



wwPDB EM Validation Summary Report ⓘ

Sep 29, 2025 – 12:24 PM EDT

PDB ID : 9NMR / pdb_00009nmr
EMDB ID : EMD-49538
Title : Structure of mouse RyR1 (including auxiliary transmembrane helix TMx; EGTA-only dataset)
Authors : Weninger, G.; Marks, A.R.
Deposited on : 2025-03-04
Resolution : 2.91 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:

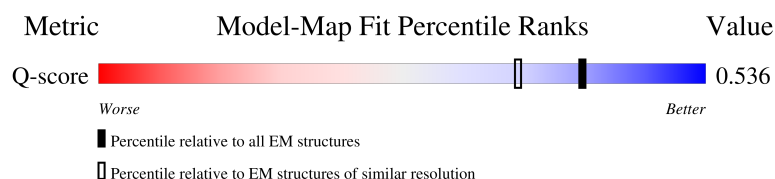
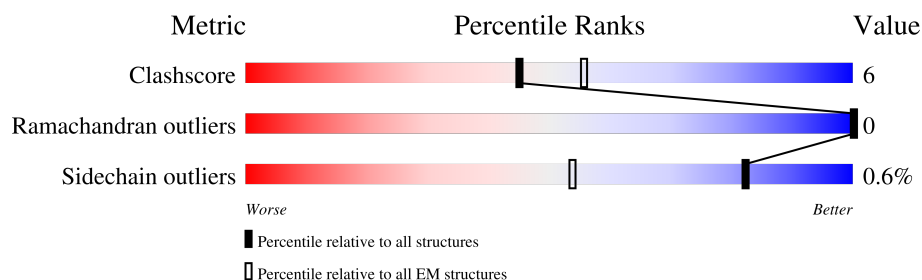
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.91 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	12972 (2.41 - 3.41)

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	5035	<div> <div>8%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
1	B	5035	<div> <div>8%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
1	C	5035	<div> <div>8%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>
1	D	5035	<div> <div>8%</div> <div>74%</div> <div>13%</div> <div>13%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	108	<div><div></div><div>91%</div><div>8%</div><div></div></div>
2	F	108	<div><div></div><div>89%</div><div>10%</div><div></div></div>
2	G	108	<div><div></div><div>90%</div><div>9%</div><div></div></div>
2	H	108	<div><div></div><div>91%</div><div>8%</div><div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 143684 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4397	Total	C	N	O	S	1	0
			34983	22250	6021	6475	237		
1	B	4397	Total	C	N	O	S	1	0
			34983	22250	6021	6475	237		
1	C	4397	Total	C	N	O	S	1	0
			34983	22250	6021	6475	237		
1	D	4397	Total	C	N	O	S	1	0
			34983	22250	6021	6475	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

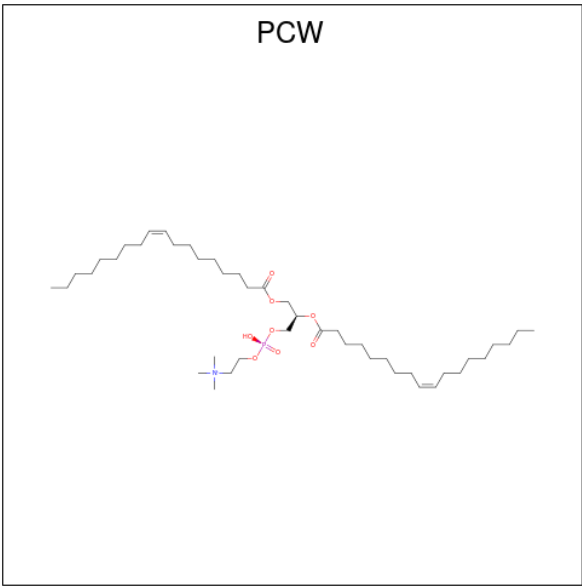
Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	F	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	G	107	Total	C	N	O	S	0	0
			829	526	145	155	3		
2	H	107	Total	C	N	O	S	0	0
			829	526	145	155	3		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

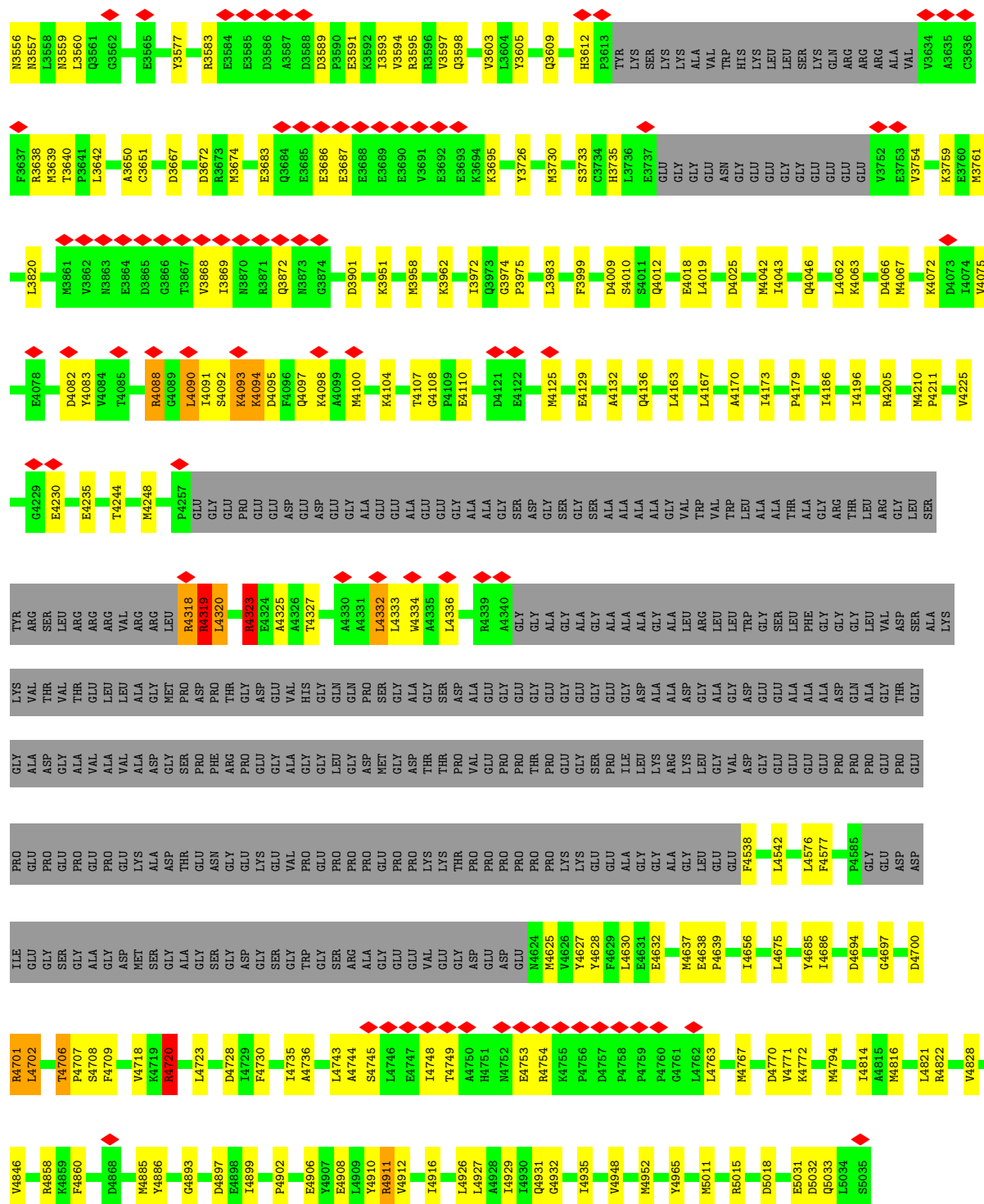
- Molecule 4 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PCW)

(formula: C₄₄H₈₅NO₈P).

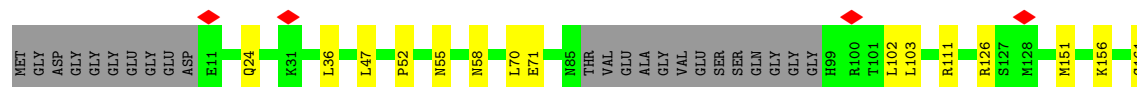
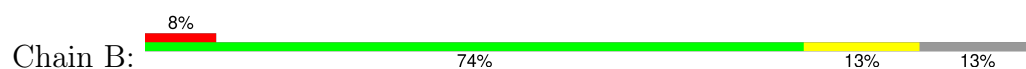


Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	A	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	B	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	C	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	D	1	Total	C	N	O	P	0
			54	44	1	8	1	
4	D	1	Total	C	N	O	P	0
			54	44	1	8	1	





