



wwPDB EM Validation Summary Report ⓘ

Nov 14, 2022 – 06:50 PM JST

PDB ID : 6JIY
EMDB ID : EMD-9837
Title : Structure of RyR2 (F/A/C/H-Ca²⁺/Ca²⁺+CaM dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-24
Resolution : 3.90 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

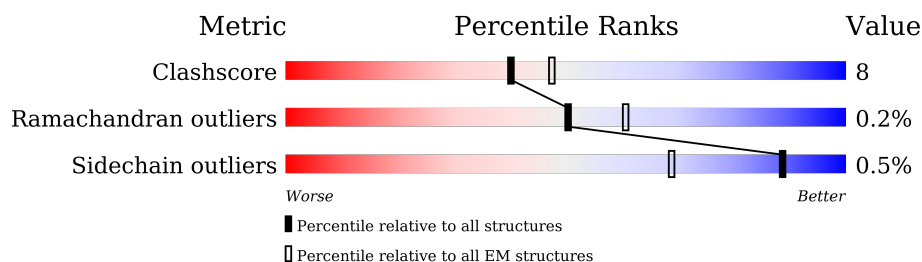
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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.



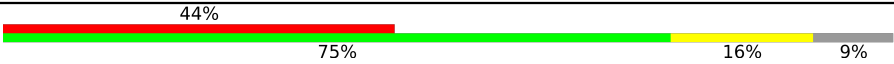

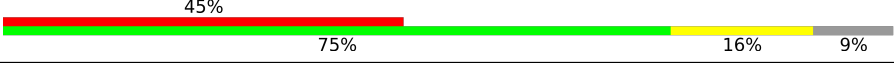
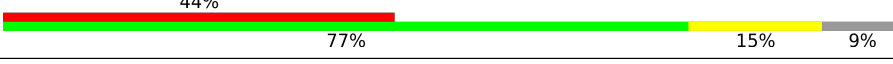
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	4968	
1	D	4968	
1	G	4968	
1	J	4968	
2	B	108	
2	E	108	
2	H	108	
2	K	108	

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Mol	Chain	Length	Quality of chain
3	C	149	
3	F	149	
3	I	149	
3	L	149	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 115288 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	D	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	G	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		
1	J	3521	Total	C	N	O	S	0	0
			26877	17119	4610	4988	160		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	K	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	F	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	I	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		
3	L	136	Total	C	N	O	S	0	0
			1075	663	173	230	9		

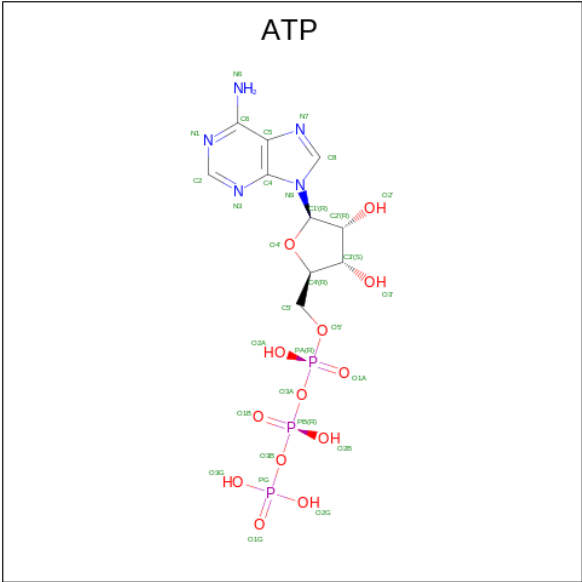
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	J	1	Total 1	Zn 1	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

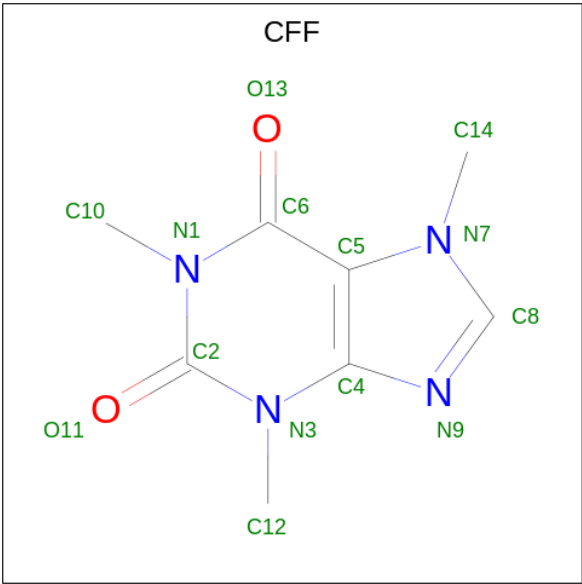
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	C	4	Total 4	Ca 4	0
5	D	1	Total 1	Ca 1	0
5	F	4	Total 4	Ca 4	0
5	G	1	Total 1	Ca 1	0
5	I	4	Total 4	Ca 4	0
5	J	1	Total 1	Ca 1	0
5	L	4	Total 4	Ca 4	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	G	1	Total	C	N	O	P	0
			31	10	5	13	3	
6	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 7 is CAFFEINE (three-letter code: CFF) (formula: C₈H₁₀N₄O₂).

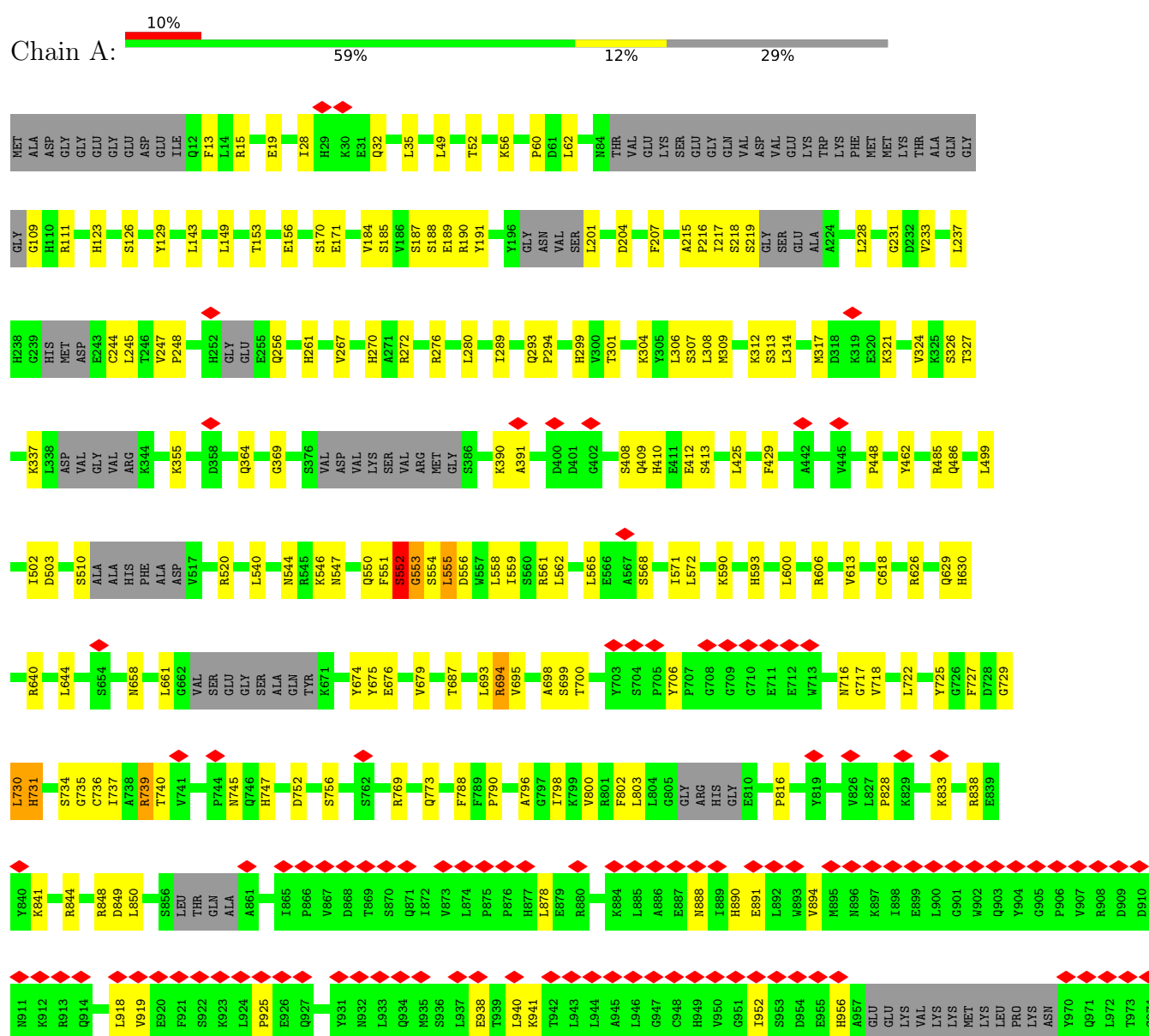


Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 4	O 2	0
7	D	1	Total 14	C 8	N 4	O 2	0
7	G	1	Total 14	C 8	N 4	O 2	0
7	J	1	Total 14	C 8	N 4	O 2	0

