



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 09:52 AM UTC

PDB ID : 9CGP / pdb_00009cgp
EMDB ID : EMD-45584
Title : RyR1 disease mutant Y523S with FKBP12.6, nanodisc and inhibitor dantrolene in the absence of calcium with refined P1 domain
Authors : Iyer, K.A.; Samso, M.
Deposited on : 2024-06-30
Resolution : 3.34 Å(reported)
Based on initial model : 7T64

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:

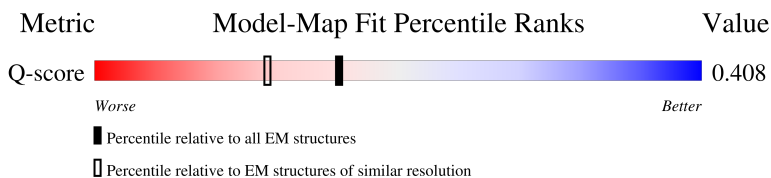
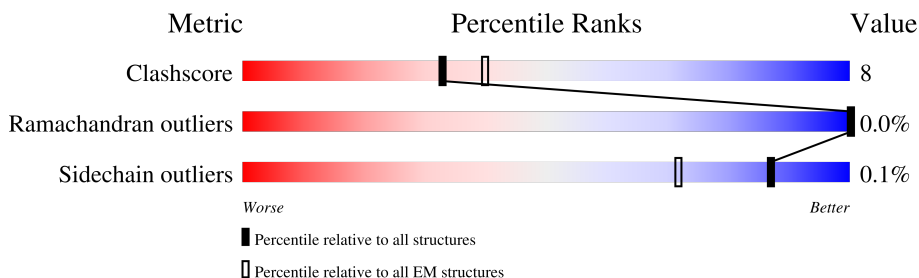
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.34 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.



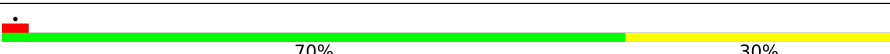
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14446 (2.84 - 3.84)

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	5037	8% 68% 16% 15%
1	B	5037	8% 69% 15% 15%
1	C	5037	8% 69% 16% 15%
1	D	5037	8% 69% 16% 15%

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Mol	Chain	Length	Quality of chain
2	E	107	 70%30%
2	F	107	 75%25%
2	G	107	 71%29%
2	H	107	 70%30%

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
5	U1C	A	5103	-	X	-	-
5	U1C	B	5103	-	X	-	-
5	U1C	C	5103	-	X	-	-
5	U1C	D	5103	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 132860 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	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	B	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	C	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0
1	D	4258	Total 32374	C 20609	N 5541	O 6025	S 199	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	TYR	engineered mutation	UNP P11716
B	523	SER	TYR	engineered mutation	UNP P11716
C	523	SER	TYR	engineered mutation	UNP P11716
D	523	SER	TYR	engineered mutation	UNP P11716

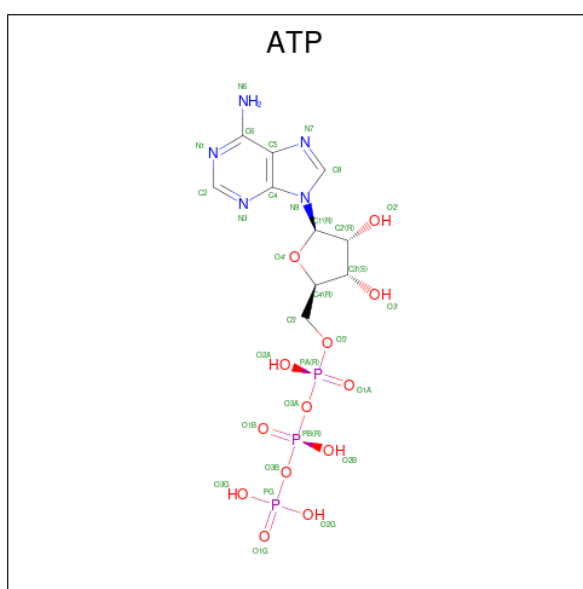
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	F	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	G	107	Total 786	C 498	N 137	O 148	S 3	0	0
2	H	107	Total 786	C 498	N 137	O 148	S 3	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

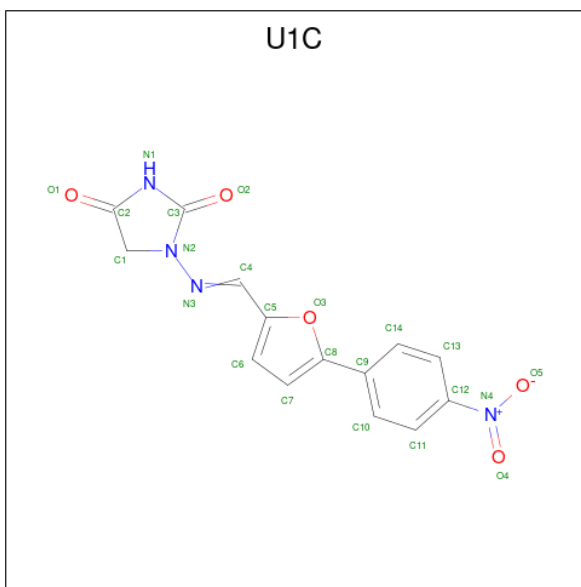
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	C	1	Total	Zn	0
			1	1	
3	D	1	Total	Zn	0
			1	1	

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is Dantrolene (CCD ID: U1C) (formula: $C_{14}H_{10}N_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	A	1	23	14	4	5	0
5	B	1	23	14	4	5	0
5	C	1	23	14	4	5	0
5	D	1	23	14	4	5	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: Ryanodine receptor 1



D1028	F1139	L1283	THR	PRO	M1527	R1656	GLU	K2013	V2098	D2282	H2420	D2516
K1032	G1140	V1284	ALA	HIS	T1530	L1657	GLU	D2017	V2102	N2283	A2421	H2520
N1035	V1148	F1288	LYS	ASP	T1530	D1658	GLU	E2018	R2103	L2286	M2422	V2524
R1036	G1151	L1289	GLY	VAL	E1535	N1678	GLU	C2021	E2108	S2309	S2424	V2524
L1039	M1152	Q1299	THR	PRO	S1536	D1700	GLU	P2022	R2118	C2310	D2431	L2527
R1044	T1153	HIS	PRO	ALA	N1537	P1703	GLU	L2023	R2125	M2312	R2435	M2530
L1047	D1154	PHE	THR	ARG	N1545	P1704	GLU	P2024	L2124	L2313	C2436	R2531
G1048	T1156	ARG	PRO	CYS	L1548	L1707	GLU	L2031	H2125	Y2318	A2437	L2536
N1052	I1160	THR	PRO	THR	F1549	R1708	GLU	H2035	Q2127	P2319	M2440	L2536
I1053	I1161	ALA	GLY	ALA	P1550	A1708	GLU	E2047	D2149	D2320	H2441	A2547
E1054	L1169	GLY	VAL	GLY	A1551	S1717	GLU	GLY	E2150	I2321	I2442	L2550
PRO	M1170	THR	ALA	ALA	V1554	E1721	GLU	GLU	S2153	P2326	Q2444	N2551
ASP	S1171	GLN	GLN	THR	L1555	T1742	GLU	ASP	Q2154	S2345	R2452	L2556
GLN	D1172	LEU	PRO	VAL	H1558	K1753	GLU	GLU	R2159	R2355	I2453	L2556
TRP	F1179	ALA	ARG	ARG	V1561	V1767	GLU	GLU	L2179	R2359	R2454	L2556
A1077	E1180	PRO	ASN	ASN	I1562	T1768	GLU	PRO	M2188	L2368	D2464	L2561
E1078	E1181	GLY	GLY	GLY	Q1563	T1769	GLU	GLU	F2191	R2369	L2472	I2562
K1079	G1189	GLY	LYS	LYS	F1564	R1772	GLU	GLU	M2198	G2370	P2473	I2563
S1080	P1189	PRO	ASP	ASP	I1572	R1772	GLU	GLU	R2199	S2374	L2474	K2564
R1087	E1201	ALA	GLU	GLU	S1576	A1788	GLU	LEU	M2198	E2388	L2476	L2566
W1088	Q1206	ASP	THR	THR	D1456	A1789	GLU	LEU	L2198	D2389	Q2475	L2566
Y1089	D1207	PRO	THR	THR	V1457	G1790	GLU	GLU	R2199	P2390	P2477	L2566
E1093	V1208	ASP	LYS	LYS	M1462	V1791	GLU	GLU	L2201	A2391	T2478	L2566
W1104	S1210	TYR	ALA	ALA	R1470	A1792	GLU	GLU	V2212	P2395	LEU	C2606
P1107	L1211	ASP	ALA	ALA	A1471	E1793	GLU	GLU	N2213	GLY	GLY	L2607
R1110	G1219	PRO	ASP	ASP	G1477	E1805	GLU	VAL	N2214	VAL	ALA	M2608
D1112	F1223	TYR	PRO	PRO	D1478	R1808	GLU	ARG	G2218	VAL	LEU	C2608
D1118	T1230	LYS	ALA	ALA	M1482	L1815	GLU	ARG	T2223	ARG	VAL	L2614
M1125	M1230	ALA	ARG	ARG	S1486	S1833	GLU	LEU	M2228	ASP	ARG	A2491
G1126	S1241	SER	MET	MET	W1494	E1835	GLU	GLU	L2236	ARG	ASP	I2614
W1132	P1253	THR	THR	THR	G1504	F1836	GLU	GLU	T2242	ARG	ARG	A2492
	H1254	GLY	GLN	GLN	Q1505	V1845	GLU	LYS	R2244	GLU	ARG	S2493
	T1263	TRP	PRO	PRO	R1508	T1847	GLU	LYS	Q2245	HTS	GLU	F2494
	T1266	GLY	ALA	ALA	I1509	L1848	GLU	GLU	N2246	PHE	GLY	D2497
	L1270	GLY	ALA	ALA	G1517	V1851	GLU	LEU	M2250	GLY	GLY	A2500
	L1276	GLY	LEU	LEU	C1518	M1851	GLU	ALA	Y2256	GLU	GLU	L2506
	W1277	ARG	PRO	PRO	L1519	P1868	GLU	GLU	L2257	PRO	PRO	D2507
			LEU	LEU	D1521	T1872	GLU	GLU	L2258	GLU	GLU	V2508
					T1524	E1873	GLU	GLU	V2276	ASN	ASN	Y2510
						E1874	GLU	GLU				G2511
							GLU	GLU				I2512
							GLU	GLU				R2650
							GLU	GLU				C2651
							GLU	GLU				W2652
							GLU	GLU				K2653
							GLU	GLU				Y2654

