



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 06:40 AM UTC

PDB ID : 8UXG / pdb_00008uxg
EMDB ID : EMD-42763
Title : Structure of PKA phosphorylated human RyR2-R420W in the closed state in the presence of ARM210
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.08 Å(reported)
Based on initial model : 7UA5

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:

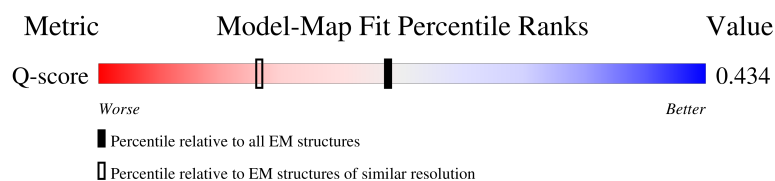
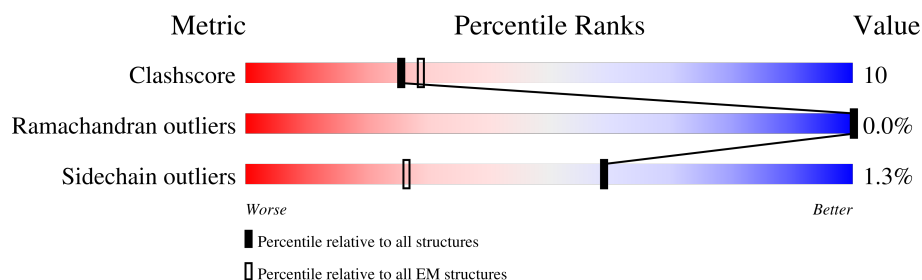
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.08 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	14000 (2.58 - 3.58)

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	4967	 65% 19% 15%
1	B	4967	 65% 19% 15%
1	C	4967	 65% 19% 15%
1	D	4967	 65% 19% 15%

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Mol	Chain	Length	Quality of chain
2	E	108	 81% 17% ..
2	F	108	 79% 19% ..
2	G	108	 81% 18% ..
2	H	108	 79% 19% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 138712 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	B	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	C	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0
1	D	4224	Total 33774	C 21521	N 5743	O 6280	S 230	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	420	TRP	ARG	variant	UNP Q92736
B	420	TRP	ARG	variant	UNP Q92736
C	420	TRP	ARG	variant	UNP Q92736
D	420	TRP	ARG	variant	UNP Q92736

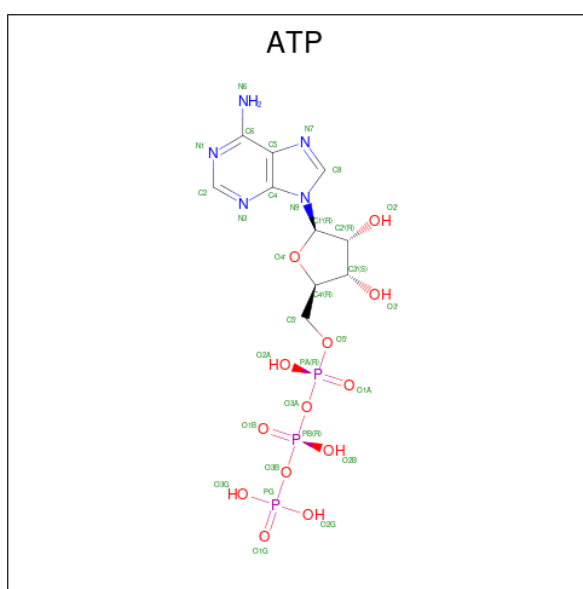
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	F	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	G	107	Total 818	C 516	N 144	O 154	S 4	0	0
2	H	107	Total 818	C 516	N 144	O 154	S 4	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).



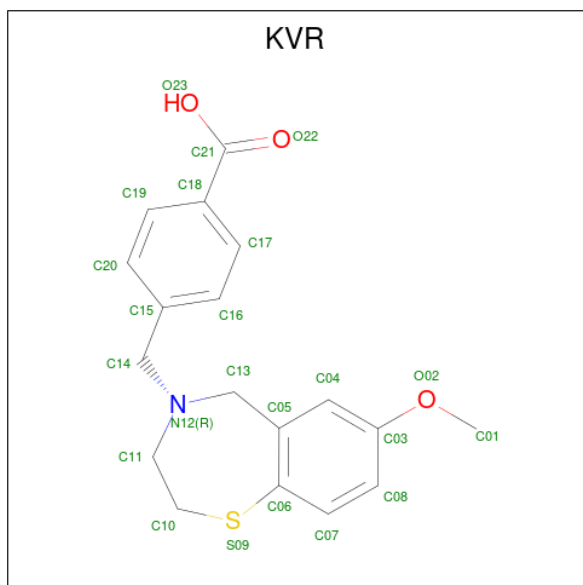
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	D	1	Total	C	N	O	P	0
			31	10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

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

- Molecule 5 is 4-[(7-methoxy-2,3-dihydro-1,4-benzothiazepin-4(5H)-yl)methyl]benzoic acid (CCD ID: KVR) (formula: C₁₈H₁₉NO₃S) (labeled as "Ligand of Interest" by depositor).



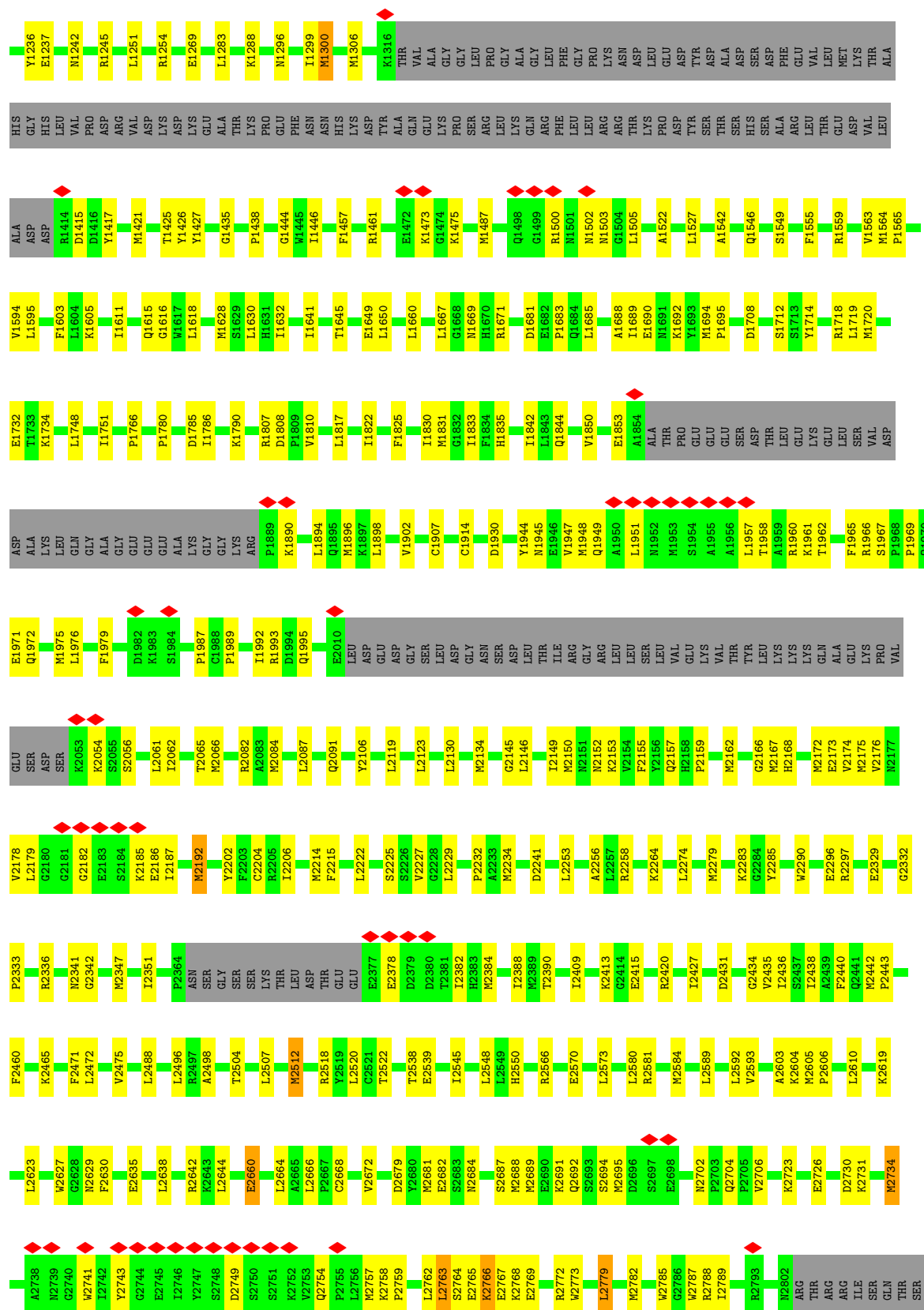
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
5	A	1	23	18	1	3	1	0
5	B	1	23	18	1	3	1	0
5	C	1	23	18	1	3	1	0
5	D	1	23	18	1	3	1	0

3 Residue-property plots

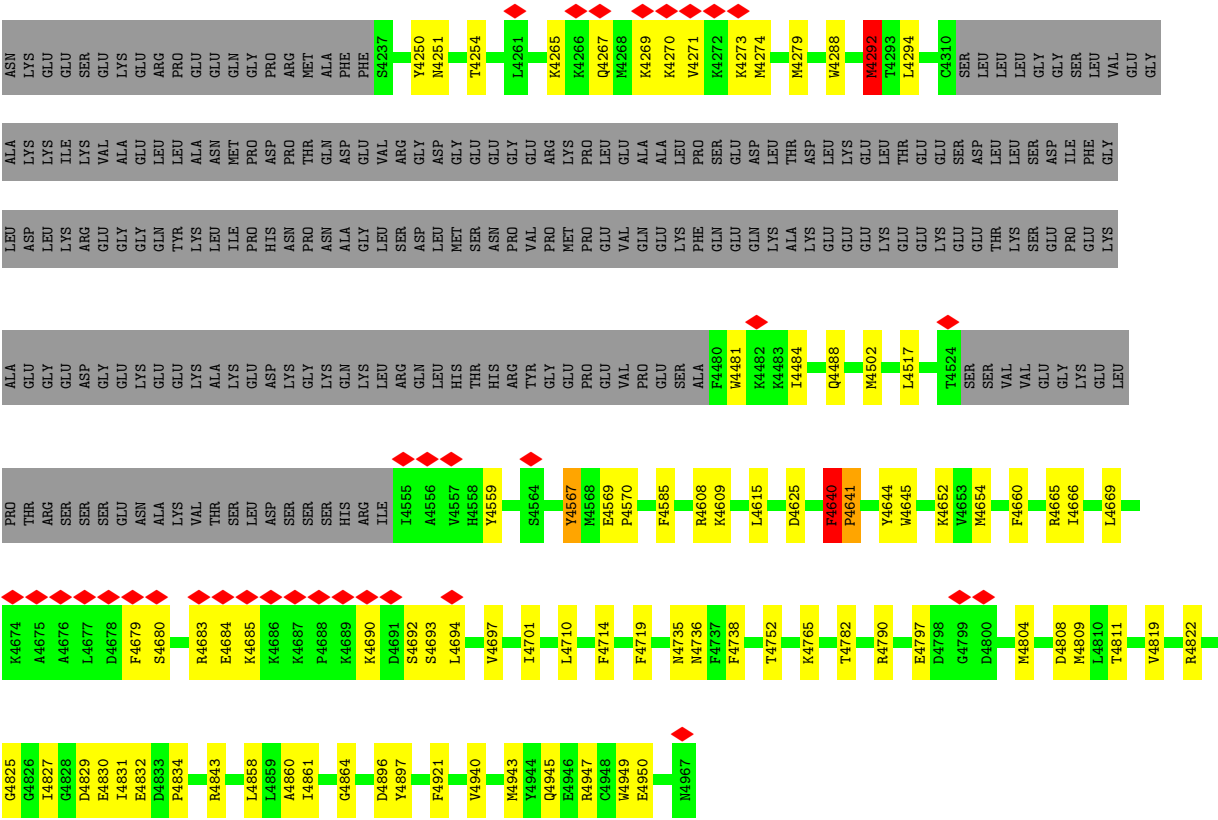
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Ryanodine receptor 2