3 Residue-property plots [i](#)

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: RyR2





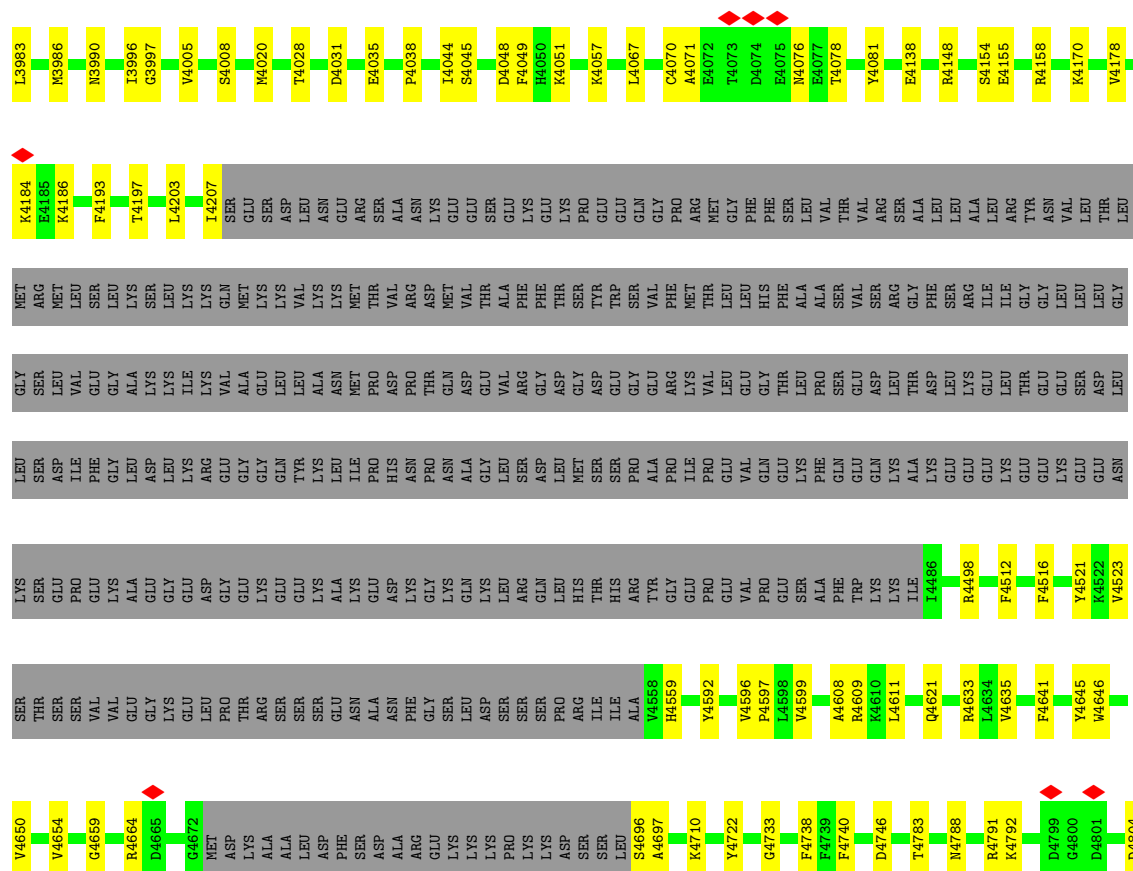




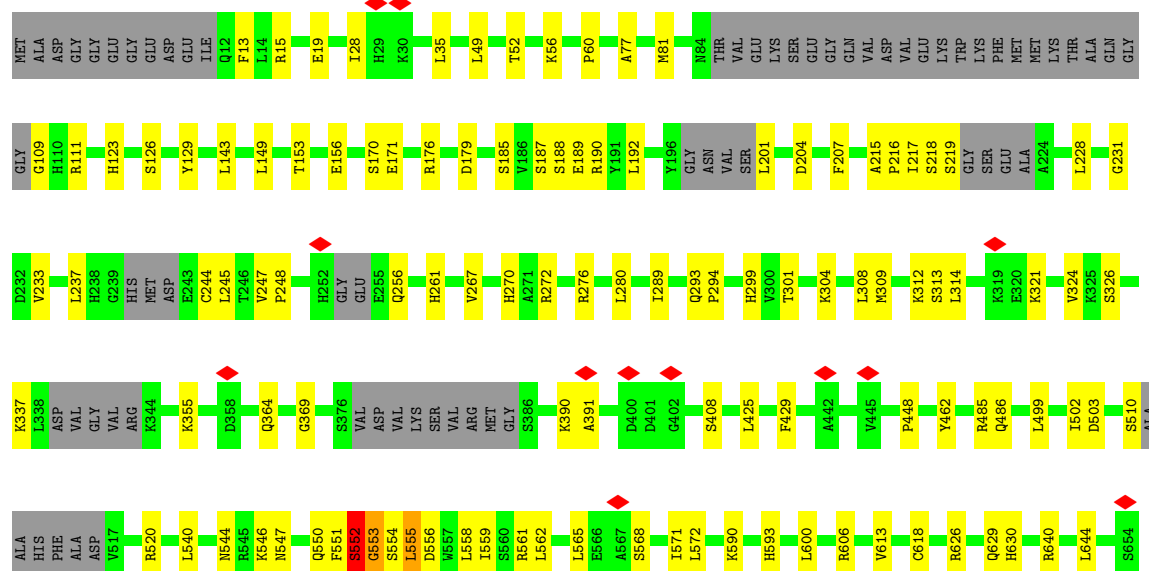
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D1160	V1161	M1168	M1174	F1175	T1176	L1177	N1178	L1182	L1183	D1184	D1185	S1188	E1189	L1190	K1193	S1206	L1207	G1208	V1209	A1210	Q1211	R1214	K1219	D1220	K1225	I1229	C1230	G1231	L1232	Q1233	Y1236	E1237	A1240	V1241	W1250	L1251	S1252	K1253	R1254	Q1257	F1258	L1259	Q1260																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
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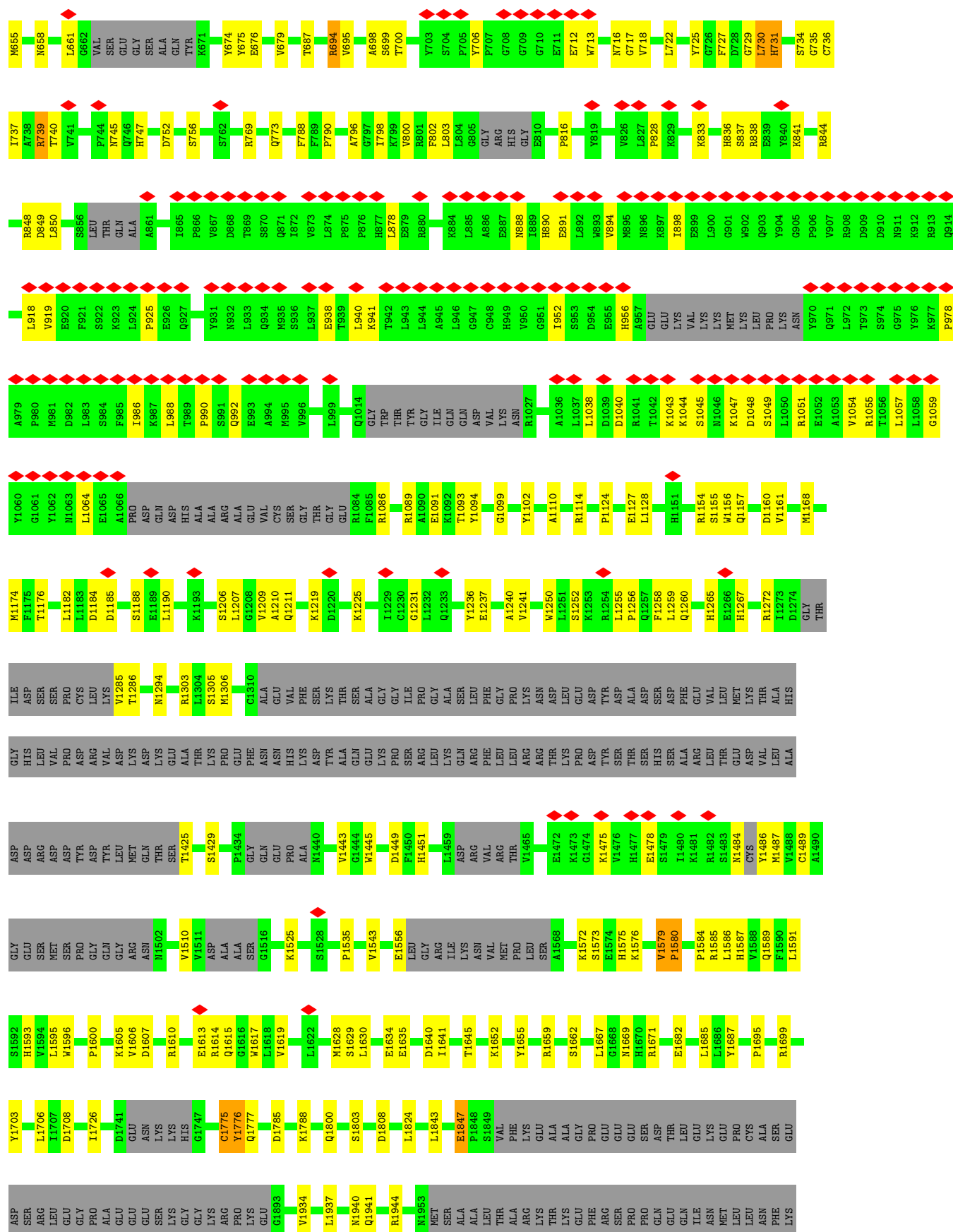


G3825	HIS	CYS	ASP	GLN	GLU	LYS	LYS	ALA	ASN	TYR	TYR	PRO	LYS	ASP	GLU	ASP	SER	VAL	SER
K3829	GLU	ARG	ILE	GLY	ASN	PRO	LYS	LEU	ILE	VAL	VAL	GLY	VAL	GLY	ALA	ASP	ASP	D2876	
T3837	ASP	TYR	SER	LYS	GLU	GLY	VAL	GLY	LEU	GLY	GLY	THR	THR	THR	THR	THR	THR	D2877	
F3841	ASP	TYR	ILE	LYS	ASP	GLY	VAL	GLY	LEU	GLY	GLY	THR	THR	THR	THR	THR	THR	L2878	
Q3845	GLY	SER	HIS	ARG	ASP	GLY	VAL	GLY	LEU	GLY	GLY	THR	THR	THR	THR	THR	THR	T2879	
L3846	GLU	VAL	LEU	ARG	GLY	ASP	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	A2880	
L3847	GLU	GLY	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	G2881	
S3853	VAL	HIS	LYS	TYR	TYR	VAL	VAL	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	V2882	
D3854	LYS	GLN	GLU	SER	GLY	ALA	LEU	ILE	ASP	VAL	VAL	ASP	ASP	ASP	ASP	ASP	ASP	S2883	
N3857	LYS	ARG	PRO	GLN	GLY	GLY	LEU	ILE	ASP	GLY	GLY	THR	THR	THR	THR	THR	THR	P2884	
T3875	LYS	LYS	ALA	THR	THR	THR	GLY	VAL	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	R2885	
L3879	GLY	ARG	ARG	ILE	THR	THR	GLY	VAL	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	D2886	
Q3883	GLY	LYS	TRP	ILE	VAL	VAL	GLY	VAL	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	L2887	
E3884	GLY	GLY	ALA	VAL	ALA	ALA	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	D2888	
S3885	GLY	GLY	ALA	VAL	ALA	ALA	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	G2889	
Y3893	GLY	GLY	TYR	ILE	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	A2890	
T3899	GLY	GLY	ASP	ARG	ARG	ARG	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	Q2891	
E3901	GLY	GLY	PRO	ILE	THR	THR	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	D2892	
R3906	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	L2893	
T3920	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	K2894	
E3923	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	L2895	
Y3924	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	K2896	
L3925	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	F2896	
N3932	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	L2897	
Q3933	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	Q2898	
S3934	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	K2899	
S3935	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	L2899	
L3936	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	Q2901	
S3939	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	Y2902	
R3940	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	A2903	
L3941	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	V2904	
A3944	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	S2905	
G3947	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	R2906	
M3955	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	E2847	
Q3956	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	N2848	
L3959	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	Y2849	
S3960	GLY	GLY	GLY	VAL	VAL	VAL	GLY	GLY	GLY	GLY	GLY	THR	THR	THR	THR	THR	THR	H2850	
																		G2851	
																		L2852	
																		G2853	
																		A2854	
																		K2855	
																		K2856	
																		K2857	
																		R2858	
																		L2859	
																		E2860	
																		L2861	
																		E2862	
																		S2863	
																		K2864	
																		G2865	
																		G2866	
																		G2867	
																		N2868	
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																		V2873	
																		P2874	



