



wwPDB EM Validation Summary Report ⓘ

Mar 15, 2026 – 08:31 AM UTC

PDB ID : 7TZC / pdb_00007tzc
EMDB ID : EMD-26205
Title : A drug and ATP binding site in type 1 ryanodine receptor
Authors : Melville, Z.; Dridi, H.; Yuan, Q.; Reiken, S.; Anetta, W.; Liu, Y.; Clarke, O.B.; Marks, A.R.
Deposited on : 2022-02-15
Resolution : 2.45 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

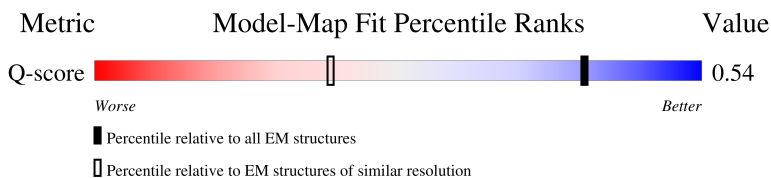
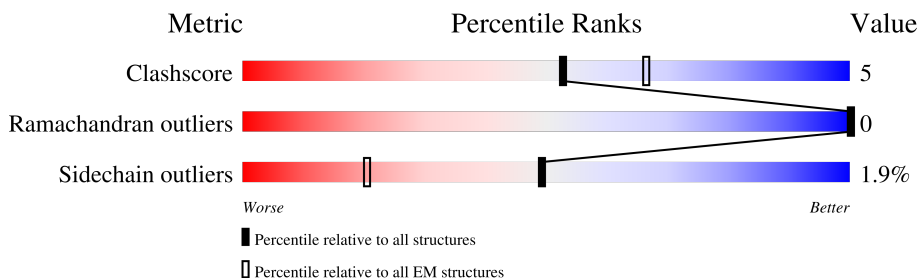
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.45 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.



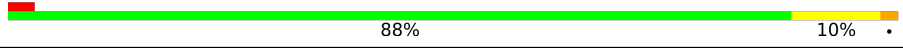
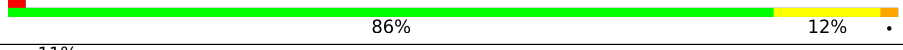
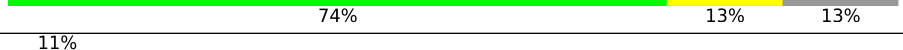
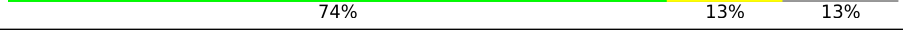
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5931 (1.96 - 2.95)

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	C	150	
1	D	150	
1	E	150	
1	K	150	

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Mol	Chain	Length	Quality of chain
2	F	107	
2	H	107	
2	J	107	
2	O	107	
3	A	5037	
3	B	5037	
3	G	5037	
3	I	5037	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CFF	I	5105	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 149472 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 Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	D	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	E	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		
1	C	149	Total	C	N	O	S	0	0
			1174	719	190	255	10		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP P0DP23
D	-1	HIS	-	expression tag	UNP P0DP23
E	-1	HIS	-	expression tag	UNP P0DP23
C	-1	HIS	-	expression tag	UNP P0DP23

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	J	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	O	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

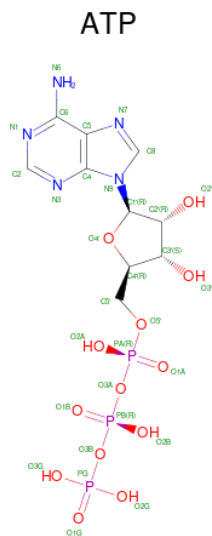
- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	G	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
3	I	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
4	K	4	Total	Ca	0
			4	4	
4	D	4	Total	Ca	0
			4	4	
4	E	4	Total	Ca	0
			4	4	
4	C	4	Total	Ca	0
			4	4	
4	A	1	Total	Ca	0
			1	1	
4	B	1	Total	Ca	0
			1	1	
4	G	1	Total	Ca	0
			1	1	
4	I	1	Total	Ca	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

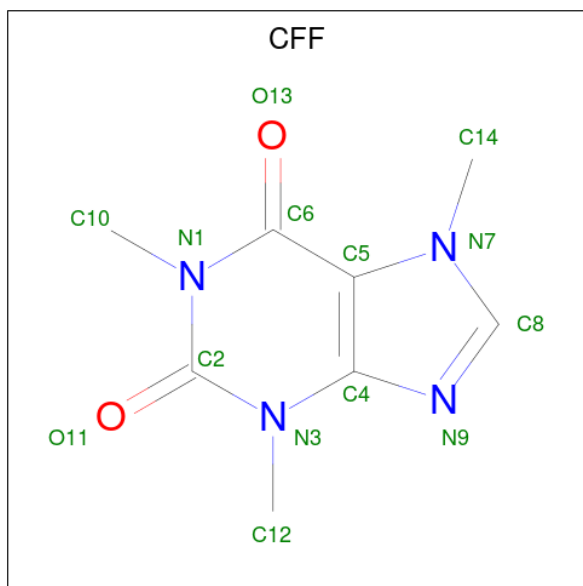


Mol	Chain	Residues	Atoms					AltConf
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	A	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	B	1	Total 31	C 10	N 5	O 13	P 3	0
5	G	1	Total 31	C 10	N 5	O 13	P 3	0
5	G	1	Total 31	C 10	N 5	O 13	P 3	0
5	I	1	Total 31	C 10	N 5	O 13	P 3	0
5	I	1	Total 31	C 10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

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

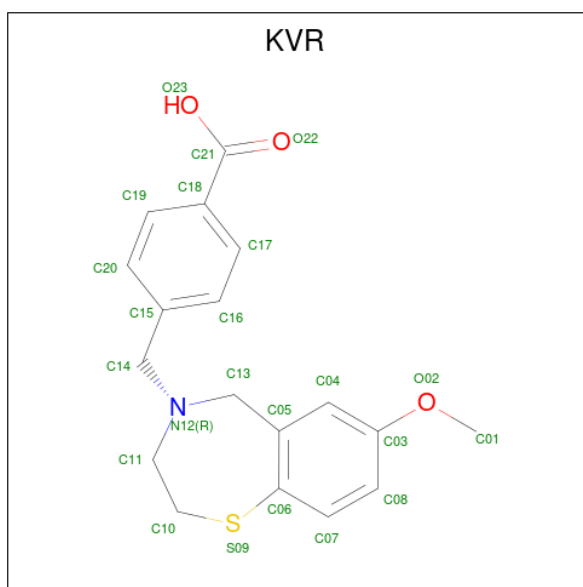
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Zn 1 1	0
6	B	1	Total Zn 1 1	0
6	G	1	Total Zn 1 1	0
6	I	1	Total Zn 1 1	0

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: $C_8H_{10}N_4O_2$).



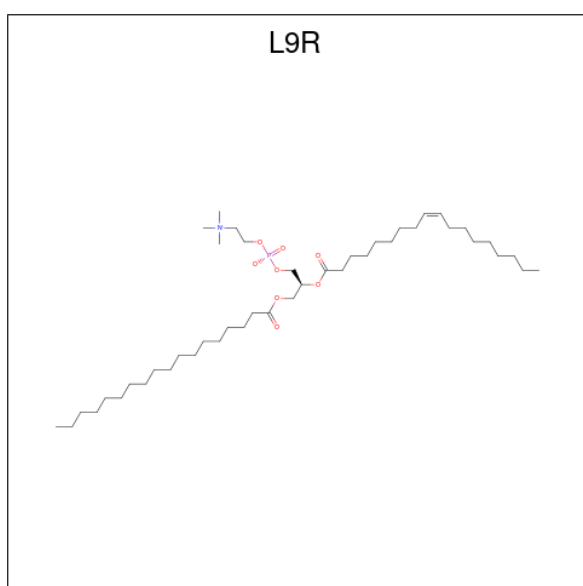
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	4	2	
7	B	1	Total	C	N	O	0
			14	8	4	2	
7	G	1	Total	C	N	O	0
			14	8	4	2	
7	I	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 8 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (CCD ID: KVR) (formula: $C_{18}H_{19}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	B	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	G	1	Total	C	N	O	S	0
			23	18	1	3	1	
8	I	1	Total	C	N	O	S	0
			23	18	1	3	1	

- Molecule 9 is (2S)-3-(octadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylamm onio)ethyl phosphate (CCD ID: L9R) (formula: C₄₄H₈₆NO₈P).

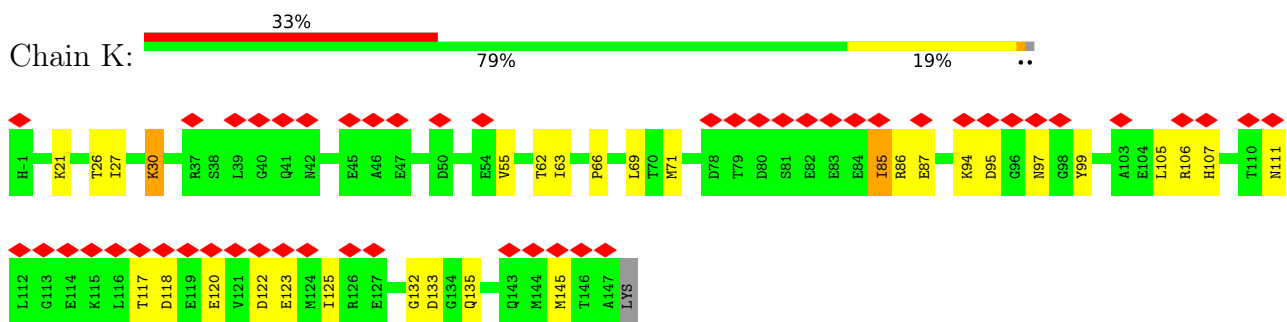


Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total 54	C 44	N 1	O 8	P 1	0
9	A	1	Total 54	C 44	N 1	O 8	P 1	0
9	B	1	Total 54	C 44	N 1	O 8	P 1	0
9	B	1	Total 54	C 44	N 1	O 8	P 1	0
9	G	1	Total 54	C 44	N 1	O 8	P 1	0
9	G	1	Total 54	C 44	N 1	O 8	P 1	0
9	I	1	Total 54	C 44	N 1	O 8	P 1	0
9	I	1	Total 54	C 44	N 1	O 8	P 1	0

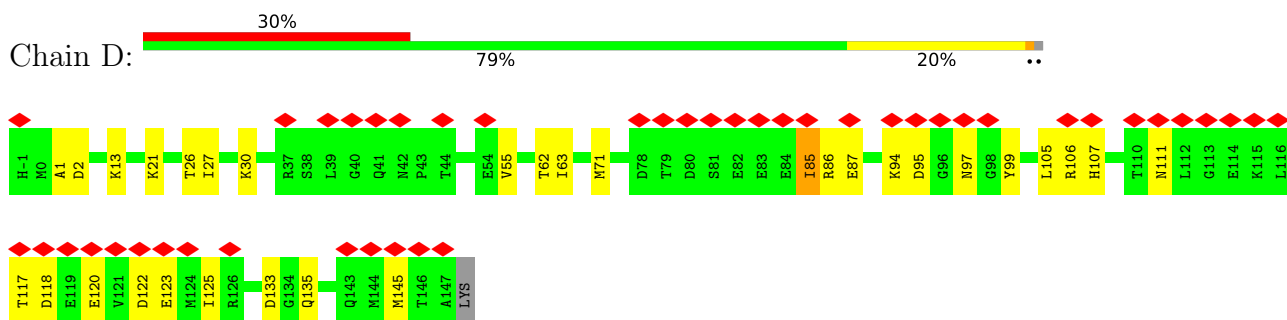
3 Residue-property plots

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.

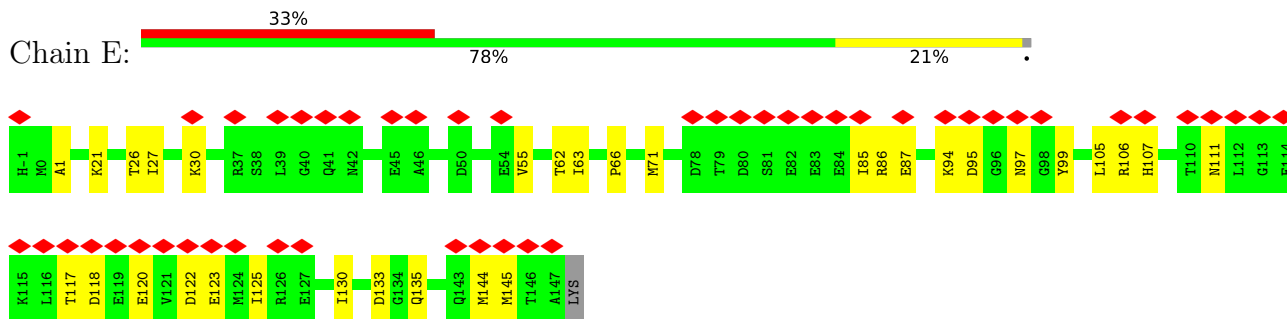
• Molecule 1: Calmodulin-1



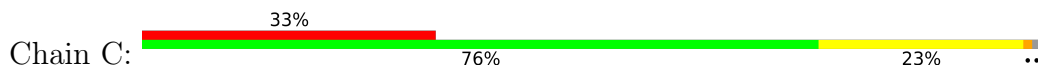
• Molecule 1: Calmodulin-1

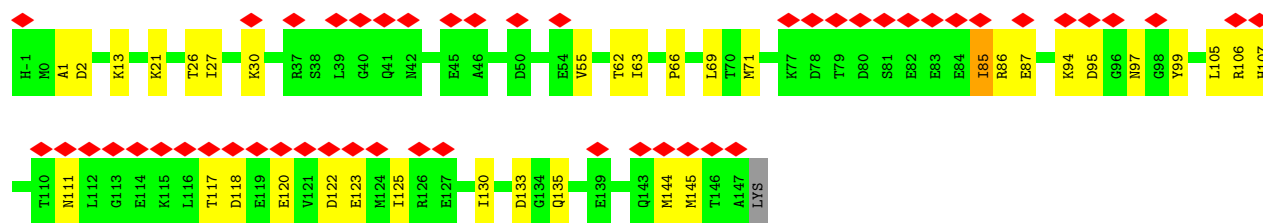


• Molecule 1: Calmodulin-1

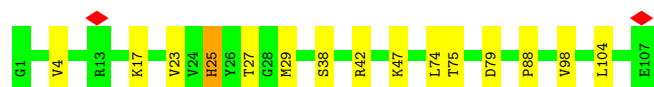
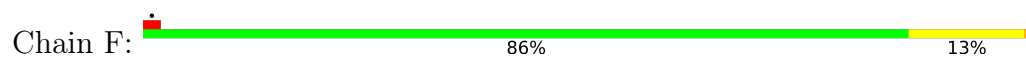


• Molecule 1: Calmodulin-1

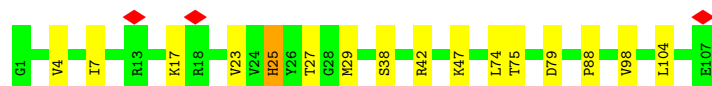
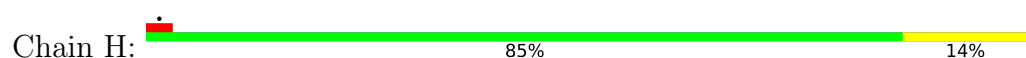




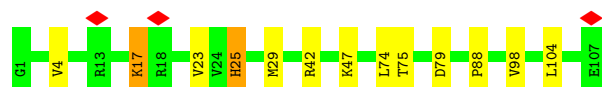
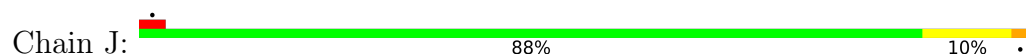
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



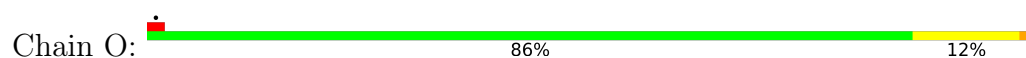
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



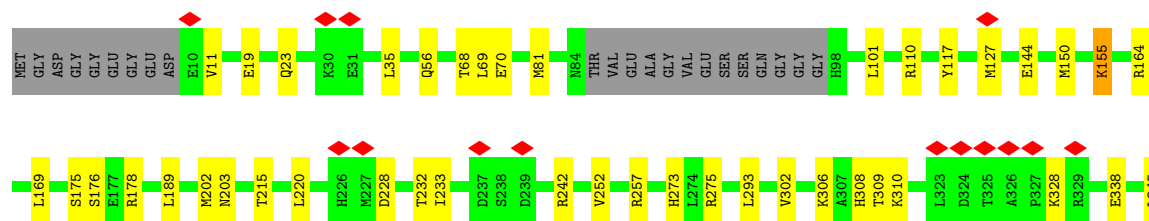
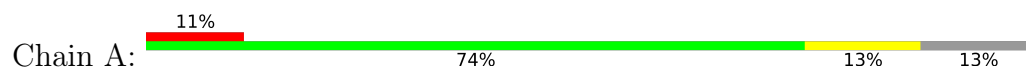
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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