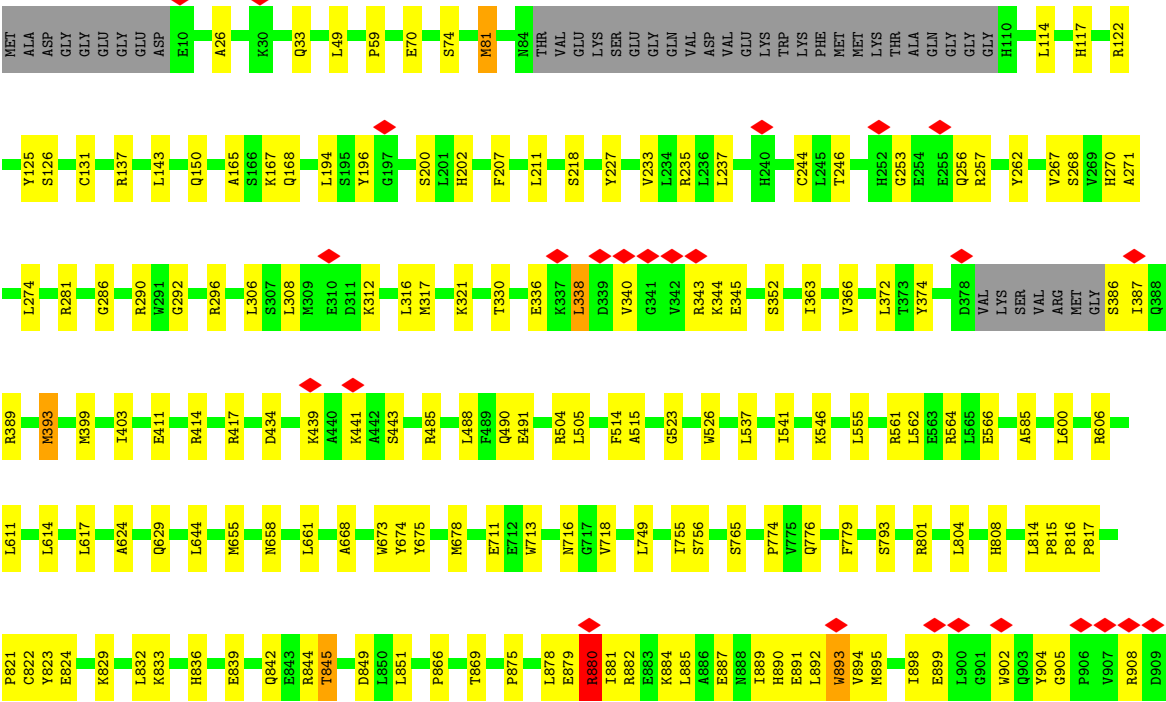




F4048	A4051	M4052	H4055	T4059	Q4060	S4061	E4062	T4063	E4064	F4065	L4066	A4070	E4071	T4072	D4073	E4074	N4075	K4085	R4086	F4087	H4088	E4089	P4090	D4093	T4094	E4137	R4147	R4170	E4179	E4182	K4183	E4187	E4194	A4203	T4206	S4209	ASP	LEU	ASN	ASN	GLU	ARG	SER	ALA				
G3926	P3927	D3942	R3943	V3944	V3945	G3946	V3950	M3954	Q3955	R3956	K3957	L3958	I3965	E3966	L3967	K3968	E3970	L3971	M3972	Q3975	V3979	V3980	M3981	M3985	M3999	S4006	M4019	K4022	L4026	T4027	S4028	K4033	E4034	Y4035	D4036	P4037	D4038	G4039	K4040	G4041	V4042	I4043	S4044	K4045				
M3719	A3729	R3730	L3731	H3732	M3739	L3793	L3796	M3797	A3807	L3817	G3818	M3819	V3820	T3821	E3822	G3824	S3825	G3826	E3827	K3828	Q3831	F3835	L3846	F3854	I3870	V3881	Q3882	E3883	I3885	Y3891	Y3892	K3895	D3899	N3918	T3919	L3920	T3921	I3924	Q3925									
TRP	HIS	LEU	LEU	SER	LYS	GLN	ARG	ARG	ALA	V3599	V3600	A3601	F3602	F3603	R3604	M3605	R3615	K3639	I3640	I3641	A3649	E3650	F3651	P3652	E3653	E3654	D3655	E3656	G3657	T3658	K3659	L3664	I3668	F3671	L3687	K3697	S3698	C3699	H3700	D3701	E3702	GLU	ASP	ASP	GLY	GLU	GLU	E3710
GLN	MET	ALA	LEU	TYR	ASP	LEU	PRO	ARG	THR	ASP	THR	SER	ASP	PRO	GLY	LYS	THR	GLU	ALA	ASP	ILE	VAL	LEU	VAL	PHE	HIS	LEU	GLN	LYS	SER	LYS	VAL	GLY	LEU	VAL	GLY	HIS	PRO	GLN	THR	LYS	LYS	ALA	VAL				
SER	LYS	SER	HIS	ASN	PHE	LEU	ARG	GLN	ASN	PHE	VAL	VAL	ASN	GLN	ALA	ASP	ILE	GLU	ALA	ASP	THR	ILE	THR	ASP	THR	LYS	THR	LEU	ASP	GLN	ASP	ILE	ARG	GLY	ASP	ARG	TYR	VAL	ALA	GLU	THR	ILE	LEU	ARG	ILE			
ASP	MET	SER	GLU	ALA	GLU	LEU	ILE	LEU	ASP	THR	THR	THR	GLU	ARG	ASP	LEU	ALA	PHE	TYR	PRO	LEU	LEU	ILE	LEU	ASP	TYR	ASN	LYS	TRP	LEU	LYS	GLU	PRO	ASN	GLU	PRO	GLU	PRO	GLU	ASP	VAL	ALA	HIS	LEU	ALA	ARG	GLY	
N3269	S3270	E3271	M3272	H3273	L3276	L3277	I3280	L3281	I3284	Y3285	G3288	G3289	I3290	E3291	M3296	L3299	Q3304	I3307	L3314	L3315	K3316	T3317	H3318	F3319	L3320	P3321	L3322	M3323	G3324	K3325	L3326	K3327	K3328	T3332	V3333	V3334	E3337	ASP	HIS	LEU	LYS	ALA	GLU	ARG	GLY			
P3167	V3168	L3171	H3174	L3175	T3183	Y3184	K3187	S3188	S3189	R3190	R3192	P3198	V3204	L3211	E3212	K3213	L3214	M3215	G3216	E3217	I3218	V3219	E3223	R3227	Y3228	T3229	Q3230	H3233	V3234	M3235	I3238	L3239	P3240	M3241	Y3245	R3248	M3249	K3250	E3251	M3256	R3260	T3266						
Q3079	F3080	T3081	HIS	THR	ARG	ASN	GLN	PRO	K3088	Y3096	L3102	P3103	M3104	L3108	F3109	I3112	H3115	Q3116	F3117	G3118	E3119	T3122	L3123	D3125	V3126	Q3127	V3128	S3129	I3133	L3134	T3135	S3136	L3137	Y3138	K3144	V3148	E3149	R3150	R3152	L3155	L3159	F3162	F3166					
L2983	R2988	P2989	S2997	E3000	K3001	E3002	T3005	S3006	L3011	L3014	R3018	I3019	S3020	L3021	F3022	D3025	I3029	L3033	H3034	I3035	Q3038	T3039	L3040	D3041	A3042	R3043	T3044	V3045	M3046	K3047	L3050	E3051	S3052	V3053	K3054	A3059	M3063	K3070	T3071	K3072	E3073	N3074	L2970	R2979	F2982			
D2891	I2892	K2893	K2894	F2895	L2896	S2904	R2905	K2908	D2909	L2910	L2911	L2912	D2913	T2914	P2915	S2916	I2917	E2918	K2919	R2920	F2921	Q2927	R2931	D2934	Q2938	E2942	F2943	D2944	G2945	G2946	S2947	R2948	G2949	K2950	G2951	E2952	H2953	F2954	Y2955	E2957	L2960	V2966	P2969	L2970	R2979	F2982		
SER	VAL	ASP	ALA	HIS	G2820	Y2821	S2822	F2823	R2824	K2825	I2826	M2830	V2831	T2832	L2833	S2834	R2835	E2836	L2837	M2840	M2844	H2849	V2852	K2853	K2854	K2855	K2856	K2857	E2858	E2859	L2860	E2861	G2864	G2865	G2866	V2867	H2868	Y2874	D2875	T2876	L2877	T2878	E2881	K2884	R2885	E2887	Q2890	