- Molecule 1: Ryanodine receptor 1





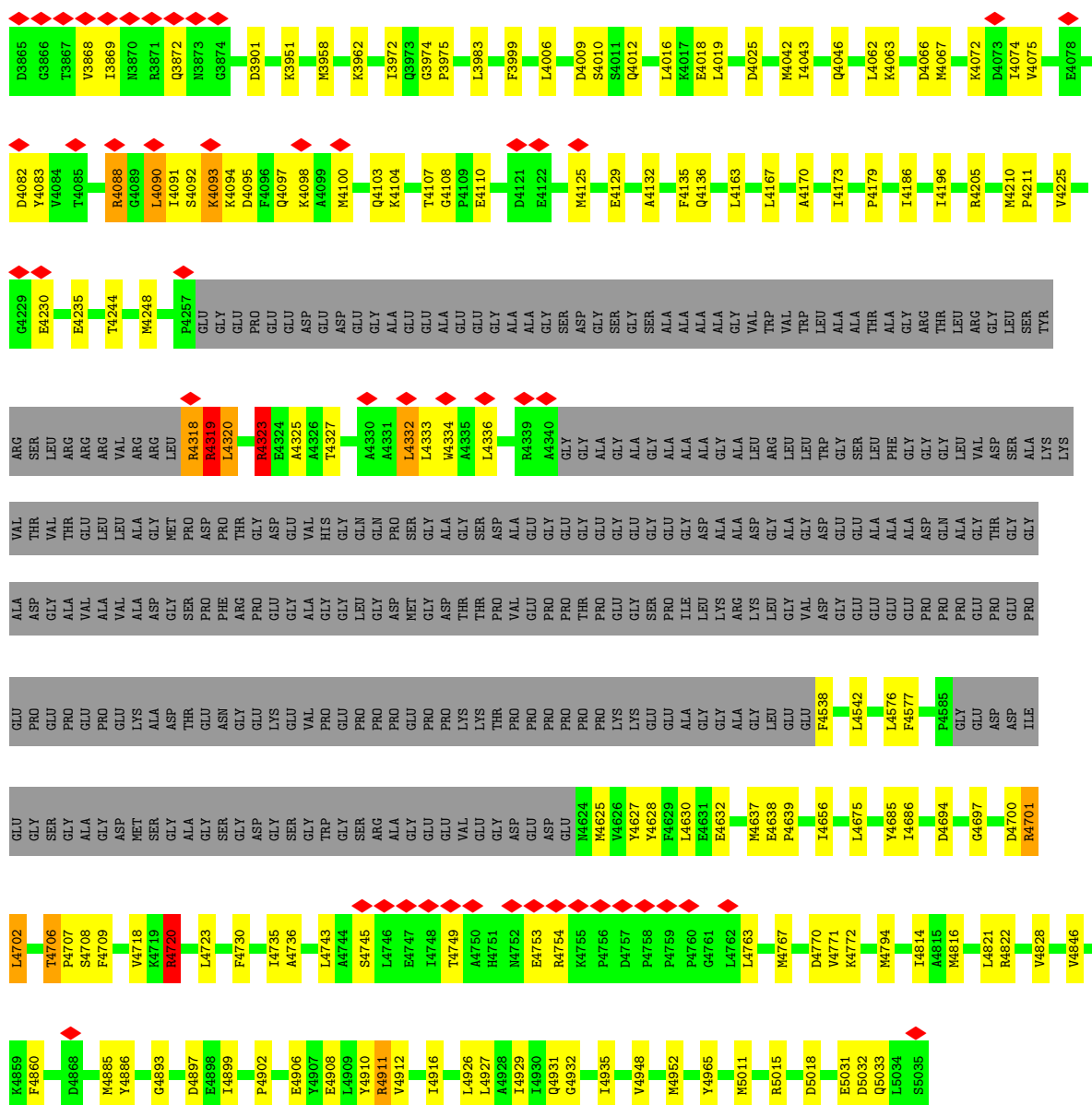








D3672	E3683	ALA	V3373	R3188	M3013	D2920	F2860	P2740	Q2516	L2308	L2183
R3673	E3584	GLY	E3377	L3195	V3025	R2921	K2801	V2741	D2517	C2327	M2187
R3674	E3585	VAL	E3377	L3195	V3025	E2922	D2802	E2742	L2520	R2331	F2191
E3683	D3586	GLN	L3380	E3208	K3037	K2923	K2803	T2743	V2525	R2337	F2192
Q3684	A3587	SER	R3381	E3227	T3040	Q2925	E2804	L2744	Q2526	R2356	N2197
E3685	D3588	GLY	L3382	R3228	T3041	E2926	E2805	N2745	L2537	R2356	L2198
D3589	D3589	SER	E3383	A3229	T3041	E2926	E2806	V2746	L2537	R2356	N2199
P3590	P3590	ASP	A3384	R3229	T3041	E2926	E2807	L2747	L2563	E2383	R2200
E3591	E3591	GLN	A3385	N3235	V3051	L2927	R2807	L2748	L2563	E2383	N2204
K3592	K3592	GLU	K3385	N3236	V3051	L2928	E2808	P2749	P2570	R2386	
I3593	I3593	ARG	V3386	V3237	L3057	K2929	P2809	E2750	R2576	P2391	T2207
V3594	V3594	THR	E3387	E3238	L3057	F2930	K2811	K2751	A2392	A2392	V2208
R3595	R3595	LYS	E3387	E3238	V3065	L2931	K2811	K2751	V2398	V2398	M2209
R3596	R3596	LYS	E3388	M3240	D3077	Q2932	E2812	D2752	D2581	ARG	
V3597	V3597	LYS	E3389	D3243	D3077	M2933	E2812	D2752	D2582	ASP	
Q3598	Q3598	ARG	G3391	I3244	V3081	M2934	E2813	D2753	D2583	ARG	
V3603	V3603	GLY	F3399	L3250	M3082	Q2935	E2815	S2754	M2584	ASP	
L3604	L3604	GLY	L3406	E3253	M3082	Q2935	E2816	F2755	L2585	ARG	
Y3605	Y3605	ARG	L3406	E3253	M3082	Q2935	E2816	N2756	L2596	ARG	
Q3609	Q3609	ARG	F3399	E3253	M3082	Q2935	E2817	K2758	L2604	ARG	
H3612	H3612	ARG	Y3410	L3257	V3089	V2938	E2818	F2759	L2604	GLU	
P3613	P3613	TYR	P3411	L3278	V3089	V2938	E2819	E2760	L2611	HIS	
L3614	L3614	LYS	I3414	L3282	V3089	V2938	E2820	A2761	L2627	GLY	
SER	SER	LYS	R3421	P3283	E3109	L2942	E2821	Y2762	L2627	GLU	
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2822	Y2762	L2627	GLU	
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2823	T2763	P2641	GLU	
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2824	H2764	L2645	P2411	
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2825	E2765	L2645	P2412	
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2826	K2766	L2679	E2413	
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LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2828	A2768	R2698	E2415	
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2829	F2769	R2698	R2416	
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LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2834	N2774	K2723	C2238	
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2835	N2775	T2724	R2249	
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LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2838	Y2778	LYS		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2839	G2779	ALA		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2840	E2780	THR		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2841	E2781	VAL		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2842	N2781	ASP		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2843	L2782	ALA		
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LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2845	E2784	GLN		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2846	E2785	GLN		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2847	L2786	TYR		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2848	K2787	ASP		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2849	T2788	PRO		
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2850	K2788	ARG		
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LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2915				
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2916				
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2917				
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2918				
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LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2921				
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2922				
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2923				
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2924				
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2925				
LYS	LYS	LYS	P3283	P3283	E3109	L2942	E2926				



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain E: 91% 8%




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain F: 89% 10%




• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain G:  90% 9% .



● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A

Chain H:  91% 8% .



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	129073	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.613	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	427.008, 427.008, 427.008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.834, 0.834, 0.834	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PCW, 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	0.23	0/35776	0.41	5/48462 (0.0%)
1	B	0.23	0/35776	0.41	5/48462 (0.0%)
1	C	0.23	0/35776	0.41	5/48462 (0.0%)
1	D	0.23	0/35776	0.41	5/48462 (0.0%)
2	E	0.18	0/847	0.32	0/1142
2	F	0.18	0/847	0.32	0/1142
2	G	0.18	0/847	0.31	0/1142
2	H	0.18	0/847	0.31	0/1142
All	All	0.23	0/146492	0.40	20/198416 (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	8
1	B	0	8
1	C	0	8
1	D	0	8
All	All	0	32

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	B	2238	CYS	CA-CB-SG	9.06	135.23	114.40
1	A	2238	CYS	CA-CB-SG	9.05	135.21	114.40
1	D	2238	CYS	CA-CB-SG	9.05	135.21	114.40
1	C	2238	CYS	CA-CB-SG	9.04	135.19	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2238	CYS	CB-CA-C	6.19	120.63	110.17

There are no chirality outliers.

5 of 32 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2238	CYS	Peptide
1	A	4088	ARG	Sidechain
1	A	4318	ARG	Sidechain
1	A	4319	ARG	Sidechain
1	A	4323	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	34983	0	34589	445	0
1	B	34983	0	34589	438	0
1	C	34983	0	34589	437	0
1	D	34983	0	34589	432	0
2	E	829	0	826	8	0
2	F	829	0	826	10	0
2	G	829	0	826	9	0
2	H	829	0	826	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	108	0	168	0	0
4	B	108	0	168	0	0
4	C	108	0	168	0	0
4	D	108	0	168	0	0
All	All	143684	0	142332	1748	0

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

The worst 5 of 1748 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:C:2752:LEU:HD13	1:C:2814:LEU:HD21	1.43	1.00
1:B:2752:LEU:HD13	1:B:2814:LEU:HD21	1.43	0.98
1:C:1991:GLU:OE2	1:C:1995:ARG:NH1	1.97	0.97
1:D:2752:LEU:HD13	1:D:2814:LEU:HD21	1.43	0.97
1:A:1991:GLU:OE2	1:A:1995:ARG:NH1	1.97	0.96

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	4368/5035 (87%)	4233 (97%)	135 (3%)	0	100	100
1	B	4368/5035 (87%)	4233 (97%)	135 (3%)	0	100	100
1	C	4368/5035 (87%)	4233 (97%)	135 (3%)	0	100	100
1	D	4368/5035 (87%)	4234 (97%)	134 (3%)	0	100	100
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17892/20572 (87%)	17337 (97%)	555 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	3823/4296 (89%)	3801 (99%)	22 (1%)	84	94
1	B	3823/4296 (89%)	3801 (99%)	22 (1%)	84	94
1	C	3823/4296 (89%)	3801 (99%)	22 (1%)	84	94
1	D	3823/4296 (89%)	3801 (99%)	22 (1%)	84	94
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15648/17544 (89%)	15560 (99%)	88 (1%)	82	94

5 of 88 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4332	LEU
1	D	4094	LYS
1	C	4576	LEU
1	C	4772	LYS
1	D	4129	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 169 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2992	HIS
1	D	1939	GLN
1	C	3598	GLN
1	D	242	GLN
1	D	2499	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 12 ligands modelled in this entry, 4 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
4	PCW	A	8003	-	53,53,53	1.24	7 (13%)	59,61,61	1.03	3 (5%)
4	PCW	D	5101	-	53,53,53	1.24	7 (13%)	59,61,61	1.03	3 (5%)
4	PCW	B	8002	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
4	PCW	C	8003	-	53,53,53	1.24	7 (13%)	59,61,61	1.03	3 (5%)
4	PCW	B	8003	-	53,53,53	1.24	7 (13%)	59,61,61	1.03	3 (5%)
4	PCW	D	5103	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
4	PCW	A	8002	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)
4	PCW	C	8002	-	53,53,53	1.25	7 (13%)	59,61,61	1.04	3 (5%)

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
4	PCW	A	8003	-	-	25/57/57/57	-
4	PCW	D	5101	-	-	25/57/57/57	-
4	PCW	B	8002	-	-	33/57/57/57	-
4	PCW	C	8003	-	-	25/57/57/57	-
4	PCW	B	8003	-	-	25/57/57/57	-
4	PCW	D	5103	-	-	33/57/57/57	-
4	PCW	A	8002	-	-	33/57/57/57	-
4	PCW	C	8002	-	-	33/57/57/57	-

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8003	PCW	O3-C11	3.02	1.42	1.33
4	C	8003	PCW	O3-C11	3.02	1.42	1.33
4	D	5101	PCW	O3-C11	3.02	1.42	1.33
4	A	8003	PCW	O3-C11	2.99	1.42	1.33
4	A	8002	PCW	O3-C11	2.96	1.42	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	8002	PCW	C21-C20-C19	3.88	153.88	124.83
4	B	8002	PCW	C21-C20-C19	3.88	153.88	124.83
4	C	8002	PCW	C21-C20-C19	3.88	153.88	124.83
4	D	5103	PCW	C21-C20-C19	3.88	153.88	124.83
4	A	8003	PCW	C21-C20-C19	3.81	153.38	124.83

There are no chirality outliers.

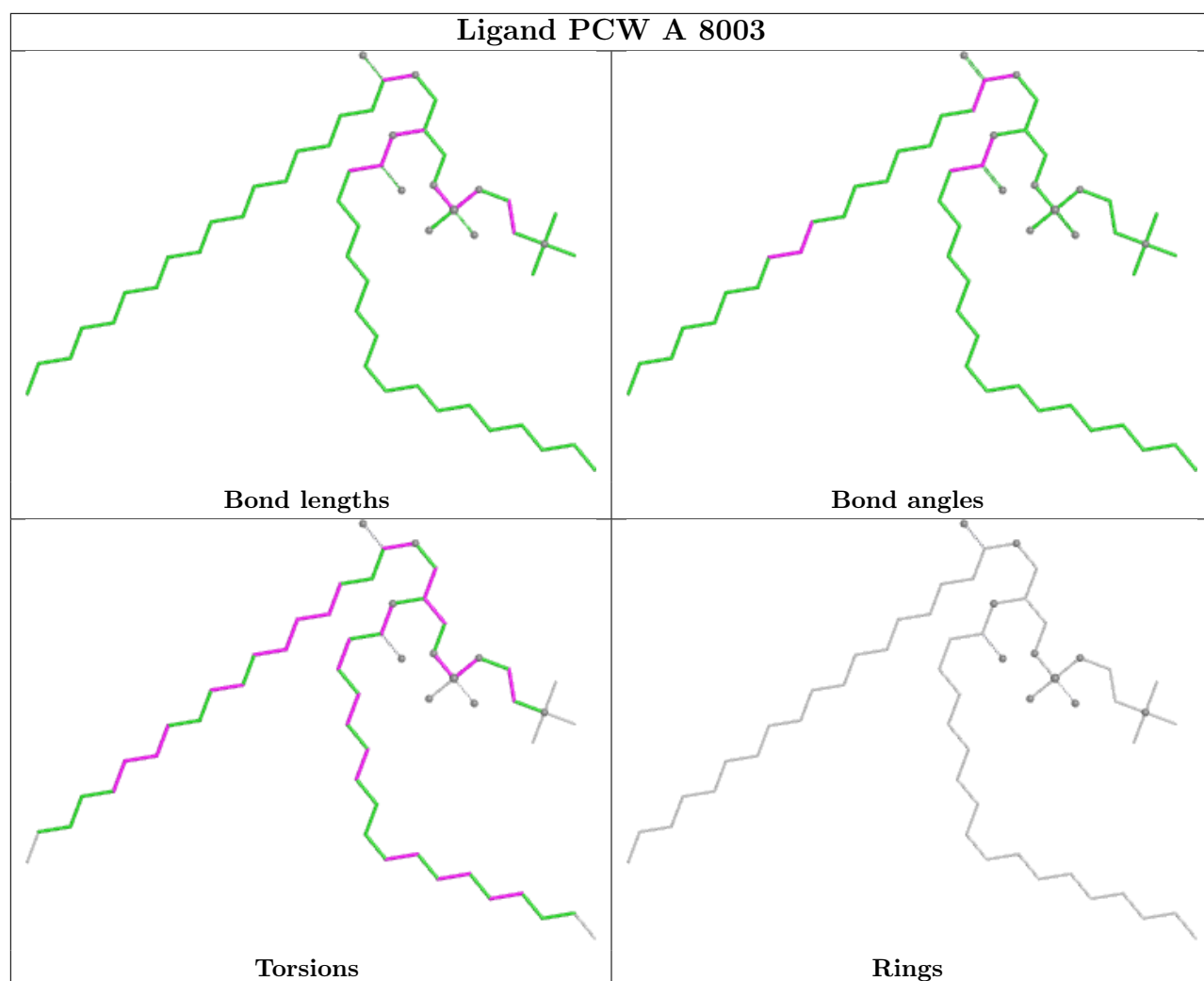
5 of 232 torsion outliers are listed below:

