



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 02:28 AM JST

PDB ID : 6JRR
EMDB ID : EMD-9879
Title : Structure of RyR2 (*F/A/C/L-Ca²⁺ dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-04-05
Resolution : 3.90 Å(reported)

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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

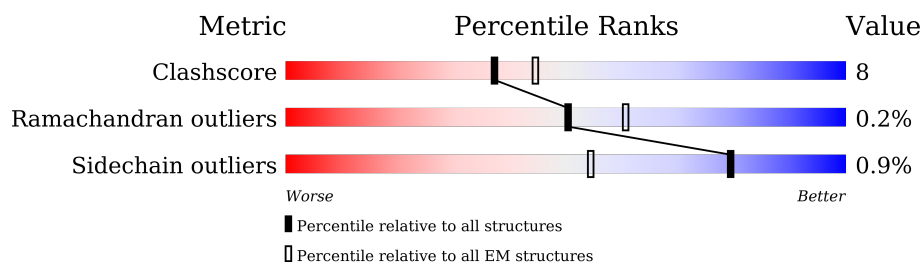
1 Overall quality at a glance

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	 9% 57% 12% 30%
1	C	4968	 9% 57% 12% 30%
1	E	4968	 9% 57% 12% 30%
1	G	4968	 9% 57% 12% 30%
2	B	108	 74% 25% .
2	D	108	 75% 24% .
2	F	108	 73% 26% .
2	H	108	 75% 24% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 109132 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	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	C	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	E	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		
1	G	3460	Total	C	N	O	S	0	0
			26417	16833	4528	4900	156		

- 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	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	F	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		

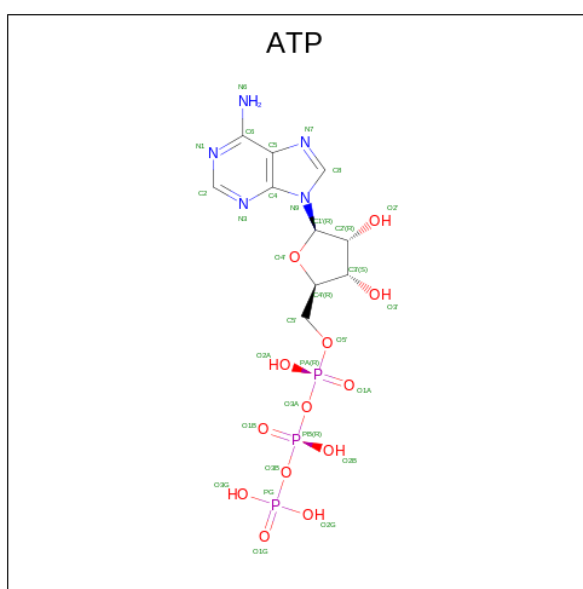
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	
3	G	1	Total	Zn	0
			1	1	

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

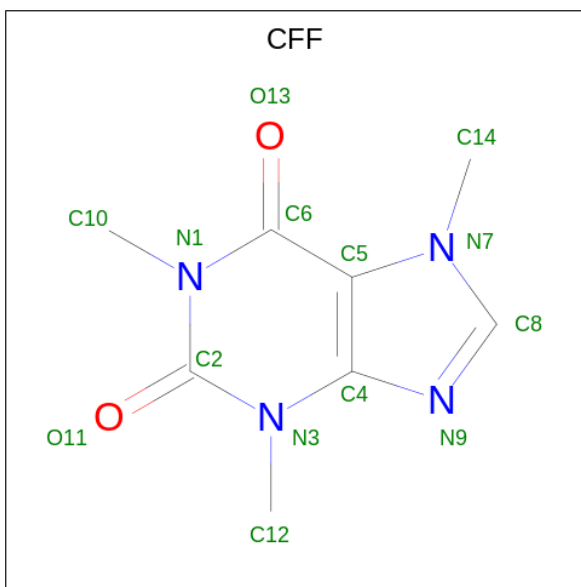
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Ca	0
			1	1	
4	C	1	Total	Ca	0
			1	1	
4	E	1	Total	Ca	0
			1	1	
4	G	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$).

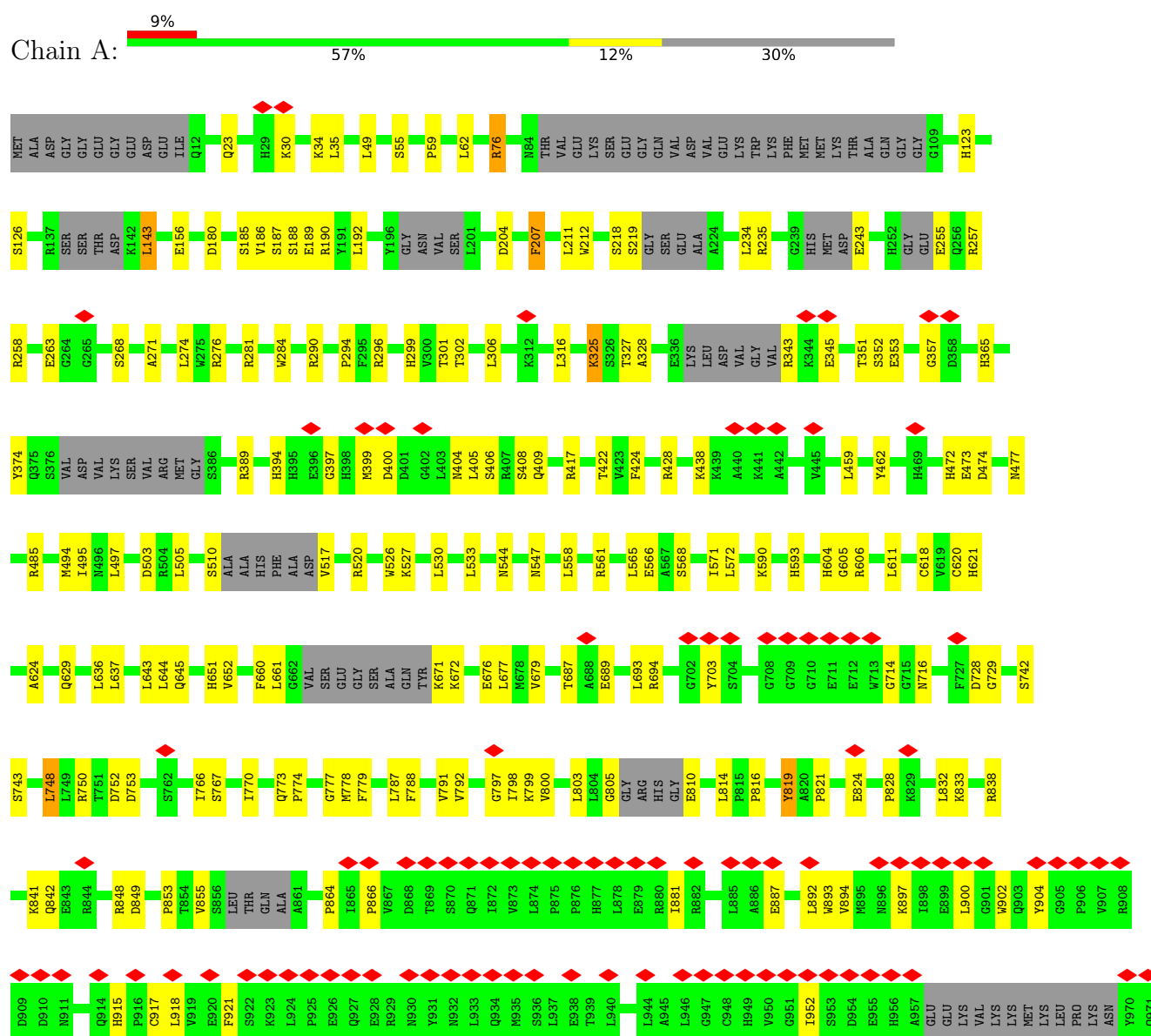


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	4	2	
6	C	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	

3 Residue-property plots

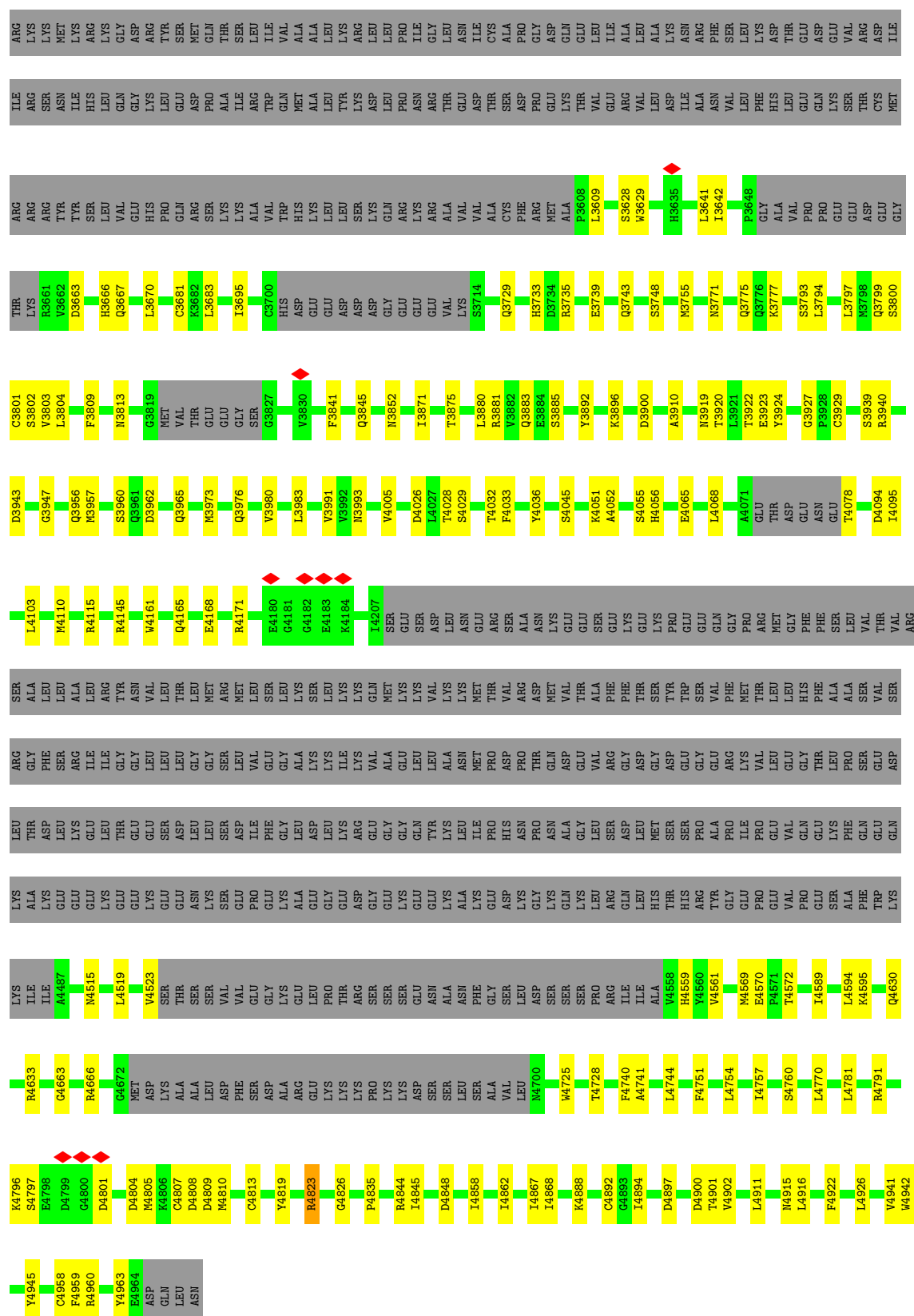
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: RyR2