● Molecule 1: Ryanodine receptor 2

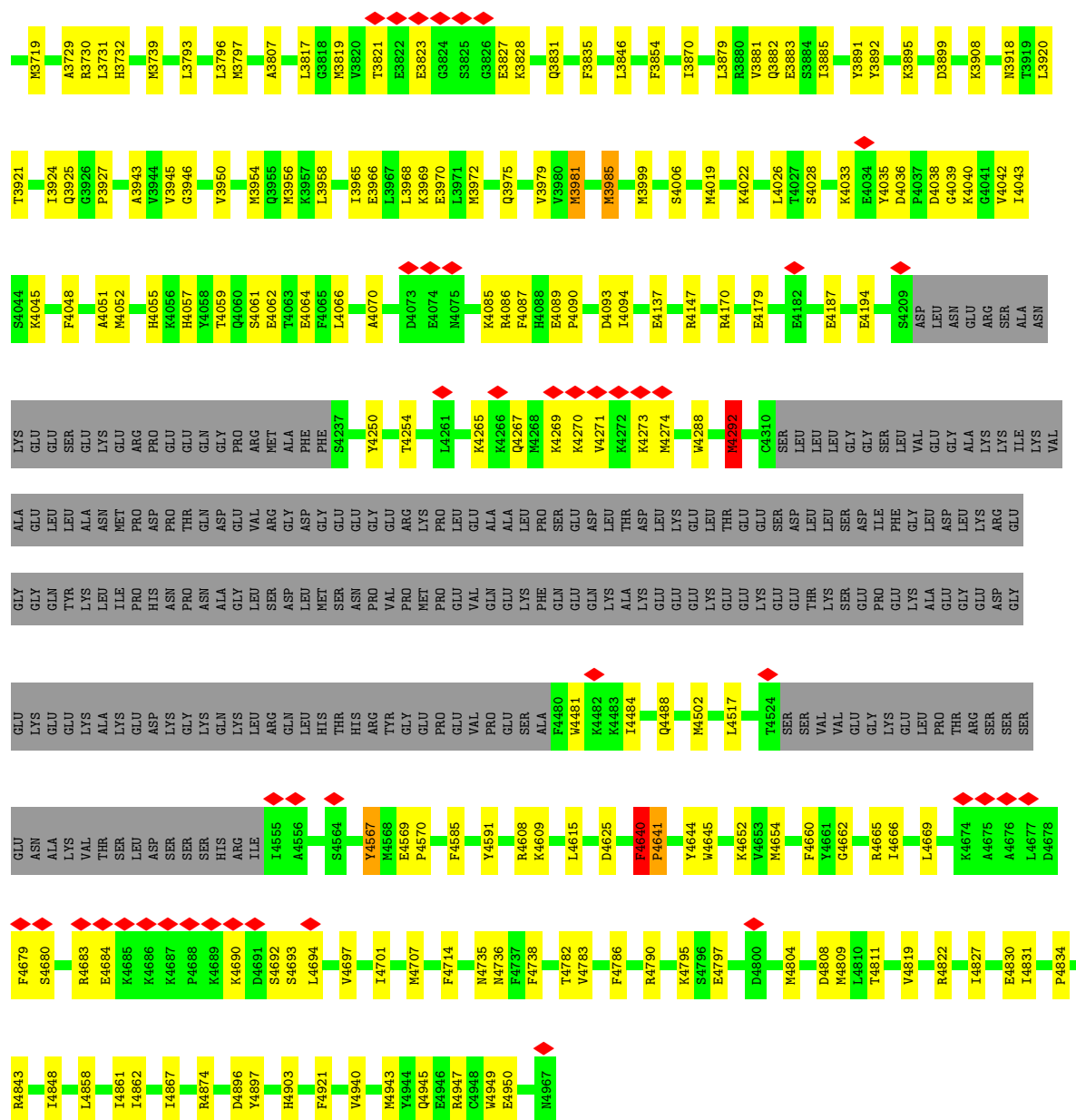


G2284	Y2285	W2290	E2296	R2297	R2326	E2329	G2332	P2333	R2336	N2341	G2342	M2347	I2351	P2364	ASN	SER	GLY	SER	SER	LYS	THR	LEU	ASP	THR	GLY	E2377	E2378	D2379	D2380	I2382	H2383	M2384	L2388	M2389	T2390	I2409	K2413	G2414	E2415	R2420	L2427														
G2166	M2167	H2168	M2172	E2173	V2174	M2175	V2176	N2177	V2178	L2179	G2180	G2181	G2182	E2183	S2184	K2185	E2186	I2187	M2192	Y2202	F2203	C2204	R2205	I2206	M2214	F2215	L2222	S2225	V2227	G2228	L2229	P2232	M2234	D2241	L2253	A2256	L2257	R2258	E2259	K2264	G2414	E2415	R2420	L2427											
LYS	LYS	GLN	ALA	GLU	PRO	VAL	GLU	SER	ASP	SER	K2053	K2054	S2055	S2056	L2061	L2062	T2065	M2066	R2082	A2083	M2084	L2087	R2090	Q2091	L2095	Y2106	L2119	L2123	L2123	L2130	M2134	G2145	I2149	M2150	N2151	N2152	V2154	F2155	V2156	Q2157	H2158	P2159	M2162												
T1962	F1965	R1966	S1967	P1968	P1969	Q1970	E1971	Q1972	M1975	L1976	F1979	D1982	K1983	S1984	P1987	C1988	P1989	I1992	R1993	D1994	Q1995	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	THR	ILE	ARG	GLY	ARG	LEU	SER	LEU	VAL	GLU	LYS	VAL	THR	LYS											
LEU	GLU	LYS	GLN	LEU	SER	VAL	ASP	ALA	LYS	LEU	GLN	GLY	ALA	GLY	GLU	GLU	ALA	LYS	ARG	P1889	K1890	L1894	K1895	M1896	L1897	L1898	V1902	C1907	C1914	D1930	Y1944	N1945	E1946	V1947	M1948	Q1949	A1950	L1951	N1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	K1961							
D1708	S1712	S1713	Y1714	R1718	L1719	M1720	E1732	L1733	K1734	P1766	S1767	F1768	P1780	D1785	I1786	K1790	R1807	D1808	F1809	V1810	L1817	I1822	F1825	I1830	M1831	G1832	F1834	H1835	I1842	L1843	Q1844	V1850	E1853	A1854	ALA	THR	PRO	GLU	GLU	GLU	SER	ASP	THR												
S1549	P1550	N1551	F1555	R1569	V1563	M1564	P1565	V1594	L1595	F1603	L1604	K1605	T1611	Q1615	G1616	V1617	L1618	M1628	S1629	L1630	H1631	I1632	I1641	T1645	E1649	L1650	L1660	L1667	G1668	N1669	D1681	E1682	P1683	Q1684	L1685	A1688	I1689	E1690	N1691	L1692	Y1693	M1694	P1695												
HIS	SER	ALA	ARG	THR	GLU	ASP	VAL	LEU	ALA	ASP	R1414	D1415	D1416	Y1417	M1421	T1425	Y1426	Y1427	G1435	P1438	F1444	G1445	I1446	F1457	R1461	E1472	K1473	G1474	K1475	M1487	Q1498	G1499	R1500	M1501	N1502	N1503	G1504	L1505	A1522	L1527	A1542	Q1546													
SER	ASP	PHE	VAL	LEU	MET	LYS	THR	HIS	ALA	GLY	ASP	VAL	PRO	ASP	VAL	LYS	ASP	LYS	GLU	ALA	THR	PRO	PHE	ASN	HIS	LYS	ASP	TYR	ALA	GLN	GLY	PRO	LEU	LYS	ALA	GLN	PHE	LEU	LEU	ARG	ARG	THR	LYS	PRO	ASP	GLU	GLY	TYR	ASP	ALA	ASP				
K1044	S1045	N1046	K1047	D1048	S1049	L1050	R1051	R1055	T1056	L1057	L1058	G1059	Y1060	P1067	D1068	Q1069	D1070	H1071	A1072	A1073	R1074	A1075	E1076	V1077	C1078	T1081	I1012	R1013	Q1014	G1015	A1098	G1099	R1100	Y1102	M1113	P1124	G1129	E1132	F1140	K1141	R1144	M1145	H1146	Q1147	W1156	M1165	M1168								
S974	Q975	Y976	K977	P978	A979	P980	M981	D982	L983	P986	K987	G988	Q992	E993	A994	M995	V996	D997	K998	L999	N1005	V1006	W1007	A1008	E938	R1009	D1010	R1011	I1012	R1013	Q1014	G1015	W1016	T1017	I1020	R1021	Q1022	D1023	V1024	K1025	N1026	R1027	R1028	M1029	P1030	R1031	L1032	V1033	P1034	Y1035	T1036	L1037	R1041	T1042	K1043
D910	N911	K912	R913	Q914	H915	P916	C917	L918	V919	E920	F921	S922	K923	L924	P925	E926	Q927	E928	R929	N932	L933	Q934	M935	S936	L937	E938	T939	D1010	R1011	T941	T942	L946	G947	C948	I952	S953	D954	E955	H956	A957	E958	D959	K960	V961	K962	M963	M964	K965	L966	P967	K968	N969	Y970	Q971	L972



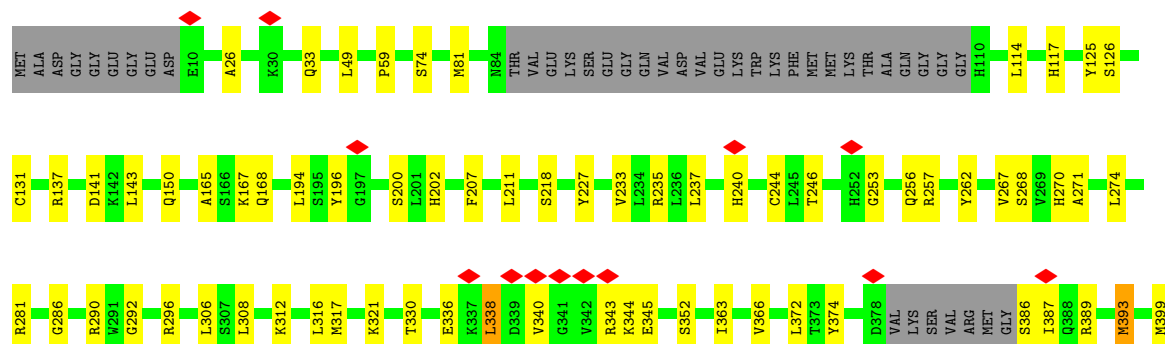






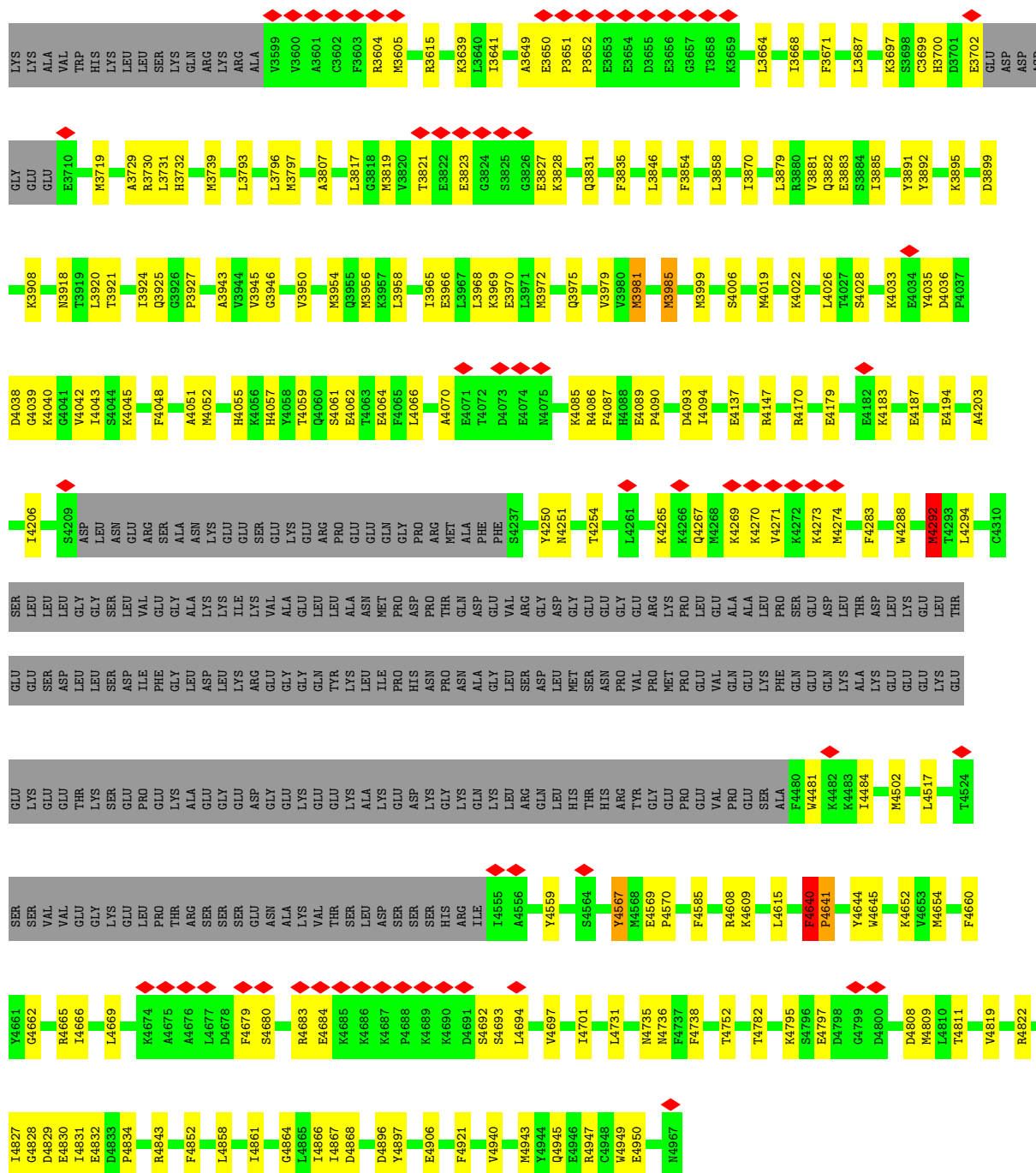
• Molecule 1: Ryanodine receptor 2

Chain D: 65% 19% 15%



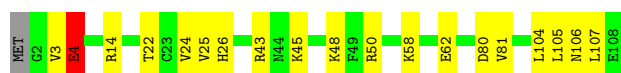






- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:

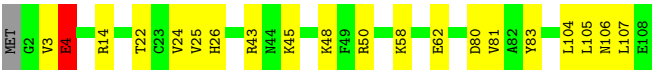
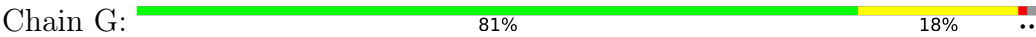


- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

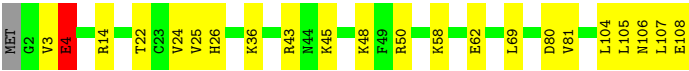
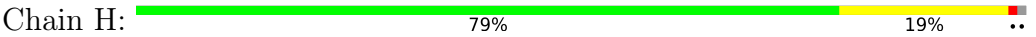
Chain F:



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	181724	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 ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.623	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	430.592, 430.592, 430.592	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.841, 0.841, 0.841	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/34516	0.44	10/46623 (0.0%)
1	B	0.17	0/34516	0.44	10/46623 (0.0%)
1	C	0.17	0/34516	0.44	10/46623 (0.0%)
1	D	0.17	0/34516	0.44	10/46623 (0.0%)
2	E	0.15	0/834	0.40	1/1123 (0.1%)
2	F	0.15	0/834	0.40	1/1123 (0.1%)
2	G	0.14	0/834	0.40	1/1123 (0.1%)
2	H	0.14	0/834	0.40	1/1123 (0.1%)
All	All	0.17	0/141400	0.44	44/190984 (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	5
1	B	0	5
1	C	0	5
1	D	0	5
All	All	0	20

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	943	LEU	CA-CB-CG	7.87	143.83	116.30
1	C	943	LEU	CA-CB-CG	7.86	143.81	116.30
1	D	943	LEU	CA-CB-CG	7.86	143.81	116.30
1	B	943	LEU	CA-CB-CG	7.85	143.78	116.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2734	MET	CA-CB-CG	7.46	129.03	114.10

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2766	LYS	Peptide
1	A	439	LYS	Peptide
1	A	4640	PHE	Peptide
1	A	879	GLU	Peptide
1	A	880	ARG	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	33774	0	33452	708	0
1	B	33774	0	33452	712	0
1	C	33774	0	33452	715	0
1	D	33774	0	33452	719	0
2	E	818	0	821	12	0
2	F	818	0	821	15	0
2	G	818	0	821	13	0
2	H	818	0	821	15	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	62	0	24	2	0
4	B	62	0	24	2	0
4	C	62	0	24	2	0
4	D	62	0	24	2	0
5	A	23	0	0	1	0
5	B	23	0	0	1	0
5	C	23	0	0	1	0
5	D	23	0	0	1	0
All	All	138712	0	137188	2838	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 10.