- Molecule 3: Ryanodine receptor 1

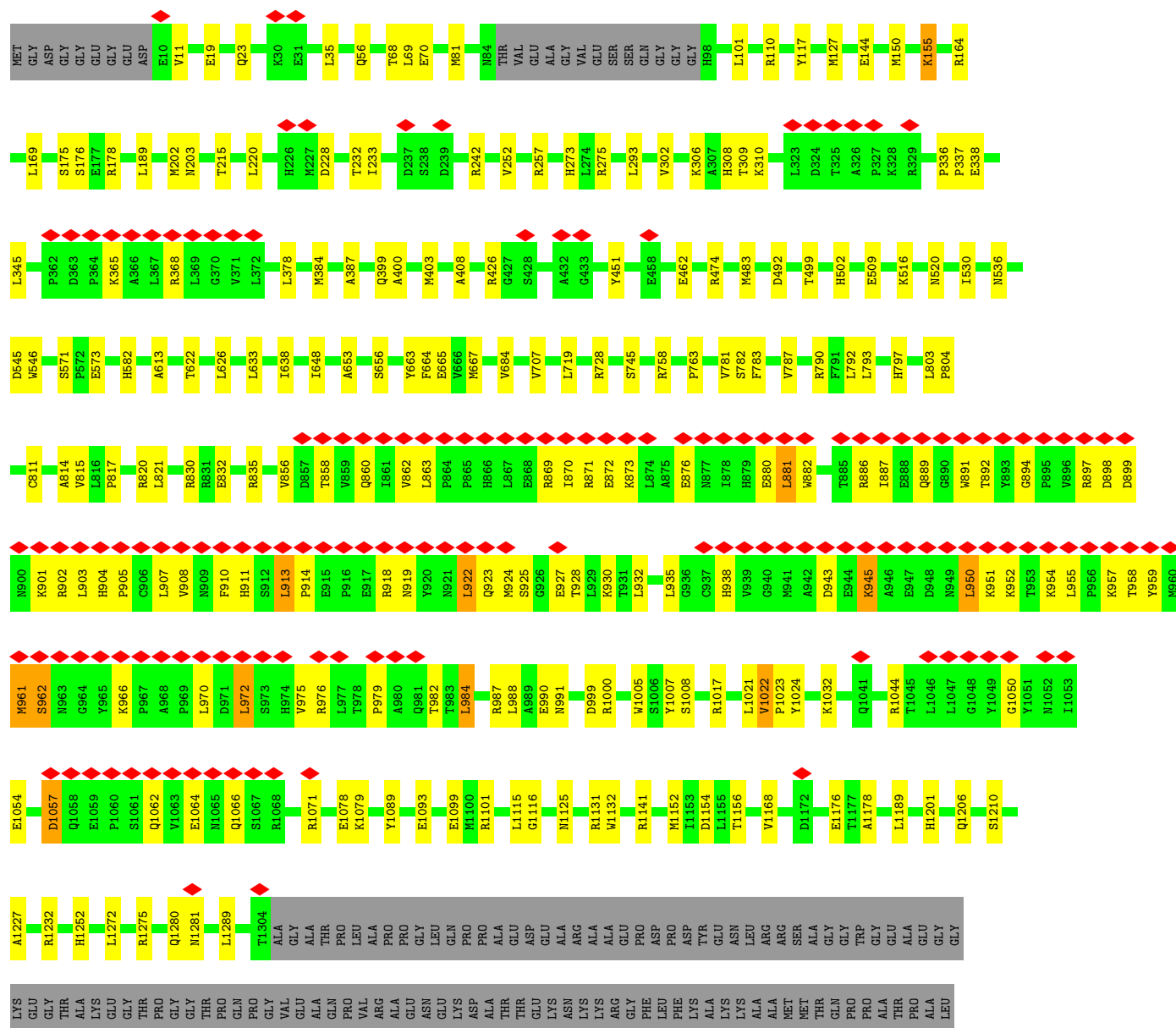




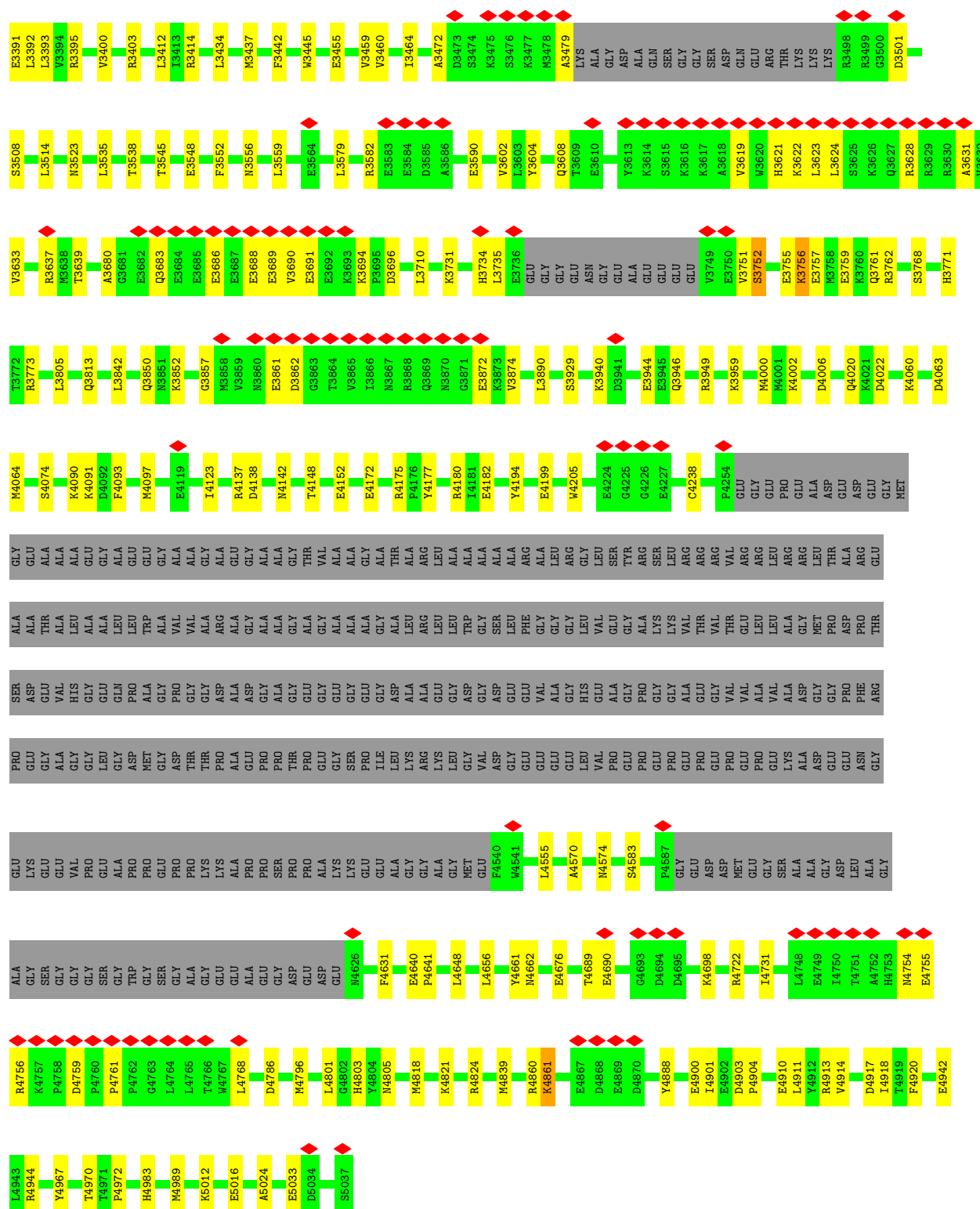




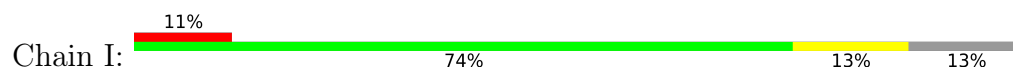




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L3249	L3112	R2920	P2859	E2799	P2739	G2264	G2264	ARG	T1985	E1873	M1636	ARG
Y3263	G3113	E2921	F2860	K2800	V2740	T2538	D2282	LEU	M1986	E1874	L1639	LEU
V3269	K3114	K2922	D2861	D2801	E2741	F2541	Y2256	LYS	S1987	GLU	L1639	HIS
I3270	V3115	A2923	L2862	K2802	T2742	R2576	Q2308	LYS	A1988	GLU	L1653	ASP
T3273	S3116	Q2924	S2863	E2803	L2743	R2576	S2309	GLU	A1989	GLU	S1694	VAL
L3274	GLN	E2925	G2864	T2804	N2744	M2578	D2320	LYS	E1990	GLU	Q1660	VAL
L3277	ALA	L2926	V2865	R2805	V2745	V2579	T2321	PRO	T1991	GLU	L1676	PRO
W3284	THR	L2927	T2866	R2806	I2746	D2580	V2341	GLU	R1993	GLU	L1676	ALA
G3288	GLN	K2928	L2867	V2807	I2747	L2614	R2355	LEU	T1994	GLU	R1680	ALA
F3293	VAL	F2929	S2868	P2808	P2748	M2618	R2355	PRO	E1997	GLU	R1680	ALA
P3294	K3123	L2930	R2869	T2809	E2749	P2618	E2382	ALA	F1998	GLU	D1690	ALA
A3295	G3124	Q2931	E2870	K2810	K2750	H2621	E2382	GLU	R1999	GLU	Q1693	ALA
L3296	V3125	M2932	L2871	E2811	L2751	L2626	R2385	GLU	S2000	GLU	L1694	ALA
P3297	T3132	N2933	Q2872	S2812	D2752	L2626	P2390	GLU	P2001	GLU	L1715	ALA
G3298	V3133	G2934	A2873	L2813	S2753	L2633	A2391	ASP	Q2005	ASP	I1716	ALA
A3300	V3134	Y2935	M2874	K2814	P2754	L2633	R2392	GLU	E2016	GLU	E1721	ALA
P3303	A3135	A2936	A2875	A2815	T2755	P2640	R2392	GLU	E2017	GLU	E1733	ALA
T3305	L3136	V2937	E2876	M2816	N2756	L2644	Y2397	ARG	E2018	GLU	G1751	ALA
L3316	L3137	T2938	Q2877	L2817	K2757	L2644	ARG	ASP	D2019	GLU	R1752	ALA
V3324	I3147	R2939	L2878	A2818	F2758	W2661	ARG	ARG	D2020	GLU	K1753	ALA
I3329	F3152	GLU	N2881	E2820	E2760	L2678	GLU	ARG	C2021	GLU	G1754	ALA
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H3335	L3158	ASP	H2883	T2822	T2762	D2716	P2411	GLU	Q2029	GLU	N1756	ALA
F3341	L3159	MET	N2884	L2823	H2763	P2664	E2412	GLU	D2037	GLU	A1757	ALA
Q3343	D3160	GLU	T2885	E2824	E2764	G2665	E2413	GLU	Q2045	GLU	R1758	ALA
V3345	V3161	L2946	W2886	K2825	K2765	L2678	N2414	GLU	L2046	GLU	L1771	ALA
V3346	L3169	D2947	G2887	A2826	W2766	K2689	E2415	GLU	GLU	GLU	P1780	ALA
I3359	C3170	S2970	R2888	R2827	A2767	D2716	R2449	GLU	GLU	GLU	A1788	ALA
A3360	S3171	F2973	K2889	E2828	F2768	S2720	R2452	GLU	GLU	GLU	A1789	ALA
T3361	S3174	T2974	K2890	G2829	D2769	K2721	R2452	GLU	GLU	GLU	G1790	ALA
F3363	K3179	A2975	K2891	E2830	K2770	E2724	E2449	GLU	GLU	GLU	V1791	ALA
A3364	L3186	E2978	E2893	GLU	I2771	K2725	R2452	GLU	GLU	GLU	A1792	ALA
Q3343	L3186	S2982	L2894	ARG	Q2772	ALA	V2461	GLU	GLU	GLU	E1793	ALA
V3345	L3194	S2983	E2895	THR	N2773	ALA	D2482	GLU	GLU	GLU	A1794	ALA
V3346	L3194	G2984	A2896	GLU	N2774	THR	G2483	GLU	GLU	GLU	E1805	ALA
I3359	P3208	R2985	K2897	LYS	W2775	VAL	V2495	GLU	GLU	GLU	K1810	ALA
F3360	R3225	V2986	G2898	LYS	S2776	ALA	V2495	GLU	GLU	GLU	M1814	ALA
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A3363	A3228	K2988	G2900	LYS	G2778	THR	G2483	GLU	GLU	GLU	L1980	ALA
K3383	I3229	T2901	T2901	ILE	E2779	ASP	H2498	GLU	GLU	GLU	V1819	ALA
K3384	L3003	H2902	H2902	GLN	W2781	GLU	H2498	GLU	GLU	GLU	R1820	ALA
A3385	P3004	P2903	P2903	GLN	D2782	GLU	H2498	GLU	GLU	GLU	Q1824	ALA
E3386	F3017	L2904	L2905	ALA	E2783	GLU	E2513	GLU	GLU	GLU	D1828	ALA
A3387	T3020	L2906	V2906	GLN	E2784	THR	V2514	GLU	GLU	GLU		ALA
F3388	T3023	P2907	T2907	TYR	L2785	THR	V2514	GLU	GLU	GLU		ALA
E3389	K3023	Y2908	Y2908	ASP	K2786	THR	D2516	GLU	GLU	GLU		ALA
G3390	K3036	D2909	D2909	PRO	T2787	THR	D2516	GLU	GLU	GLU		ALA
	R3053	L2911	L2911	ARG	H2788	THR	D2516	GLU	GLU	GLU		ALA
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		A2913	W2856	P2857	M2790	THR	D2516	GLU	GLU	GLU		ALA
		K2914	K2914		L2791	THR	D2516	GLU	GLU	GLU		ALA
		E2915	K2915		T2794	THR	D2516	GLU	GLU	GLU		ALA
		K2916	K2916		T2796	THR	D2516	GLU	GLU	GLU		ALA
		A2917	K2918		F2797	THR	D2516	GLU	GLU	GLU		ALA



• Molecule 3: Ryanodine receptor 1







P4904	G4699	GLY	GLY	ALA	LYS	VAL	LEU	ALA	ALA	LEU	D4046
E4910	R4722	SER	ALA	ASP	ALA	ASP	ALA	GLY	ARG	ALA	D4063
L4911		ALA	ASP	GLY	GLY	GLY	PRO	MET	ARG	GLY	M4064
Y4912	I4731	ALA	GLU	GLY	PRO	GLY	ASP	THR	ALA	GLY	D4070
R4913	L4748	GLY	LEU	ASN	PHE	ARG	THR	GLY	GLY	MET	D4070
V4914	E4749	ASP	GLY	GLY	GLY	GLY	ALA	SER	ALA	GLY	S4074
	L4750	ALA	GLY	LYS	GLY	GLY	ASP	ALA	GLY	GLY	D4086
D4917	T4751	ALA	GLY	GLY	GLY	ALA	VAL	THR	ALA	ALA	K4090
I4918	A4752	SER	GLY	VAL	VAL	GLY	GLY	HIS	LEU	ALA	K4091
T4919	H4753	GLY	GLY	PRO	PRO	GLY	GLY	GLY	ALA	GLY	E4092
F4920	M4754	GLY	ALA	GLY	GLY	GLY	GLN	LEU	ALA	GLY	F4093
	E4755	SER	PRO	PRO	ASP	ASP	PRO	LEU	GLY	GLY	M4097
I4931	R4756	GLY	GLY	MET	ALA	ALA	GLY	TSP	GLY	GLY	D4098
E4942	K4757	TRP	GLY	GLY	GLY	GLY	PRO	ALA	ALA	GLY	E4119
L4943	P4758	SER	GLY	ASP	THR	THR	VAL	GLY	ALA	ALA	I4123
R4944	D4759	SER	GLY	PRO	LYS	THR	GLY	GLY	ALA	GLY	R4137
Y4967	P4760	ALA	LYS	LYS	PRO	PRO	ARG	ASP	ALA	ALA	D4138
T4970	P4761	GLY	PRO	ALA	ALA	ALA	ASP	GLY	GLY	GLY	M4142
T4971	P4762	GLY	GLY	PRO	PRO	PRO	GLY	GLY	GLY	ALA	T4148
P4972	G4763	ALA	GLY	SER	SER	PRO	GLY	GLY	ALA	ALA	R4159
H4983	L4764	GLY	GLY	ALA	ALA	GLY	GLY	GLY	ALA	ALA	E4172
M4989	L4765	ASP	GLY	LYS	LYS	GLY	LEU	LEU	ALA	ALA	R4175
K5012	L4768	GLY	GLY	LYS	GLY	GLY	LEU	LEU	ALA	ALA	Y4177
E5016	M4769	ASP	GLY	LYS	LYS	SER	GLY	TRP	ALA	ALA	R4180
A5024	D4786	GLY	GLY	ALA	ALA	ILE	GLY	ALA	ALA	GLY	I4181
E5033	M4796		M4626	GLY	GLY	LEU	ASP	THR	ALA	ALA	E4182
S5037	L4801		E4631	GLY	GLY	LYS	ALA	LEU	ARG	ARG	P4176
	G4802		E4640	ALA	ALA	LYS	ALA	LEU	LEU	LEU	Y4177
	H4803		P4641	GLY	ALA	LYS	GLY	LEU	LEU	ALA	R4180
	L4813		L4648	GLY	GLY	GLY	ASP	TRP	ALA	ALA	E4182
	M4818		L4656	ALA	GLY	GLY	GLY	GLY	ALA	ALA	E4199
	G4819		Y4661	GLY	GLY	GLY	VAL	GLY	LEU	LEU	K4205
	V4820		Y4661	GLY	GLY	GLY	VAL	GLY	ARG	ARG	G4226
	K4821		M4662	GLY	GLY	LEU	GLY	GLY	GLY	GLY	E4227
	R4824		E4676	GLY	GLY	VAL	GLY	GLY	VAL	LEU	C4238
	R4860		Y4687	GLY	GLY	PRO	ALA	GLY	GLY	TYR	T4241
	K4861		L4688	GLY	GLY	PRO	PRO	GLY	ARG	ARG	M4245
	E4867		T4689	GLY	GLY	PRO	GLY	GLY	LEU	ARG	P4254
	D4868		E4690	GLY	GLY	PRO	GLY	VAL	GLY	ARG	GLY
	E4869		G4693	GLY	GLY	GLY	VAL	THR	VAL	ARG	GLY
	D4870		D4694	ASP	ASP	PRO	VAL	THR	VAL	ARG	GLY
	M4880		D4695	ASP	ASP	PRO	VAL	THR	VAL	ARG	GLY
	Y4888		K4698	MET	MET	PRO	ALA	LEU	ARG	ARG	PRO
	I4901										
	E4902										
	D4903										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	153840	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 ($e^-/\text{\AA}^2$)	57.65	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.887	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.013	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	426.496, 426.496, 426.496	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: L9R, KVR, ATP, CA, CFF, 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	C	0.10	0/1187	0.24	0/1594
1	D	0.09	0/1187	0.24	0/1594
1	E	0.09	0/1187	0.24	0/1594
1	K	0.09	0/1187	0.24	0/1594
2	F	0.33	0/850	0.49	0/1146
2	H	0.33	0/850	0.49	0/1146
2	J	0.33	0/850	0.49	0/1146
2	O	0.33	0/850	0.49	0/1146
3	A	0.15	0/35977	0.30	3/48726 (0.0%)
3	B	0.15	0/35977	0.30	3/48726 (0.0%)
3	G	0.15	0/35977	0.30	3/48726 (0.0%)
3	I	0.15	0/35977	0.30	3/48726 (0.0%)
All	All	0.15	0/152056	0.30	12/205864 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	4920	PHE	N-CA-C	-5.60	105.17	112.23
3	I	4920	PHE	N-CA-C	-5.58	105.20	112.23
3	A	4920	PHE	N-CA-C	-5.58	105.20	112.23
3	B	4920	PHE	N-CA-C	-5.56	105.23	112.23
3	B	4970	THR	CA-C-N	5.08	130.59	120.94