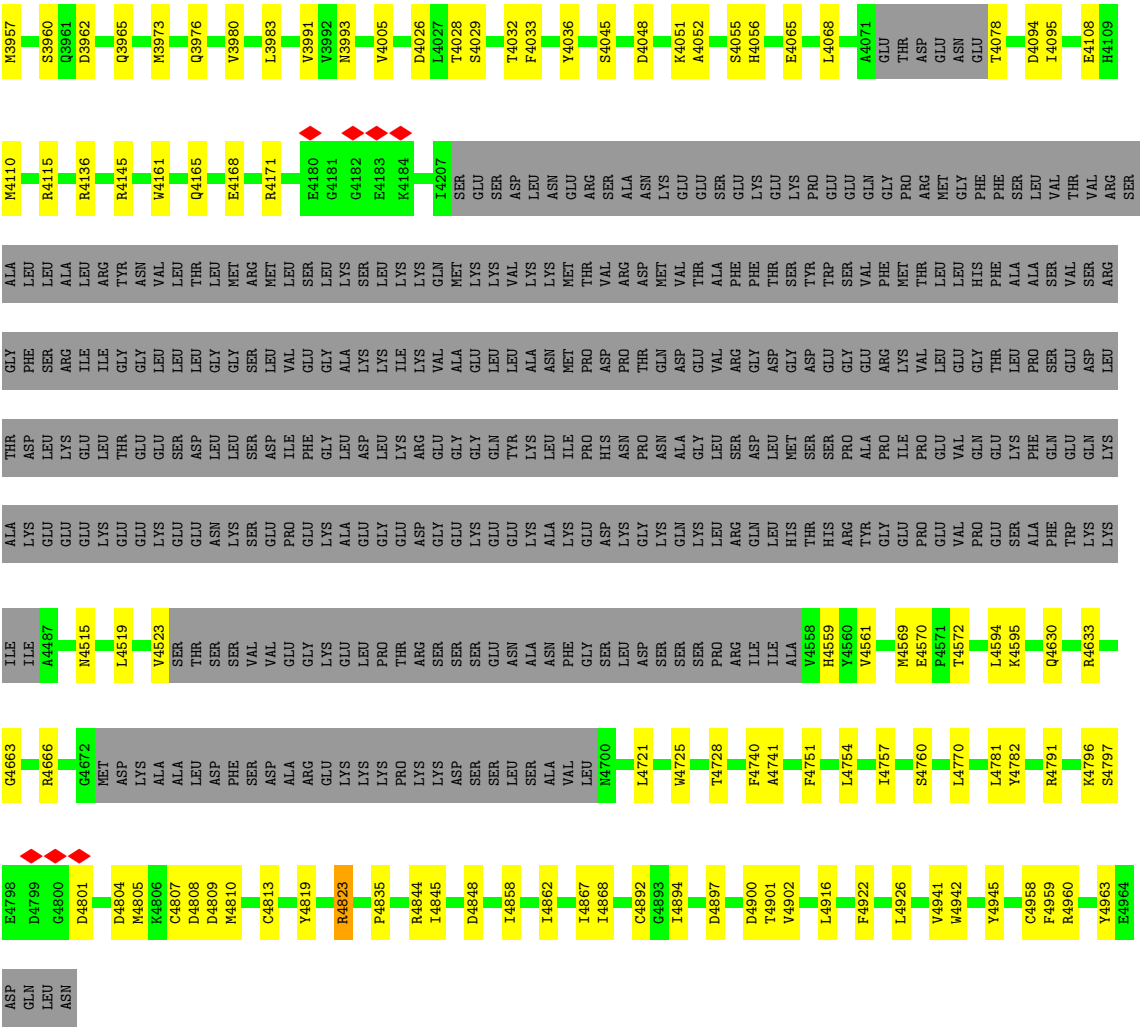
• Molecule 1: RyR2



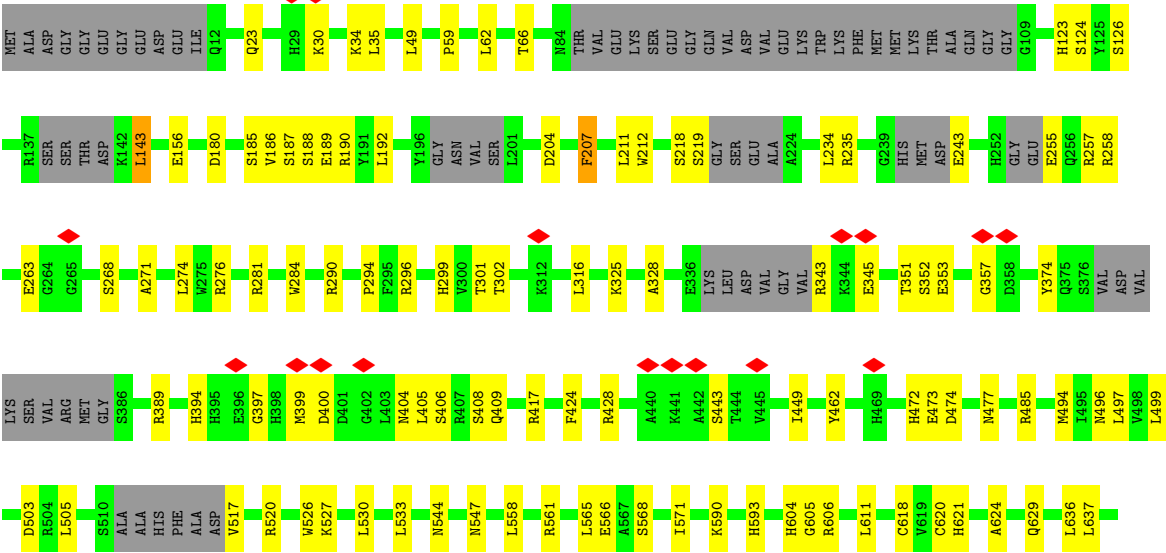








● Molecule 1: RyR2



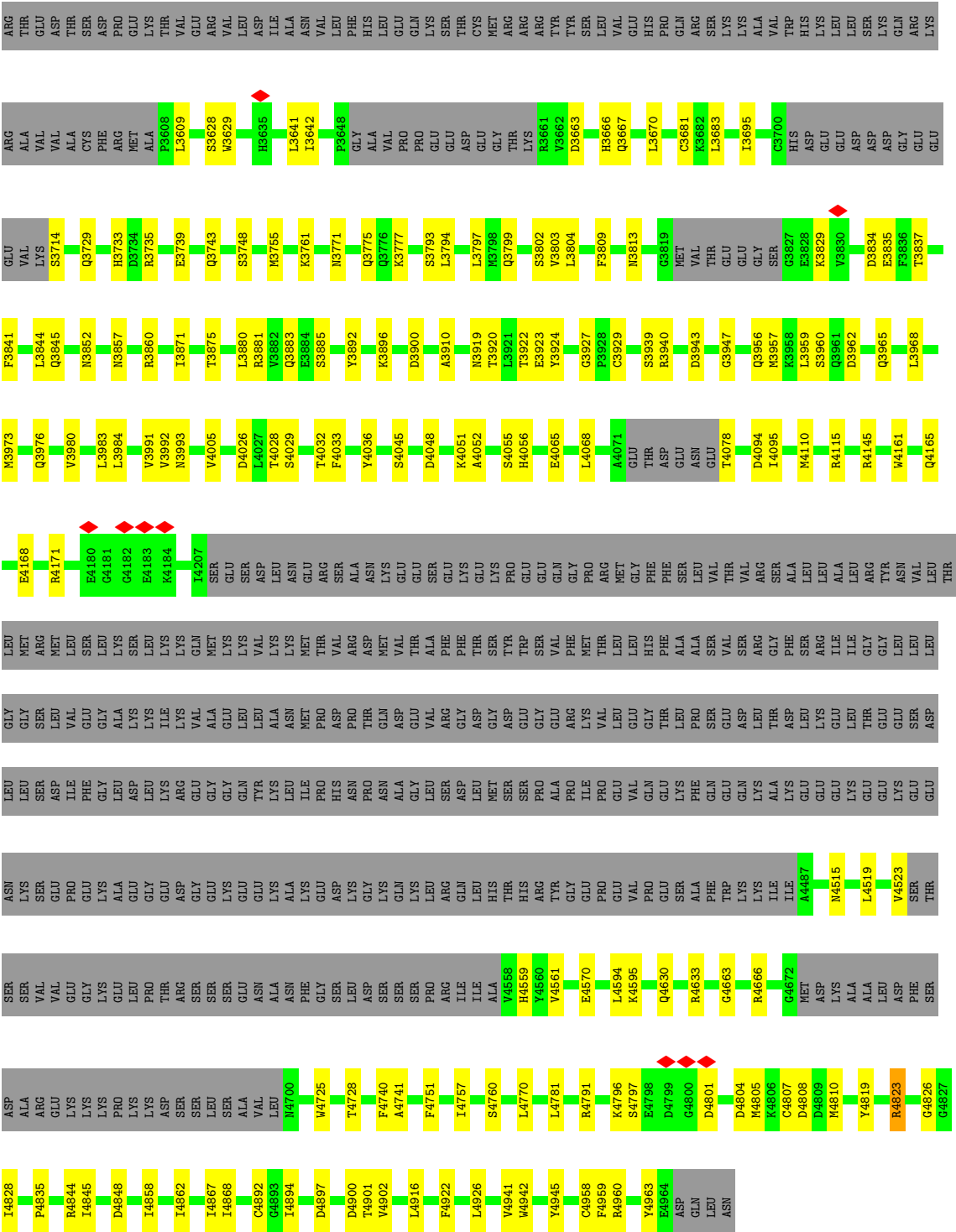
L643	L644	Q645	H651	V652	F660	L661	G662	VAL	SER	GLU	GLY	SER	ALA	GLN	TYR	K671	K672	E676	L677	M678	V679	T687	A688	E689	L693	R694	G702	Y703	S704	G708	G709	E711	E712	W713	G714	G715	W716	F727	D728	G729	S742	S743	L748	L749	R750	T751	D752	D753																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	