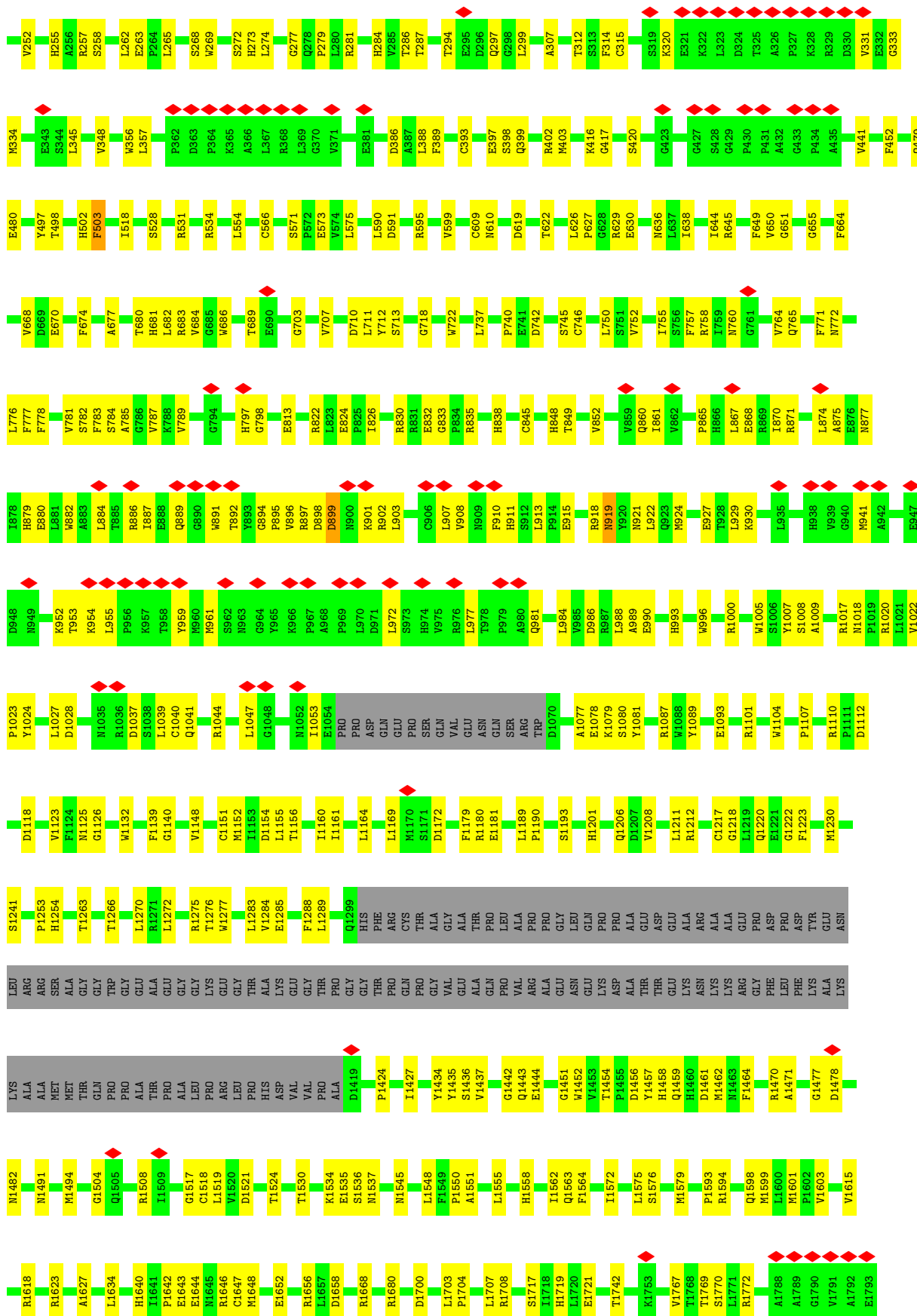
L3866	H3699	R3595	A3332	F3096	R2985	A2917	P2857	F2797	P2737	L2657
N3867	Q3700	P3612	T3353	E3097	V2986	R2918	Q2858	S2798	R2738	P2658
R3868	L3701	T3612	W3334	S3098	E2987	D2919	P2859	E2799	P2739	T2659
R3869	L3716	L3716	L3338	A3099	R2988	R2920	P2860	K2800	V2740	N2663
N3870	D3719	SER	S3347	E3101	S2989	E2921	L2861	D2801	E2741	
N3875	G3738	A3876	V3245	V3107	L3003	K2922	L2862	K2802	T2742	L2672
D3877	GLY	ALA	V3236	L3110	P3004	A2923	S2863	E2803	L2743	K2677
	GLY	ASP	E3237	L3112	Y3016	Q2924	Q2864	T2804	N2744	
Q3889	GLN	TRP	V3245	R3111	F3017	E2925	V2865	R2806	V2745	G2681
L3890	GLY	HIS	L3246	L3112	L3018	L2926	T2866	W2807	I2747	K2690
	GLY	LEU	D3247	G3113	S3019	L2927	L2867	P2808	P2748	TYR
Q3927	ALA	LEU	R3248	LYS	T3020	K2928	S2868	T2809	E2749	GLN
E3928	GLY	SER	L3249	VAL	Y3020	F2929	S2869	K2810	K2750	ASP
S3929	GLY	LYS	L3253	GLN	K3023	L2930	E2870	E2811	K2751	LEU
	GLY	ARG	E3366	ALA	V3024	Q2931	L2871	E2812	L2752	TYR
L3965	GLN	ARG	Y3263	ARG	L3025	M2932	Q2872	S2812	S2753	ARG
T3966	ARG	ARG	E3264	THR	G3026	M2933	A2873	K2814	F2754	MET
E3967	GLY	ASP	E3265	GLN	S3027	Q2934	M2874	A2815	I2755	ALA
Y3968	VAL	ARG	M3266	VAL	S3027	Q2934	A2875	A2816	K2756	PRO
L3969	VAL	VAL	P3267	LYS	G3028	Y2935	Q2877	M2817	N2757	CYS
Q3970	TYR	VAL	I3270	GLY	G3029	A2936	E2878	L2817	F2758	LEU
G3971	SER	VAL	F3271	VAL	H3030	V2937	Q2877	A2818	A2759	CYS
P3972	VAL	VAL	I3272	G3126	A3031	T2938	L2878	W2819	E2760	ALA
C3973	GLN	GLN	I3274	Q3127	S3032	T2938	L2879	E2820	I2761	ALA
L3980	ARG	ARG	L3277	N3128	E3035	R2939	A2879	E2821	Y2762	GLY
S3983	ARG	ARG	Y3415	L3129	K3036	Q2940	E2880	E2822	T2763	ALA
R3984	M3617	Y3416	V3416	T3133	E3037	L2941	M2881	W2821	H2763	LEU
L3985	L3518	D3417	N3418	V3134	H3038	K2942	Y2882	I2823	E2764	PRO
G3991	P3519	N3418	N3419	A3135	I3039	D2943	H2883	E2824	K2765	ASP
					S3041	M2944	N2884	A2825	W2766	TYR
V3995	M3524	L3424	L3424	V3139	L3049	E2945	T2885	A2826	A2767	VAL
	C3525	L3434	L3434	L3140	L3049	D2947	T2886	R2827	F2768	ALA
M3999	A3526	L3434	L3434	T3141	H3052	T2948	R2888	G2828	D2769	ASP
M4000	P3527	V3438	V3438	Q3145	H3052	S2949	K2889	G2829	K2770	SER
L4003	T3528	T3441	T3441	F3152	L3056	S2950	K2890	E2830	I2771	TYR
S4008	L3535	K3447	K3447	G3153	V3065	I2951	K2891	GLU	Q2772	SER
Q4009	T3545	E3458	E3458	L3156	L3068	E2952	Q2892	GLU	N2773	LYS
L4012	E3548	R3453	R3453	D3159	H3069	K2953	E2893	THR	N2774	ALA
L4016	L3579	E2454	E2454	L3159	I3070	R2954	L2894	GLU	W2775	LYS
	E3685	N3457	N3457	S3171	L3070	G2958	E2895	LYS	S2776	ALA
L4030	GLU	T3471	T3471	I3172	D3076	Q2961	A2896	LYS	Y2777	THR
L4031	GLU	ALA	ALA	L3175	A3077	Q2962	K2897	ARG	G2778	VAL
E4032	GLU	ASP	ASP	L3175	R3078	L2963	G2898	THR	E2779	ASP
G4033	VAL	SER	SER	L3194	T3079	L2964	G2899	ILE	ALA	ALA
M4034	ASN	LYS	LYS	L3194	V3080	W2966	G2900	SER	N2780	GLY
M4044	GLU	LYS	LYS	A3198	M3081	M2967	T2901	GLN	V2781	GLY
	ASP	ALA	ALA	A3199	V3081	D2968	T2902	THR	D2782	N2734
V4049	THR	MET	MET	A3200	V3088	L2969	P2903	ALA	E2783	F2735
				P3208	G3091	S2970	L2905	THR	E2784	D2736
S4052					L3092	L2974	V2906	TYR	L2785	
					F3095	E2978	P2907	ASP	K2786	
							Y2908	ARG	T2787	
							D2909	GLU	H2788	
							T2910	GLY	P2789	
							L2911	GLY	M2790	
							T2912	GLY	L2791	
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							E2915	GLY	K2795	
									T2796	



