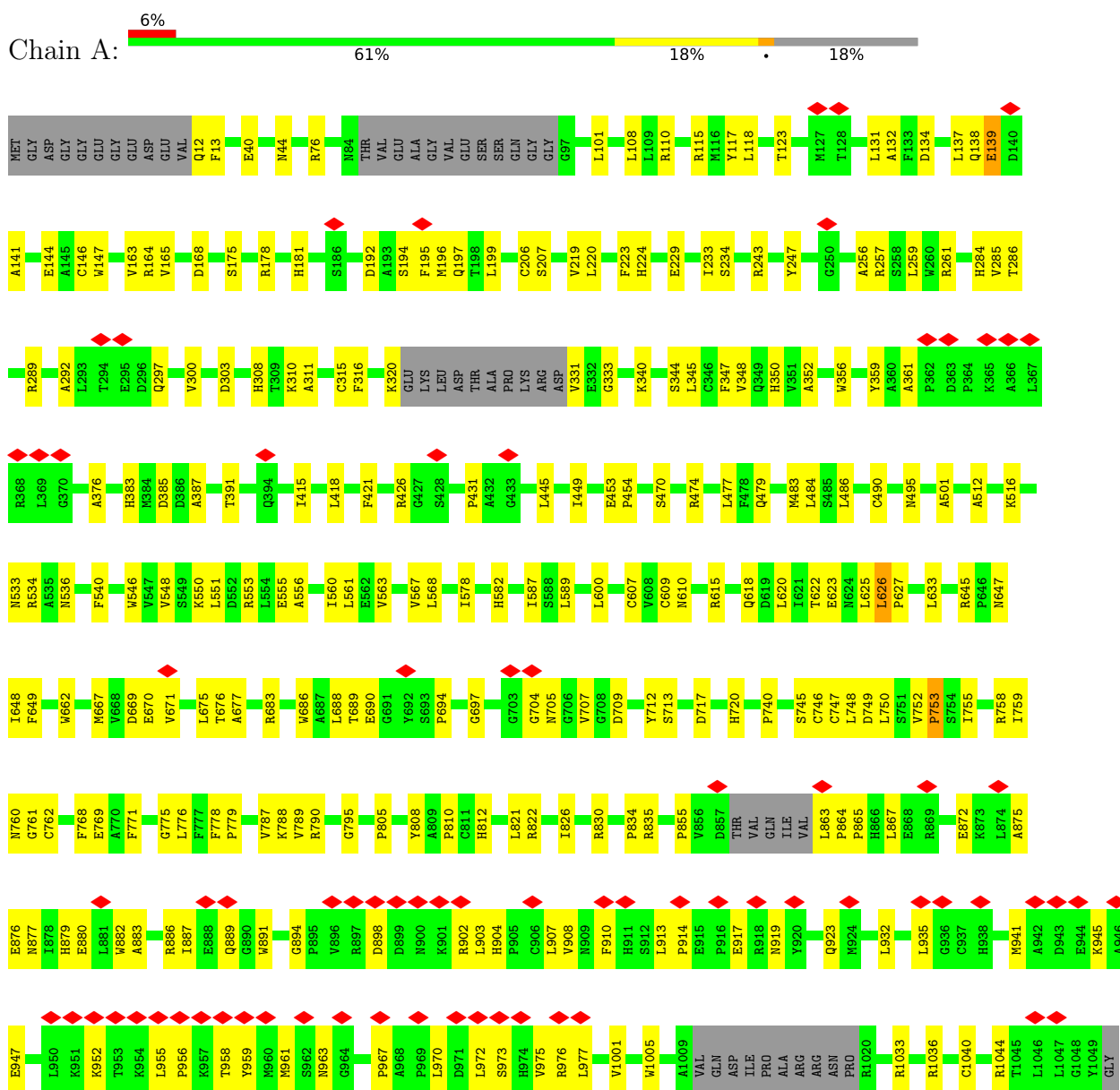


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	D	1	Total	C	N	O	0
			14	8	4	2	
7	C	1	Total	C	N	O	0
			14	8	4	2	
7	B	1	Total	C	N	O	0
			14	8	4	2	

3 Residue-property plots

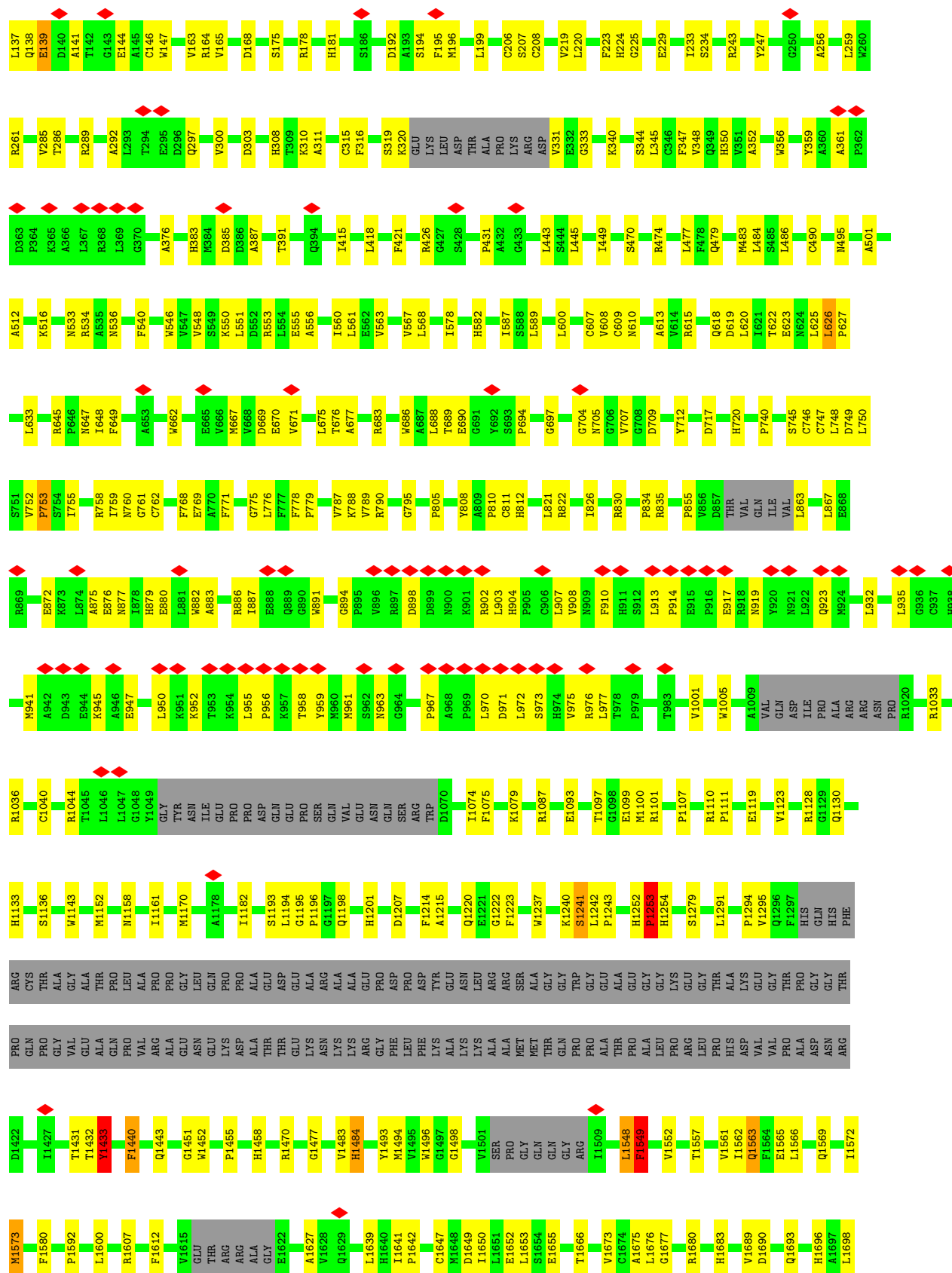
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 1



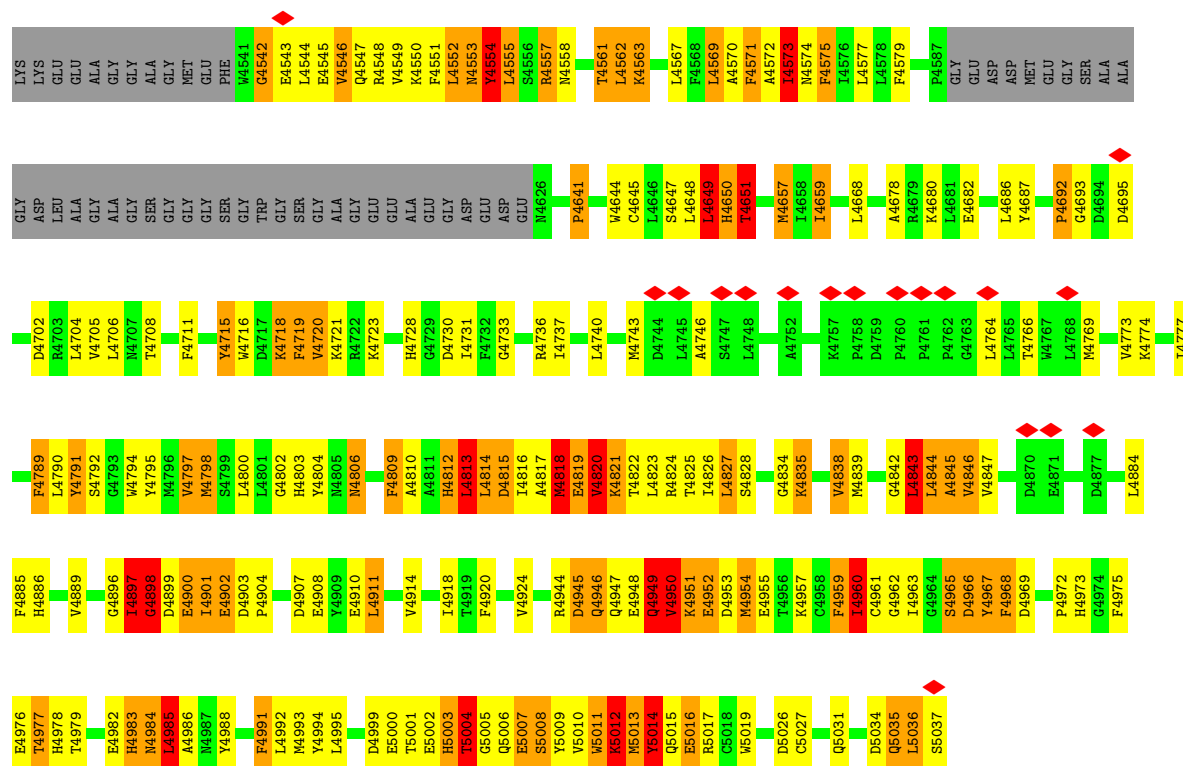
S2459	V2346	N2196	L1922	T1847	I1716	R1607	Q1443	PRO	LEU	ALA	PRO	ALA	ASN	ASP	GLN	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
I2470	E2347	R2199	Q1928	G1855	L1720	F1612	G1451	ARG	ALA	PRO	ARG	ALA	ASN	ASP	GLN	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
L2479	R2355	M2203	L1937	D1856	S1722	V1615	W1452	GLU	GLU	GLY	GLY	GLU	LEU	LEU	LEU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
GLY	L2356	E2209	F1946	D1858	A1723	GLU	P1455	THR	THR	THR	THR	THR	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
LYS	A2367	N2213	C1947	V1859	C1724	ARG	H1458	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
ALA	L2368	G2217	D1948	L1863	R1728	GLY	R1477	GLY	GLY	GLY	GLY	GLY	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
VAL	S2374	G2218	L1951	E1874	M1730	ALA	V1484	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
VAL	A2378	G2219	Q1952	L1863	M1730	ALA	V1484	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
VAL	E2382	T2220	E1956	E1874	S1732	GLY	G1477	GLY	GLY	GLY	GLY	GLY	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
L2386	E2382	K2221	L1969	E1874	E1733	ALA	V1484	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
D2393	D2394	F2235	R1976	GLU	L1738	ALA	Y1493	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
G2394	P2395	Q2247	Y1977	GLU	R1752	ALA	M1494	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
GLY	VAL	L2257	M1981	GLU	K1753	ALA	W1495	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
ARG	ARG	L2258	R1982	GLU	L1762	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
ARG	ARG	E2259	T1985	GLU	V1767	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
ASP	ASP	N2260	M1986	GLU	S1770	ALA	W1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
ARG	ARG	L2265	A1988	GLU	L1771	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
ARG	ARG	L2265	A1989	GLU	R1772	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
ARG	ARG	T2271	T1995	ASP	H1776	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
GLU	GLU	P2272	T1996	GLU	F1782	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
HIS	HIS	L2273	E1997	GLU	A1788	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
PHE	PHE	D2274	E1997	GLU	ALA	GLY	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
GLY	GLY	V2275	E1997	GLU	ALA	VAL	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
GLU	GLU	A2276	L2009	GLU	E1793	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
PRO	PRO	S2279	F2012	GLU	A1788	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
PRO	PRO	V2280	P2022	GLU	ALA	VAL	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
GLU	GLU	N2284	L2023	GLU	E1793	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
Q2291	E2292	Q2293	E2025	GLU	A1796	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
Q2293	E2292	Q2293	E2025	GLU	A1796	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
E2296	K2297	E2296	E2025	GLU	A1796	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
K2297	E2296	E2296	E2025	GLU	A1796	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
P2311	L2314	P2311	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
L2314	L2314	L2314	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
E2604	E2604	E2604	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
P2616	S2617	P2616	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
M2618	M2618	M2618	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
L2622	L2622	L2622	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
R2625	R2625	R2625	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
V2630	V2630	V2630	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
P2631	P2631	P2631	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR
I2456	I2456	I2456	E2047	GLU	R1808	ALA	H1496	ALA	ALA	ALA	ALA	ALA	GLU	GLU	GLU	PRO	PRO	ASP	GLN	ASN	ILE	ASN	TYR