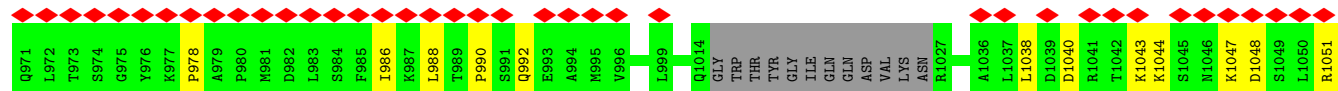
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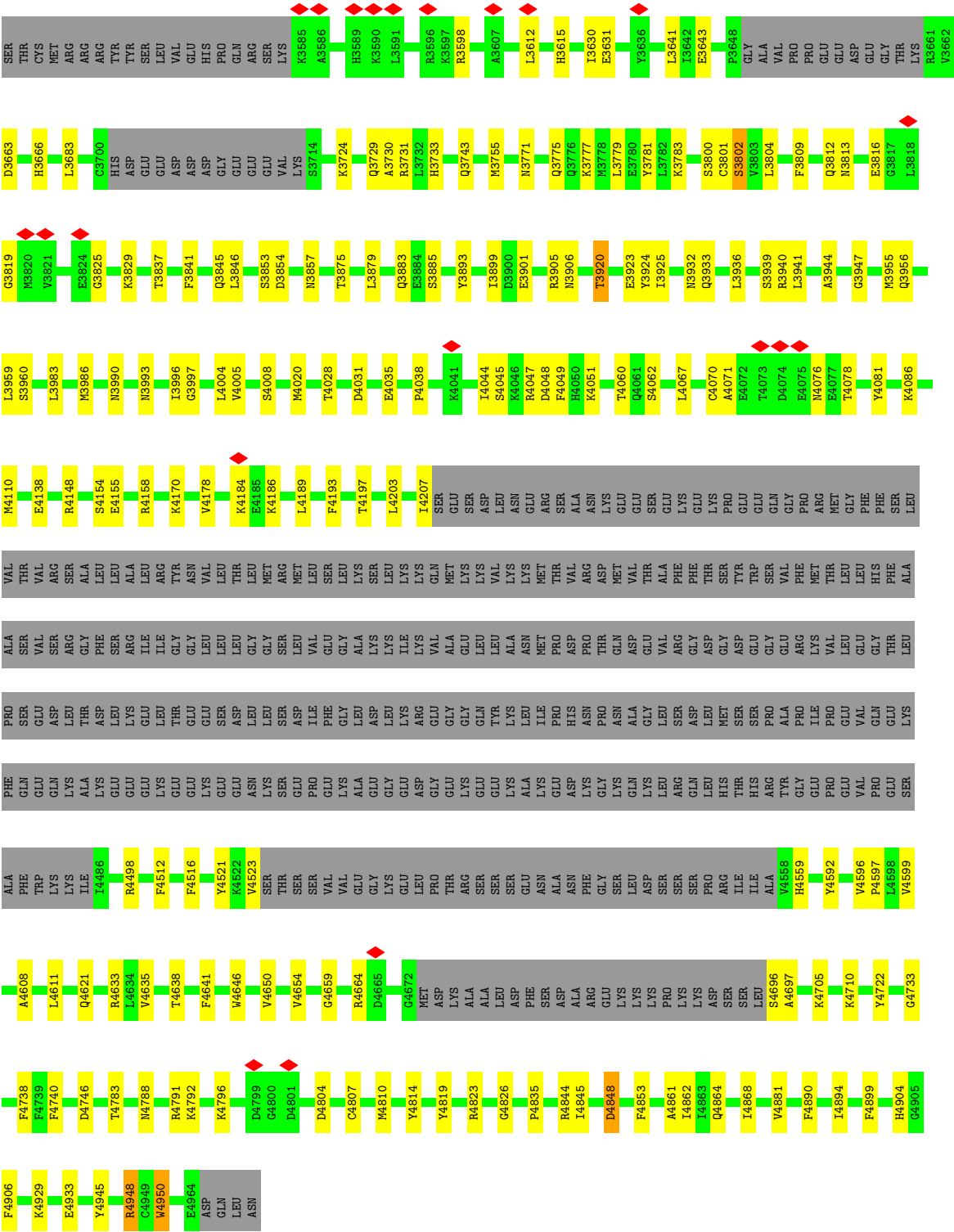




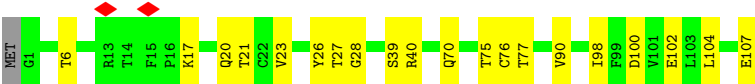
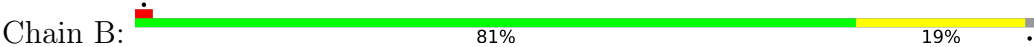









● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B




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

Chain E: 




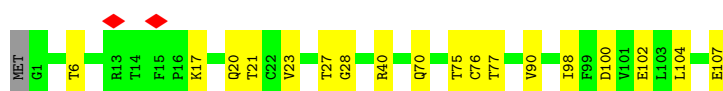
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




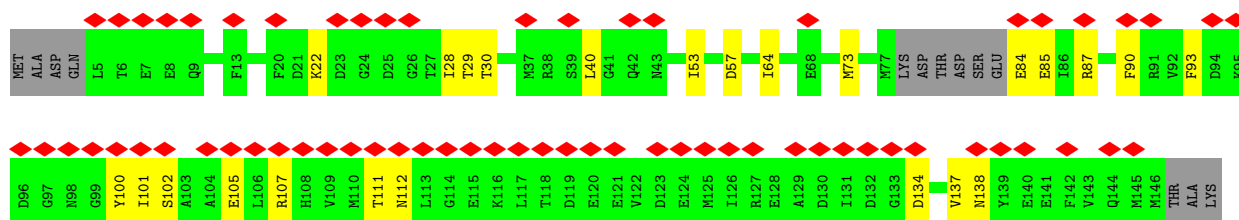
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K: 




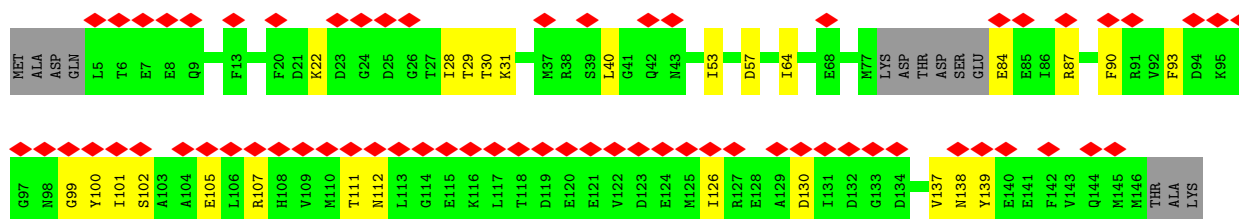
- Molecule 3: Calmodulin-1

Chain C: 




- Molecule 3: Calmodulin-1

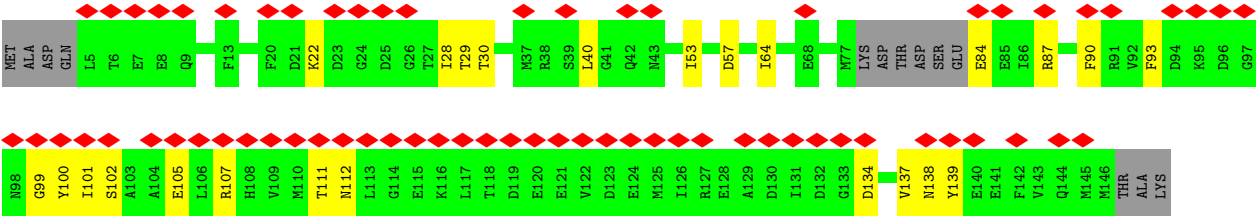
Chain F: 



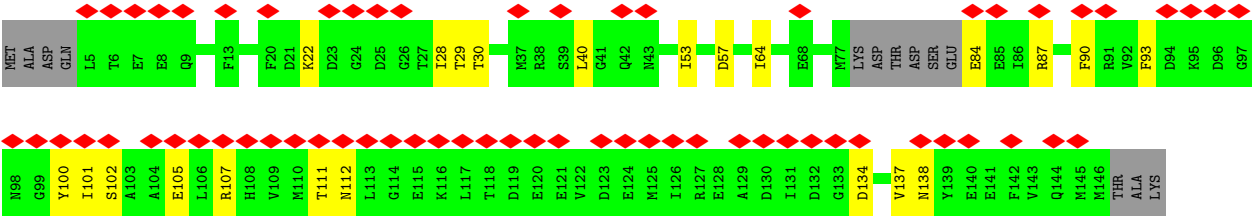
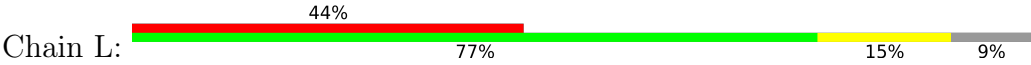
- Molecule 3: Calmodulin-1

Chain I: 





• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	96158	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.062	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.40	2/27385 (0.0%)	0.57	7/37042 (0.0%)
1	D	0.40	2/27385 (0.0%)	0.57	7/37042 (0.0%)
1	G	0.40	2/27385 (0.0%)	0.57	7/37042 (0.0%)
1	J	0.40	2/27385 (0.0%)	0.57	7/37042 (0.0%)
2	B	0.35	0/835	0.55	0/1123
2	E	0.35	0/835	0.55	0/1123
2	H	0.35	0/835	0.55	0/1123
2	K	0.35	0/835	0.55	0/1123
3	C	0.28	0/1086	0.48	0/1456
3	F	0.28	0/1086	0.48	0/1456
3	I	0.28	0/1086	0.48	0/1456
3	L	0.28	0/1086	0.48	0/1456
All	All	0.39	8/117224 (0.0%)	0.57	28/158484 (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	A	0	19
1	D	0	19
1	G	0	19
1	J	0	19
All	All	0	76