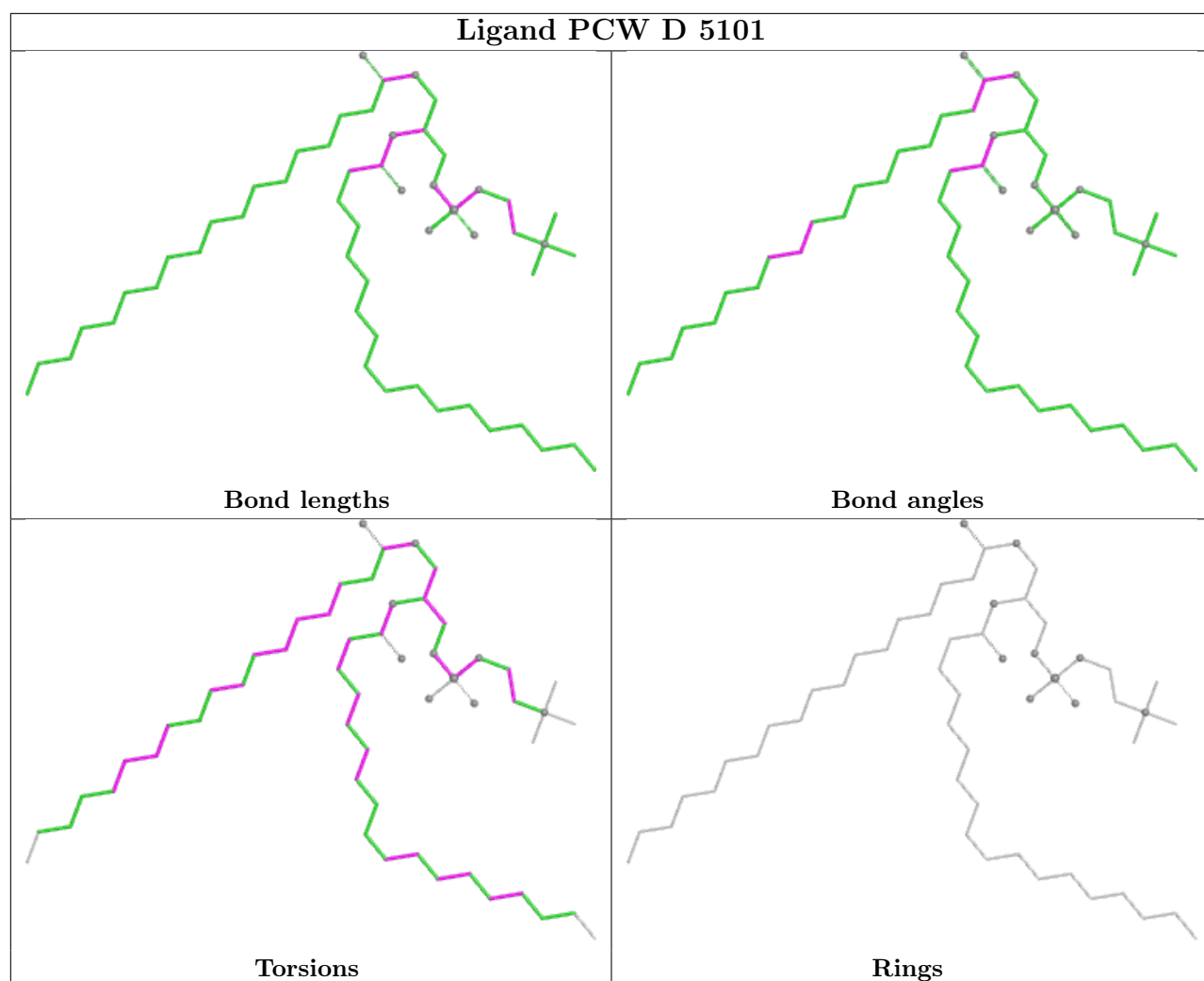
Mol	Chain	Res	Type	Atoms
4	A	8002	PCW	C32-C31-O2-C2
4	A	8002	PCW	C1-O3P-P-O1P
4	A	8002	PCW	C1-O3P-P-O2P
4	A	8002	PCW	C1-O3P-P-O4P
4	A	8002	PCW	C4-O4P-P-O1P

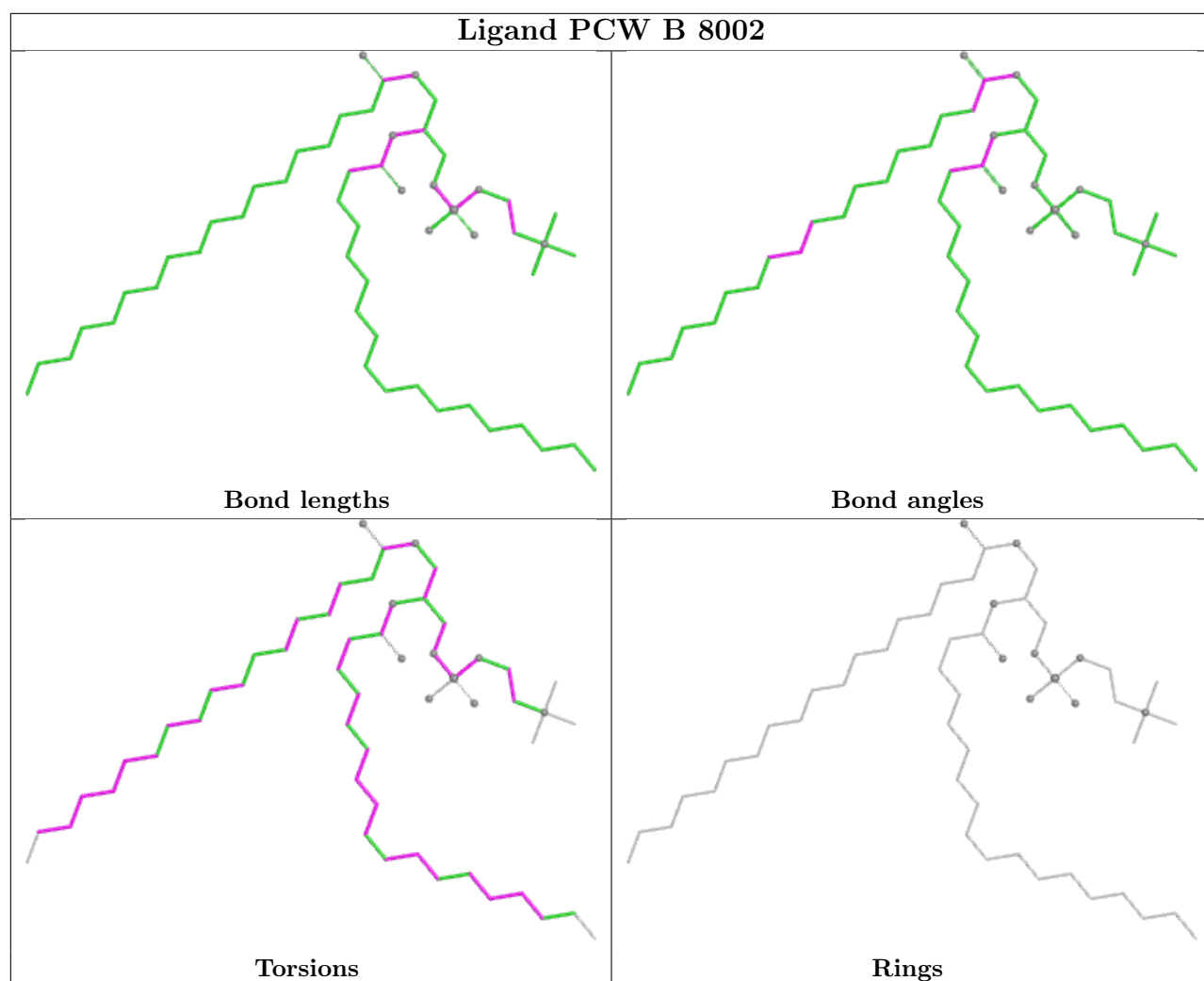
There are no ring outliers.

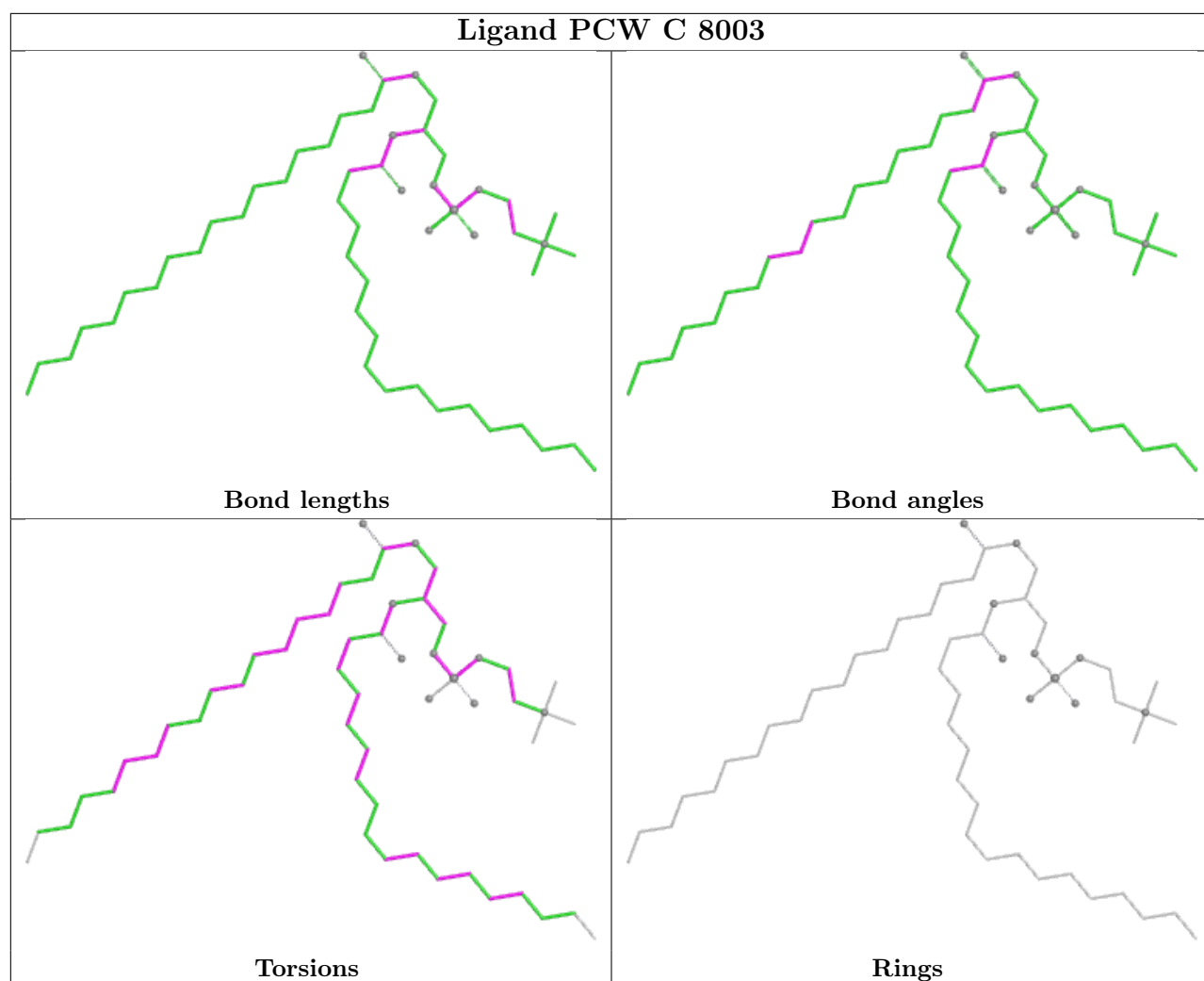
No monomer is involved in short contacts.

