



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 07:22 AM UTC

PDB ID : 8Y40 / pdb_00008y40
EMDB ID : EMD-38908
Title : Structure of chimeric RyR-I4657M/G4819E complex with chlorantraniliprole
Authors : Lin, L.; Wang, C.; Wang, W.; Jiang, H.; Yuchi, Z.
Deposited on : 2024-01-29
Resolution : 3.58 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

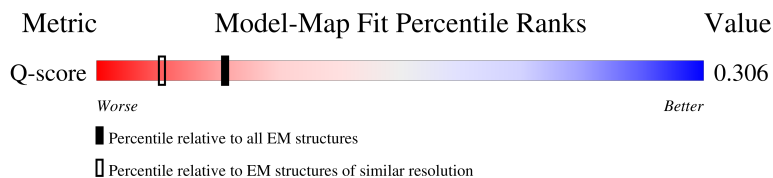
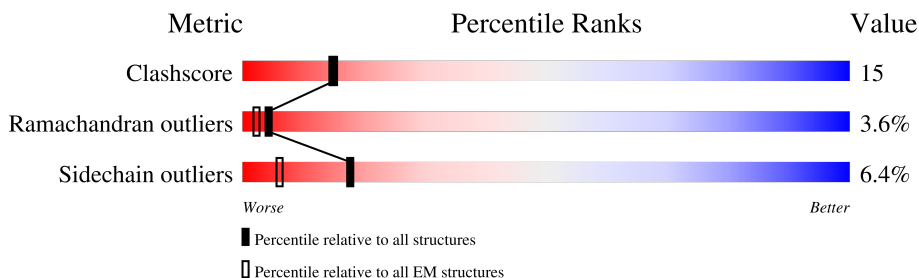
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.58 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	12629 (3.08 - 4.08)

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	E	107	
1	F	107	
1	G	107	
1	H	107	

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Mol	Chain	Length	Quality of chain
2	I	149	
2	J	149	
2	K	149	
2	L	149	
3	A	5037	
3	B	5037	
3	C	5037	
3	D	5037	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 123925 atoms, of which 88 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	H	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	G	107	Total	C	N	O	S	0	0
			804	510	144	146	4		
1	F	107	Total	C	N	O	S	0	0
			804	510	144	146	4		

- Molecule 2 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	139	Total	C	N	O	S	0	0
			1023	633	172	209	9		
2	L	139	Total	C	N	O	S	0	0
			1023	633	172	209	9		
2	K	139	Total	C	N	O	S	0	0
			1023	633	172	209	9		
2	J	139	Total	C	N	O	S	0	0
			1023	633	172	209	9		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23
K	32	ALA	GLU	engineered mutation	UNP P0DP23

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Chain	Residue	Modelled	Actual	Comment	Reference
K	68	ALA	GLU	engineered mutation	UNP P0DP23
K	105	ALA	GLU	engineered mutation	UNP P0DP23
K	141	ALA	GLU	engineered mutation	UNP P0DP23
J	32	ALA	GLU	engineered mutation	UNP P0DP23
J	68	ALA	GLU	engineered mutation	UNP P0DP23
J	105	ALA	GLU	engineered mutation	UNP P0DP23
J	141	ALA	GLU	engineered mutation	UNP P0DP23

- Molecule 3 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	4121	Total	C	N	O	S	0	0
			29056	18435	5131	5332	158		
3	B	4121	Total	C	N	O	S	0	0
			29059	18438	5131	5332	158		
3	C	4121	Total	C	N	O	S	0	0
			29059	18438	5131	5332	158		
3	D	4121	Total	C	N	O	S	0	0
			29055	18436	5131	5330	158		

There are 20 discrepancies between the modelled and reference sequences:

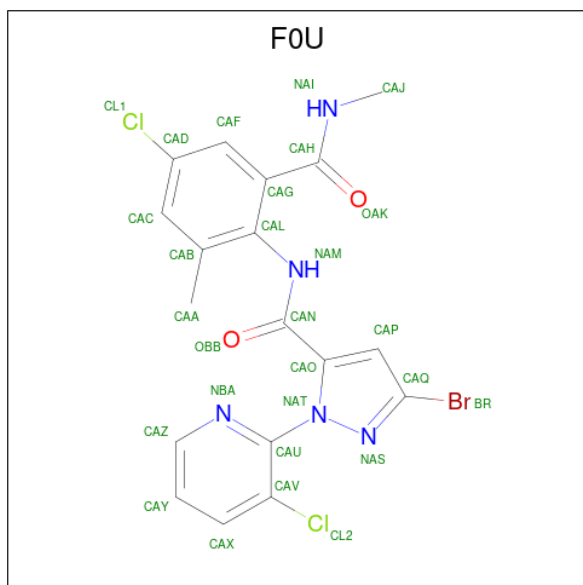
Chain	Residue	Modelled	Actual	Comment	Reference
A	4563	LYS	ARG	engineered mutation	UNP P11716
A	4564	TYR	PHE	engineered mutation	UNP P11716
A	4657	MET	CYS	engineered mutation	UNP P11716
A	4792	SER	LEU	engineered mutation	UNP P11716
A	4819	GLU	GLY	engineered mutation	UNP P11716
B	4563	LYS	ARG	engineered mutation	UNP P11716
B	4564	TYR	PHE	engineered mutation	UNP P11716
B	4657	MET	CYS	engineered mutation	UNP P11716
B	4792	SER	LEU	engineered mutation	UNP P11716
B	4819	GLU	GLY	engineered mutation	UNP P11716
C	4563	LYS	ARG	engineered mutation	UNP P11716
C	4564	TYR	PHE	engineered mutation	UNP P11716
C	4657	MET	CYS	engineered mutation	UNP P11716
C	4792	SER	LEU	engineered mutation	UNP P11716
C	4819	GLU	GLY	engineered mutation	UNP P11716
D	4563	LYS	ARG	engineered mutation	UNP P11716
D	4564	TYR	PHE	engineered mutation	UNP P11716
D	4657	MET	CYS	engineered mutation	UNP P11716
D	4792	SER	LEU	engineered mutation	UNP P11716

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Chain	Residue	Modelled	Actual	Comment	Reference
D	4819	GLU	GLY	engineered mutation	UNP P11716

- Molecule 4 is 5-bromanyl-N-[4-chloranyl-2-methyl-6-(methylcarbamoyl)phenyl]-2-(3-chloranypyridin-2-yl)pyrazole-3-carboxamide (CCD ID: F0U) (formula: $C_{18}H_{14}BrCl_2N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
4	A	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
4	B	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
4	C	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	
4	D	1	Total	Br	C	Cl	N	O	0
			28	1	18	2	5	2	

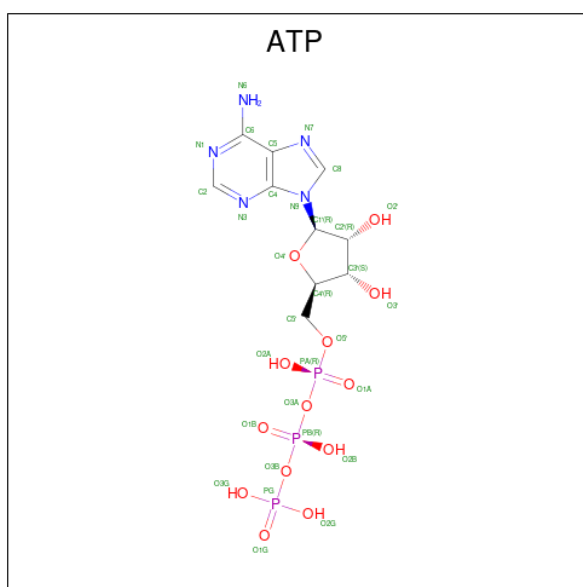
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

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

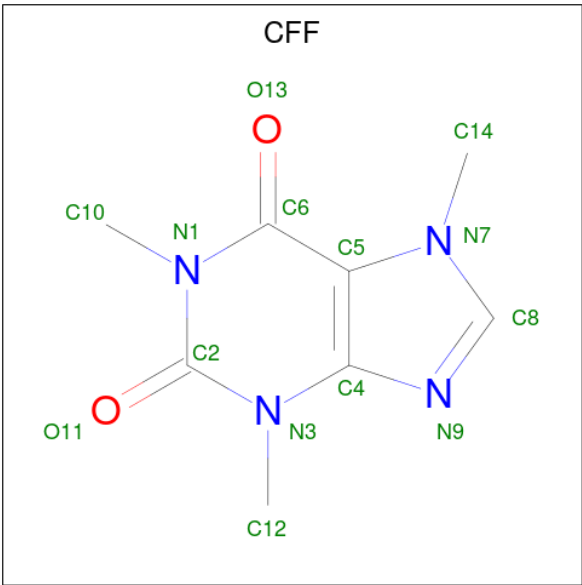
Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total 1	Ca 1	0
6	B	1	Total 1	Ca 1	0
6	C	1	Total 1	Ca 1	0
6	D	1	Total 1	Ca 1	0

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



Mol	Chain	Residues	Atoms						AltConf
7	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	C	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
7	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

- Molecule 8 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂) (labeled as "Ligand of Interest" by depositor).

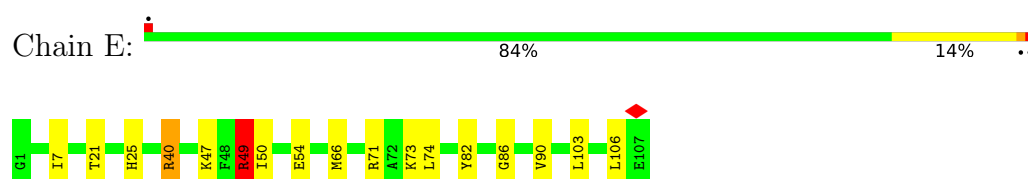


Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	H	N	O	0
			24	8	10	4	2	
8	B	1	Total	C	H	N	O	0
			24	8	10	4	2	
8	C	1	Total	C	H	N	O	0
			24	8	10	4	2	
8	D	1	Total	C	H	N	O	0
			24	8	10	4	2	

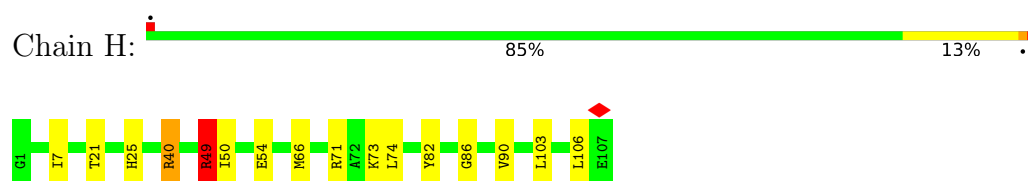
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

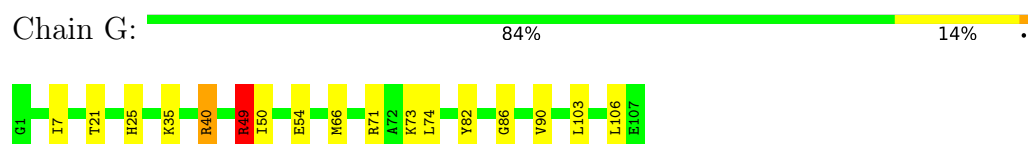
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



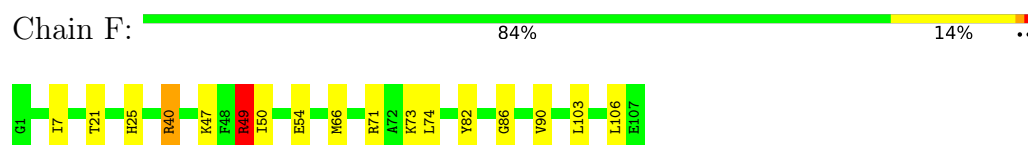
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



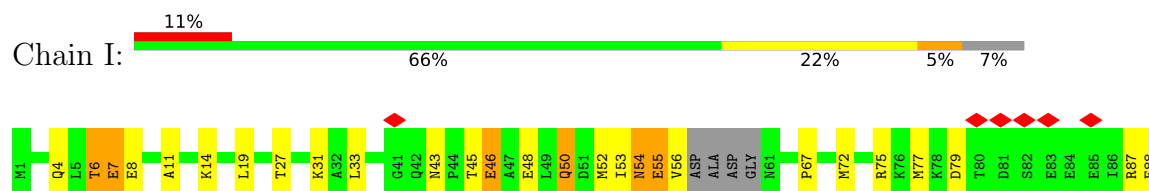
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Calmodulin-1

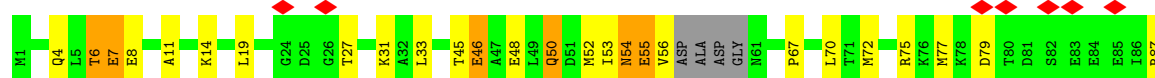




• Molecule 2: Calmodulin-1



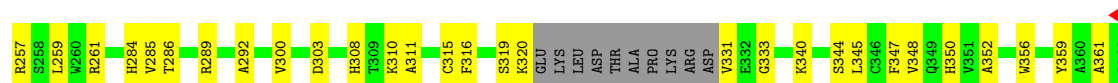
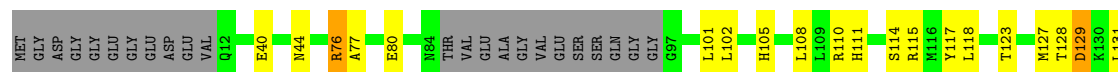
• Molecule 2: Calmodulin-1