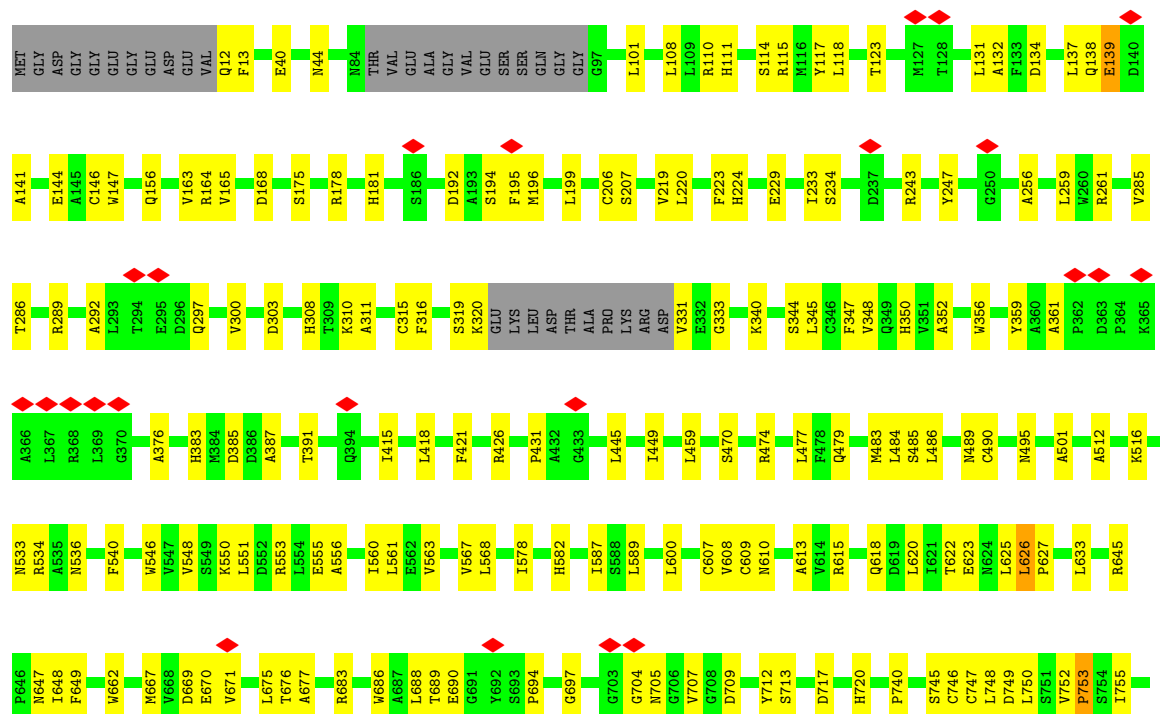




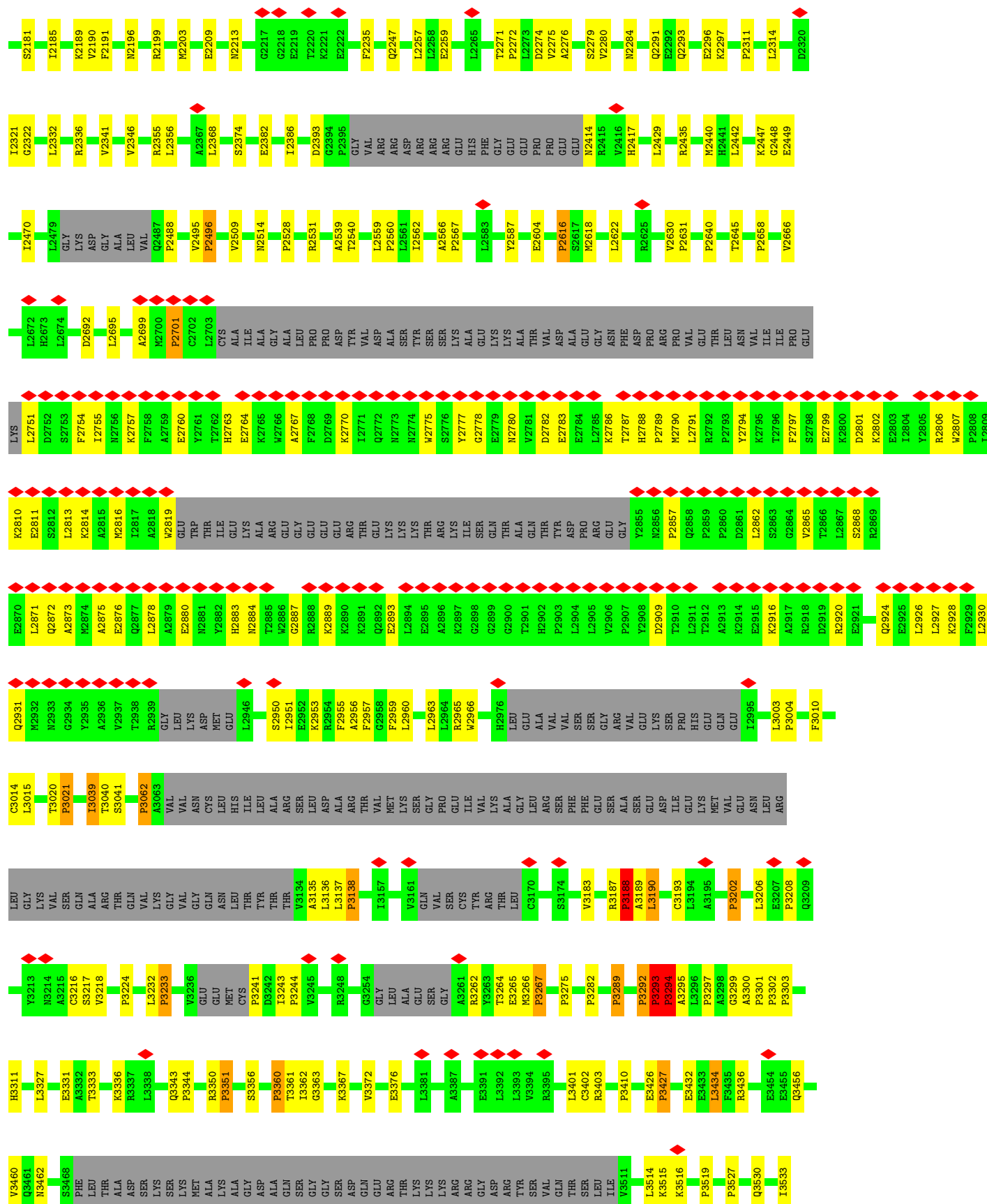




• Molecule 1: Ryanodine receptor 1





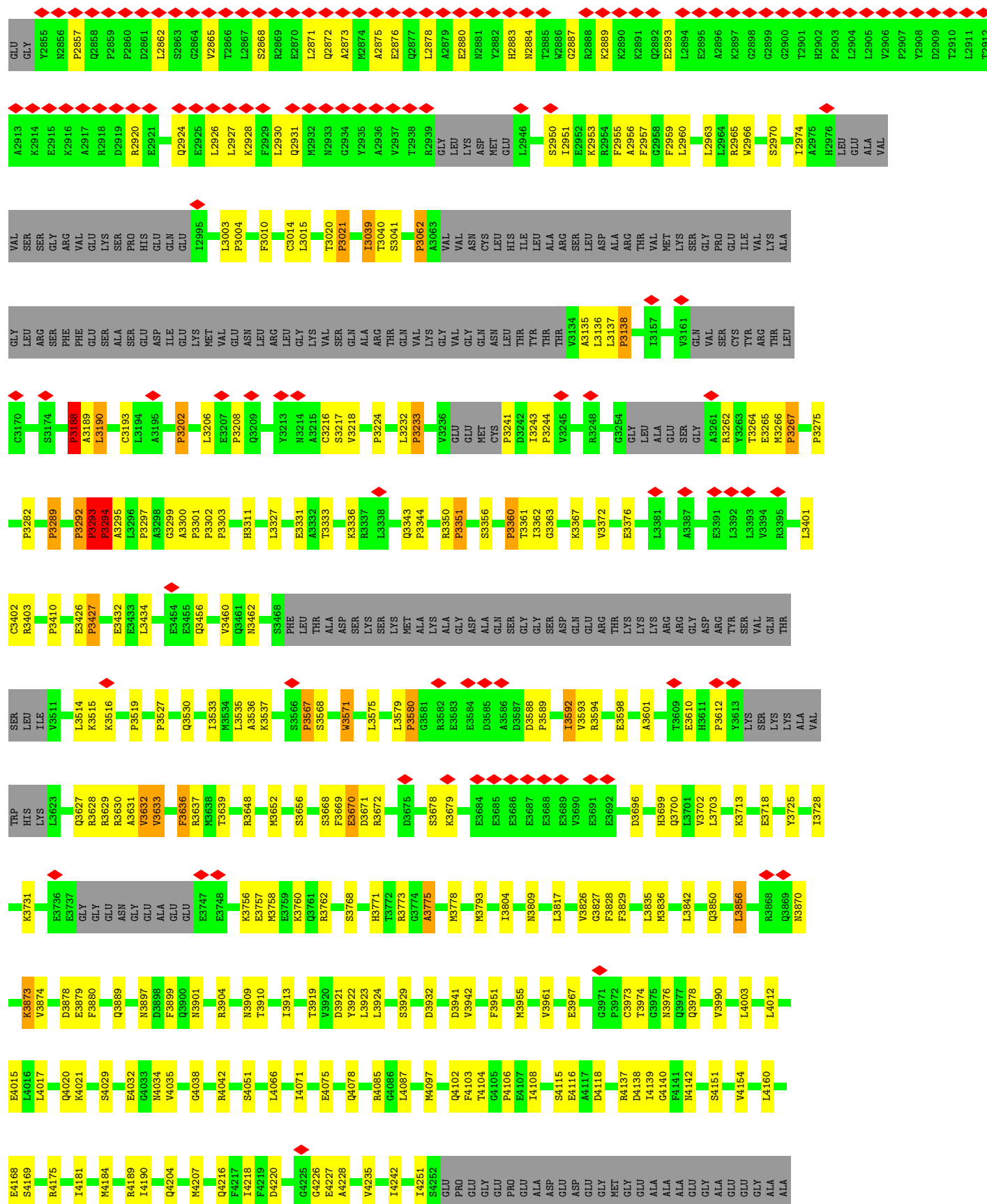




Chain B: 6% 61% 18% 18%

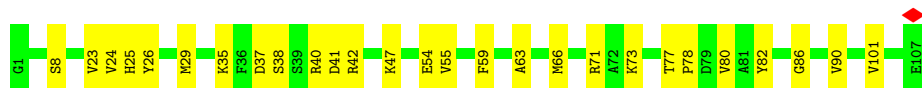
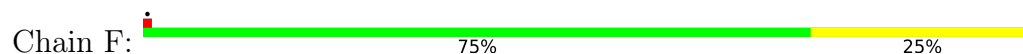




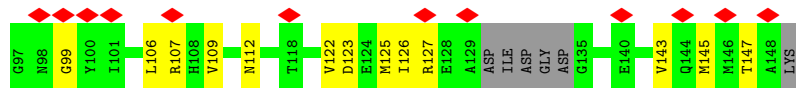
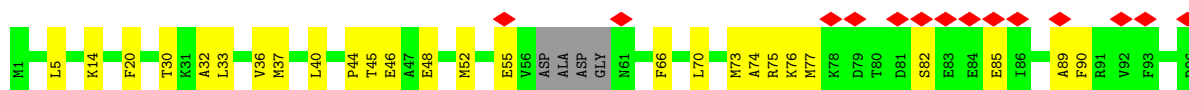




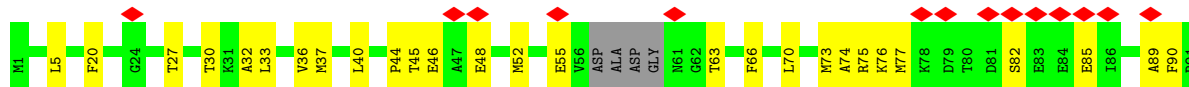
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