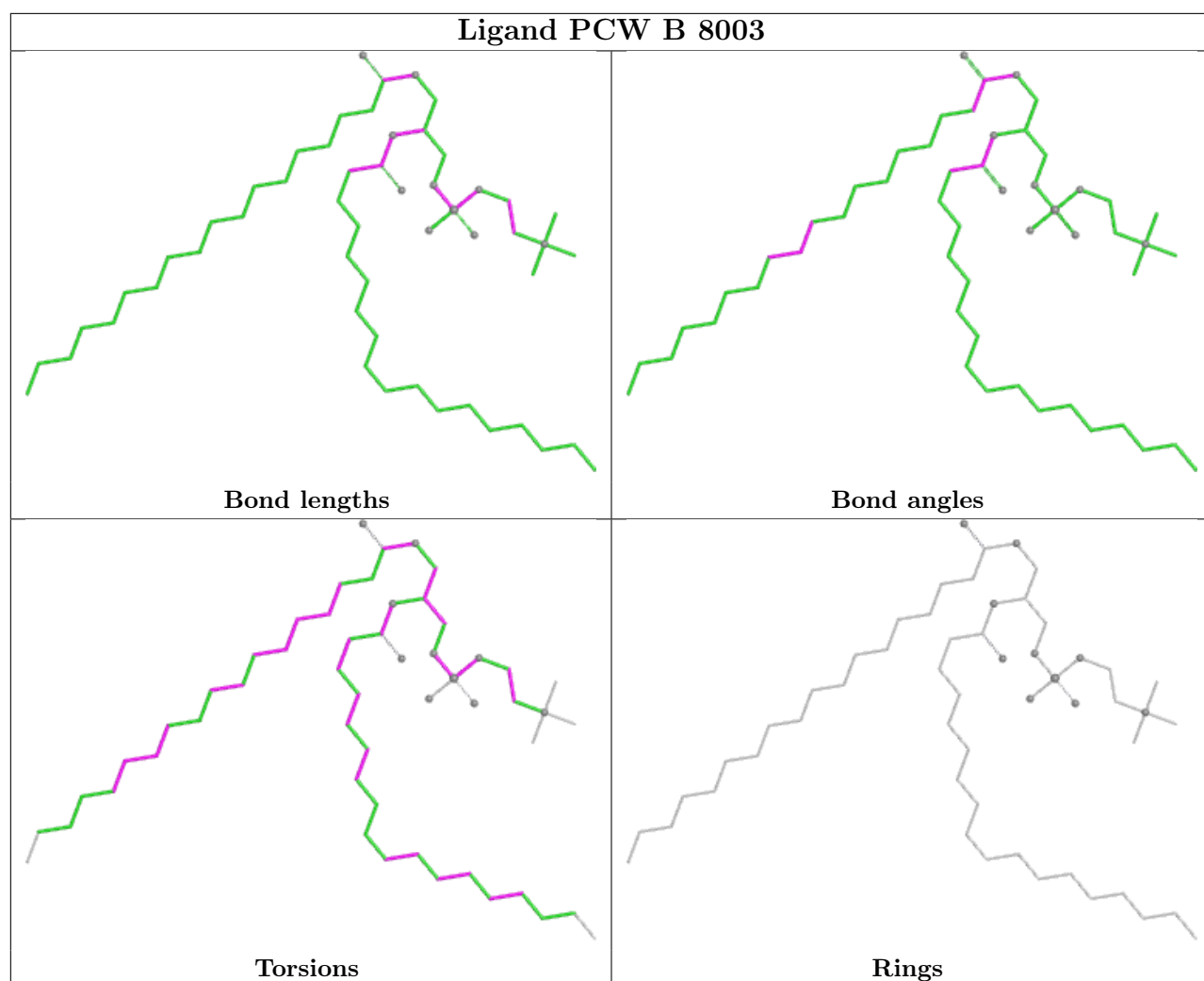
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

