



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:18 AM UTC

PDB ID : 8DUJ / pdb_00008duj
EMDB ID : EMD-27721
Title : Global map in C1 of RyR1 particles in complex with ImperaCalcin
Authors : Haji-Ghassemi, O.; Van Petegm, F.
Deposited on : 2022-07-27
Resolution : 3.70 Å (reported)
Based on initial model : 6M2W

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:

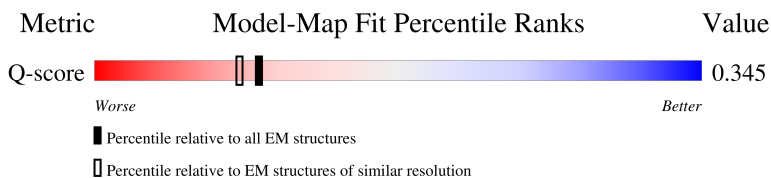
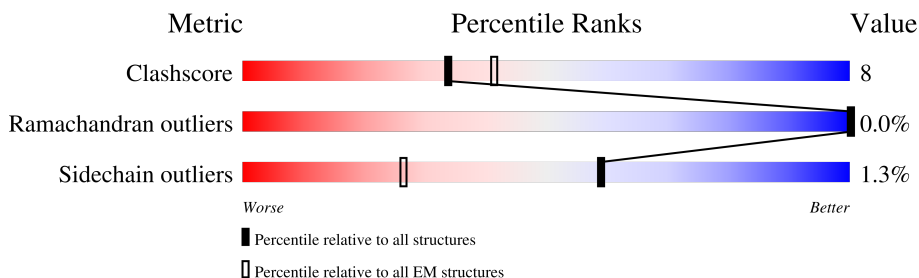
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD 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 3.70 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	11569 (3.20 - 4.20)

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	M	33	24% 67% 33%
2	A	5037	11% 64% 12% 24%
2	D	5037	15% 68% 8% 23%
2	G	5037	8% 66% 12% 22%

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Mol	Chain	Length	Quality of chain
2	J	5037	
3	B	107	
3	E	107	
3	H	107	
3	K	107	
4	C	149	
4	F	149	
4	I	149	
4	L	149	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 106156 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 Imperacalcin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	33	Total	C	N	O	S	33	0
			514	296	116	90	12		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	3933	Total	C	N	O	S	0	0
			26285	16856	4666	4625	138		
2	A	3823	Total	C	N	O	S	1	0
			24845	15885	4439	4407	114		
2	D	3865	Total	C	N	O	S	1	0
			23336	14719	4259	4281	77		
2	J	3892	Total	C	N	O	S	0	0
			25245	16153	4530	4440	122		

- Molecule 3 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	107	Total	C	N	O	S	0	0
			759	483	134	138	4		
3	B	107	Total	C	N	O	S	0	0
			735	465	130	136	4		
3	E	106	Total	C	N	O	S	0	0
			657	415	115	125	2		
3	K	106	Total	C	N	O	S	0	0
			758	483	135	136	4		

- Molecule 4 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	I	138	Total	C	N	O	S	0	0
			711	431	139	139	2		

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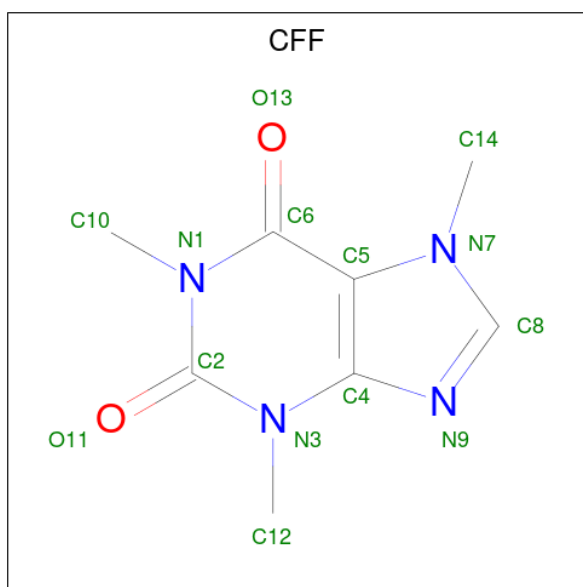
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Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	137	Total	C	N	O	S	0	0
			707	430	137	139	1		
4	F	137	Total	C	N	O		0	0
			710	434	137	139			
4	L	139	Total	C	N	O	S	0	0
			706	427	139	139	1		

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
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	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

- Molecule 5 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).

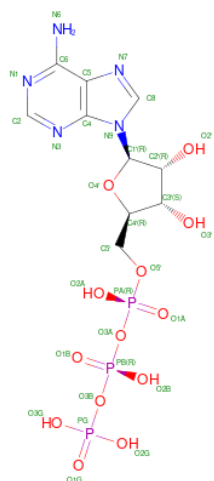


Mol	Chain	Residues	Atoms				AltConf
5	G	1	Total	C	N	O	0
			14	8	4	2	
5	A	1	Total	C	N	O	0
			14	8	4	2	
5	D	1	Total	C	N	O	0
			14	8	4	2	
5	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
6	G	1	Total	Ca	0
			1	1	
6	A	1	Total	Ca	0
			1	1	
6	D	1	Total	Ca	0
			1	1	
6	J	1	Total	Ca	0
			1	1	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

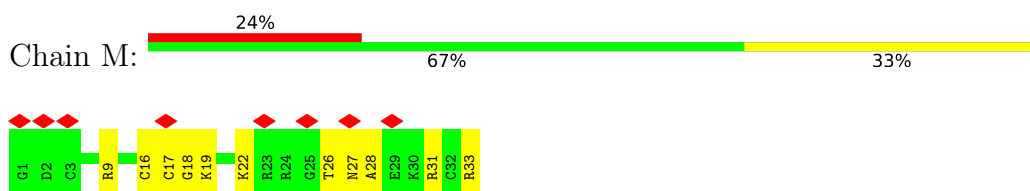
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

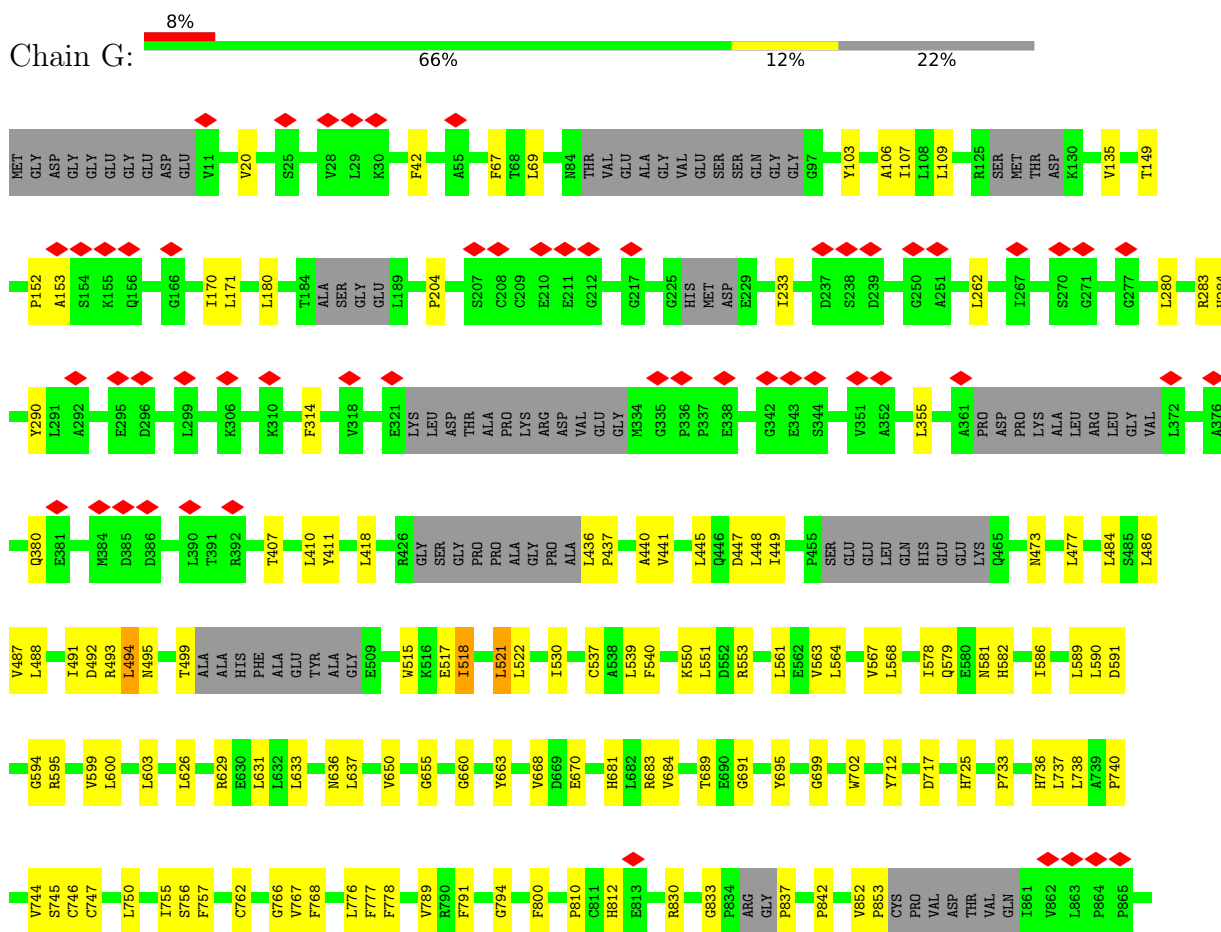
3 Residue-property plots

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: Imperacalcin

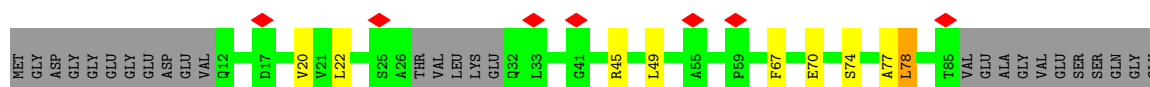
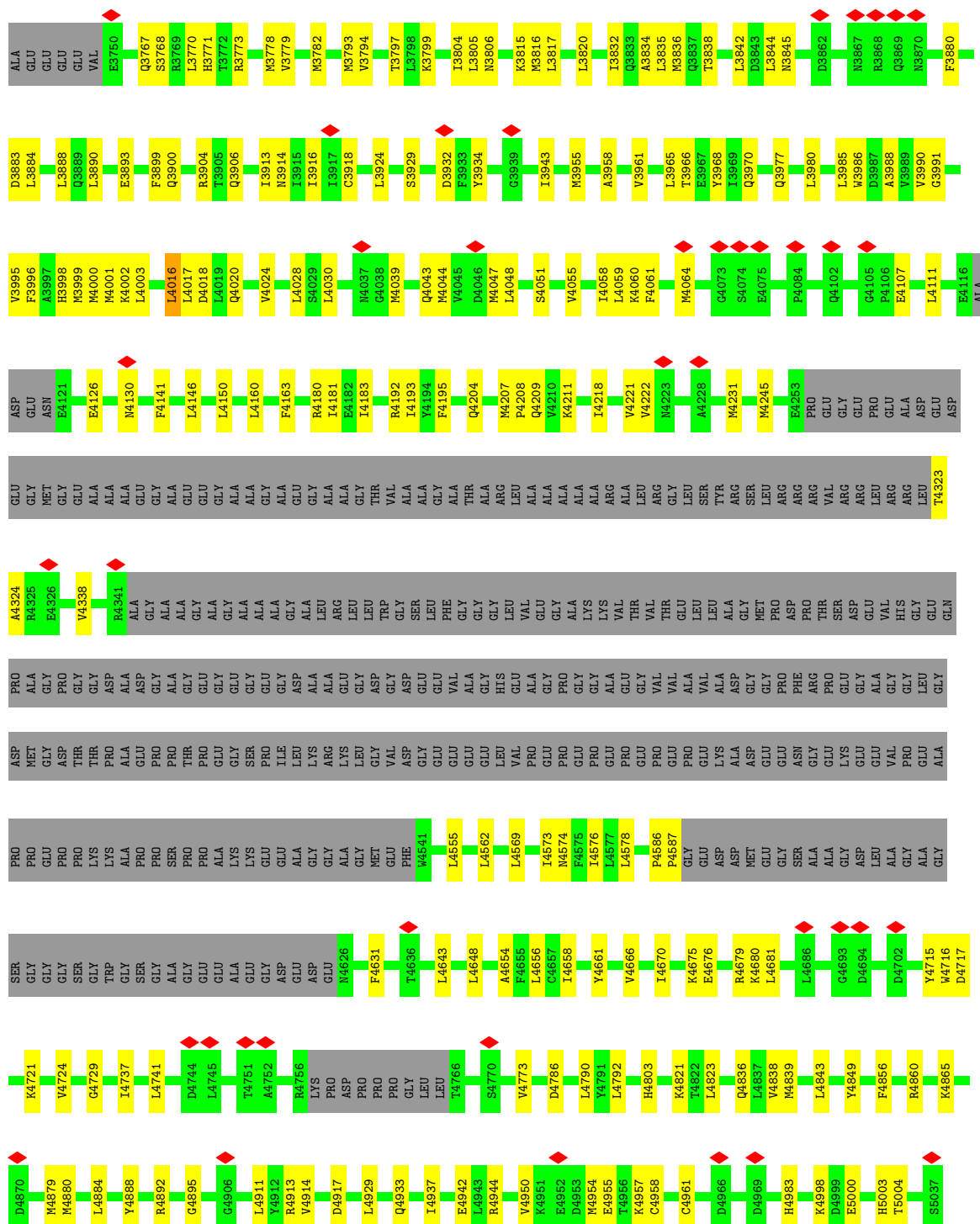