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4950	TRP	CB-CG	-6.13	1.39	1.50
1	G	4950	TRP	CB-CG	-6.13	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	4950	TRP	CB-CG	-6.13	1.39	1.50
1	D	4950	TRP	CB-CG	-6.09	1.39	1.50
1	G	2198	CYS	CB-SG	-5.54	1.72	1.81

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	3612	LEU	CA-CB-CG	7.47	132.49	115.30
1	G	3612	LEU	CA-CB-CG	7.47	132.49	115.30
1	A	3612	LEU	CA-CB-CG	7.47	132.48	115.30
1	J	3612	LEU	CA-CB-CG	7.46	132.46	115.30
1	G	2517	LEU	CA-CB-CG	6.33	129.85	115.30

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	551	PHE	Peptide
1	A	552	SER	Peptide
1	A	729	GLY	Peptide
1	A	731	HIS	Peptide
1	A	739	ARG	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26877	0	25382	455	0
1	D	26877	0	25382	463	0
1	G	26877	0	25382	458	0
1	J	26877	0	25382	454	0
2	B	819	0	824	11	0
2	E	819	0	824	9	0
2	H	819	0	824	9	0
2	K	819	0	824	11	0
3	C	1075	0	1011	16	0
3	F	1075	0	1011	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	1075	0	1011	16	0
3	L	1075	0	1011	14	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	C	4	0	0	0	0
5	D	1	0	0	0	0
5	F	4	0	0	0	0
5	G	1	0	0	0	0
5	I	4	0	0	0	0
5	J	1	0	0	0	0
5	L	4	0	0	0	0
6	A	31	0	12	1	0
6	D	31	0	12	1	0
6	G	31	0	12	1	0
6	J	31	0	12	1	0
7	A	14	0	10	2	0
7	D	14	0	10	2	0
7	G	14	0	10	2	0
7	J	14	0	10	2	0
All	All	115288	0	108956	1705	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 8.

The worst 5 of 1705 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:G:4862:ILE:HG22	1:J:4868:ILE:CD1	1.57	1.35
1:A:4868:ILE:CD1	1:J:4862:ILE:HG22	1.58	1.34
1:D:4862:ILE:HG22	1:G:4868:ILE:CD1	1.59	1.30
1:A:4862:ILE:HG22	1:D:4868:ILE:CD1	1.60	1.30
1:G:4862:ILE:CG2	1:J:4868:ILE:HD13	1.64	1.28

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	3405/4968 (68%)	2973 (87%)	423 (12%)	9 (0%)	41	75
1	D	3405/4968 (68%)	2974 (87%)	422 (12%)	9 (0%)	41	75
1	G	3405/4968 (68%)	2973 (87%)	423 (12%)	9 (0%)	41	75
1	J	3405/4968 (68%)	2974 (87%)	422 (12%)	9 (0%)	41	75
2	B	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	E	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	H	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
2	K	105/108 (97%)	91 (87%)	14 (13%)	0	100	100
3	C	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	F	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	I	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
3	L	132/149 (89%)	123 (93%)	9 (7%)	0	100	100
All	All	14568/20900 (70%)	12750 (88%)	1782 (12%)	36 (0%)	50	79

5 of 36 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	553	GLY
1	A	1776	TYR
1	D	553	GLY
1	D	1776	TYR
1	G	553	GLY

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	2701/4355 (62%)	2687 (100%)	14 (0%)	88	93
1	D	2700/4355 (62%)	2685 (99%)	15 (1%)	86	91
1	G	2700/4355 (62%)	2685 (99%)	15 (1%)	86	91
1	J	2700/4355 (62%)	2685 (99%)	15 (1%)	86	91
2	B	88/89 (99%)	88 (100%)	0	100	100
2	E	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
2	K	88/89 (99%)	88 (100%)	0	100	100
3	C	116/127 (91%)	116 (100%)	0	100	100
3	F	116/127 (91%)	116 (100%)	0	100	100
3	I	116/127 (91%)	116 (100%)	0	100	100
3	L	116/127 (91%)	116 (100%)	0	100	100
All	All	11617/18284 (64%)	11558 (100%)	59 (0%)	89	93

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4853	PHE
1	J	3920	THR
1	G	1176	THR
1	J	3879	LEU
1	J	990	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 153 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	32	GLN
1	J	4076	ASN
1	J	544	ASN
1	J	1684	GLN
1	J	4937	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 24 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	D	6002	-	26,33,33	0.87	0	31,52,52	1.55	5 (16%)
7	CFF	D	6003	-	8,15,15	2.74	4 (50%)	8,23,23	1.21	1 (12%)
7	CFF	A	6003	-	8,15,15	2.74	4 (50%)	8,23,23	1.21	1 (12%)
6	ATP	A	6002	-	26,33,33	0.87	1 (3%)	31,52,52	1.55	5 (16%)
6	ATP	J	6002	-	26,33,33	0.87	1 (3%)	31,52,52	1.55	5 (16%)
6	ATP	G	6002	-	26,33,33	0.86	1 (3%)	31,52,52	1.55	5 (16%)
7	CFF	G	6003	-	8,15,15	2.73	4 (50%)	8,23,23	1.20	1 (12%)
7	CFF	J	6003	-	8,15,15	2.74	4 (50%)	8,23,23	1.21	1 (12%)

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	D	6002	-	-	5/18/38/38	0/3/3/3
7	CFF	D	6003	-	-	-	0/2/2/2
7	CFF	A	6003	-	-	-	0/2/2/2
6	ATP	A	6002	-	-	5/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ATP	J	6002	-	-	5/18/38/38	0/3/3/3
6	ATP	G	6002	-	-	5/18/38/38	0/3/3/3
7	CFF	G	6003	-	-	-	0/2/2/2
7	CFF	J	6003	-	-	-	0/2/2/2

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	6003	CFF	C5-C4	-4.77	1.33	1.39
7	D	6003	CFF	C5-C4	-4.77	1.33	1.39
7	J	6003	CFF	C5-C4	-4.77	1.33	1.39
7	G	6003	CFF	C6-N1	-4.74	1.31	1.38
7	A	6003	CFF	C6-N1	-4.73	1.31	1.38

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	6002	ATP	PB-O3B-PG	-3.84	119.66	132.83
6	A	6002	ATP	PB-O3B-PG	-3.84	119.66	132.83
6	G	6002	ATP	PB-O3B-PG	-3.84	119.66	132.83
6	J	6002	ATP	PB-O3B-PG	-3.83	119.67	132.83
6	J	6002	ATP	PA-O3A-PB	-3.57	120.59	132.83

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O1A
6	A	6002	ATP	C5'-O5'-PA-O2A
6	D	6002	ATP	C5'-O5'-PA-O1A
6	D	6002	ATP	C5'-O5'-PA-O2A
6	G	6002	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

8 monomers are involved in 12 short contacts:

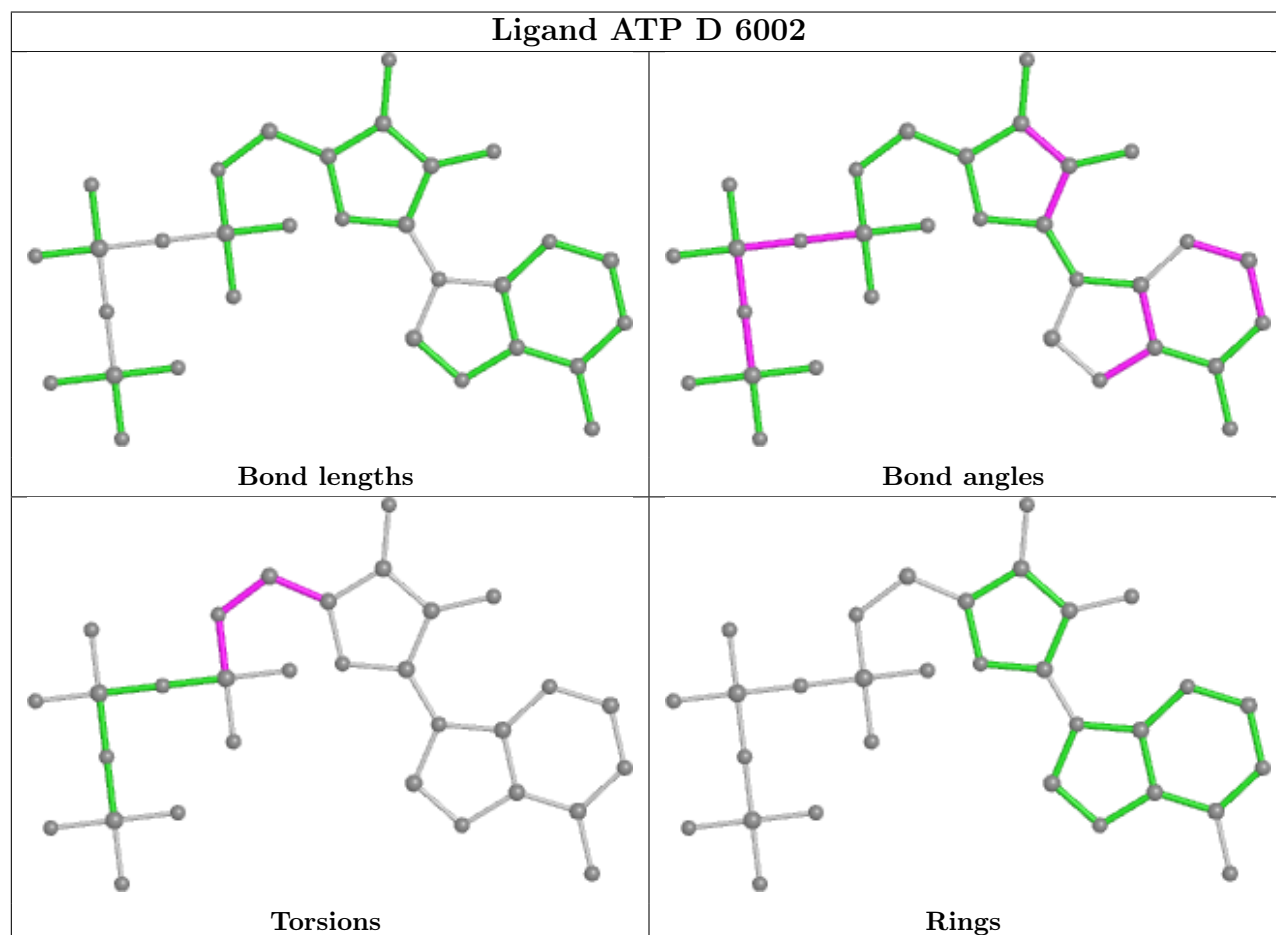
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	6002	ATP	1	0
7	D	6003	CFF	2	0
7	A	6003	CFF	2	0