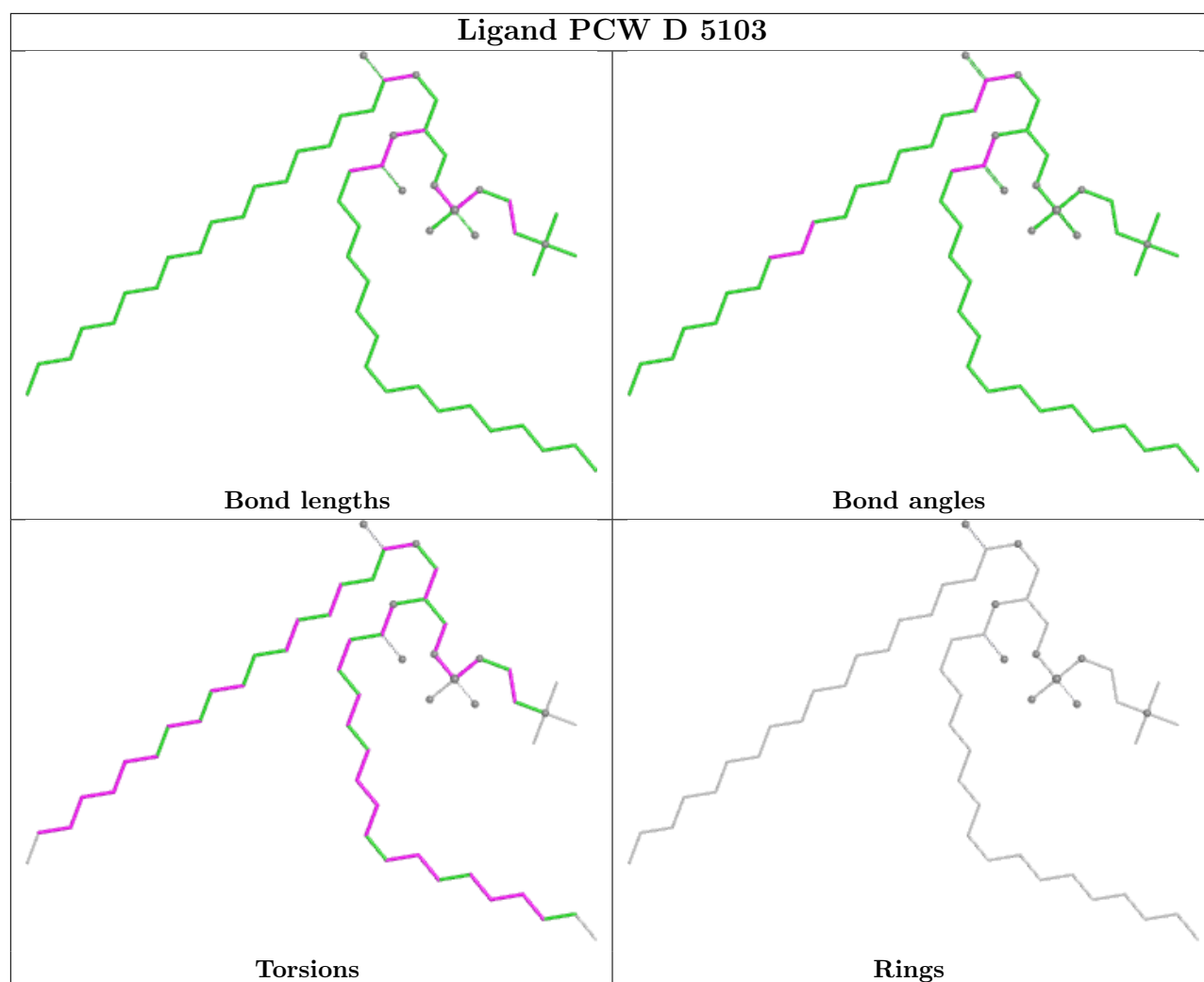


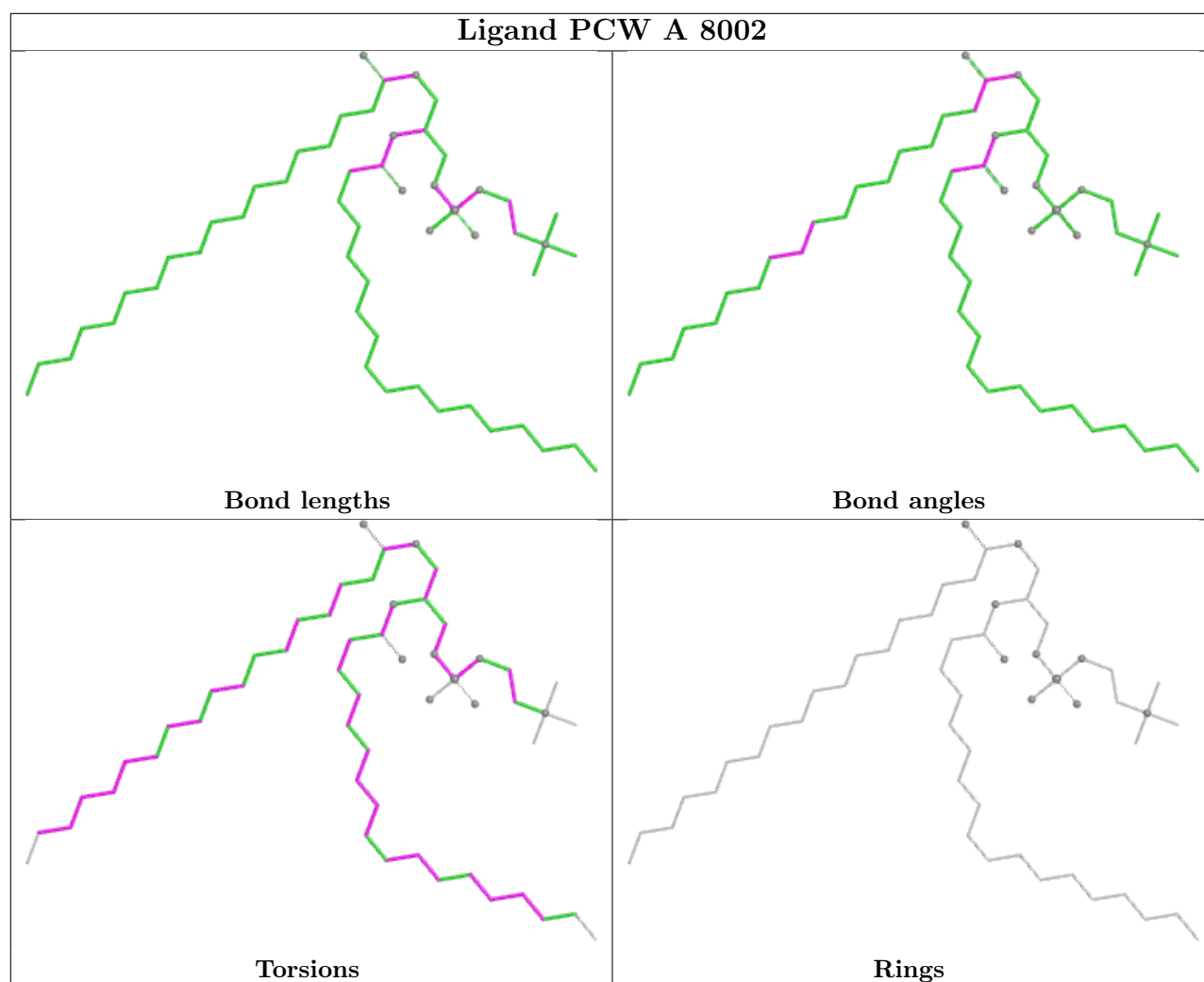


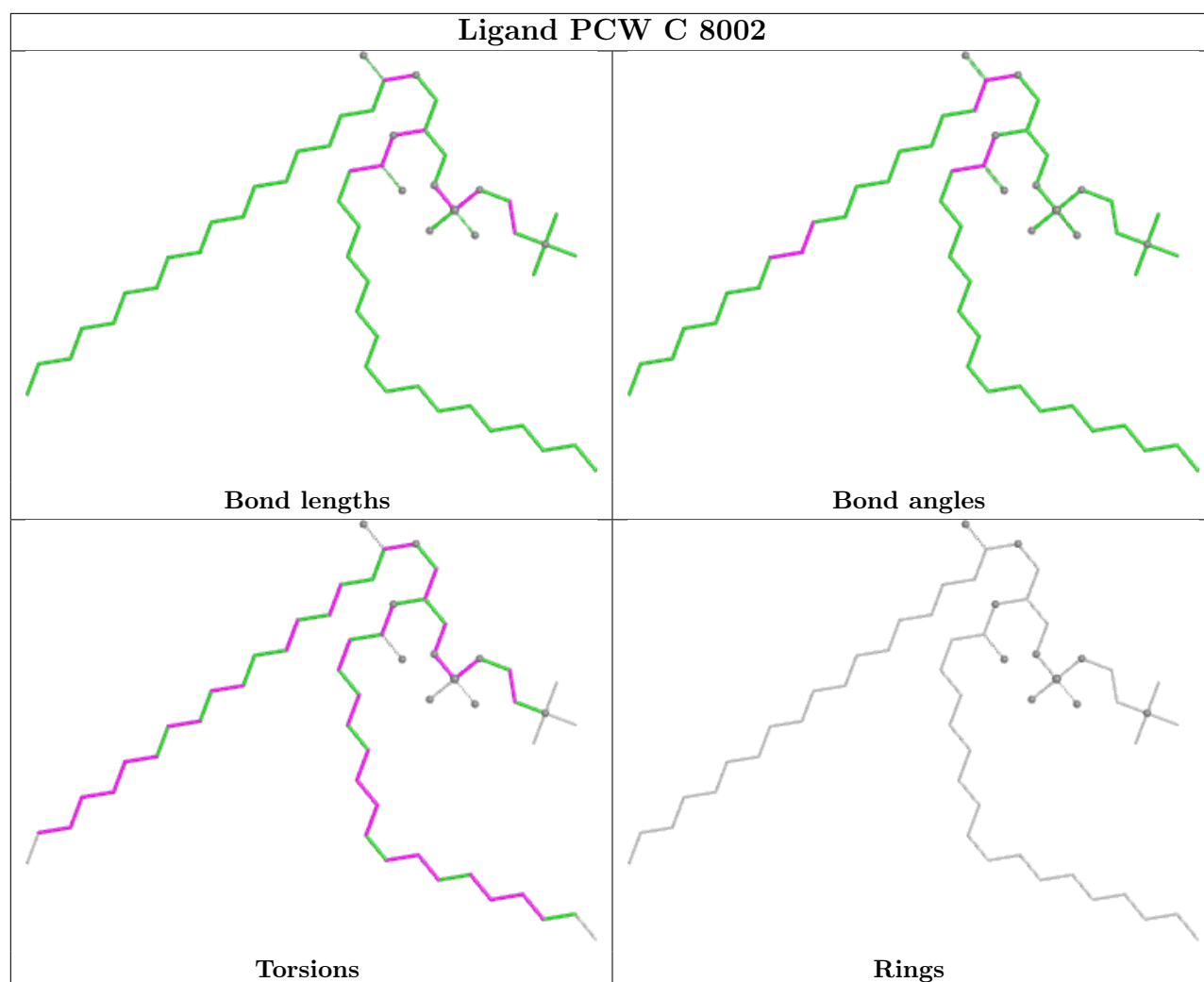












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

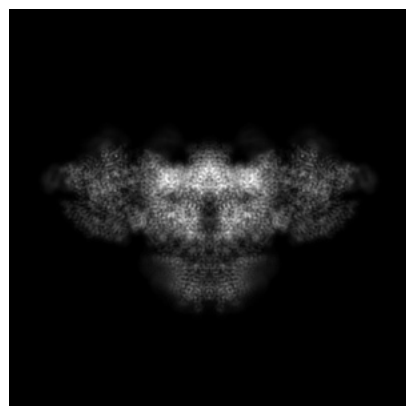
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49538. These allow visual inspection of the internal detail of the map and identification of artifacts.

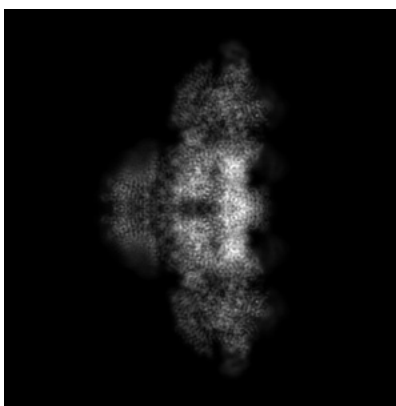
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

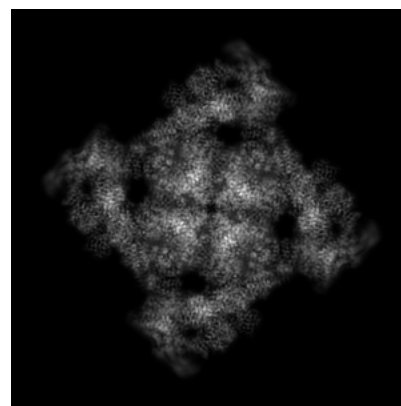
6.1.1 Primary map



X

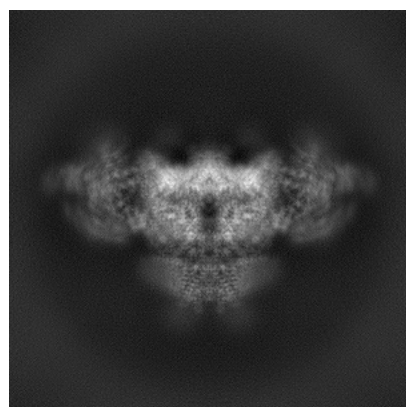


Y

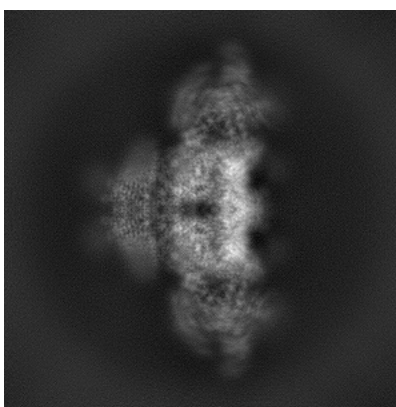


Z

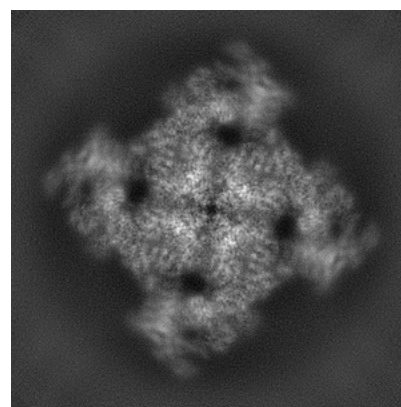
6.1.2 Raw map



X



Y



Z

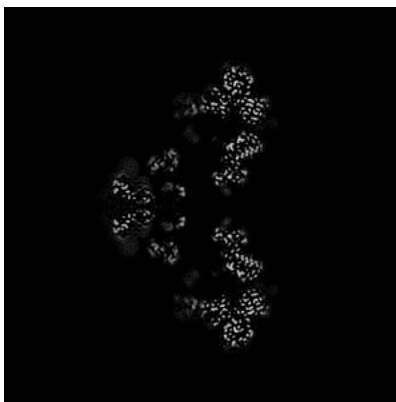
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

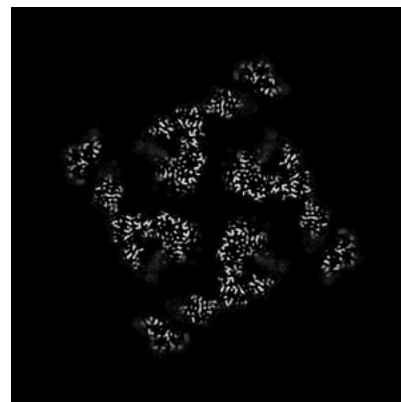
6.2.1 Primary map



X Index: 256

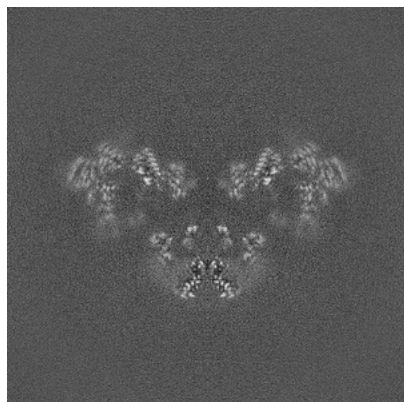


Y Index: 256

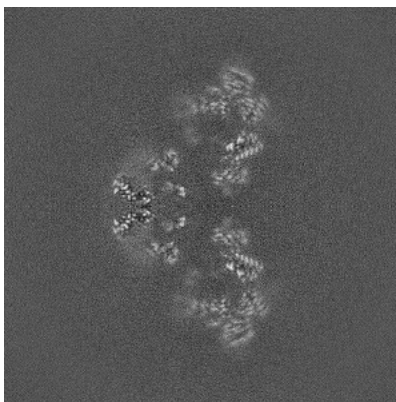


Z Index: 256

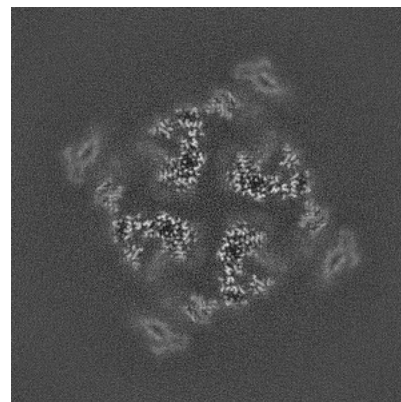
6.2.2 Raw map



X Index: 256



Y Index: 256



Z Index: 256

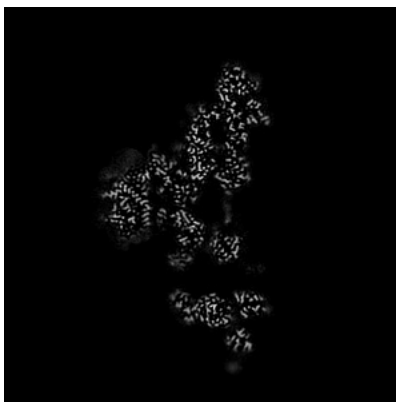
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