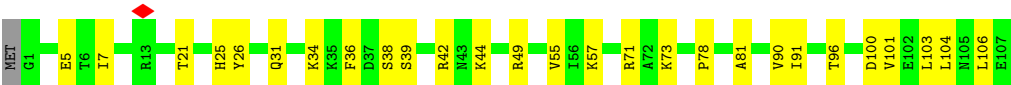
L3103	F3104	H3105	N3106	S3107	S3108	L3109	F3110	I3113	Q3117	F3118	GLY	GLU	ASP	LEU	ILE	L3124	E3125	D3126	V3127	Q3128	V3129	S3130	R3133	L3134	L3135	T3136	S3137	L3138	V3139	A3140	L3141	G3142	T3143	S3144	LYS	SER	ILE	TYR	V3149	E3150	R3151	A3155	A3164	Q3165	A3166	PHE	PRO	VAL	A3170	F3171	T3174	H3175
K3178	H3179	N3180	I3181	Y3182	S3183	ILE	TYR	ASN	THR	LYS	SER	SER	GLU	ARG	GLY	ASN	ASN	PRO	LYS	THR	ALA	ASN	VAL	CYS	PRO	ASN	ILE	PRO	GLU	SER	GLU	MET	GLU	ASP	LYS	ILE	TYR	SER	GLY	ILE	ARG	TYR	THR	GLN	MET	PRO	ALA	HIS	VAL	MET	GLU	
VAL	VAL	LEU	PRO	MET	LEU	CYS	SER	TYR	ILE	SER	ASN	TRP	GLU	HIS	GLY	PRO	ASN	PRO	ARG	ALA	GLU	VAL	ASP	GLY	LYS	LYS	ALA	SER	GLU	GLY	THR	LEU	ASP	GLY	ILE	VAL	ARG	ASN	ASN	LEU	GLY	ILE	GLY	ASP	GLY	GLU	ALA	TRP	ILE	MET		
LYS	ARG	LEU	ALA	VAL	PHE	LEU	SER	GLN	PRO	ILE	VAL	LYS	GLN	LEU	PRO	GLY	ILE	ARG	ILE	LEU	GLU	PHE	THR	GLY	LYS	LYS	ALA	VAL	VAL	THR	GLY	ASP	GLY	ILE	VAL	ARG	ASN	ASN	LEU	GLY	ASP	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY			
GLN	ASN	PHE	VAL	VAL	CYS	ASN	GLN	GLY	ILE	ASN	MET	SER	PHE	ILE	ASN	ASP	THR	LYS	THR	ARG	ALA	VAL	SER	GLY	LYS	SER	PRO	GLY	VAL	VAL	GLY	GLN	ASP	GLY	ARG	TYR	SER	ILE	VAL	VAL	GLN	MET	ALA	ALA	LEU	TYR	LYS	ASP	LEU	ASN		
GLY	LEU	ASN	ILE	ILE	ALA	PRO	GLY	ALA	GLY	GLN	ILE	ALA	LEU	LYS	ASN	ARG	PHE	THR	ASP	ALA	GLU	PRO	ASP	ILE	ILE	ILE	SER	ARG	GLY	GLN	GLY	GLY	LYS	ARG	GLY	THR	ILE	VAL	GLN	MET	ALA	ALA	LEU	TYR	LYS	ASP	LEU	PRO	ASN			
ARG	THR	GLU	ASP	THR	SER	ASP	PRO	ASP	GLU	LYS	THR	VAL	ARG	GLY	ASN	VAL	VAL	PHE	LEU	ASP	ILE	ALA	ASN	VAL	VAL	GLN	SER	THR	ASP	THR	GLY	GLY	GLY	GLY	VAL	THR	GLN	HIS	LYS	LEU	LEU	SER	LYS	GLN	ARG	LYS						
ARG	ALA	VAL	VAL	CYS	PHE	ARG	MET	ALA	L3608	L3609	S3628	W3629	H3635	L3641	I3642	P3643	GLY	ALA	VAL	PRO	PRO	GLU	GLY	THR	LYS	R3651	V3652	D3653	H3666	Q3667	L3670	C3681	K3682	L3683	I3695	C3700	HIS	ASP	GLY	GLY	GLY	ASP	ASP	GLY	GLY	GLY						
GLU	VAL	L3714	Q3729	H3733	D3734	R3735	E3739	Q3743	S3748	M3755	N3771	Q3775	Q3776	K3777	Q3799	S3802	V3803	L3804	F3809	E3810	R3811	N3813	G3819	MET	VAL	THR	GLY	GLY	GLY	SER	G3827	E3828	K3829	V3830	F3841	L3844	Q3845	N3852	N3857	R3860												
L3871	T3875	L3880	R3881	V3882	Q3883	E3884	S3885	V3891	Y3892	K3896	D3900	A3910	N3919	T3920	L3921	T3922	E3923	Y3924	G3927	P3928	C3929	S3939	R3940	D3943	G3947	Q3956	M3957	S3960	Q3961	D3962	Q3965	M3973	Q3976	V3980	L3983	V3991	V3992	N3993														
V4005	D4026	L4027	T4028	S4029	T4032	F4033	Y4036	S4045	D4048	K4051	A4052	S4055	H4056	E4065	L4068	A4071	THR	ASP	GLY	ASN	GLU	T4078	D4094	I4095	M4110	R4115	R4145	W4161	Q4165	E4168	R4171	E4180	Q4181	G4182	E4183	K4184	I4207	SER														
GLU	SER	ASP	LEU	ASN	GLY	THR	ARG	THR	GLU	GLU	THR	GLU	GLU	GLY	THR	GLY	PHE	THR	GLY	VAL	THR	VAL	VAL	LEU	LEU	LEU	LEU	ASN	VAL	LEU	GLY	MET	MET	LEU	LEU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
MET	LYS	VAL	VAL	LYS	MET	THR	MET	VAL	THR	ALA	PHE	ASP	PHE	THR	GLY	TYR	GLY	THR	GLY	ASP	GLY	GLY	GLY	GLY	ALA	ALA	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
ALA	GLU	LEU	LEU	ALA	ASN	MET	PRO	ASP	GLU	GLU	VAL	ARG	GLY	ASP	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
GLY	GLY	GLN	TYR	LYS	ILE	PRO	HIS	ASN	GLY	GLY	ALA	LEU	HIS	THR	PRO	GLY	GLY	VAL	GLY	VAL	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL			
GLU	LYS	GLU	GLU	ALA	LYS	GLY	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
GLU	LYS	GLU	GLU	ALA	LYS	GLY	GLY	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				








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



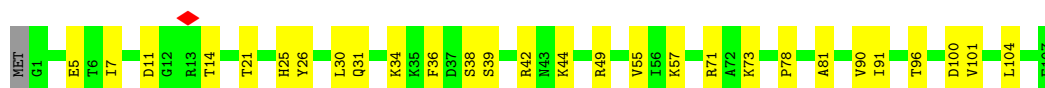
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D:  75% 24%




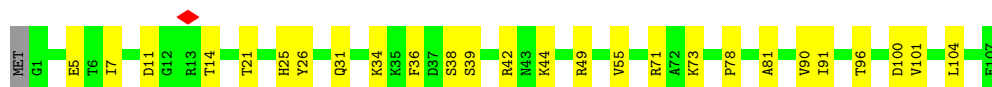
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:  73% 26%



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

Chain H:  75% 24%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	149212	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	0.141	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.022	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

5.1 Standard geometry

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

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	0.47	0/26913	0.60	5/36395 (0.0%)
1	C	0.47	0/26913	0.60	5/36395 (0.0%)
1	E	0.47	0/26913	0.60	5/36395 (0.0%)
1	G	0.47	0/26913	0.60	5/36395 (0.0%)
2	B	0.41	0/835	0.58	0/1123
2	D	0.41	0/835	0.58	0/1123
2	F	0.41	0/835	0.58	0/1123
2	H	0.41	0/835	0.58	0/1123
All	All	0.47	0/110992	0.60	20/150072 (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	15
1	C	0	15
1	E	0	15
1	G	0	15
All	All	0	60

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2430	LEU	CA-CB-CG	7.00	131.39	115.30
1	C	2430	LEU	CA-CB-CG	7.00	131.39	115.30
1	E	2430	LEU	CA-CB-CG	7.00	131.39	115.30
1	G	2430	LEU	CA-CB-CG	7.00	131.39	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	3681	CYS	CA-CB-SG	5.68	124.22	114.00

There are no chirality outliers.