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	C	1174	0	1099	22	0
1	D	1174	0	1099	18	0
1	E	1174	0	1099	18	0
1	K	1174	0	1099	19	0
2	F	831	0	831	7	0
2	H	831	0	831	8	0
2	J	831	0	831	7	0
2	O	831	0	831	8	0
3	A	35150	0	34797	374	0
3	B	35150	0	34797	371	0
3	G	35150	0	34797	373	0
3	I	35150	0	34797	378	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	G	1	0	0	0	0
4	I	1	0	0	0	0
4	K	4	0	0	0	0
5	A	62	0	24	2	0
5	B	62	0	24	2	0
5	G	62	0	24	2	0
5	I	62	0	24	2	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	G	1	0	0	0	0
6	I	1	0	0	0	0
7	A	14	0	10	0	0
7	B	14	0	10	0	0
7	G	14	0	10	0	0
7	I	14	0	10	0	0
8	A	23	0	0	0	0
8	B	23	0	0	0	0
8	G	23	0	0	0	0
8	I	23	0	0	0	0
9	A	108	0	172	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	108	0	172	6	0
9	G	108	0	172	9	0
9	I	108	0	172	8	0
All	All	149472	0	147732	1564	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 5.

The worst 5 of 1564 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)
3:I:4904:PRO:HB3	3:I:4913:ARG:HG2	1.57	0.86
3:G:4904:PRO:HB3	3:G:4913:ARG:HG2	1.57	0.86
3:A:4904:PRO:HB3	3:A:4913:ARG:HG2	1.57	0.84
3:B:4904:PRO:HB3	3:B:4913:ARG:HG2	1.57	0.83
3:A:2779:GLU:HG3	3:A:2792:ARG:HG2	1.66	0.78

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	C	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	D	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	E	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
1	K	147/150 (98%)	146 (99%)	1 (1%)	0	100	100
2	F	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	H	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
2	J	105/107 (98%)	103 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	105/107 (98%)	103 (98%)	2 (2%)	0	100	100
3	A	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	B	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
3	G	4385/5037 (87%)	4274 (98%)	111 (2%)	0	100	100
3	I	4385/5037 (87%)	4273 (97%)	112 (3%)	0	100	100
All	All	18548/21176 (88%)	18089 (98%)	459 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	C	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	D	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	E	127/128 (99%)	123 (97%)	4 (3%)	35	50
1	K	127/128 (99%)	123 (97%)	4 (3%)	35	50
2	F	89/89 (100%)	85 (96%)	4 (4%)	24	37
2	H	89/89 (100%)	85 (96%)	4 (4%)	24	37
2	J	89/89 (100%)	85 (96%)	4 (4%)	24	37
2	O	89/89 (100%)	85 (96%)	4 (4%)	24	37
3	A	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	B	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	G	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
3	I	3836/4276 (90%)	3768 (98%)	68 (2%)	51	65
All	All	16208/17972 (90%)	15904 (98%)	304 (2%)	49	64

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	881	LEU
3	I	4821	LYS
3	I	913	LEU
3	I	2153	MET
2	O	17	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	2933	ASN
3	I	3667	HIS
3	B	963	ASN
3	B	938	HIS
3	I	3761	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 48 ligands modelled in this entry, 24 are monoatomic - leaving 24 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	ATP	I	5102	-	32,33,33	0.28	0	48,52,52	0.39	0
5	ATP	B	5301	-	32,33,33	0.28	0	48,52,52	0.39	0
8	KVR	G	5107	-	24,25,25	1.41	3 (12%)	31,34,34	1.56	4 (12%)
8	KVR	B	5306	-	24,25,25	1.42	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	I	5108	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
5	ATP	A	5305	-	32,33,33	0.25	0	48,52,52	0.29	0
9	L9R	B	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
9	L9R	I	5101	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
5	ATP	G	5102	-	32,33,33	0.28	0	48,52,52	0.39	0
9	L9R	G	5108	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
9	L9R	A	5307	-	53,53,53	1.24	5 (9%)	59,61,61	1.12	3 (5%)
7	CFF	A	5304	-	15,15,15	1.77	4 (26%)	23,23,23	2.95	11 (47%)
5	ATP	I	5106	-	32,33,33	0.26	0	48,52,52	0.29	0
9	L9R	A	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
7	CFF	I	5105	-	15,15,15	1.77	5 (33%)	23,23,23	2.95	11 (47%)
5	ATP	B	5305	-	32,33,33	0.26	0	48,52,52	0.29	0
5	ATP	A	5301	-	32,33,33	0.28	0	48,52,52	0.39	0
7	CFF	B	5304	-	15,15,15	1.77	4 (26%)	23,23,23	2.96	11 (47%)
5	ATP	G	5106	-	32,33,33	0.25	0	48,52,52	0.29	0
8	KVR	A	5306	-	24,25,25	1.41	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	B	5308	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
8	KVR	I	5107	-	24,25,25	1.41	3 (12%)	31,34,34	1.55	4 (12%)
9	L9R	G	5101	-	53,53,53	1.21	4 (7%)	59,61,61	1.12	2 (3%)
7	CFF	G	5105	-	15,15,15	1.76	4 (26%)	23,23,23	2.95	11 (47%)

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	ATP	I	5102	-	-	8/22/38/38	0/3/3/3
5	ATP	B	5301	-	-	8/22/38/38	0/3/3/3
8	KVR	G	5107	-	-	2/10/20/20	0/2/3/3
8	KVR	B	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	I	5108	-	-	30/57/57/57	-
5	ATP	A	5305	-	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	L9R	B	5307	-	-	30/57/57/57	-
9	L9R	I	5101	-	-	34/57/57/57	-
5	ATP	G	5102	-	-	8/22/38/38	0/3/3/3
9	L9R	G	5108	-	-	30/57/57/57	-
9	L9R	A	5307	-	-	30/57/57/57	-
7	CFF	A	5304	-	-	-	0/2/2/2
5	ATP	I	5106	-	-	8/22/38/38	0/3/3/3
9	L9R	A	5308	-	-	34/57/57/57	-
7	CFF	I	5105	-	-	-	0/2/2/2
5	ATP	B	5305	-	-	8/22/38/38	0/3/3/3
5	ATP	A	5301	-	-	8/22/38/38	0/3/3/3
7	CFF	B	5304	-	-	-	0/2/2/2
5	ATP	G	5106	-	-	8/22/38/38	0/3/3/3
8	KVR	A	5306	-	-	2/10/20/20	0/2/3/3
9	L9R	B	5308	-	-	34/57/57/57	-
8	KVR	I	5107	-	-	2/10/20/20	0/2/3/3
9	L9R	G	5101	-	-	34/57/57/57	-
7	CFF	G	5105	-	-	-	0/2/2/2

The worst 5 of 65 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	5306	KVR	C06-S09	4.92	1.82	1.77
8	I	5107	KVR	C06-S09	4.91	1.82	1.77
8	A	5306	KVR	C06-S09	4.88	1.82	1.77
8	G	5107	KVR	C06-S09	4.86	1.82	1.77
7	B	5304	CFF	C6-N1	-3.78	1.32	1.40

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	5105	CFF	C14-N7-C8	-8.45	110.47	126.28
7	A	5304	CFF	C14-N7-C8	-8.43	110.51	126.28
7	B	5304	CFF	C14-N7-C8	-8.42	110.52	126.28
7	G	5105	CFF	C14-N7-C8	-8.41	110.54	126.28
7	I	5105	CFF	C14-N7-C5	5.78	141.53	127.77

There are no chirality outliers.

5 of 328 torsion outliers are listed below:

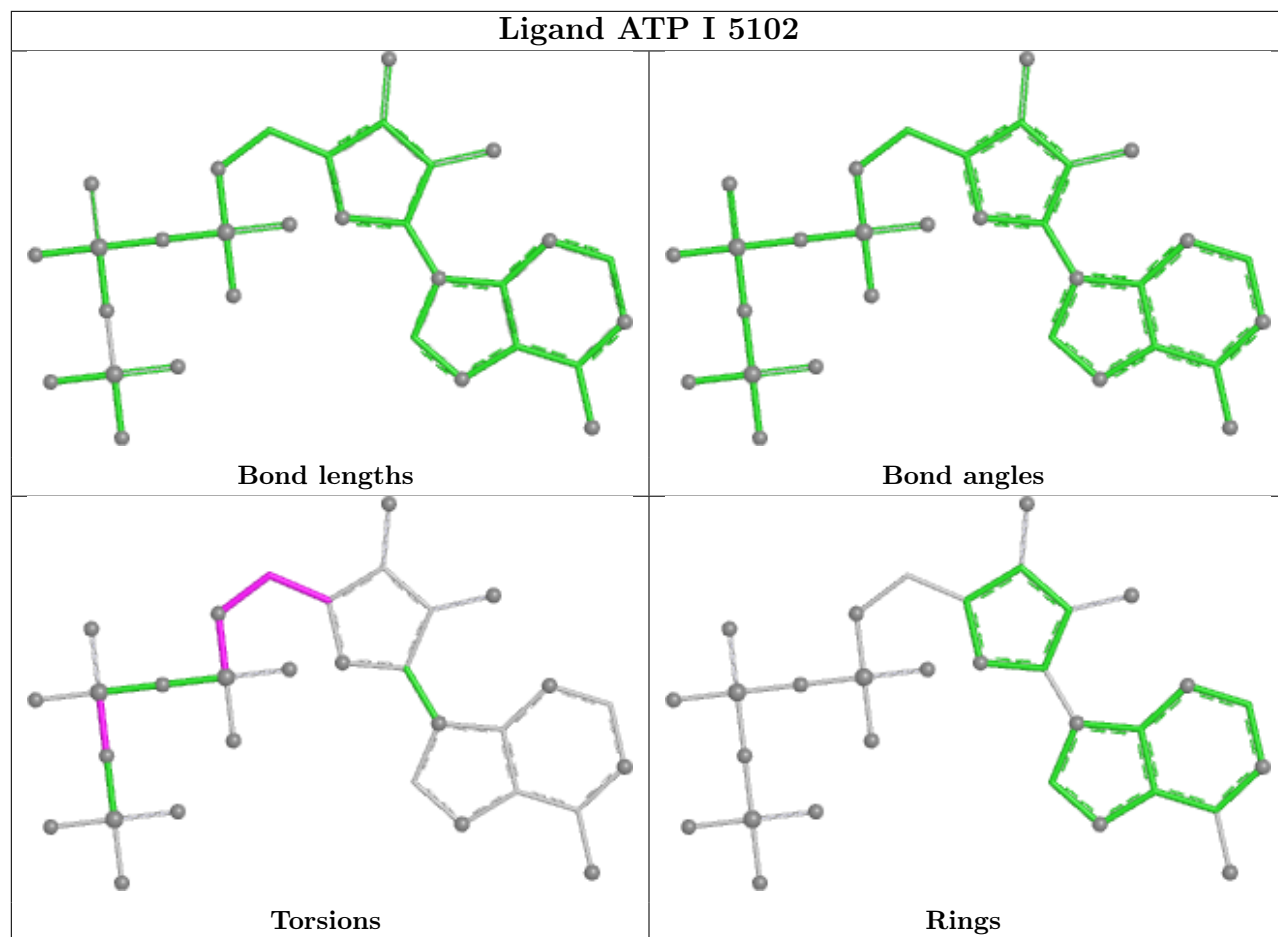
Mol	Chain	Res	Type	Atoms
5	A	5301	ATP	C5'-O5'-PA-O1A
5	A	5301	ATP	C5'-O5'-PA-O2A
5	A	5301	ATP	C5'-O5'-PA-O3A
5	A	5305	ATP	C5'-O5'-PA-O2A
5	A	5305	ATP	C5'-O5'-PA-O3A

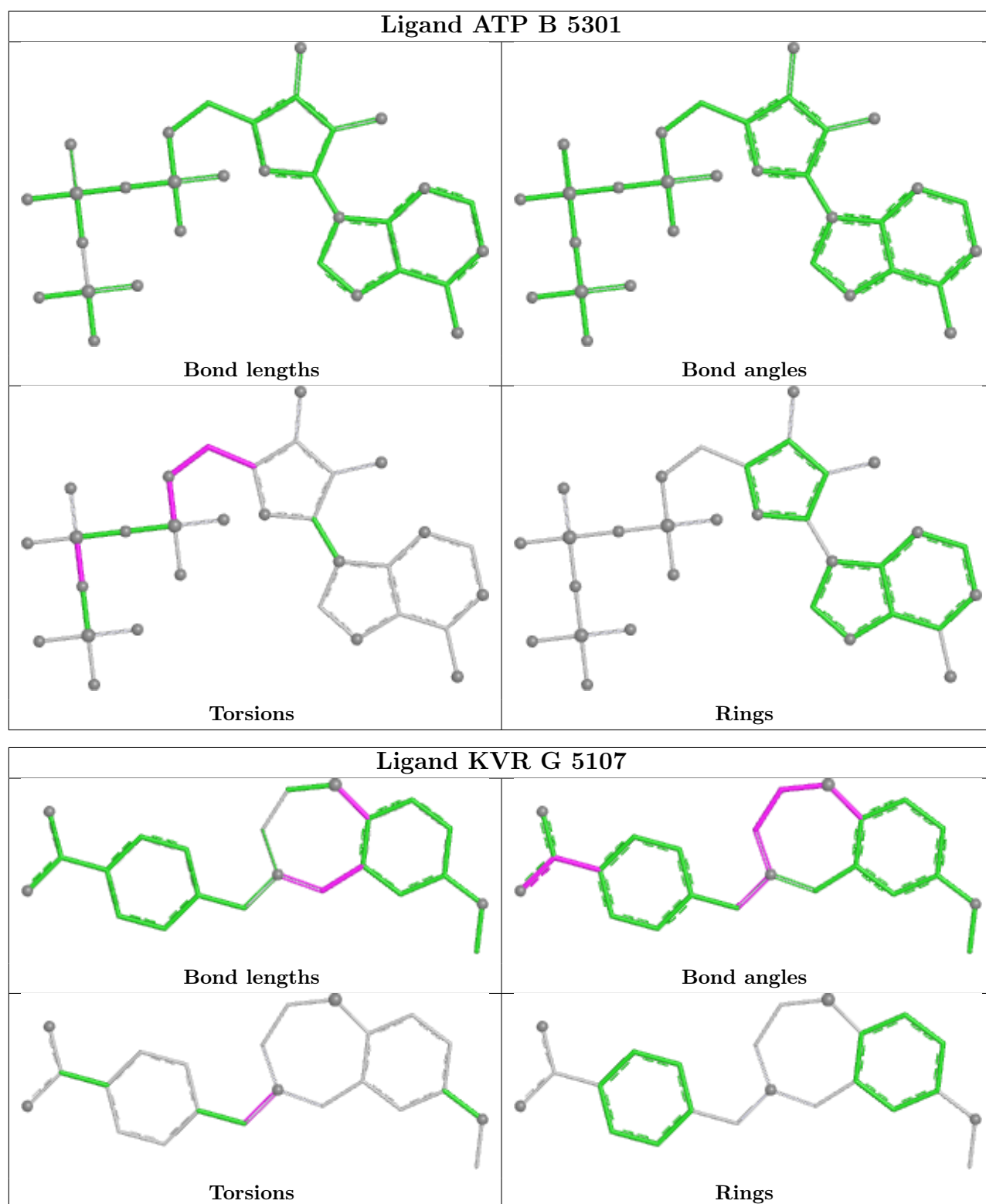
There are no ring outliers.