• Molecule 2: Ryanodine receptor 1











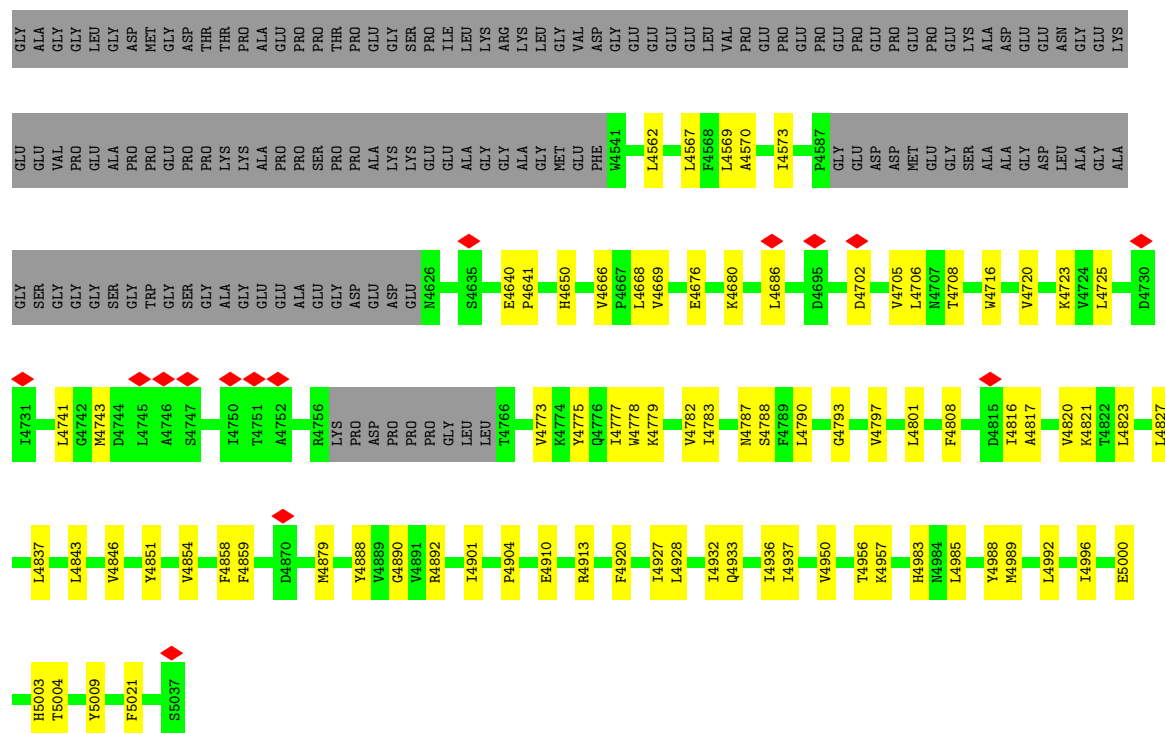


F3951	I3832	A3726	E3607	K3537	LYS	E3309	ILE	THR	ARG	LEU	SER
S3952	L3835	L3735	Q3608	T3538	ALA	D3310	PRO	TTR	LEU	SER	SER
K3953	L3836	GLU	T3609	R3539	LYS	A3385	VAL	VAL	GLY	ILE	GLY
A3954	M3836	GLU	E3610	Y3540	ALA	E3386	ASP	LYS	VAL	GLY	LYS
M3955	C3839	GLY	H3611	A3541	ASP	L3316	ARG	ARG	GLN	SER	ARG
S3956	S3940	GLU	PRO	L3542	ALA	G3317	LEU	LEU	ALA	ALA	F2965
V3957	V3941	ASN	TYR	T3545	ALA	N3318	MET	ARG	ALA	SER	
A3958	L3842	GLY	LYS	D3546	GLN	E3389	ALA	ALA	ASN	ASN	W2966
K3959	L3842	GLY	SER	D3547	GLY	G3390	ASP	ILE	THR	LYS	W2967
Q3960	ALA	GLY	LYS	E3548	GLY	E3391	ILE	GLY	VAL	GLN	D2968
	ALA	GLY	ASP	E3549	ASP	L3322	GLY	E3192	VAL	LYS	I2969
N3963	VAL	VAL	TRP	V3549	GLN	I3323	ALA	R3196	VAL	GLY	
T3974	GLU	VAL	HIS	R3550	ARG	V3324	ALA	ALA	GLU	GLU	E2972
G3975	GLU	VAL	LYS	E3551	THR	N3325	SER	ALA	GLU	GLU	F2973
N3976	VAL	E3750	LEU	PHE	LYS	N3326	GLY	ALA	VAL	ALA	I2974
Q3977	VAL	Q3767	LEU	LEU	LYS	GLY	GLU	ALA	VAL	ALA	
Q3978	VAL	Q3768	LEU	GLN	LYS	ILE	GLU	ALA	VAL	VAL	
S3979	VAL	S3768	LEU	ASN	LYS	ASP	GLY	ALA	VAL	VAL	
L3980	VAL	S3788	LEU	GLN	LYS	ILE	GLY	ALA	VAL	VAL	
A3981	VAL	H3771	LEU	ASN	LYS	ASP	GLY	ALA	VAL	VAL	
R3984	VAL	A3775	LEU	LEU	LYS	THR	PRO	PHE	VAL	VAL	
L3985	VAL	A3776	LEU	HIS	ASP	TRP	HIS	LEU	SER	SER	
W3986	VAL	M3778	LEU	GLN	ARG	M3335	VAL	GLU	LEU	SER	
V3989	VAL	V3779	LEU	GLY	TYR	K3336	VAL	PRO	PHE	LEU	
V3990	VAL	L3780	LEU	LYS	SER	K3336	ILE	PRO	GLY	GLY	
G3991	VAL	Q3781	LEU	VAL	VAL	A3339	ILE	LEU	THR	THR	
F3992	VAL	M3782	LEU	GLY	THR	R3413	THR	GLU	ALA	ALA	
L3993	VAL	Q3788	LEU	GLY	SER	Y415	LEU	TYR	ASN	PRO	
H3994	VAL	E3789	LEU	SER	LEU	A3342	ASN	ASN	ALA	ALA	
V3995	VAL	E3790	LEU	PRO	ILE	Q3343	CYS	CYS	VAL	VAL	
F3996	VAL	K3658	LEU	SER	VAL	P3344	SER	VAL	SER	GLU	
L4016	VAL	I3662	LEU	ARG	ARG	ILE	VAL	THR	THR	THR	
L4017	VAL	G3681	LEU	TRP	TRP	SER	GLU	LYS	GLN	GLN	
Q4020	VAL	L3798	LEU	GLN	GLN	ARG	ARG	THR	PHE	E2994	
K4021	VAL	K3799	LEU	MET	MET	ALA	GLY	LYS	GLY	I2995	
D4022	VAL	L3800	LEU	ALA	ALA	ARG	PRO	PRO	ASP	I2996	
M4023	VAL	G3801	LEU	LEU	LEU	ALA	ALA	PRO	SER	F2997	
V4024	VAL	L3802	LEU	TYR	ARG	PRO	ALA	GLY	ASP	K3000	
	VAL	S3803	LEU	GLY	GLY	LEU	PRO	GLU	ASP	I3001	
L4031	VAL	L3804	LEU	LEU	LEU	L3354	PRO	GLU	ASP	L3002	
	VAL	L3805	LEU	PRO	PRO	H3355	PRO	GLU	ASP	L3003	
A4041	VAL	N3806	LEU	GLY	GLY	G3362	ALA	ILE	LEU	F3004	
M4044	VAL	N3809	LEU	GLY	GLY	G3363	ALA	GLY	ASP	L3005	
V4045	VAL	E3811	LEU	ASP	ASP	R3364	ALA	GLY	ASP	I3006	
M4047	VAL	V3812	LEU	ALA	ALA	L3365	ALA	PRO	ASP	H3013	
L4048	VAL	M3816	LEU	ASP	ASP	R3366	ALA	GLY	ASP	CYS	
V4049	VAL	S3706	LEU	ASP	ASP	K3367	ALA	PRO	ASP	LEU	
E4050	VAL	R3707	LEU	PRO	PRO	V3373	ASN	GLU	GLY	TYR	
S4051	VAL	D3719	LEU	PRO	PRO	A3374	ILE	GLU	GLY	PHE	
S4052	VAL	E3590	LEU	ASN	ASN	E3375	ASN	GLU	GLY	LEU	
S4053	VAL	I3592	LEU	ASN	ASN	E3376	THR	GLU	GLY	SER	
N4054	VAL	V3593	LEU	ASN	ASN	E3377	VAL	GLU	GLY	THR	
	VAL	R3594	LEU	ASN	ASN	Q3378	CYS	GLU	GLY	PRO	
	VAL	A3724	LEU	ASN	ASN	L3379	GLY	GLU	GLY	ALA	
	VAL	Y3725	LEU	ASN	ASN	R3380	GLY	GLU	GLY	LYS	
	VAL		LEU	ASN	ASN	L3381	GLY	GLU	GLY	VAL	
	VAL		LEU	ASN	ASN	E3382	GLY	GLU	GLY	VAL	