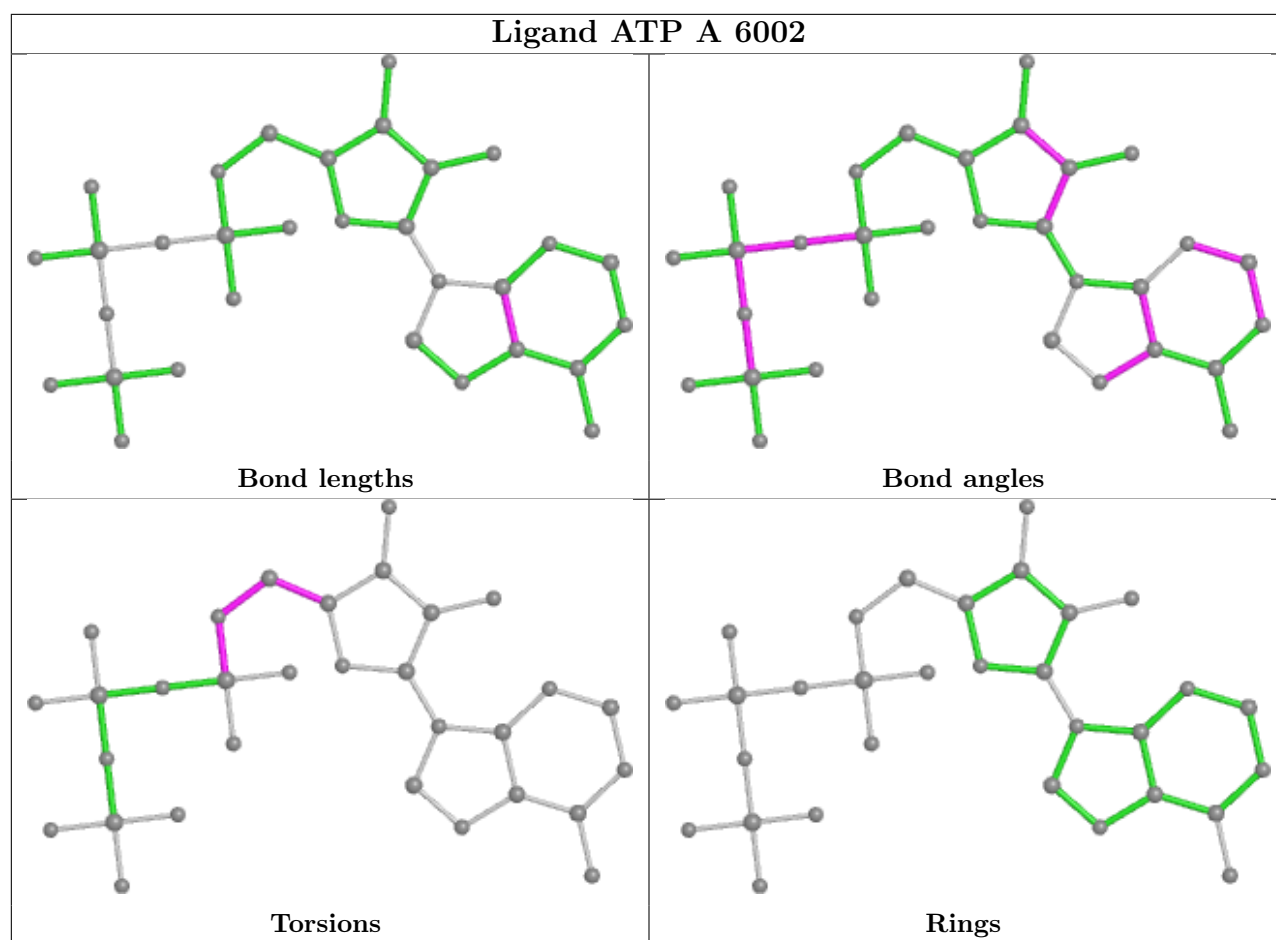
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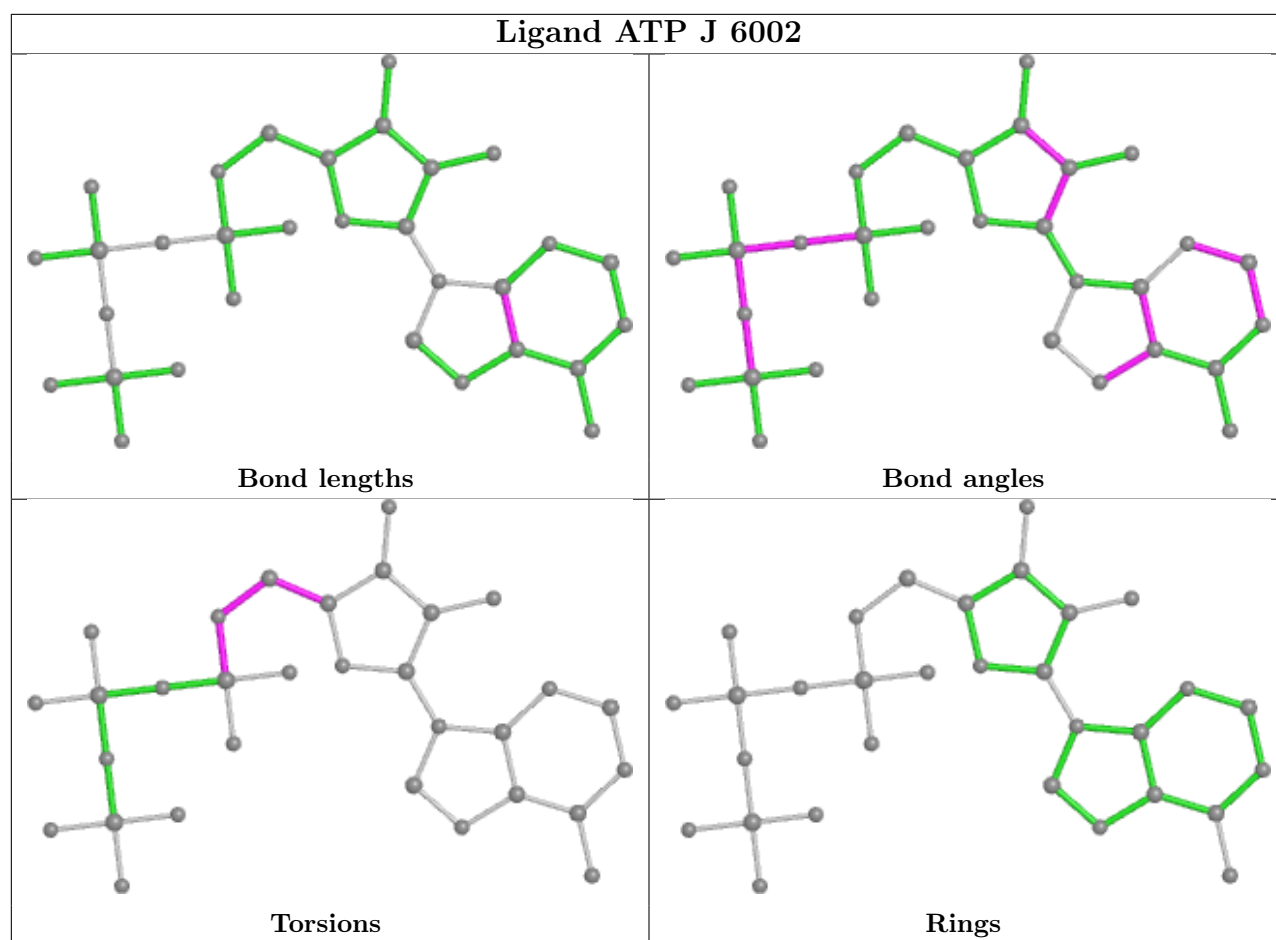
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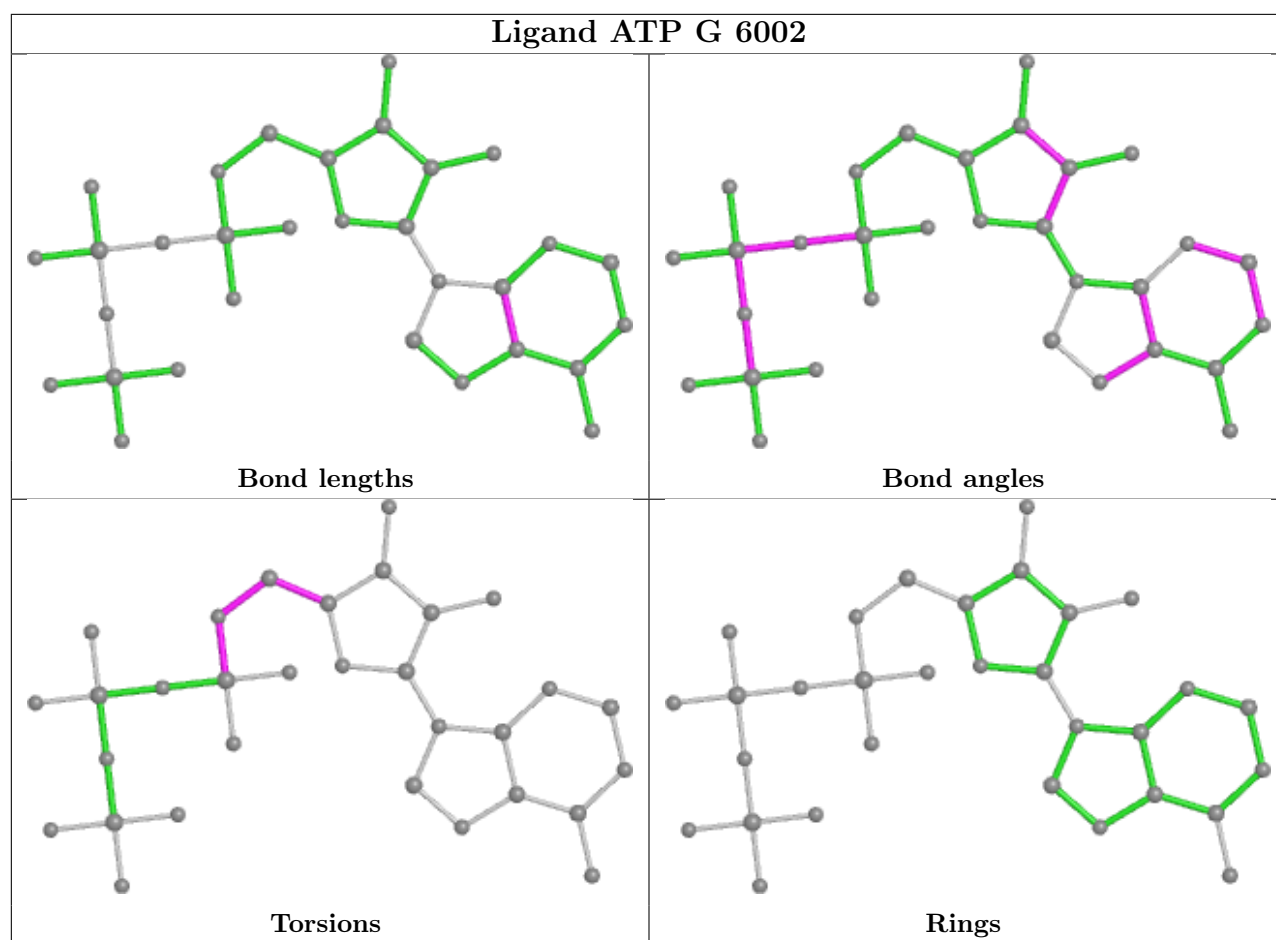
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	6002	ATP	1	0
6	J	6002	ATP	1	0
6	G	6002	ATP	1	0
7	G	6003	CFE	2	0
7	J	6003	CFE	2	0

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









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.