The worst 5 of 2838 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2779:LEU:HA	1:A:2782:MET:HG3	1.56	0.88
1:B:2779:LEU:HA	1:B:2782:MET:HG3	1.56	0.87
1:D:2779:LEU:HA	1:D:2782:MET:HG3	1.56	0.86
1:C:2779:LEU:HA	1:C:2782:MET:HG3	1.56	0.85
2:F:4:GLU:OE1	2:F:4:GLU:N	2.13	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4198/4967 (84%)	4098 (98%)	98 (2%)	2 (0%)	100	100
1	B	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
1	C	4198/4967 (84%)	4100 (98%)	96 (2%)	2 (0%)	100	100
1	D	4198/4967 (84%)	4099 (98%)	97 (2%)	2 (0%)	100	100
2	E	105/108 (97%)	105 (100%)	0	0	100	100
2	F	105/108 (97%)	105 (100%)	0	0	100	100
2	G	105/108 (97%)	105 (100%)	0	0	100	100
2	H	105/108 (97%)	105 (100%)	0	0	100	100
All	All	17212/20300 (85%)	16816 (98%)	388 (2%)	8 (0%)	100	100

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3927	PRO

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Mol	Chain	Res	Type
1	A	4641	PRO
1	B	3927	PRO
1	B	4641	PRO
1	C	3927	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	3708/4358 (85%)	3660 (99%)	48 (1%)	61	74
1	B	3708/4358 (85%)	3660 (99%)	48 (1%)	61	74
1	C	3708/4358 (85%)	3659 (99%)	49 (1%)	61	74
1	D	3708/4358 (85%)	3660 (99%)	48 (1%)	61	74
2	E	88/89 (99%)	87 (99%)	1 (1%)	65	76
2	F	88/89 (99%)	87 (99%)	1 (1%)	65	76
2	G	88/89 (99%)	87 (99%)	1 (1%)	65	76
2	H	88/89 (99%)	87 (99%)	1 (1%)	65	76
All	All	15184/17788 (85%)	14987 (99%)	197 (1%)	59	74

5 of 197 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1011	ARG
1	C	3956	MET
1	C	1025	LYS
1	C	1720	MET
1	D	338	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 148 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	658	ASN

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Mol	Chain	Res	Type
1	D	4088	HIS
1	D	1014	GLN
1	D	2890	GLN
1	B	1014	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 16 ligands modelled in this entry, 4 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	$\# Z > 2$
4	ATP	B	5002	-	32,33,33	0.27	0	48,52,52	0.30	0
5	KVR	B	5004	-	24,25,25	0.51	0	31,34,34	0.99	2 (6%)
4	ATP	D	5003	-	32,33,33	0.57	0	48,52,52	0.55	0
4	ATP	A	5002	-	32,33,33	0.27	0	48,52,52	0.30	0
5	KVR	C	5004	-	24,25,25	0.51	0	31,34,34	0.99	2 (6%)
4	ATP	D	5002	-	32,33,33	0.27	0	48,52,52	0.30	0
4	ATP	A	5003	-	32,33,33	0.57	0	48,52,52	0.55	0
5	KVR	A	5004	-	24,25,25	0.51	0	31,34,34	0.99	2 (6%)
4	ATP	C	5003	-	32,33,33	0.57	0	48,52,52	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	KVR	D	5004	-	24,25,25	0.52	0	31,34,34	1.00	2 (6%)
4	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	B	5003	-	32,33,33	0.58	0	48,52,52	0.55	0

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	B	5002	-	-	8/22/38/38	0/3/3/3
5	KVR	B	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	D	5003	-	-	5/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	8/22/38/38	0/3/3/3
5	KVR	C	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	D	5002	-	-	8/22/38/38	0/3/3/3
4	ATP	A	5003	-	-	5/22/38/38	0/3/3/3
5	KVR	A	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	C	5003	-	-	5/22/38/38	0/3/3/3
5	KVR	D	5004	-	-	6/10/20/20	0/2/3/3
4	ATP	C	5002	-	-	8/22/38/38	0/3/3/3
4	ATP	B	5003	-	-	5/22/38/38	0/3/3/3

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	5004	KVR	C10-S09-C06	3.36	107.46	102.71
5	C	5004	KVR	C10-S09-C06	3.34	107.44	102.71
5	A	5004	KVR	C10-S09-C06	3.34	107.44	102.71
5	B	5004	KVR	C10-S09-C06	3.33	107.42	102.71
5	D	5004	KVR	C14-N12-C11	2.99	115.95	111.09

There are no chirality outliers.

5 of 76 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3B-PG-O3G

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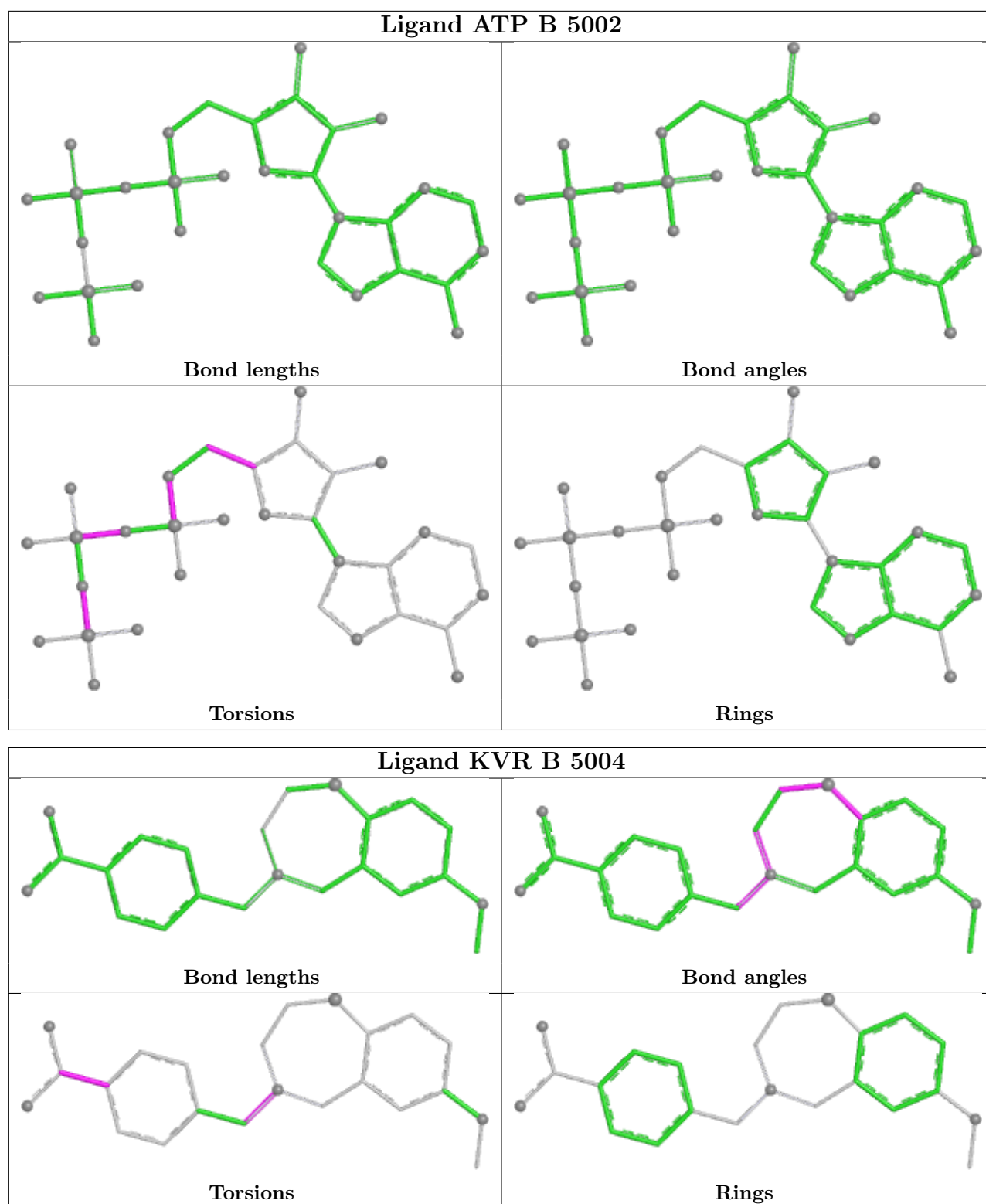
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	C4'-C5'-O5'-PA

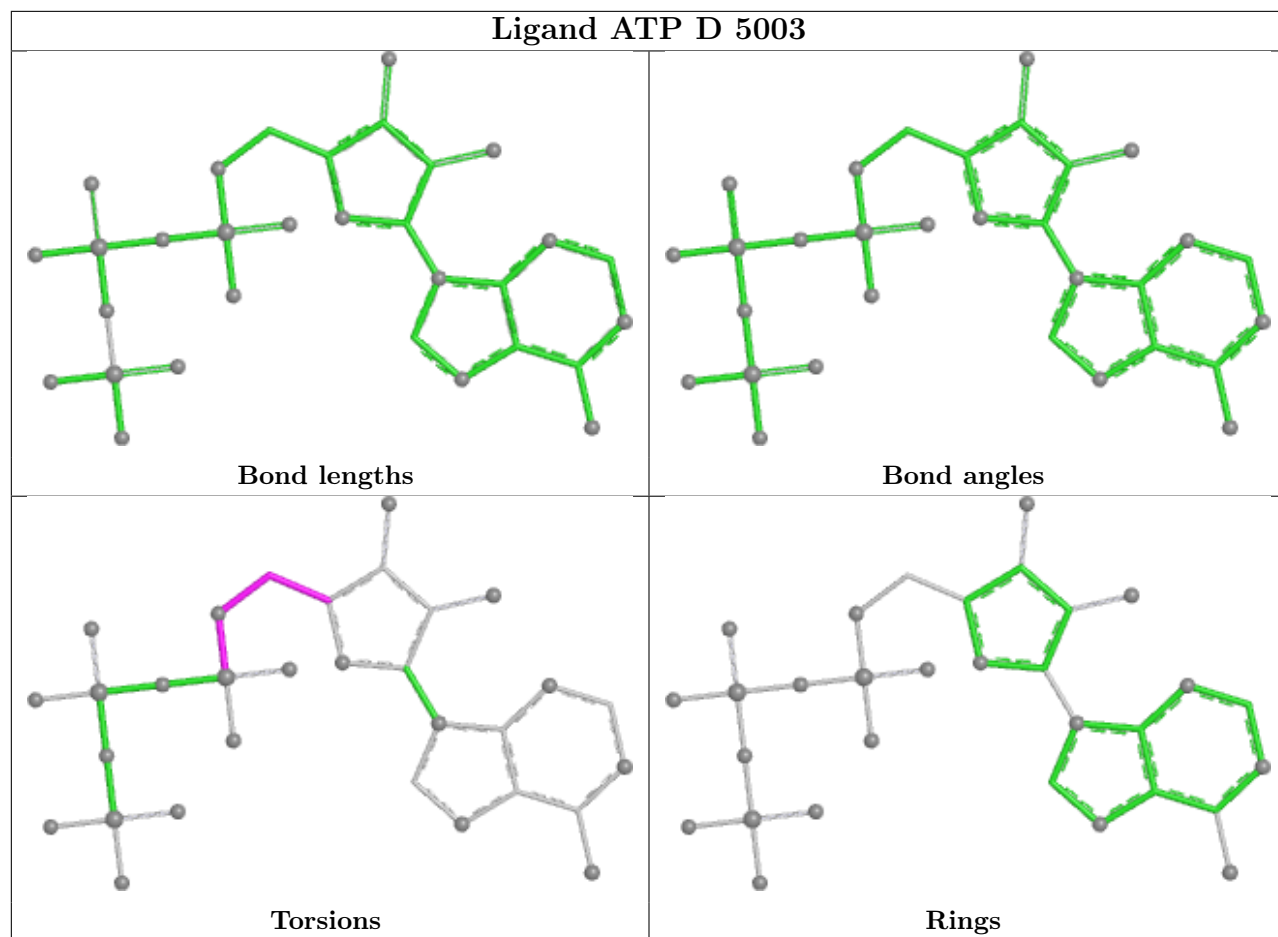
There are no ring outliers.