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	729	GLY	Peptide
1	A	791	VAL	Peptide
1	A	814	LEU	Peptide
1	A	816	PRO	Peptide
1	A	819	TYR	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	26417	0	24909	474	0
1	C	26417	0	24909	487	0
1	E	26417	0	24909	466	0
1	G	26417	0	24909	457	0
2	B	819	0	824	18	0
2	D	819	0	824	18	0
2	F	819	0	824	19	0
2	H	819	0	824	18	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	31	0	12	1	0
5	C	31	0	12	1	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
6	A	14	0	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	14	0	10	2	0
6	E	14	0	10	2	0
6	G	14	0	10	2	0
All	All	109132	0	103020	1741	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 1741 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:A:2427:LEU:HD13	1:G:143:LEU:CB	1.41	1.51
1:E:143:LEU:CB	1:G:2427:LEU:HD13	1.41	1.49
1:A:143:LEU:CB	1:C:2427:LEU:HD13	1.41	1.48
1:C:143:LEU:CB	1:E:2427:LEU:HD13	1.43	1.47
1:A:2427:LEU:CD1	1:G:143:LEU:HB3	1.48	1.42

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	A	3336/4968 (67%)	2981 (89%)	347 (10%)	8 (0%)	47	79
1	C	3336/4968 (67%)	2982 (89%)	345 (10%)	9 (0%)	41	75
1	E	3336/4968 (67%)	2980 (89%)	347 (10%)	9 (0%)	41	75
1	G	3336/4968 (67%)	2980 (89%)	348 (10%)	8 (0%)	47	79
2	B	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	D	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	13764/20304 (68%)	12323 (90%)	1407 (10%)	34 (0%)	50	79

5 of 34 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2328	ARG
1	A	4901	THR
1	C	2328	ARG
1	C	4901	THR
1	E	2328	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	2650/4355 (61%)	2627 (99%)	23 (1%)	78	87
1	C	2650/4355 (61%)	2625 (99%)	25 (1%)	78	87
1	E	2648/4355 (61%)	2623 (99%)	25 (1%)	78	87
1	G	2650/4355 (61%)	2628 (99%)	22 (1%)	81	89
2	B	88/89 (99%)	88 (100%)	0	100	100
2	D	88/89 (99%)	88 (100%)	0	100	100
2	F	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
All	All	10950/17776 (62%)	10855 (99%)	95 (1%)	79	87

5 of 95 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1013	ARG
1	E	4823	ARG
1	E	1466	THR
1	E	2327	ARG

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Mol	Chain	Res	Type
1	G	325	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 149 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	394	HIS
1	G	4880	GLN
1	G	550	GLN
1	G	1836	ASN
1	C	914	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 monosaccharides 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	CFF	E	6003	-	8,15,15	2.91	4 (50%)	8,23,23	1.32	1 (12%)
6	CFF	G	6003	-	8,15,15	2.93	4 (50%)	8,23,23	1.30	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CFF	A	6003	-	8,15,15	2.93	4 (50%)	8,23,23	1.30	1 (12%)
5	ATP	E	6002	-	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)
5	ATP	G	6002	-	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)
5	ATP	A	6002	-	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)
6	CFF	C	6003	-	8,15,15	2.93	4 (50%)	8,23,23	1.30	1 (12%)
5	ATP	C	6002	-	26,33,33	0.91	1 (3%)	31,52,52	1.66	6 (19%)

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	CFF	E	6003	-	-	-	0/2/2/2
6	CFF	G	6003	-	-	-	0/2/2/2
6	CFF	A	6003	-	-	-	0/2/2/2
5	ATP	E	6002	-	-	4/18/38/38	0/3/3/3
5	ATP	G	6002	-	-	4/18/38/38	0/3/3/3
5	ATP	A	6002	-	-	4/18/38/38	0/3/3/3
6	CFF	C	6003	-	-	-	0/2/2/2
5	ATP	C	6002	-	-	4/18/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	6003	CFF	C5-C4	-5.46	1.32	1.39
6	C	6003	CFF	C5-C4	-5.46	1.32	1.39
6	G	6003	CFF	C5-C4	-5.46	1.32	1.39
6	E	6003	CFF	C5-C4	-5.39	1.32	1.39
6	A	6003	CFF	C6-N1	-4.45	1.31	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	6002	ATP	PA-O3A-PB	-4.88	116.07	132.83
5	A	6002	ATP	PA-O3A-PB	-4.87	116.11	132.83
5	C	6002	ATP	PA-O3A-PB	-4.87	116.11	132.83
5	G	6002	ATP	PA-O3A-PB	-4.86	116.15	132.83
5	A	6002	ATP	N3-C2-N1	-3.63	123.01	128.68

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

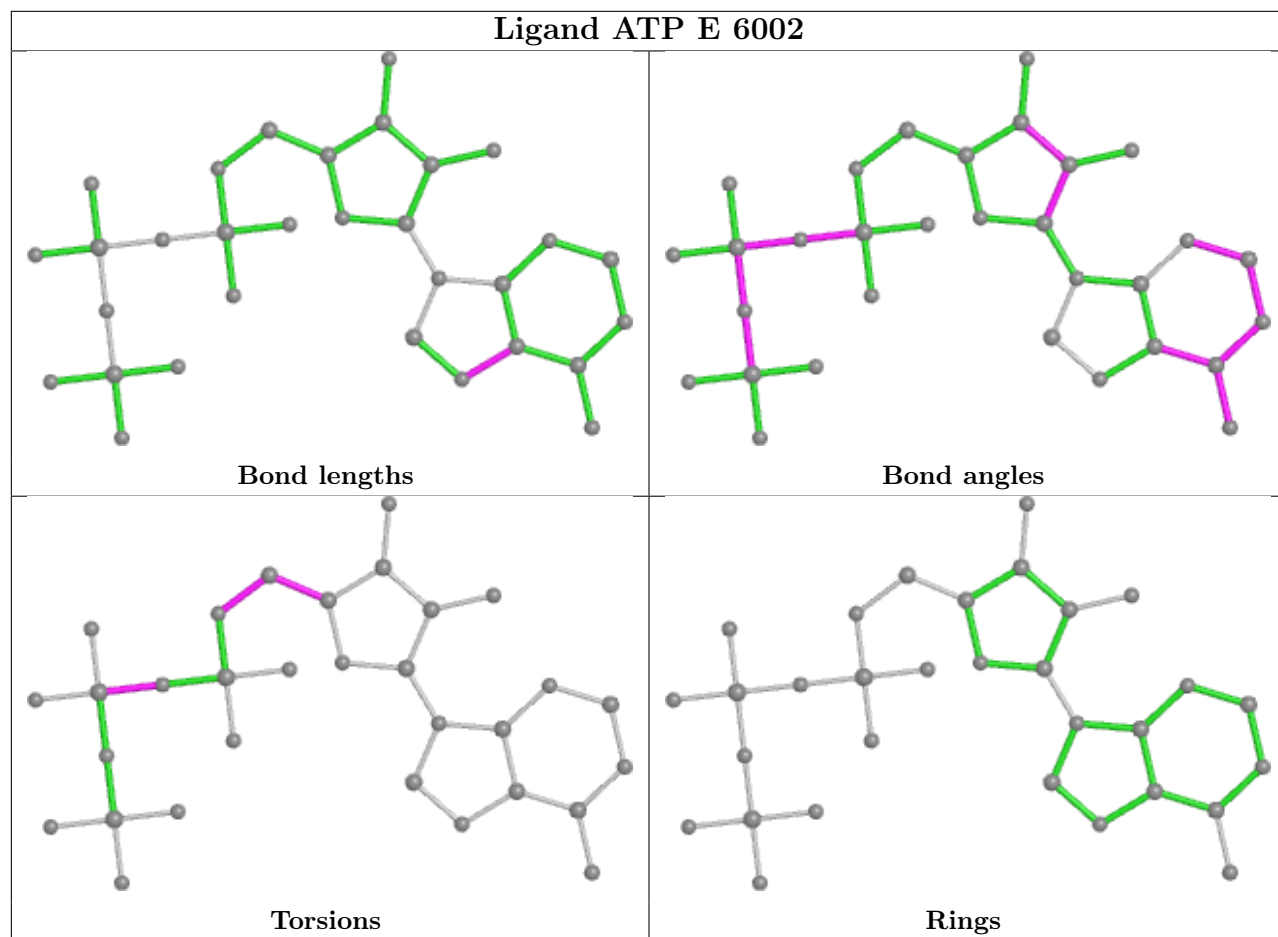
Mol	Chain	Res	Type	Atoms
5	A	6002	ATP	C3'-C4'-C5'-O5'
5	C	6002	ATP	C3'-C4'-C5'-O5'
5	E	6002	ATP	C3'-C4'-C5'-O5'
5	G	6002	ATP	C3'-C4'-C5'-O5'
5	A	6002	ATP	O4'-C4'-C5'-O5'

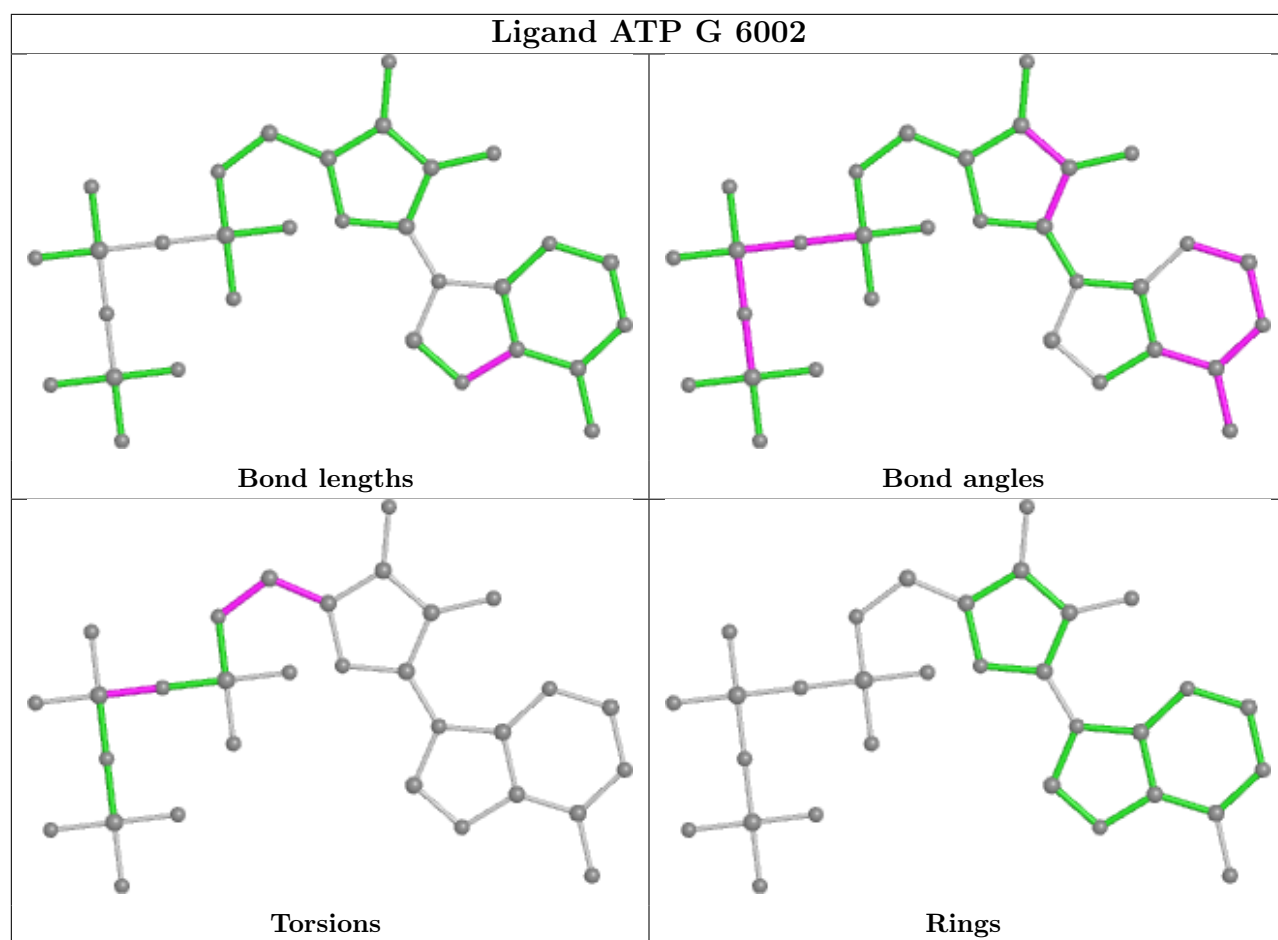
There are no ring outliers.