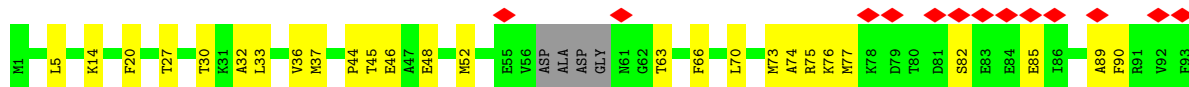
- Molecule 3: Calmodulin-1



- Molecule 3: Calmodulin-1

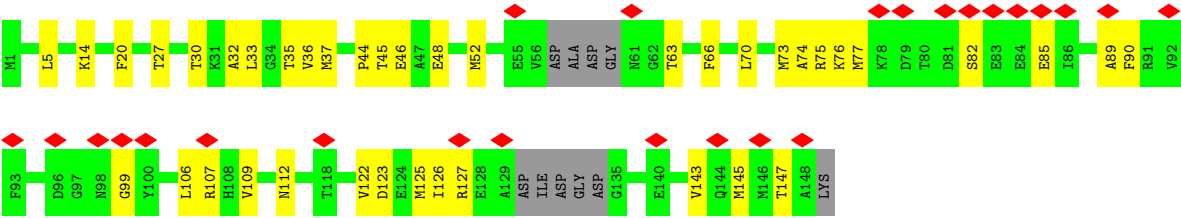


- Molecule 3: Calmodulin-1



- Molecule 3: Calmodulin-1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28189	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.354	Depositor
Minimum map value	-0.808	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.135	Depositor
Map size (Å)	502.80002, 502.80002, 502.80002	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0475, 1.0475, 1.0475	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ZN, CFF, ATP

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	0.44	17/29778 (0.1%)	0.77	106/40610 (0.3%)
1	B	0.45	17/29778 (0.1%)	0.77	106/40610 (0.3%)
1	C	0.45	17/29778 (0.1%)	0.77	109/40610 (0.3%)
1	D	0.45	17/29778 (0.1%)	0.77	109/40610 (0.3%)
2	E	0.15	0/820	0.43	0/1105
2	F	0.15	0/820	0.43	0/1105
2	G	0.15	0/820	0.43	0/1105
2	H	0.15	0/820	0.43	0/1105
3	I	0.16	0/1042	0.42	0/1404
3	J	0.16	0/1042	0.42	0/1404
3	K	0.16	0/1042	0.42	0/1404
3	L	0.16	0/1042	0.42	0/1404
All	All	0.43	68/126560 (0.1%)	0.76	430/172476 (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	7
1	B	0	8
1	C	0	7
1	D	0	7
All	All	0	29

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4910	GLU	CA-C	-8.54	1.45	1.52
1	C	4910	GLU	CA-C	-8.54	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	855	PRO	CG-CD	-7.94	1.23	1.50
1	C	855	PRO	CG-CD	-7.94	1.23	1.50
1	A	855	PRO	CG-CD	-7.93	1.23	1.50

The worst 5 of 430 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4791	TYR	N-CA-C	-14.66	93.74	114.12
1	D	4791	TYR	N-CA-C	-14.65	93.75	114.12
1	C	4791	TYR	N-CA-C	-14.65	93.75	114.12
1	B	4791	TYR	N-CA-C	-14.65	93.75	114.12
1	D	4949	GLN	N-CA-C	-12.57	96.63	112.72

There are no chirality outliers.

5 of 29 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	GLU	Peptide
1	A	1432	THR	Mainchain
1	A	1796	ALA	Peptide
1	A	4553	ASN	Mainchain
1	A	752	VAL	Peptide

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	29207	0	25765	674	0
1	B	29207	0	25765	678	0
1	C	29207	0	25765	678	0
1	D	29207	0	25765	677	0
2	E	804	0	812	15	0
2	F	804	0	812	16	0
2	G	804	0	812	16	0
2	H	804	0	812	16	0
3	I	1033	0	958	31	0
3	J	1033	0	958	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	1033	0	958	30	0
3	L	1033	0	958	32	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	31	0	12	1	0
6	B	31	0	12	1	0
6	C	31	0	12	1	0
6	D	31	0	12	1	0
7	A	14	0	10	0	0
7	B	14	0	10	0	0
7	C	14	0	10	0	0
7	D	14	0	10	0	0
All	All	124364	0	110228	2849	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 12.

The worst 5 of 2849 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1698:LEU:HD12	1:B:1814:MET:HE1	1.53	0.90
1:C:1698:LEU:HD12	1:C:1814:MET:HE1	1.53	0.89
1:A:1698:LEU:HD12	1:A:1814:MET:HE1	1.53	0.89
1:D:1698:LEU:HD12	1:D:1814:MET:HE1	1.53	0.88
1:D:1484:HIS:ND1	1:D:1484:HIS:O	2.07	0.86

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	4081/5037 (81%)	3348 (82%)	598 (15%)	135 (3%)	3	21
1	B	4081/5037 (81%)	3348 (82%)	598 (15%)	135 (3%)	3	21
1	C	4081/5037 (81%)	3351 (82%)	596 (15%)	134 (3%)	3	21
1	D	4081/5037 (81%)	3348 (82%)	598 (15%)	135 (3%)	3	21
2	E	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	F	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	G	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
2	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	I	133/149 (89%)	129 (97%)	4 (3%)	0	100	100
3	J	133/149 (89%)	129 (97%)	4 (3%)	0	100	100
3	K	133/149 (89%)	129 (97%)	4 (3%)	0	100	100
3	L	133/149 (89%)	129 (97%)	4 (3%)	0	100	100
All	All	17276/21172 (82%)	14307 (83%)	2430 (14%)	539 (3%)	5	22

5 of 539 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	626	LEU
1	A	1215	ALA
1	A	1241	SER
1	A	1291	LEU
1	A	1708	ARG

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	2516/4277 (59%)	2456 (98%)	60 (2%)	43	60
1	B	2516/4277 (59%)	2456 (98%)	60 (2%)	43	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	2516/4277 (59%)	2455 (98%)	61 (2%)	43	60
1	D	2516/4277 (59%)	2455 (98%)	61 (2%)	43	60
2	E	84/88 (96%)	84 (100%)	0	100	100
2	F	84/88 (96%)	84 (100%)	0	100	100
2	G	84/88 (96%)	84 (100%)	0	100	100
2	H	84/88 (96%)	84 (100%)	0	100	100
3	I	102/123 (83%)	102 (100%)	0	100	100
3	J	102/123 (83%)	102 (100%)	0	100	100
3	K	102/123 (83%)	102 (100%)	0	100	100
3	L	102/123 (83%)	102 (100%)	0	100	100
All	All	10808/17952 (60%)	10566 (98%)	242 (2%)	45	62

5 of 242 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4985	LEU
1	B	4843	LEU
1	C	4668	LEU
1	B	4838	VAL
1	B	4985	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 123 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	4836	GLN
1	B	3889	GLN
1	C	1560	ASN
1	B	3814	GLN
1	B	4946	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](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
6	ATP	B	5103	-	32,33,33	1.30	4 (12%)	48,52,52	1.77	12 (25%)
6	ATP	A	5103	-	32,33,33	1.31	4 (12%)	48,52,52	1.76	12 (25%)
7	CFF	D	5104	-	15,15,15	0.71	0	23,23,23	0.90	0
7	CFF	A	5104	-	15,15,15	0.73	0	23,23,23	0.92	0
6	ATP	C	5103	-	32,33,33	1.31	4 (12%)	48,52,52	1.76	12 (25%)
7	CFF	B	5104	-	15,15,15	0.73	0	23,23,23	0.91	0
7	CFF	C	5104	-	15,15,15	0.73	0	23,23,23	0.93	0
6	ATP	D	5103	-	32,33,33	1.30	4 (12%)	48,52,52	1.76	13 (27%)

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
6	ATP	B	5103	-	-	3/22/38/38	0/3/3/3
6	ATP	A	5103	-	-	3/22/38/38	0/3/3/3
7	CFF	D	5104	-	-	-	0/2/2/2
7	CFF	A	5104	-	-	-	0/2/2/2
6	ATP	C	5103	-	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CFF	B	5104	-	-	-	0/2/2/2
7	CFF	C	5104	-	-	-	0/2/2/2
6	ATP	D	5103	-	-	3/22/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5103	ATP	C5-C4	3.77	1.45	1.39
6	A	5103	ATP	C5-C4	3.74	1.45	1.39
6	B	5103	ATP	C5-C4	3.74	1.45	1.39
6	D	5103	ATP	C5-C4	3.72	1.45	1.39
6	A	5103	ATP	C4-N9	-2.90	1.31	1.37

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	5103	ATP	C5-C4-N3	-4.45	120.59	126.72
6	A	5103	ATP	C5-C4-N3	-4.45	120.59	126.72
6	B	5103	ATP	C5-C4-N3	-4.45	120.59	126.72
6	D	5103	ATP	C5-C4-N3	-4.43	120.62	126.72
6	B	5103	ATP	N3-C2-N1	-3.73	122.94	128.58

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

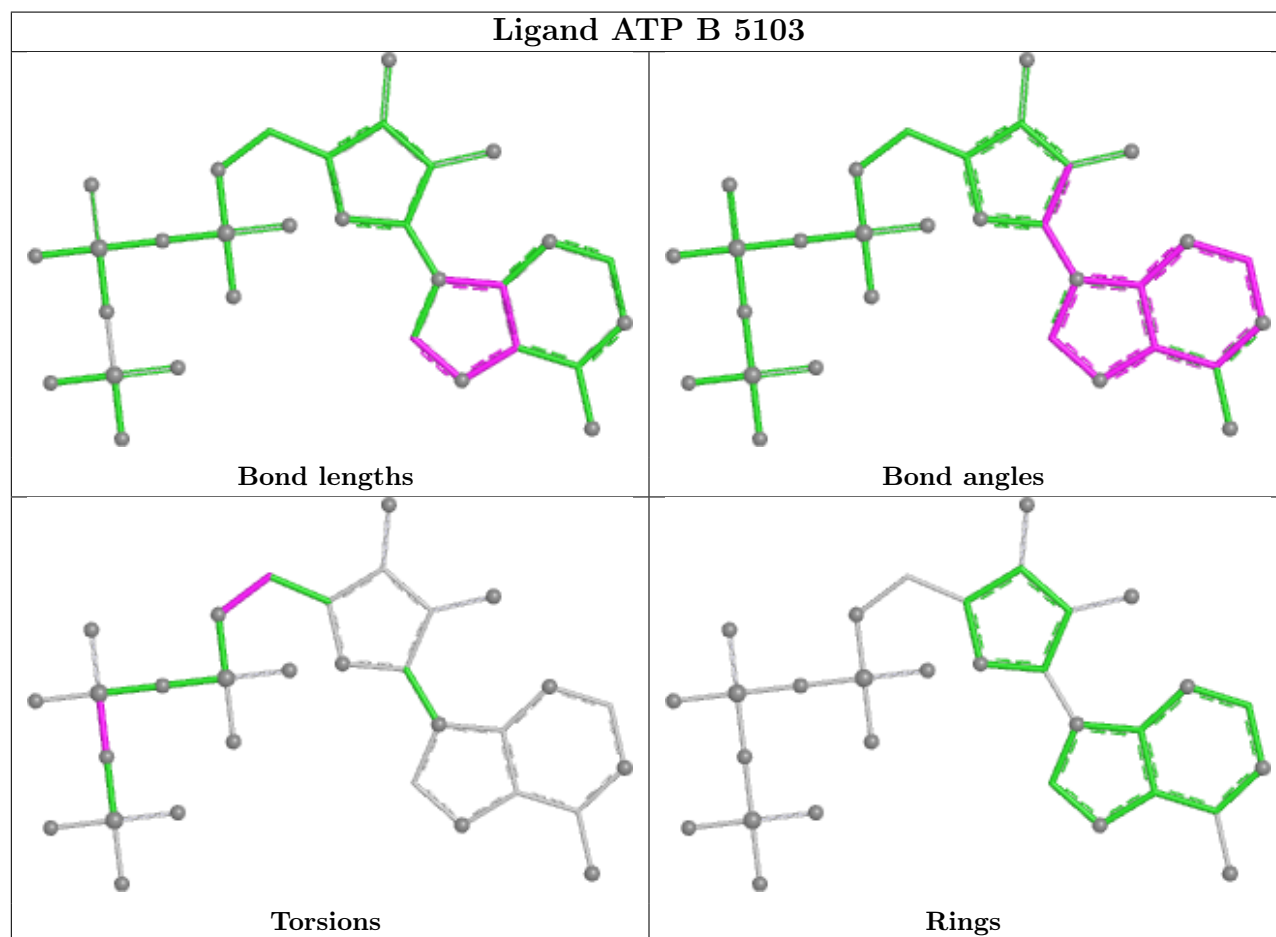
Mol	Chain	Res	Type	Atoms
6	A	5103	ATP	C4'-C5'-O5'-PA
6	D	5103	ATP	C4'-C5'-O5'-PA
6	C	5103	ATP	C4'-C5'-O5'-PA
6	B	5103	ATP	C4'-C5'-O5'-PA
6	A	5103	ATP	PG-O3B-PB-O1B