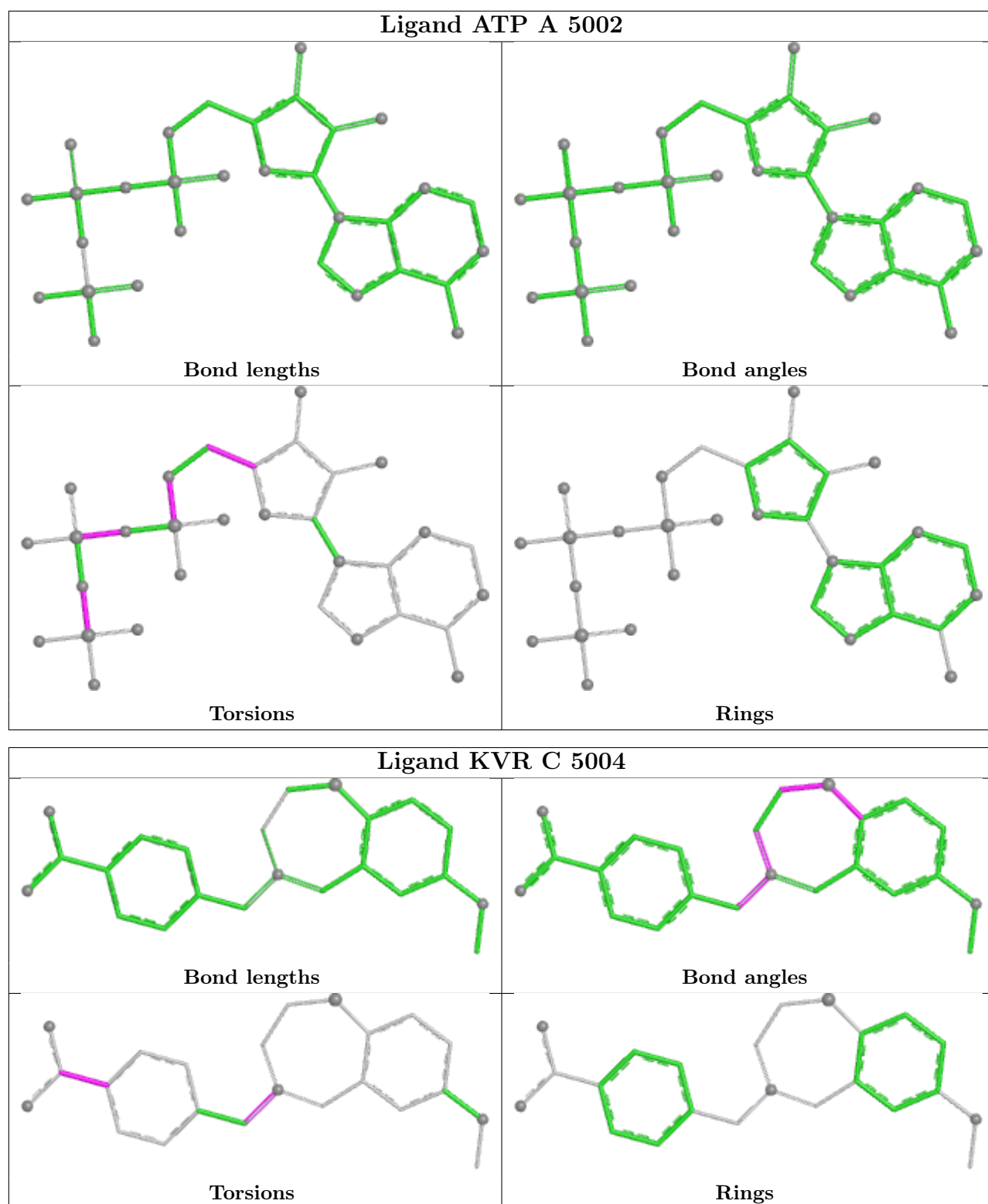
12 monomers are involved in 12 short contacts:

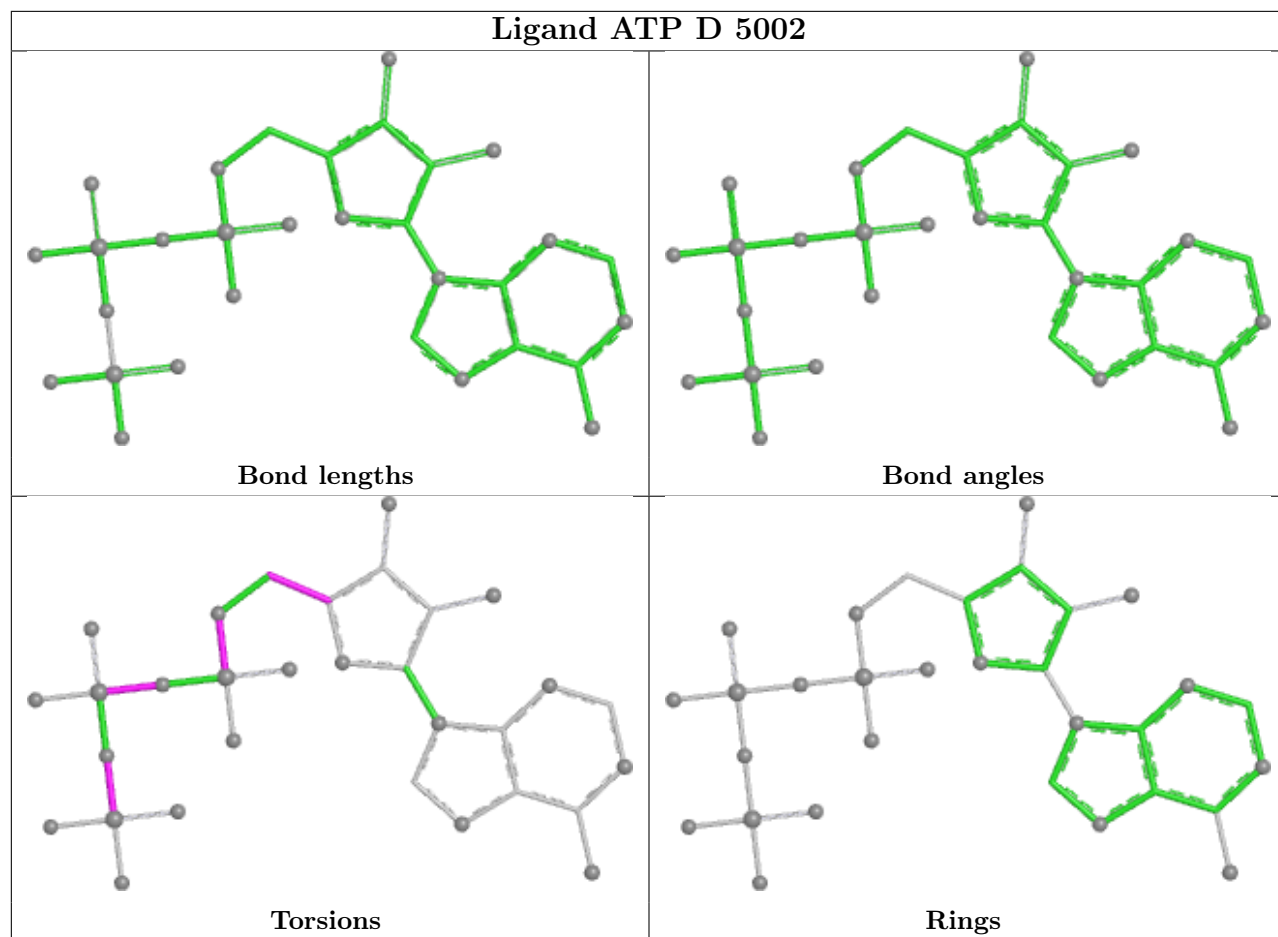
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5002	ATP	1	0
5	B	5004	KVR	1	0
4	D	5003	ATP	1	0
4	A	5002	ATP	1	0
5	C	5004	KVR	1	0
4	D	5002	ATP	1	0
4	A	5003	ATP	1	0
5	A	5004	KVR	1	0
4	C	5003	ATP	1	0
5	D	5004	KVR	1	0
4	C	5002	ATP	1	0
4	B	5003	ATP	1	0

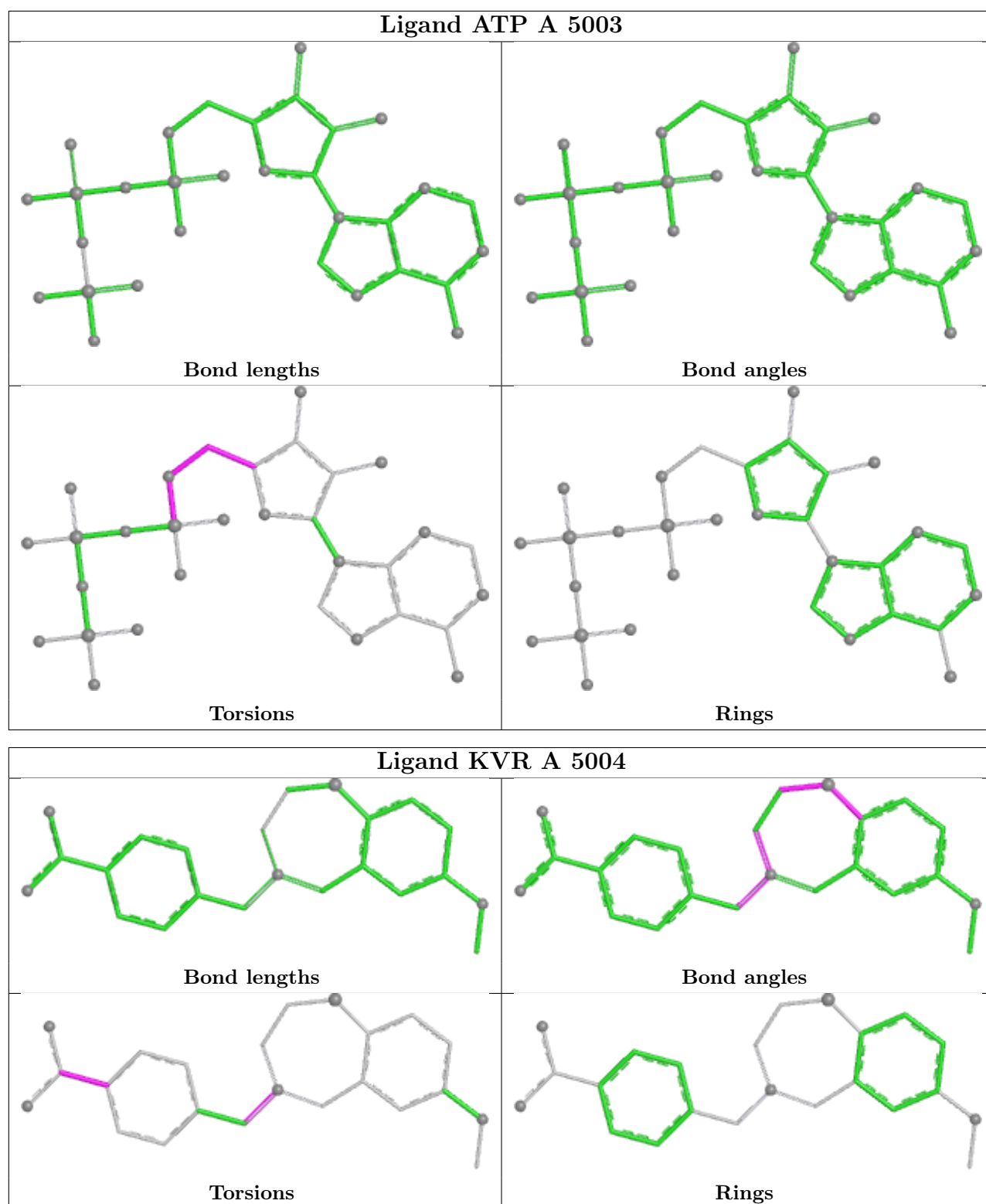
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