• Molecule 2: Calmodulin-1



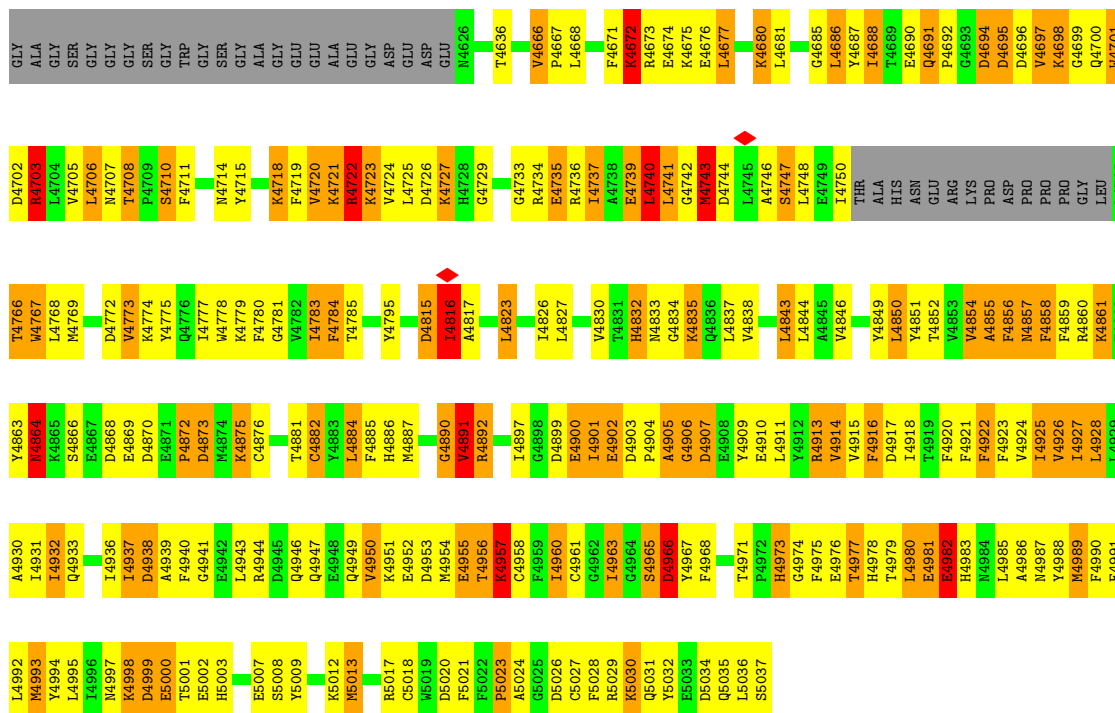
• Molecule 3: Ryanodine receptor 1



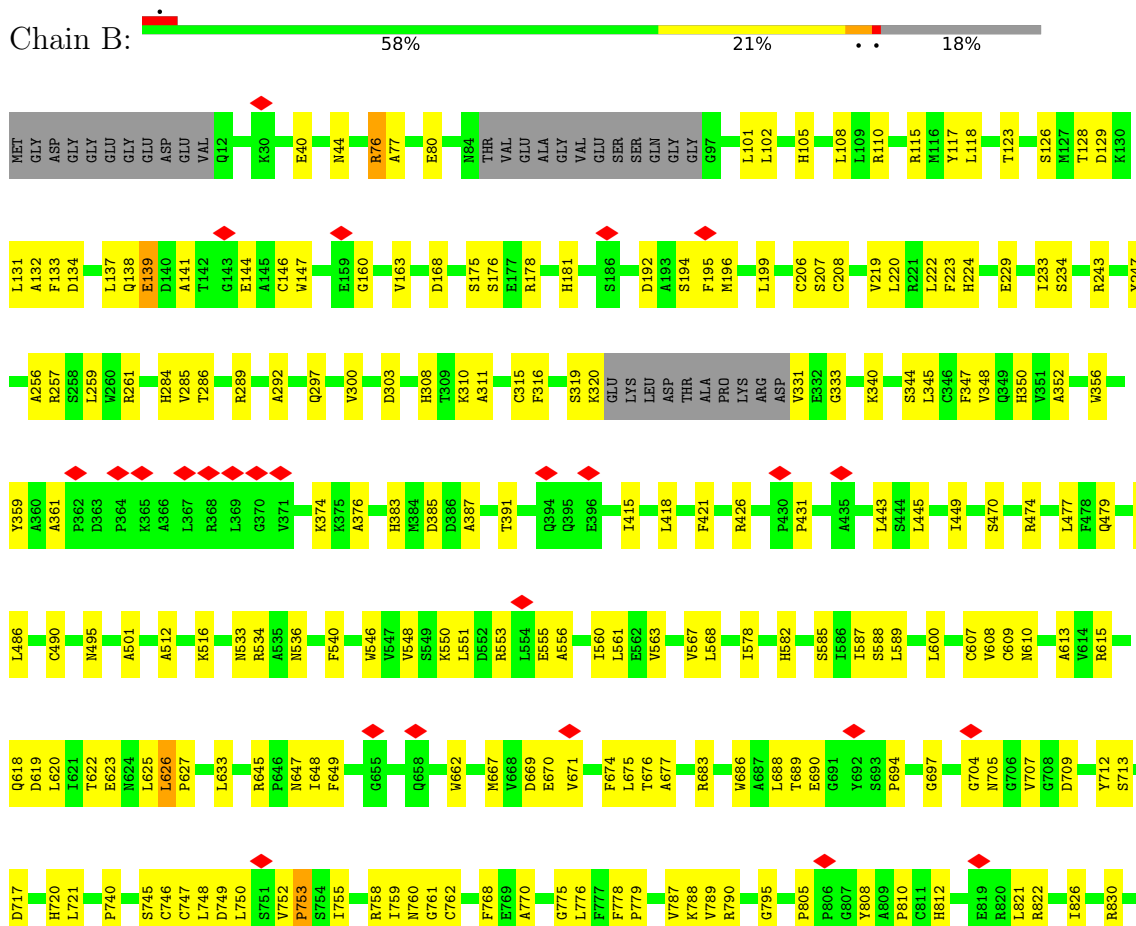


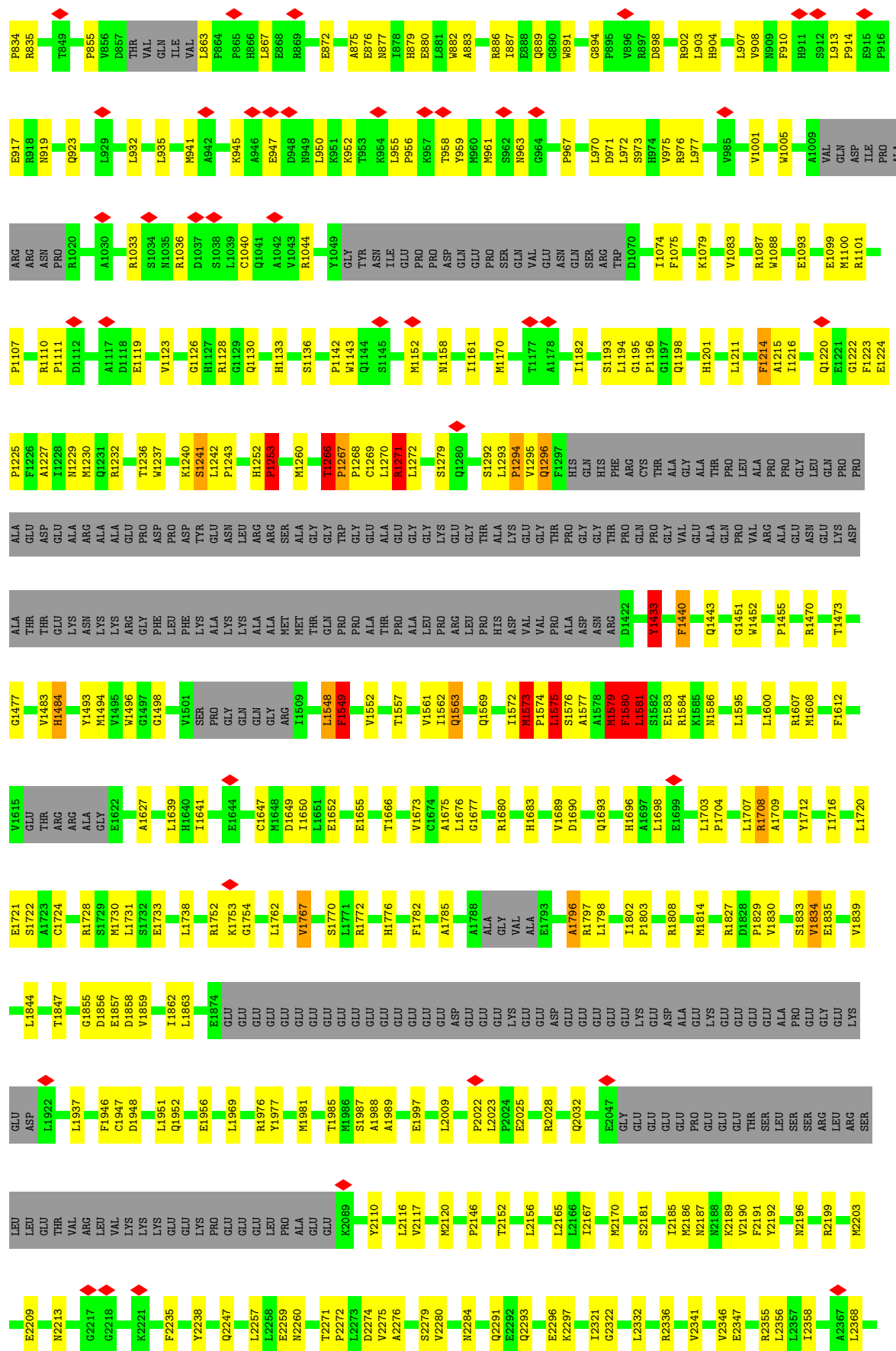






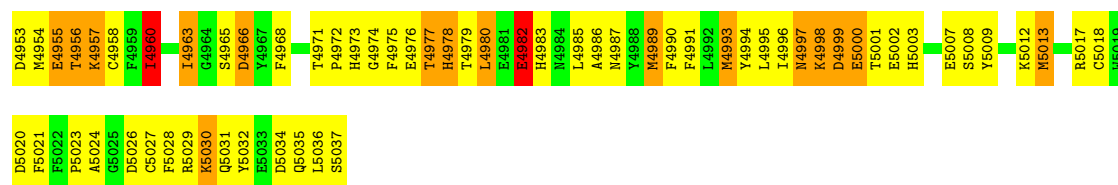
- Molecule 3: Ryanodine receptor 1



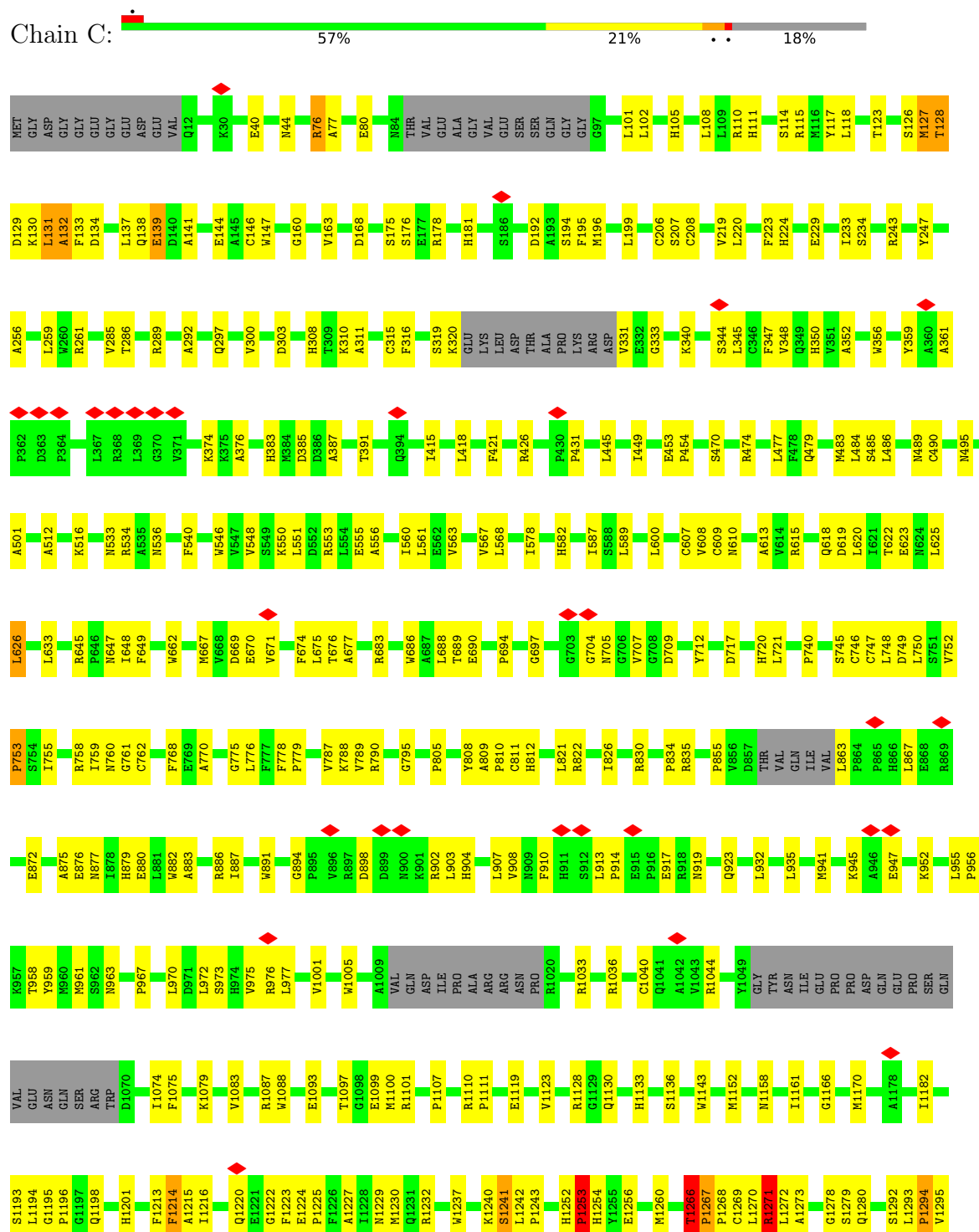






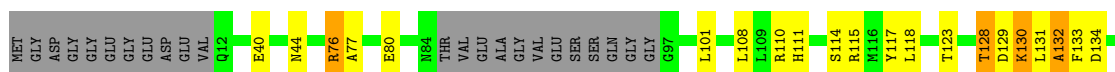


• Molecule 3: Ryanodine receptor 1











L1703	P1704	L1707	P1829	A1709	Y1712	I1716	L1720	E1721	S1722	A1723	C1724	R1728	S1729	M1730	L1731	S1732	E1733	L1738	R1752	K1753	G1754	L1762	V1767	S1770	L1771	R1772	H1776	F1782	A1785	A1788	ALA	GLY	VAL	ALA	E1793	A1796	R1797	L1798	I1802	P1803	R1808														
M1814	R1827	D1828	V1830	S1833	V1834	E1835	V1839	L1844	T1847	G1855	D1856	E1857	D1858	V1859	I1862	L1863	E1874	GLU	GLU	K1753	G1754	L1762	V1767	S1770	L1771	R1772	H1776	F1782	A1785	A1788	ALA	GLY	VAL	ALA	E1793	A1796	R1797	L1798	I1802	P1803	R1808														
GLU	LYS	GLU	GLU	GLU	ALA	PRO	GLU	GLY	GLU	L1922	E1923	Q1928	L1937	F1946	C1947	D1948	L1951	Q1952	E1956	L1969	R1976	Y1977	M1981	R1982	T1985	M1986	S1987	A1988	A1989	E1997	L2009	P2022	L2023	E2025	P2024	R2028	Q2032	E2047	GLY	GLU															
GLU	GLU	PRO	GLU	GLU	THR	SER	SER	SER	ARG	LEU	ARG	LEU	THR	VAL	ARG	VAL	LYS	LYS	GLU	LYS	PRO	GLU	GLU	GLU	PRO	ALA	GLU	GLU	Y2110	L2116	V2117	M2120	R2136	R2140	P2146	T2152	R2163	S2164	L2165	L2166															
L2167	V2168	Q2169	M2170	S2181	I2185	M2186	N2187	N2188	K2189	V2190	F2191	Y2192	N2196	R2199	M2203	E2209	N2213	G2218	E2219	T2220	K2221	F2235	Y2238	Q2247	L2257	L2258	E2259	N2260	S2261	G2262	T2271	P2272	L2273	D2274	V2275	A2276	S2279	V2280	N2284	Q2291	E2292	Q2293													
E2296	K2297	I2321	G2322	L2332	R2336	V2341	E2344	S2345	V2346	R2355	L2356	L2357	I2358	L2368	G2372	G2373	S2374	G2375	L2376	L2377	A2378	E2382	I2386	D2393	G2394	P2395	GLY	VAL	ARG	ASP	ARG	ARG	ARG	GLU	HIS	PHE	GLY	GLU	PRO	PRO	GLU	N2414	H2417												
L2429	G2434	R2435	M2440	H2441	L2442	K2447	G2448	E2449	R2452	I2456	S2459	I2470	L2479	GLY	LYS	ASP	GLY	ALA	F2754	LEU	VAL	Q2487	P2488	V2495	P2496	V2509	N2514	P2528	R2531	A2539	T2540	L2559	P2560	L2561	L2562	A2566	P2567	Y2587	V2602	L2603	E2604														
P2616	S2617	M2618	L2622	R2625	V2629	V2630	P2631	P2640	T2645	V2648	E2649	R2650	P2658	V2666	H2668	K2669	D2692	L2695	Y2696	A2699	M2700	P2701	C2702	L2703	CYS	ALA	ILE	ALA	GLY	ALA	LEU	PRO	PRO	ASP	TYR	VAL	ASP	ALA	TYR	SER	LYS	ALA	GLY	LYS											
ALA	THR	VAL	ASP	ALA	GLY	ASN	PHE	ASP	PRO	ARG	VAL	GLU	THR	ASN	VAL	ILE	ILE	PRO	GLU	LYS	L2751	D2752	S2753	F2754	I2755	K2757	F2758	A2759	E2760	H2763	E2764	K2765	C2766	A2767	K2770	I2771	Q2772	W2775	S2776	Y2777	G2778	E2779	N2780	V2781	D2782	E2783	K2786	T2787	H2788	P2789	M2790				
L2791	K2794	K2795	L2796	F2797	S2798	E2799	K2800	D2801	K2802	E2803	R2806	W2807	K2810	S2811	L2813	A2814	N2815	L2816	I2817	A2818	W2819	TRP	THR	ILE	LYS	ALA	ARG	GLU	GLY	GLU	GLU	GLU	THR	LYS	LYS	LYS	THR	ARG	LYS	ILE	GLN	ALA	GLN	THR	TYR	ASP	PRO	ARG	GLU						
GLY	Y2855	N2856	P2857	Q2858	P2859	P2860	D2861	L2862	G2863	G2864	V2865	T2866	L2867	S2868	R2869	E2870	L2871	Q2872	A2873	M2874	A2875	E2876	Q2877	L2878	A2879	E2880	H2883	N2884	G2887	R2888	K2889	K2890	K2891	Q2892	E2893	L2894	E2895	A2896	K2897	G2898	G2899	Q2900	T2901	H2902	V2903	V2906	P2907	G2908	D2909	A2913	K2916	A2917	R2920		
E2921	E2925	L2926	L2927	K2928	F2929	Q2931	L2930	L2932	N2933	G2934	Y2935	A2936	V2937	T2938	H2939	GLY	LEU	LYS	ASP	MET	L2946	D2947	S2950	I2951	F2952	K2953	A2956	F2957	G2958	F2959	L2960	L2963	L2964	R2965	W2966	S2970	I2974	A2975	H2976	LEU	GLU	ALA	ILE	VAL	VAL	SER	SER	GLY	GLU	ILE	VAL	SER	GLY	LEU	ARG
PRO	HIS	GLN	GLU	L2995	L3003	P3004	Q3008	Y3009	F3010	G3014	L3015	T3020	P3021	K3036	T3039	T3040	S3041	C3044	P3062	A3063	VAL	VAL	ASN	CYS	LEU	HIS	ILE	LEU	ALA	ARG	SER	LEU	ASP	ALA	ARG	THR	VAL	LYS	LYS	PRO	GLU	ILE	VAL	VAL	SER	ALA	GLY	LEU	ARG						