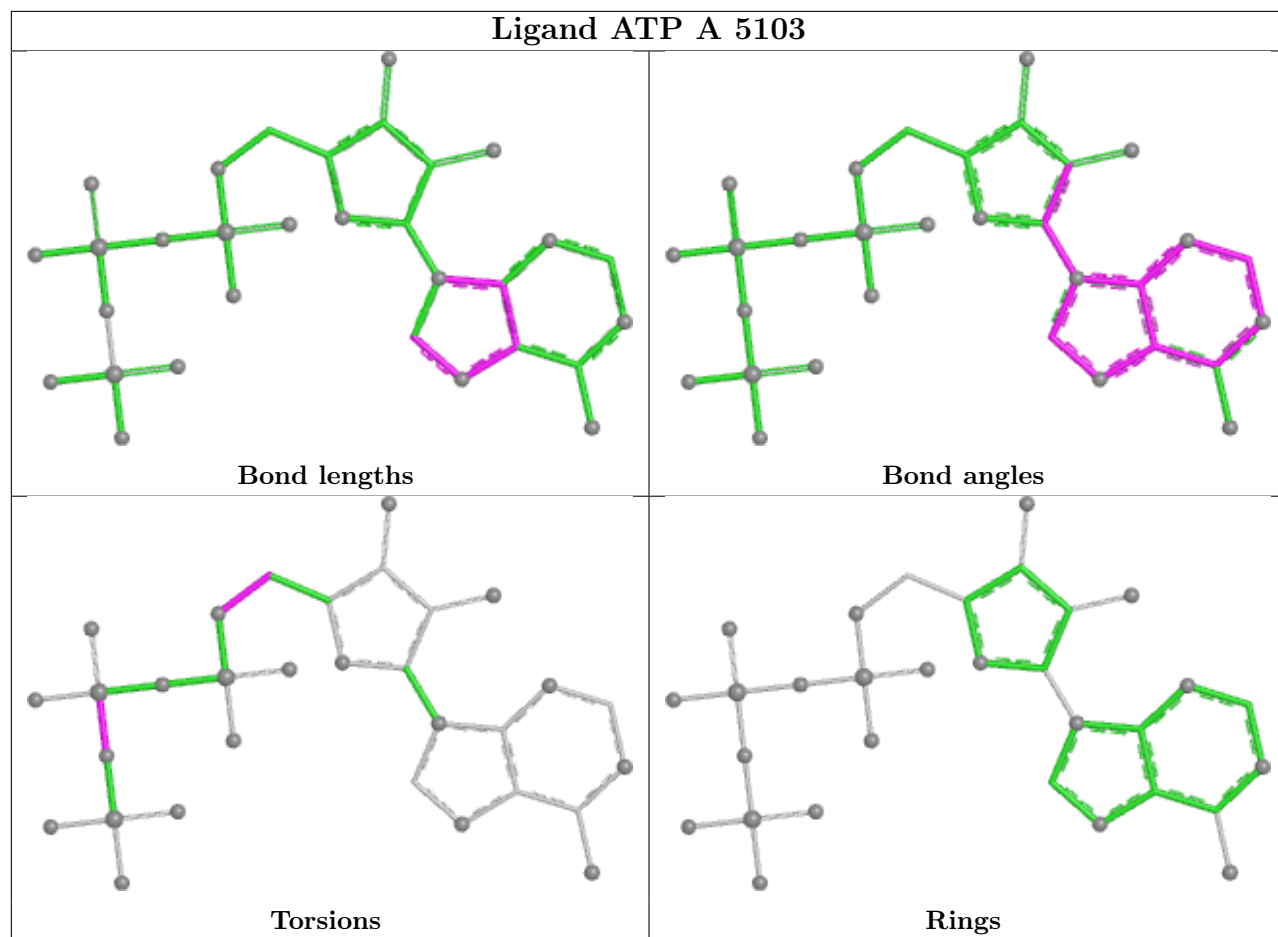
There are no ring outliers.

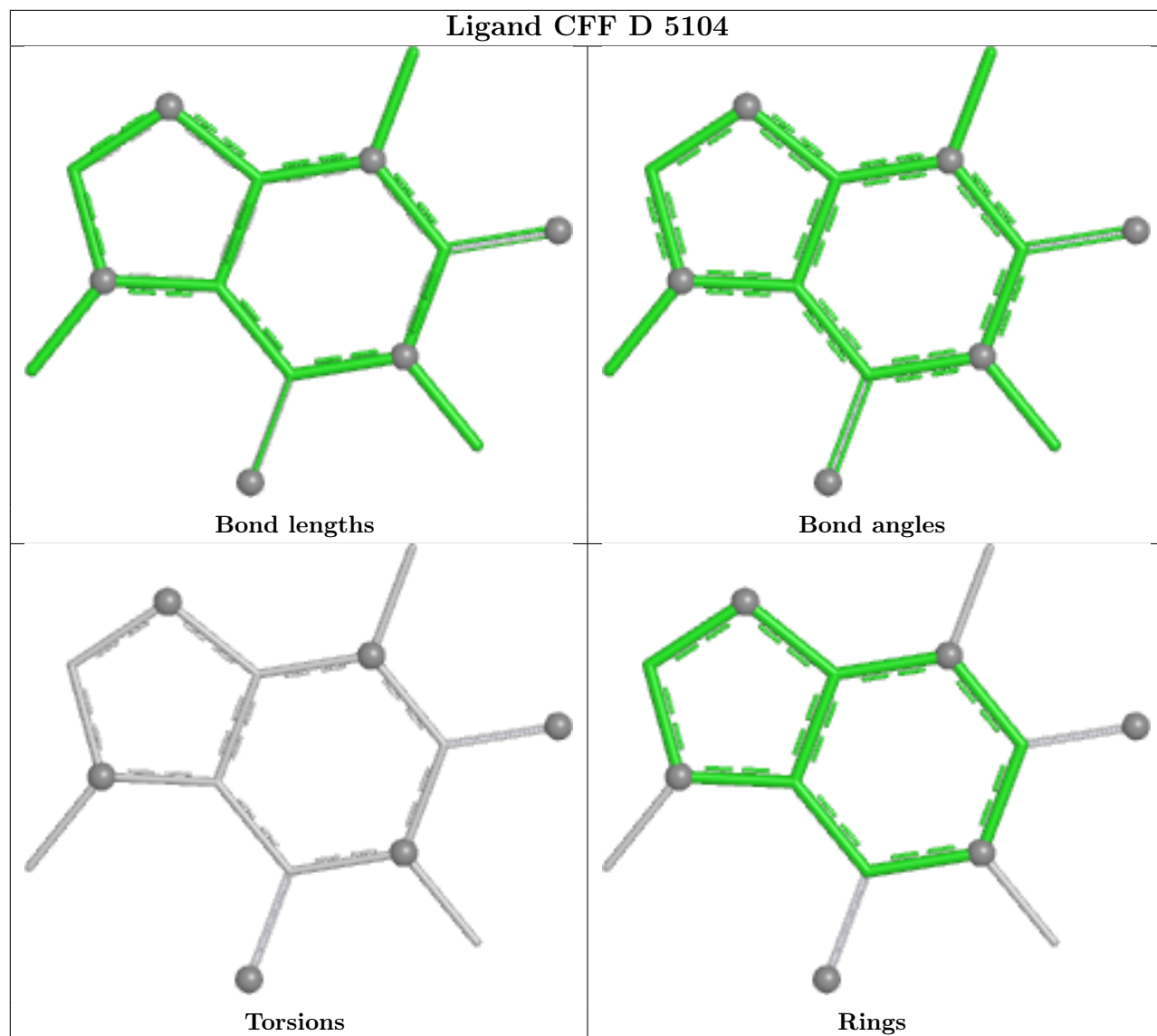
4 monomers are involved in 4 short contacts:

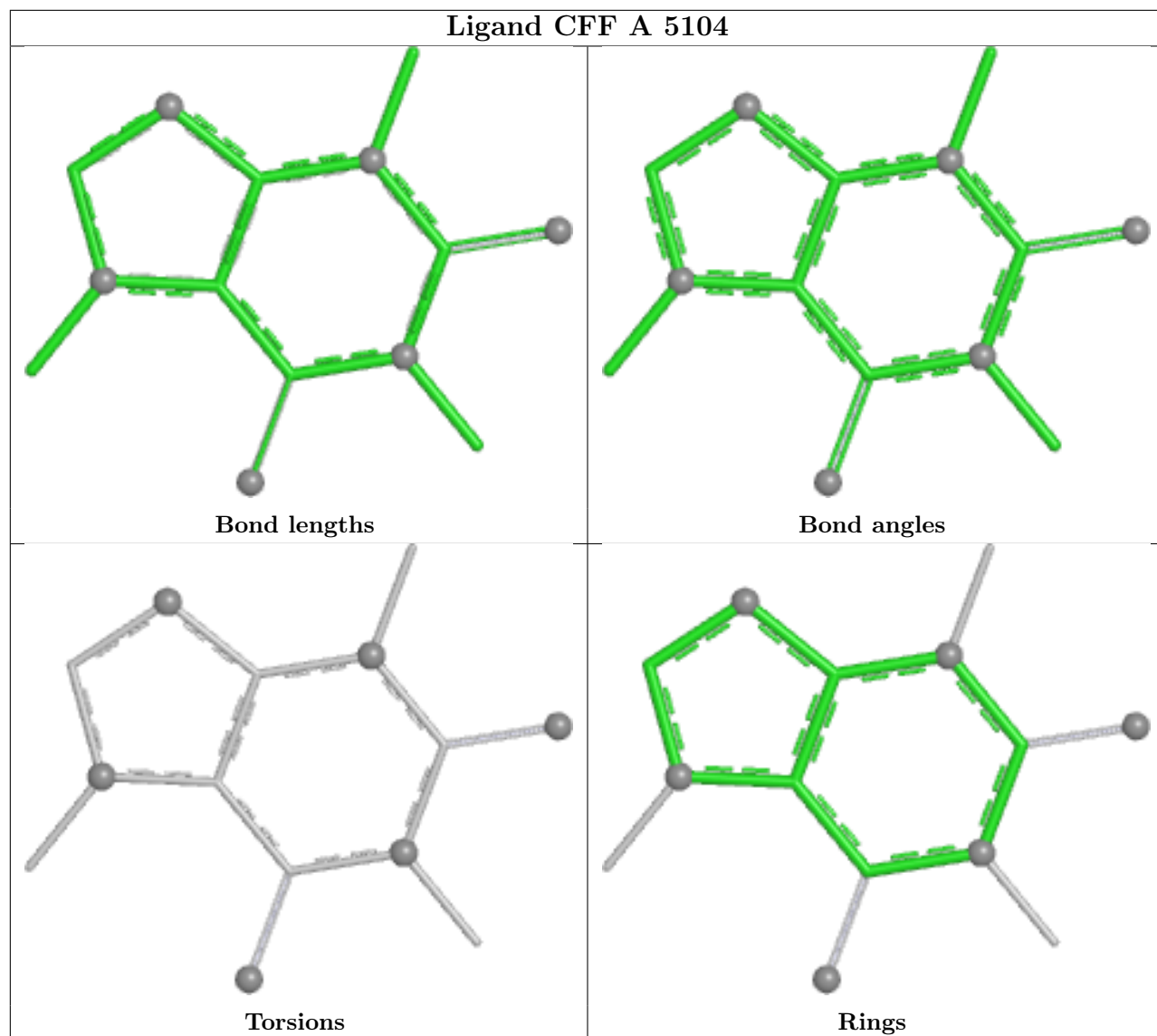
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	5103	ATP	1	0
6	A	5103	ATP	1	0
6	C	5103	ATP	1	0
6	D	5103	ATP	1	0

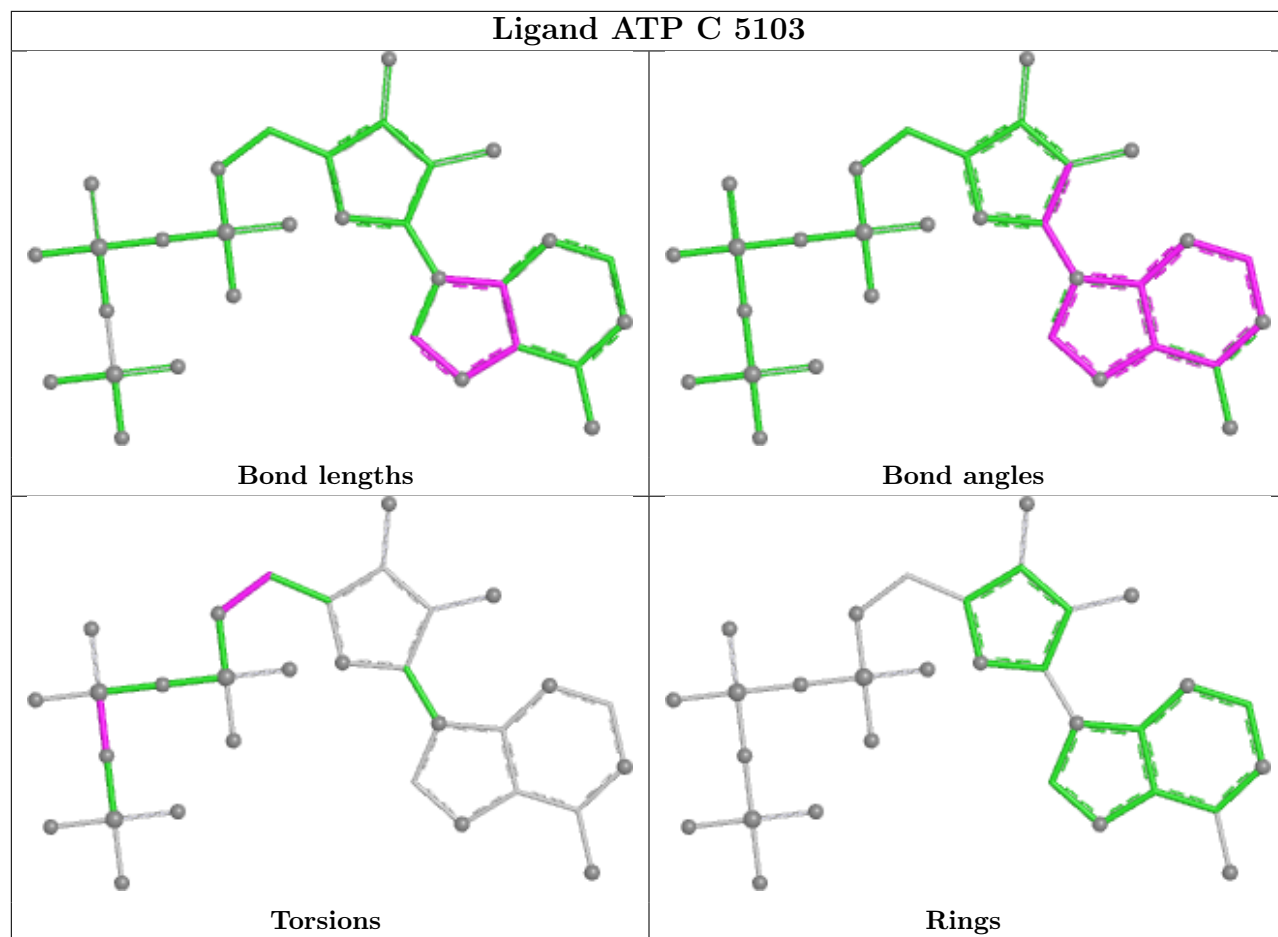
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