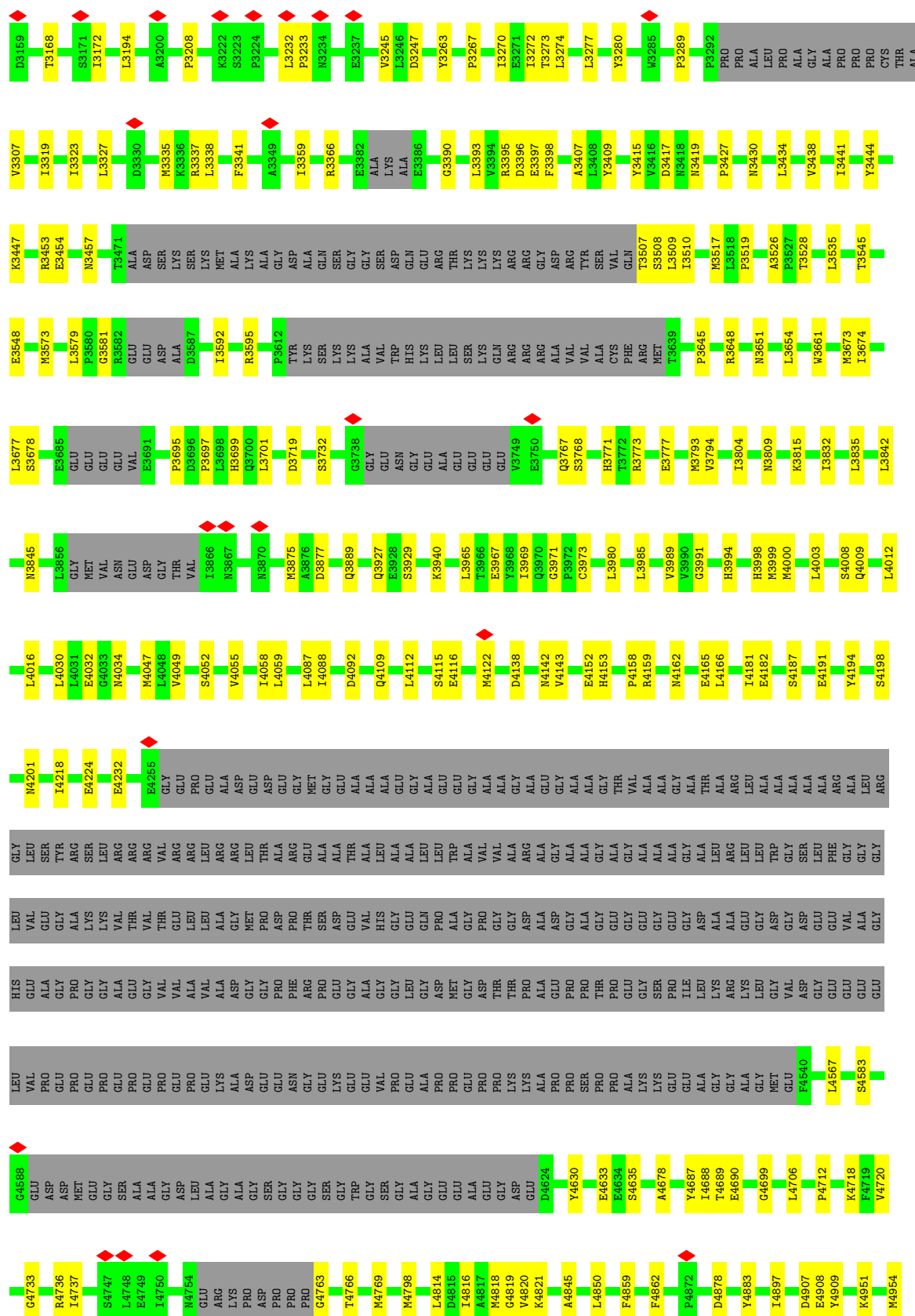




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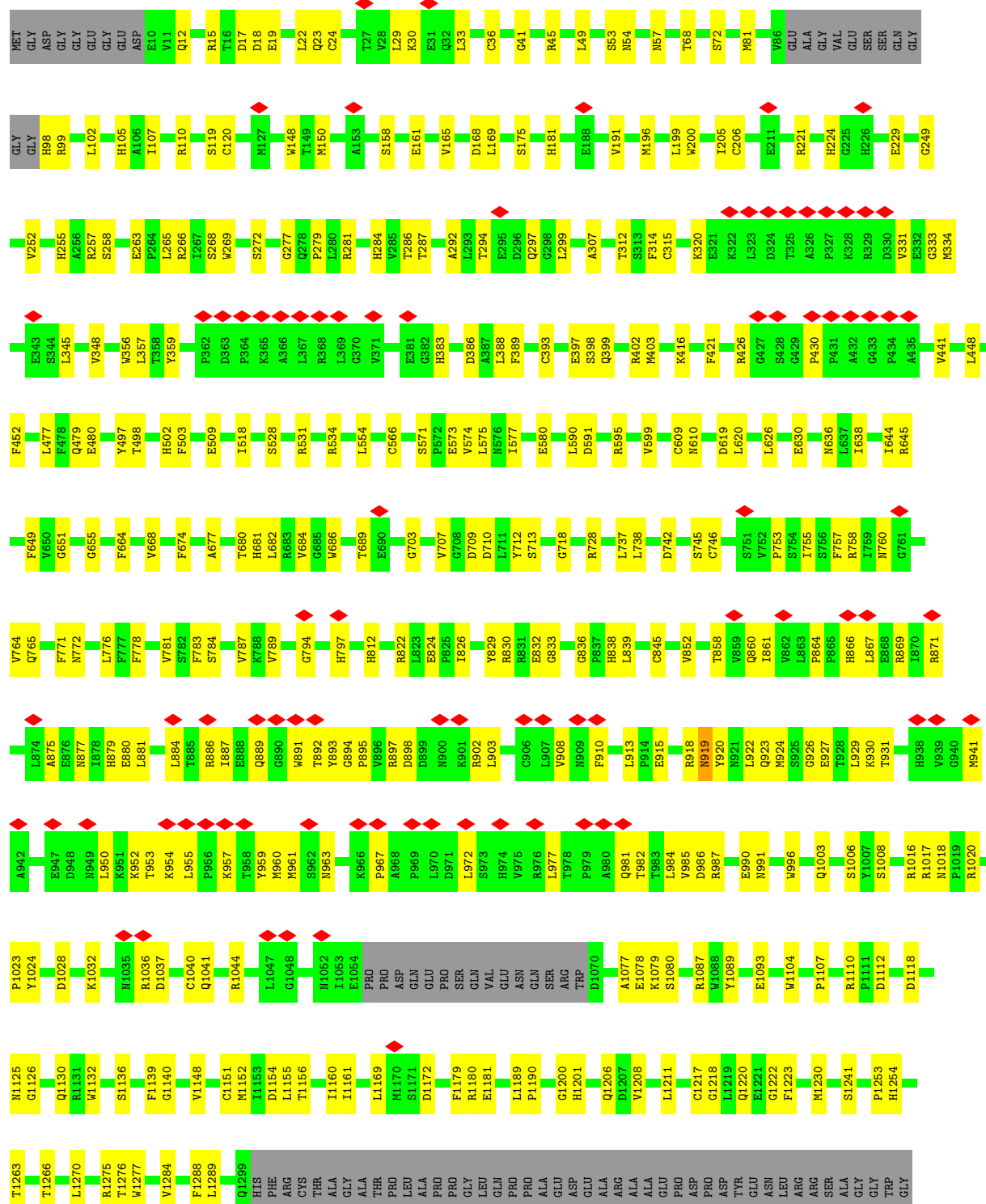






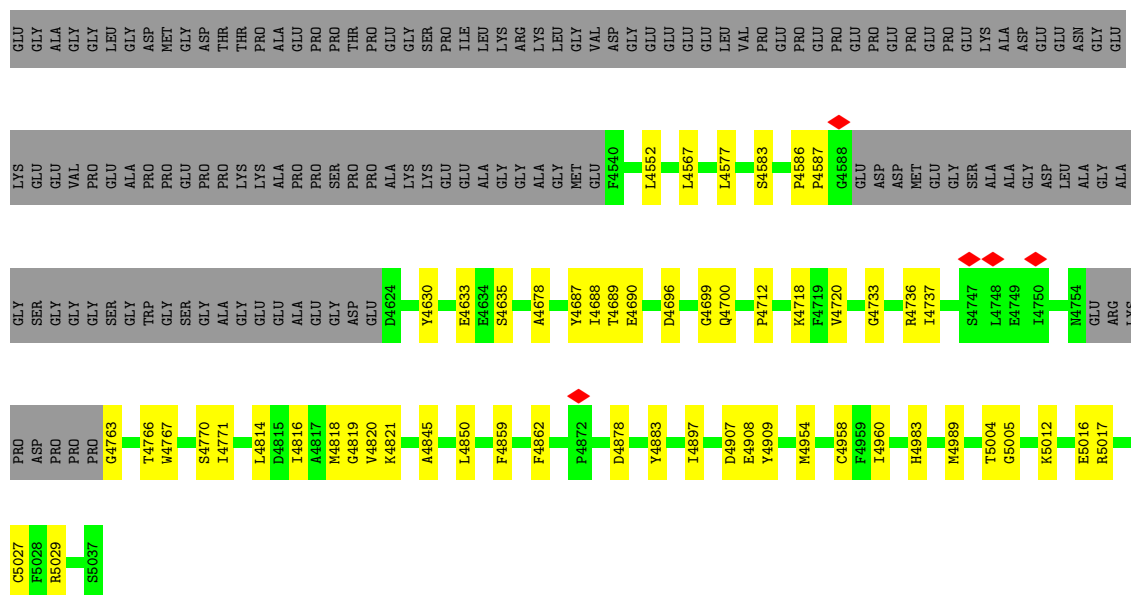


● Molecule 1: Ryanodine receptor 1



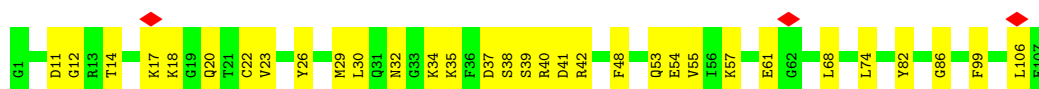
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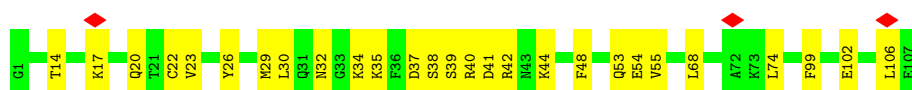
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E: 70% 30%



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

Chain F: 75% 25%



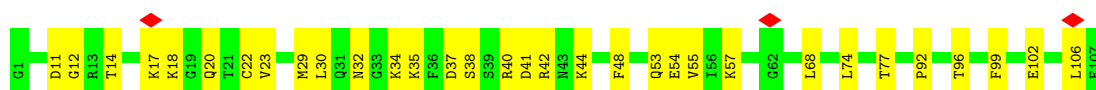
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 71% 29%



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

Chain H: 70% 30%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	249034	Depositor
Resolution determination method	OTHER	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.277	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.072	Depositor
Recommended contour level	0.32	Depositor
Map size ($\text{\AA}$)	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ZN, U1C

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	0.11	0/33082	0.29	0/45015
1	B	0.10	0/33082	0.29	0/45015
1	C	0.11	0/33082	0.29	0/45015
1	D	0.11	0/33082	0.30	2/45015 (0.0%)
2	E	0.12	0/802	0.31	0/1086
2	F	0.14	0/802	0.36	0/1086
2	G	0.13	0/802	0.37	0/1086
2	H	0.13	0/802	0.32	0/1086
All	All	0.11	0/135536	0.29	2/184404 (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	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	832	GLU	CB-CA-C	5.61	120.52	111.05
1	D	832	GLU	CB-CG-CD	5.13	121.33	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	626	LEU	Peptide
1	B	626	LEU	Peptide
1	C	626	LEU	Peptide
1	D	626	LEU	Peptide

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	32374	0	30869	532	0
1	B	32374	0	30869	511	0
1	C	32374	0	30869	533	0
1	D	32374	0	30869	537	0
2	E	786	0	766	22	0
2	F	786	0	766	20	0
2	G	786	0	766	21	0
2	H	786	0	766	26	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	31	0	12	0	0
4	B	31	0	12	0	0
4	C	31	0	12	0	0
4	D	31	0	12	0	0
5	A	23	0	0	0	0
5	B	23	0	0	0	0
5	C	23	0	0	0	0
5	D	23	0	0	0	0
All	All	132860	0	126588	2178	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 2178 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:D:830:ARG:HD3	1:D:1612:PHE:CE2	1.70	1.26
1:D:1454:THR:CG2	1:D:1456:ASP:OD1	2.09	0.99
1:D:830:ARG:CD	1:D:1612:PHE:CE2	2.45	0.99
1:D:1454:THR:HG23	1:D:1456:ASP:OD1	1.63	0.97
1:B:4763:GLY:N	1:B:4766:THR:HG1	1.64	0.94