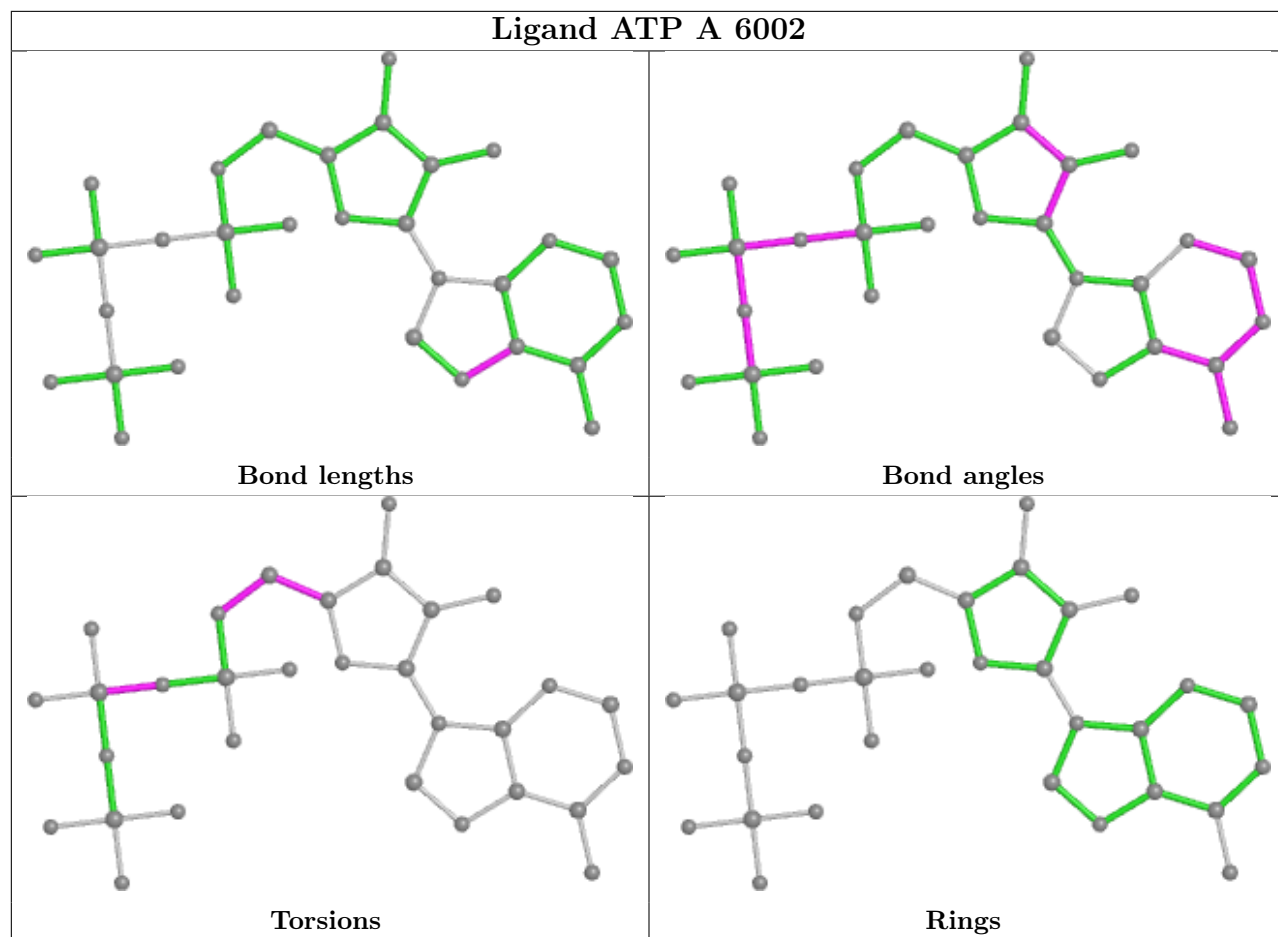
8 monomers are involved in 12 short contacts:

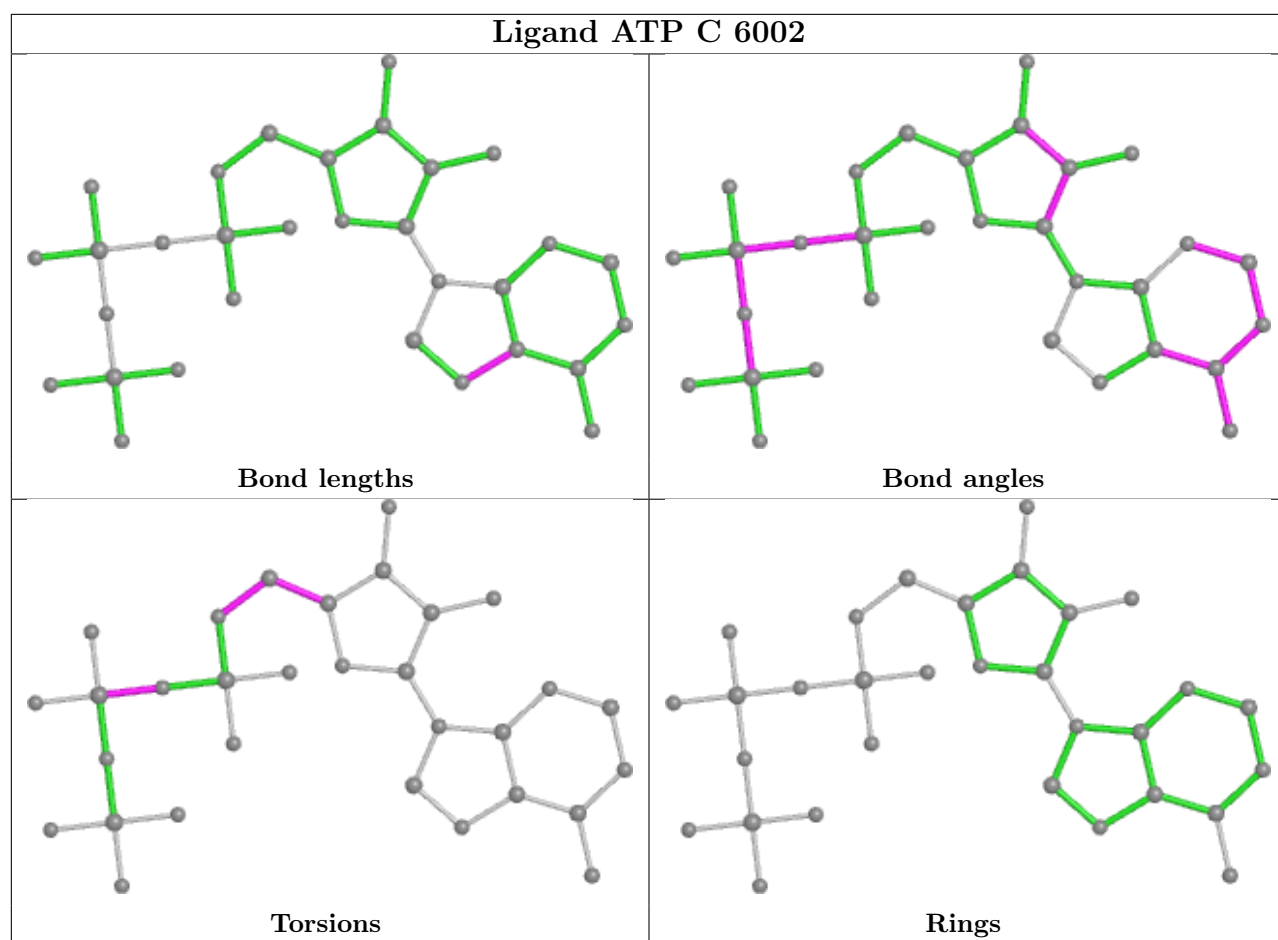
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	6003	CFF	2	0
6	G	6003	CFF	2	0
6	A	6003	CFF	2	0
5	E	6002	ATP	1	0
5	G	6002	ATP	1	0
5	A	6002	ATP	1	0
6	C	6003	CFF	2	0
5	C	6002	ATP	1	0

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.

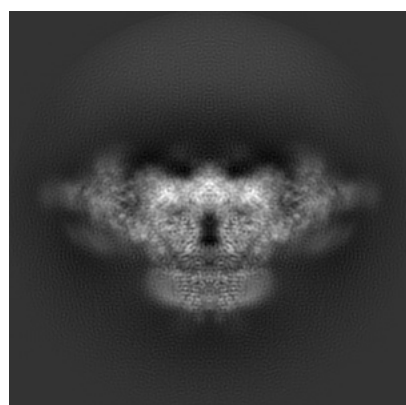
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9879. These allow visual inspection of the internal detail of the map and identification of artifacts.