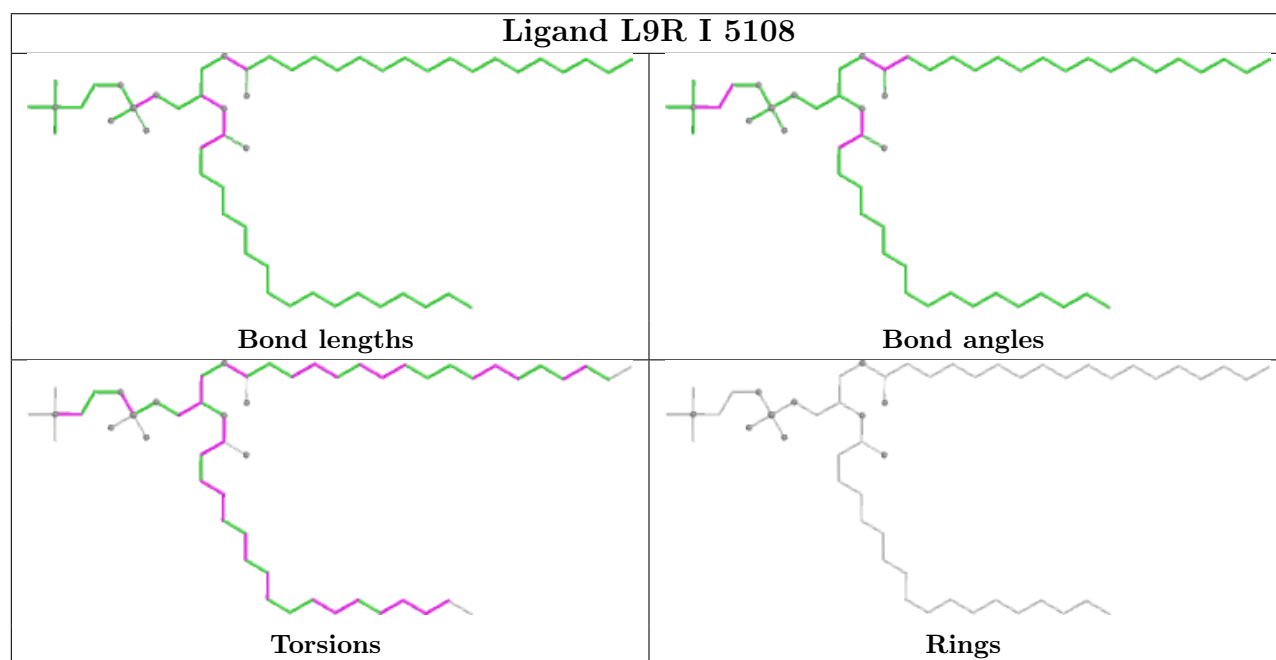
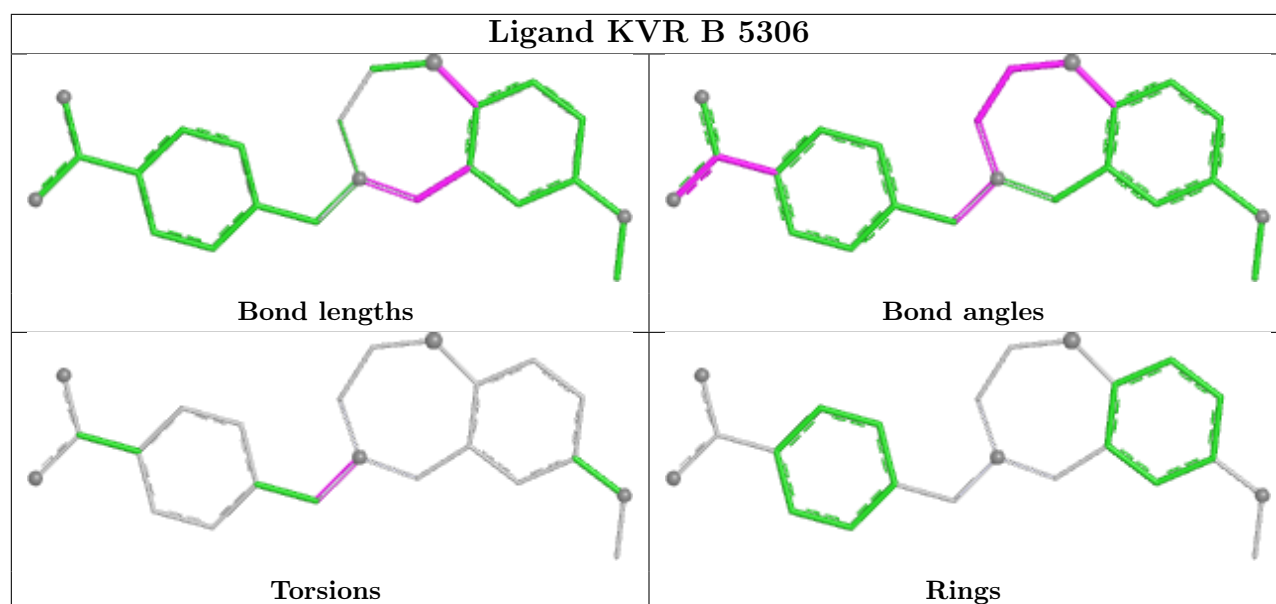
16 monomers are involved in 36 short contacts:

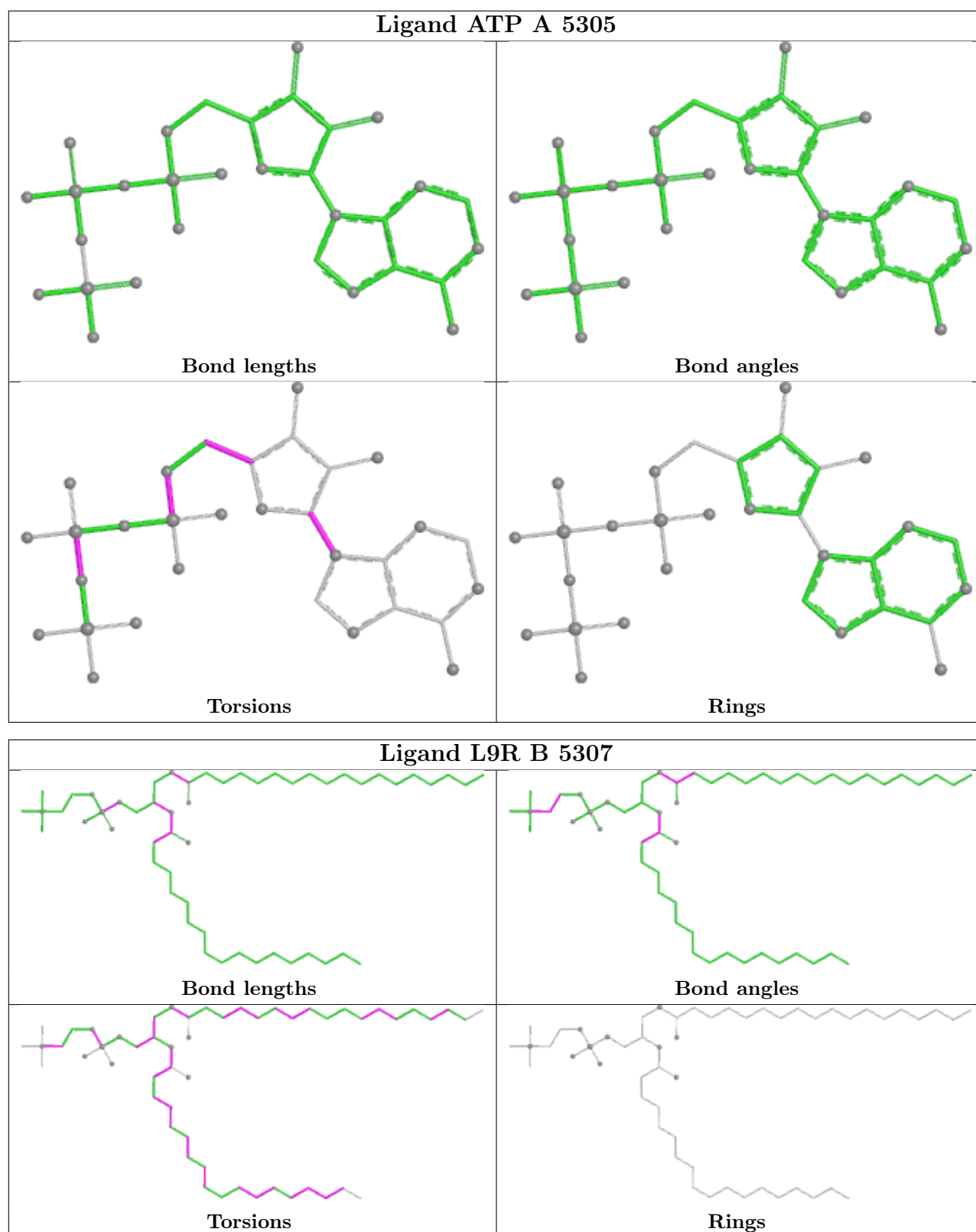
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	5102	ATP	1	0
5	B	5301	ATP	1	0
9	I	5108	L9R	3	0
5	A	5305	ATP	1	0
9	B	5307	L9R	2	0
9	I	5101	L9R	5	0
5	G	5102	ATP	1	0
9	G	5108	L9R	3	0
9	A	5307	L9R	3	0
5	I	5106	ATP	1	0
9	A	5308	L9R	6	0
5	B	5305	ATP	1	0
5	A	5301	ATP	1	0
5	G	5106	ATP	1	0
9	B	5308	L9R	4	0
9	G	5101	L9R	6	0

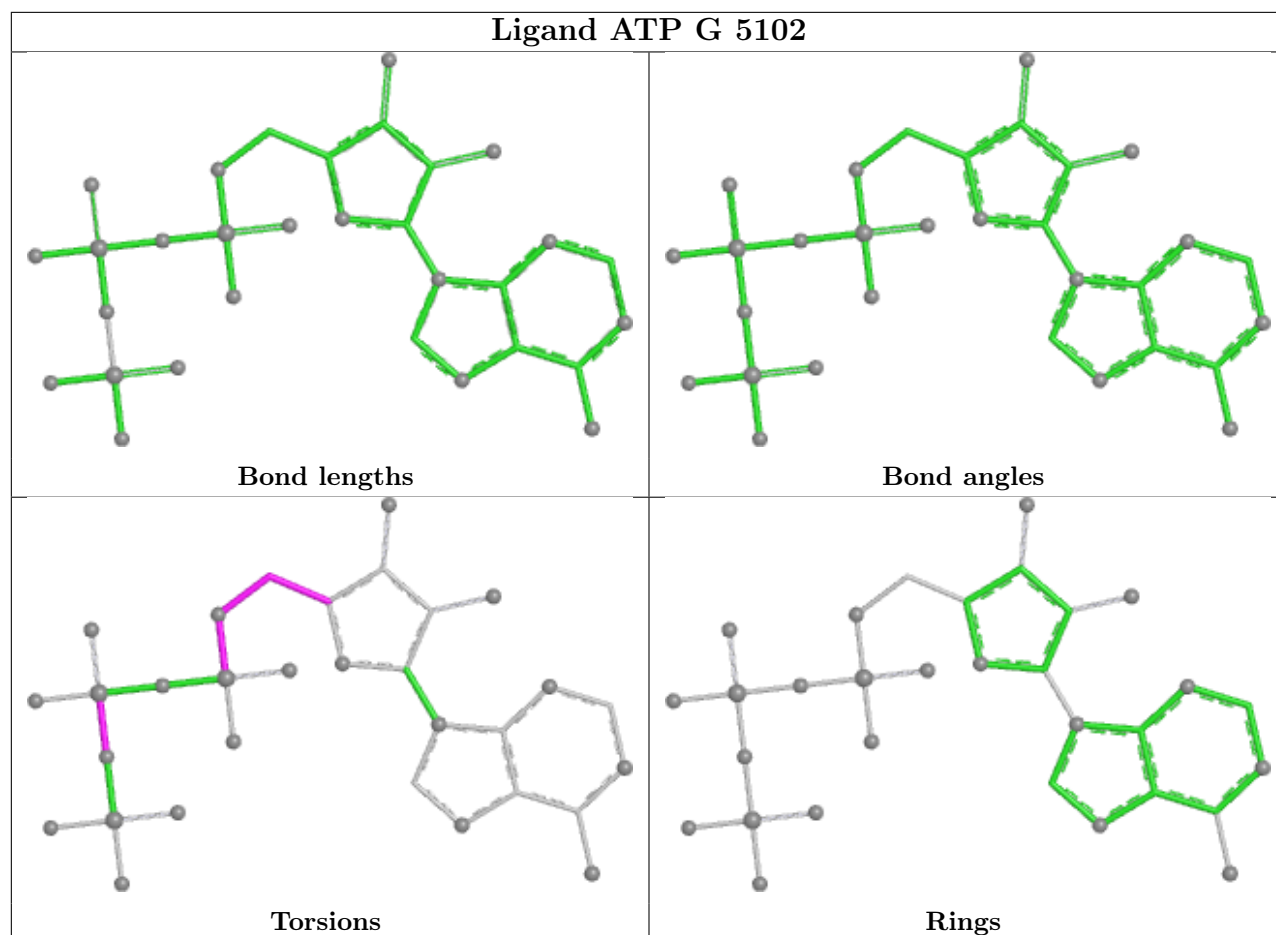
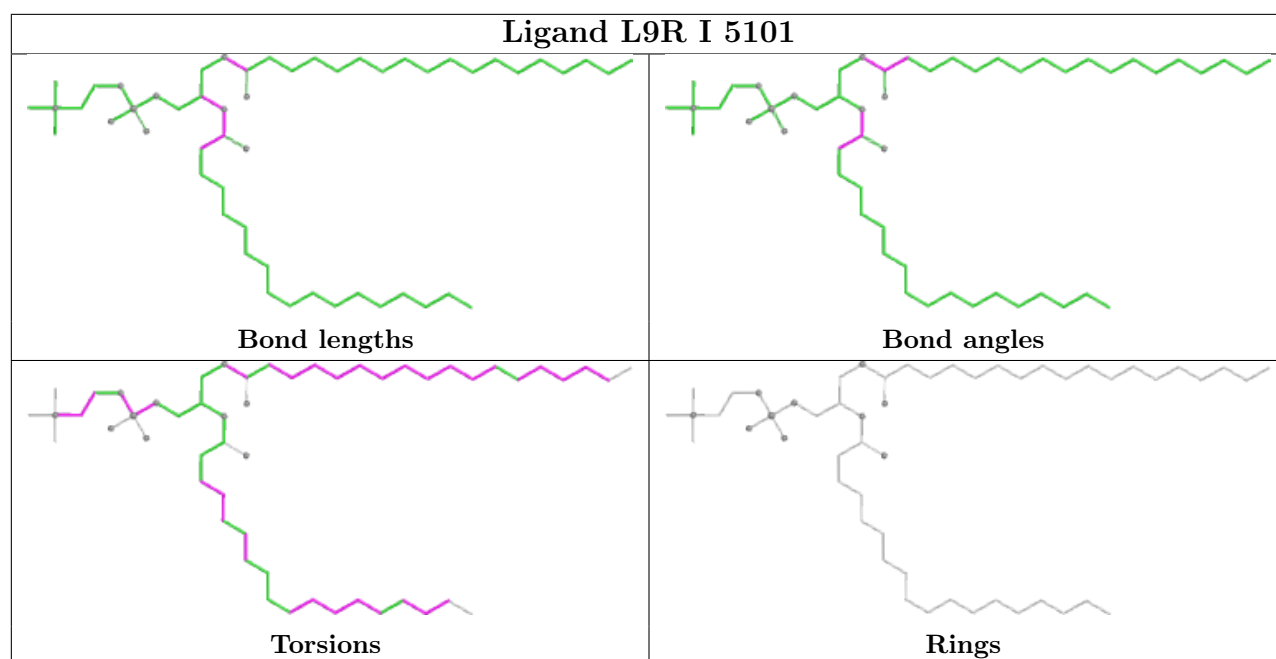
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