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	A	4214/5037 (84%)	3883 (92%)	329 (8%)	2 (0%)	100	100
1	B	4214/5037 (84%)	3873 (92%)	340 (8%)	1 (0%)	100	100
1	C	4214/5037 (84%)	3878 (92%)	334 (8%)	2 (0%)	100	100
1	D	4214/5037 (84%)	3886 (92%)	327 (8%)	1 (0%)	100	100
2	E	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
2	F	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	G	105/107 (98%)	89 (85%)	16 (15%)	0	100	100
2	H	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
All	All	17276/20576 (84%)	15878 (92%)	1392 (8%)	6 (0%)	100	100

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	862	VAL
1	C	899	ASP
1	A	1023	PRO
1	C	1023	PRO
1	D	1023	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3334/4276 (78%)	3333 (100%)	1 (0%)	100	100
1	B	3334/4276 (78%)	3328 (100%)	6 (0%)	87	87
1	C	3334/4276 (78%)	3329 (100%)	5 (0%)	88	89
1	D	3334/4276 (78%)	3330 (100%)	4 (0%)	88	89
2	E	80/88 (91%)	79 (99%)	1 (1%)	61	73
2	F	80/88 (91%)	80 (100%)	0	100	100
2	G	80/88 (91%)	79 (99%)	1 (1%)	61	73
2	H	80/88 (91%)	80 (100%)	0	100	100
All	All	13656/17456 (78%)	13638 (100%)	18 (0%)	87	89

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2382	GLU
2	G	61	GLU
2	E	61	GLU
1	C	919	ASN
1	D	1435	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 170 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	3109	ASN
1	D	2125	HIS
1	C	3850	GLN
1	D	617	ASN
1	D	2788	HIS

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 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	ATP	C	5102	-	32,33,33	0.26	0	48,52,52	0.27	0
4	ATP	D	5102	-	32,33,33	0.26	0	48,52,52	0.27	0
5	U1C	B	5103	-	25,25,25	6.18	16 (64%)	33,35,35	3.39	15 (45%)
5	U1C	D	5103	-	25,25,25	6.18	16 (64%)	33,35,35	3.38	15 (45%)
5	U1C	C	5103	-	25,25,25	6.19	16 (64%)	33,35,35	3.38	15 (45%)
4	ATP	B	5102	-	32,33,33	0.27	0	48,52,52	0.27	0
4	ATP	A	5102	-	32,33,33	0.26	0	48,52,52	0.27	0
5	U1C	A	5103	-	25,25,25	6.19	16 (64%)	33,35,35	3.39	15 (45%)

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	ATP	C	5102	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5102	-	-	9/22/38/38	0/3/3/3
5	U1C	B	5103	-	-	7/11/25/25	0/3/3/3
5	U1C	D	5103	-	-	7/11/25/25	0/3/3/3
5	U1C	C	5103	-	-	7/11/25/25	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	B	5102	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5102	-	-	9/22/38/38	0/3/3/3
5	U1C	A	5103	-	-	7/11/25/25	0/3/3/3

The worst 5 of 64 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	5103	U1C	C1-N2	-18.77	1.32	1.45
5	A	5103	U1C	C1-N2	-18.76	1.32	1.45
5	D	5103	U1C	C1-N2	-18.64	1.32	1.45
5	B	5103	U1C	C1-N2	-18.59	1.32	1.45
5	B	5103	U1C	C1-C2	-10.54	1.39	1.51

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	5103	U1C	C2-C1-N2	8.41	106.93	101.45
5	B	5103	U1C	C2-C1-N2	8.40	106.92	101.45
5	A	5103	U1C	C2-C1-N2	8.38	106.91	101.45
5	D	5103	U1C	C2-C1-N2	8.37	106.90	101.45
5	B	5103	U1C	O3-C8-C9	7.50	125.61	116.73

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

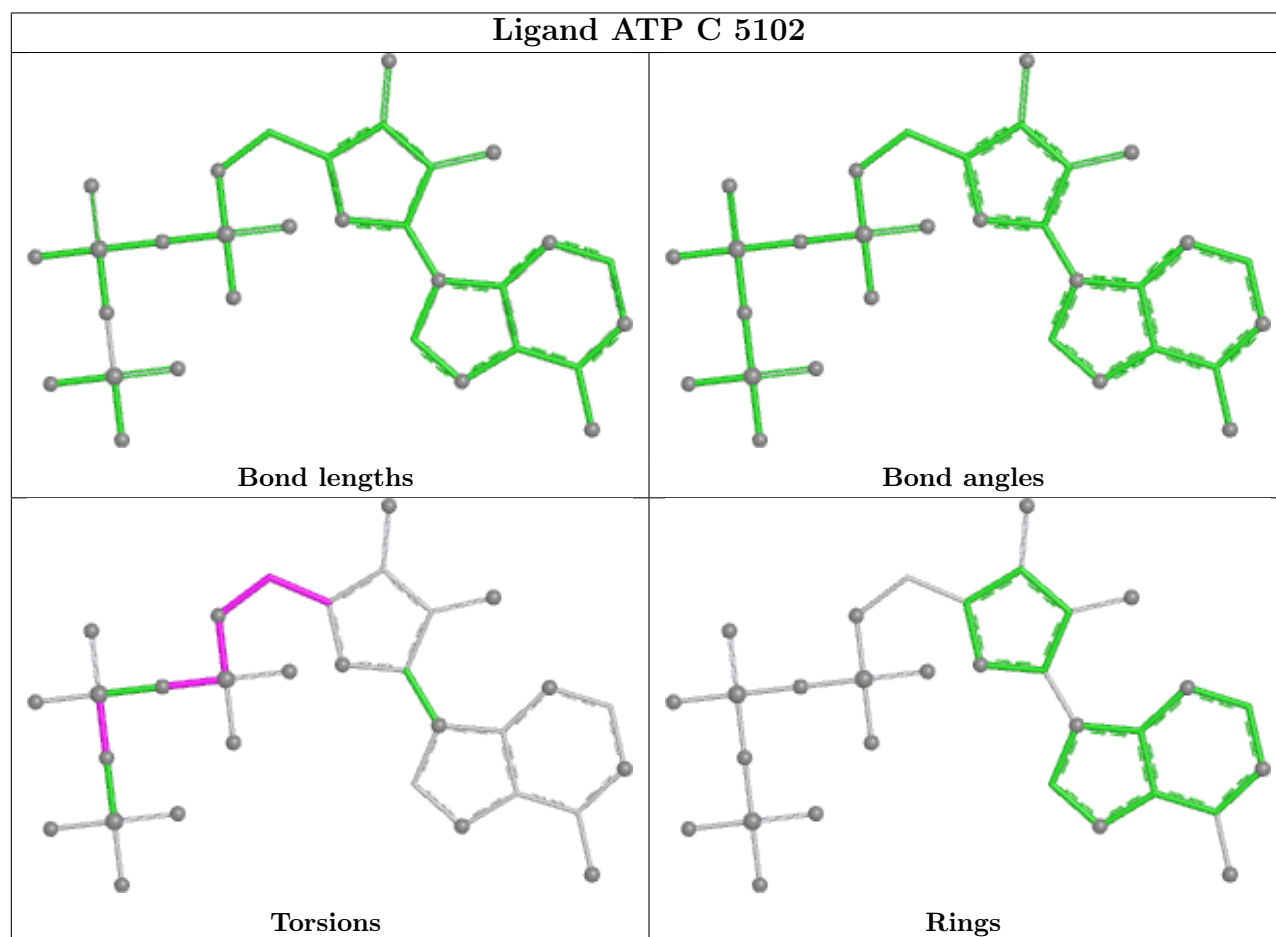
Mol	Chain	Res	Type	Atoms
4	A	5102	ATP	C5'-O5'-PA-O1A
4	A	5102	ATP	C5'-O5'-PA-O2A
4	A	5102	ATP	C5'-O5'-PA-O3A
4	A	5102	ATP	O4'-C4'-C5'-O5'
4	B	5102	ATP	C5'-O5'-PA-O1A

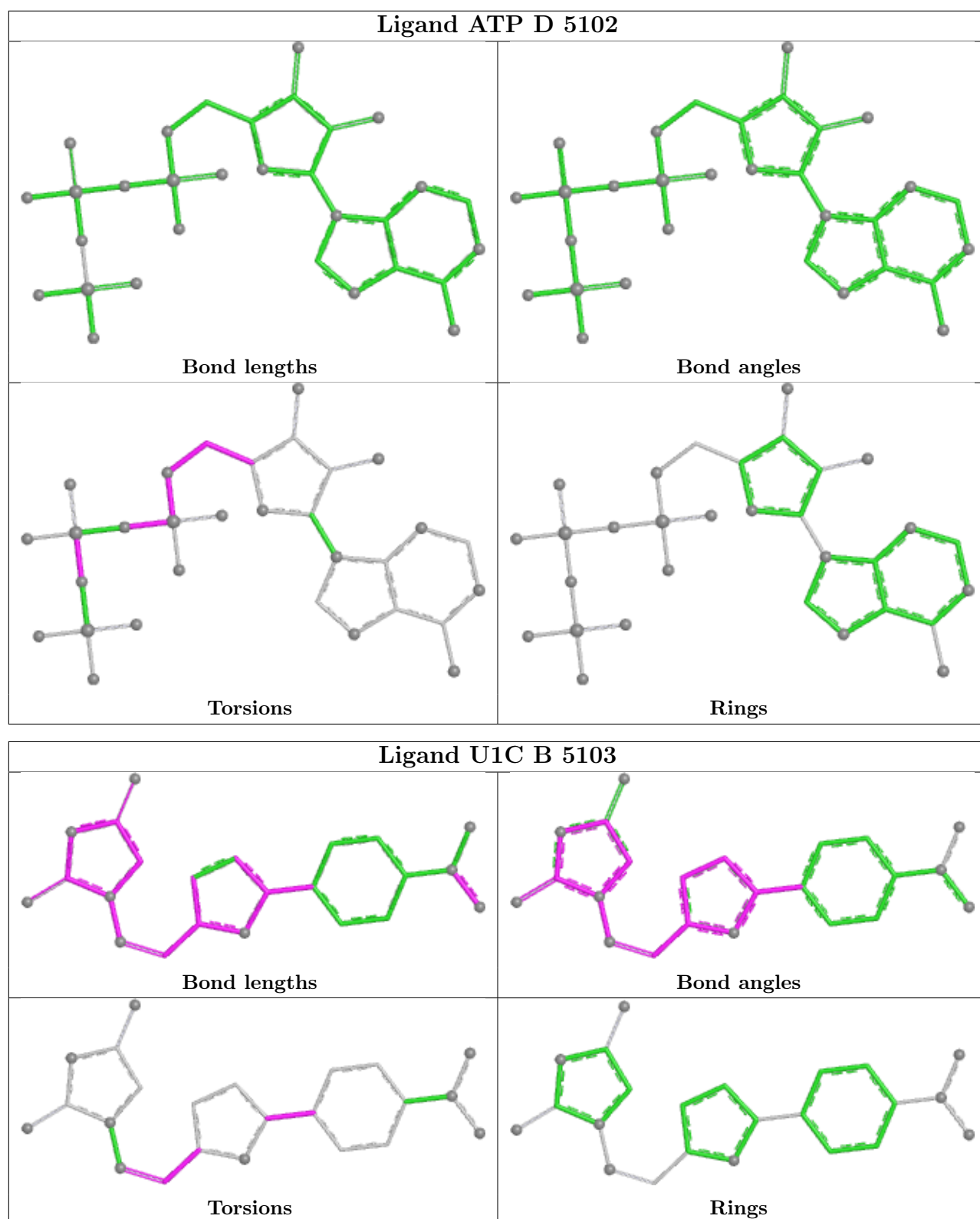
There are no ring outliers.