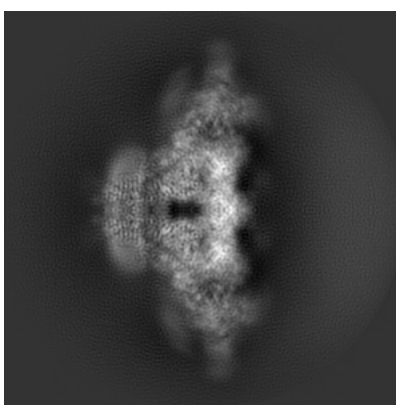
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

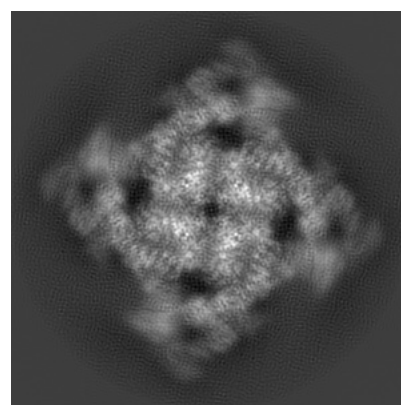
6.1.1 Primary map



X



Y

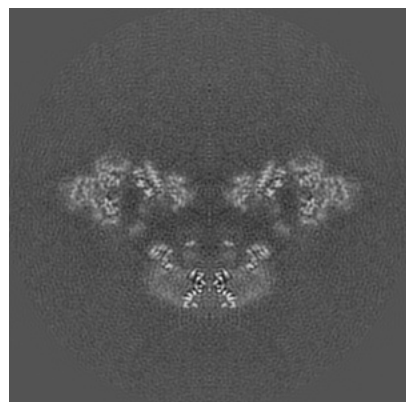


Z

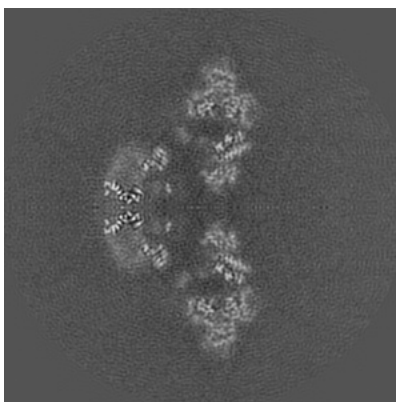
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

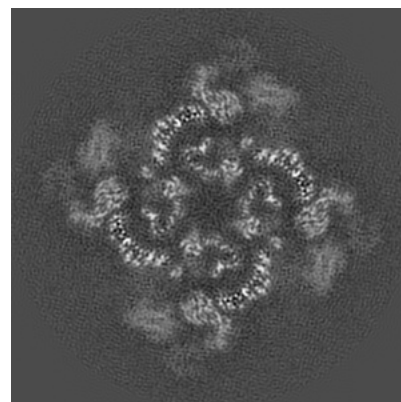
6.2.1 Primary map



X Index: 200



Y Index: 200

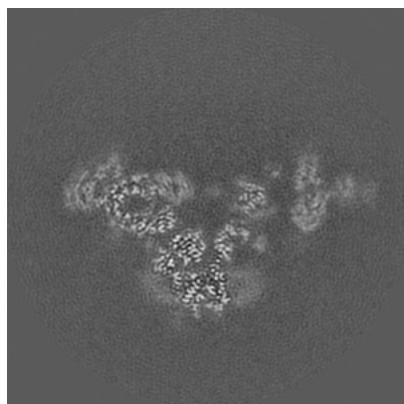


Z Index: 200

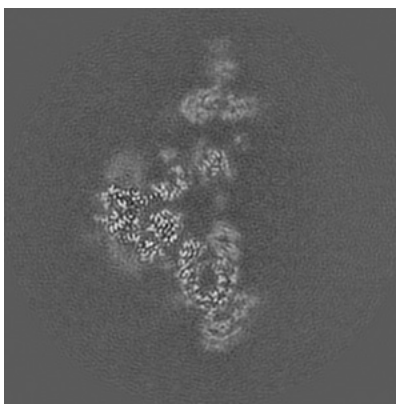
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

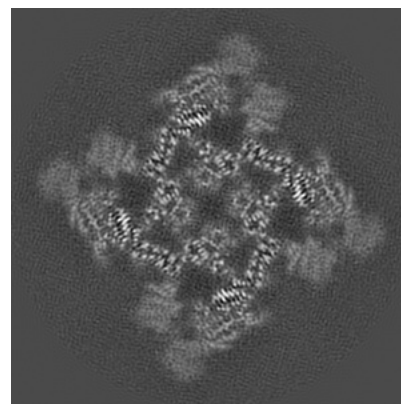
6.3.1 Primary map



X Index: 213



Y Index: 187

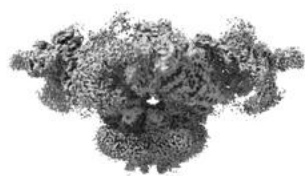


Z Index: 211

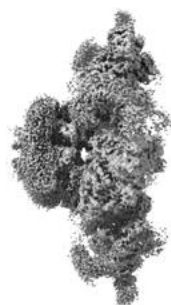
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

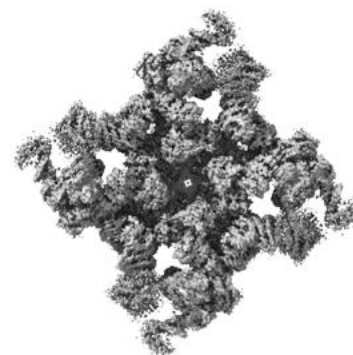
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