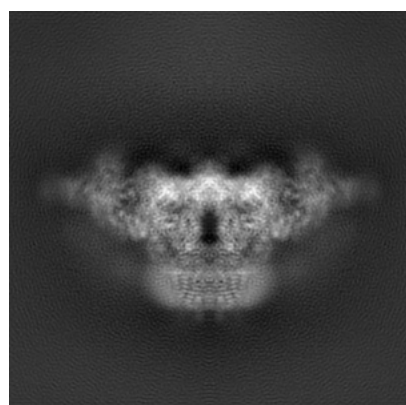
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9837. These allow visual inspection of the internal detail of the map and identification of artifacts.

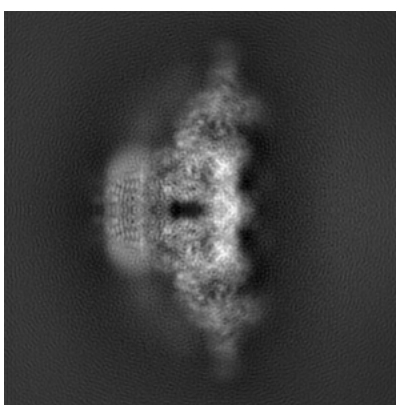
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

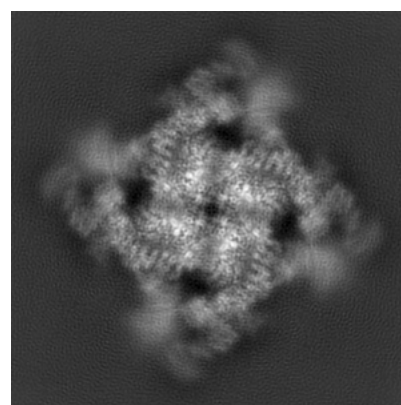
6.1.1 Primary map



X



Y

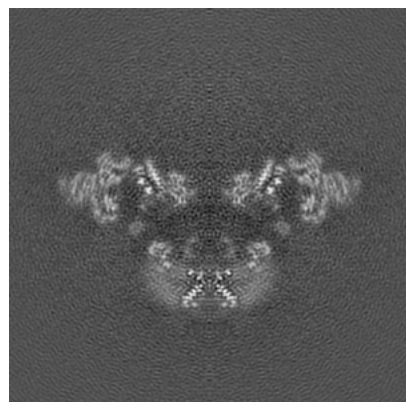


Z

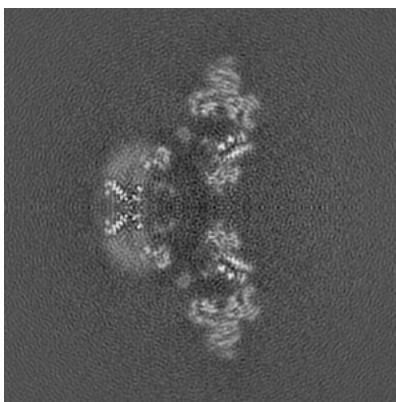
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

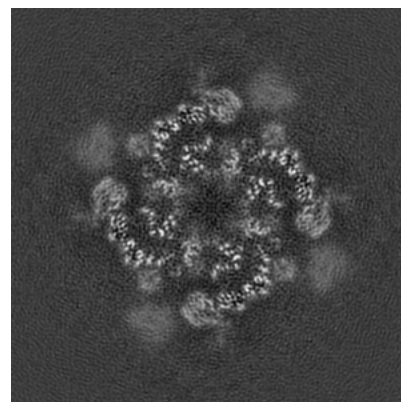
6.2.1 Primary map



X Index: 200



Y Index: 200

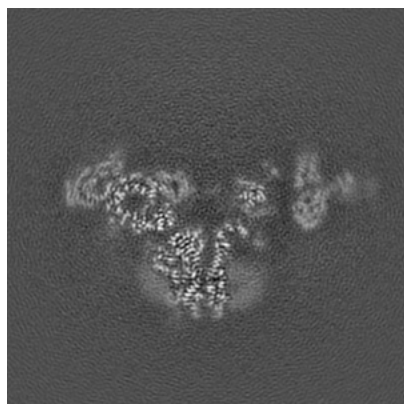


Z Index: 200

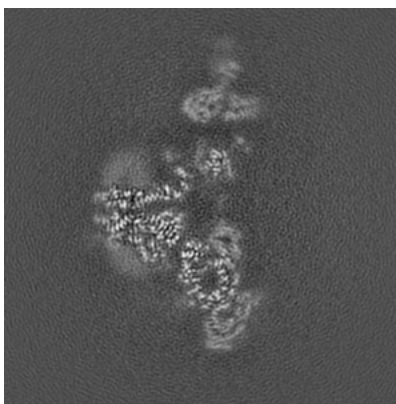
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

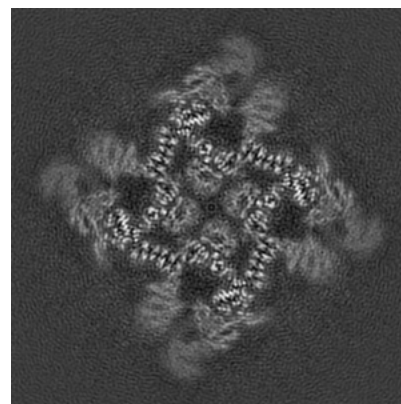
6.3.1 Primary map



X Index: 212



Y Index: 188



Z Index: 214

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

6.4 Orthogonal surface views [i](#)

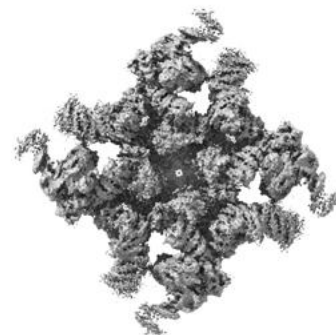
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