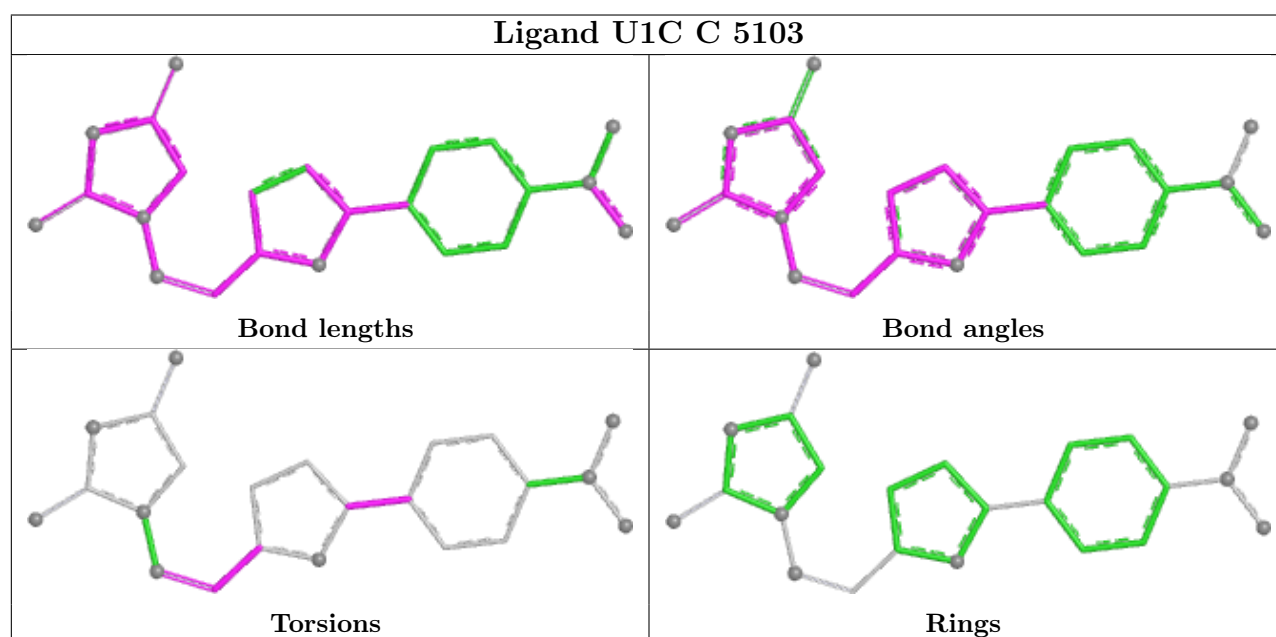
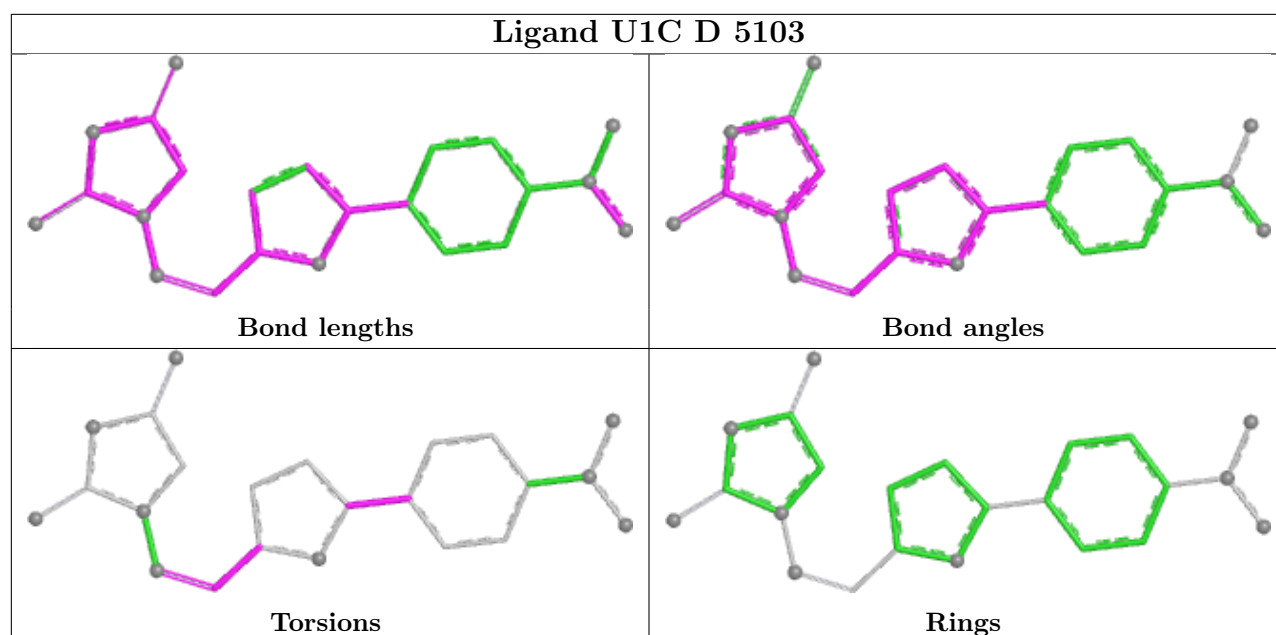
No monomer is involved in short contacts.

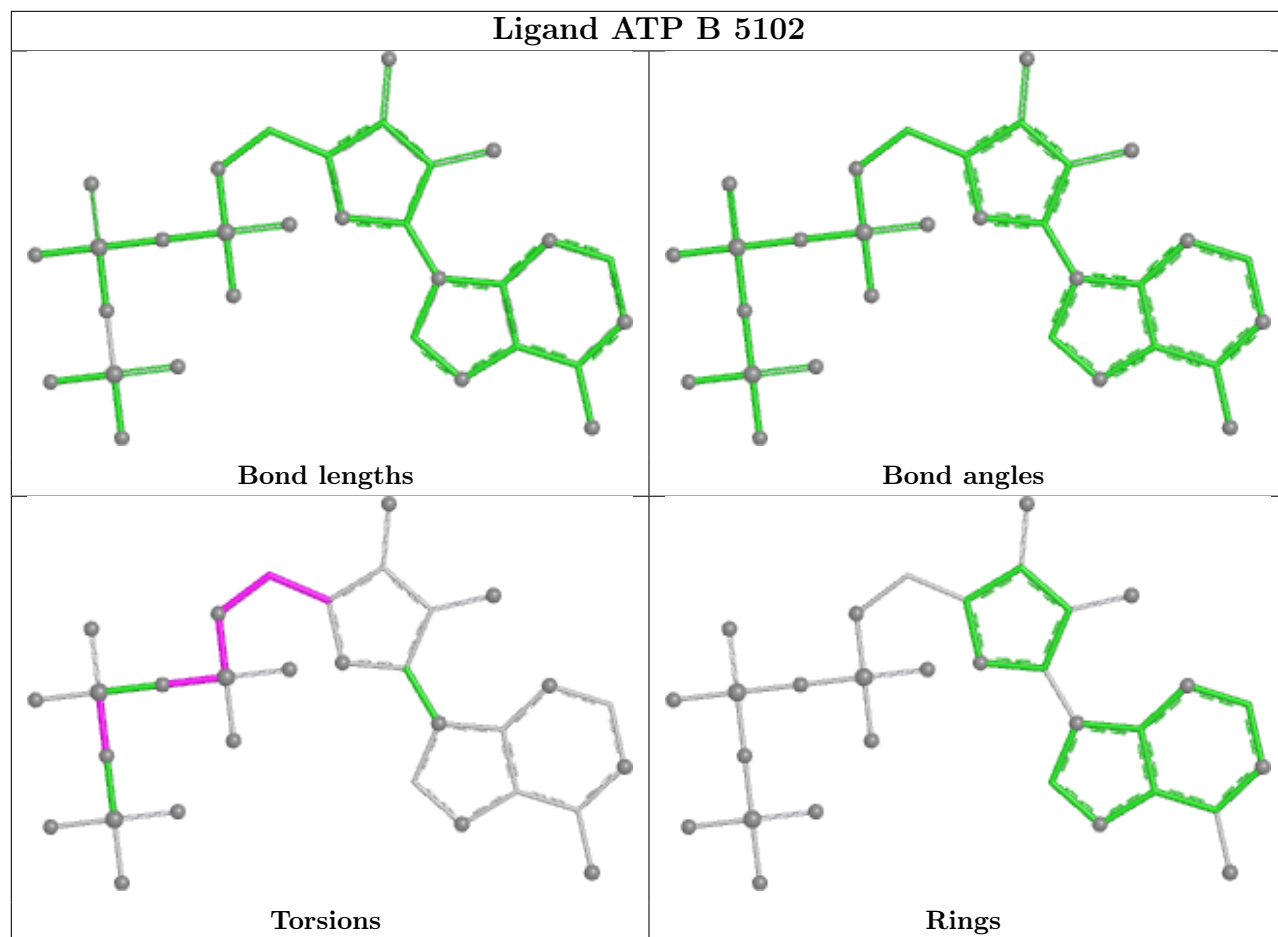
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