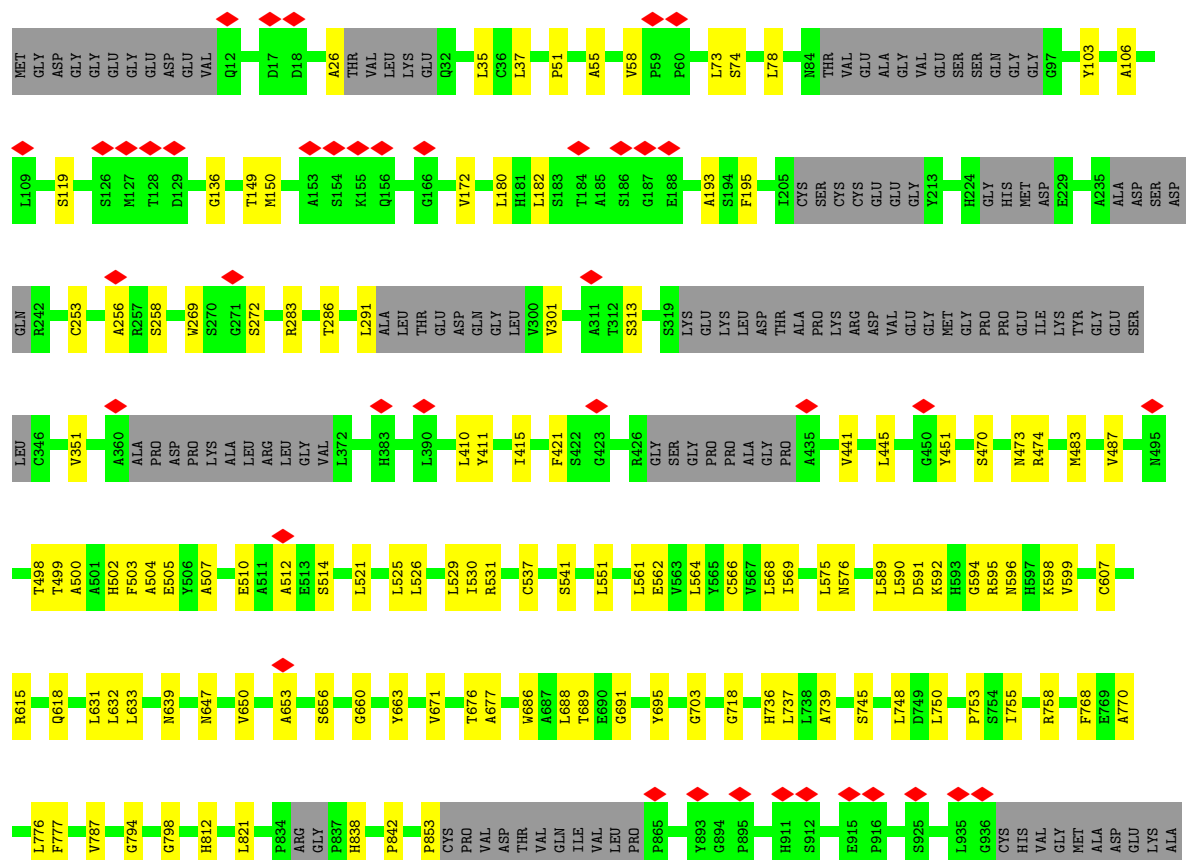






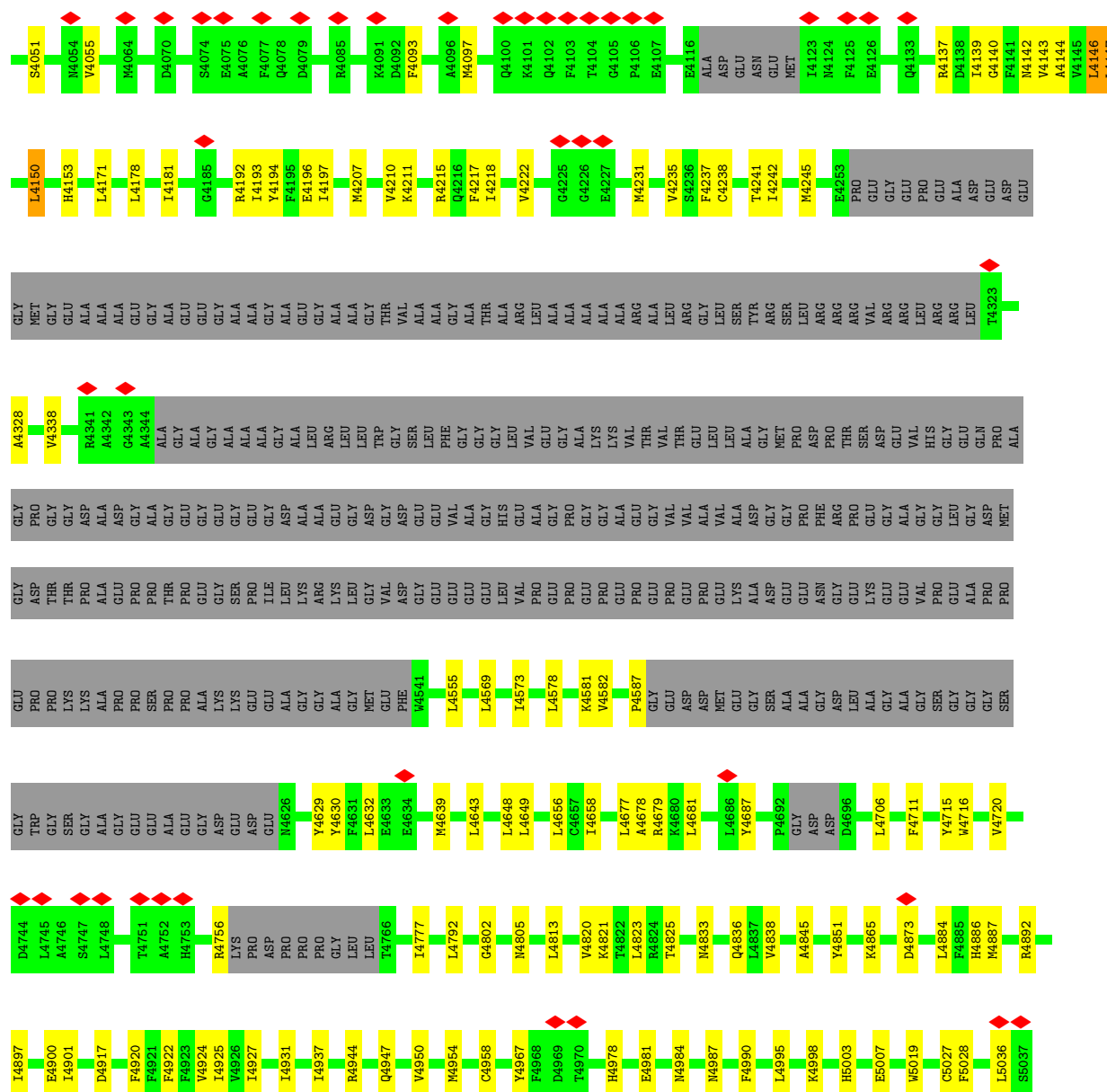


• Molecule 2: Ryanodine receptor 1





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• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 71% 28%

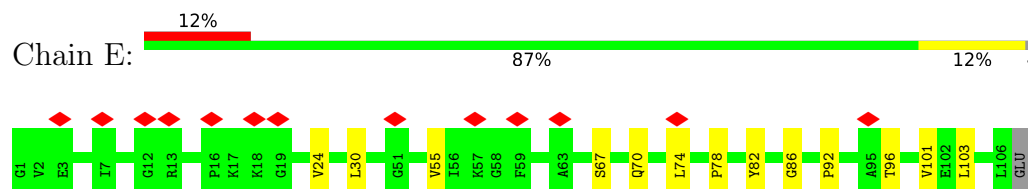


• Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B

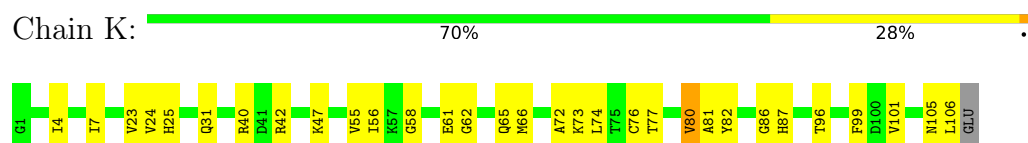
Chain B: 85% 15%



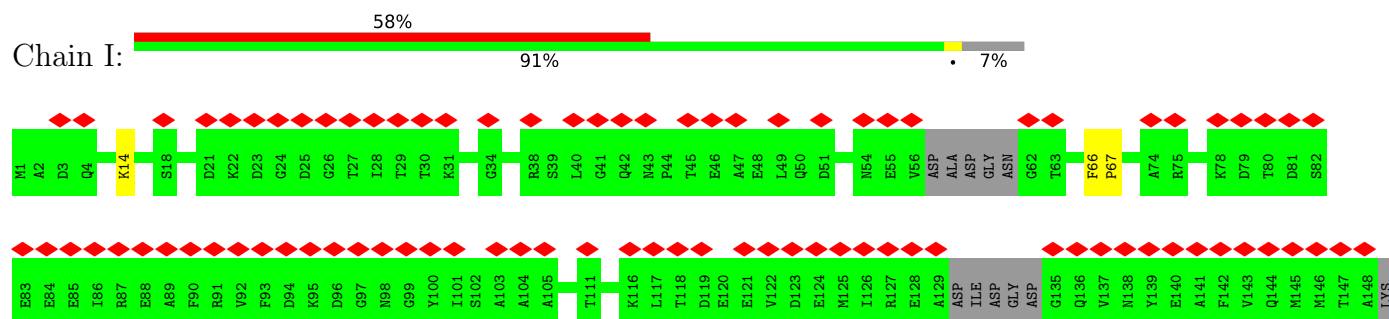
- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



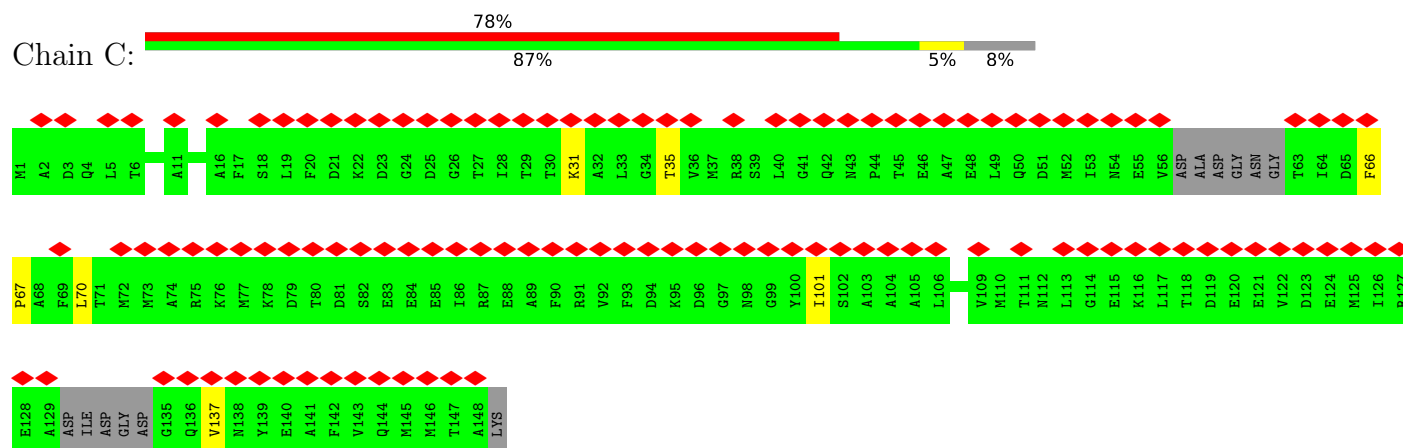
- Molecule 3: Peptidyl-prolyl cis-trans isomerase FKBP1B