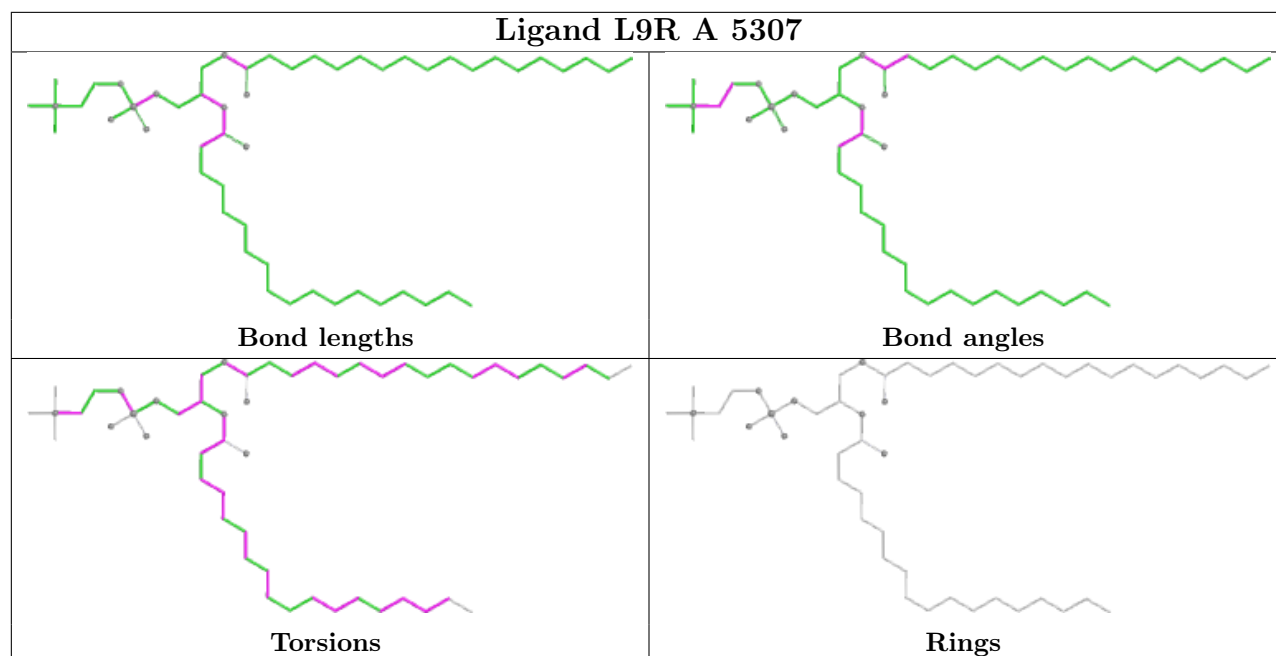
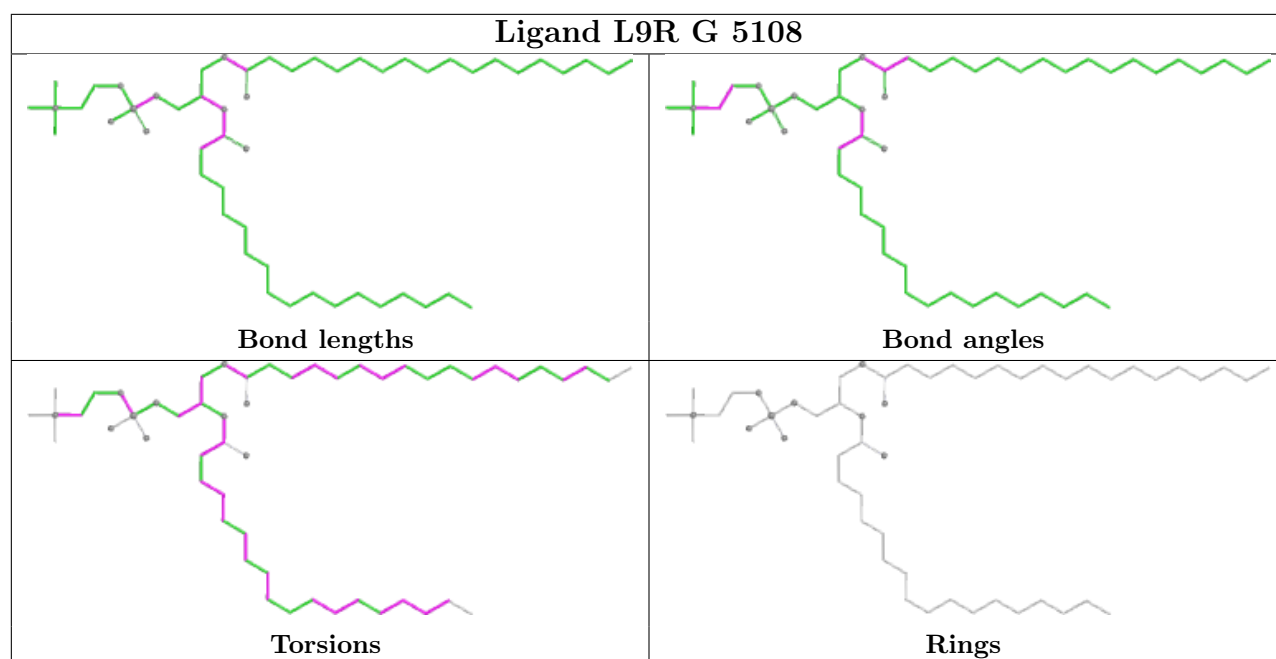