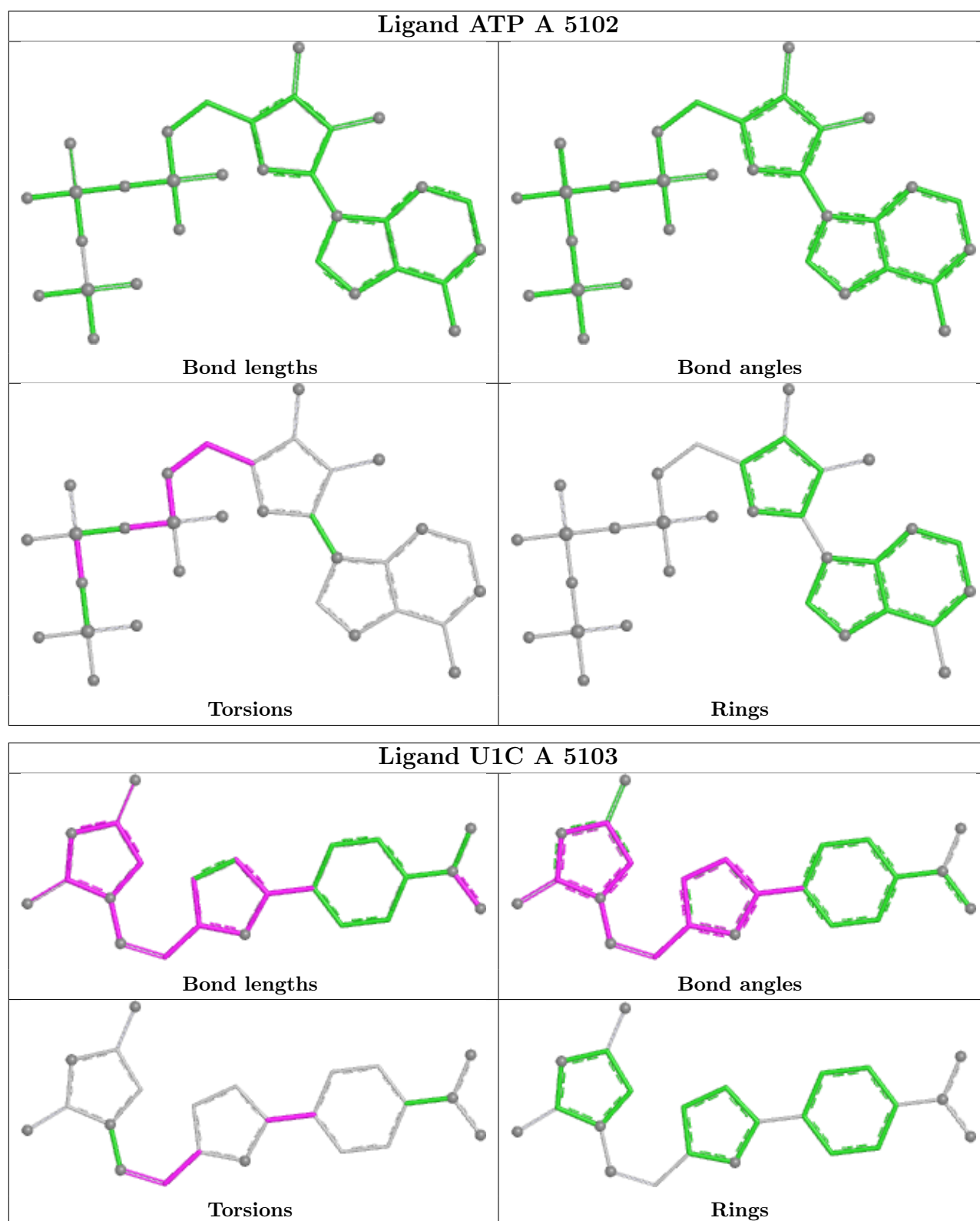
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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

There are no chain breaks in this entry.

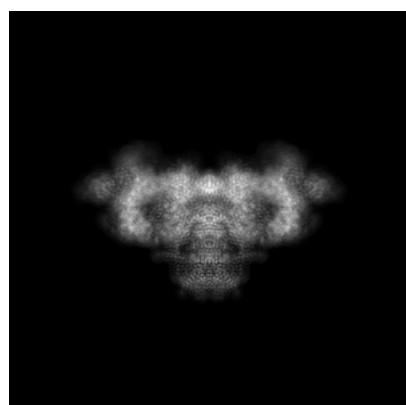
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45584. These allow visual inspection of the internal detail of the map and identification of artifacts.

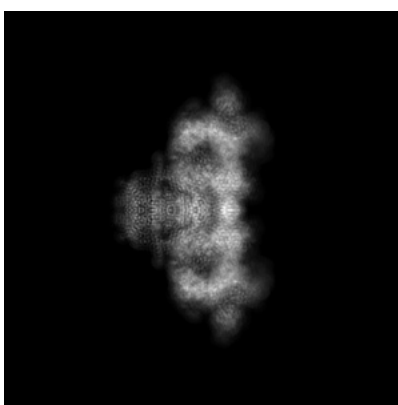
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

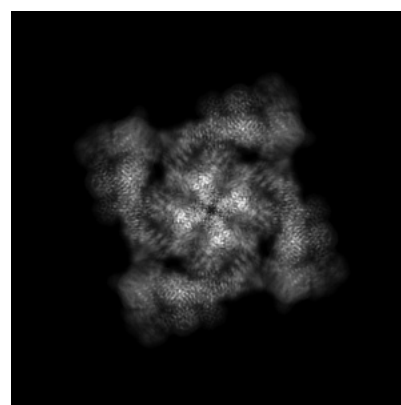
6.1.1 Primary map



X



Y

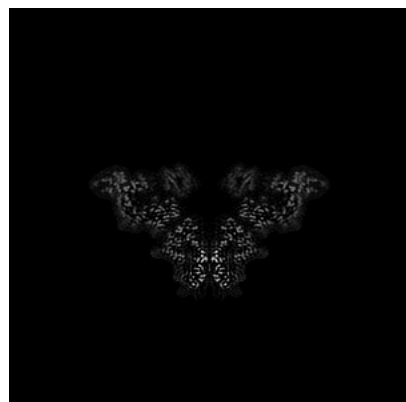


Z

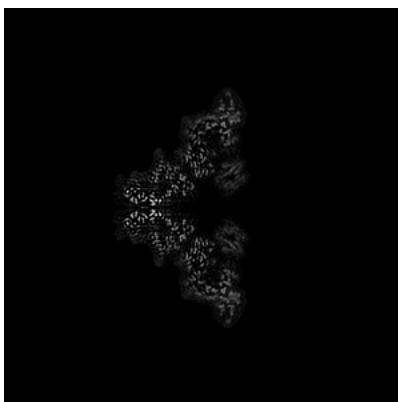
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

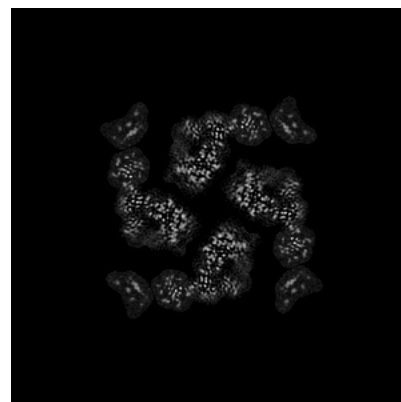
6.2.1 Primary map



X Index: 232



Y Index: 232

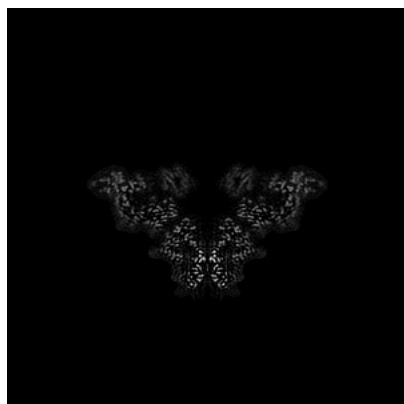


Z Index: 232

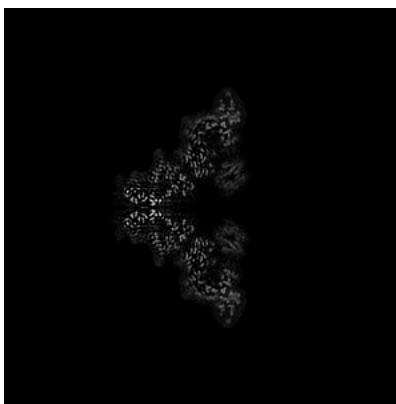
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

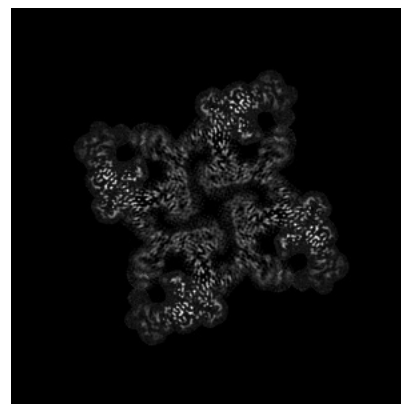
6.3.1 Primary map



X Index: 232



Y Index: 232

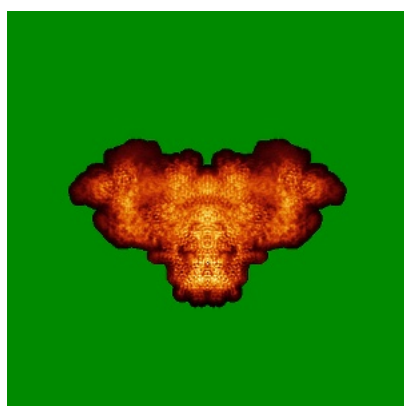


Z Index: 261

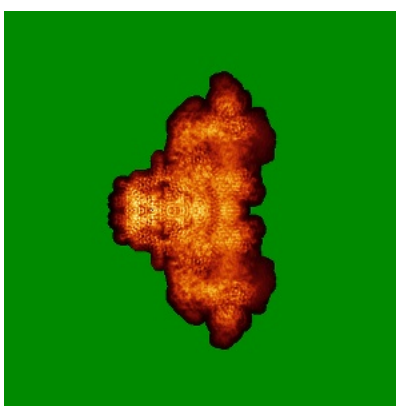
The images above show the largest variance slices of the map in three orthogonal directions.