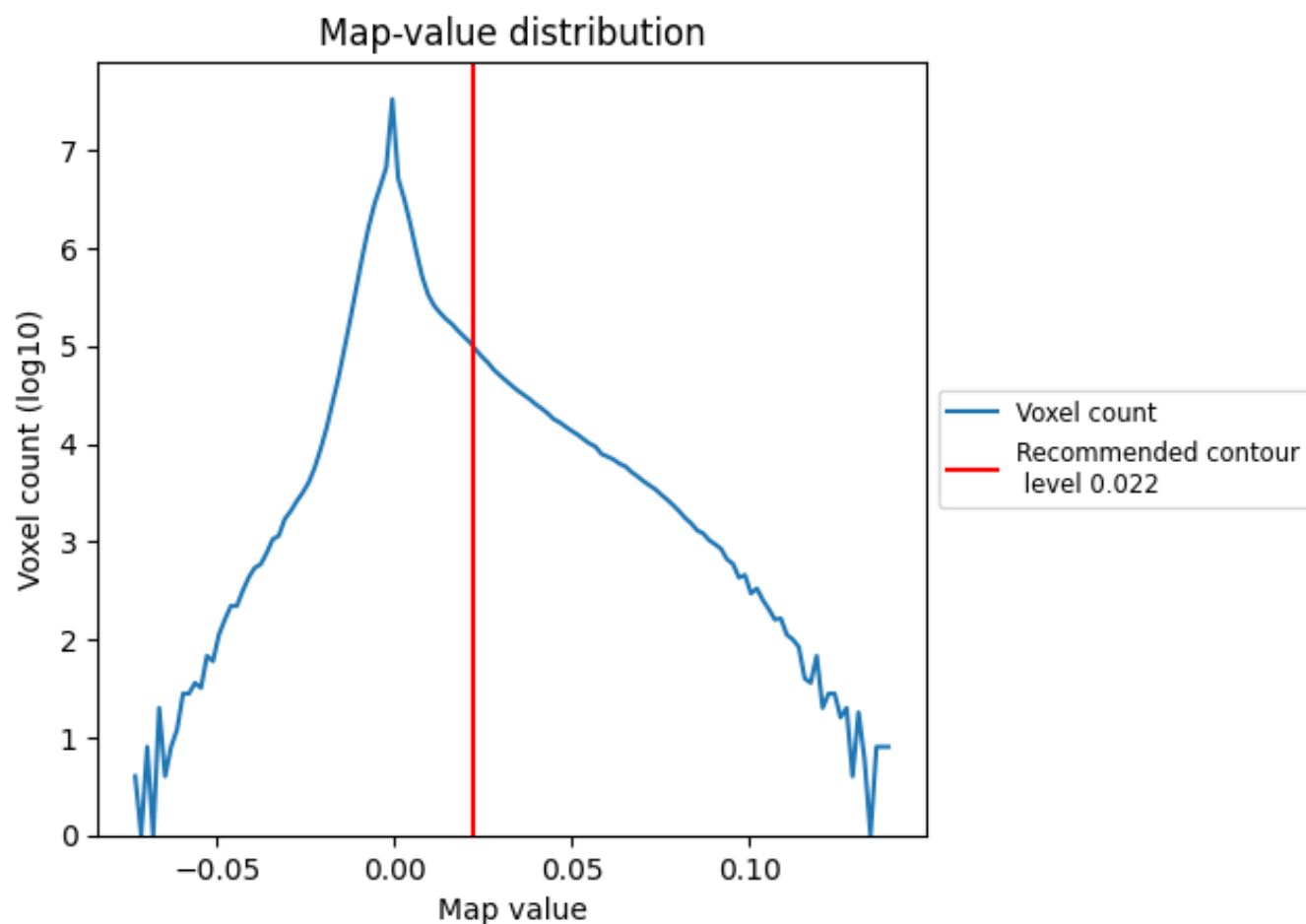
6.5 Mask visualisation

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

7 Map analysis [i](#)

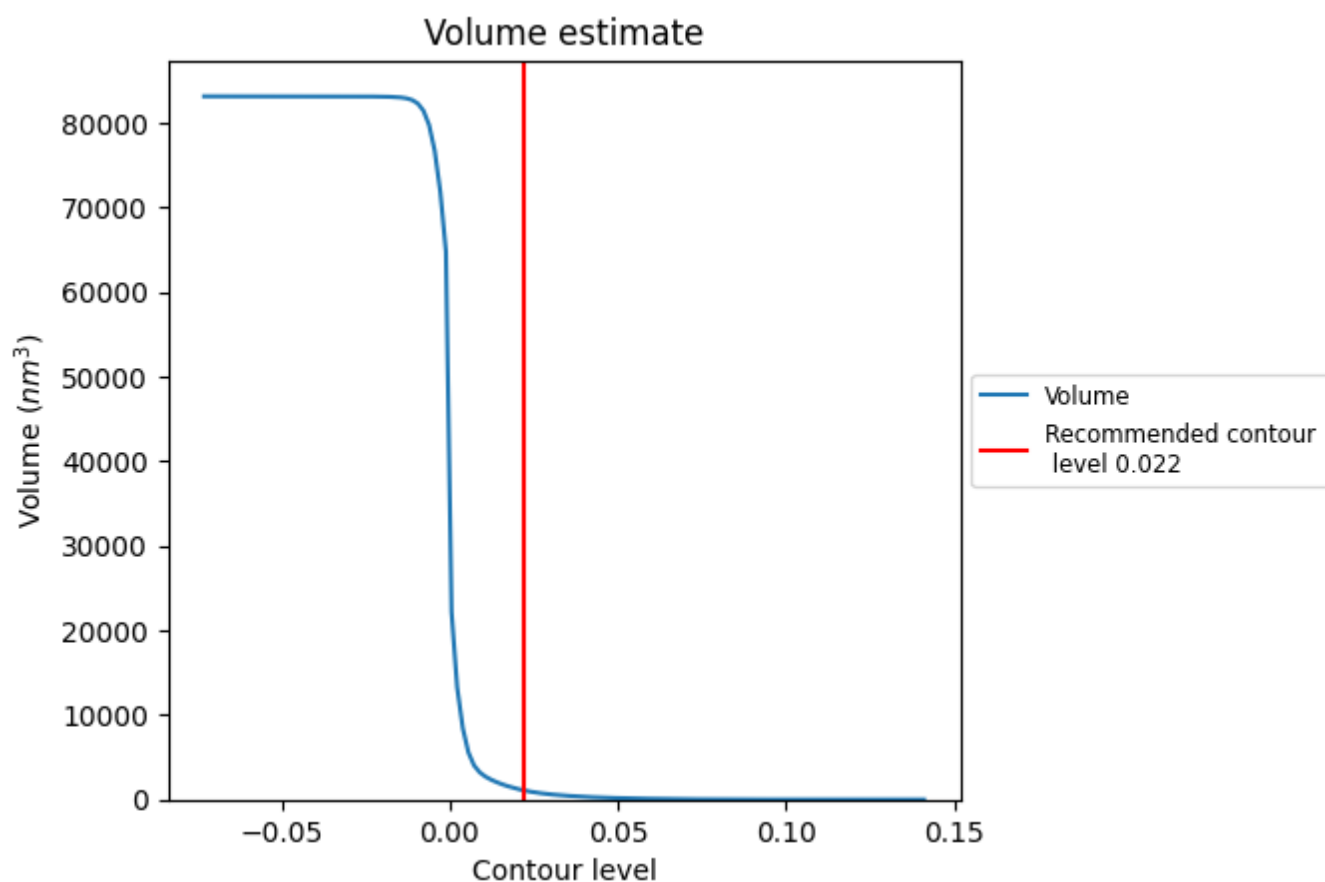
This section contains the results of statistical analysis of the map.

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.

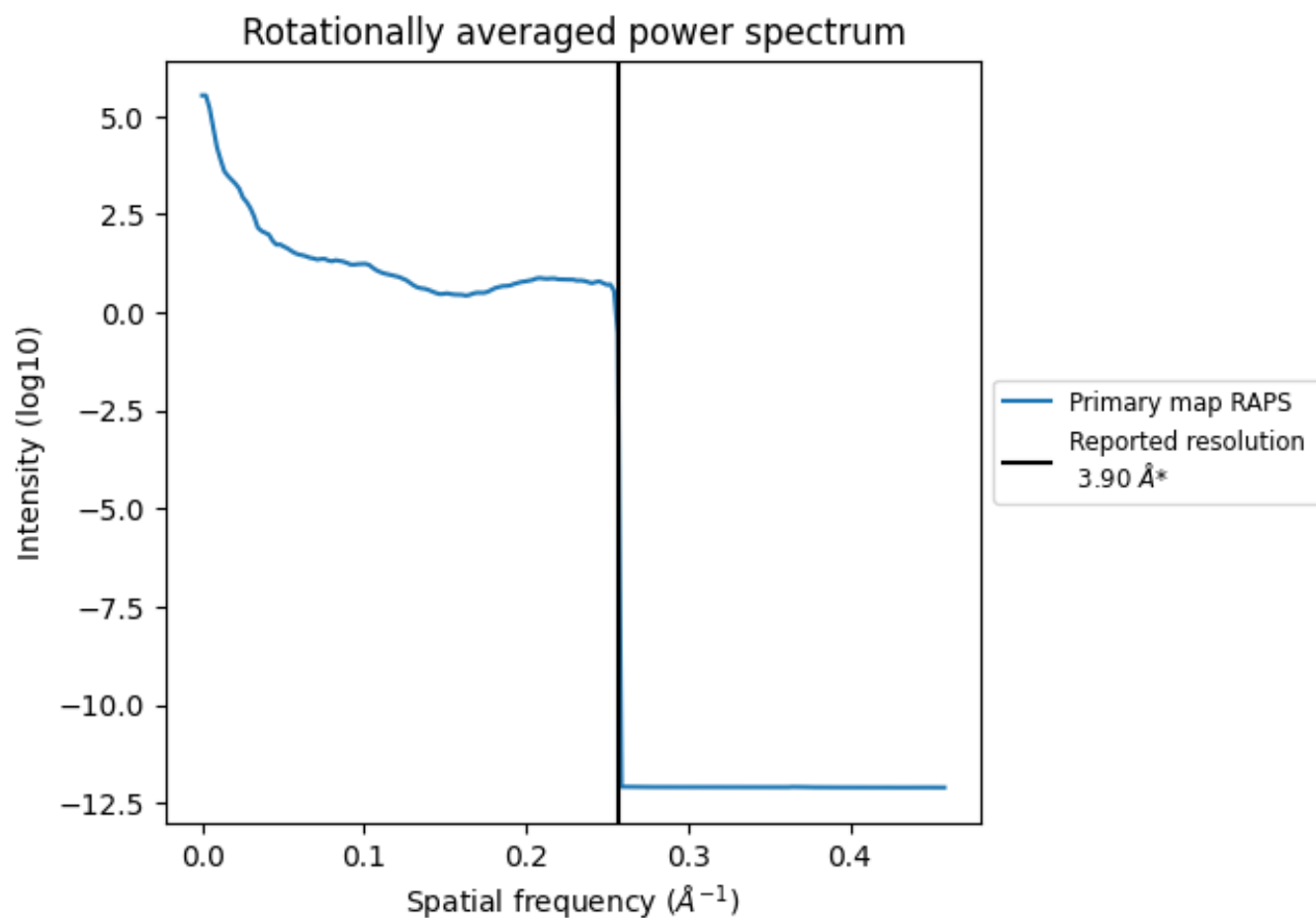
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1096 nm³; this corresponds to an approximate mass of 990 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 ⓘ

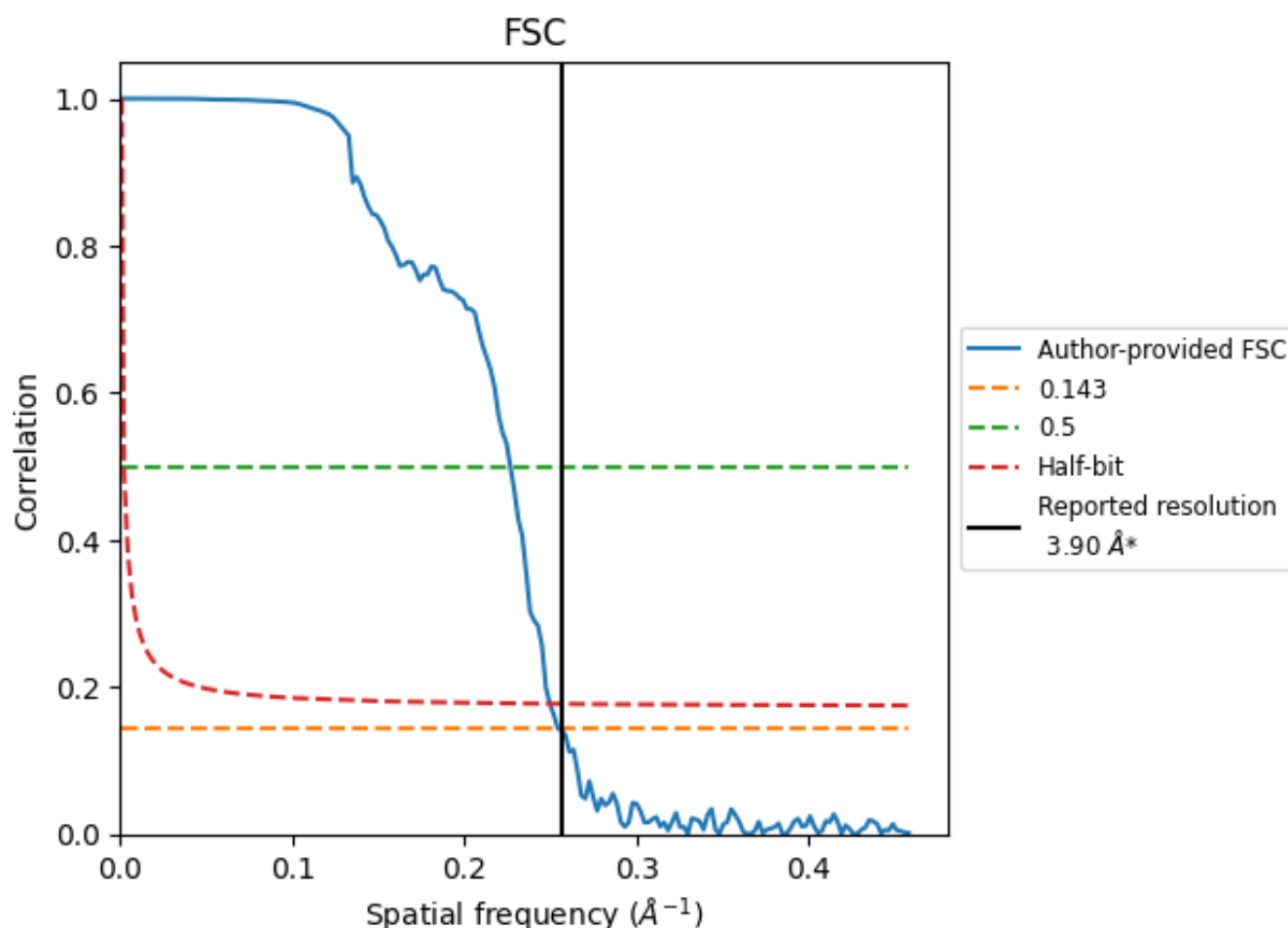


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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](#)