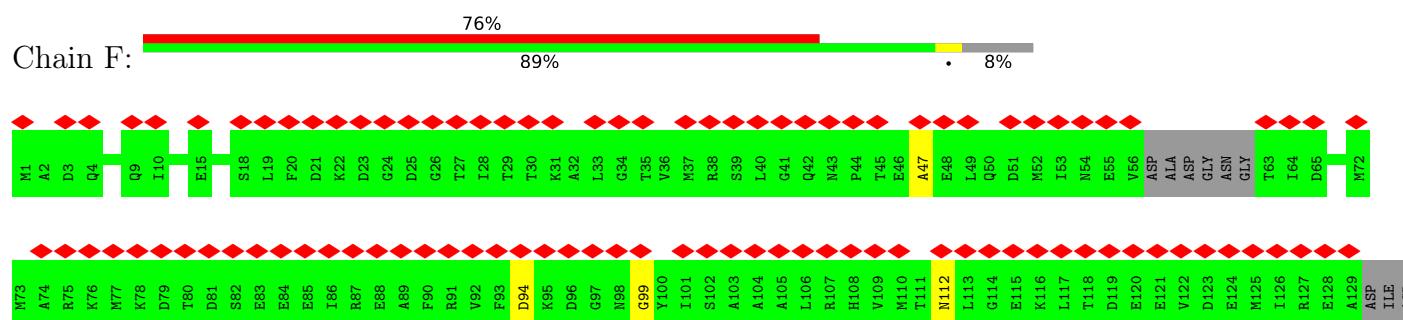
- Molecule 4: Calmodulin-1



- Molecule 4: Calmodulin-1

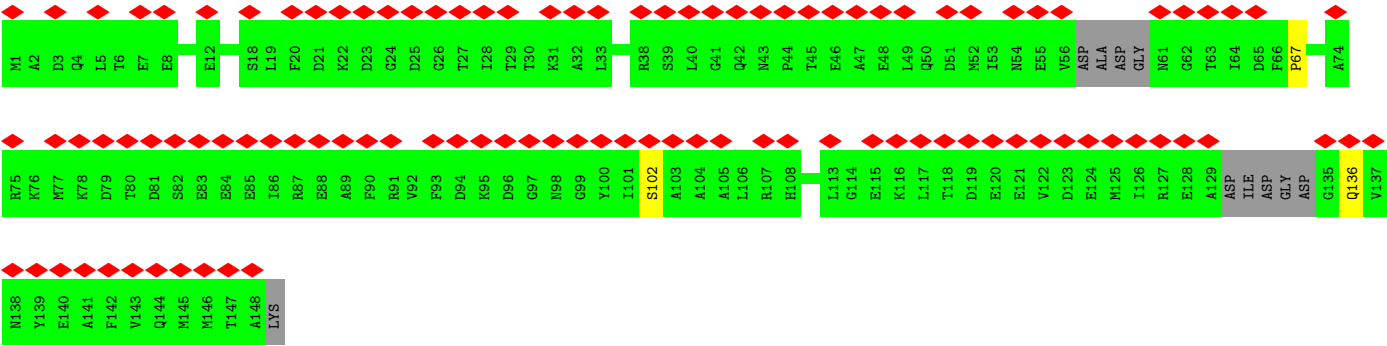
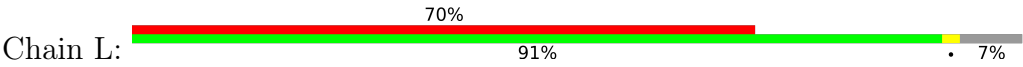


- Molecule 4: Calmodulin-1





• Molecule 4: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	144529	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)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.559	Depositor
Minimum map value	-1.060	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.066	Depositor
Recommended contour level	0.35	Depositor
Map size (Å)	479.36002, 479.36002, 479.36002	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CFF, CA, ZN, 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	M	0.10	0/516	0.27	0/672
2	A	0.20	0/25342	0.37	6/34836 (0.0%)
2	D	0.21	0/23698	0.37	4/32668 (0.0%)
2	G	0.13	0/26809	0.30	3/36763 (0.0%)
2	J	0.16	0/25729	0.31	0/35328
3	B	0.14	0/751	0.38	0/1025
3	E	0.07	0/671	0.23	0/926
3	H	0.11	0/775	0.30	0/1054
3	K	0.37	0/774	0.54	0/1051
4	C	0.08	0/707	0.22	0/978
4	F	0.07	0/711	0.16	0/984
4	I	0.07	0/711	0.18	0/981
4	L	0.07	0/706	0.18	0/976
All	All	0.17	0/107900	0.34	13/148242 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2125	HIS	N-CA-C	-8.15	102.47	111.36
2	A	4045	VAL	N-CA-C	-8.03	102.71	110.42
2	A	494	LEU	N-CA-C	-7.49	103.12	111.28
2	D	3671	ASP	N-CA-C	-7.35	103.35	111.36
2	G	4018	ASP	N-CA-C	-7.04	103.53	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	514	0	522	9	0
2	A	24845	0	19916	455	0
2	D	23336	0	16446	311	0
2	G	26285	0	21941	417	0
2	J	25245	0	20257	342	0
3	B	735	0	669	11	0
3	E	657	0	537	7	0
3	H	759	0	724	21	0
3	K	758	0	735	21	0
4	C	707	0	386	5	0
4	F	710	0	386	3	0
4	I	711	0	383	4	0
4	L	706	0	363	2	0
5	A	14	0	10	0	0
5	D	14	0	10	0	0
5	G	14	0	10	0	0
5	J	14	0	10	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	G	1	0	0	0	0
6	J	1	0	0	0	0
7	A	31	0	12	2	0
7	D	31	0	12	1	0
7	G	31	0	12	3	0
7	J	31	0	12	1	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
8	G	1	0	0	0	0
8	J	1	0	0	0	0
All	All	106156	0	83353	1556	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 1556 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:A:415:ILE:CD1	2:A:493:ARG:HD2	1.68	1.23
2:A:415:ILE:HD11	2:A:493:ARG:CD	1.68	1.21
2:D:4055:VAL:HG11	2:D:4163:PHE:CZ	1.91	1.05
2:A:4048:LEU:HD11	2:A:4055:VAL:HG21	1.36	1.03
2:A:357:LEU:HB2	2:A:378:LEU:HA	1.45	0.98

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	62/33 (188%)	56 (90%)	6 (10%)	0	100	100
2	A	3718/5037 (74%)	3668 (99%)	48 (1%)	2 (0%)	48	78
2	D	1943/5037 (39%)	1917 (99%)	26 (1%)	0	100	100
2	G	3827/5037 (76%)	3774 (99%)	53 (1%)	0	100	100
2	J	3786/5037 (75%)	3726 (98%)	60 (2%)	0	100	100
3	B	58/107 (54%)	56 (97%)	2 (3%)	0	100	100
3	E	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
3	H	105/107 (98%)	99 (94%)	6 (6%)	0	100	100
3	K	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
4	F	131/149 (88%)	130 (99%)	1 (1%)	0	100	100
4	I	132/149 (89%)	132 (100%)	0	0	100	100
4	L	133/149 (89%)	131 (98%)	2 (2%)	0	100	100
All	All	14103/21056 (67%)	13889 (98%)	212 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	4052	SER
2	A	614	VAL

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	M	56/28 (200%)	56 (100%)	0	100	100
2	A	1728/4276 (40%)	1705 (99%)	23 (1%)	61	71
2	D	1204/4276 (28%)	1180 (98%)	24 (2%)	48	64
2	G	1976/4276 (46%)	1958 (99%)	18 (1%)	70	75
2	J	1721/4276 (40%)	1703 (99%)	18 (1%)	68	74
3	B	67/88 (76%)	67 (100%)	0	100	100
3	E	49/88 (56%)	49 (100%)	0	100	100
3	H	73/88 (83%)	71 (97%)	2 (3%)	39	59
3	K	74/88 (84%)	72 (97%)	2 (3%)	39	59
4	C	9/123 (7%)	9 (100%)	0	100	100
4	F	9/123 (7%)	9 (100%)	0	100	100
4	I	8/123 (6%)	8 (100%)	0	100	100
4	L	5/123 (4%)	5 (100%)	0	100	100
All	All	6979/17976 (39%)	6892 (99%)	87 (1%)	59	72

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	4142	ASN
2	J	3721	LEU
2	D	4162	ASN
2	D	4562	LEU
2	J	3735	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	2441	HIS
2	J	1691	GLN
2	D	3833	GLN
2	J	639	ASN
2	J	2169	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
5	CFF	J	5101	-	15,15,15	0.63	0	23,23,23	0.49	0
5	CFF	A	5101	-	15,15,15	0.62	0	23,23,23	0.49	0
5	CFF	D	5101	-	15,15,15	0.62	0	23,23,23	0.48	0
7	ATP	G	5103	-	32,33,33	0.25	0	48,52,52	0.28	0
7	ATP	D	5103	-	32,33,33	0.25	0	48,52,52	0.28	0
5	CFF	G	5101	-	15,15,15	0.62	0	23,23,23	0.48	0
7	ATP	J	5103	-	32,33,33	0.26	0	48,52,52	0.29	0
7	ATP	A	5103	-	32,33,33	0.25	0	48,52,52	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CFF	J	5101	-	-	-	0/2/2/2
5	CFF	A	5101	-	-	-	0/2/2/2
5	CFF	D	5101	-	-	-	0/2/2/2
7	ATP	D	5103	-	-	12/22/38/38	0/3/3/3
7	ATP	G	5103	-	-	8/22/38/38	0/3/3/3
5	CFF	G	5101	-	-	-	0/2/2/2
7	ATP	J	5103	-	-	10/22/38/38	0/3/3/3
7	ATP	A	5103	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	5103	ATP	PB-O3B-PG-O2G
7	G	5103	ATP	C5'-O5'-PA-O2A
7	G	5103	ATP	C4'-C5'-O5'-PA
7	A	5103	ATP	PB-O3A-PA-O5'
7	A	5103	ATP	C5'-O5'-PA-O2A

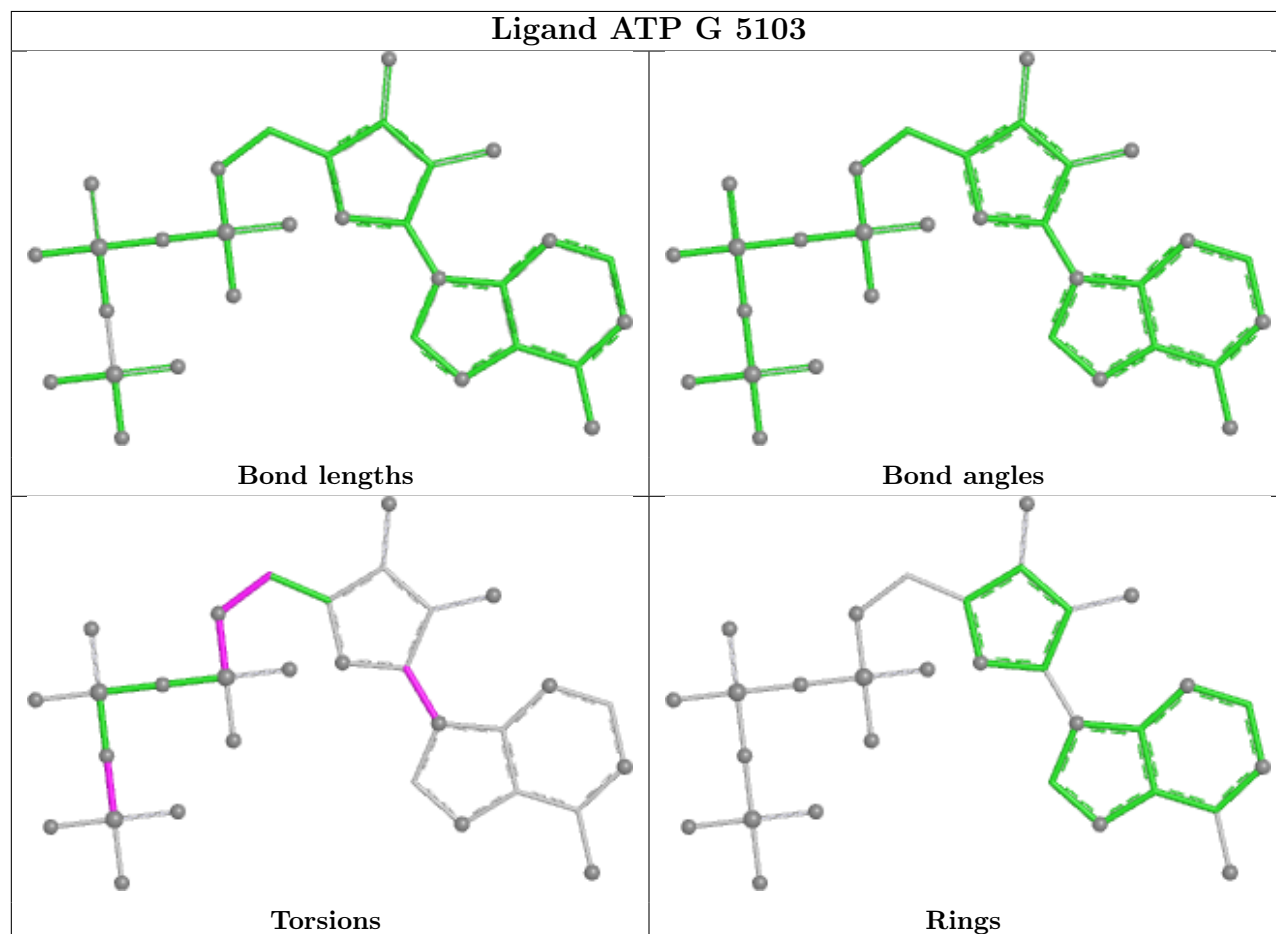
There are no ring outliers.