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

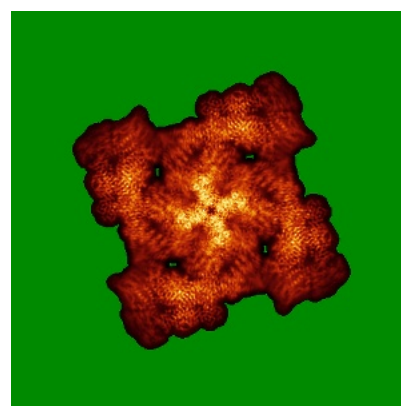
6.4.1 Primary map



X



Y

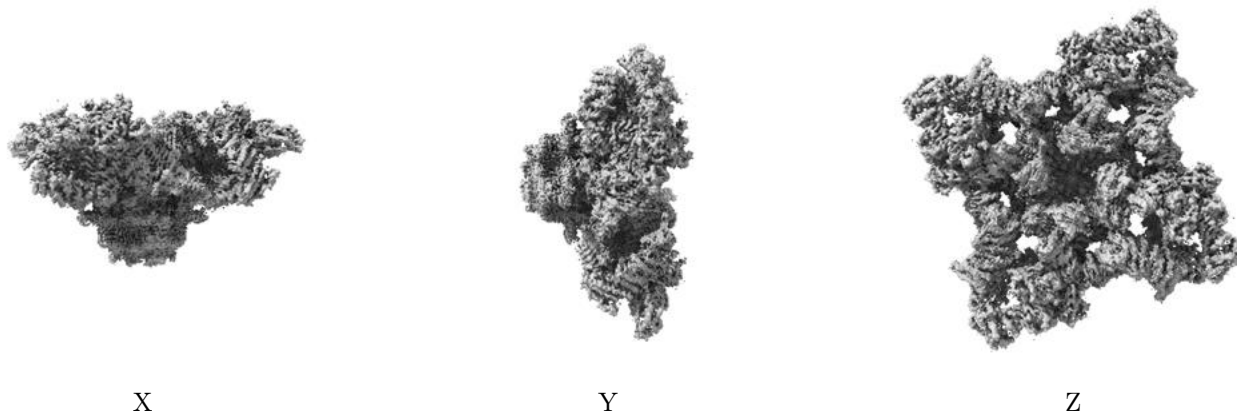


Z

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 0.32. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

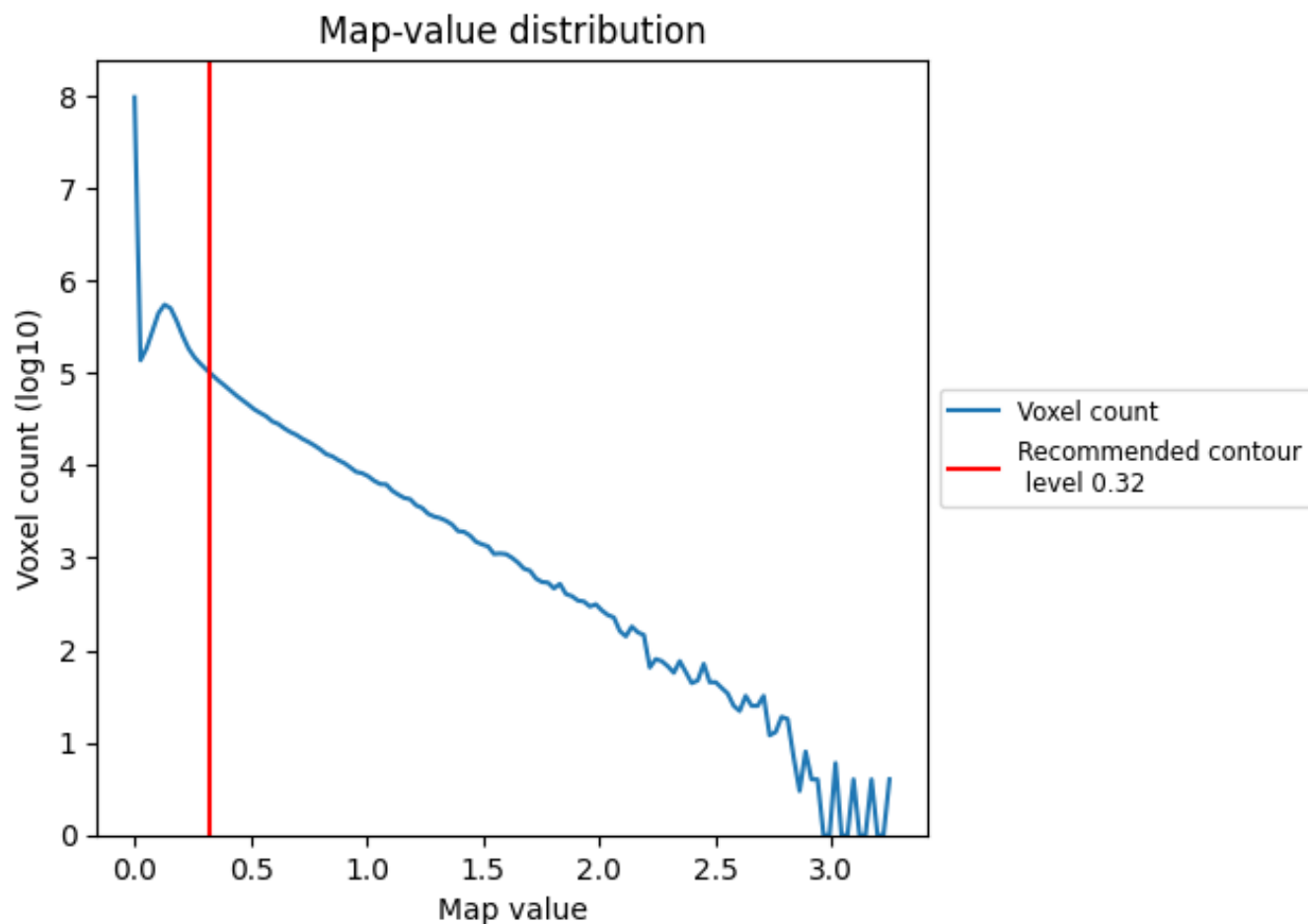
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

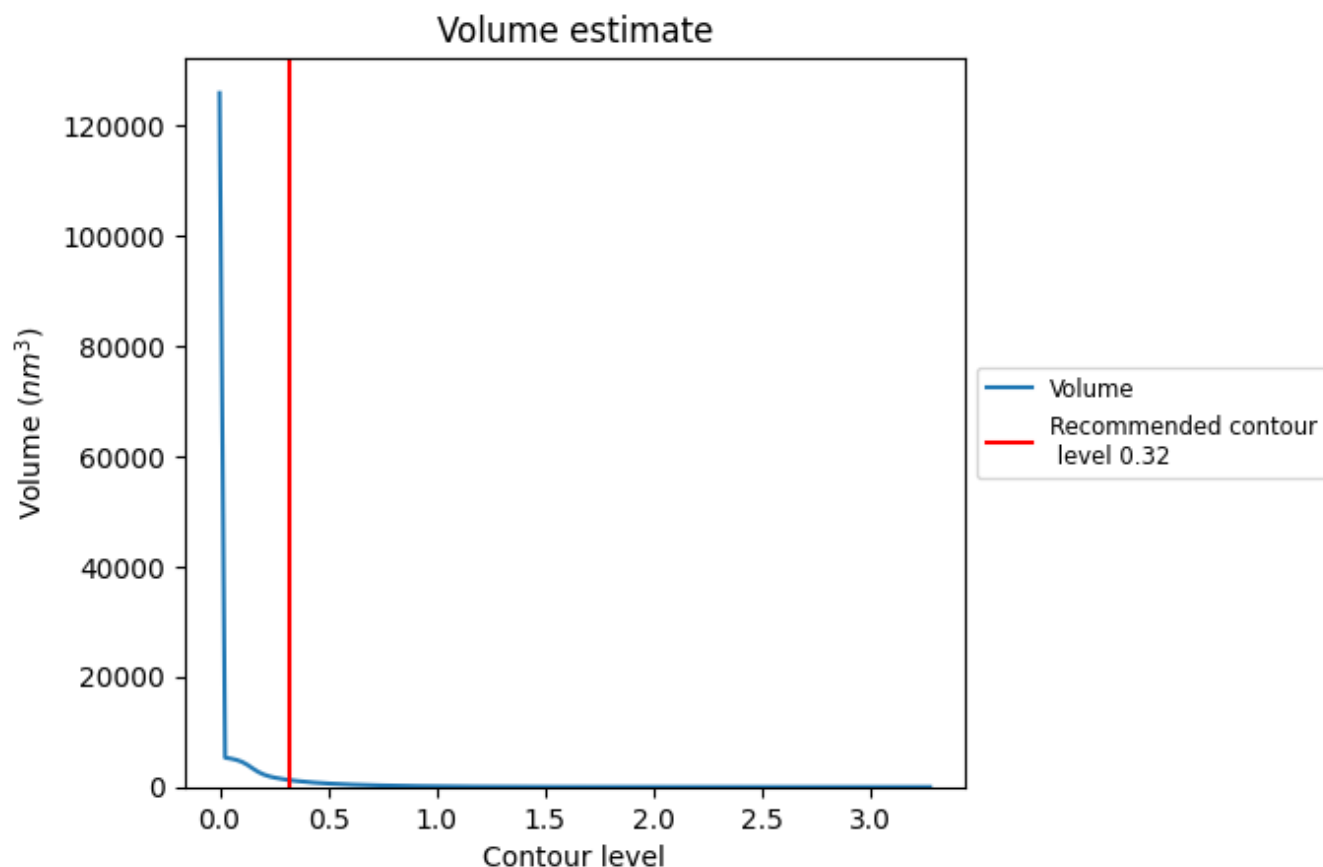
This section contains the results of statistical analysis of the map.

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.

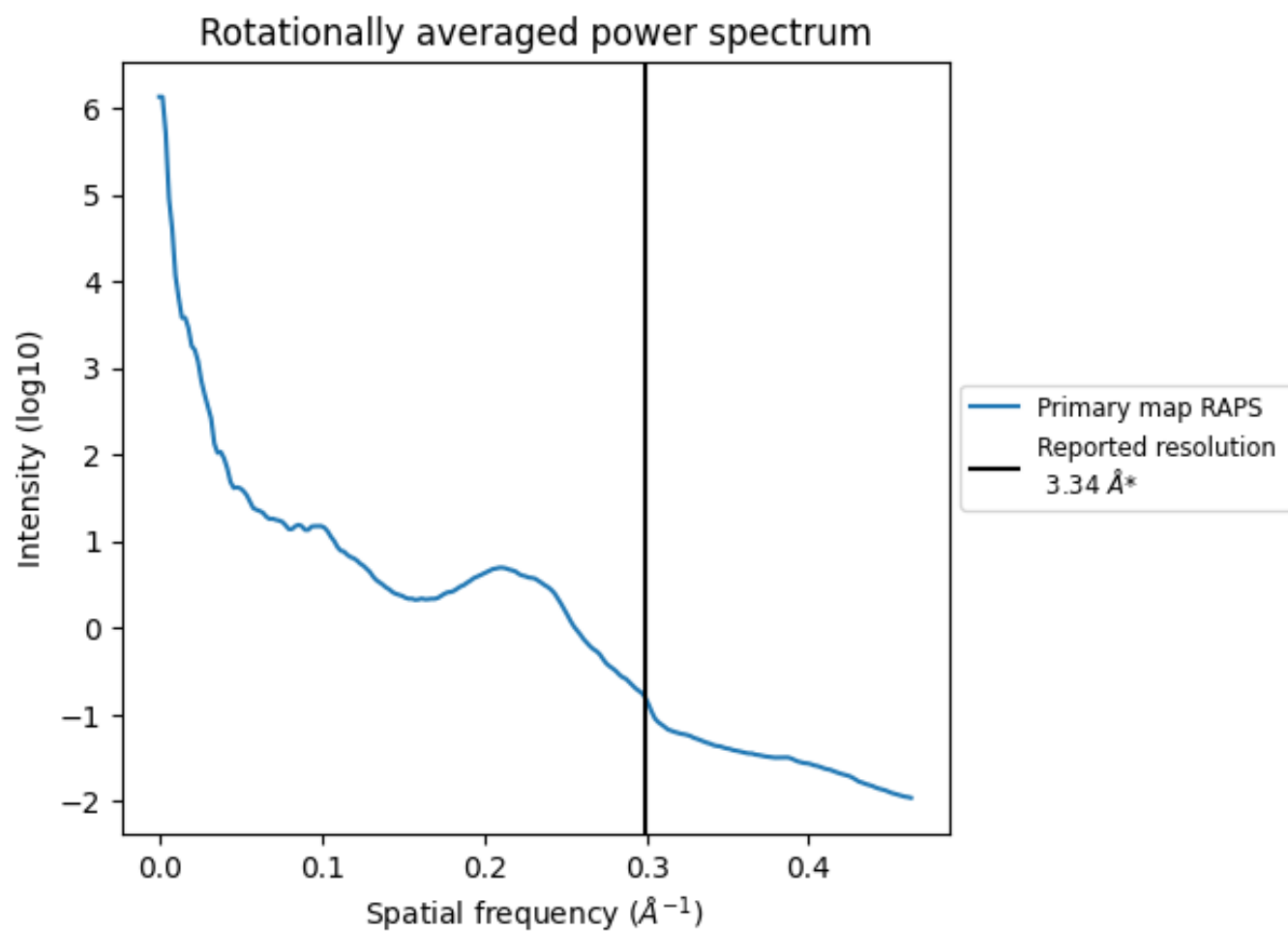
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1262 nm^3 ; this corresponds to an approximate mass of 1140 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 0.299 Å⁻¹