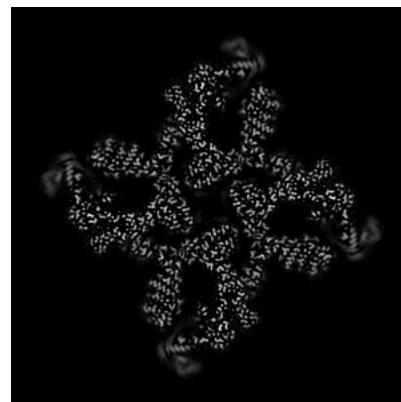
6.3.1 Primary map



X Index: 238

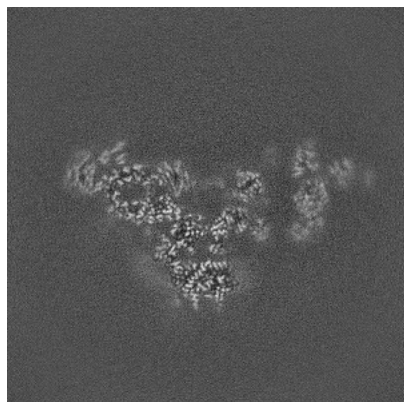


Y Index: 274

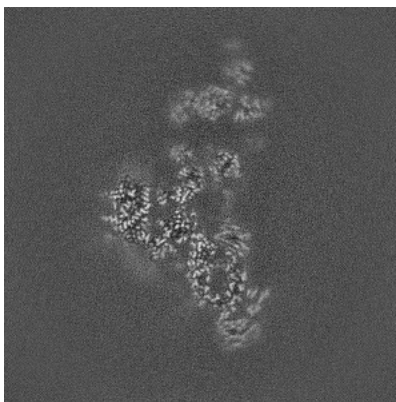


Z Index: 291

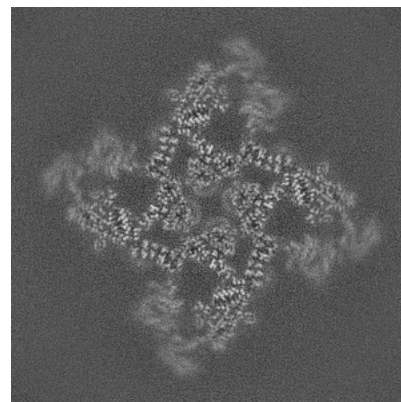
6.3.2 Raw map



X Index: 274



Y Index: 238

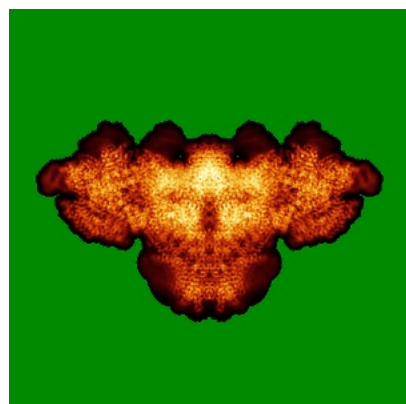


Z Index: 286

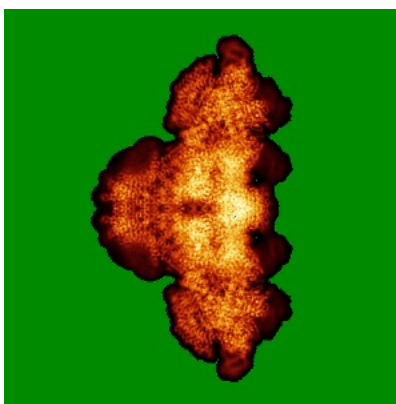
The images above show the largest variance slices of the map in three orthogonal directions.

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

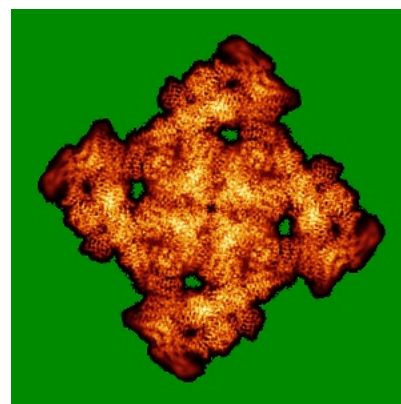
6.4.1 Primary map



X

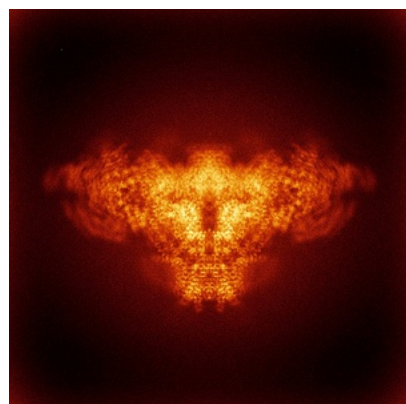


Y

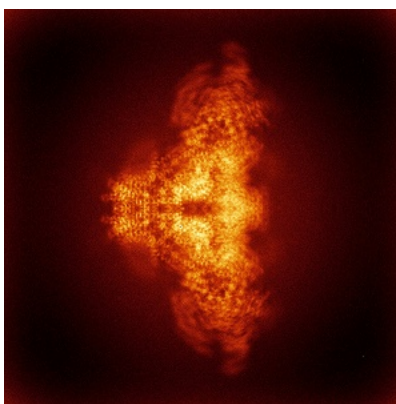


Z

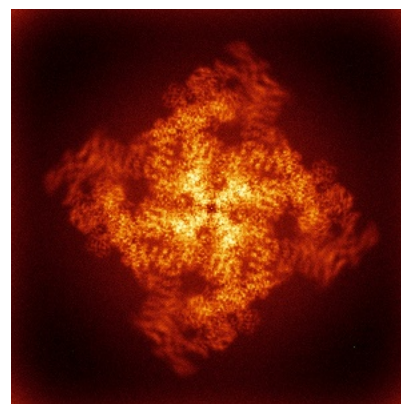
6.4.2 Raw map



X



Y

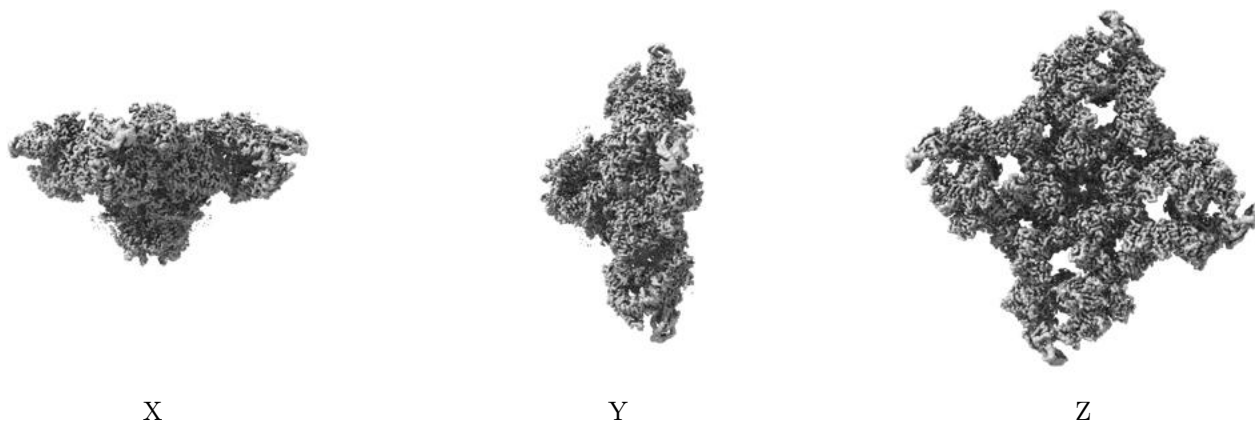


Z

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

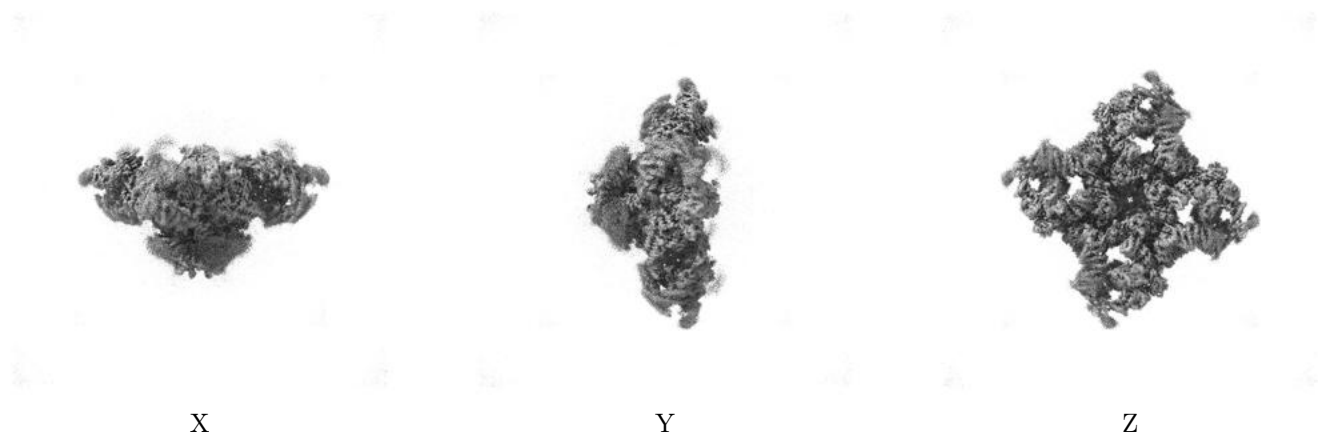
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

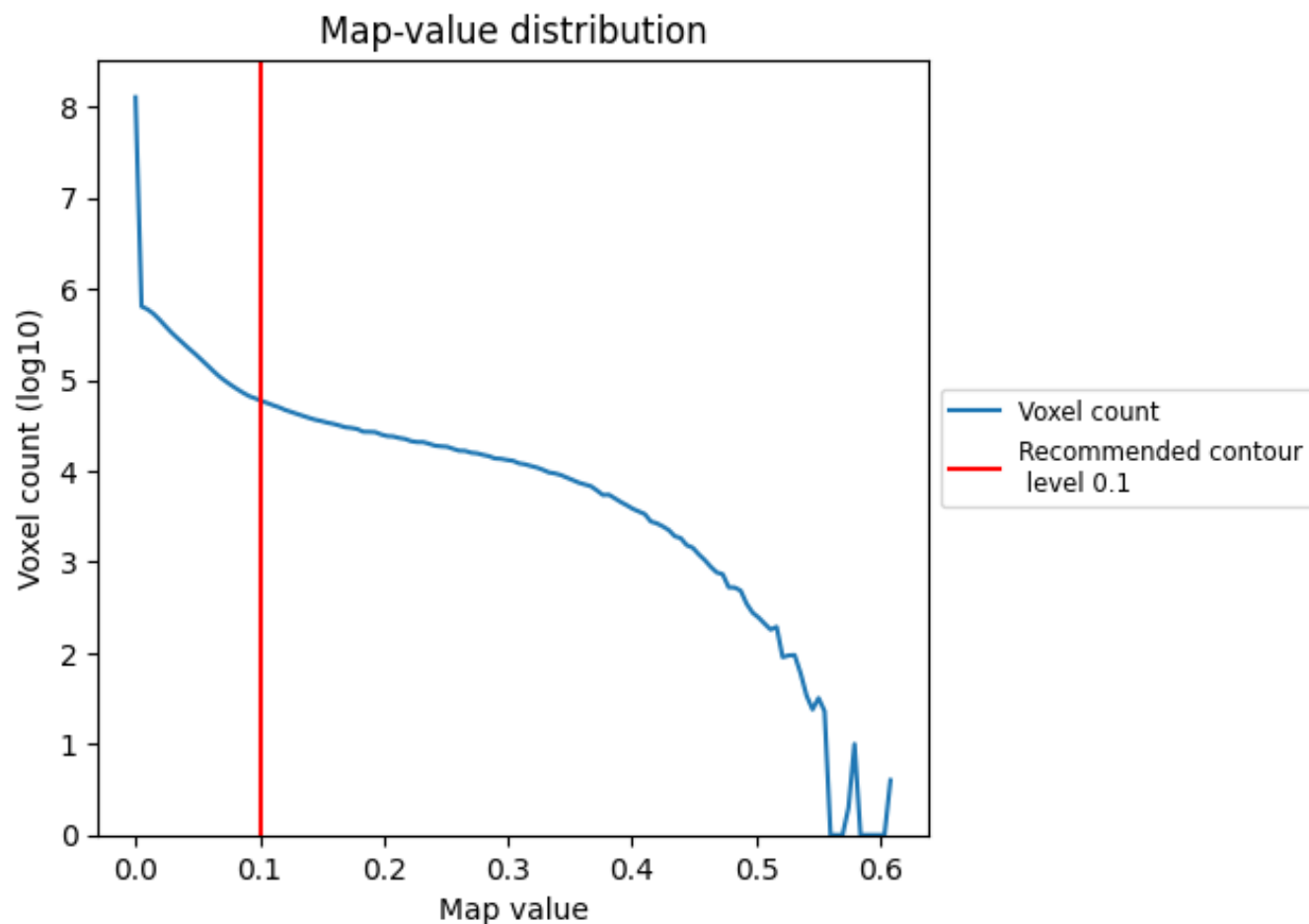
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