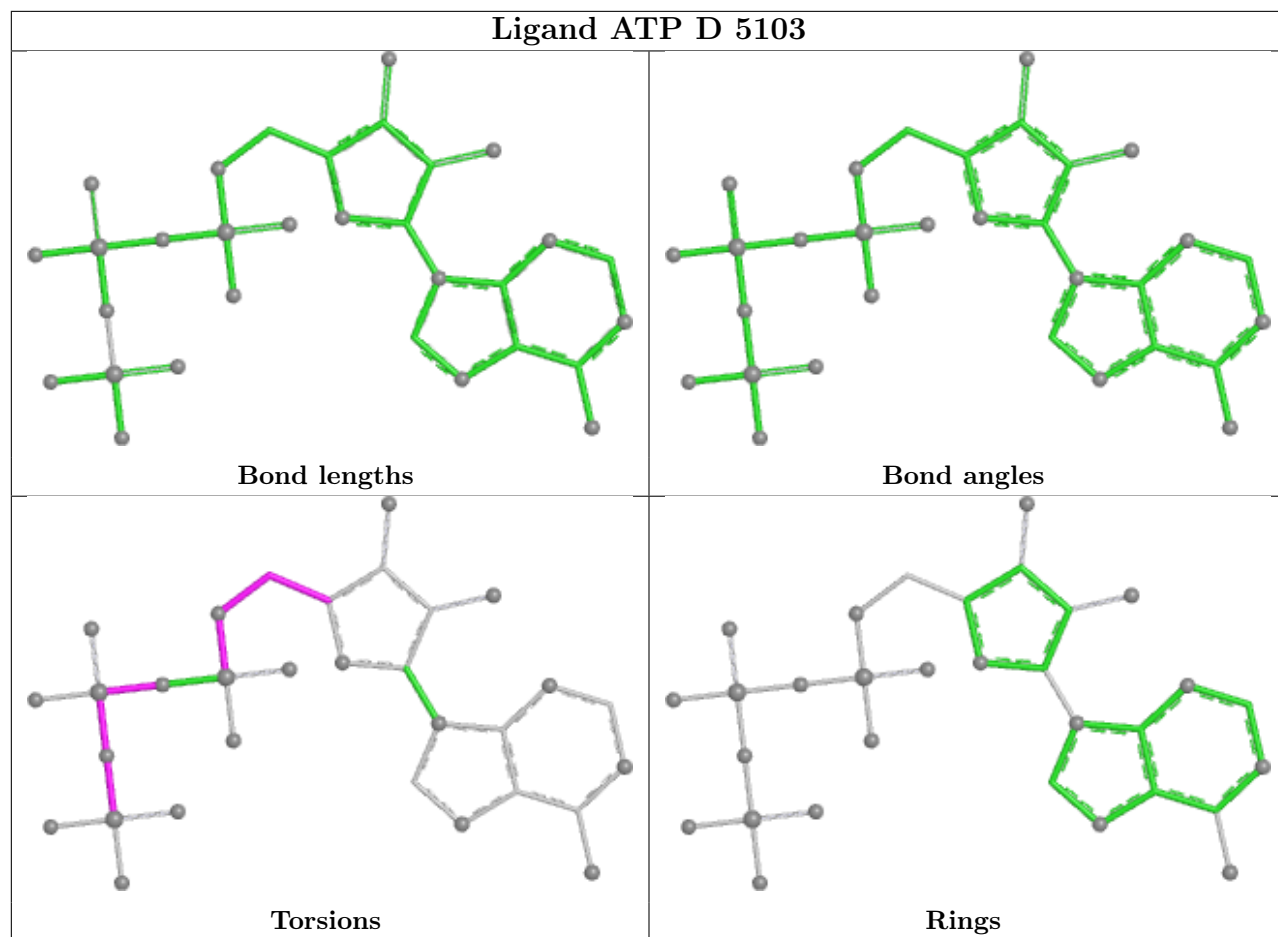
4 monomers are involved in 7 short contacts:

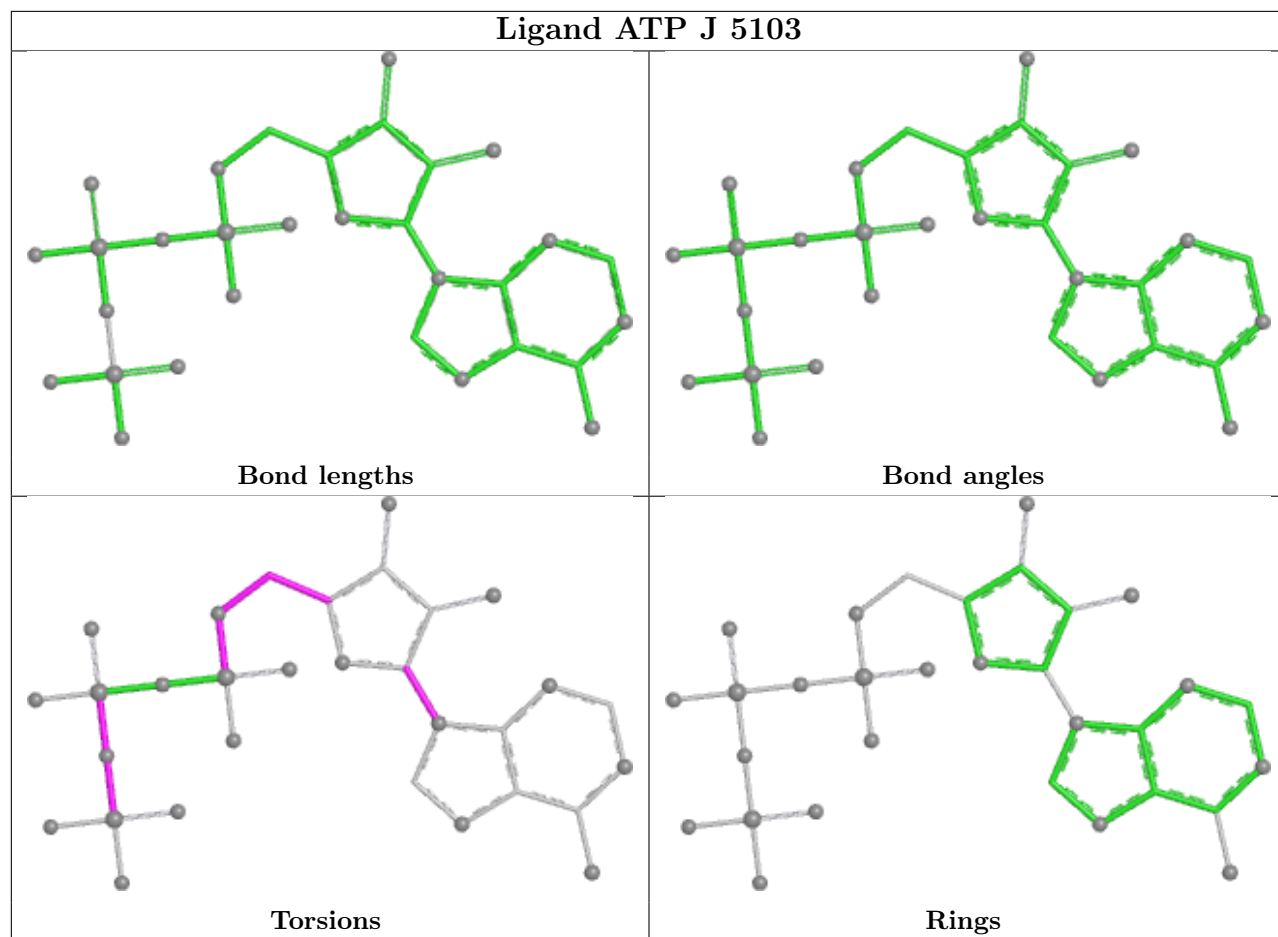
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	5103	ATP	3	0
7	D	5103	ATP	1	0
7	J	5103	ATP	1	0
7	A	5103	ATP	2	0

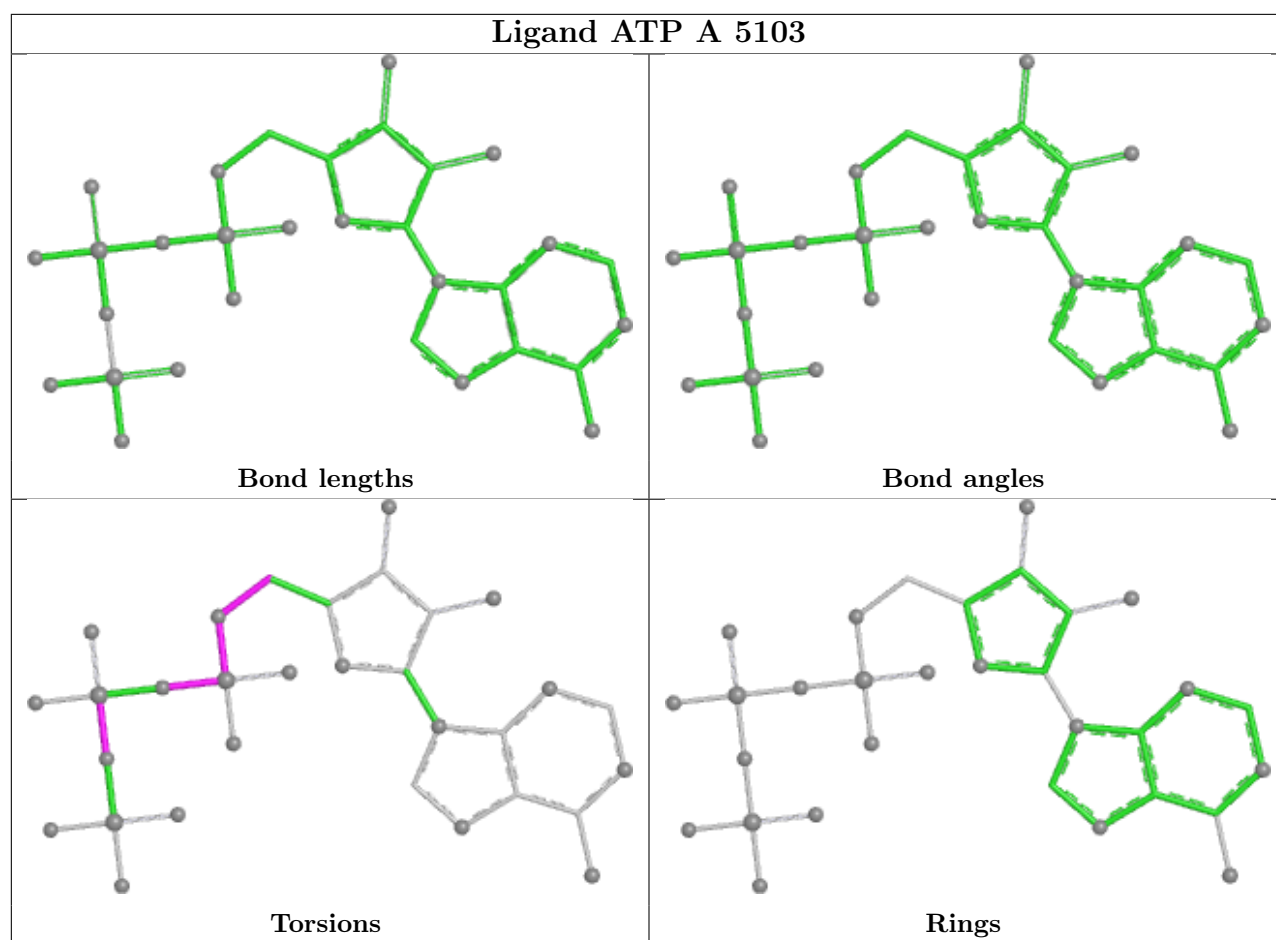
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

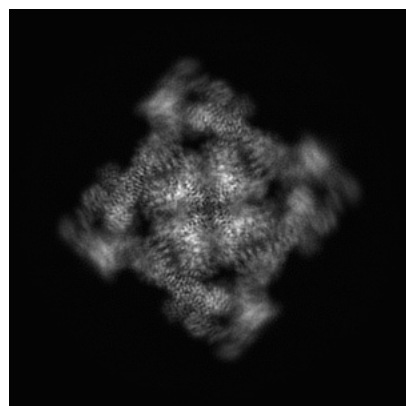
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27721. These allow visual inspection of the internal detail of the map and identification of artifacts.