V5019	D4953	V4891	L4823	H4728	N4626	PRO	GLU
D5020	M4954	R4892	R4824	G4729	T4636	ALA	GLY
F5021	E4955					LYS	GLY
F5022	T4956	G4895	L4827	G4733	P4666	GLY	GLY
A5024	C4958	I4897	H4832	R4734	P4667	PRO	ILE
G5025	F4859	G4898	M4833	R4736	L4668	ALA	LEU
D5026	I4860	D4899	G4834	T4737		LYS	ASP
C5027	C4961	E4900	K4835	A4738	F4671	ALA	ALA
F5028	G4962	I4901	K4836	E4739	K4672	ARG	ALA
R5029	I4963	E4902	L4837	L4740	R4673	GLY	GLY
K5030	G4964	D4903	V4838	L4741	E4674	LEU	GLY
Q5031	S4965	P4904	V4839	G4742	K4675	GLY	ASP
Y5032	D4866	A4905	T4840	H4743	E4676	VAL	GLY
E5033	Y4967	G4906		D4744	L4677	ASP	ASP
D5034	F4968	D4907	L4843	L4745	P4541	GLY	GLY
Q5035		E4908	L4844	L4746	R4548	GLU	GLU
L5036		E4910		A4747	K4680	VAL	ALA
S5037		E4911	V4847	S4747	L4681	GLY	GLY
		L4912	V4848	L4750	G4685	LEU	HIS
	H4973	R4913	Y4849	THR	L4686	VAL	GLU
	G4974	R4914	Y4850	ALA	P4586	GLY	ALA
	E4975	V4915	Y4851	ALA	P4587	PRO	GLY
	E4976	V4916	T4852	ASN	GLY	PRO	PRO
	T4977	F4917	V4853	HIS	T4689	GLY	GLY
	H4978	D4918	V4854	ARG	E4690	ASP	GLY
	T4979	T4919	V4855	GLY	Q4691	PRO	GLY
	L4980	T4920	F4856	LYS	P4692	GLU	ALA
	E4981	F4921	F4857	PRO	G4693	GLU	ALA
	E4982	F4922	F4858	ASP	D4694	GLY	GLU
	H4983	F4923	F4859	PRO	D4695	VAL	VAL
	M4984	F4924	F4860	PRO	D4696	VAL	VAL
	L4985	V4925	K4861	PRO	V4697	ALA	ALA
	A4986	V4926	F4862	GLY	K4698	VAL	VAL
	N4987	V4927	Y4863	LEU	G4699	GLY	GLY
	Y4988	I4928	Y4864	T4765	Q4700	ASP	ALA
	M4989	L4928	R4865	T4766	W4701	ALA	ALA
	F4990	L4929	S4866	V4767	D4702	GLY	GLY
	F4991	A4930	E4867	L4768	P4703	GLY	PRO
	L4992	I4931	G4868	M4769	L4704	ASN	PHE
	Y4994	I4932	E4869		V4705	GLY	ARG
	L4995	Q4933	E4870		L4706	GLY	PRO
	I4996		D4871		N4707	LYS	GLY
	N4997		P4872	D4772	T4708	GLY	GLY
	K4998	I4937	D4873	V4773	P4709	ALA	ALA
	D4999	D4938	P4874	Y4775	S4710	VAL	GLY
	E5000	A4939	K4875	Q4776	P4711	PRO	GLY
	T5001	F4940	C4876	I4777		GLY	LEU
	E5002	G4941	D4877	W4778	N4714	ALA	GLY
	H5003	E4942	D4878	K4779	Y4715	GLY	ASP
		L4943		F4780	K4718	ALA	MET
		R4944		G4781		GLY	GLY
	E5007	D4945	T4881	V4782	F4719	PRO	ASP
	S5008	Q4946	C4882	I4783	V4720	GLU	PRO
	Y5009	Q4947	Y4883	F4784	K4721	ALA	THR
		Q4948	L4884		GLY	LYS	LYS
	K5012	E4948	F4885	Y4795	R4722	GLY	PRO
	M5013	Q4949	H4886		K4723	ALA	ALA
		V4950	M4887	D4815	V4724	ASP	GLU
	R5017	K4951		I4816	L4725	GLU	PRO
	C5018	E4952		A4817	D4726	ASP	PRO
					K4727	GLU	THR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68897	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)	1200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.459	Depositor
Minimum map value	-0.261	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.27	0/820	0.66	1/1105 (0.1%)
1	F	0.27	0/820	0.66	1/1105 (0.1%)
1	G	0.27	0/820	0.66	1/1105 (0.1%)
1	H	0.27	0/820	0.66	1/1105 (0.1%)
2	I	0.33	0/1032	0.83	2/1392 (0.1%)
2	J	0.34	0/1032	0.83	2/1392 (0.1%)
2	K	0.34	0/1032	0.83	2/1392 (0.1%)
2	L	0.34	0/1032	0.83	2/1392 (0.1%)
3	A	0.48	52/29618 (0.2%)	0.72	98/40398 (0.2%)
3	B	0.49	54/29621 (0.2%)	0.72	101/40402 (0.2%)
3	C	0.49	53/29621 (0.2%)	0.72	102/40402 (0.3%)
3	D	0.48	54/29617 (0.2%)	0.72	98/40397 (0.2%)
All	All	0.48	213/125885 (0.2%)	0.72	411/171587 (0.2%)

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
3	A	0	5
3	B	0	6
3	C	0	5
3	D	0	5
All	All	0	21

The worst 5 of 213 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	76	ARG	CA-C	-15.46	1.32	1.52
3	B	76	ARG	CA-C	-15.43	1.32	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	76	ARG	CA-C	-15.40	1.32	1.52
3	C	76	ARG	CA-C	-15.40	1.33	1.52
3	A	3932	ASP	C-O	-11.56	1.09	1.23

The worst 5 of 411 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1267	PRO	CA-C-N	13.93	137.26	119.84
3	A	1267	PRO	C-N-CA	13.93	137.26	119.84
3	D	1267	PRO	CA-C-N	13.93	137.25	119.84
3	D	1267	PRO	C-N-CA	13.93	137.25	119.84
3	C	1267	PRO	CA-C-N	13.93	137.25	119.84

There are no chirality outliers.

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	1292	SER	Mainchain
3	A	139	GLU	Peptide
3	A	1796	ALA	Peptide
3	A	4795	TYR	Sidechain
3	A	752	VAL	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	E	804	0	812	10	0
1	F	804	0	812	10	0
1	G	804	0	812	11	0
1	H	804	0	812	9	0
2	I	1023	0	941	21	0
2	J	1023	0	941	21	0
2	K	1023	0	941	20	0
2	L	1023	0	941	21	0
3	A	29056	0	25582	871	0
3	B	29059	0	25591	883	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	29059	0	25591	910	0
3	D	29055	0	25587	866	0
4	A	28	0	0	0	0
4	B	28	0	0	0	0
4	C	28	0	0	2	0
4	D	28	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	A	31	12	12	3	0
7	B	31	12	12	3	0
7	C	31	12	12	3	0
7	D	31	12	12	2	0
8	A	14	10	10	1	0
8	B	14	10	10	3	0
8	C	14	10	10	0	0
8	D	14	10	10	0	0
All	All	123837	88	109451	3499	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 15.

The worst 5 of 3499 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:C:4820:VAL:HB	4:C:5101:F0U:BR	1.67	1.49
3:B:1271:ARG:HB2	3:B:1271:ARG:HH11	1.22	1.03
3:A:1271:ARG:HB2	3:A:1271:ARG:HH11	1.22	1.02
3:C:4820:VAL:CB	4:C:5101:F0U:BR	2.63	1.01
3:C:1271:ARG:HH11	3:C:1271:ARG:HB2	1.22	1.01

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
1	F	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
1	G	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
1	H	105/107 (98%)	98 (93%)	7 (7%)	0	100	100
2	I	133/149 (89%)	133 (100%)	0	0	100	100
2	J	133/149 (89%)	133 (100%)	0	0	100	100
2	K	133/149 (89%)	133 (100%)	0	0	100	100
2	L	133/149 (89%)	133 (100%)	0	0	100	100
3	A	4065/5037 (81%)	3275 (81%)	637 (16%)	153 (4%)	2	21
3	B	4065/5037 (81%)	3273 (80%)	636 (16%)	156 (4%)	2	21
3	C	4065/5037 (81%)	3259 (80%)	647 (16%)	159 (4%)	2	20
3	D	4065/5037 (81%)	3277 (81%)	637 (16%)	151 (4%)	2	21
All	All	17212/21172 (81%)	14008 (81%)	2585 (15%)	619 (4%)	4	22

5 of 619 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	626	LEU
3	A	1215	ALA
3	A	1241	SER
3	A	1296	GLN
3	A	1581	LEU

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	E	84/88 (96%)	77 (92%)	7 (8%)	10	35
1	F	84/88 (96%)	77 (92%)	7 (8%)	10	35
1	G	84/88 (96%)	77 (92%)	7 (8%)	10	35
1	H	84/88 (96%)	77 (92%)	7 (8%)	10	35
2	I	99/123 (80%)	76 (77%)	23 (23%)	1	6
2	J	99/123 (80%)	76 (77%)	23 (23%)	1	6
2	K	99/123 (80%)	76 (77%)	23 (23%)	1	6
2	L	99/123 (80%)	76 (77%)	23 (23%)	1	6
3	A	2499/4277 (58%)	2359 (94%)	140 (6%)	19	46
3	B	2500/4277 (58%)	2364 (95%)	136 (5%)	20	47
3	C	2500/4277 (58%)	2353 (94%)	147 (6%)	18	45
3	D	2499/4277 (58%)	2359 (94%)	140 (6%)	19	46
All	All	10730/17952 (60%)	10047 (94%)	683 (6%)	18	43

5 of 683 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	4718	LYS
3	D	4087	LEU
3	C	4743	MET
3	C	4714	ASN
3	C	4947	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	4574	ASN
3	D	2772	GLN
3	C	4946	GLN
3	D	536	ASN
3	D	4054	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 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$
8	CFF	A	5105	-	15,15,15	1.66	3 (20%)	23,23,23	1.94	7 (30%)
7	ATP	D	5104	-	32,33,33	1.35	5 (15%)	48,52,52	1.81	11 (22%)
4	F0U	B	5101	-	30,30,30	1.17	3 (10%)	43,43,43	1.73	9 (20%)
8	CFF	C	5105	-	15,15,15	1.64	3 (20%)	23,23,23	1.90	6 (26%)
4	F0U	D	5101	-	30,30,30	1.18	3 (10%)	43,43,43	1.73	9 (20%)
4	F0U	A	5101	-	30,30,30	1.18	3 (10%)	43,43,43	1.73	9 (20%)
7	ATP	C	5104	-	32,33,33	1.36	5 (15%)	48,52,52	1.82	11 (22%)
7	ATP	B	5104	-	32,33,33	1.36	5 (15%)	48,52,52	1.82	11 (22%)
4	F0U	C	5101	-	30,30,30	1.17	3 (10%)	43,43,43	1.73	9 (20%)
7	ATP	A	5104	-	32,33,33	1.36	5 (15%)	48,52,52	1.82	11 (22%)
8	CFF	D	5105	-	15,15,15	1.64	3 (20%)	23,23,23	1.92	6 (26%)
8	CFF	B	5105	-	15,15,15	1.62	3 (20%)	23,23,23	1.89	7 (30%)

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
8	CFF	A	5105	-	-	-	0/2/2/2
7	ATP	D	5104	-	-	2/22/38/38	0/3/3/3
4	F0U	B	5101	-	-	0/18/18/18	0/3/3/3
8	CFF	C	5105	-	-	-	0/2/2/2
4	F0U	D	5101	-	-	0/18/18/18	0/3/3/3
4	F0U	A	5101	-	-	0/18/18/18	0/3/3/3
7	ATP	C	5104	-	-	2/22/38/38	0/3/3/3
7	ATP	B	5104	-	-	2/22/38/38	0/3/3/3
4	F0U	C	5101	-	-	0/18/18/18	0/3/3/3
7	ATP	A	5104	-	-	2/22/38/38	0/3/3/3
8	CFF	D	5105	-	-	-	0/2/2/2
8	CFF	B	5105	-	-	-	0/2/2/2

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	5104	ATP	C5-C4	4.31	1.46	1.39
7	A	5104	ATP	C5-C4	4.30	1.46	1.39
7	B	5104	ATP	C5-C4	4.30	1.46	1.39
7	D	5104	ATP	C5-C4	4.27	1.46	1.39
8	C	5105	CFF	C5-N7	-3.13	1.32	1.38

The worst 5 of 106 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	5104	ATP	C5-C4-N3	-5.44	119.23	126.72
7	A	5104	ATP	C5-C4-N3	-5.43	119.23	126.72
7	D	5104	ATP	C5-C4-N3	-5.43	119.24	126.72
7	B	5104	ATP	C5-C4-N3	-5.42	119.26	126.72
4	A	5101	F0U	CAN-CAO-NAT	5.32	127.76	121.32

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

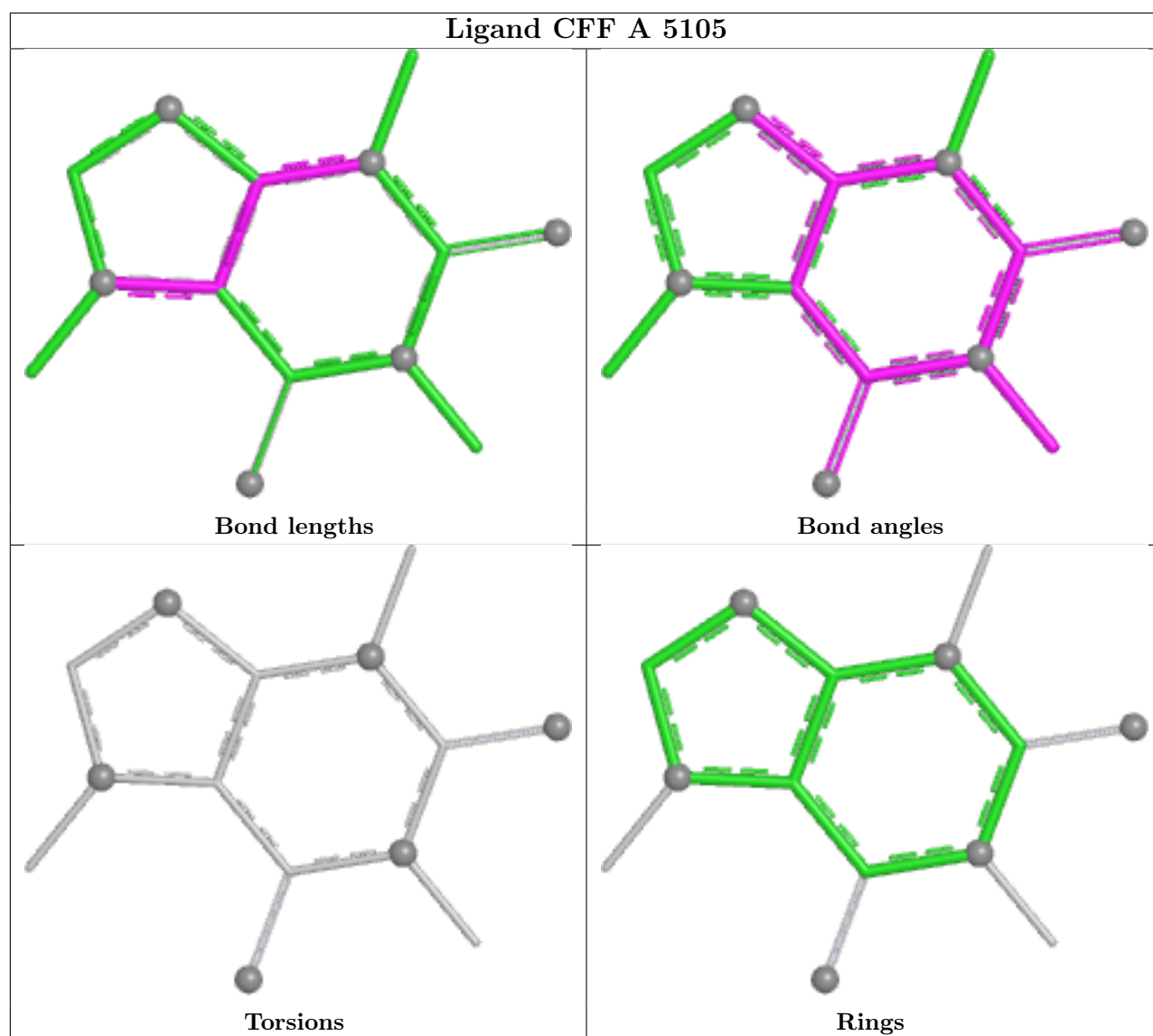
Mol	Chain	Res	Type	Atoms
7	A	5104	ATP	C5'-O5'-PA-O1A
7	B	5104	ATP	C5'-O5'-PA-O1A
7	C	5104	ATP	C5'-O5'-PA-O1A
7	D	5104	ATP	C5'-O5'-PA-O1A
7	A	5104	ATP	C5'-O5'-PA-O3A