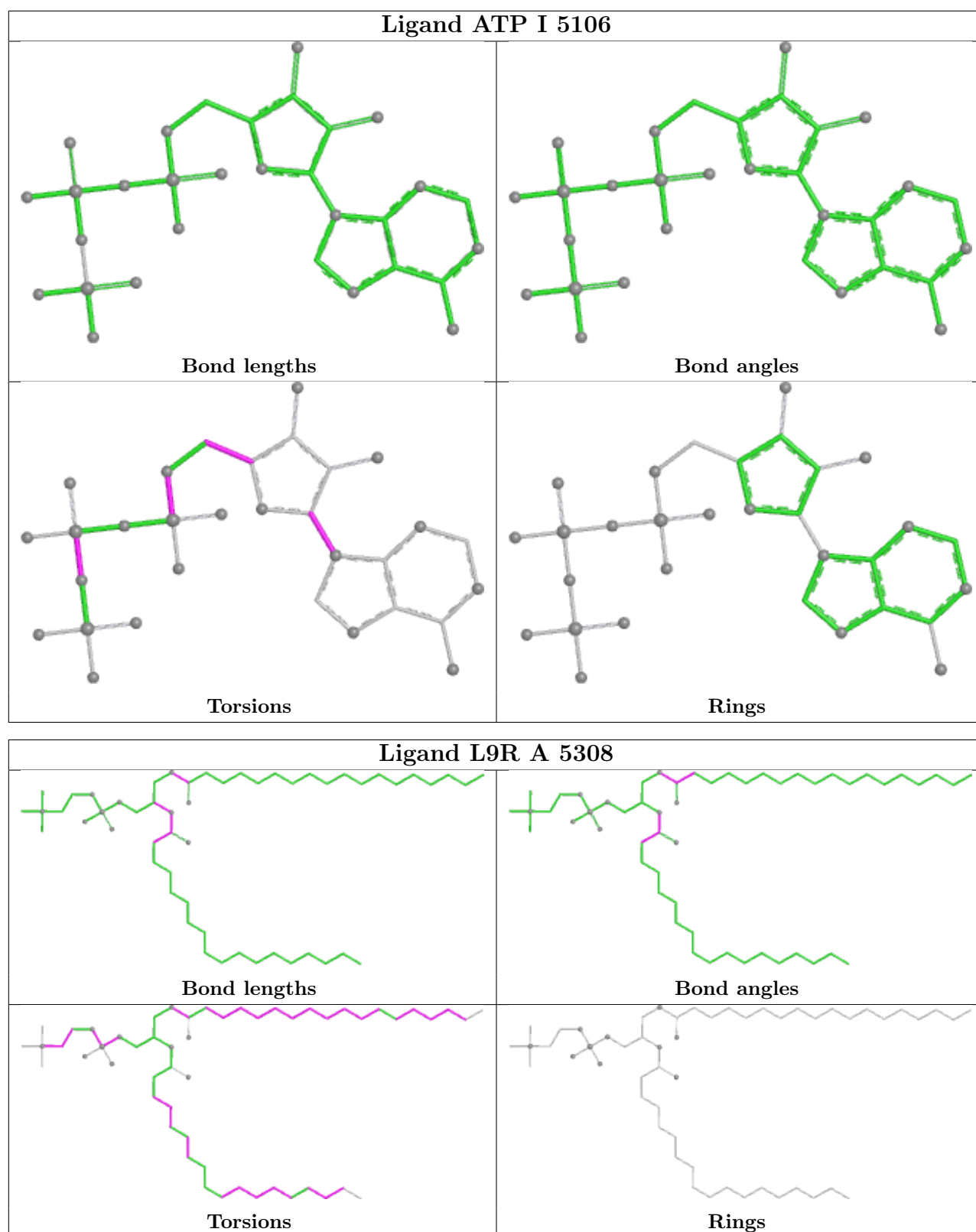


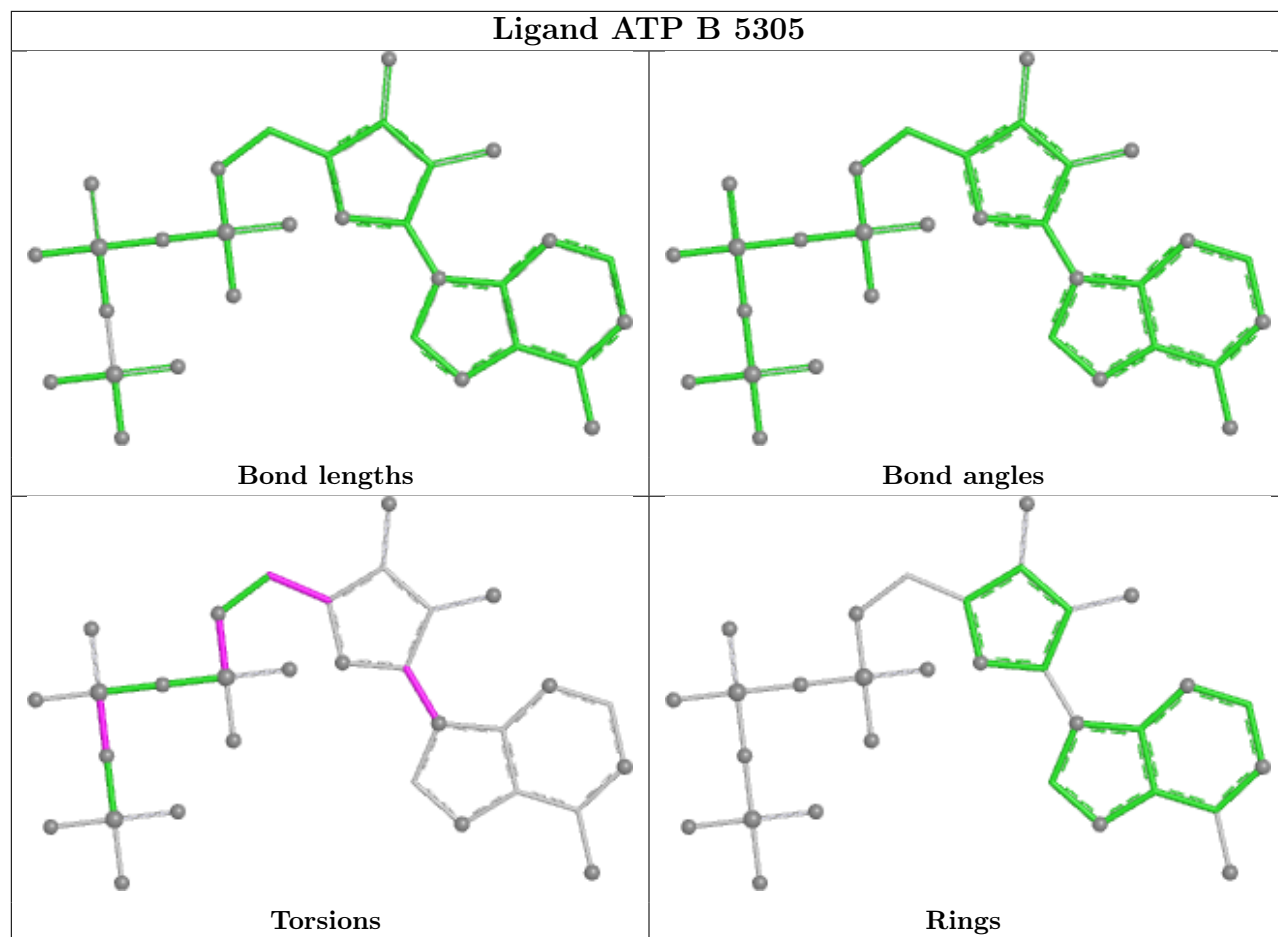


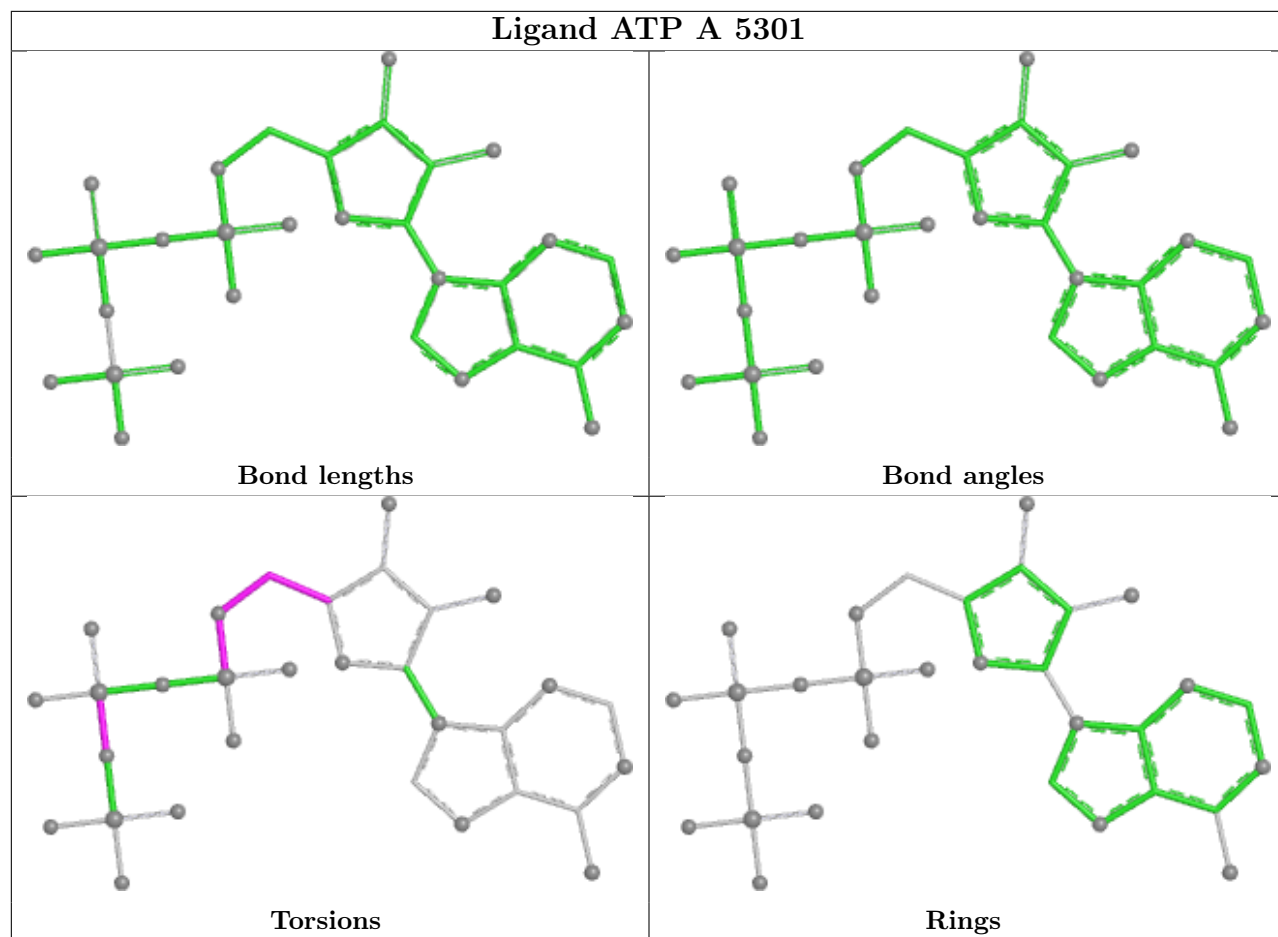


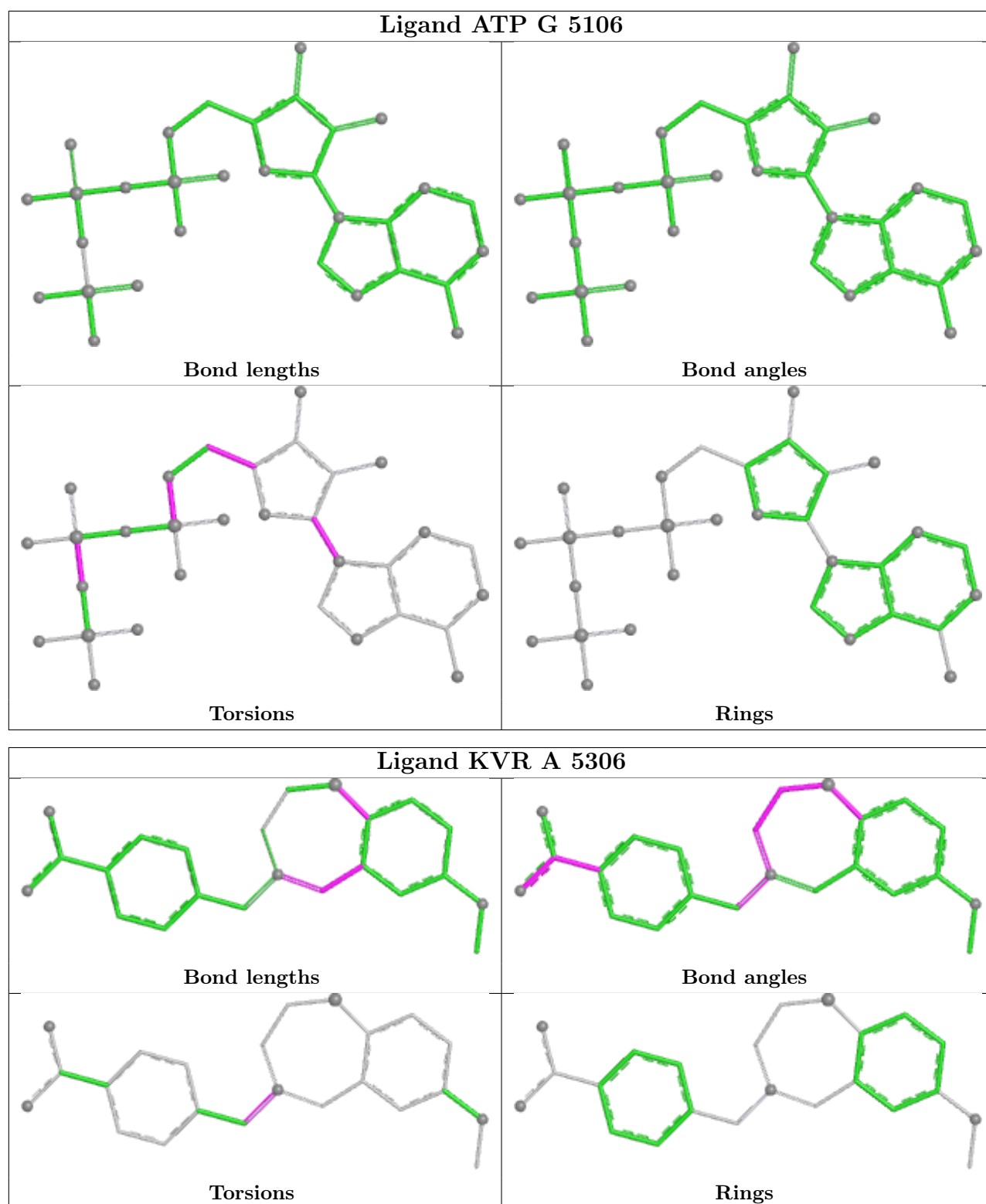


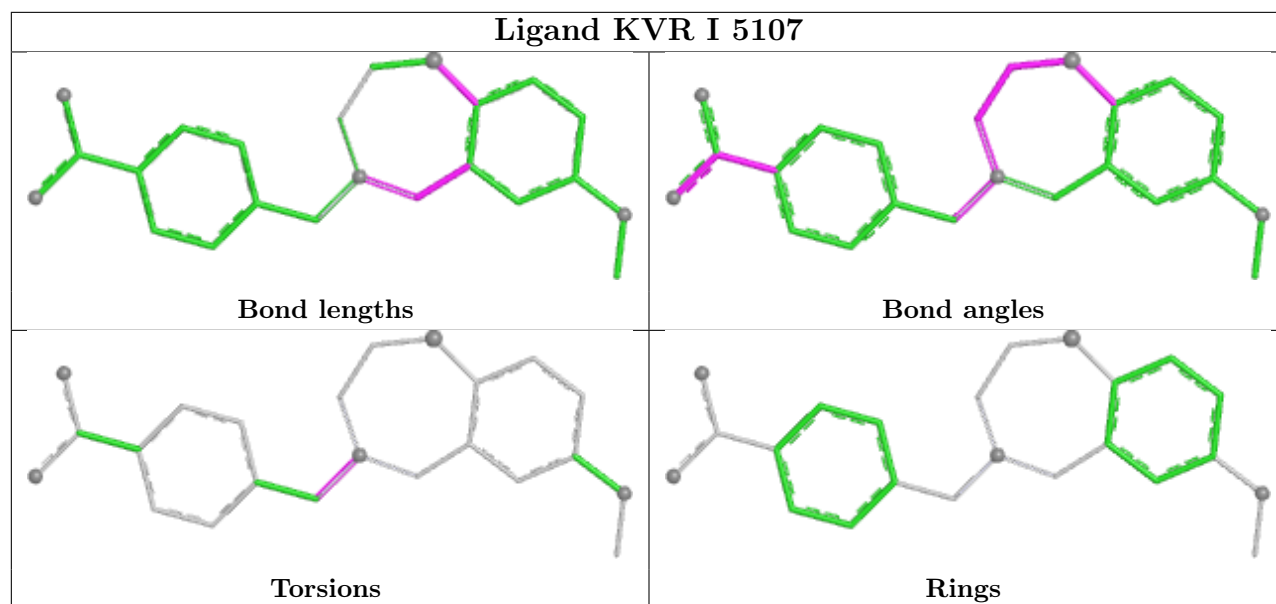
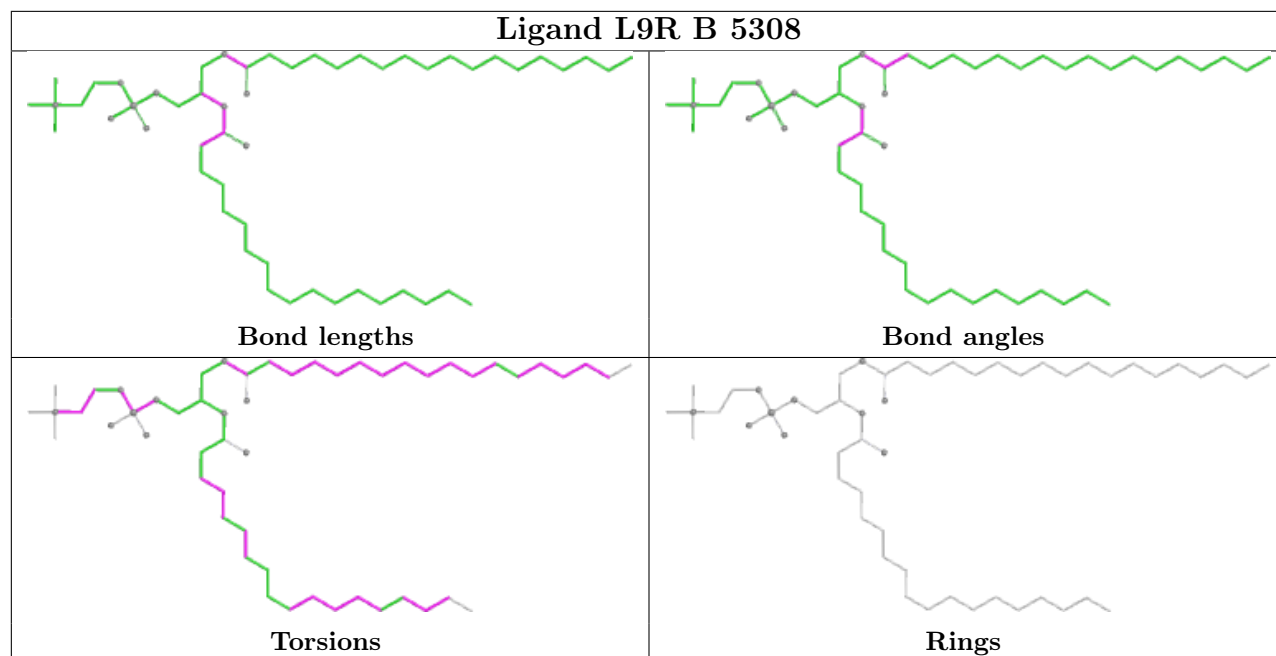


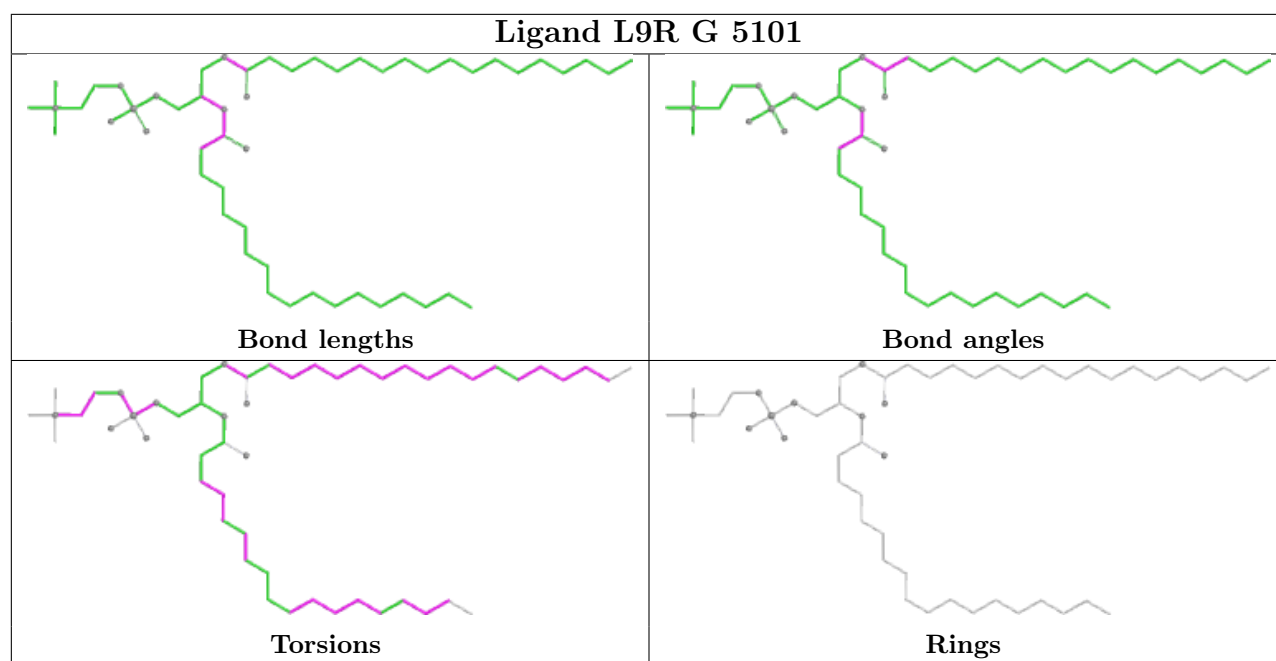












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

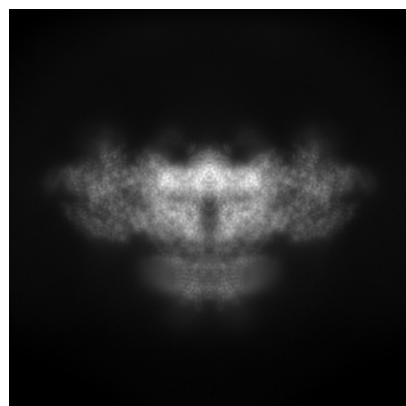
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26205. These allow visual inspection of the internal detail of the map and identification of artifacts.

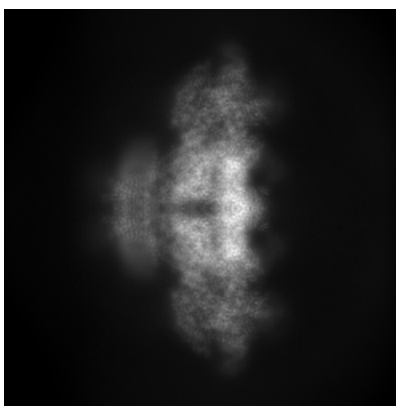
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

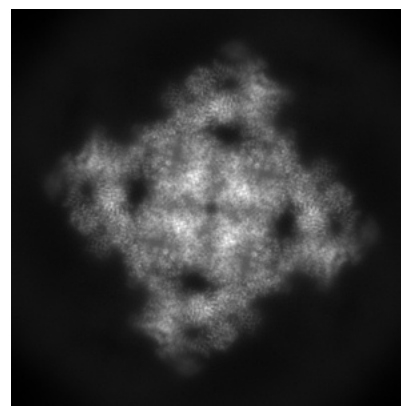
6.1.1 Primary map



X

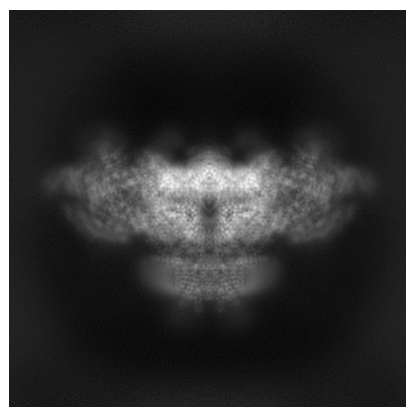


Y

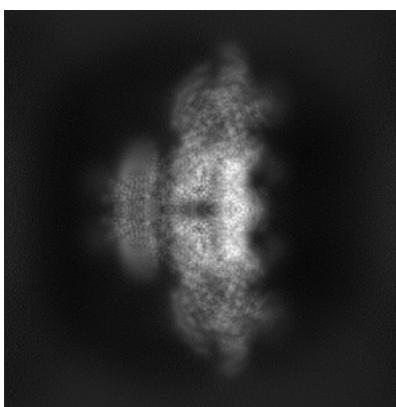


Z

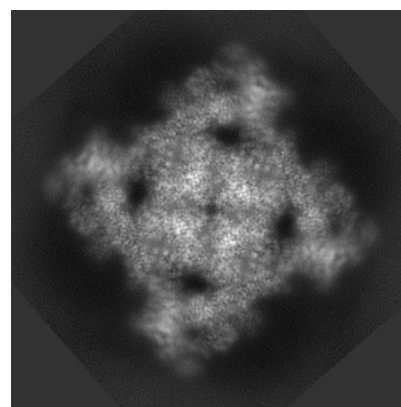
6.1.2 Raw map



X



Y



Z

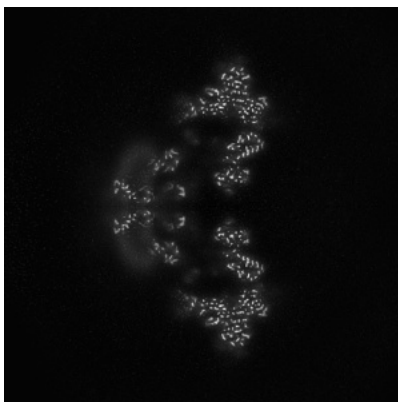
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

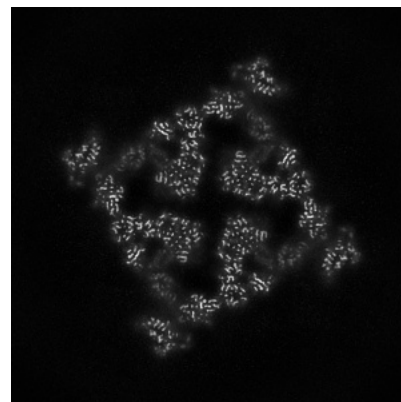
6.2.1 Primary map



X Index: 256

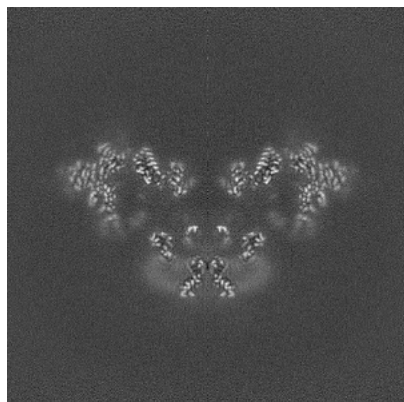


Y Index: 256

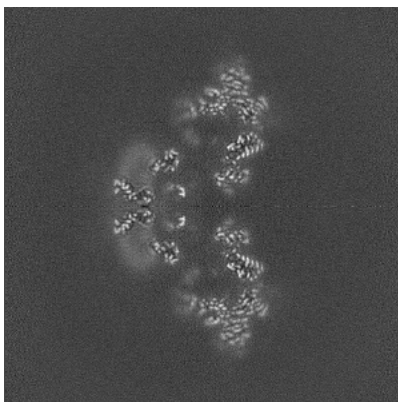


Z Index: 256

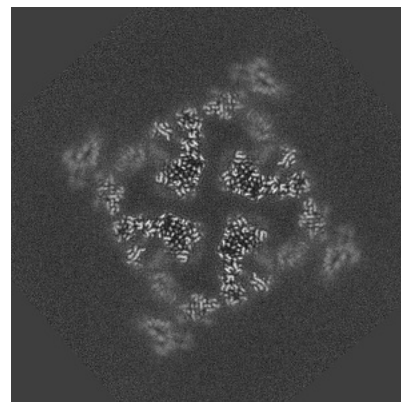
6.2.2 Raw map



X Index: 256



Y Index: 256

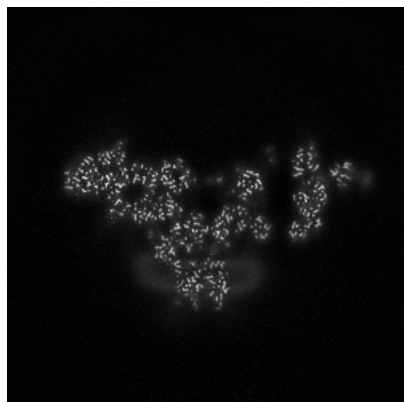


Z Index: 256

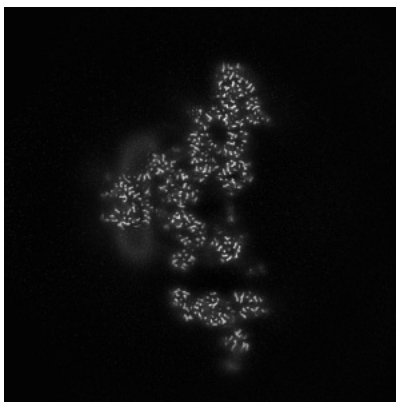
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

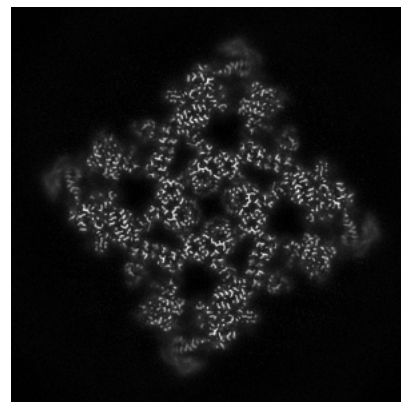
6.3.1 Primary map



X Index: 272

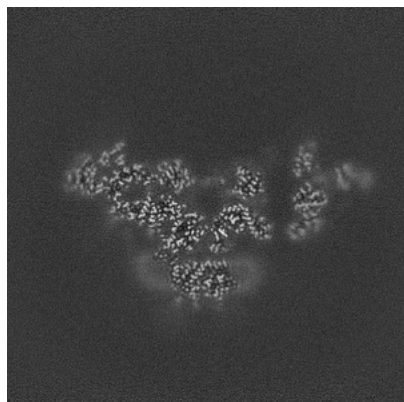


Y Index: 272

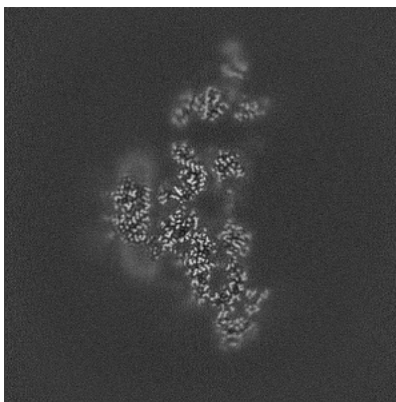


Z Index: 286

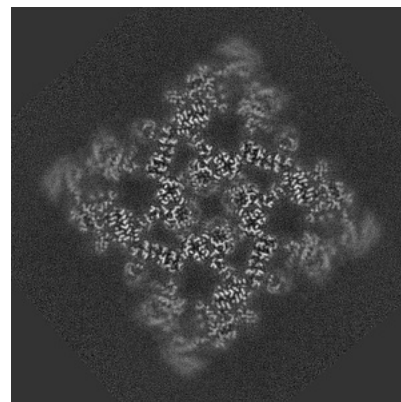
6.3.2 Raw map



X Index: 275



Y Index: 237

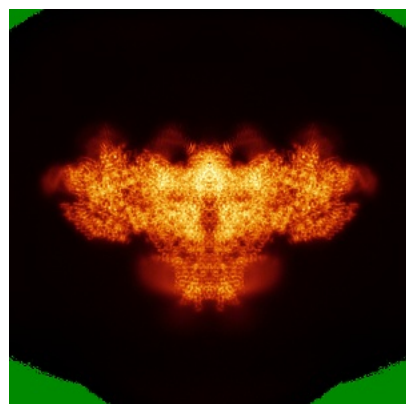


Z Index: 286

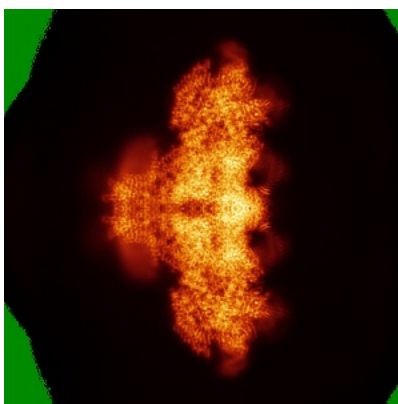
The images above show the largest variance slices of the map in three orthogonal directions.