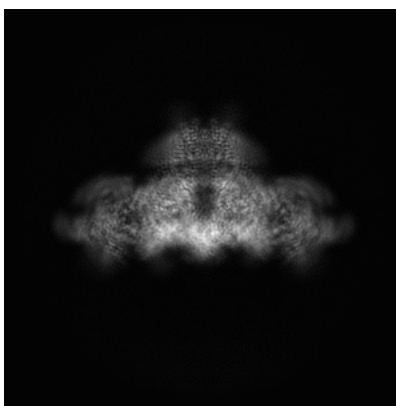
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

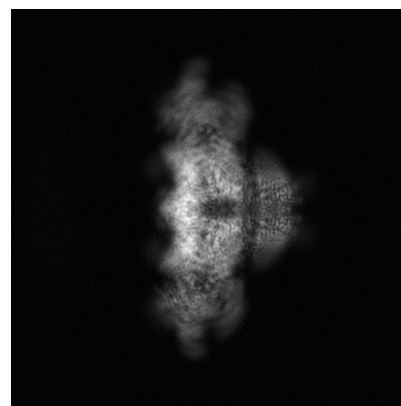
6.1.1 Primary map



X

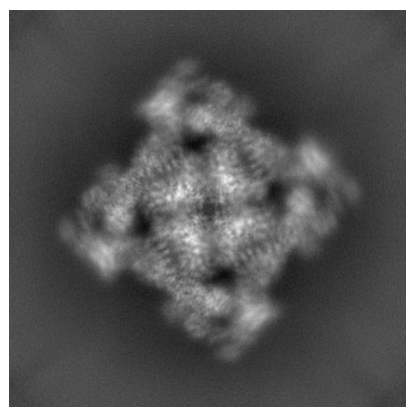


Y

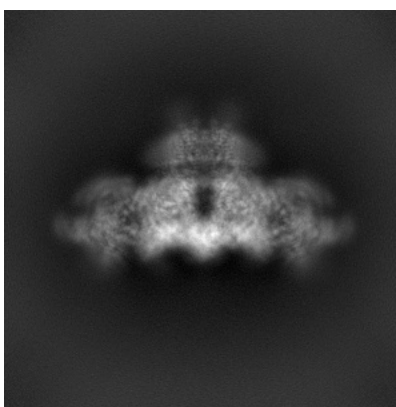


Z

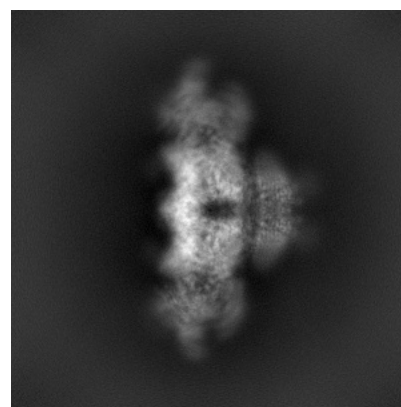
6.1.2 Raw map



X



Y

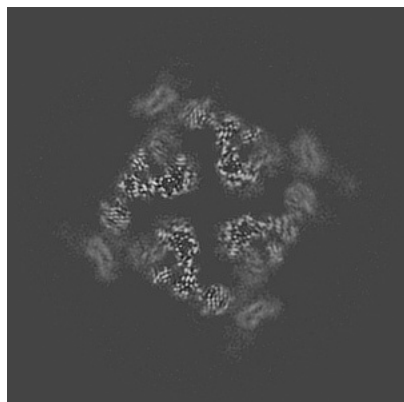


Z

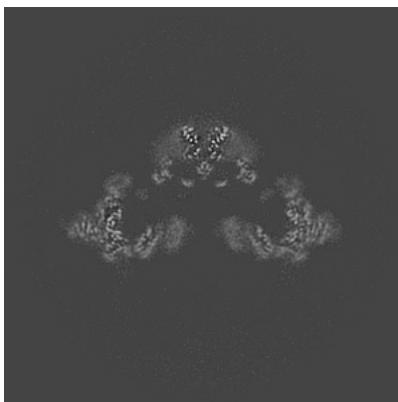
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

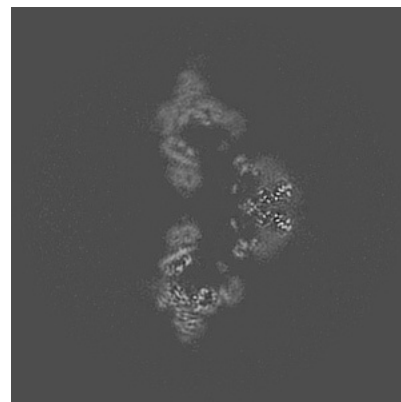
6.2.1 Primary map



X Index: 224

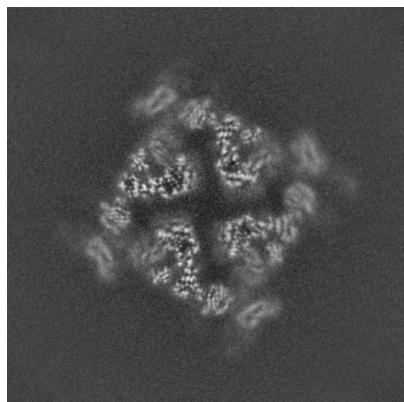


Y Index: 224

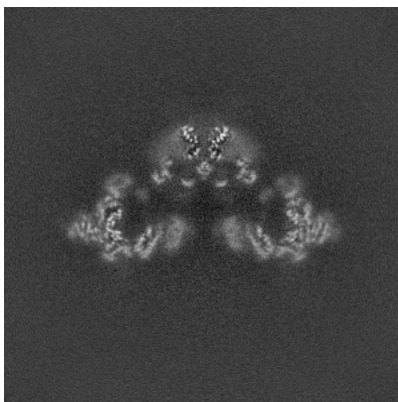


Z Index: 224

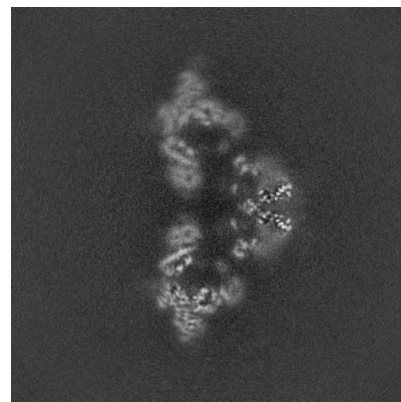
6.2.2 Raw map



X Index: 224



Y Index: 224

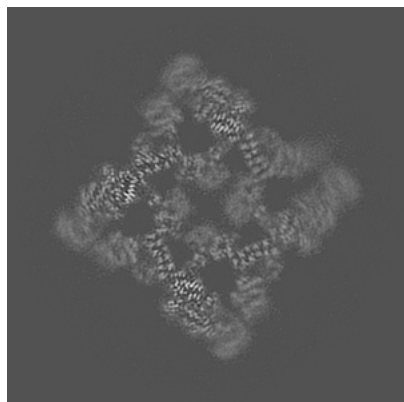


Z Index: 224

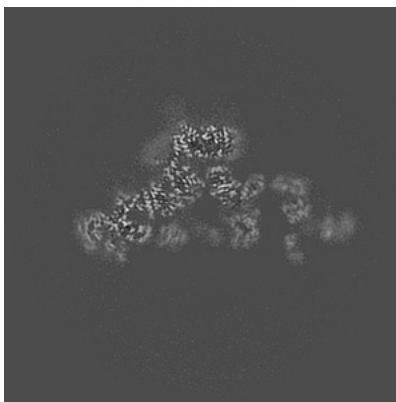
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