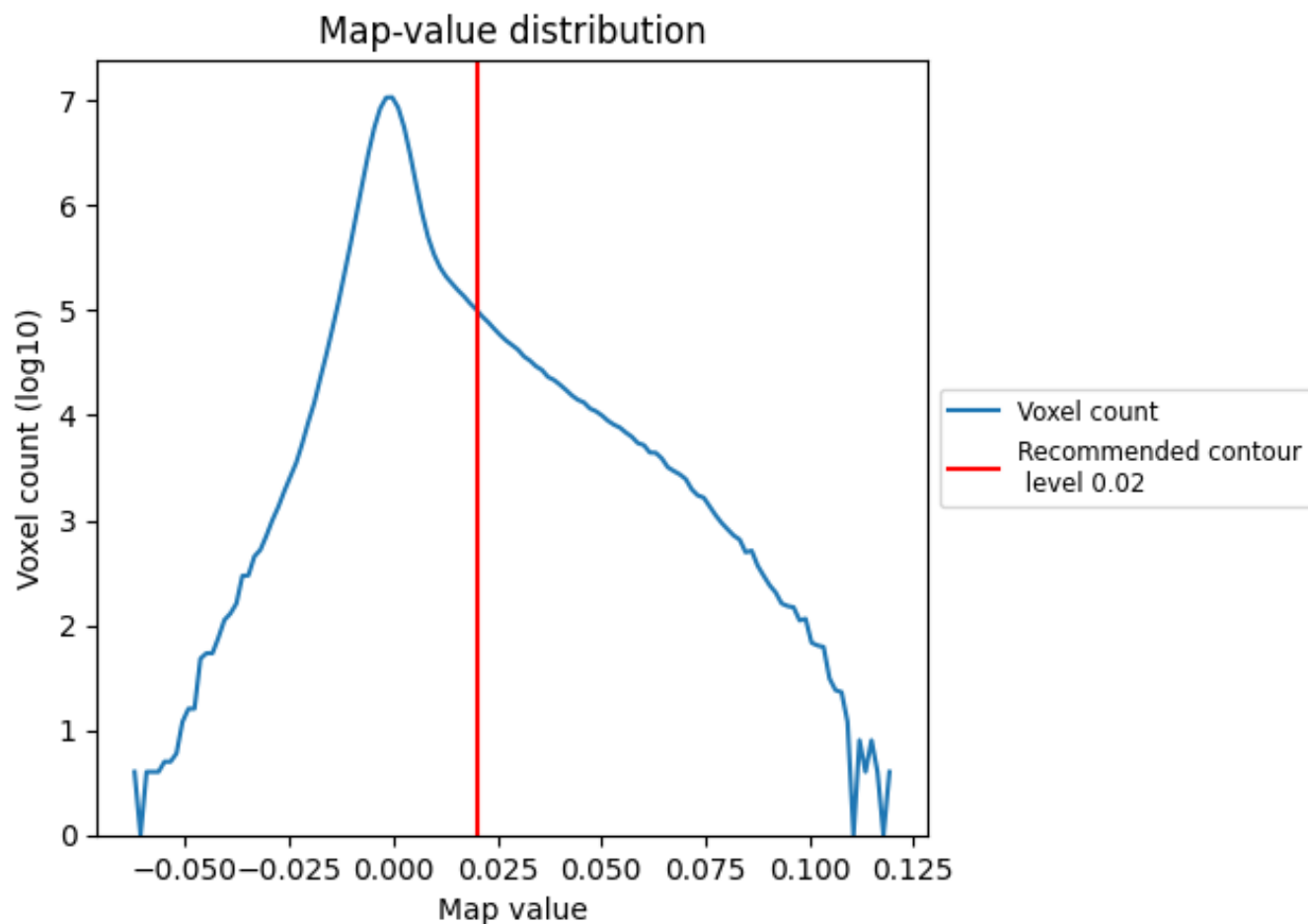
6.5 Mask visualisation

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

7 Map analysis [i](#)

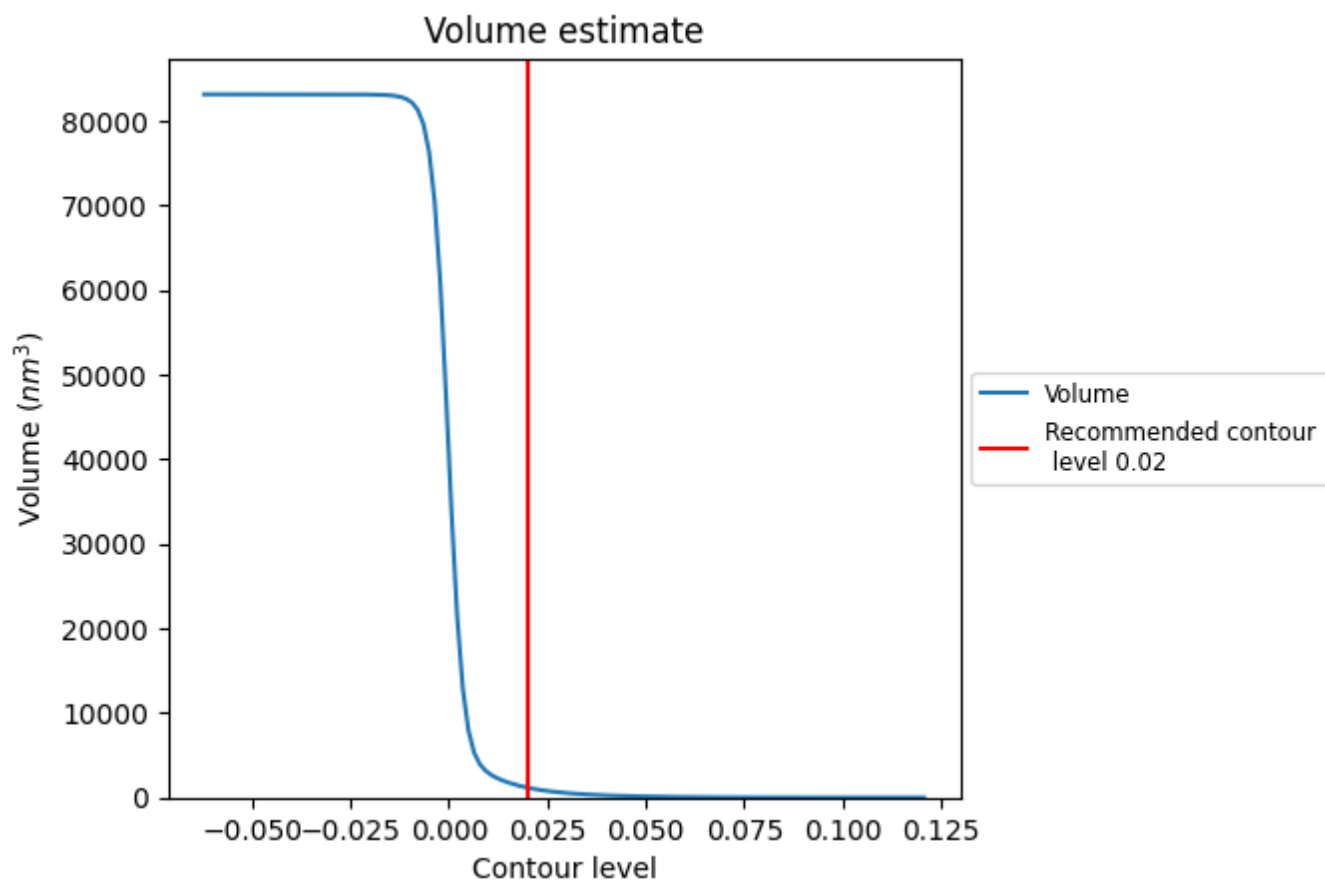
This section contains the results of statistical analysis of the map.

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.

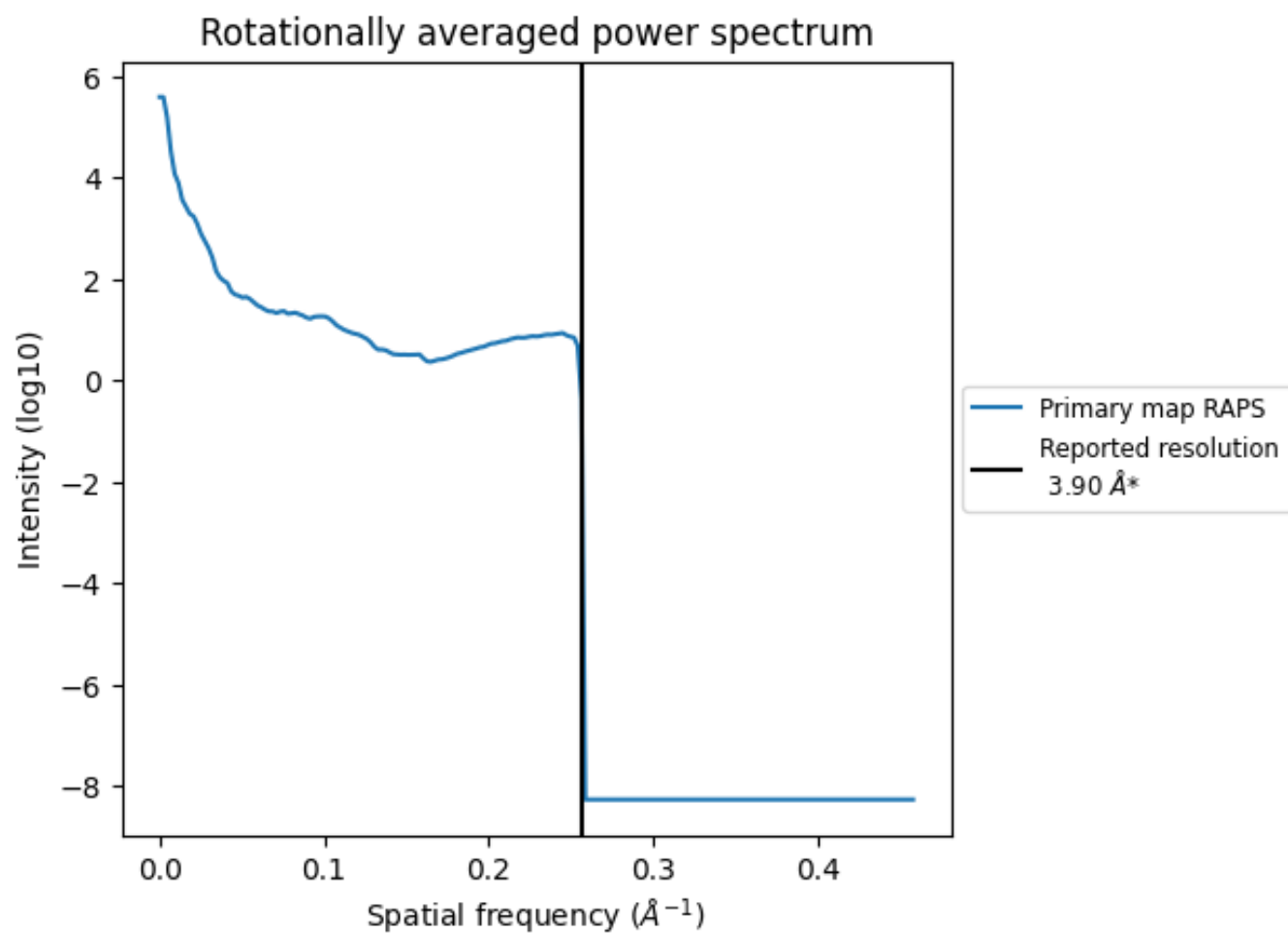
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1164 nm³; this corresponds to an approximate mass of 1051 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 ⓘ