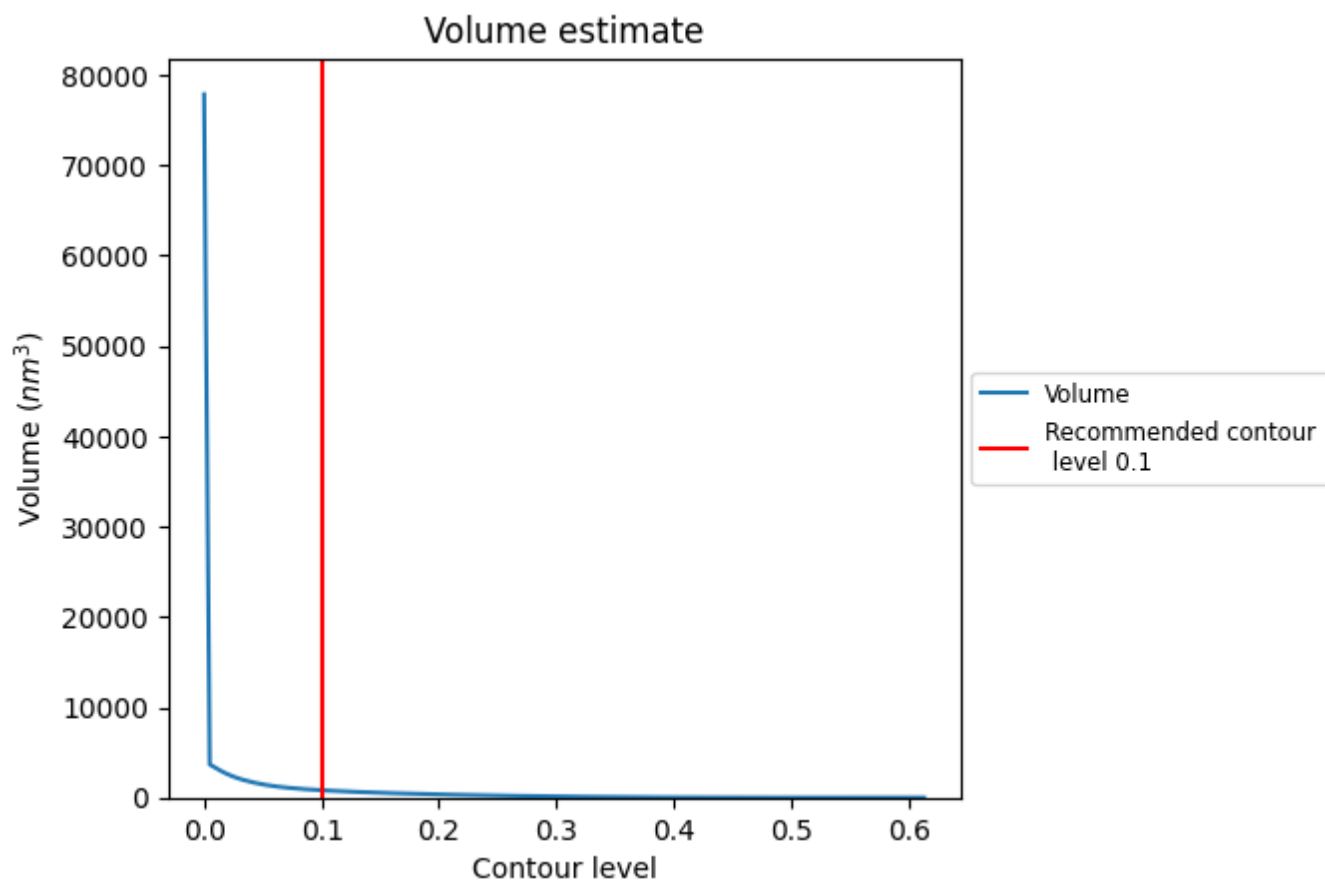
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

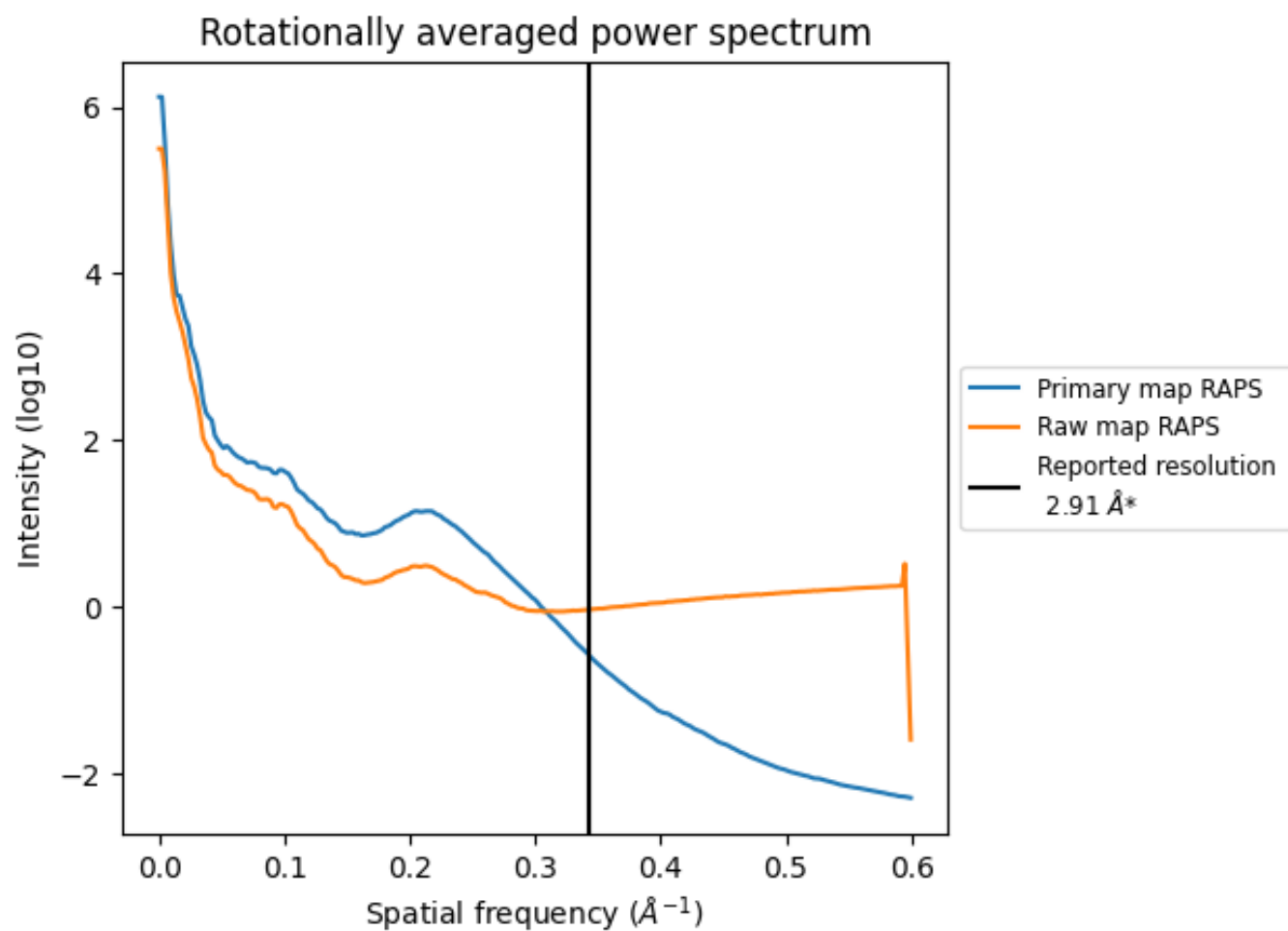
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 812 nm³; this corresponds to an approximate mass of 734 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 ⓘ