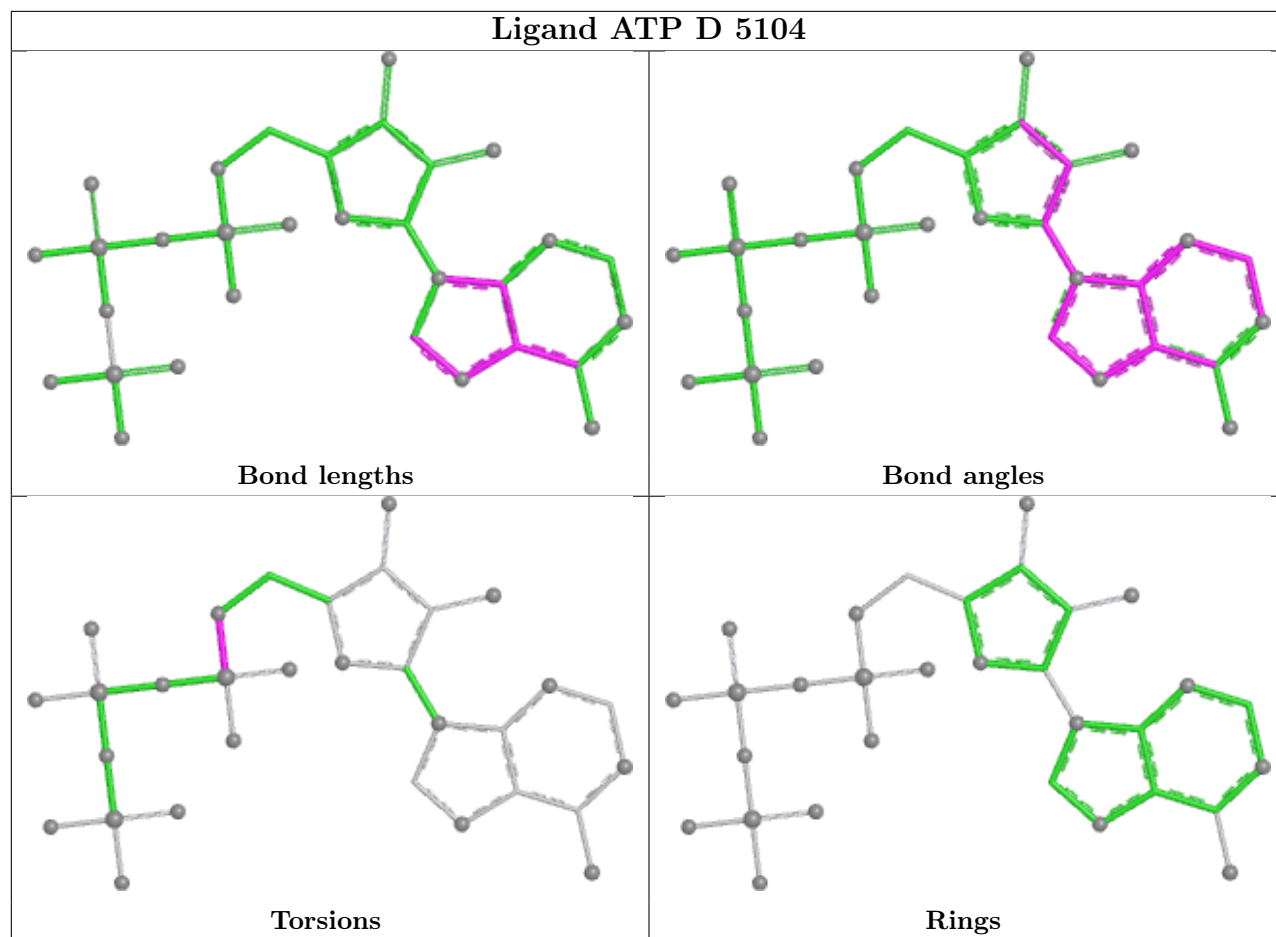
There are no ring outliers.

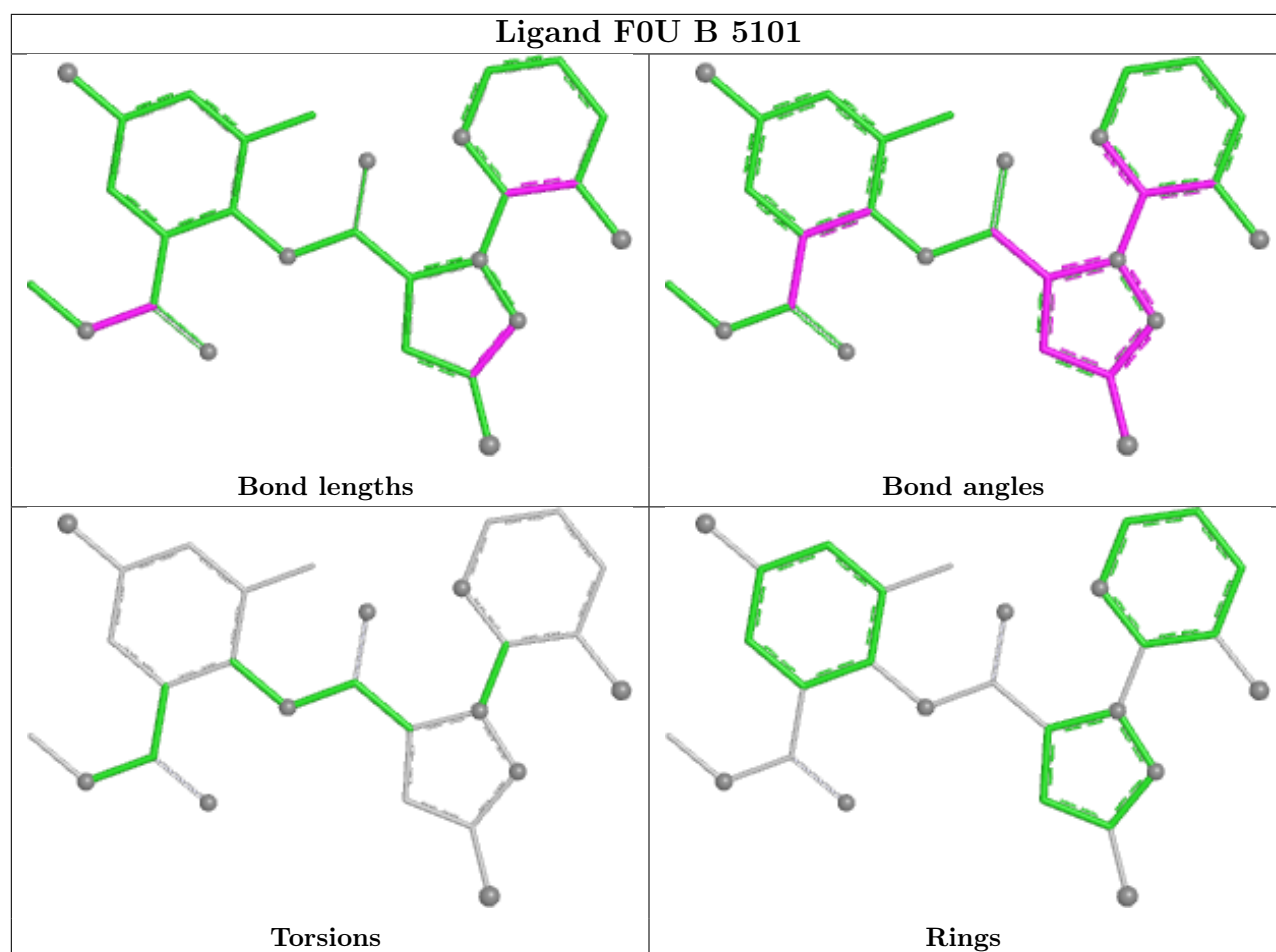
7 monomers are involved in 17 short contacts:

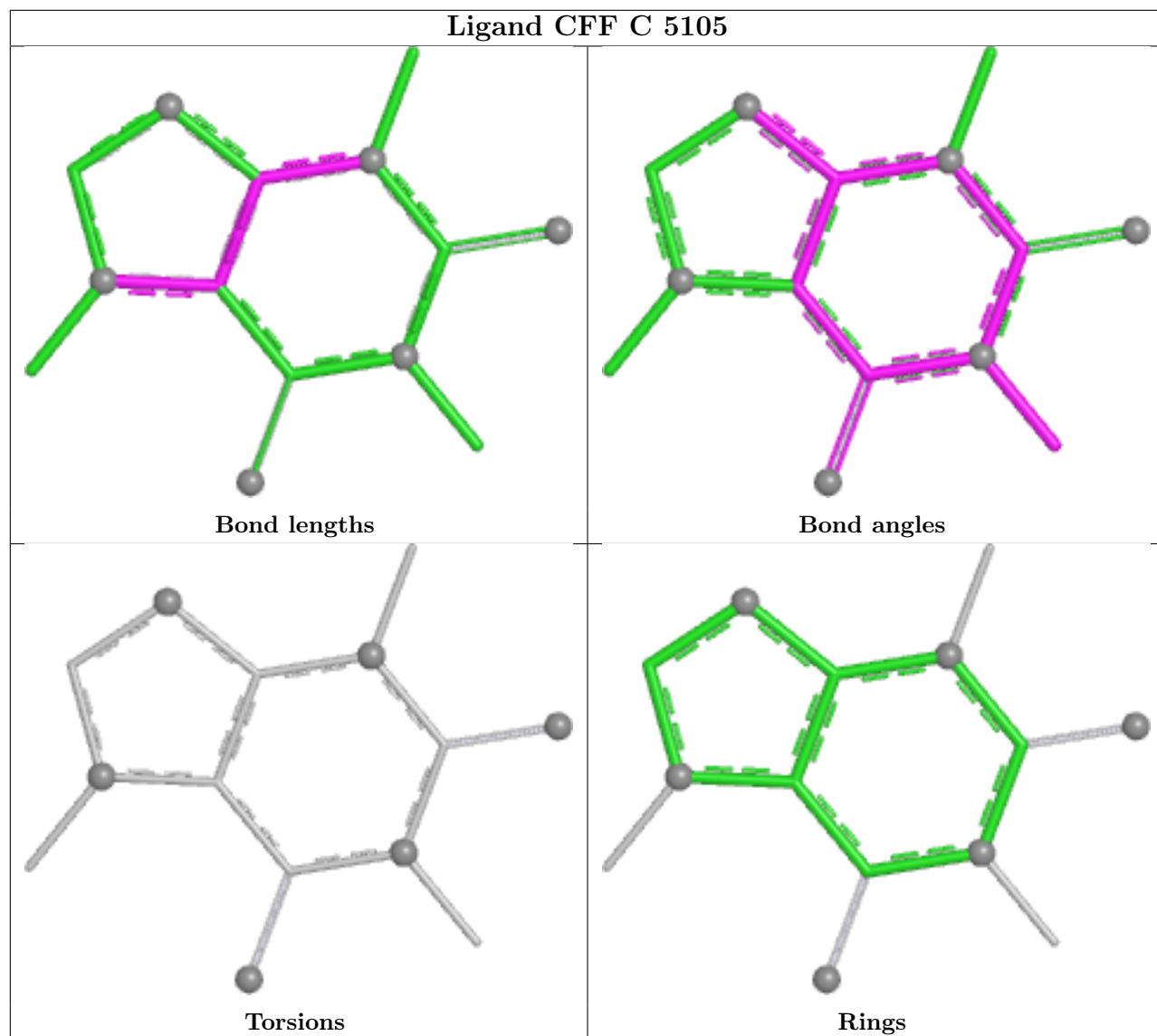
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	5105	CFF	1	0
7	D	5104	ATP	2	0
7	C	5104	ATP	3	0
7	B	5104	ATP	3	0
4	C	5101	F0U	2	0
7	A	5104	ATP	3	0
8	B	5105	CFF	3	0

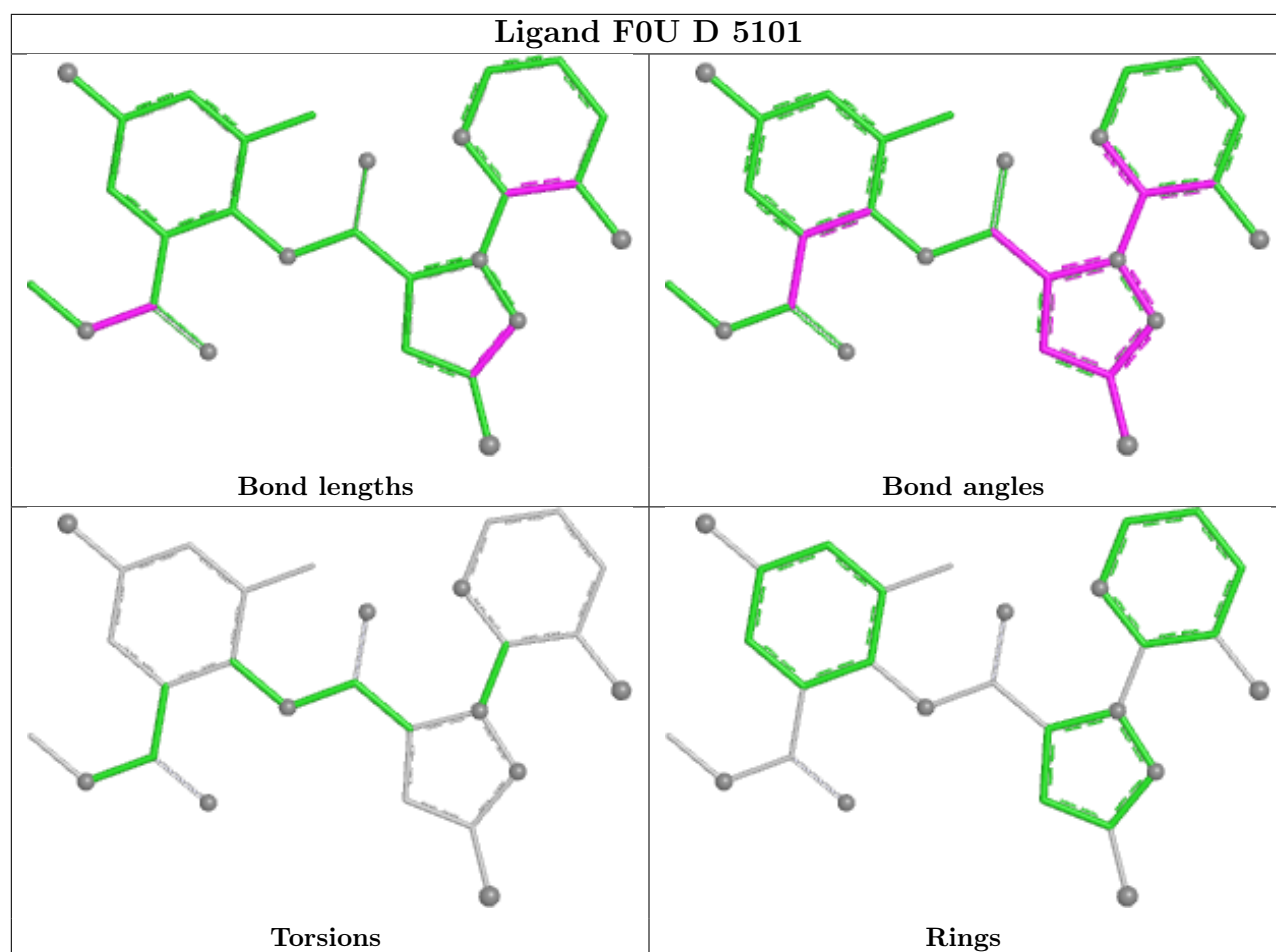
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