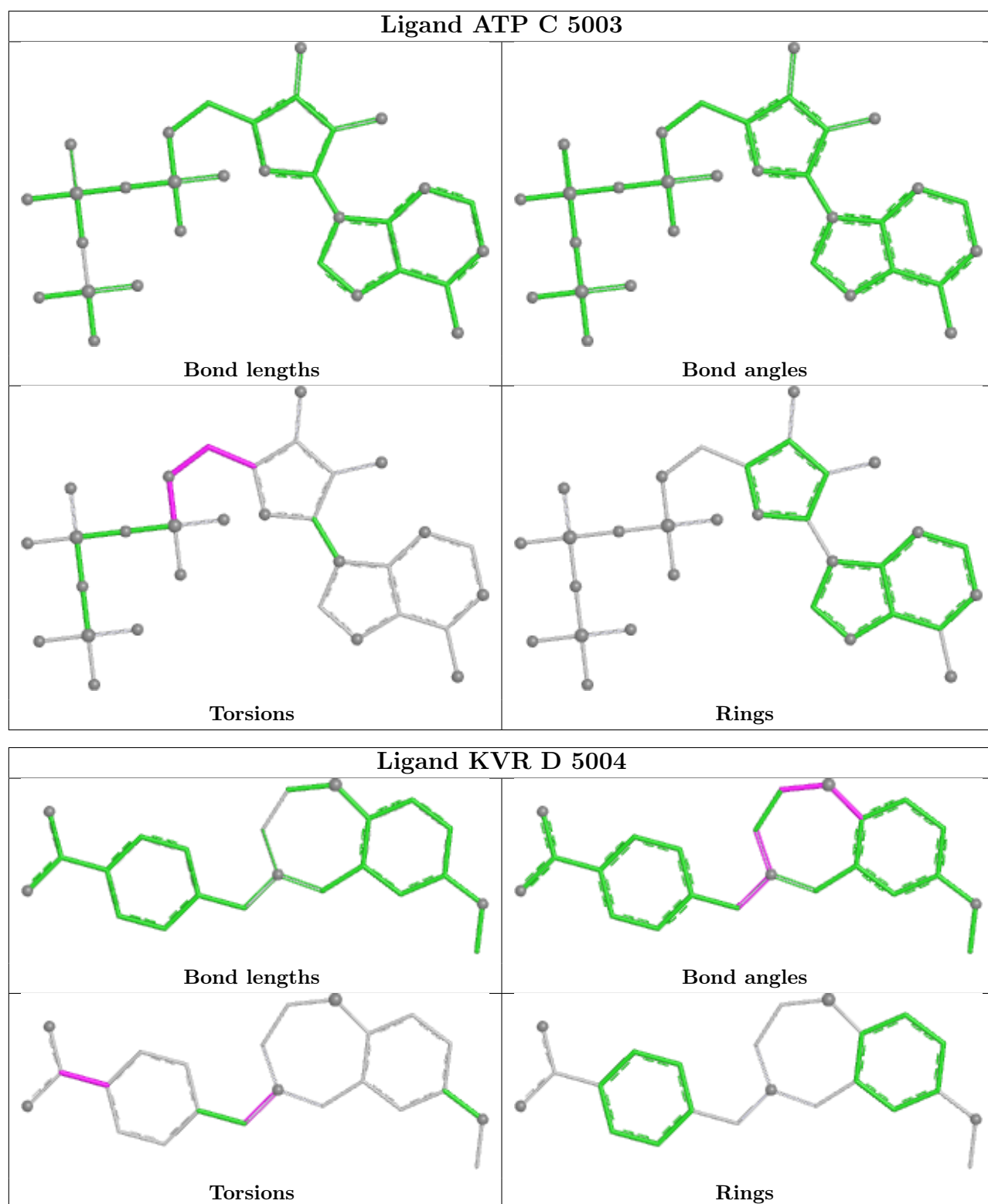


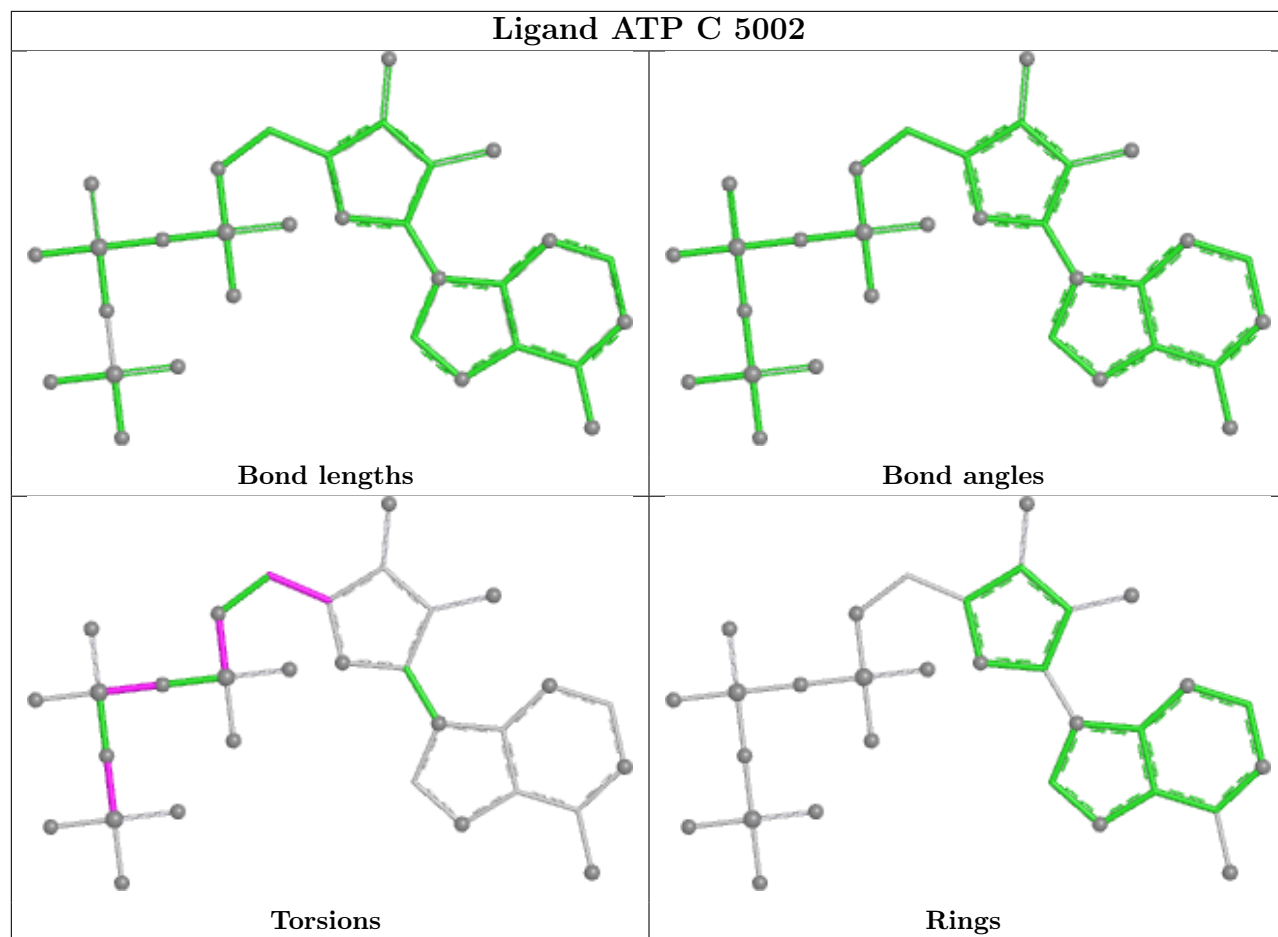


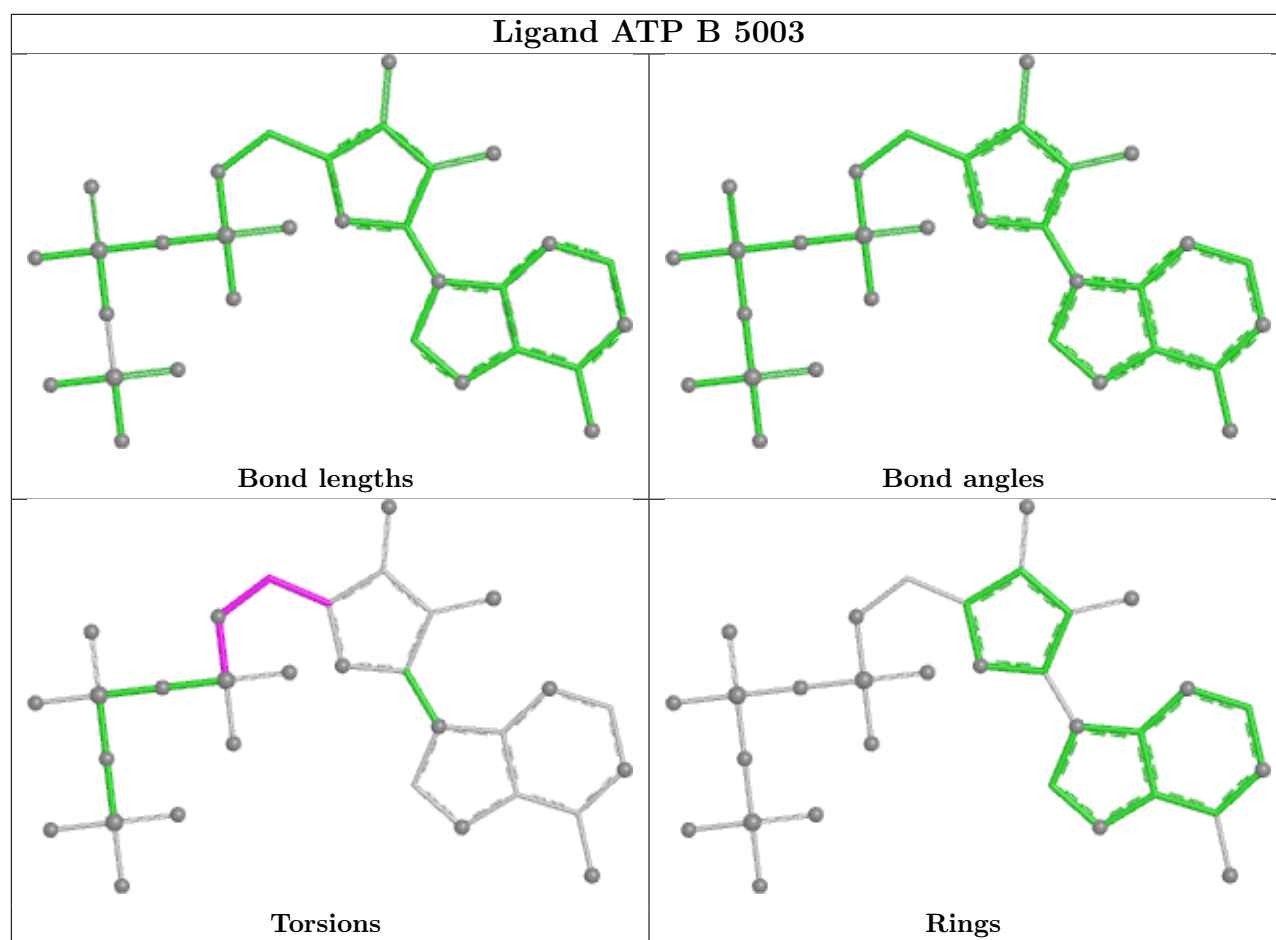












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42763. These allow visual inspection of the internal detail of the map and identification of artifacts.