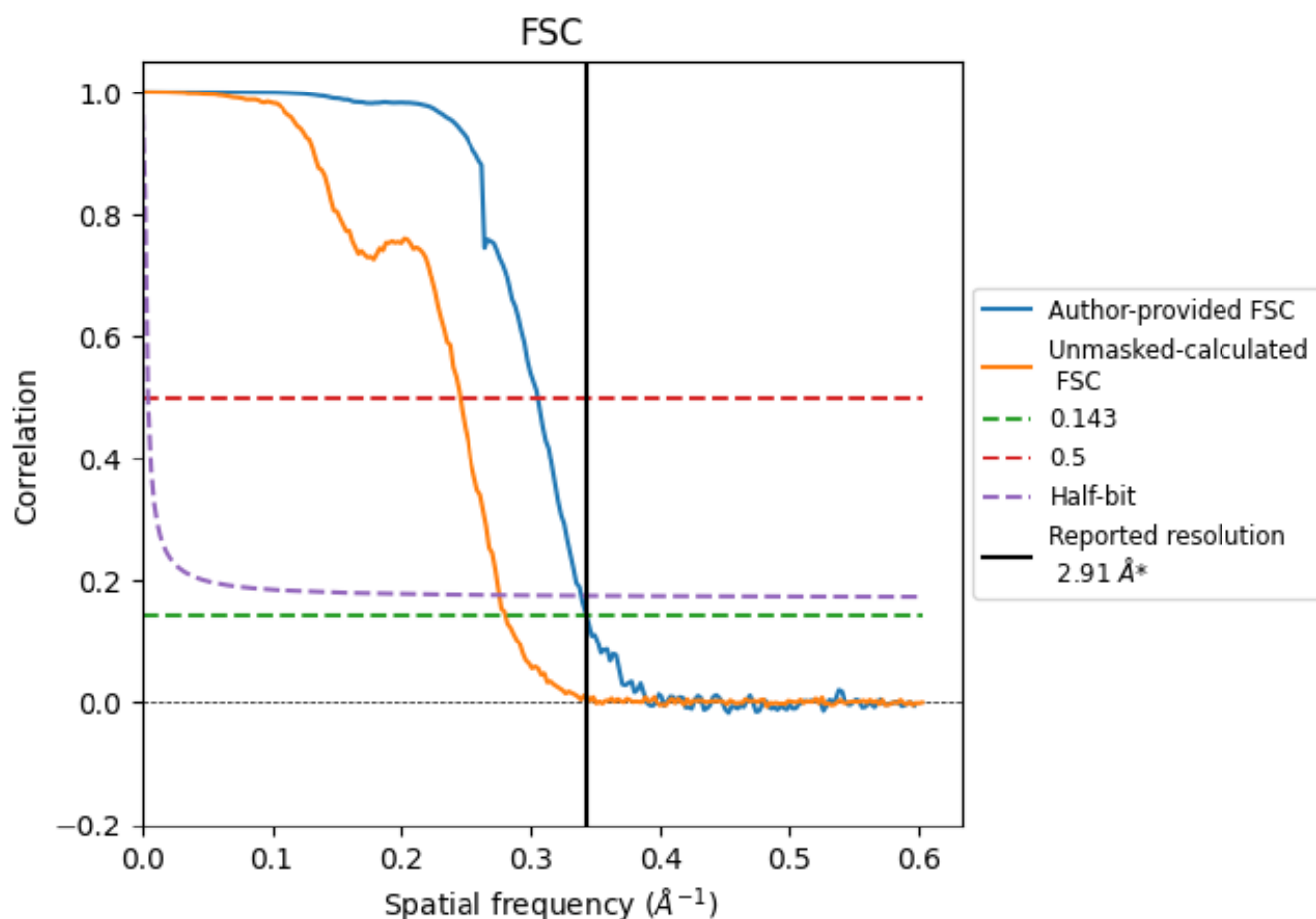


*Reported resolution corresponds to spatial frequency of 0.344 Å⁻¹

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 0.344 \AA^{-1}

8.2 Resolution estimates [i](#)

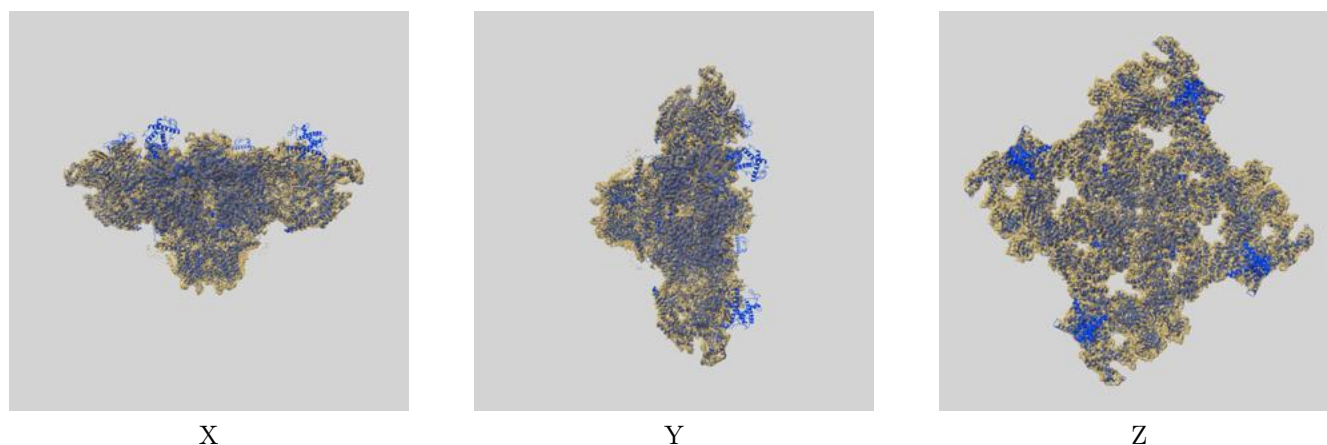
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.91	-	-
Author-provided FSC curve	2.91	3.27	2.95
Unmasked-calculated*	3.56	4.07	3.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.56 differs from the reported value 2.91 by more than 10 %

9 Map-model fit [i](#)

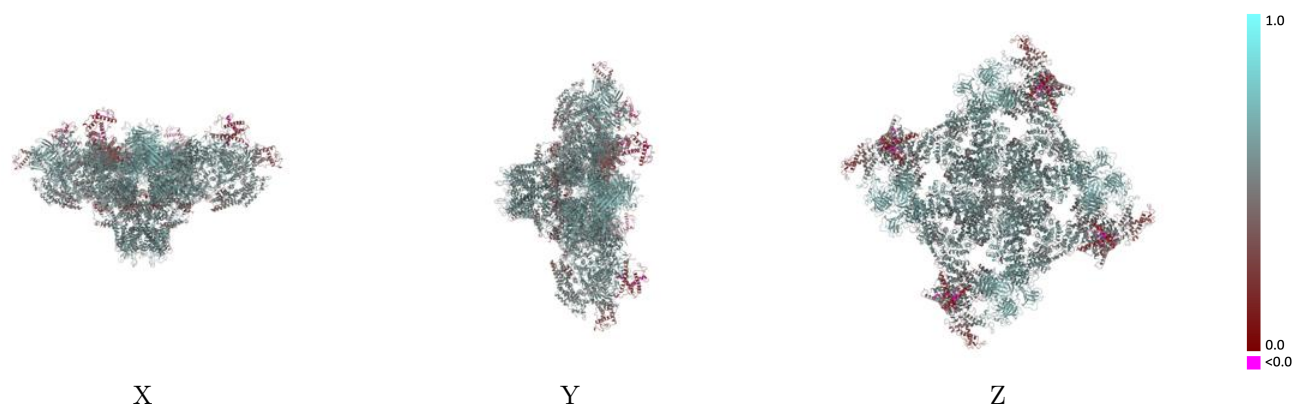
This section contains information regarding the fit between EMDB map EMD-49538 and PDB model 9NMR. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



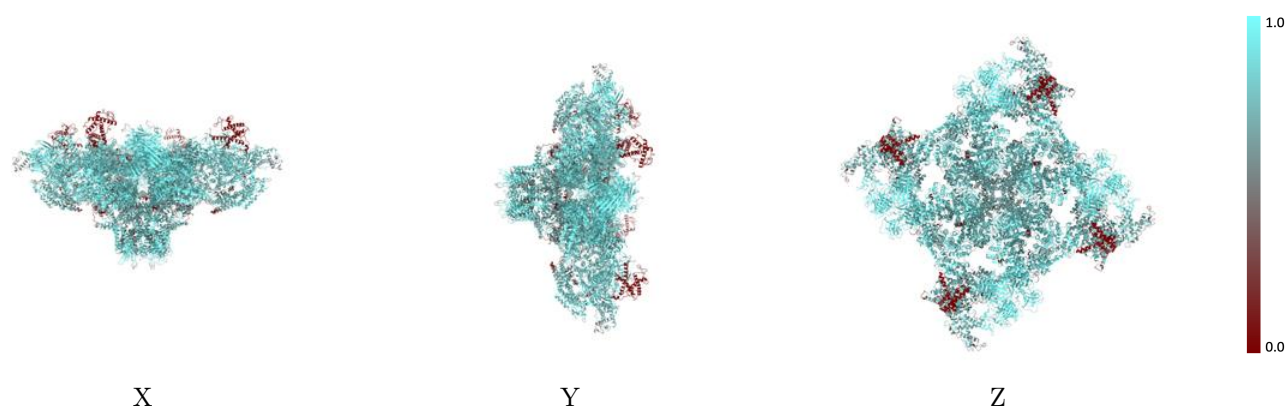
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



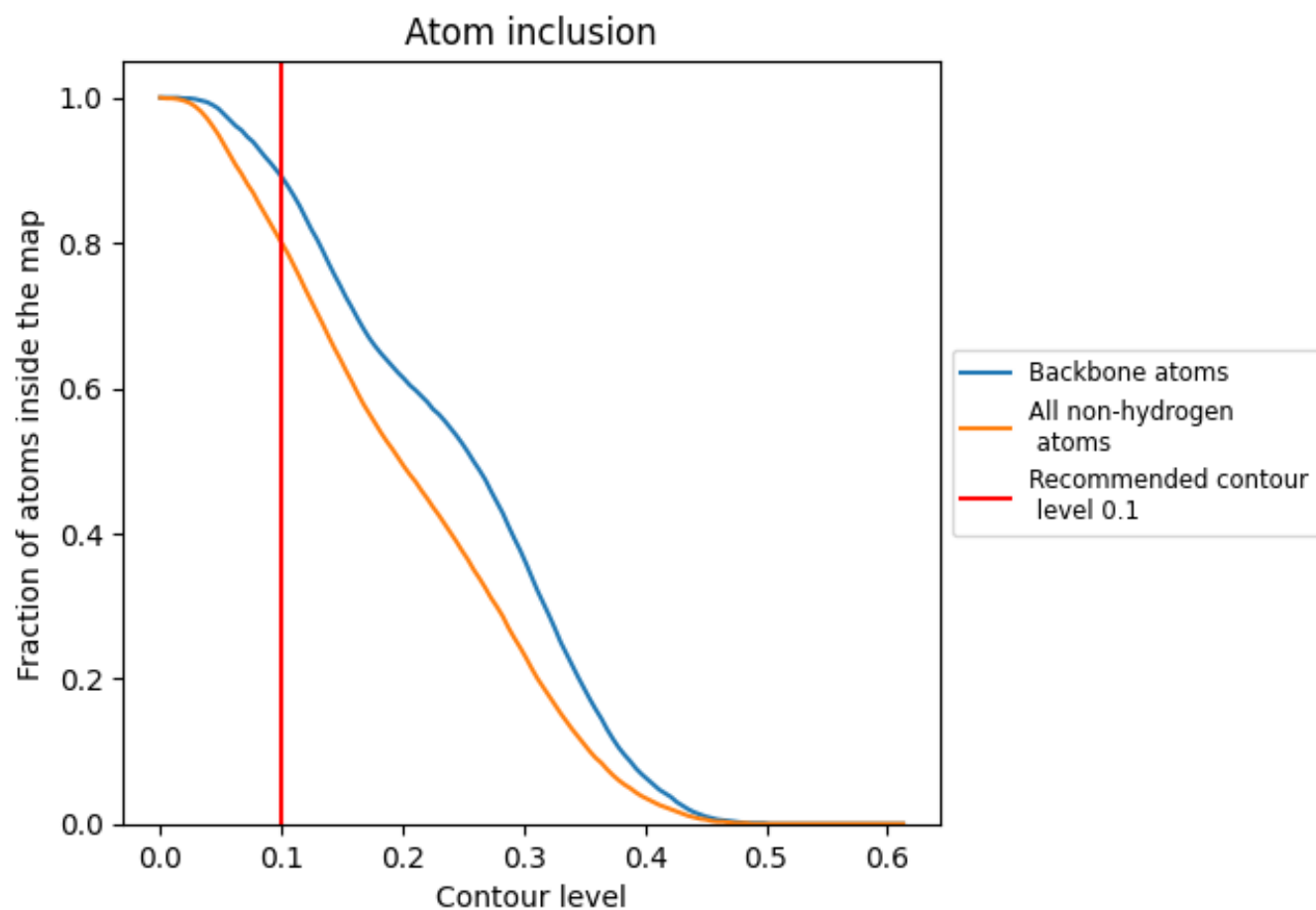
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.8000	<div><div></div></div> 0.5360
A	<div><div></div></div> 0.7980	<div><div></div></div> 0.5340
B	<div><div></div></div> 0.7980	<div><div></div></div> 0.5340
C	<div><div></div></div> 0.7970	<div><div></div></div> 0.5340
D	<div><div></div></div> 0.7980	<div><div></div></div> 0.5350
E	<div><div></div></div> 0.9050	<div><div></div></div> 0.6020
F	<div><div></div></div> 0.9000	<div><div></div></div> 0.6000
G	<div><div></div></div> 0.9040	<div><div></div></div> 0.6040
H	<div><div></div></div> 0.9020	<div><div></div></div> 0.6040

1.0

0.0

<0.0