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

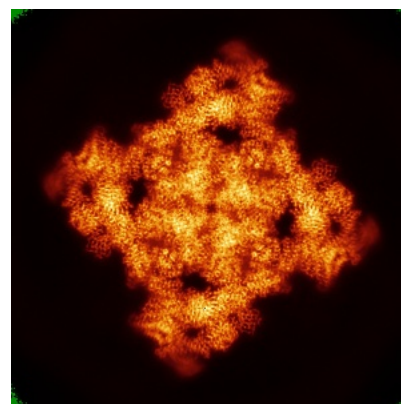
6.4.1 Primary map



X



Y

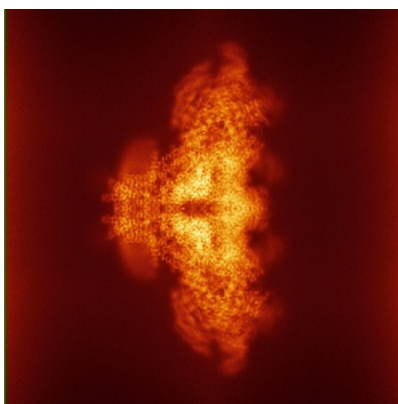


Z

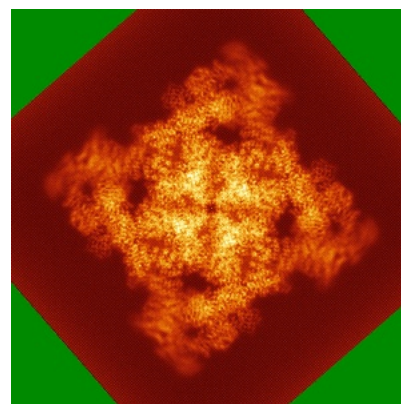
6.4.2 Raw map



X



Y

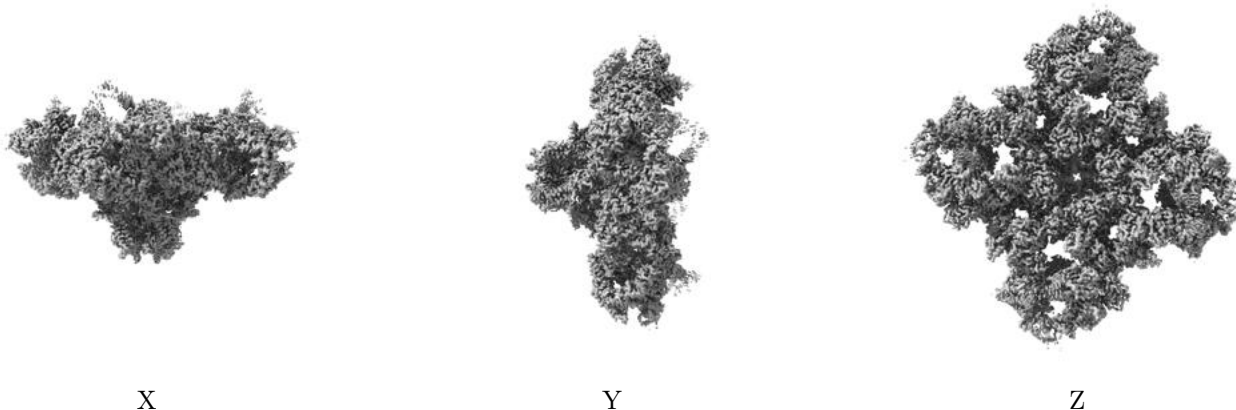


Z

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 0.15. 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.

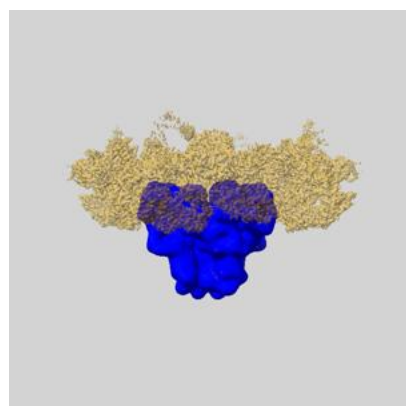
6.6 Mask visualisation [i](#)

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

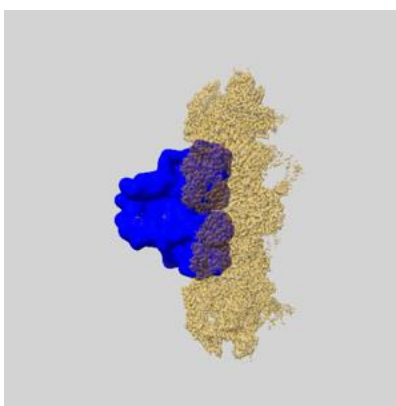
A mask typically either:

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

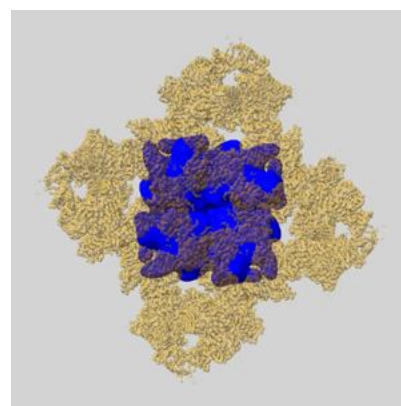
6.6.1 emd_26205_msk_1.map [i](#)



X

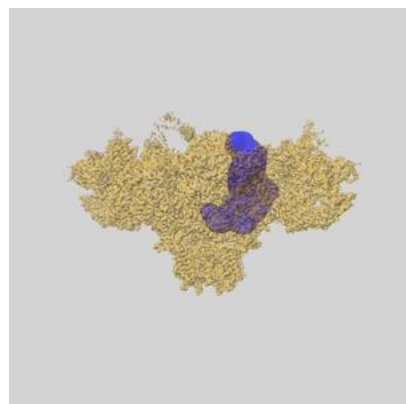


Y

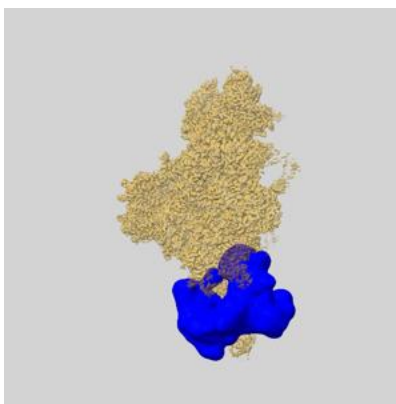


Z

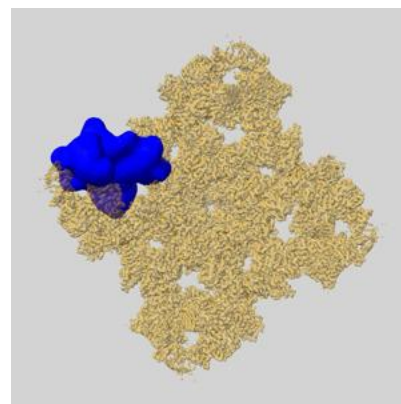
6.6.2 emd_26205_msk_2.map [i](#)



X

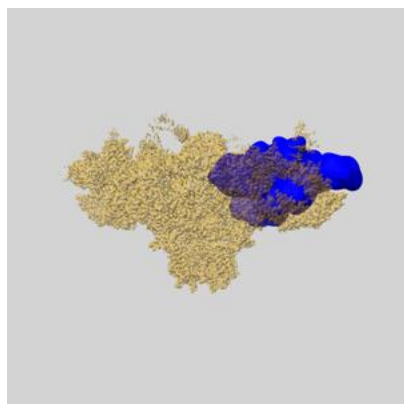


Y

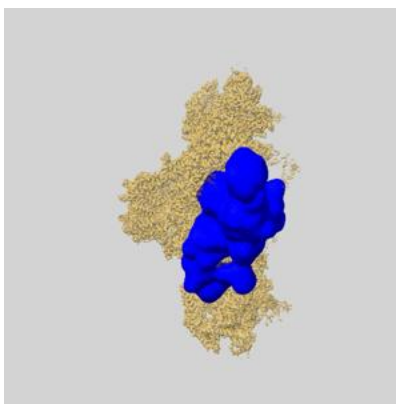


Z

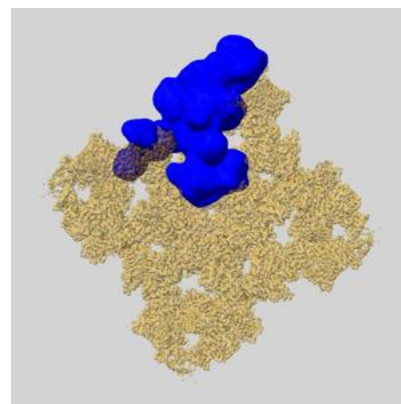
6.6.3 emd_26205_msk_3.map [i](#)



X



Y

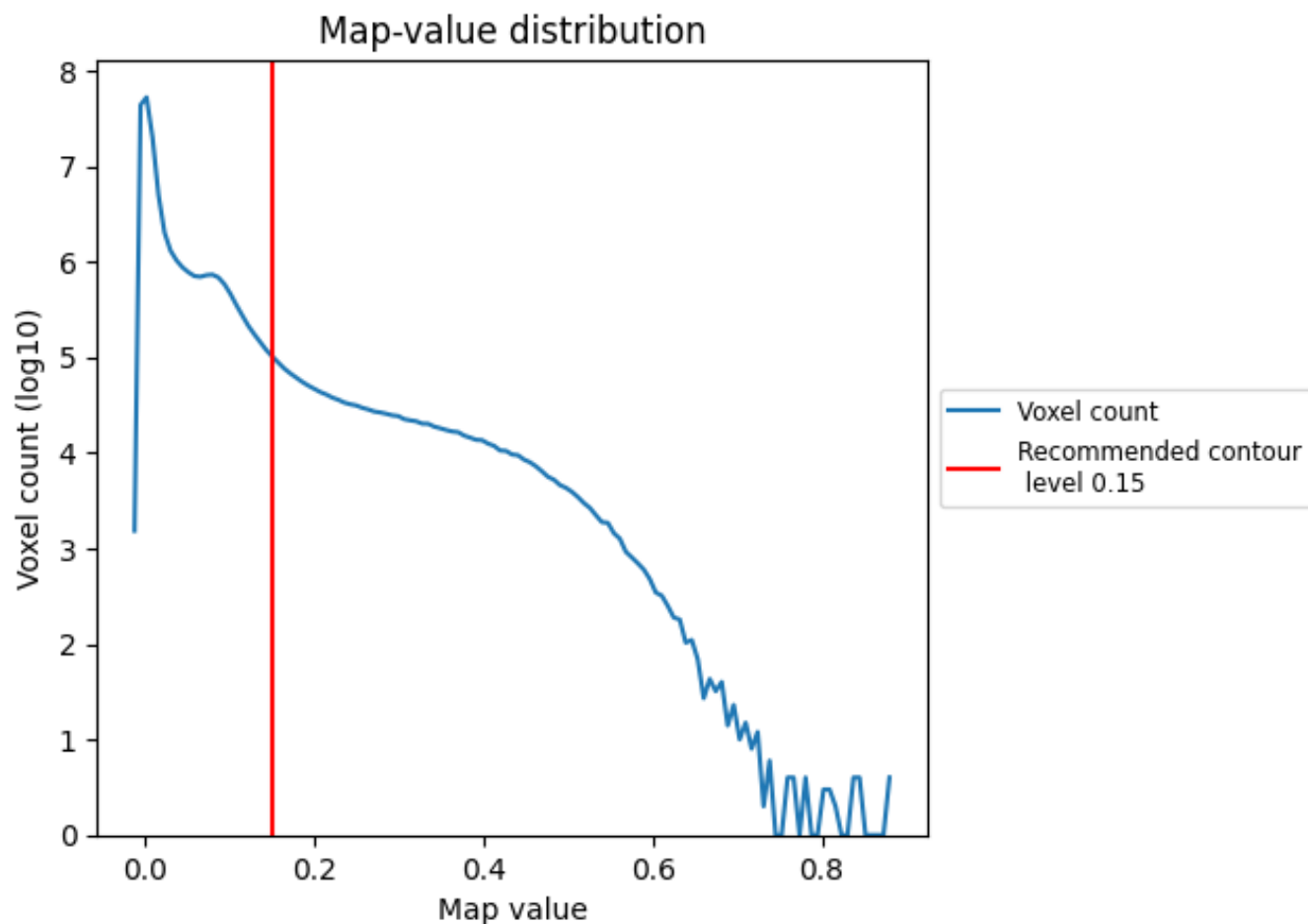


Z

7 Map analysis [i](#)

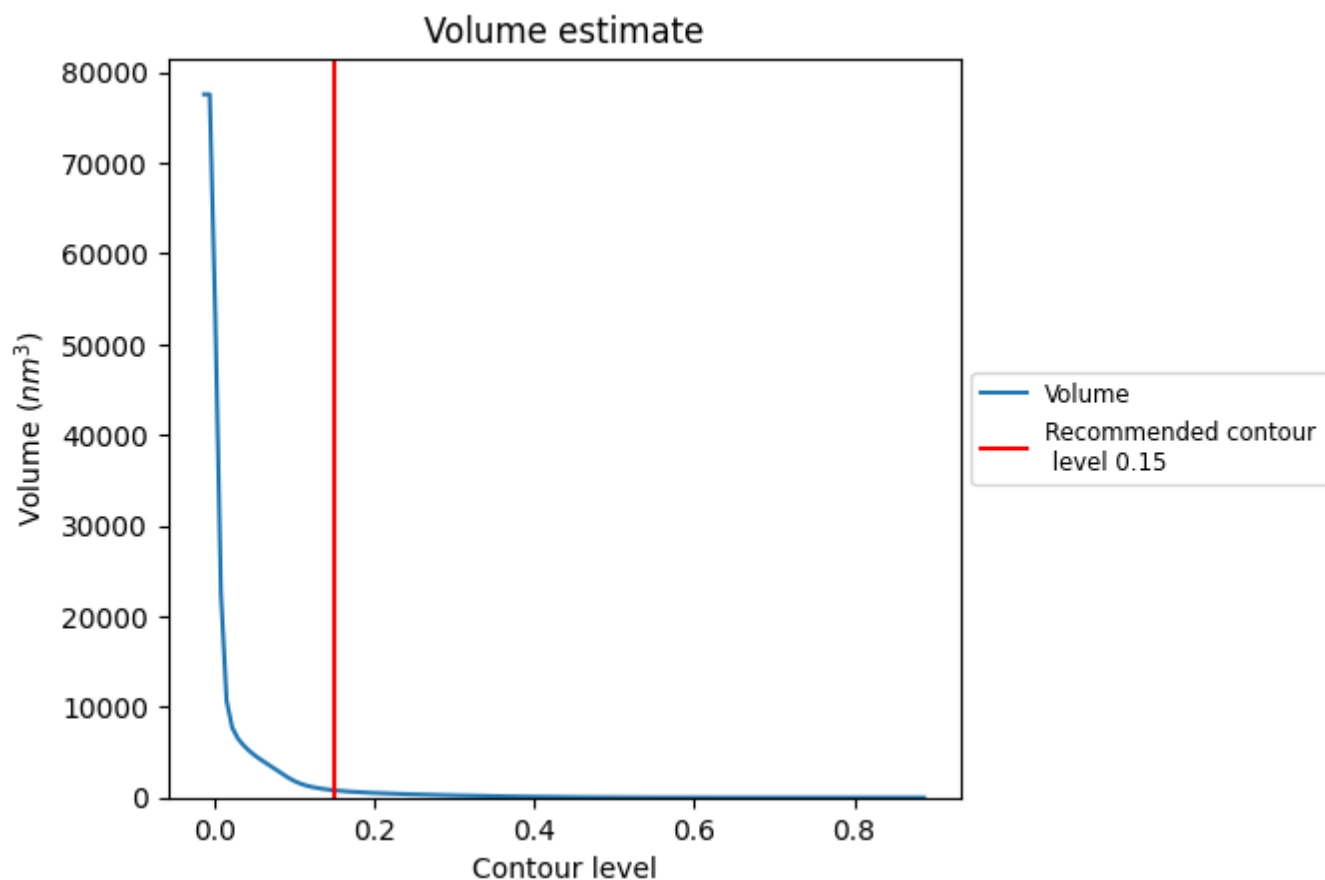
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