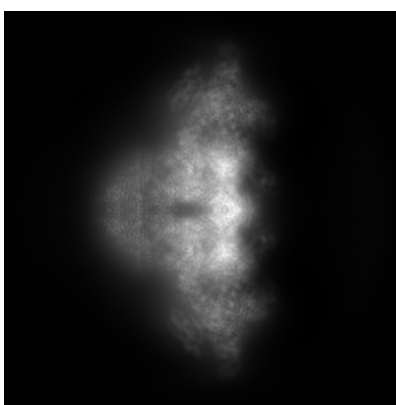
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

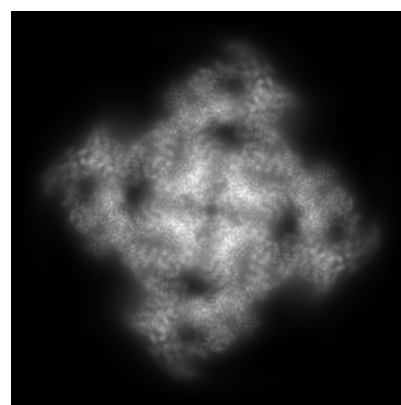
6.1.1 Primary map



X



Y



Z

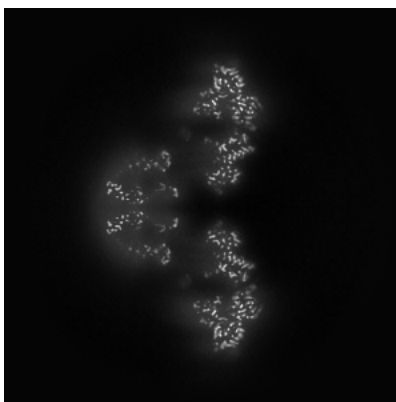
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

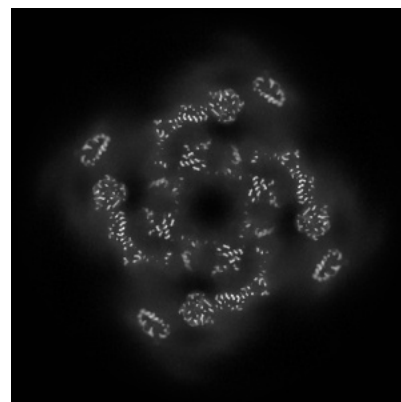
6.2.1 Primary map



X Index: 256



Y Index: 256

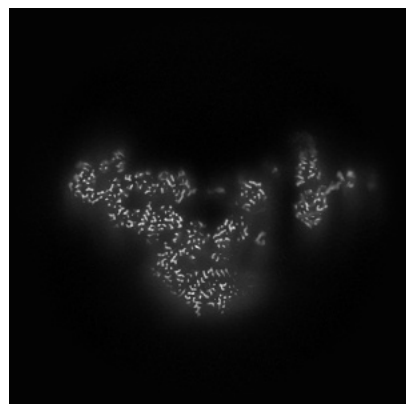


Z Index: 256

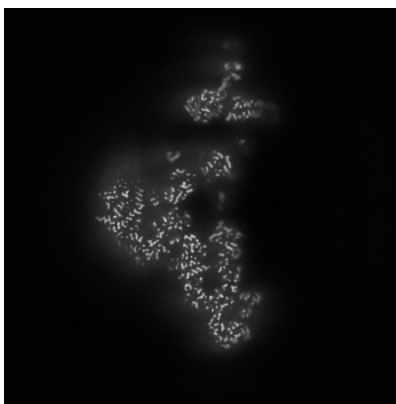
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

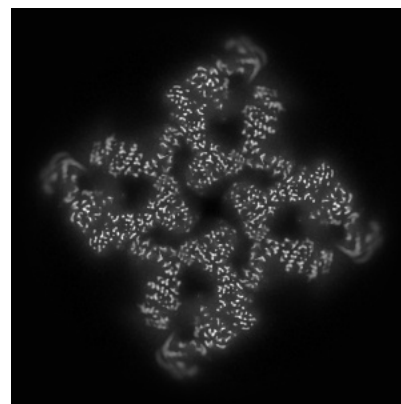
6.3.1 Primary map



X Index: 274



Y Index: 238

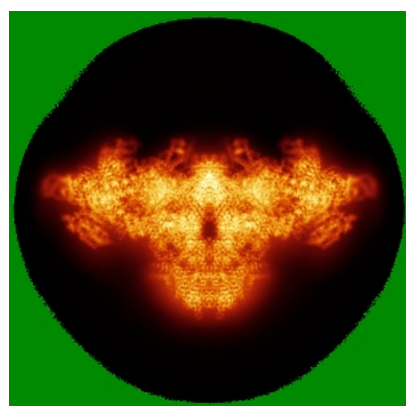


Z Index: 282

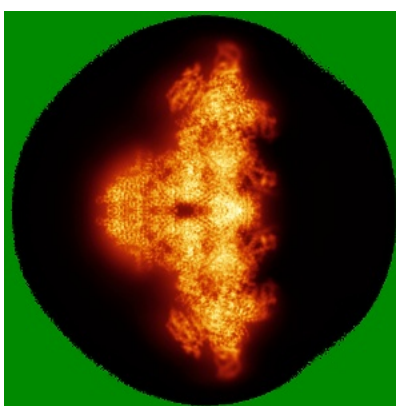
The images above show the largest variance slices of the map in three orthogonal directions.

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

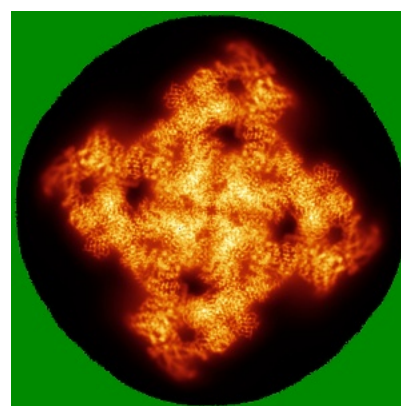
6.4.1 Primary map



X



Y

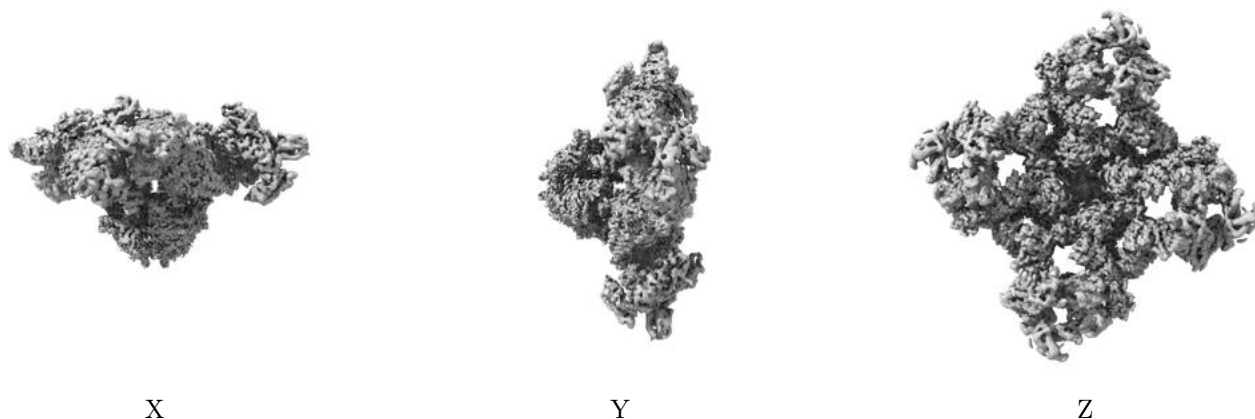


Z

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

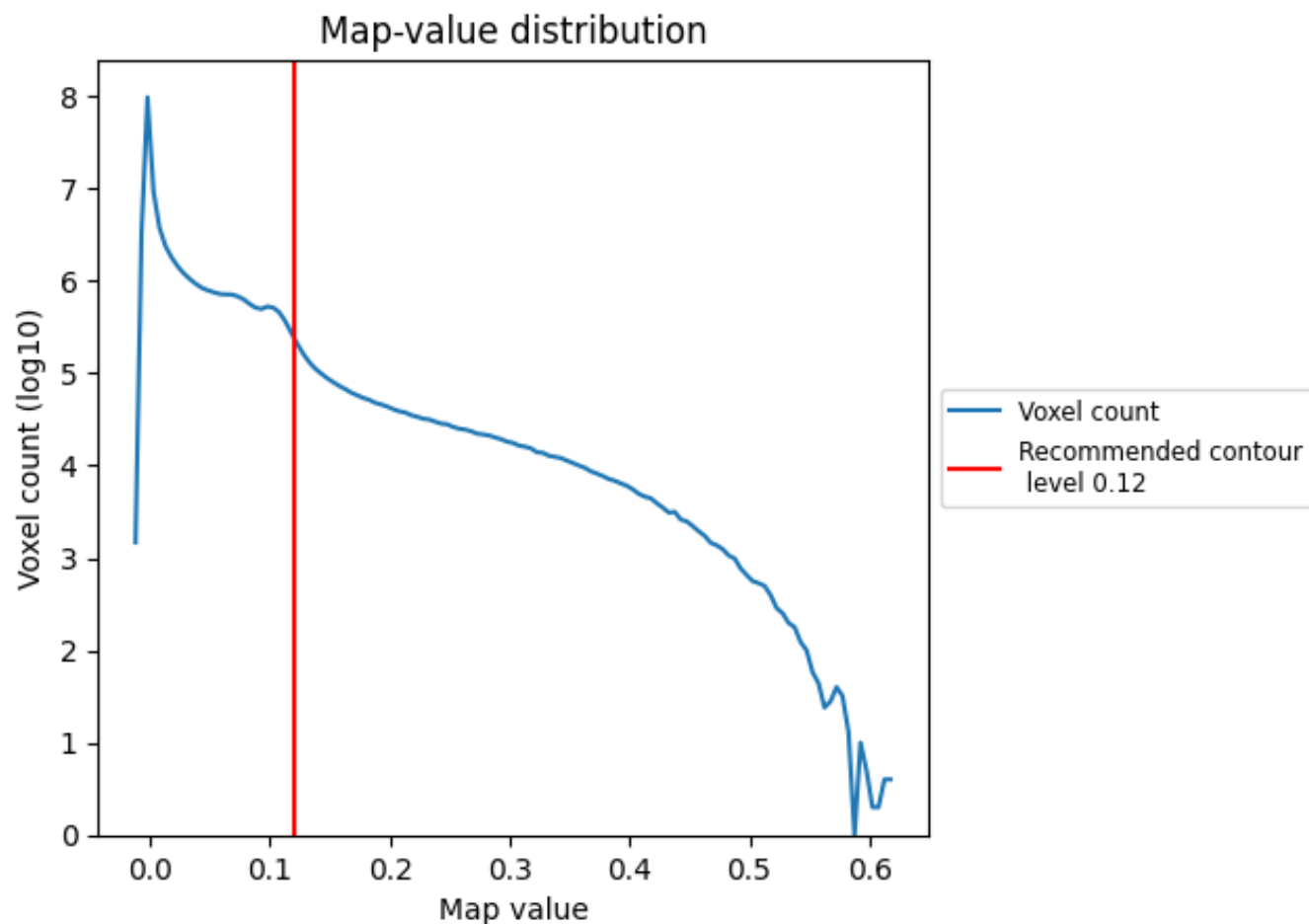
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