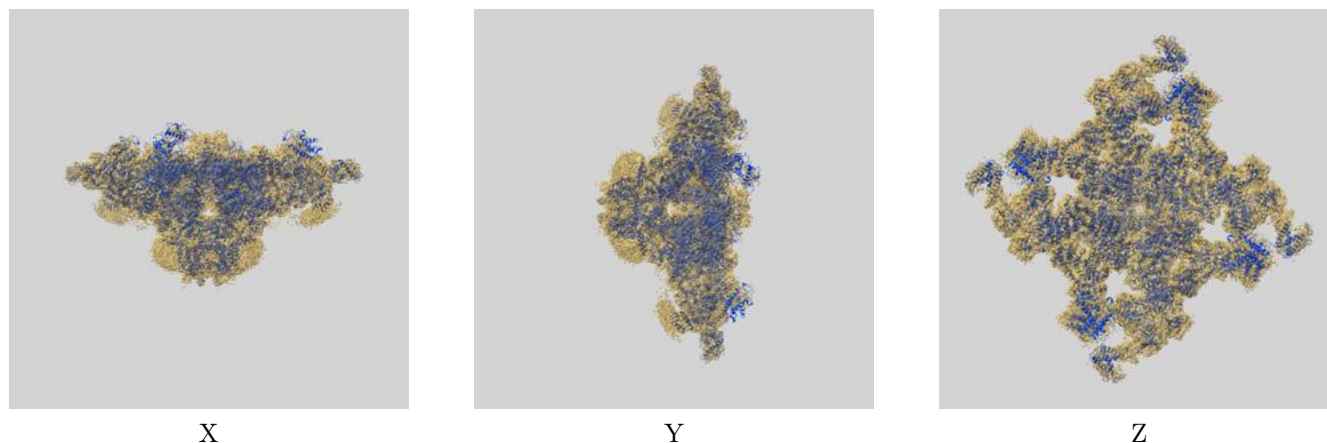
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.93	4.41	4.00
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

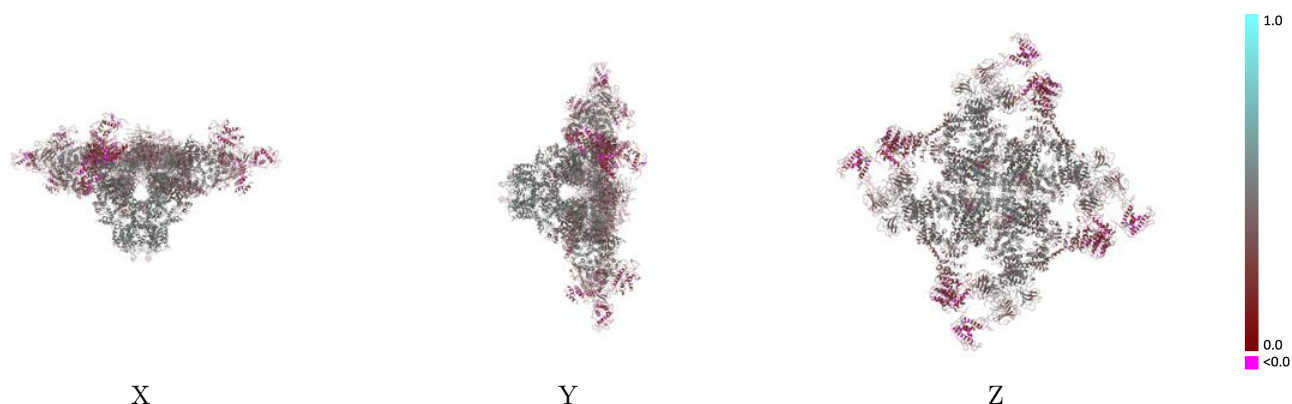
This section contains information regarding the fit between EMDB map EMD-9879 and PDB model 6JRR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



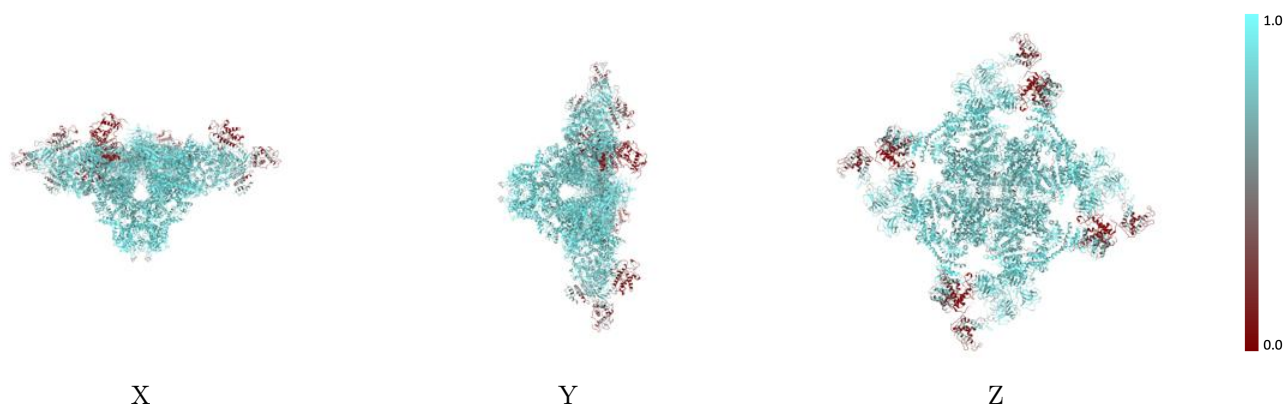
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



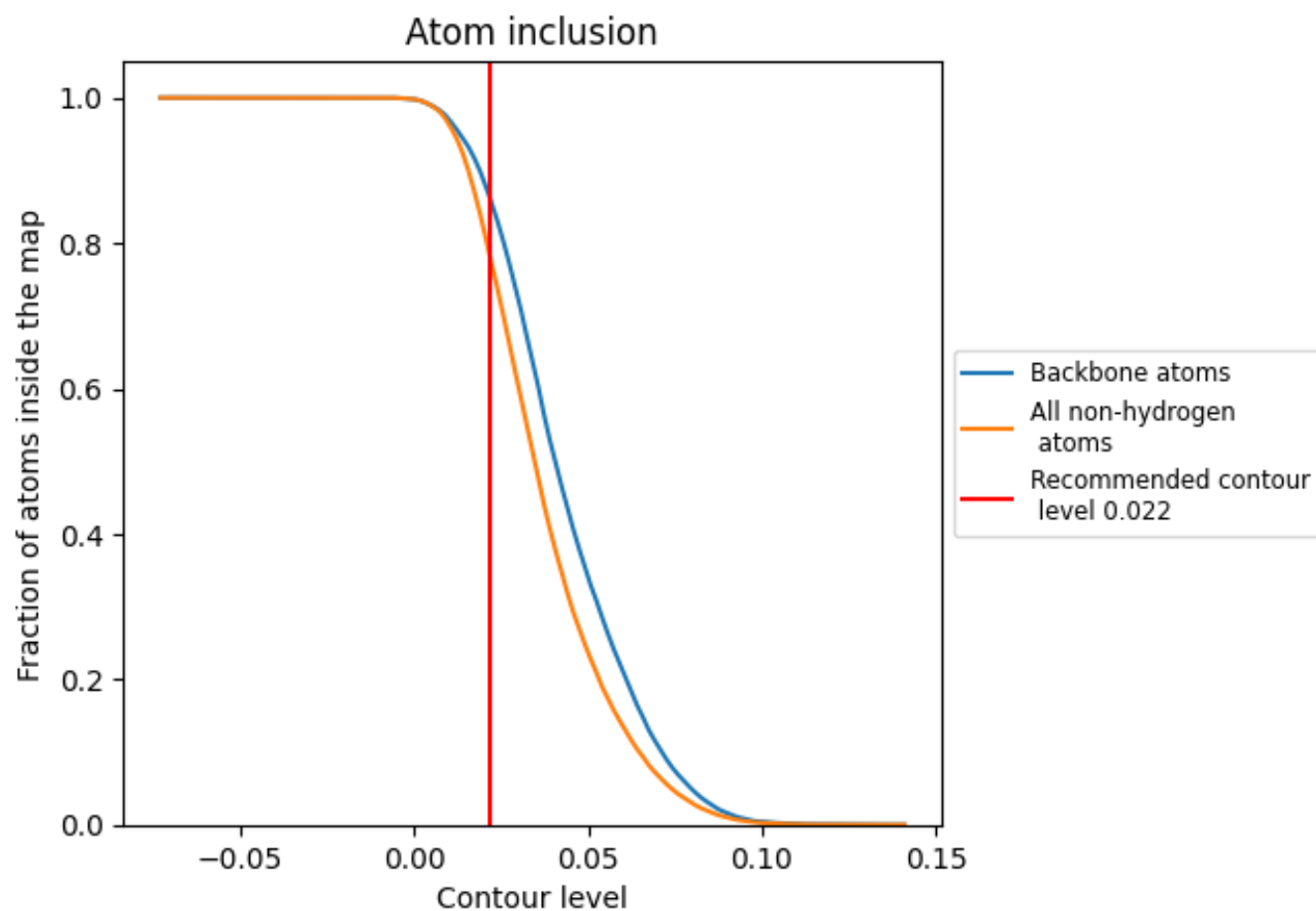
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 78% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7780	<div><div></div></div> 0.3900
A	<div><div></div></div> 0.7770	<div><div></div></div> 0.3900
B	<div><div></div></div> 0.8141	<div><div></div></div> 0.4170
C	<div><div></div></div> 0.7767	<div><div></div></div> 0.3890
D	<div><div></div></div> 0.8154	<div><div></div></div> 0.4160
E	<div><div></div></div> 0.7768	<div><div></div></div> 0.3890
F	<div><div></div></div> 0.8178	<div><div></div></div> 0.4170
G	<div><div></div></div> 0.7770	<div><div></div></div> 0.3890
H	<div><div></div></div> 0.8154	<div><div></div></div> 0.4160

1.0

0.0

<0.0