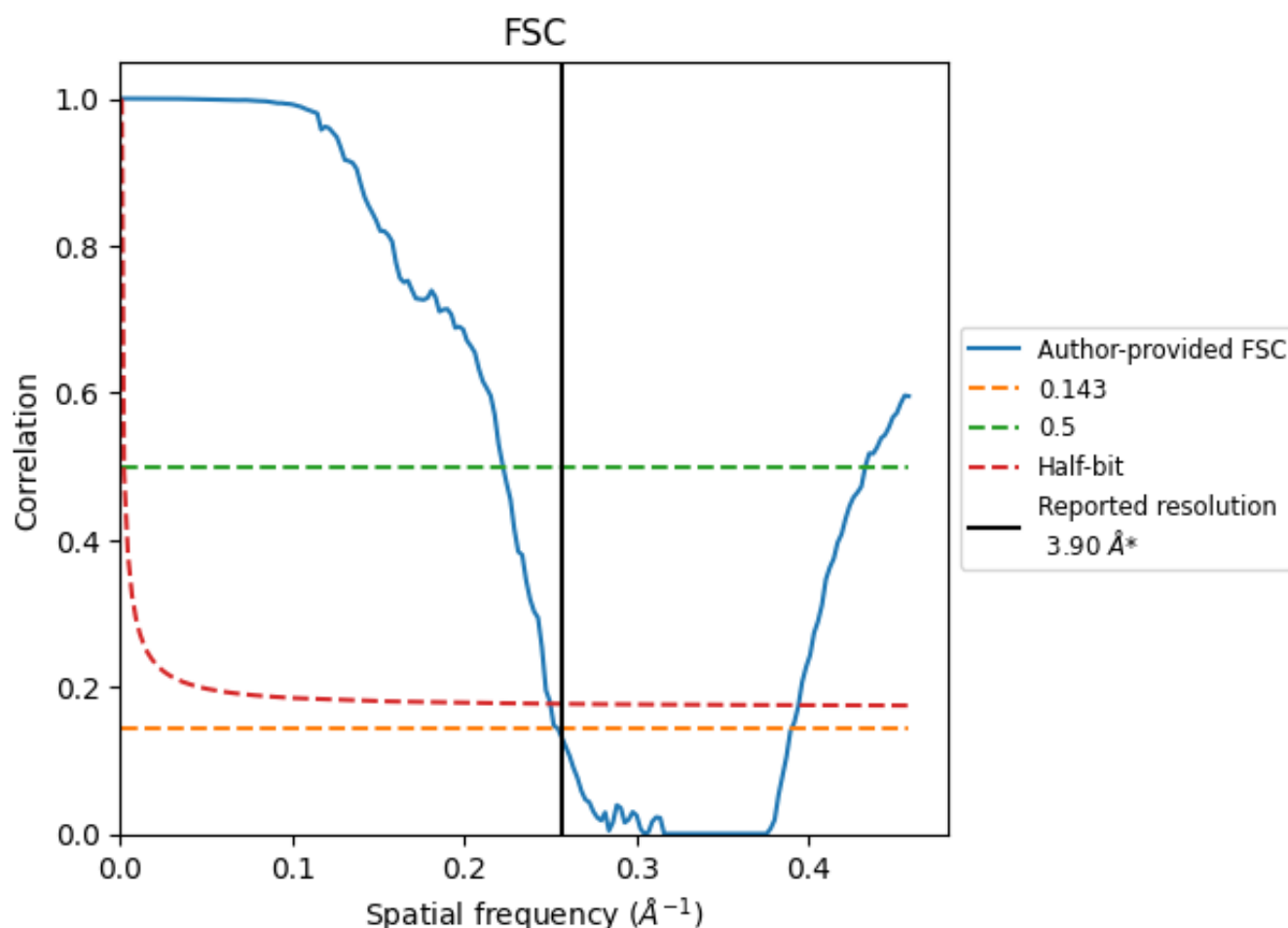


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

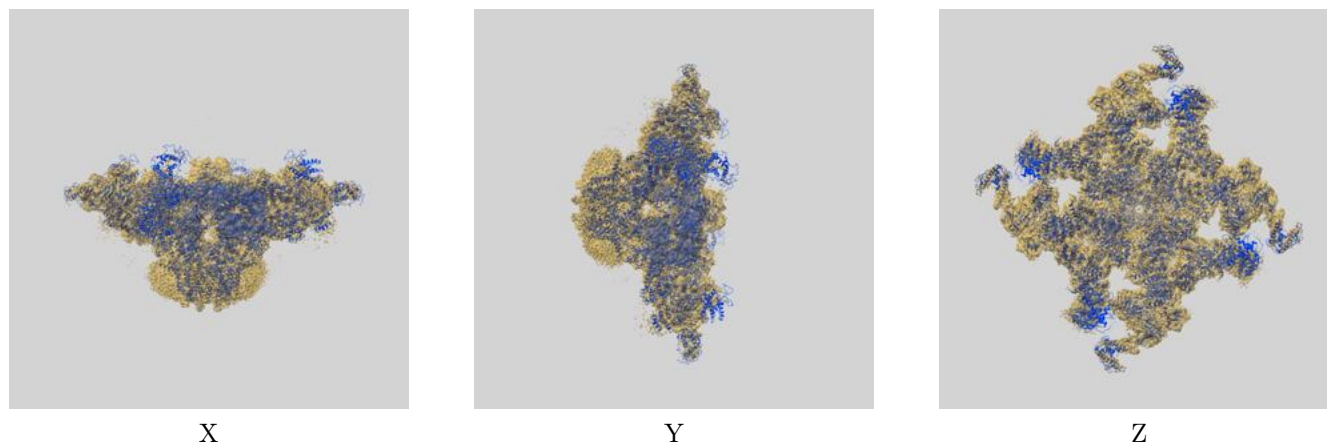
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.49	4.00
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

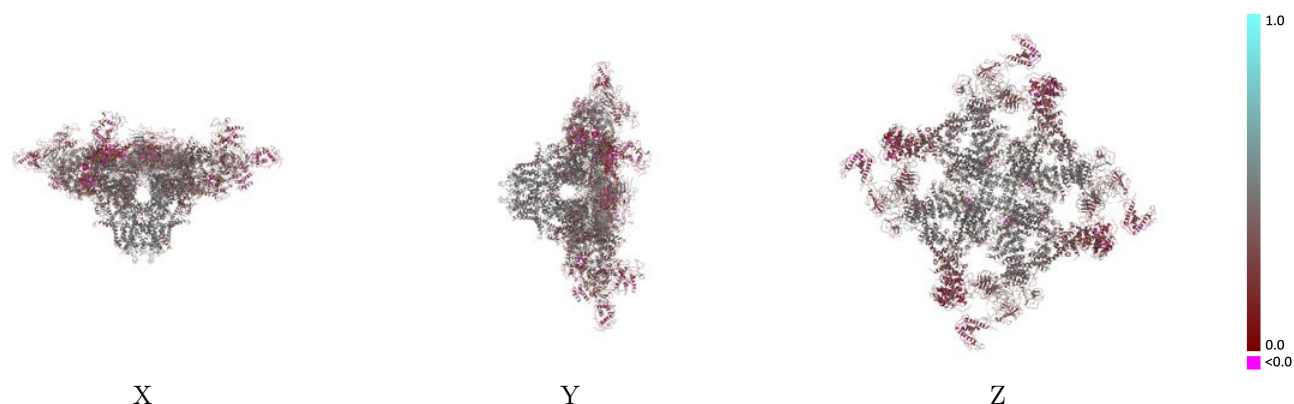
This section contains information regarding the fit between EMDB map EMD-9837 and PDB model 6JIY. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



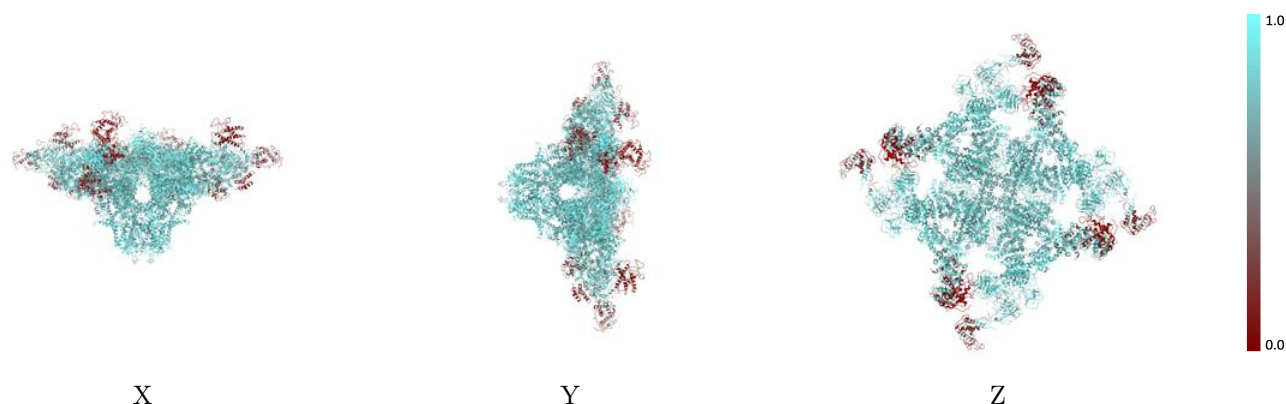
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



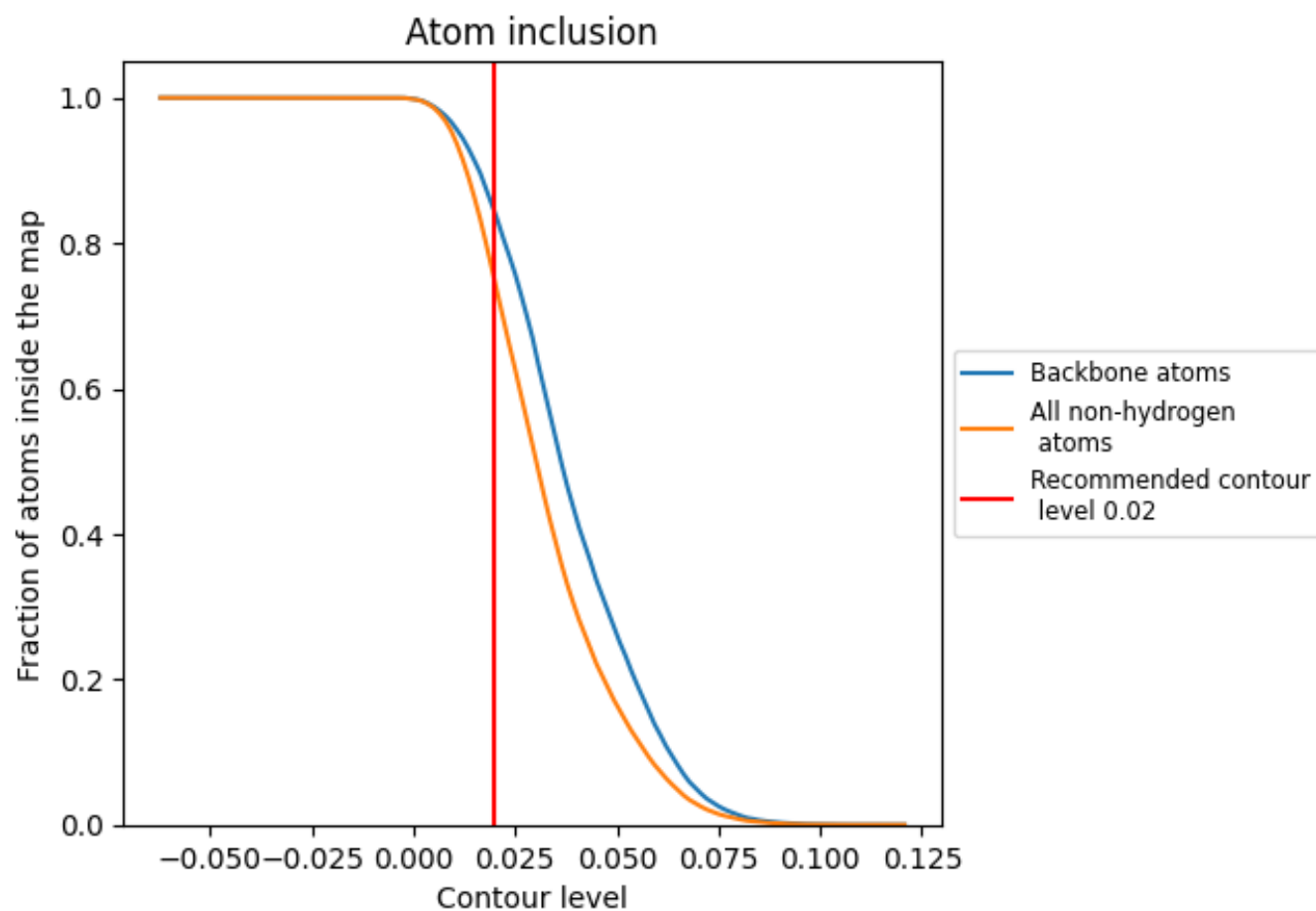
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7463	<div></div> 0.3750
A	<div></div> 0.7588	<div></div> 0.3790
B	<div></div> 0.7993	<div></div> 0.3990
C	<div></div> 0.3944	<div></div> 0.2820
D	<div></div> 0.7594	<div></div> 0.3790
E	<div></div> 0.7993	<div></div> 0.3990
F	<div></div> 0.3962	<div></div> 0.2820
G	<div></div> 0.7590	<div></div> 0.3780
H	<div></div> 0.7993	<div></div> 0.3970
I	<div></div> 0.3925	<div></div> 0.2810
J	<div></div> 0.7583	<div></div> 0.3780
K	<div></div> 0.7968	<div></div> 0.3980
L	<div></div> 0.3972	<div></div> 0.2820

1.0

0.0

<0.0