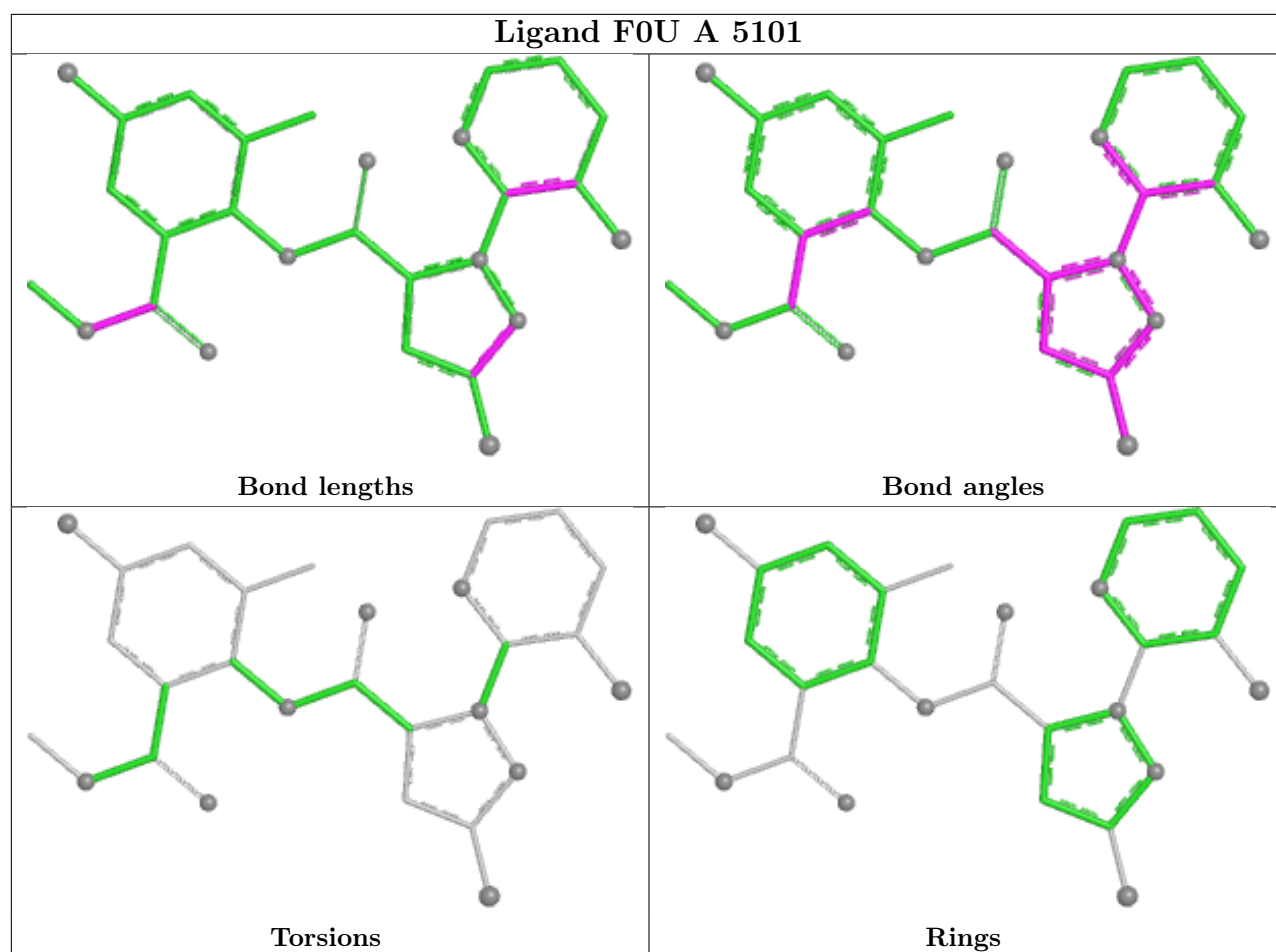


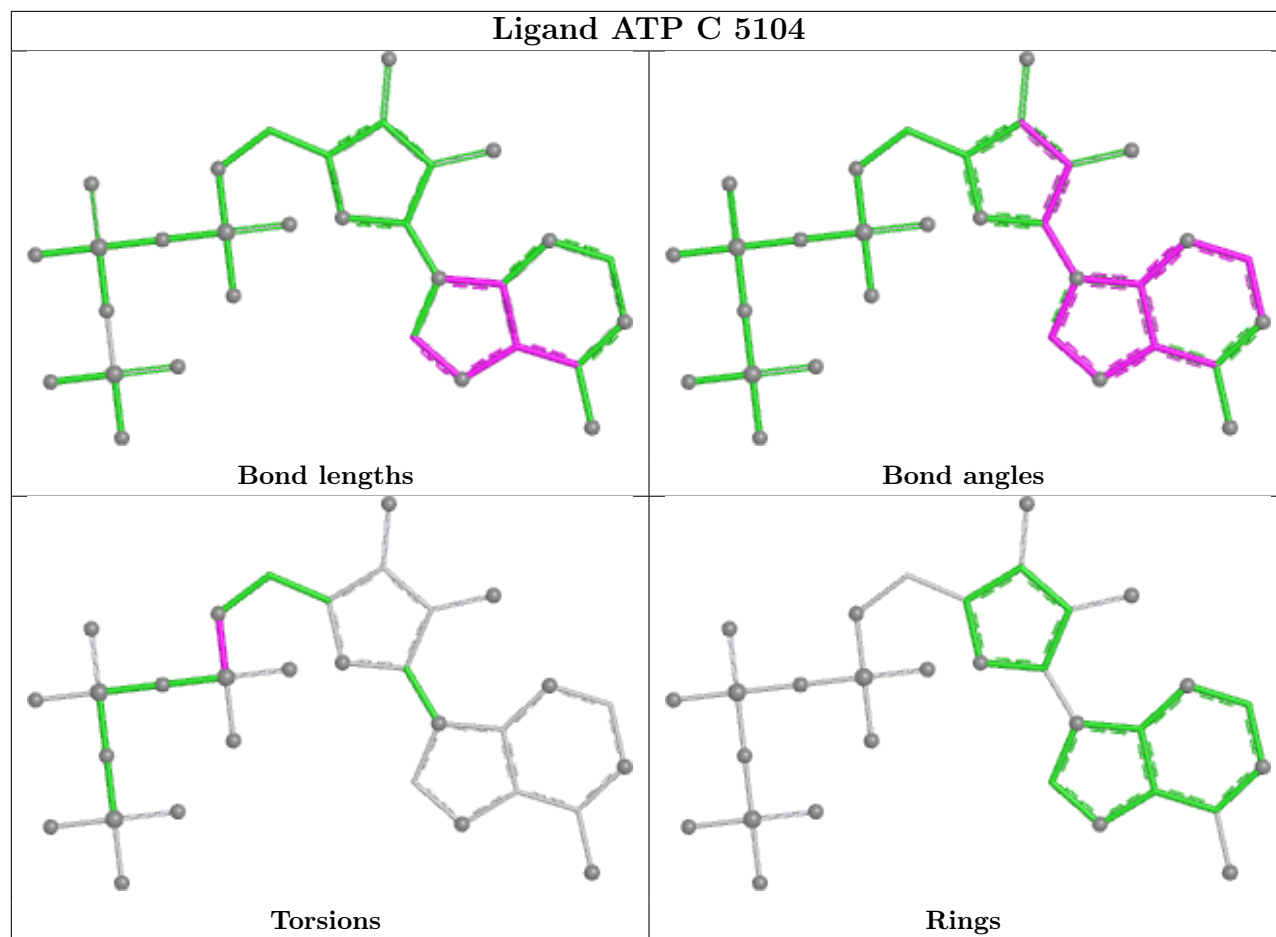


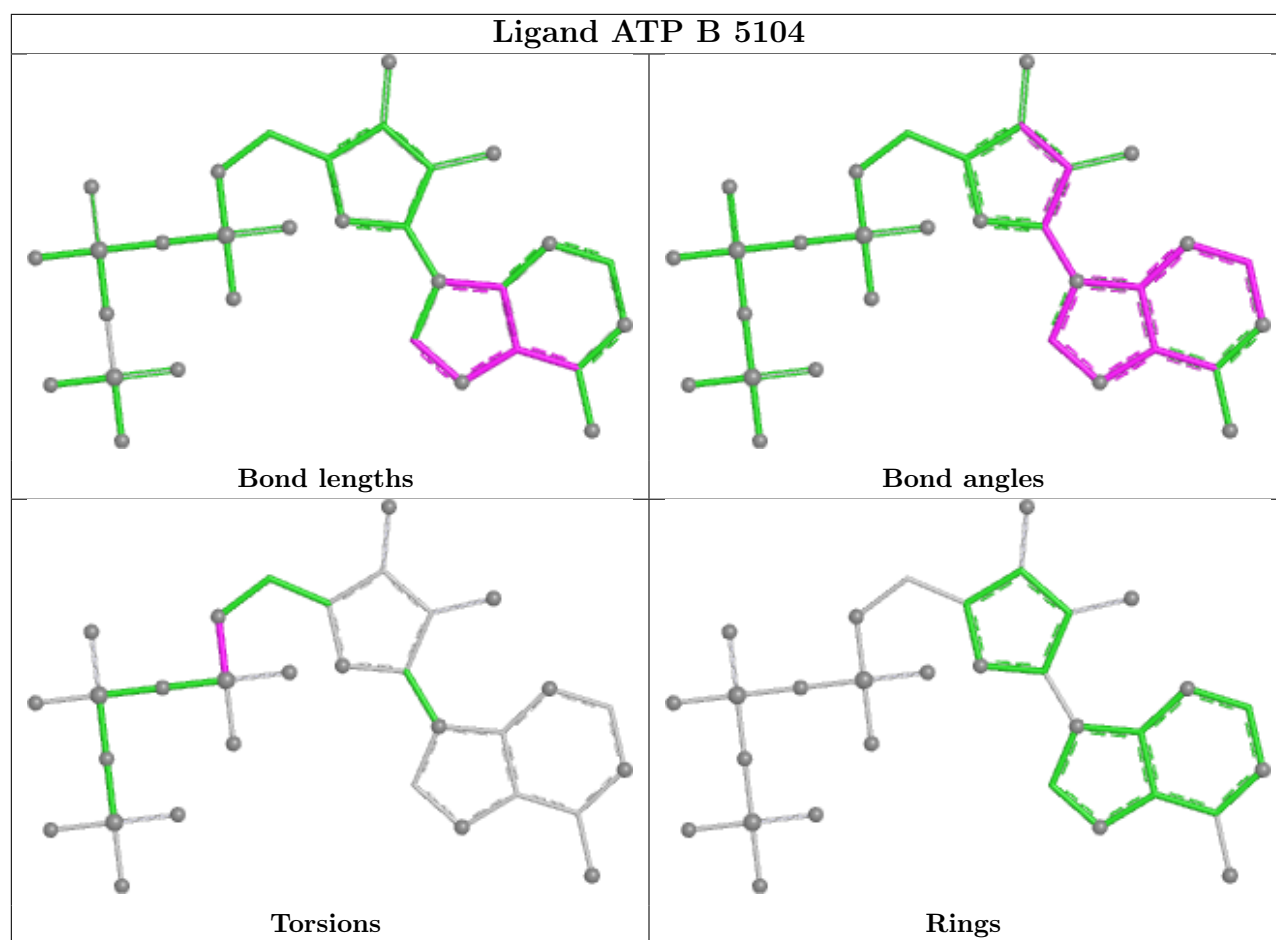


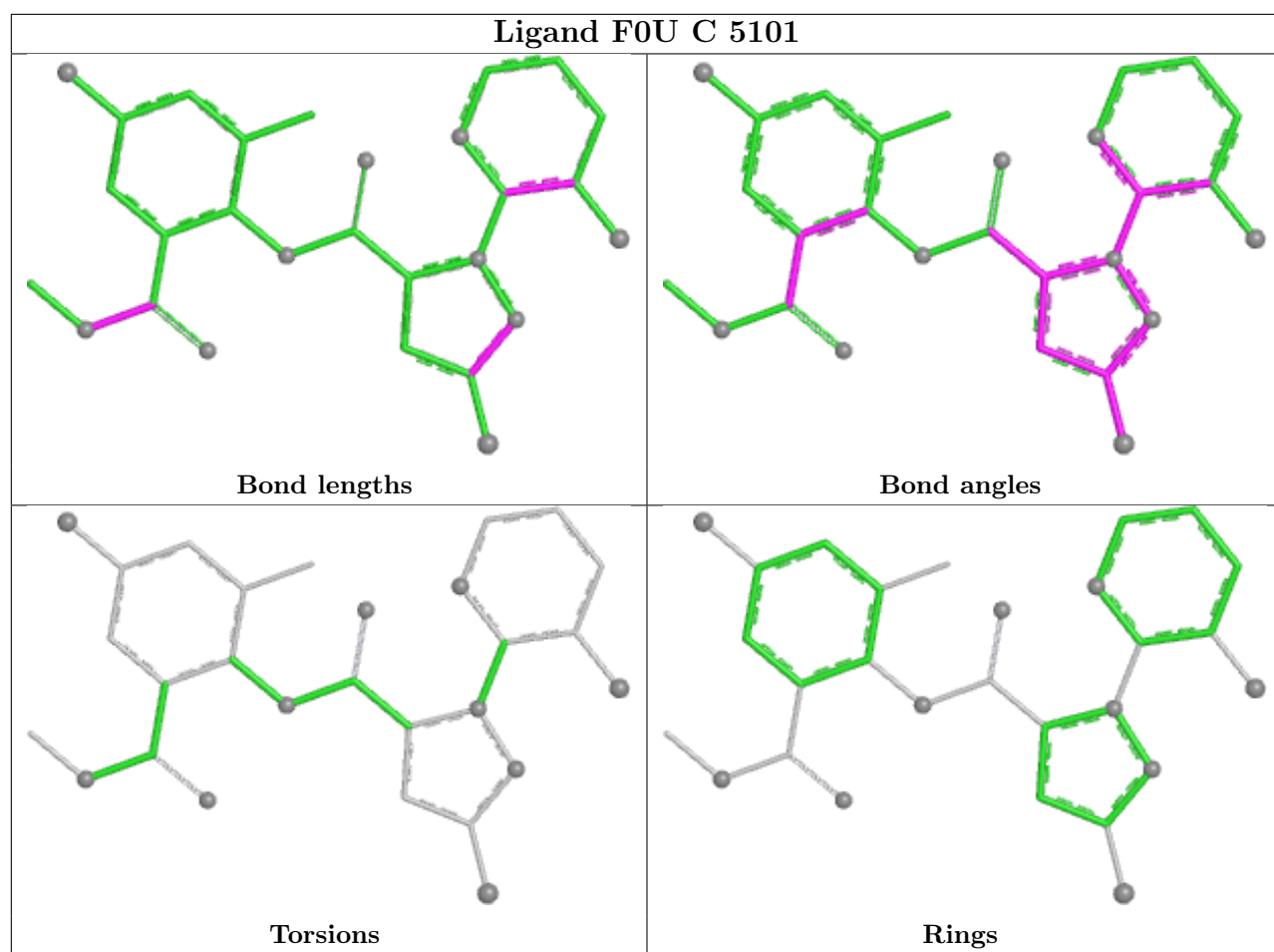


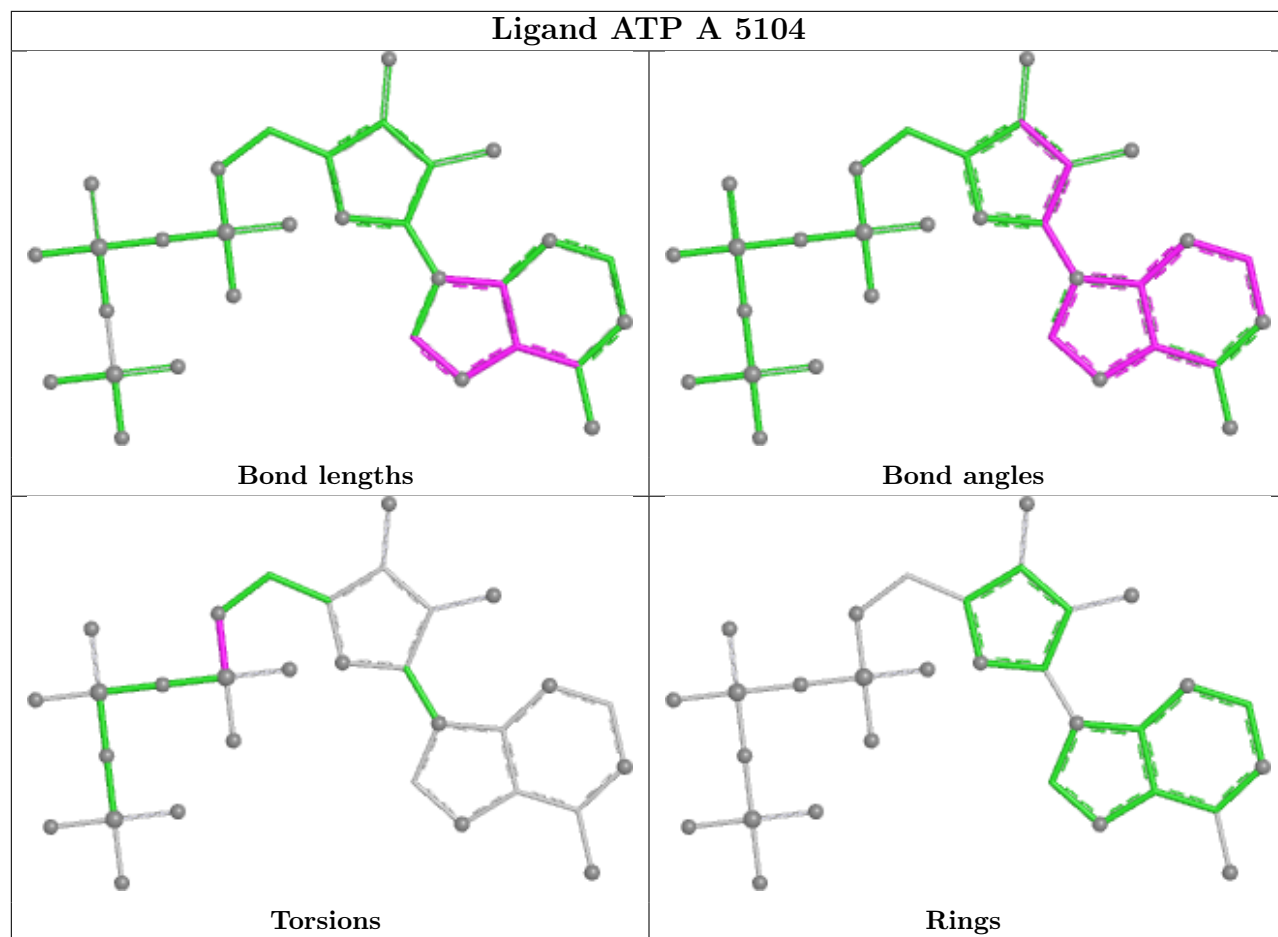


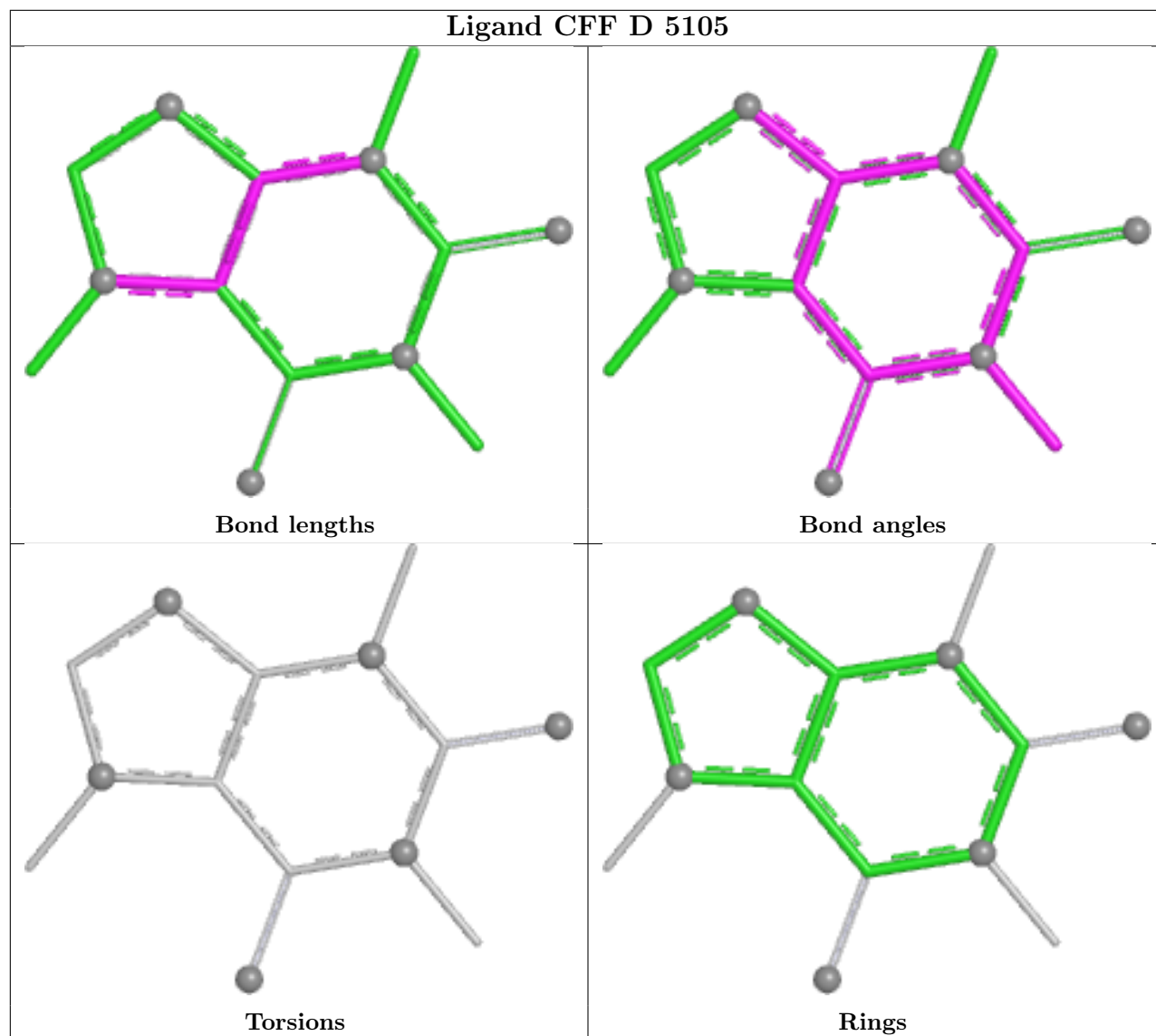


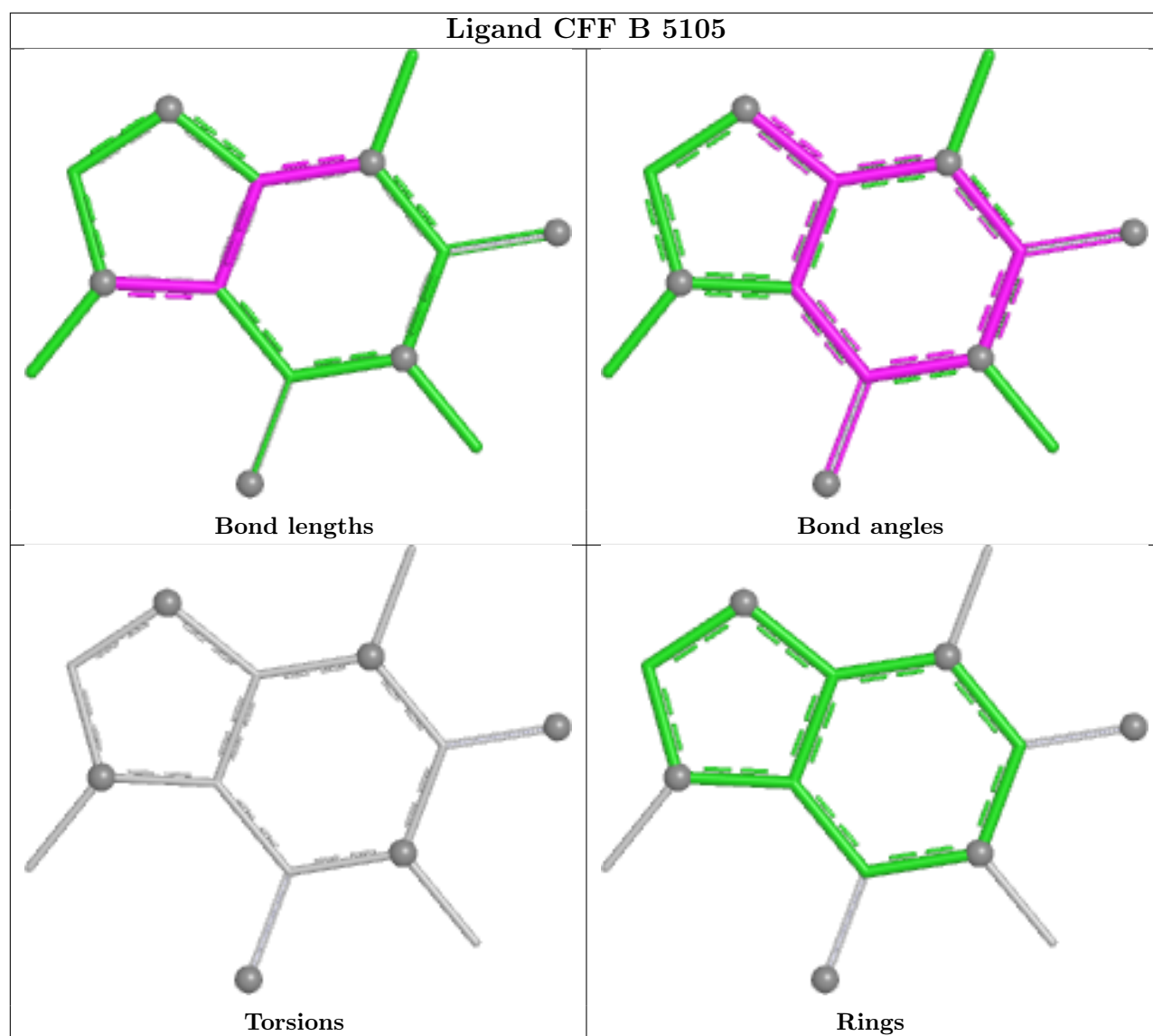












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

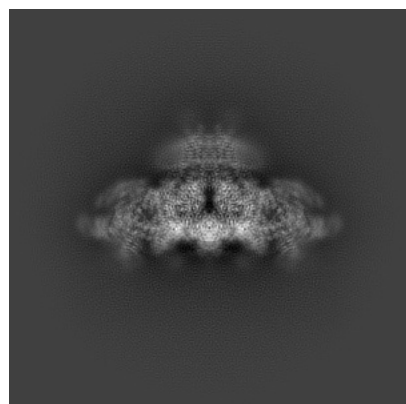
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38908. These allow visual inspection of the internal detail of the map and identification of artifacts.

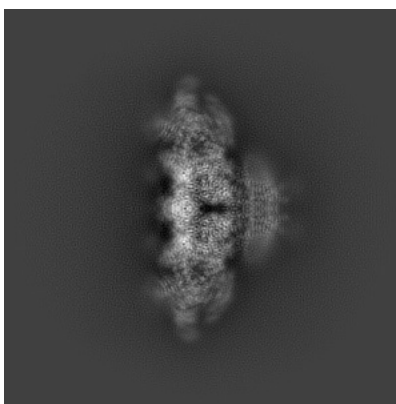
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

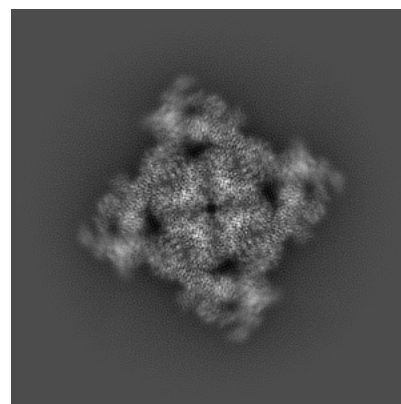
6.1.1 Primary map



X

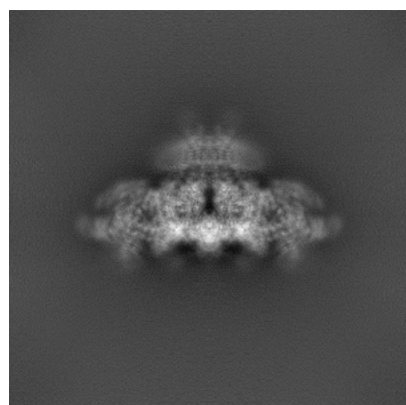


Y

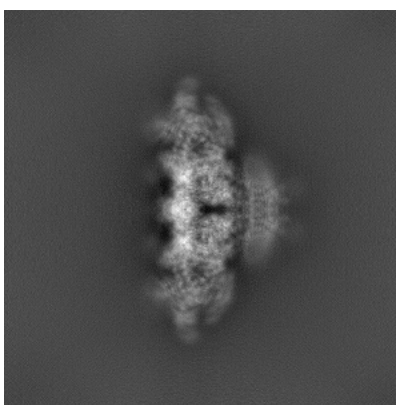


Z

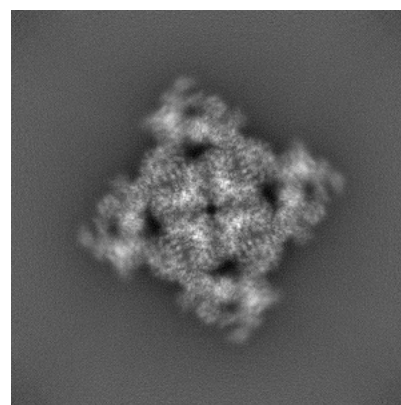
6.1.2 Raw map



X



Y

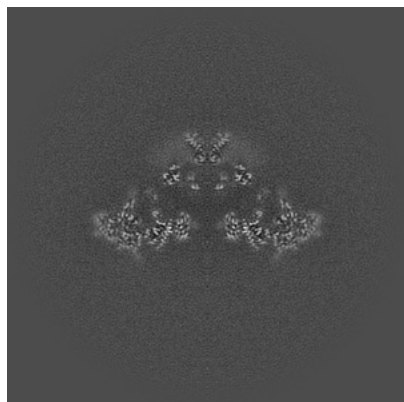


Z

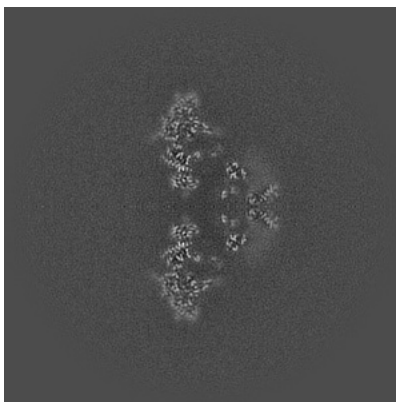