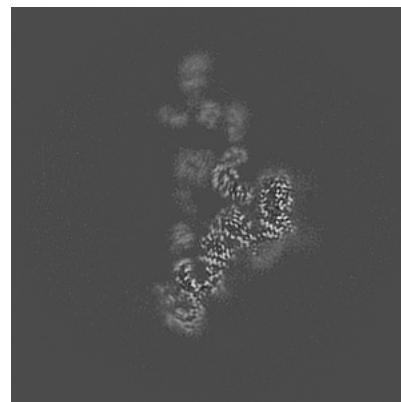
6.3.1 Primary map



X Index: 203

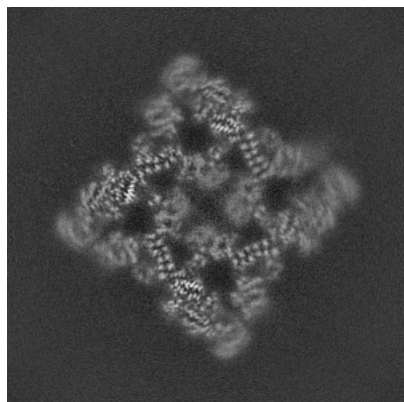


Y Index: 205

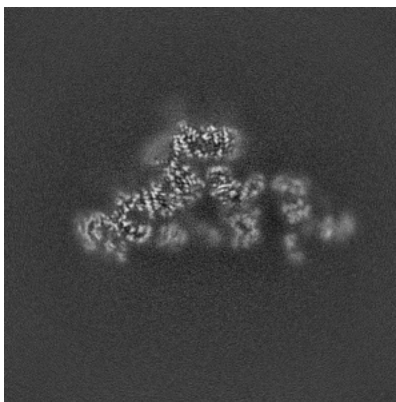


Z Index: 242

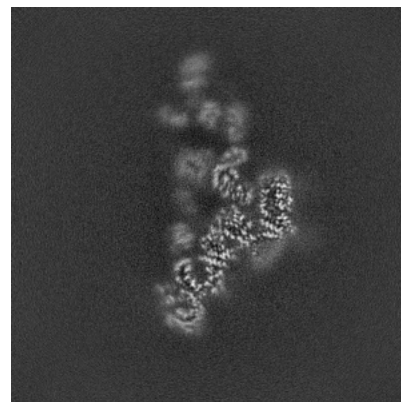
6.3.2 Raw map



X Index: 203



Y Index: 205

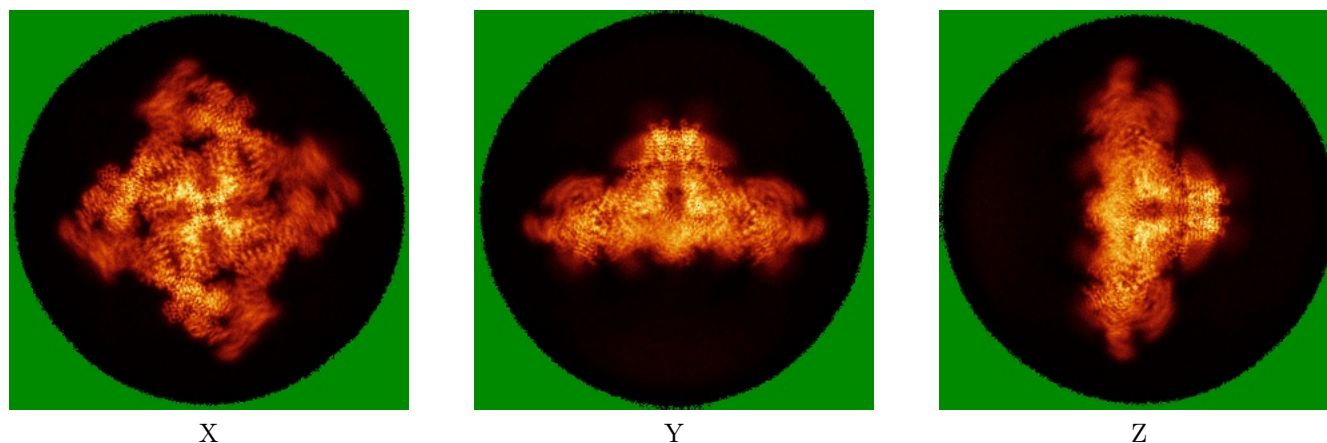


Z Index: 242

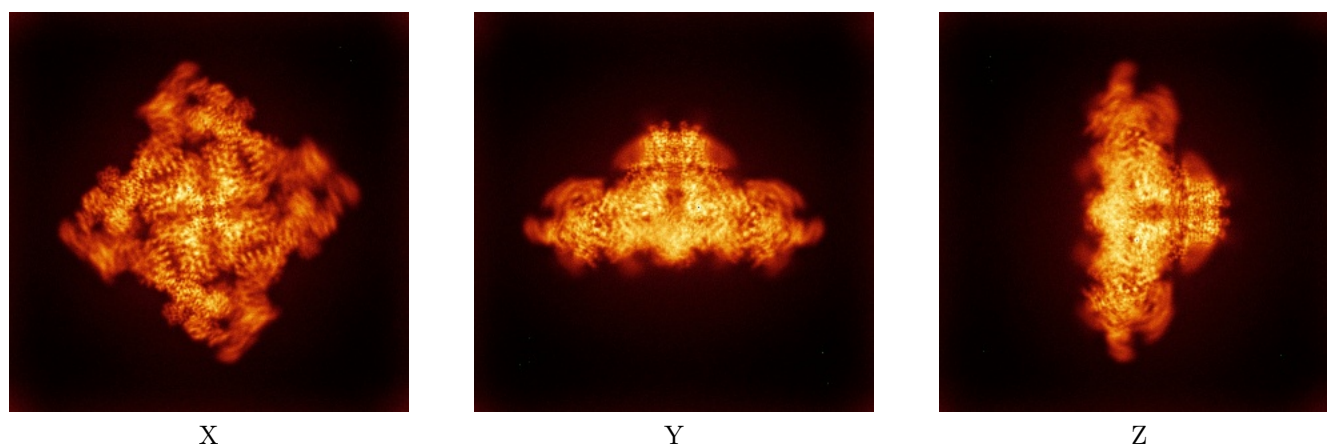
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

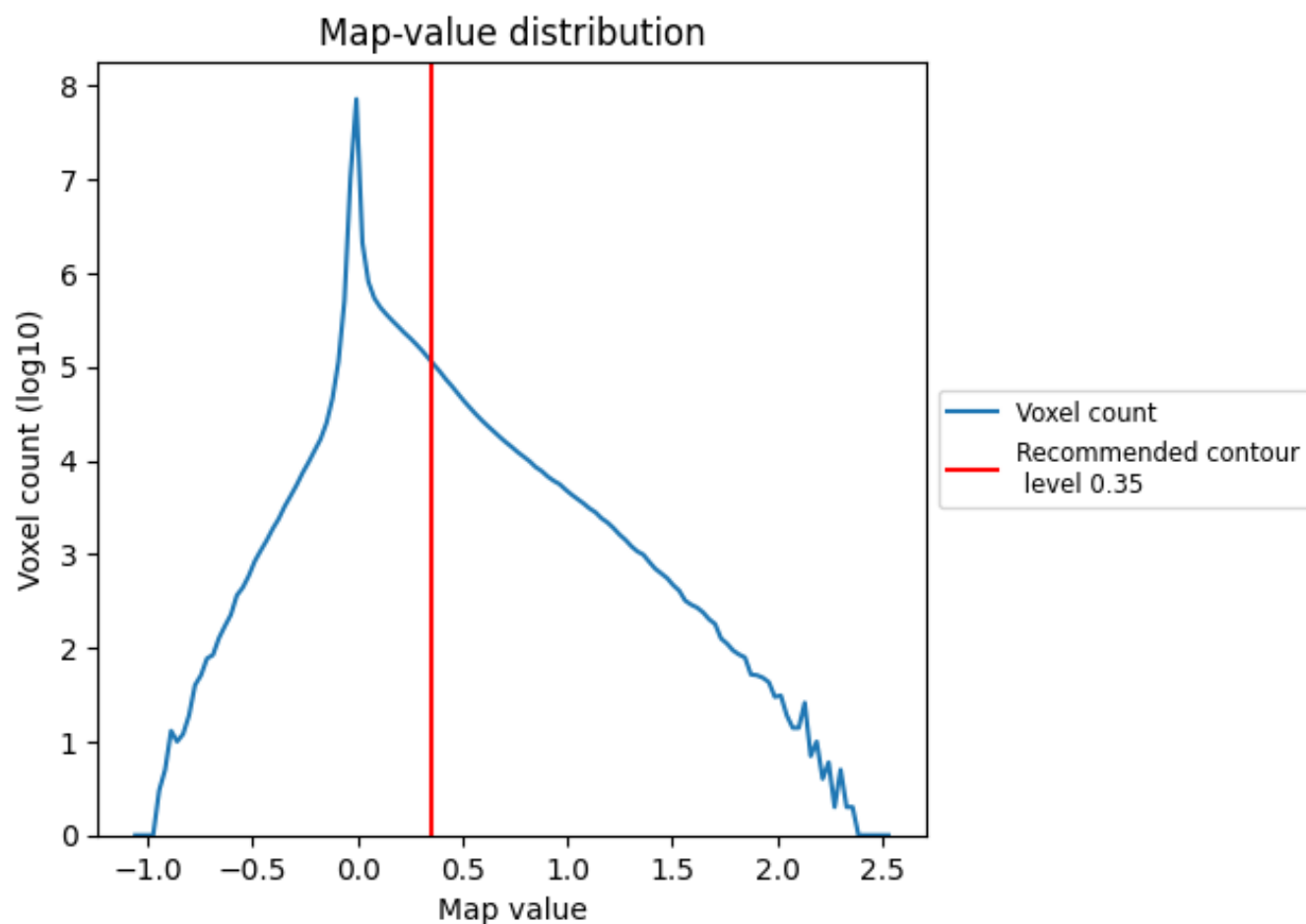
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

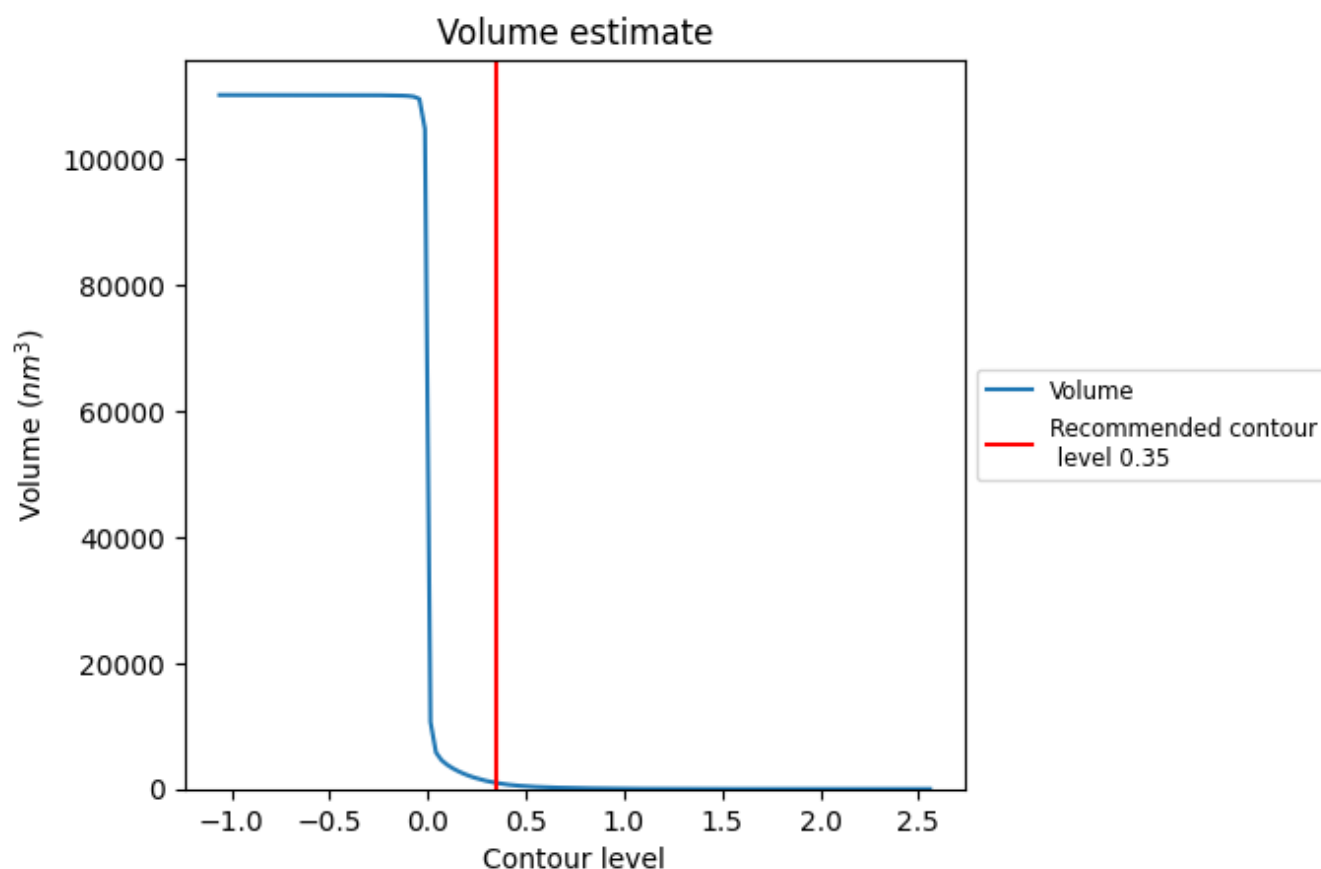
This section contains the results of statistical analysis of the map.

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.

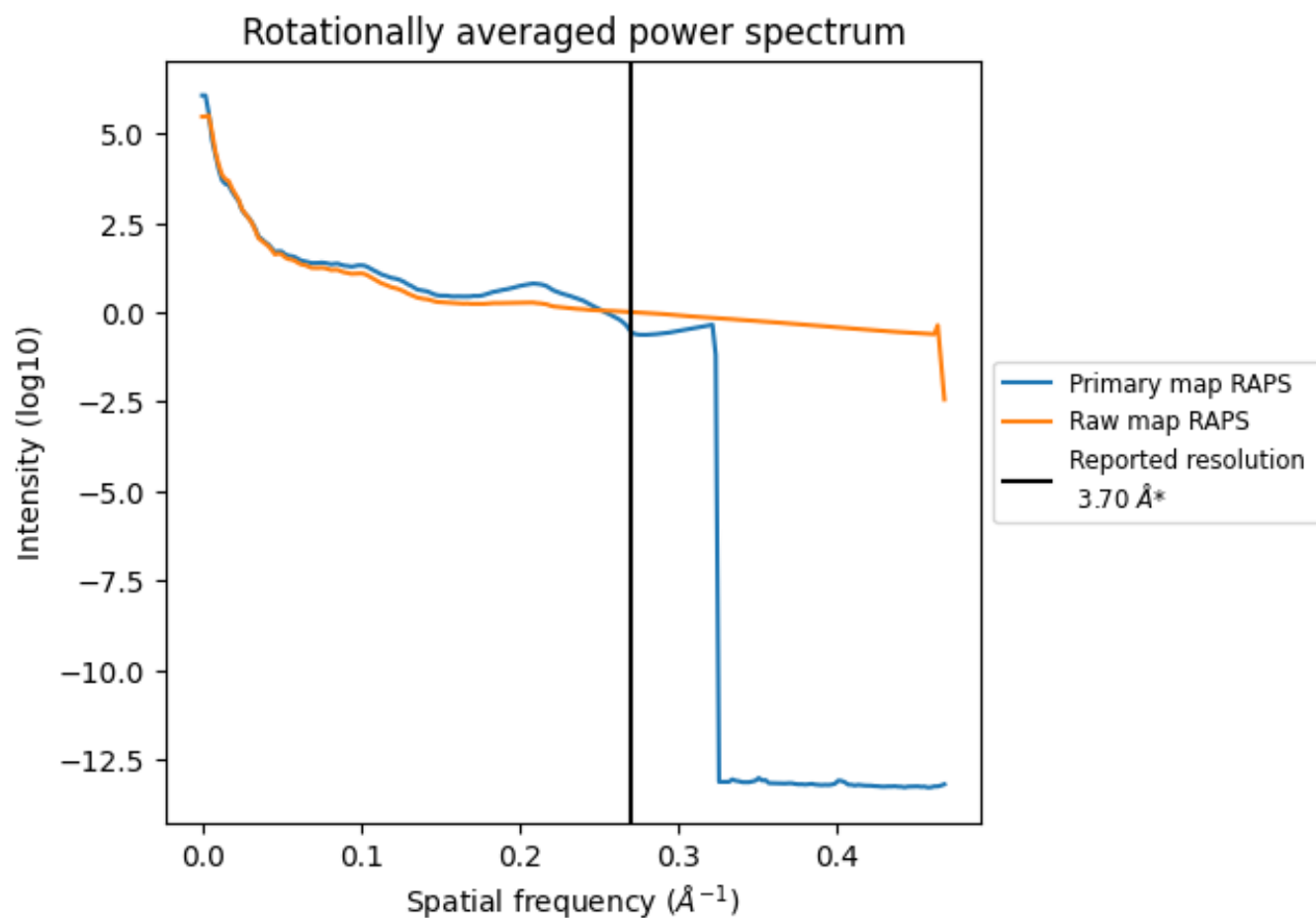
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 957 nm^3 ; this corresponds to an approximate mass of 865 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 ⓘ