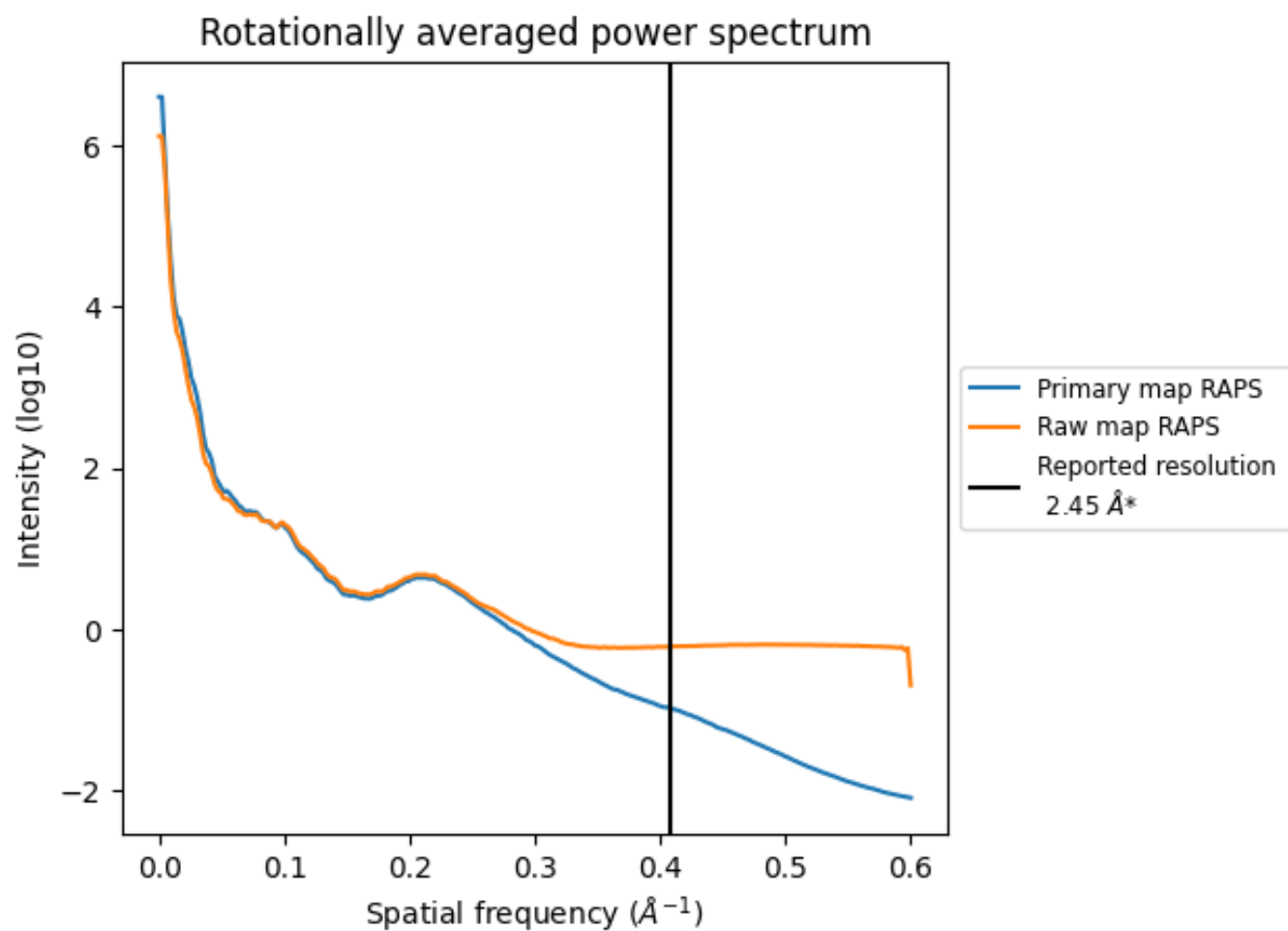
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 800 nm³; this corresponds to an approximate mass of 723 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 ⓘ

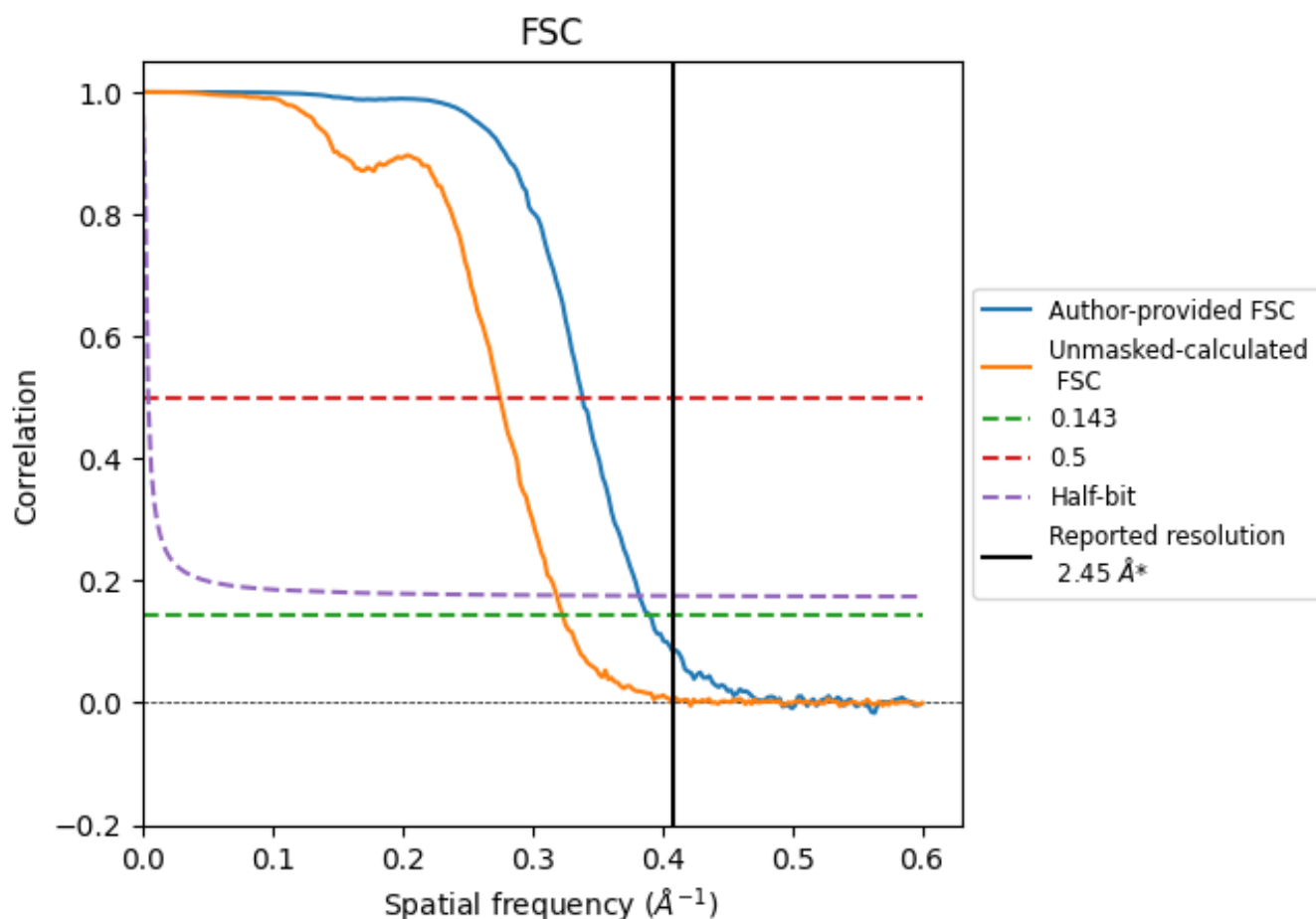


*Reported resolution corresponds to spatial frequency of 0.408 $\text{\AA}^{-1}$

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 0.408 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

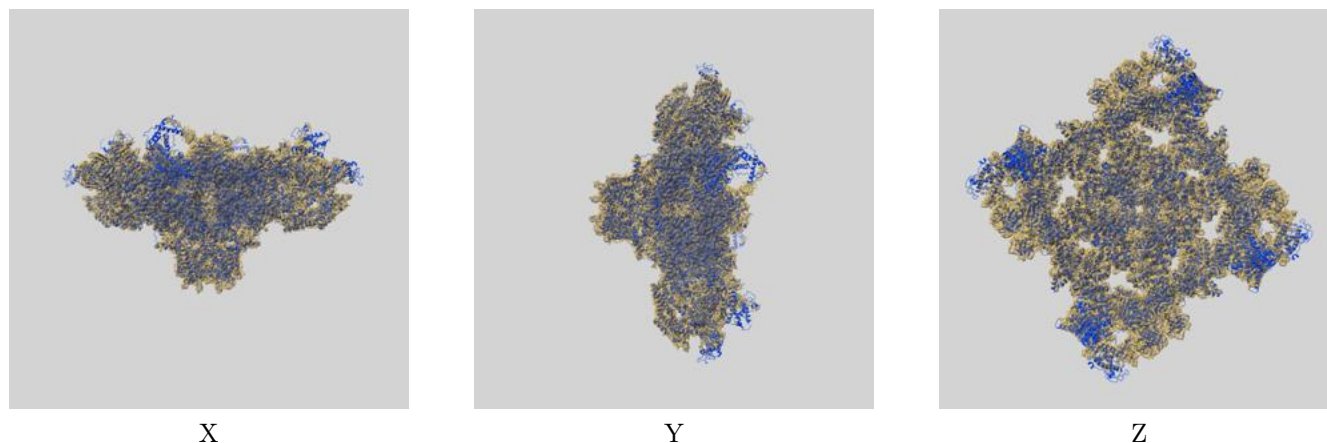
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.56	2.95	2.62
Unmasked-calculated*	3.09	3.63	3.14

*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 3.09 differs from the reported value 2.45 by more than 10 %

9 Map-model fit [i](#)

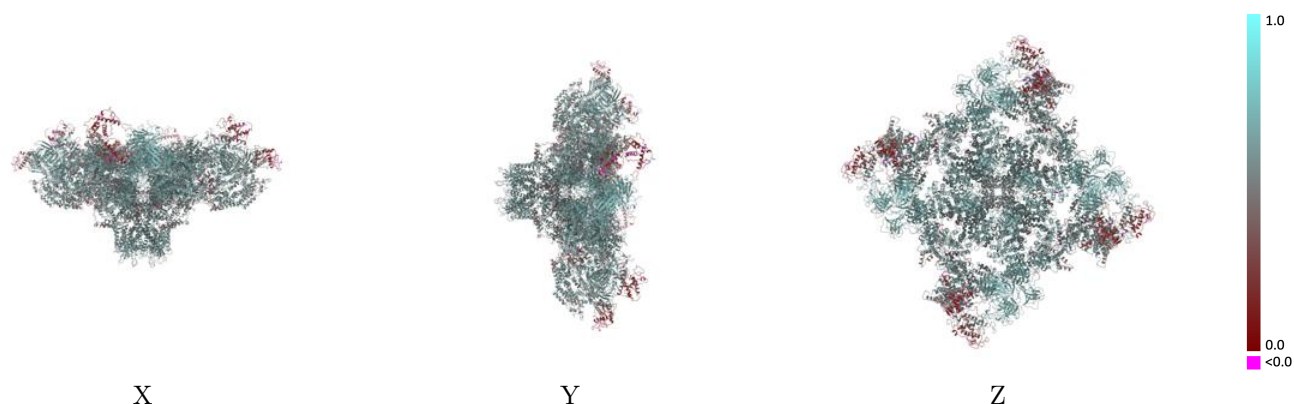
This section contains information regarding the fit between EMDB map EMD-26205 and PDB model 7TZC. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



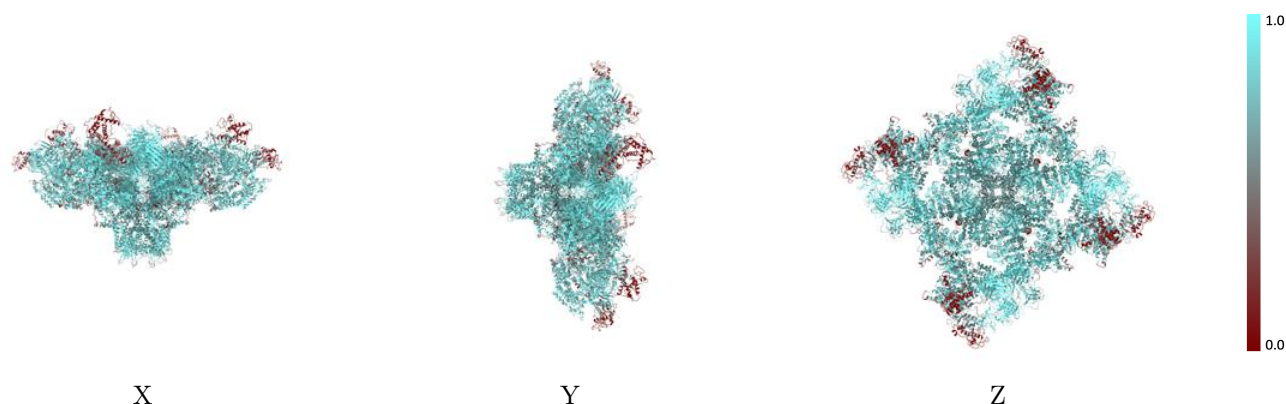
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



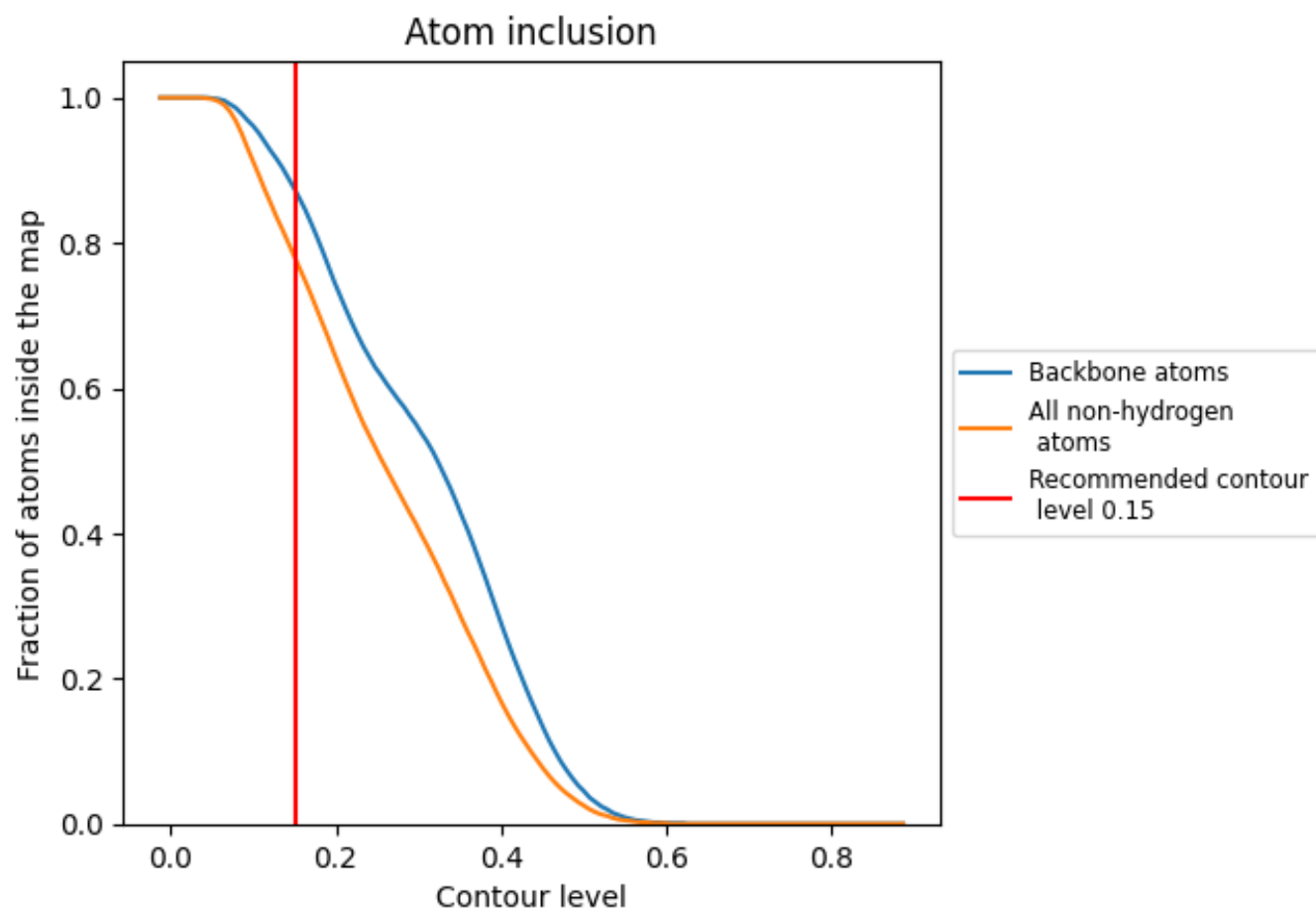
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7810	0.5400
A	0.7900	0.5430
B	0.7890	0.5400
C	0.5240	0.4370
D	0.5310	0.4320
E	0.5310	0.4390
F	0.8040	0.6020
G	0.7890	0.5410
H	0.7930	0.6020
I	0.7890	0.5420
J	0.7890	0.6020
K	0.5280	0.4400
O	0.8020	0.6030