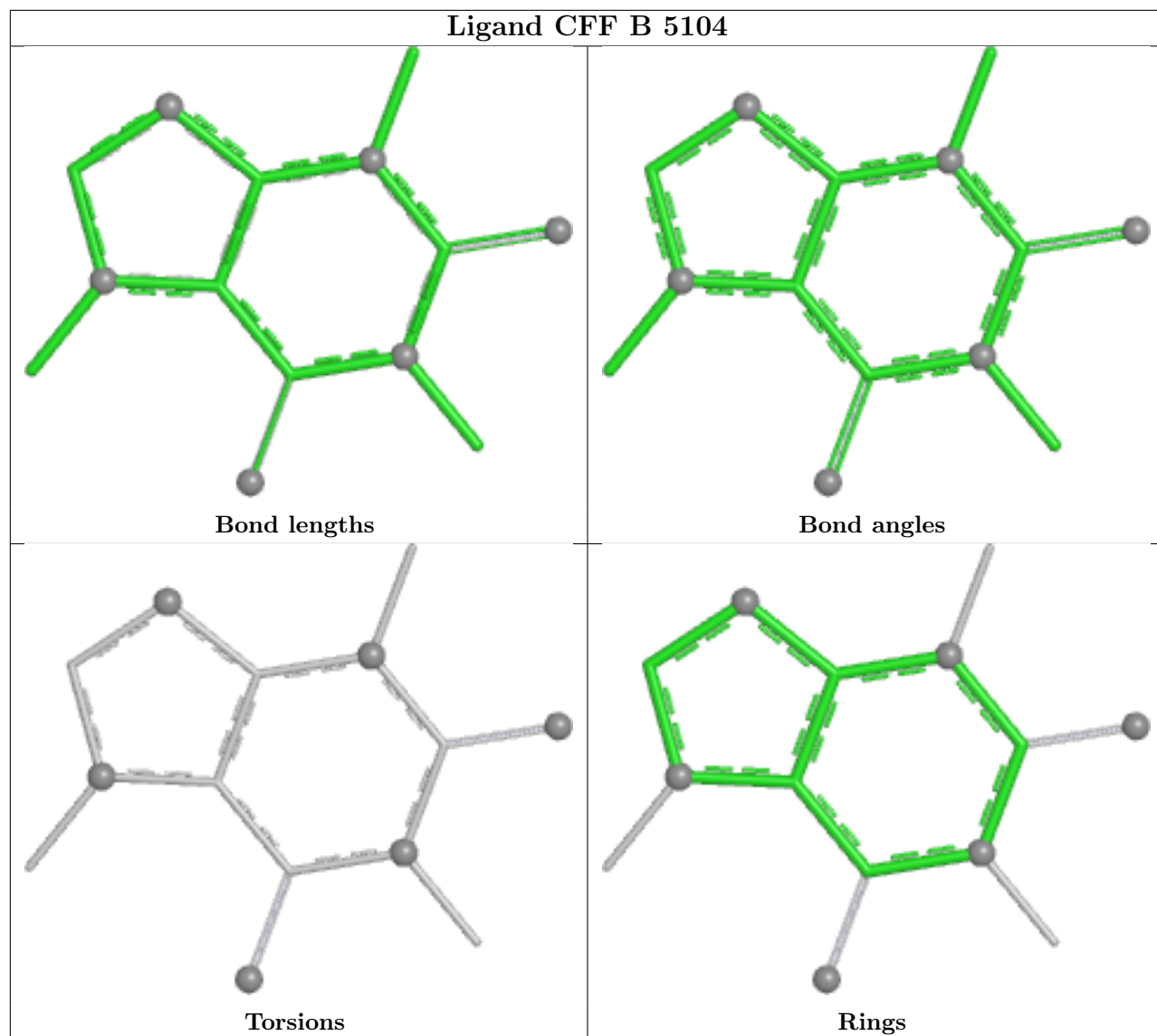


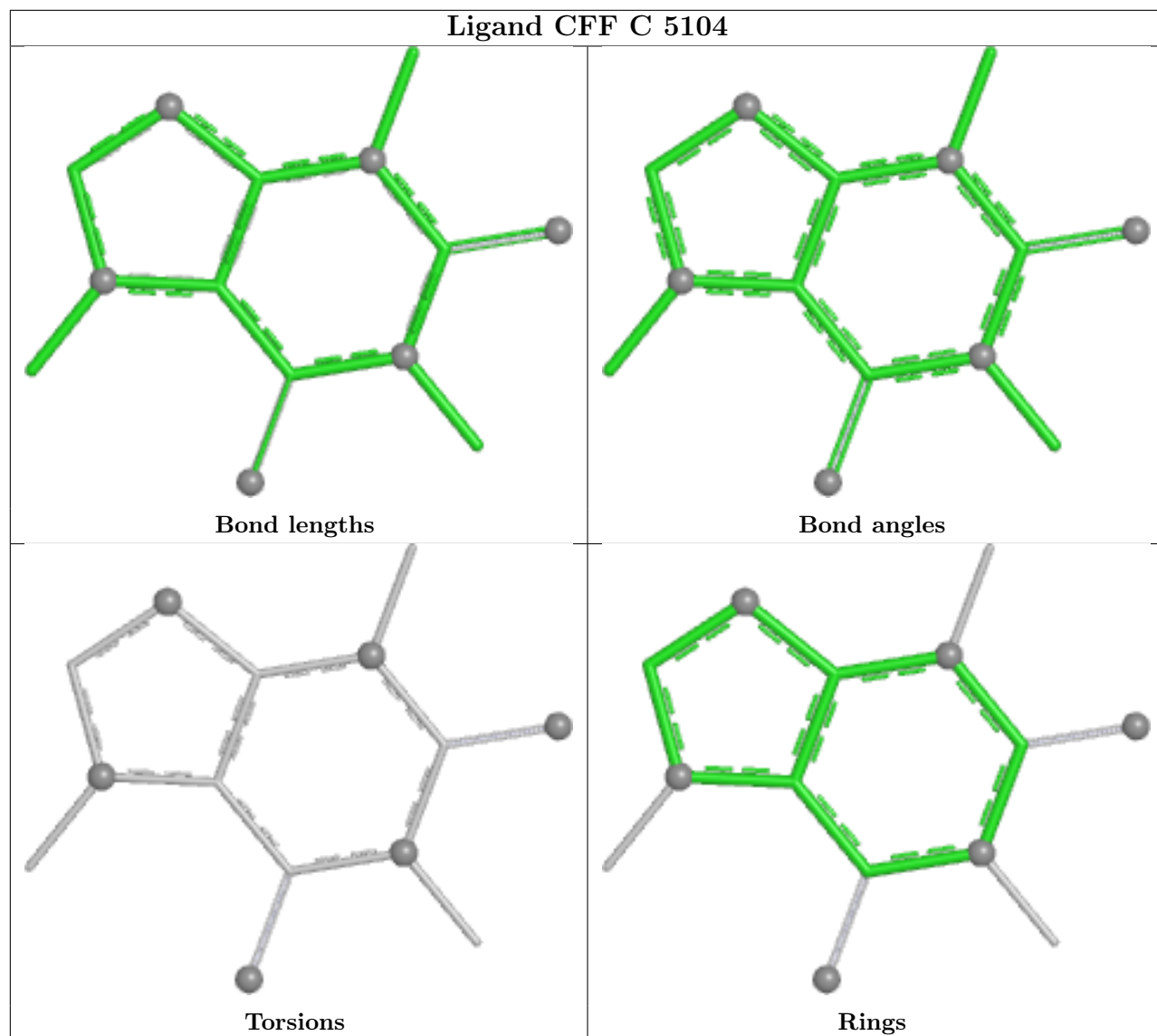


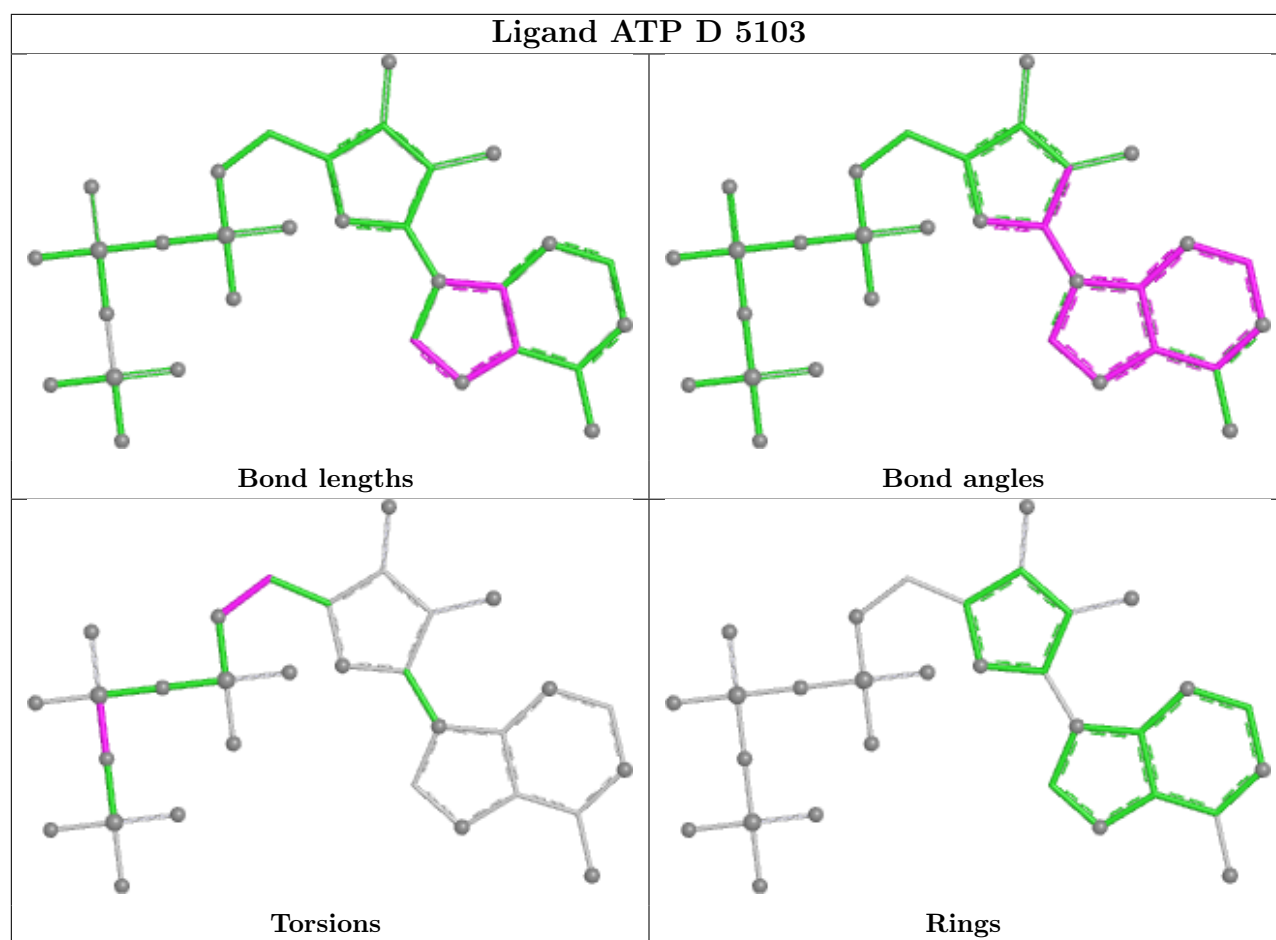












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

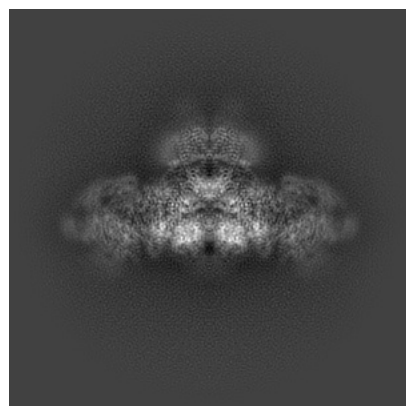
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38448. These allow visual inspection of the internal detail of the map and identification of artifacts.