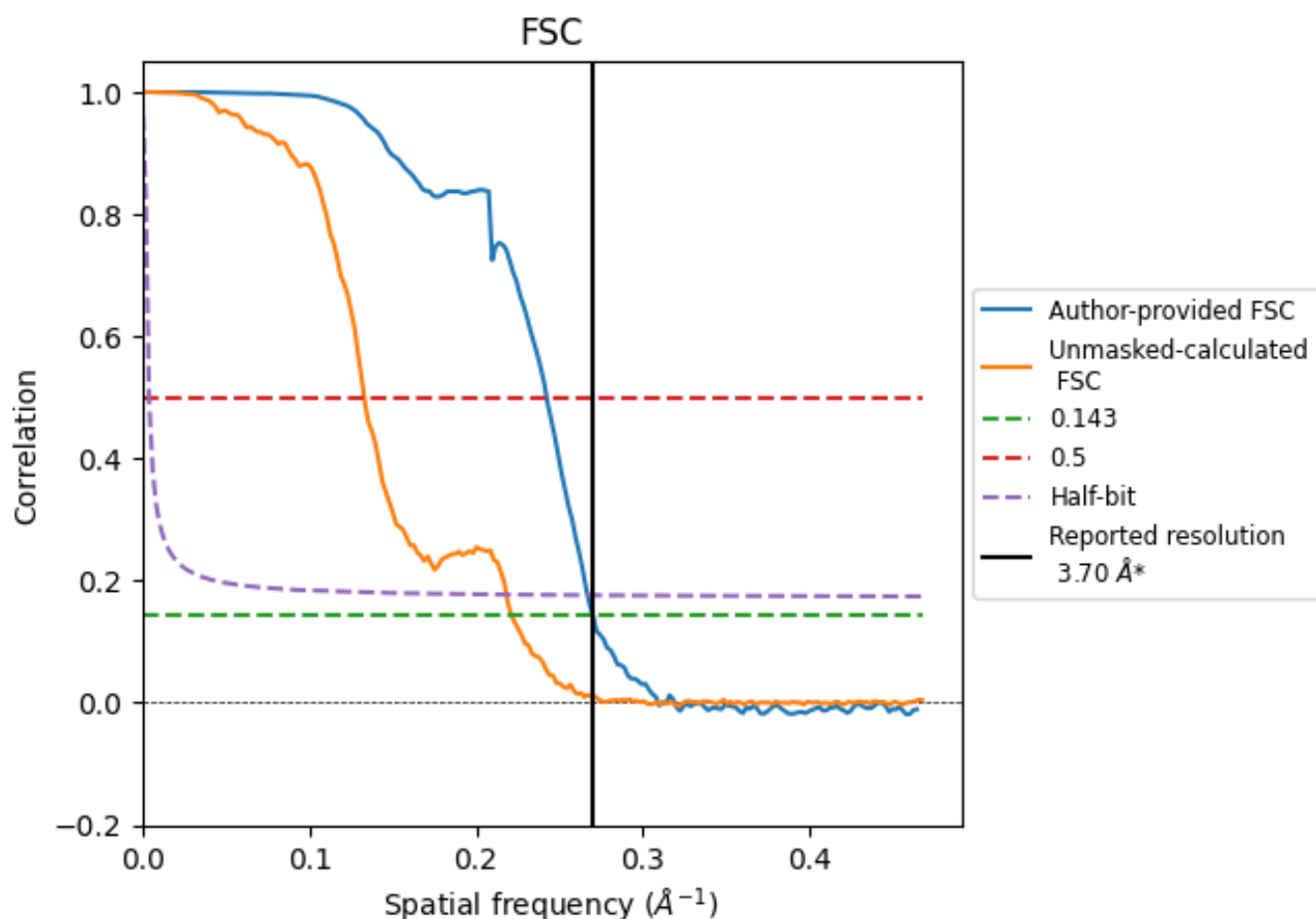


*Reported resolution corresponds to spatial frequency of $0.270 \text{ \AA}^{-1}$

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 0.270 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.13	3.75
Unmasked-calculated*	4.52	7.52	4.58

*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 4.52 differs from the reported value 3.7 by more than 10 %

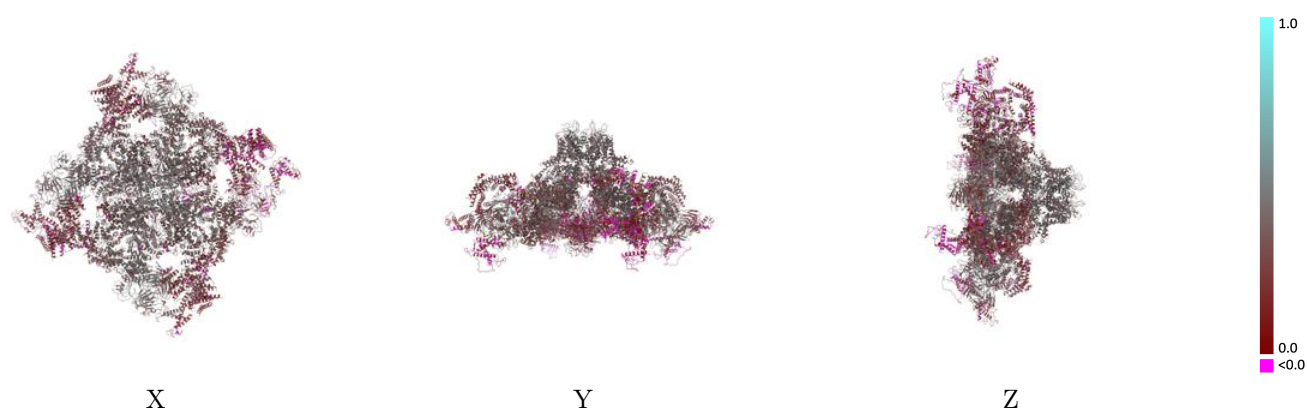
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27721 and PDB model 8DUJ. 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](#)

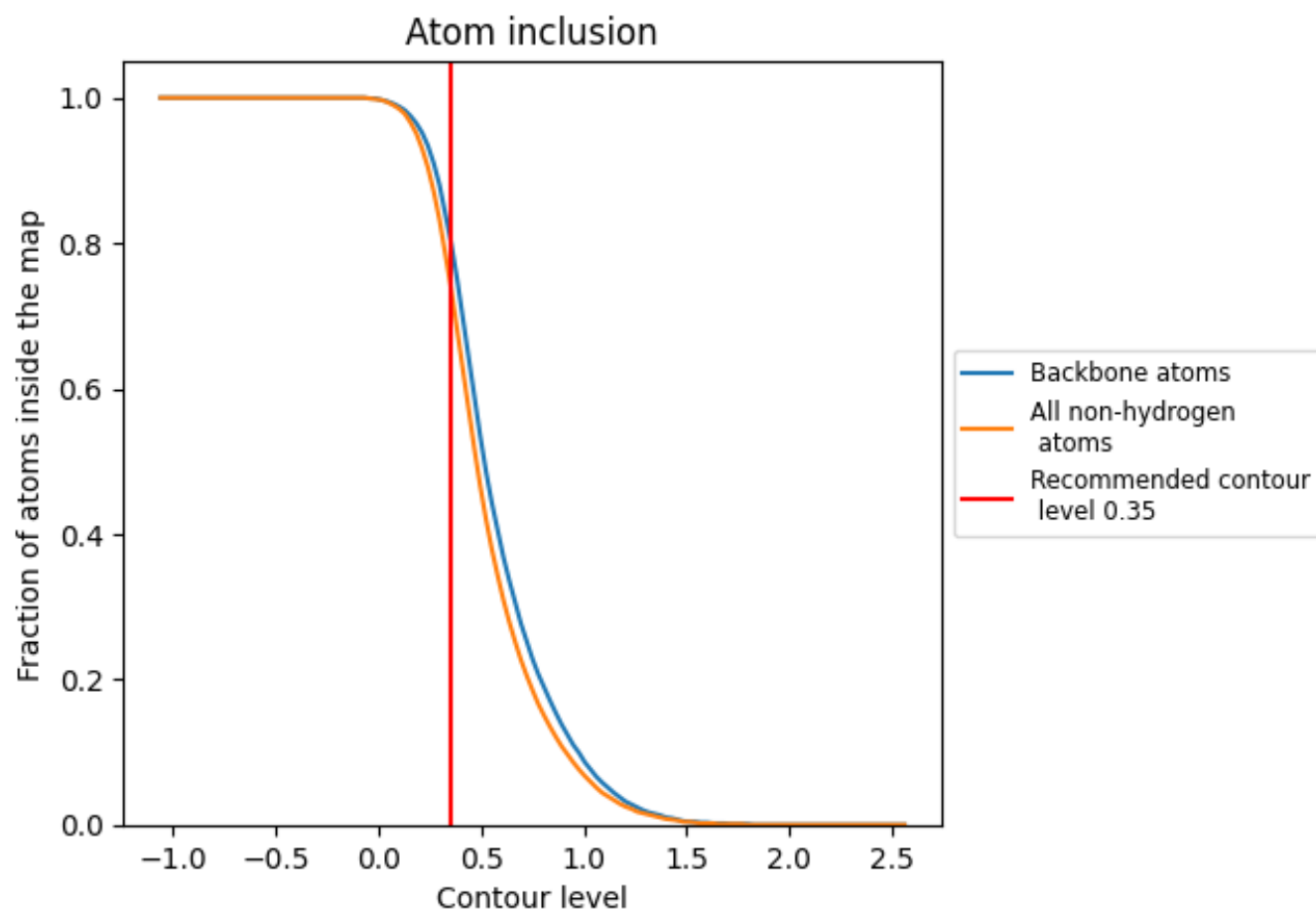


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 74% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.3450
A	 0.7390	 0.3470
B	 0.8290	 0.3980
C	 0.1920	 0.2430
D	 0.7080	 0.3050
E	 0.7030	 0.2960
F	 0.1970	 0.2240
G	 0.7760	 0.3660
H	 0.8610	 0.4330
I	 0.3760	 0.2800
J	 0.7910	 0.3640
K	 0.8640	 0.4400
L	 0.2950	 0.2410
M	 0.6070	 0.3960