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

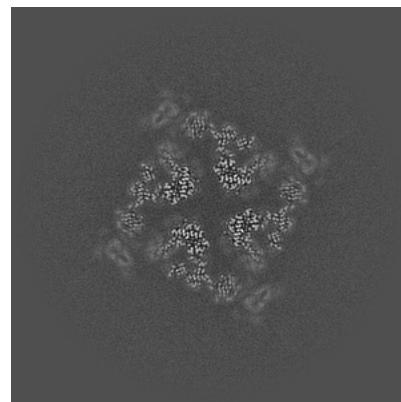
6.2.1 Primary map



X Index: 256

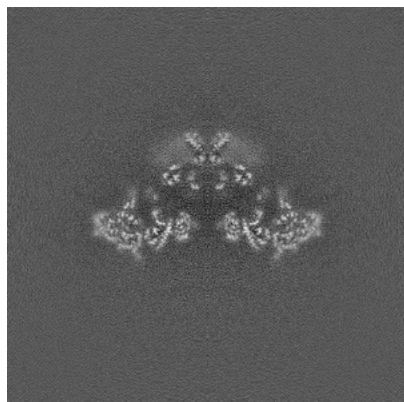


Y Index: 256

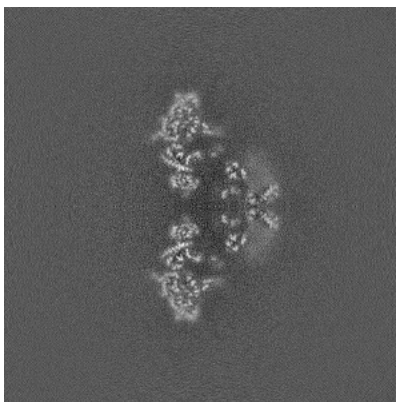


Z Index: 256

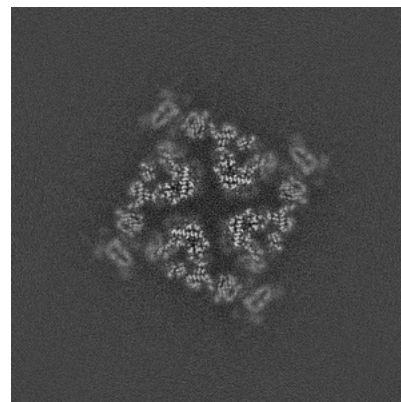
6.2.2 Raw map



X Index: 256



Y Index: 256

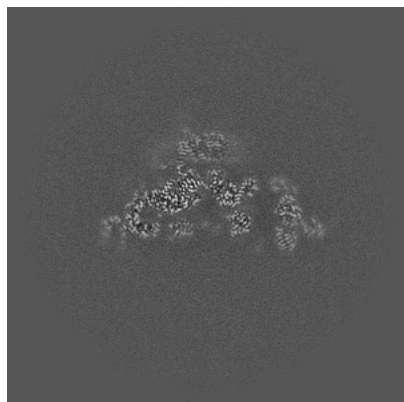


Z Index: 256

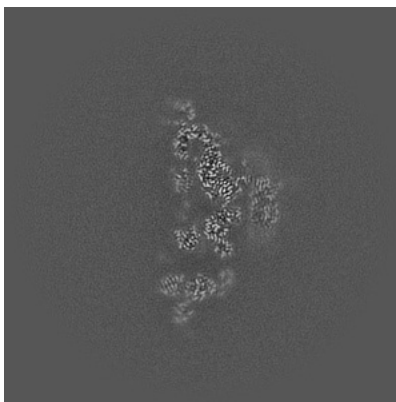
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

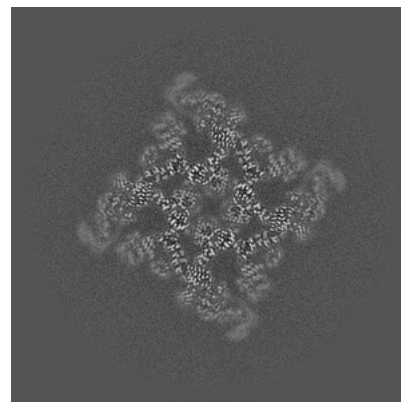
6.3.1 Primary map



X Index: 239

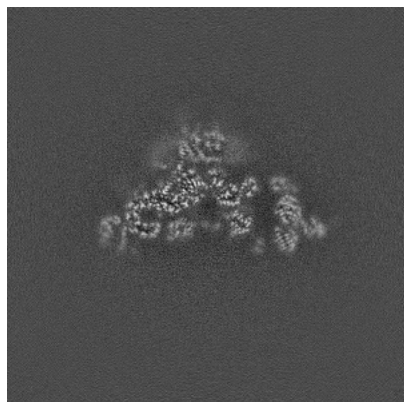


Y Index: 239

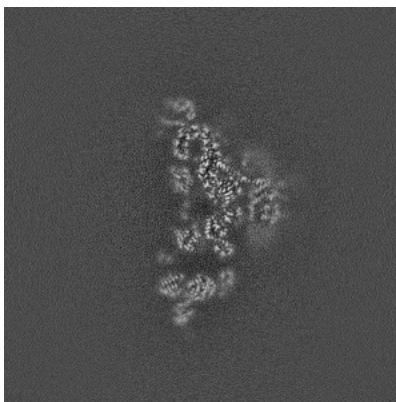


Z Index: 234

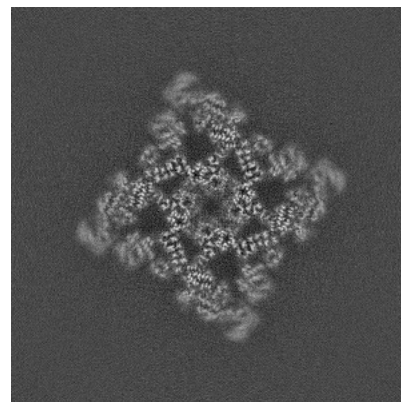
6.3.2 Raw map



X Index: 240



Y Index: 240

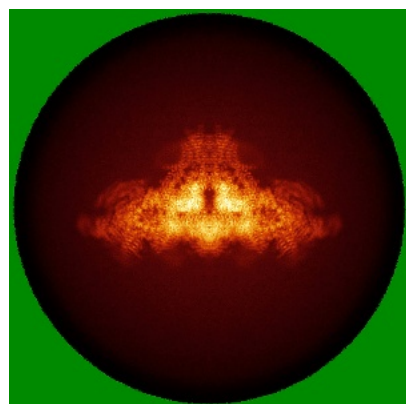


Z Index: 235

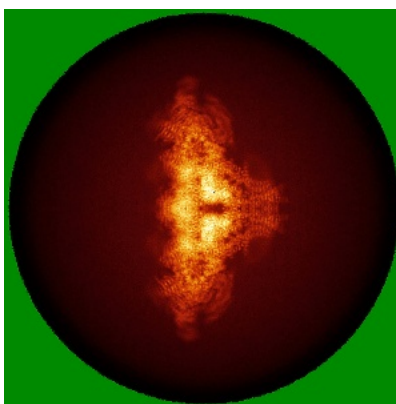
The images above show the largest variance slices of the map in three orthogonal directions.