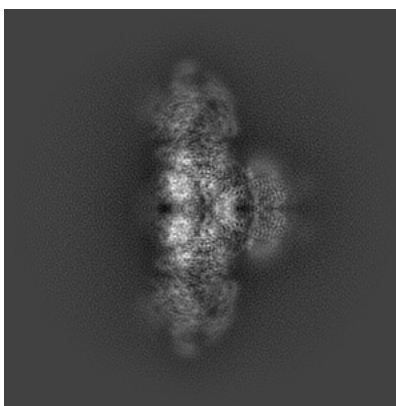
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

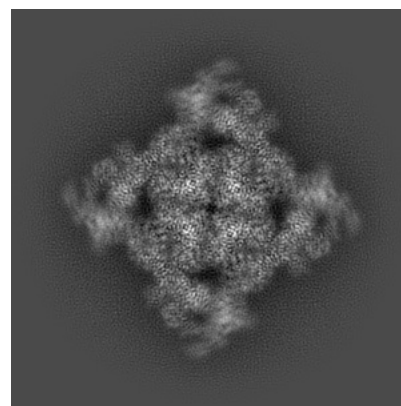
6.1.1 Primary map



X

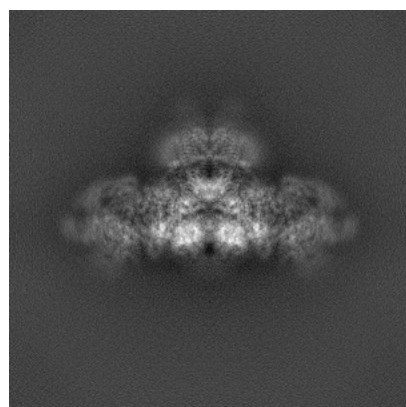


Y

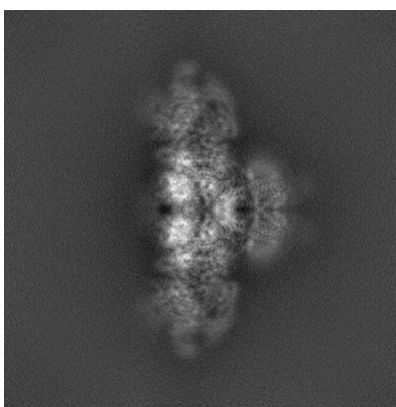


Z

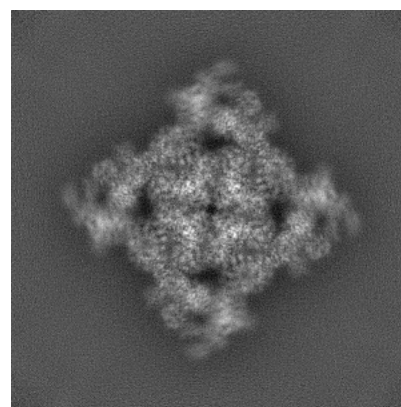
6.1.2 Raw map



X



Y

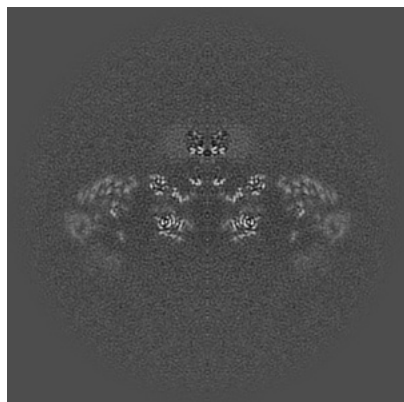


Z

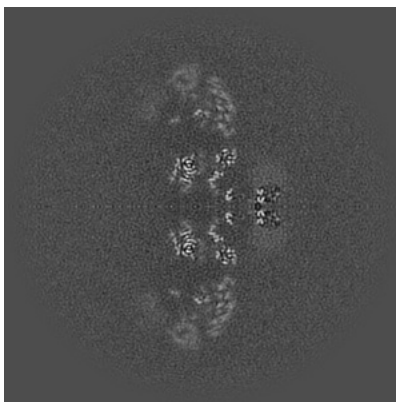
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

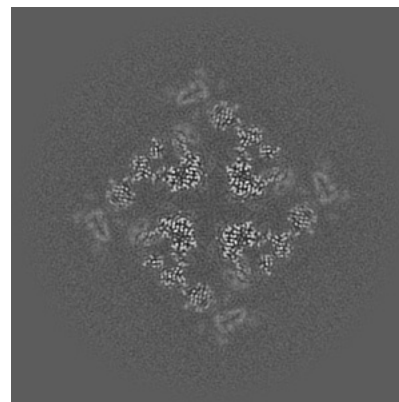
6.2.1 Primary map



X Index: 240

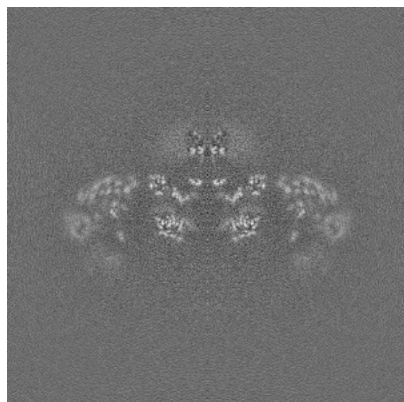


Y Index: 240

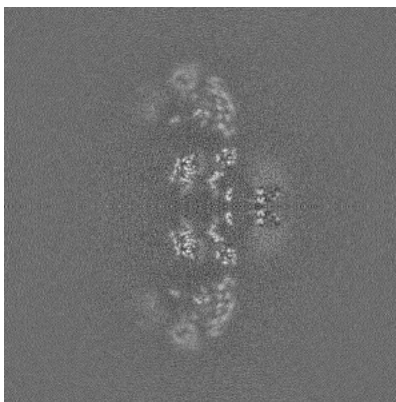


Z Index: 240

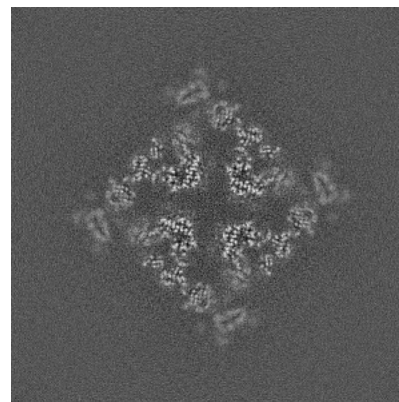
6.2.2 Raw map



X Index: 240



Y Index: 240

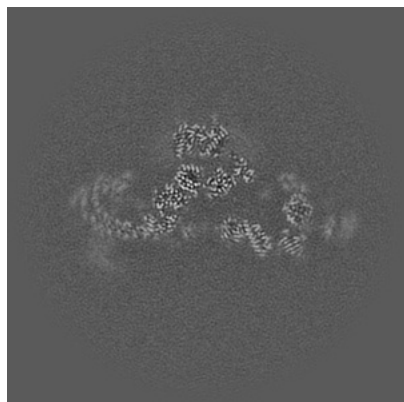


Z Index: 240

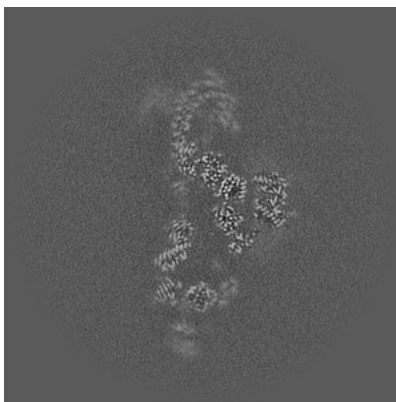
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

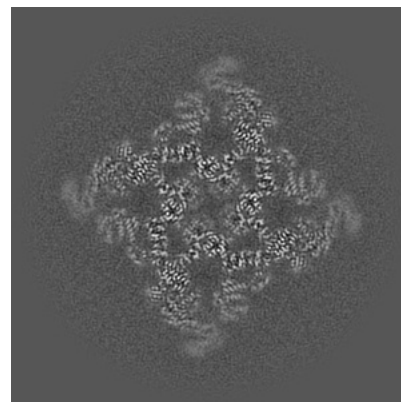
6.3.1 Primary map



X Index: 256

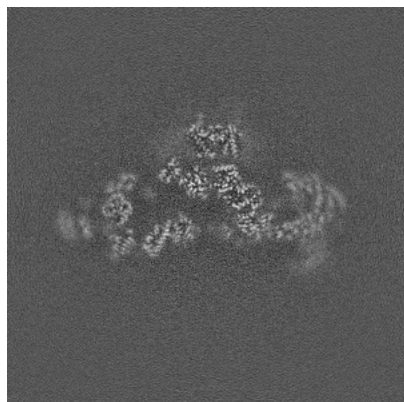


Y Index: 256

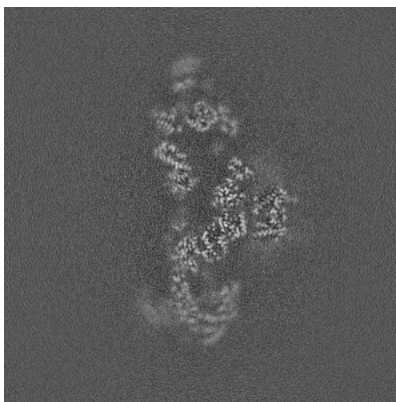


Z Index: 218

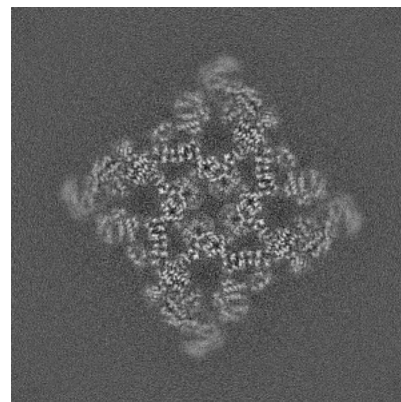
6.3.2 Raw map



X Index: 225



Y Index: 225

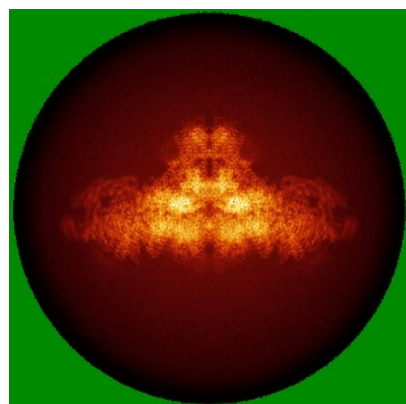


Z Index: 218

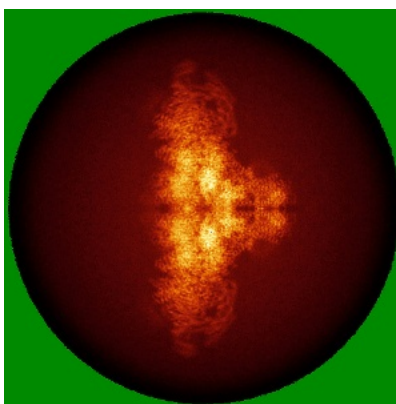
The images above show the largest variance slices of the map in three orthogonal directions.