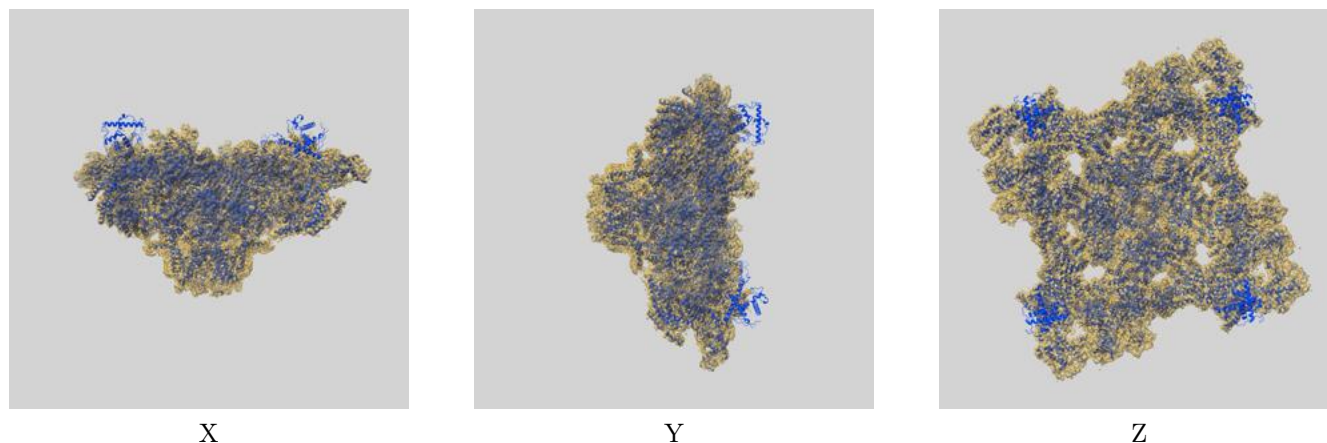
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

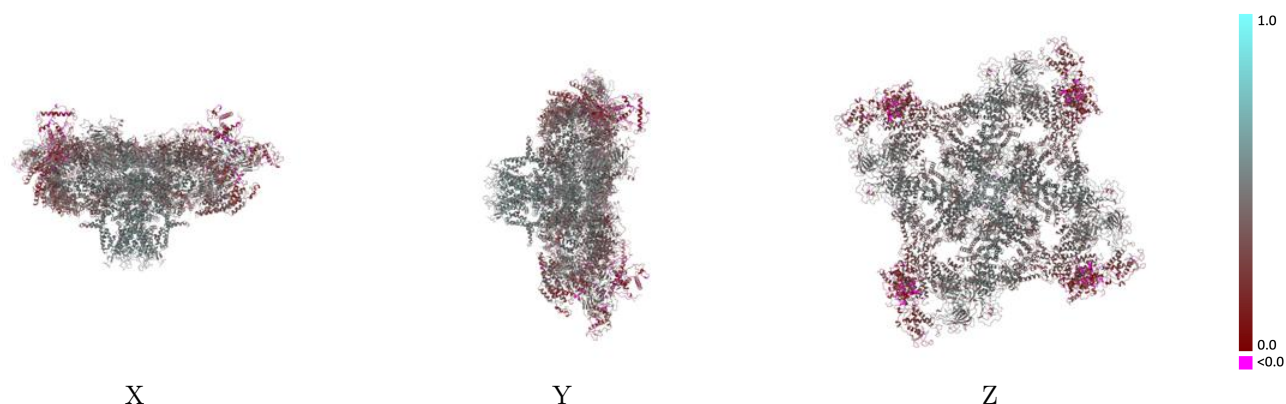
This section contains information regarding the fit between EMDB map EMD-45584 and PDB model 9CGP. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



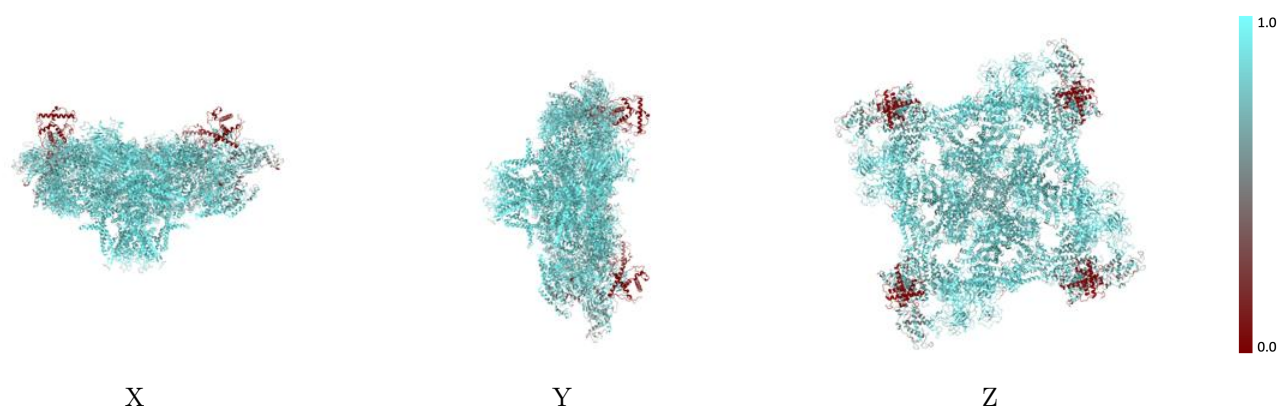
The images above show the 3D surface view of the map at the recommended contour level 0.32 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



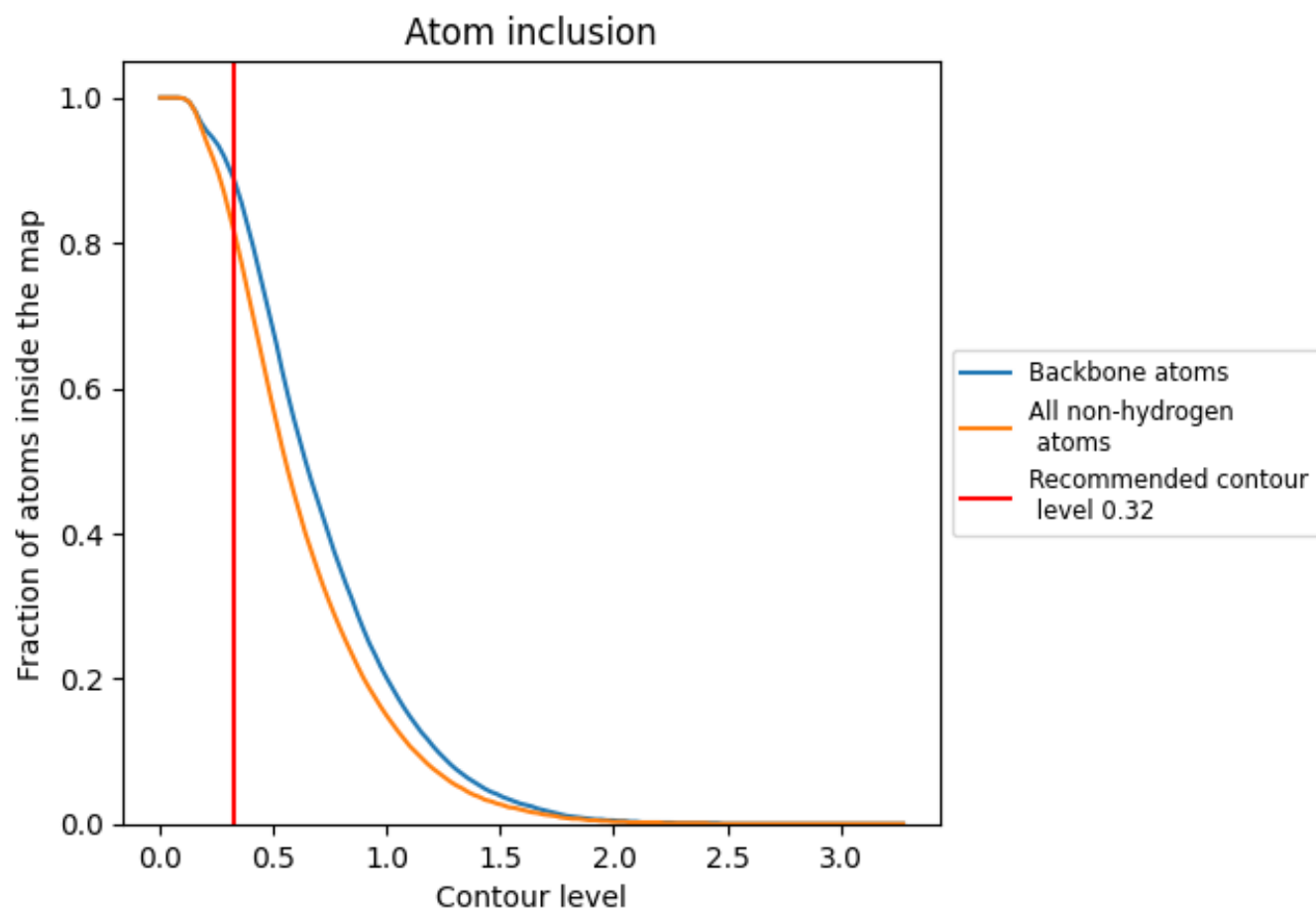
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.32).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 82% 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 (0.32) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8220	0.4080
A	0.8210	0.4070
B	0.8220	0.4080
C	0.8210	0.4070
D	0.8230	0.4080
E	0.8530	0.4190
F	0.8480	0.4210
G	0.8490	0.4200
H	0.8490	0.4230

1.0

0.0

<0.0