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

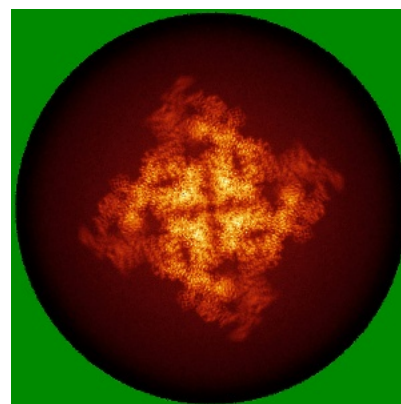
6.4.1 Primary map



X



Y

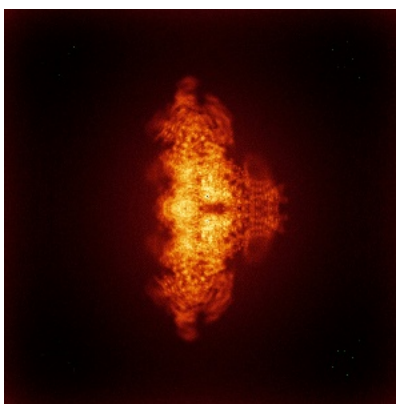


Z

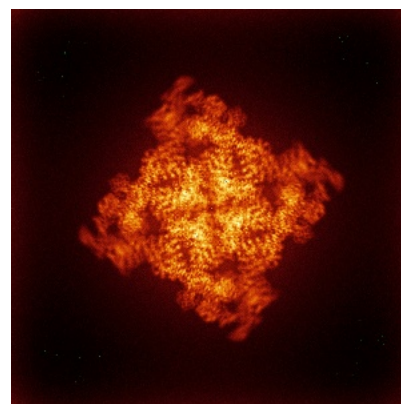
6.4.2 Raw map



X



Y

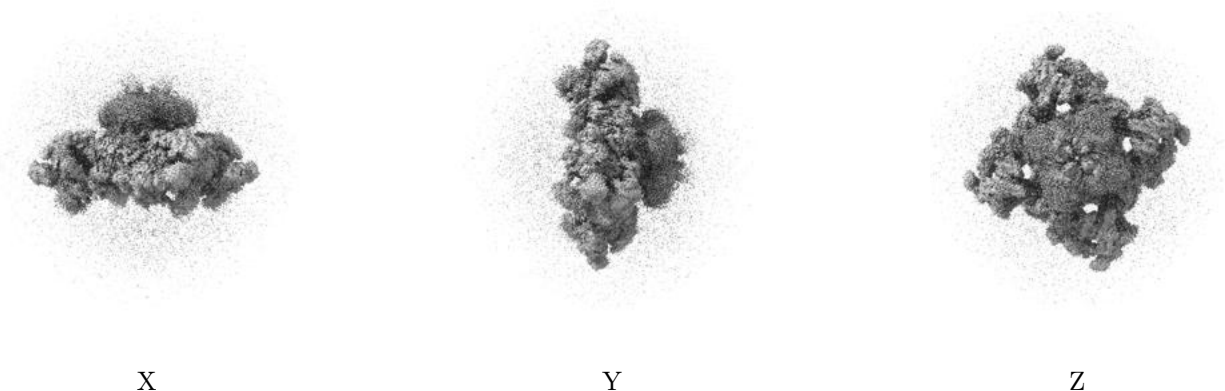


Z

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.

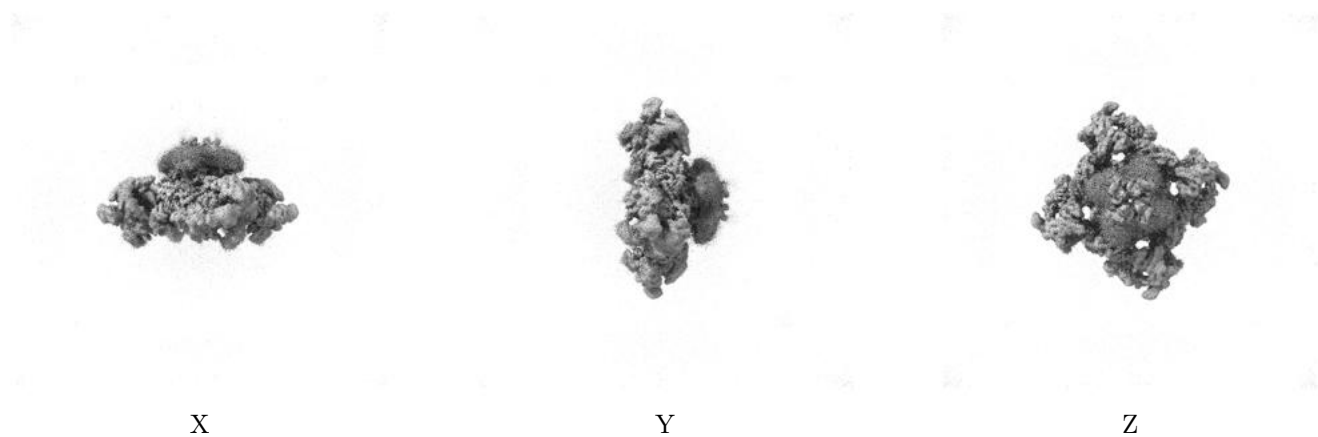
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

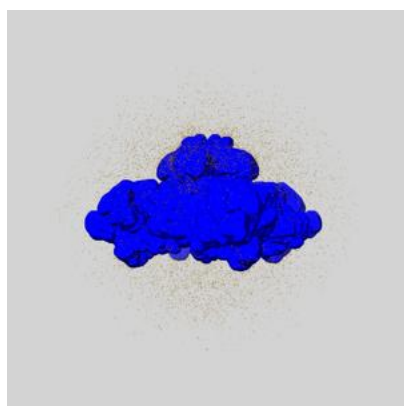
6.6 Mask visualisation [i](#)

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

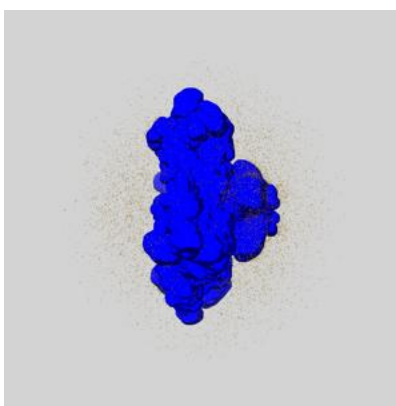
A mask typically either:

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

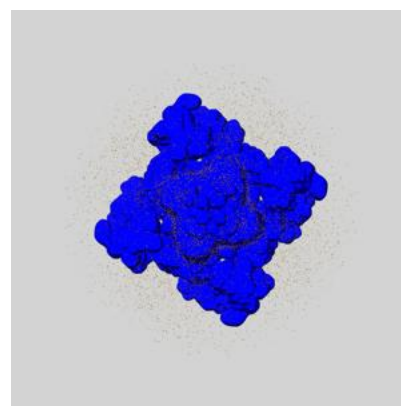
6.6.1 emd_38908_msk_1.map [i](#)



X



Y

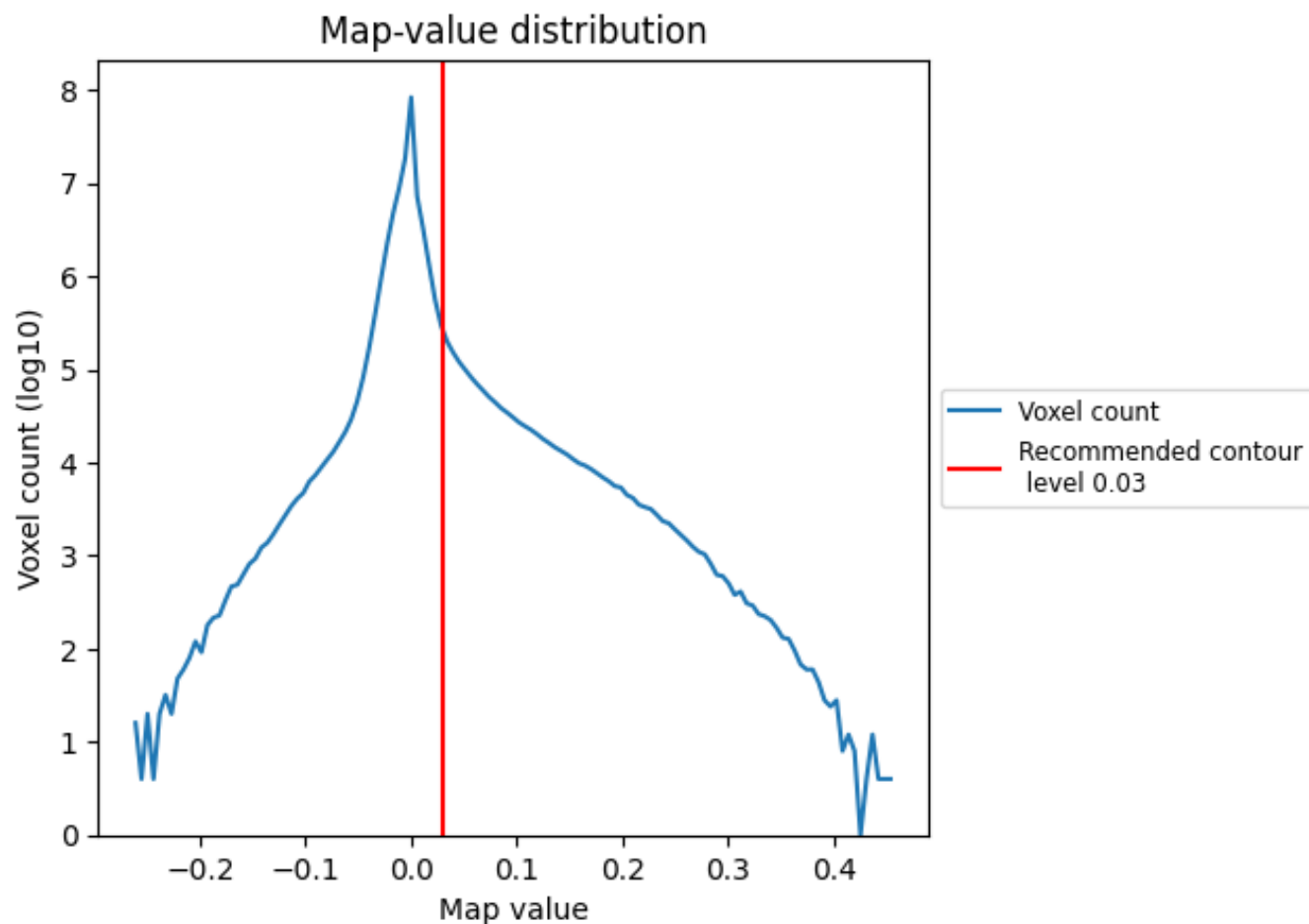


Z

7 Map analysis [i](#)

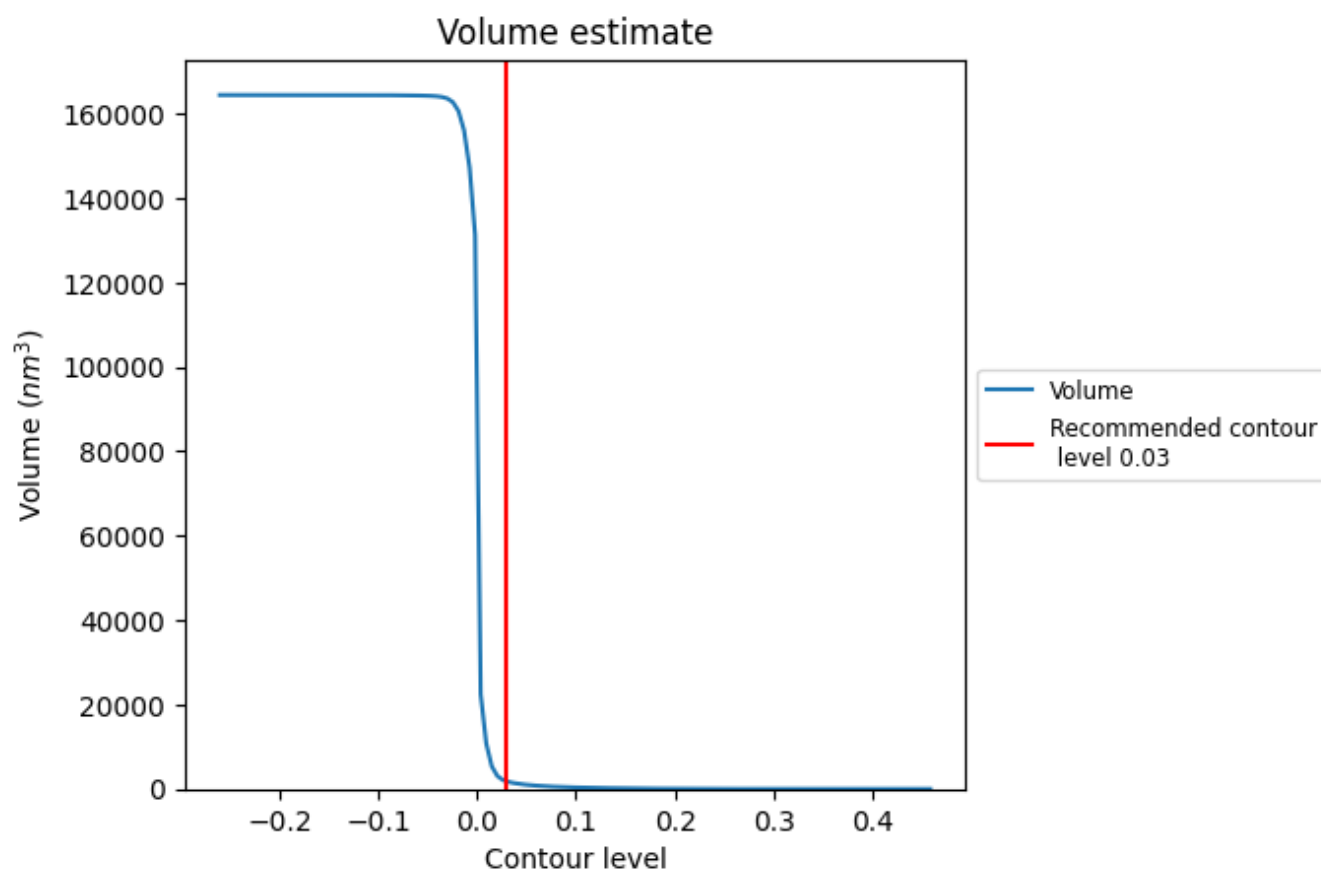
This section contains the results of statistical analysis of the map.

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.