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

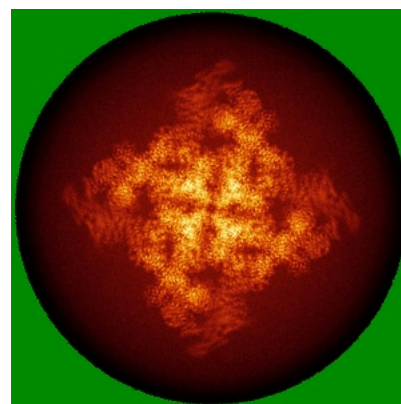
6.4.1 Primary map



X

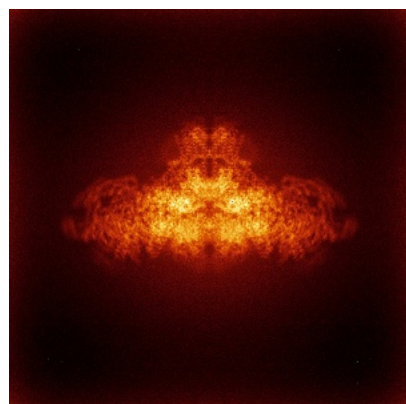


Y

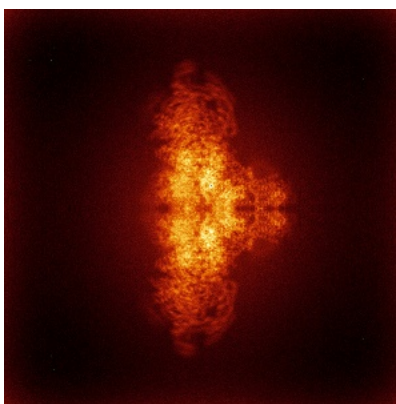


Z

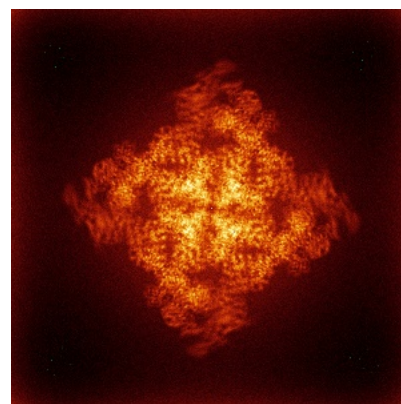
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

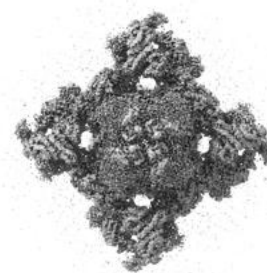
6.5.1 Primary map



X



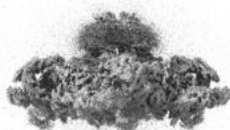
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

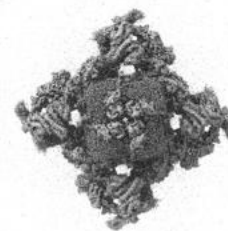
6.5.2 Raw map



X



Y



Z

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

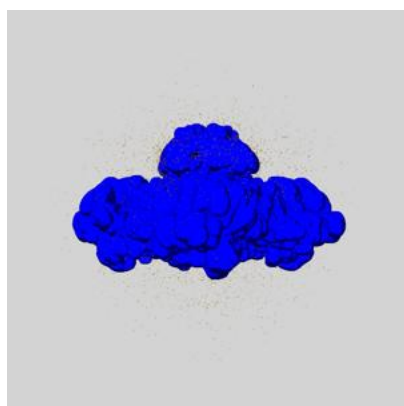
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

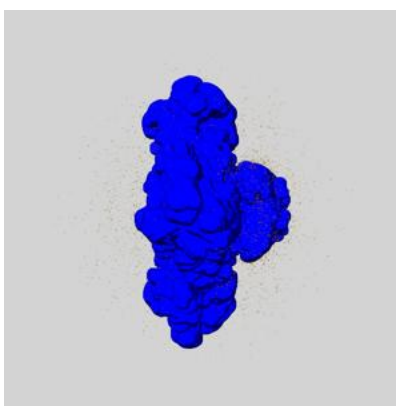
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

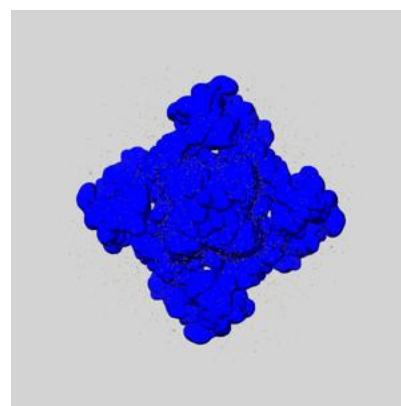
6.6.1 emd_38448_msk_1.map [i](#)



X



Y

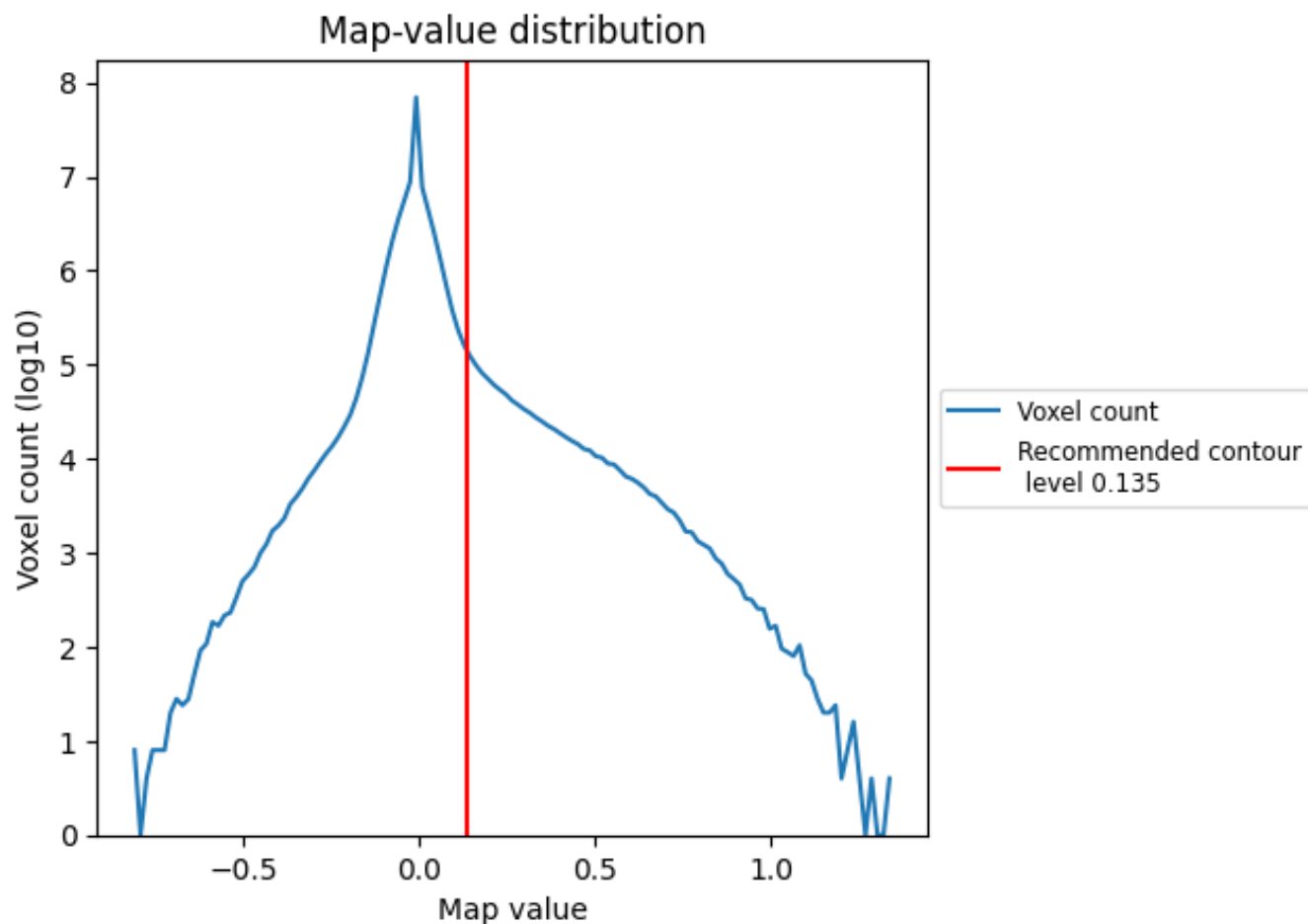


Z

7 Map analysis [i](#)

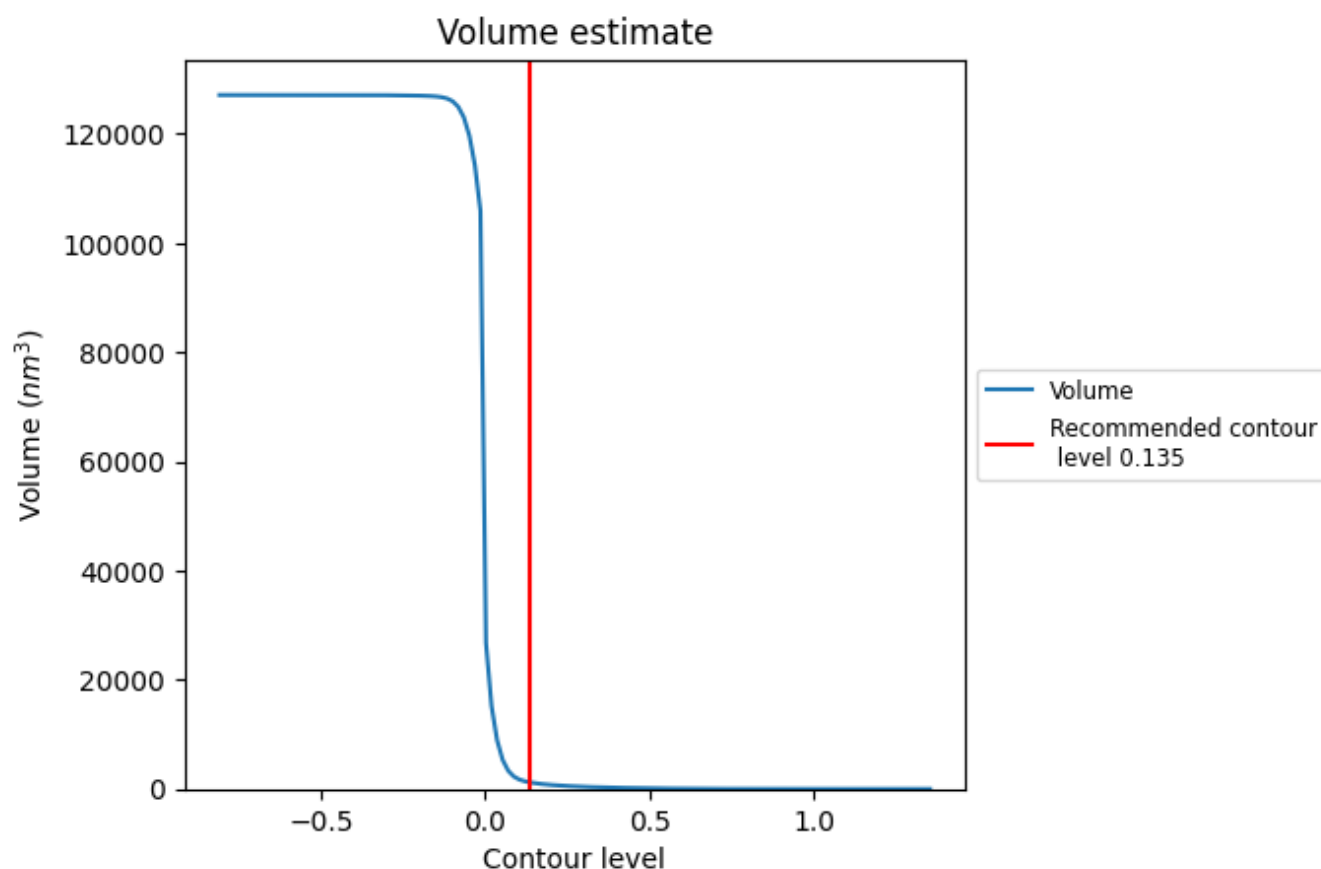
This section contains the results of statistical analysis of the map.

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.

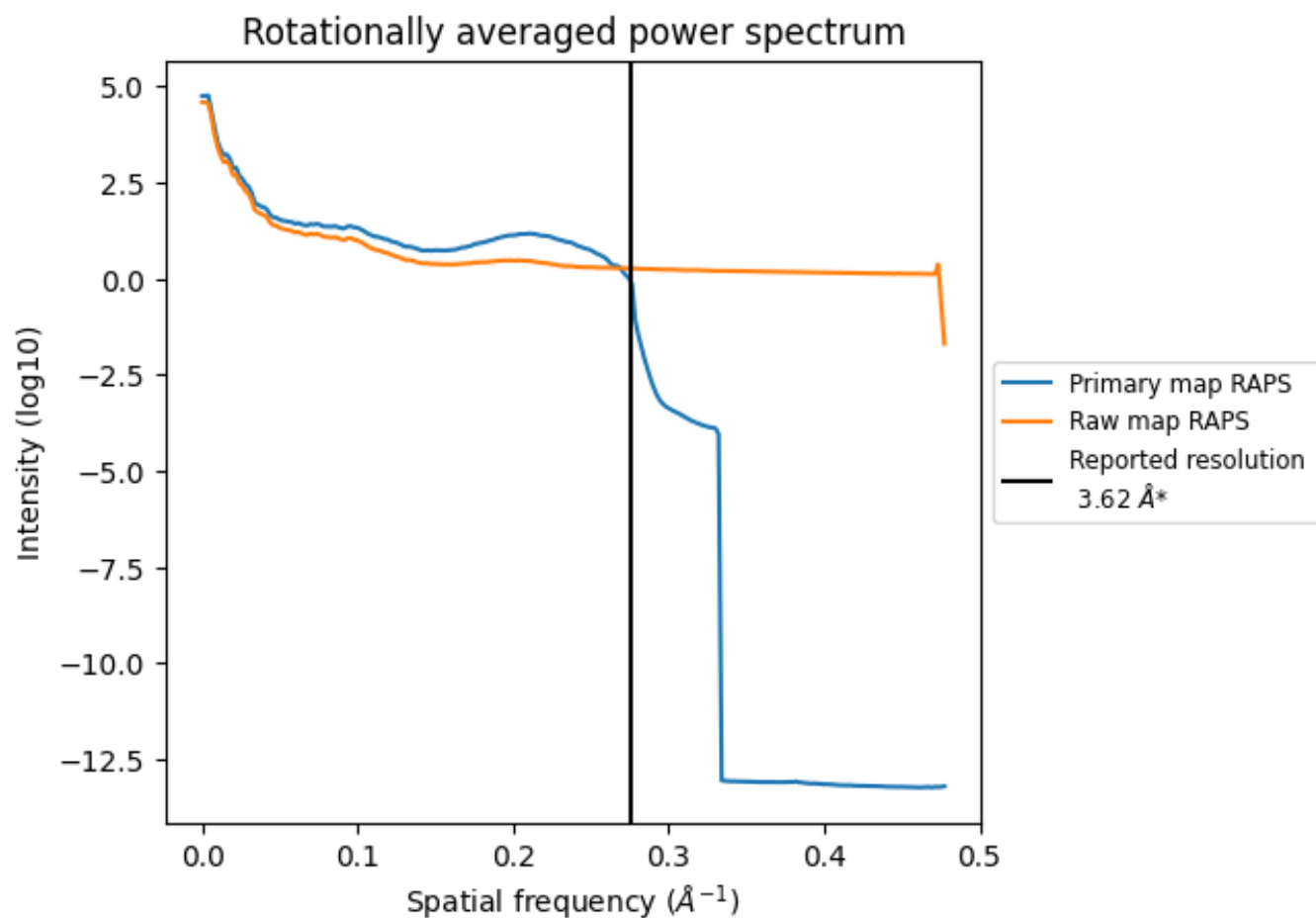
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1226 nm³; this corresponds to an approximate mass of 1107 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 ⓘ

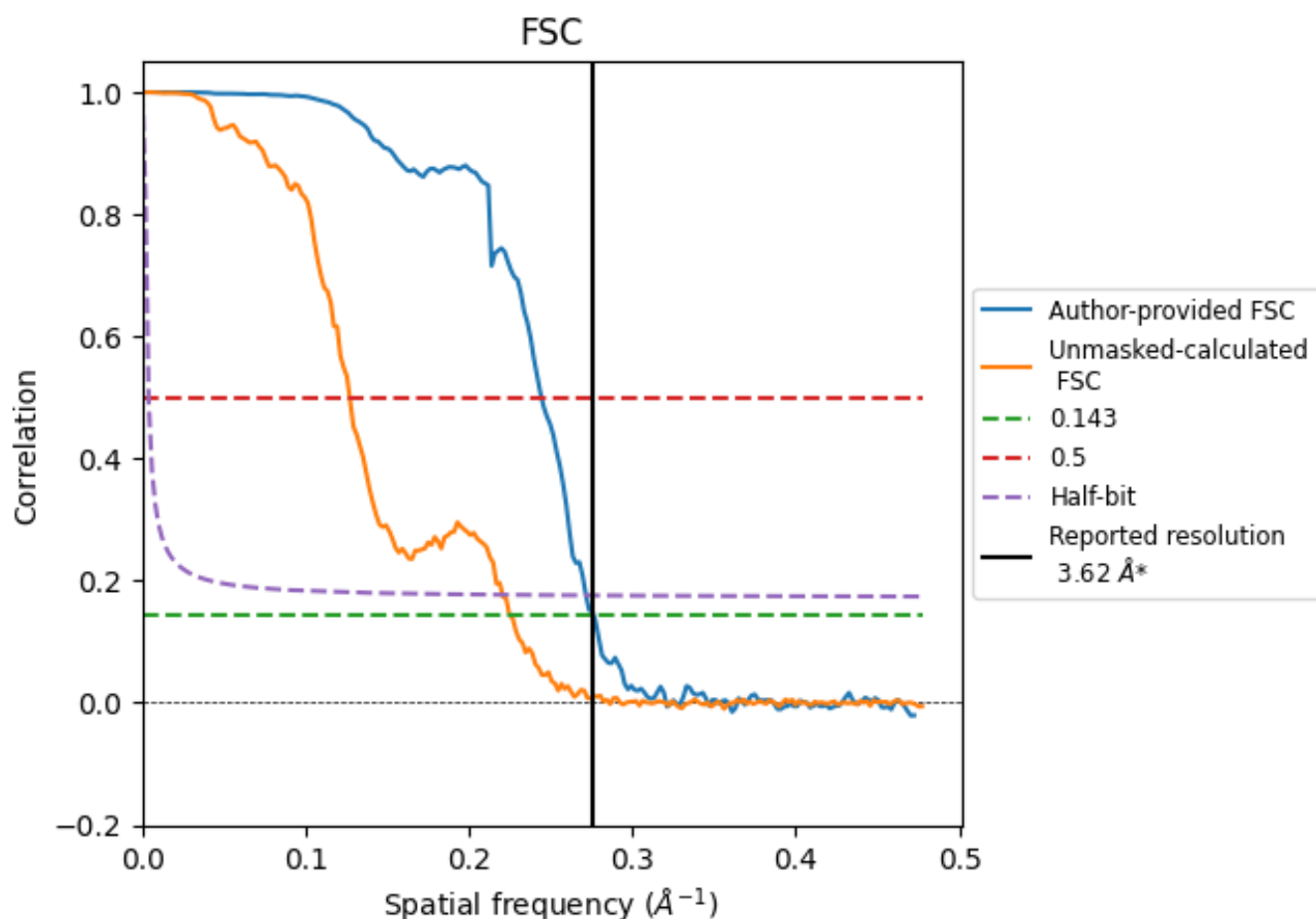


*Reported resolution corresponds to spatial frequency of 0.276 Å⁻¹

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 $0.276 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.62	4.09	3.68
Unmasked-calculated*	4.44	7.88	4.54

*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 4.44 differs from the reported value 3.62 by more than 10 %

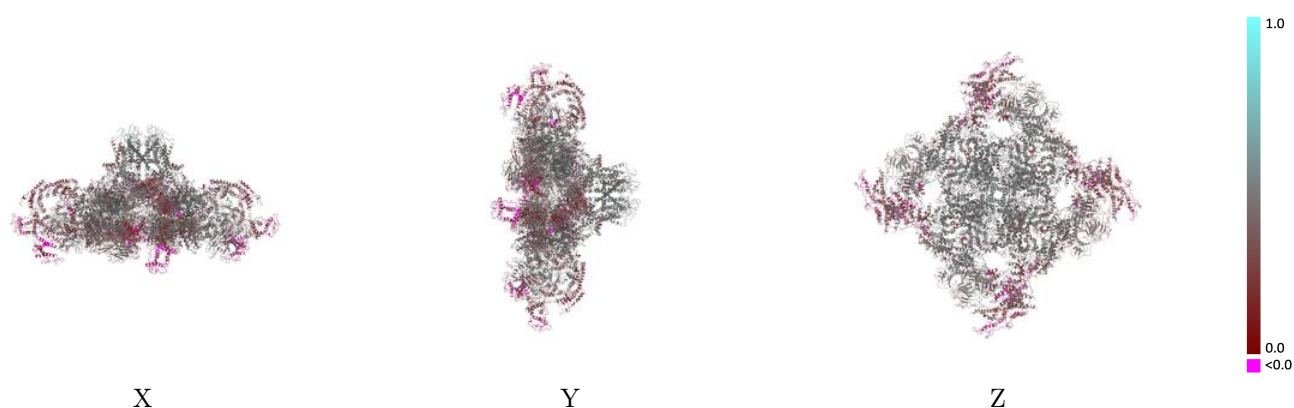
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-38448 and PDB model 8XLH. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)

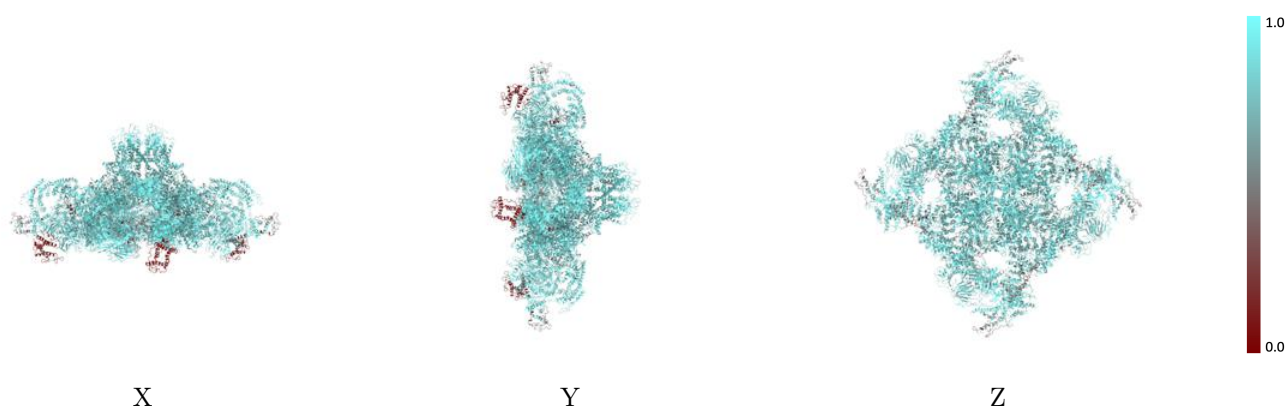
This section was not generated.

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



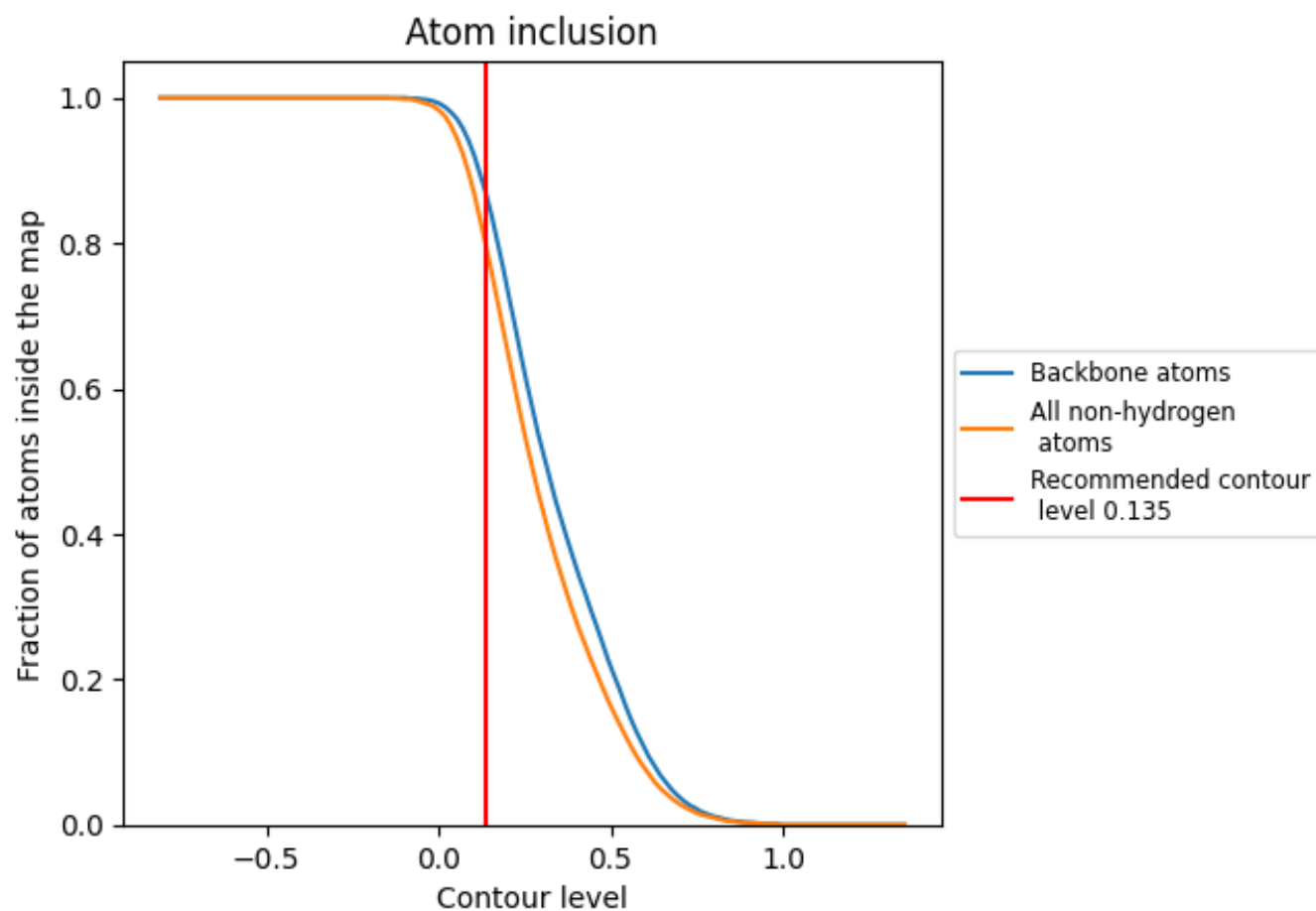
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.135).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 80% 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 (0.135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.3860
A	0.8120	0.3950
B	0.8110	0.3950
C	0.8110	0.3960
D	0.7960	0.3770
E	0.8380	0.4100
F	0.8380	0.4150
G	0.8360	0.4110
H	0.8190	0.3940
I	0.6560	0.2530
J	0.6550	0.2540
K	0.6580	0.2500
L	0.6400	0.2360