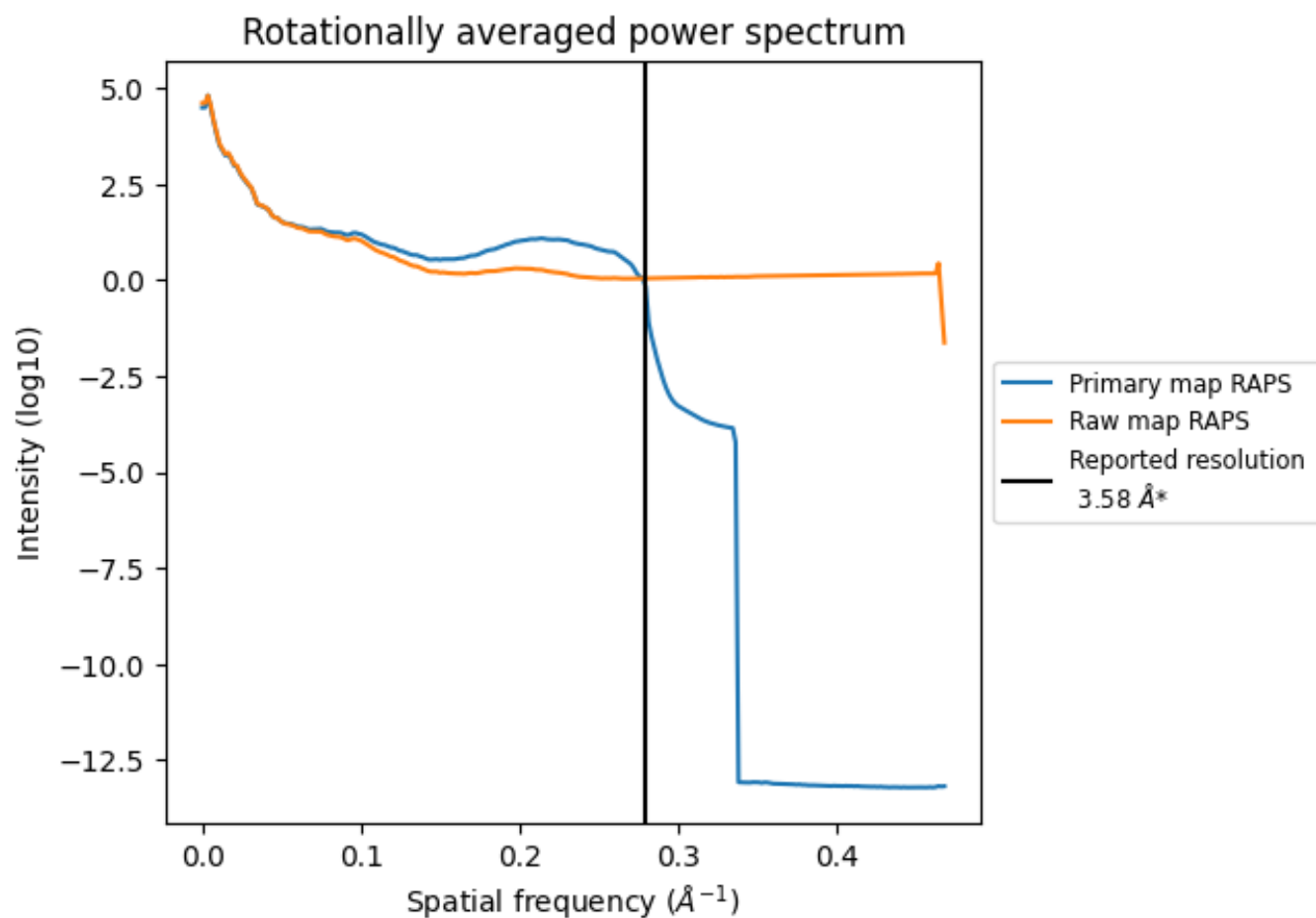
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1805 nm^3 ; this corresponds to an approximate mass of 1630 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 ⓘ

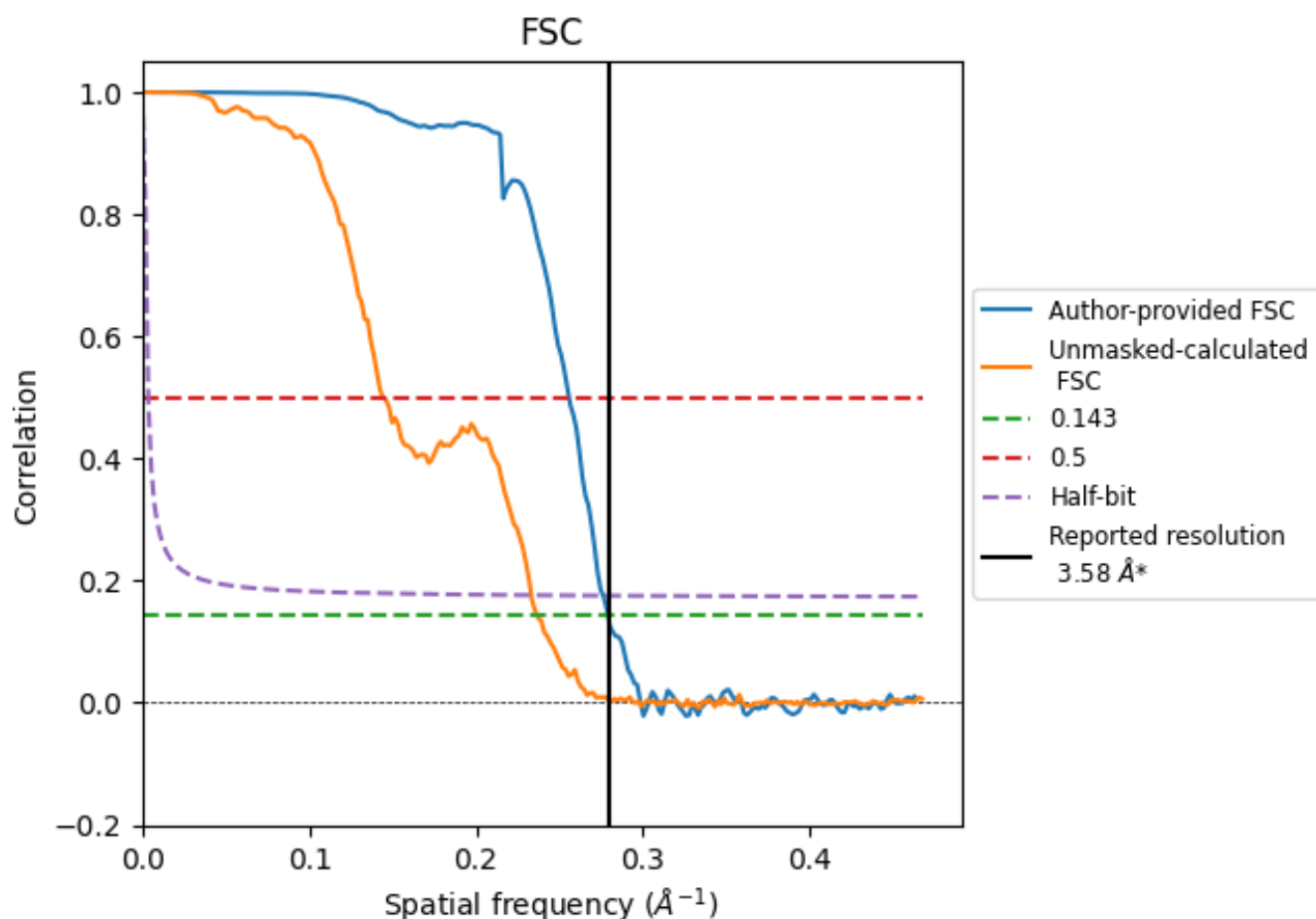


*Reported resolution corresponds to spatial frequency of 0.279 Å⁻¹

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 0.279 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

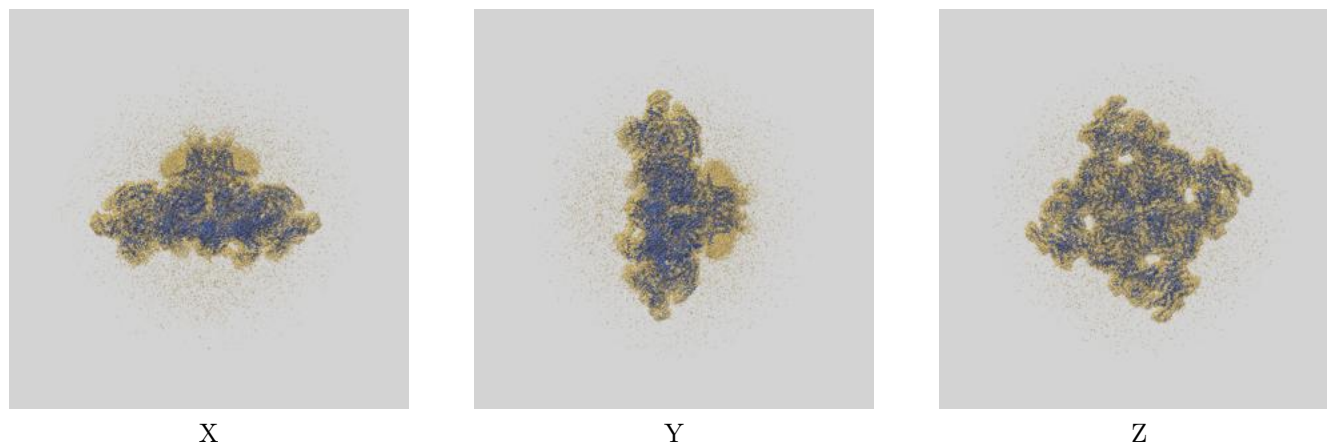
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.58	-	-
Author-provided FSC curve	3.58	3.91	3.62
Unmasked-calculated*	4.23	6.93	4.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.23 differs from the reported value 3.58 by more than 10 %

9 Map-model fit [i](#)

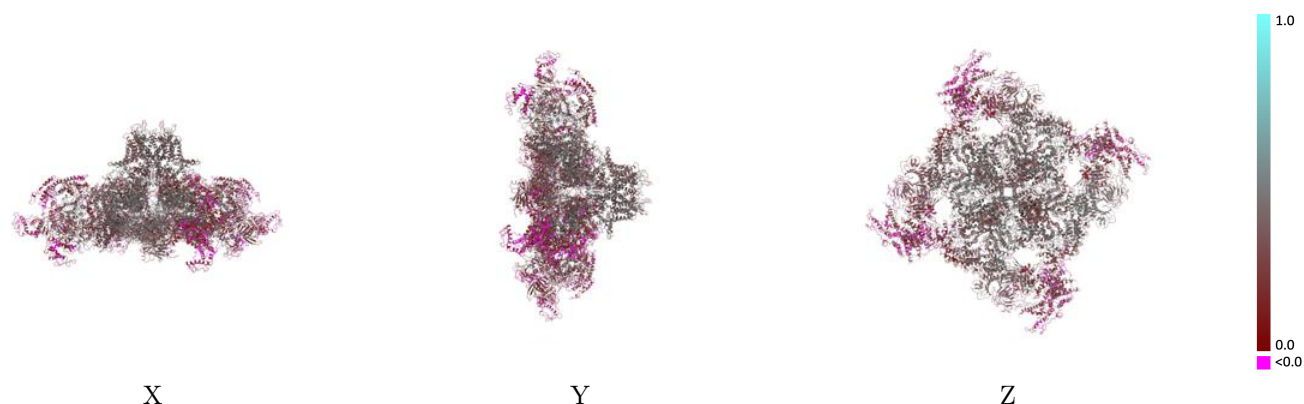
This section contains information regarding the fit between EMDB map EMD-38908 and PDB model 8Y40. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

9.1 Map-model overlay [i](#)



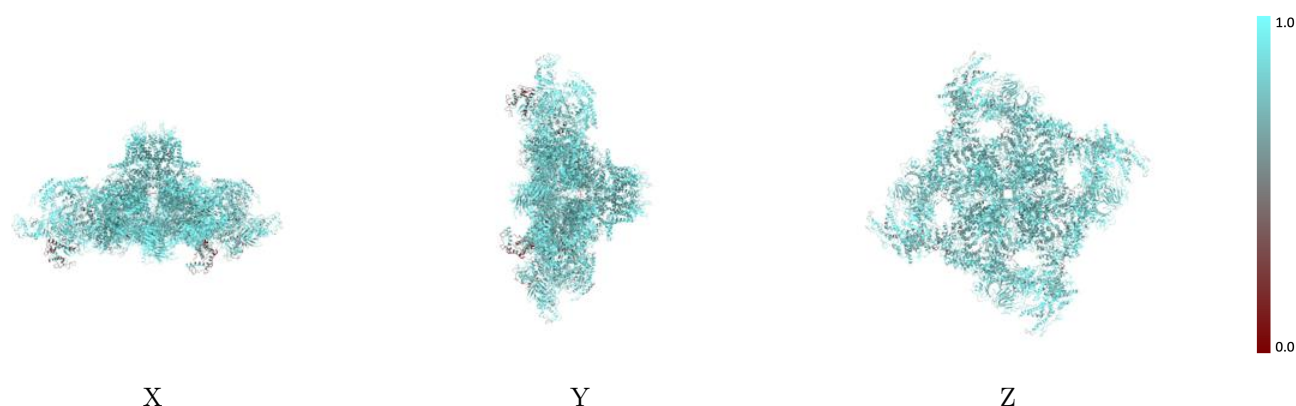
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



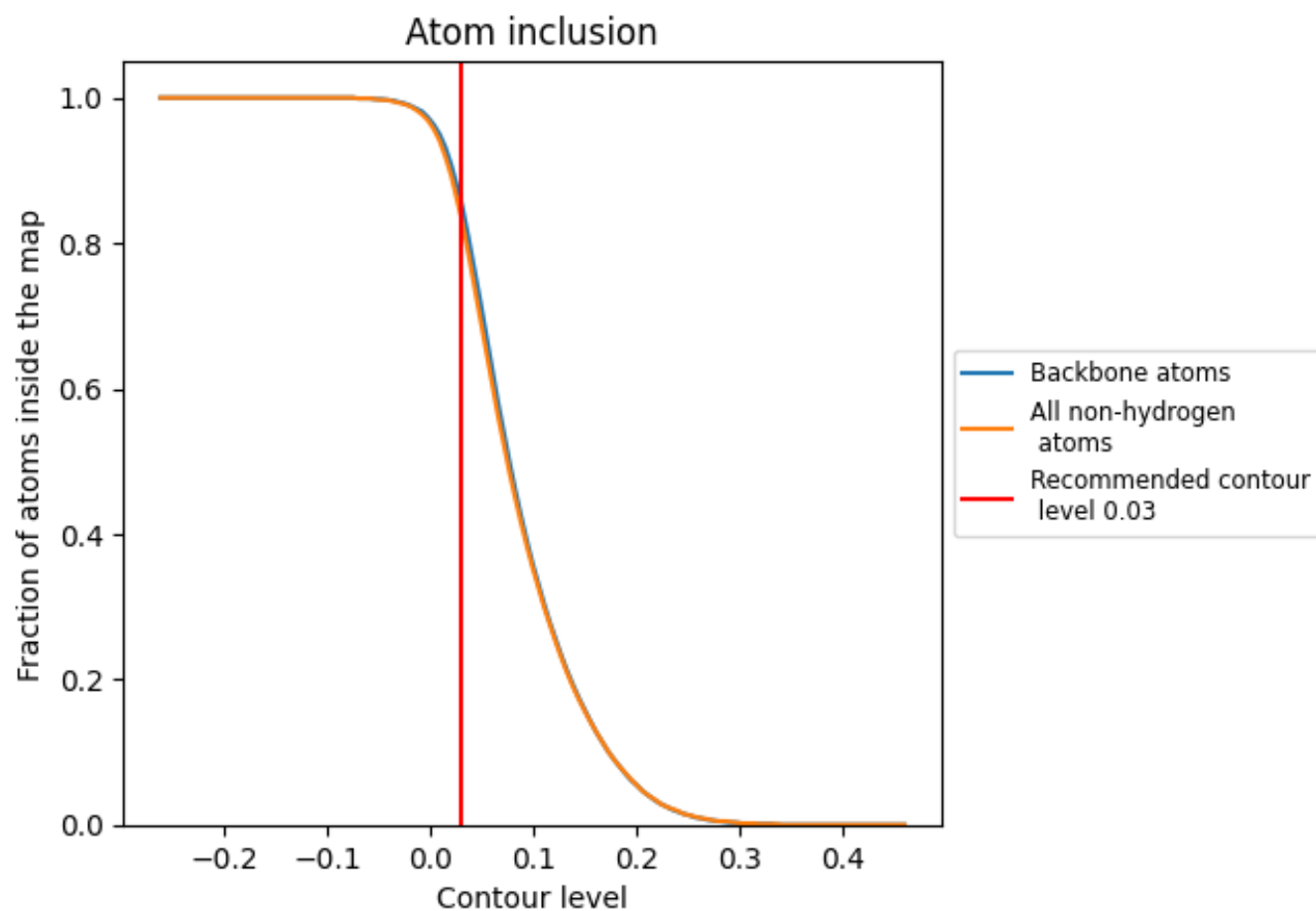
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 84% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.3060
A	0.8410	0.3060
B	0.8390	0.3020
C	0.8420	0.3140
D	0.8400	0.3120
E	0.8270	0.2460
F	0.8610	0.3230
G	0.9170	0.4220
H	0.8590	0.3010
I	0.7300	0.1900
J	0.7150	0.1800
K	0.7770	0.2500
L	0.7780	0.2510

1.0

0.0

<0.0