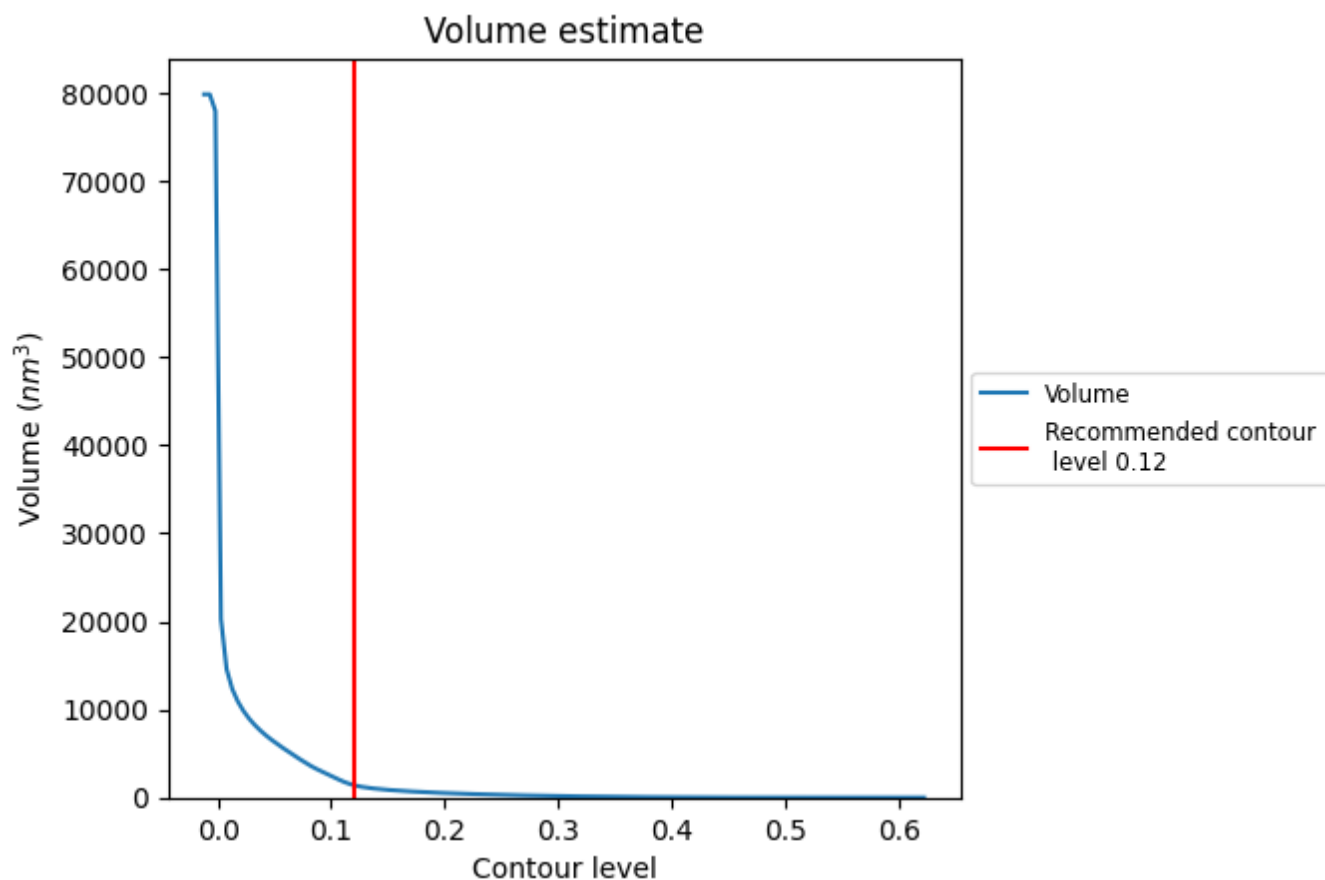
This section contains the results of statistical analysis of the map.

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.

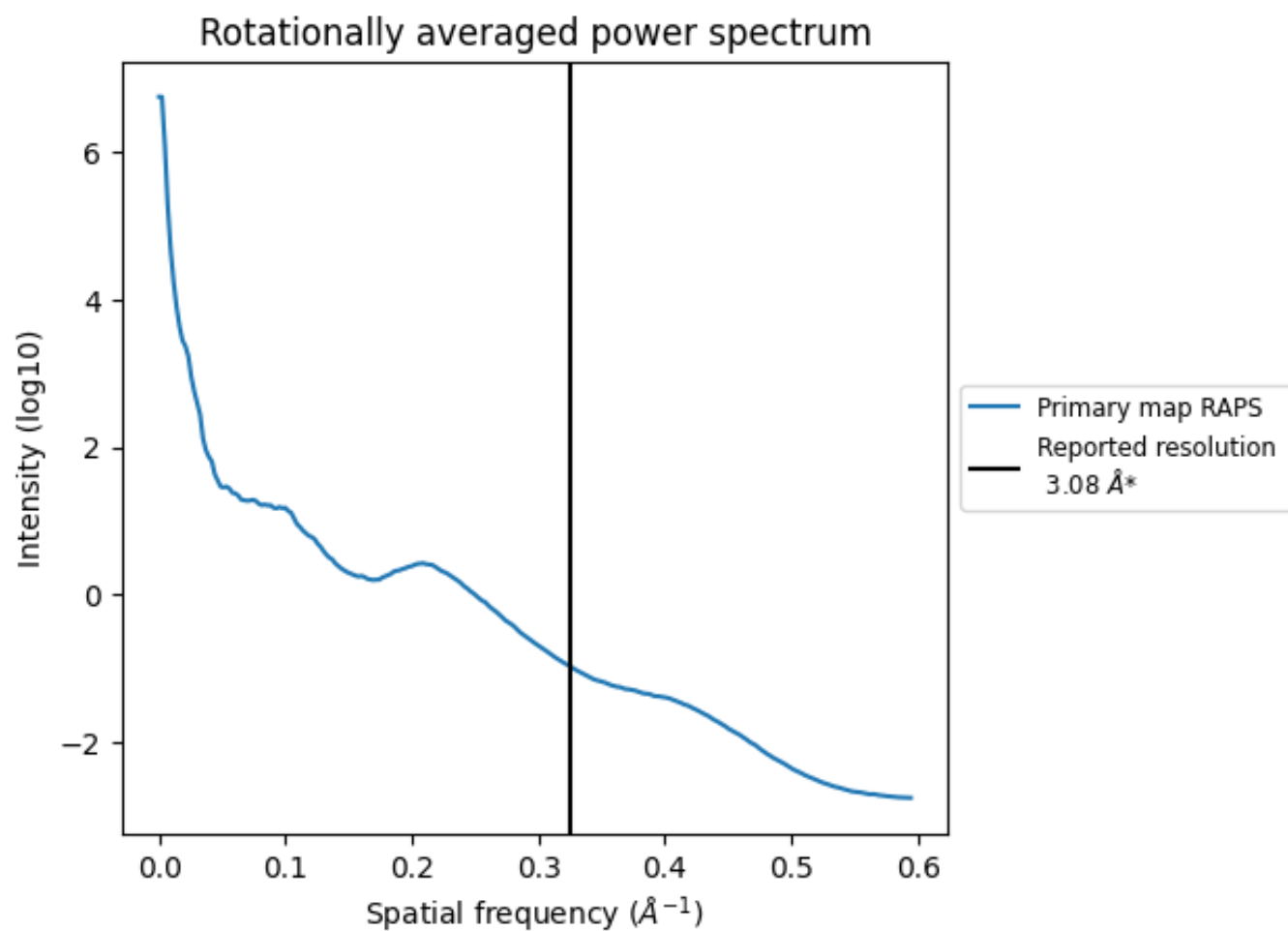
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1416 nm³; this corresponds to an approximate mass of 1279 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 0.325 Å⁻¹

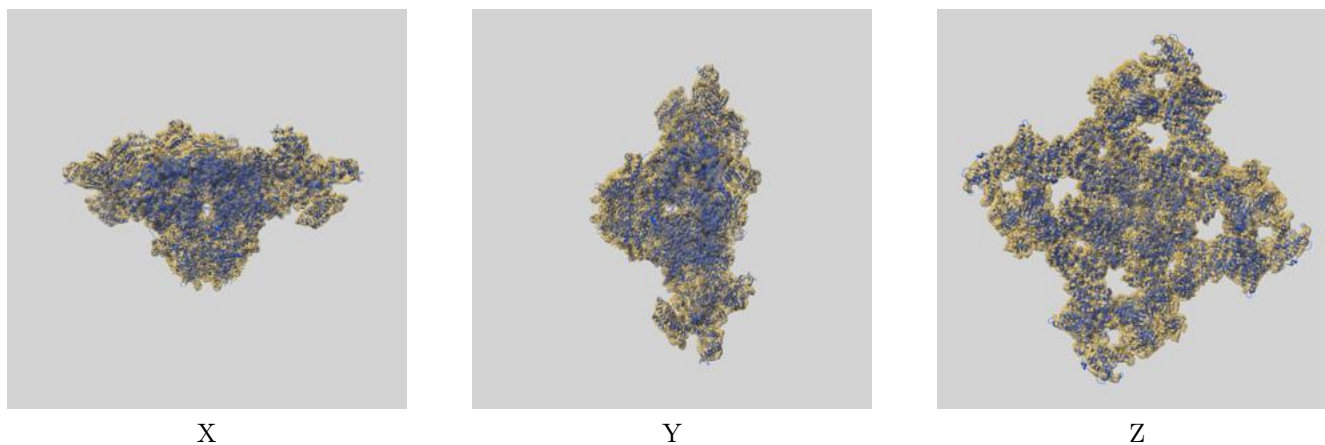
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

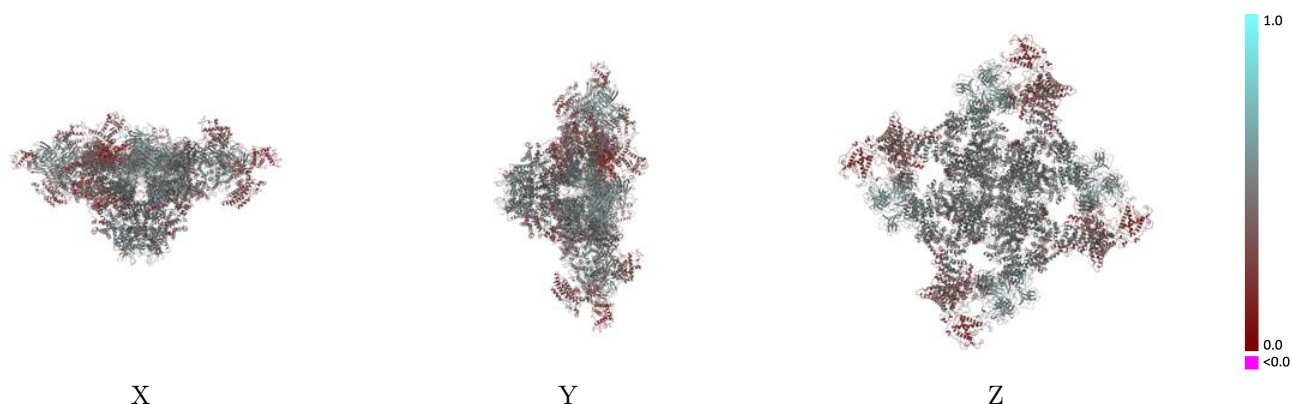
This section contains information regarding the fit between EMDB map EMD-42763 and PDB model 8UXG. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



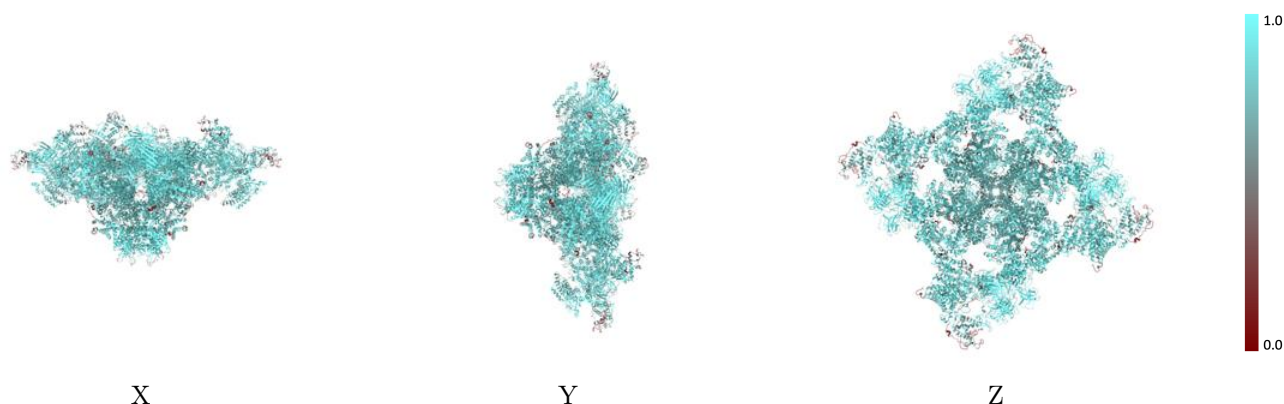
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



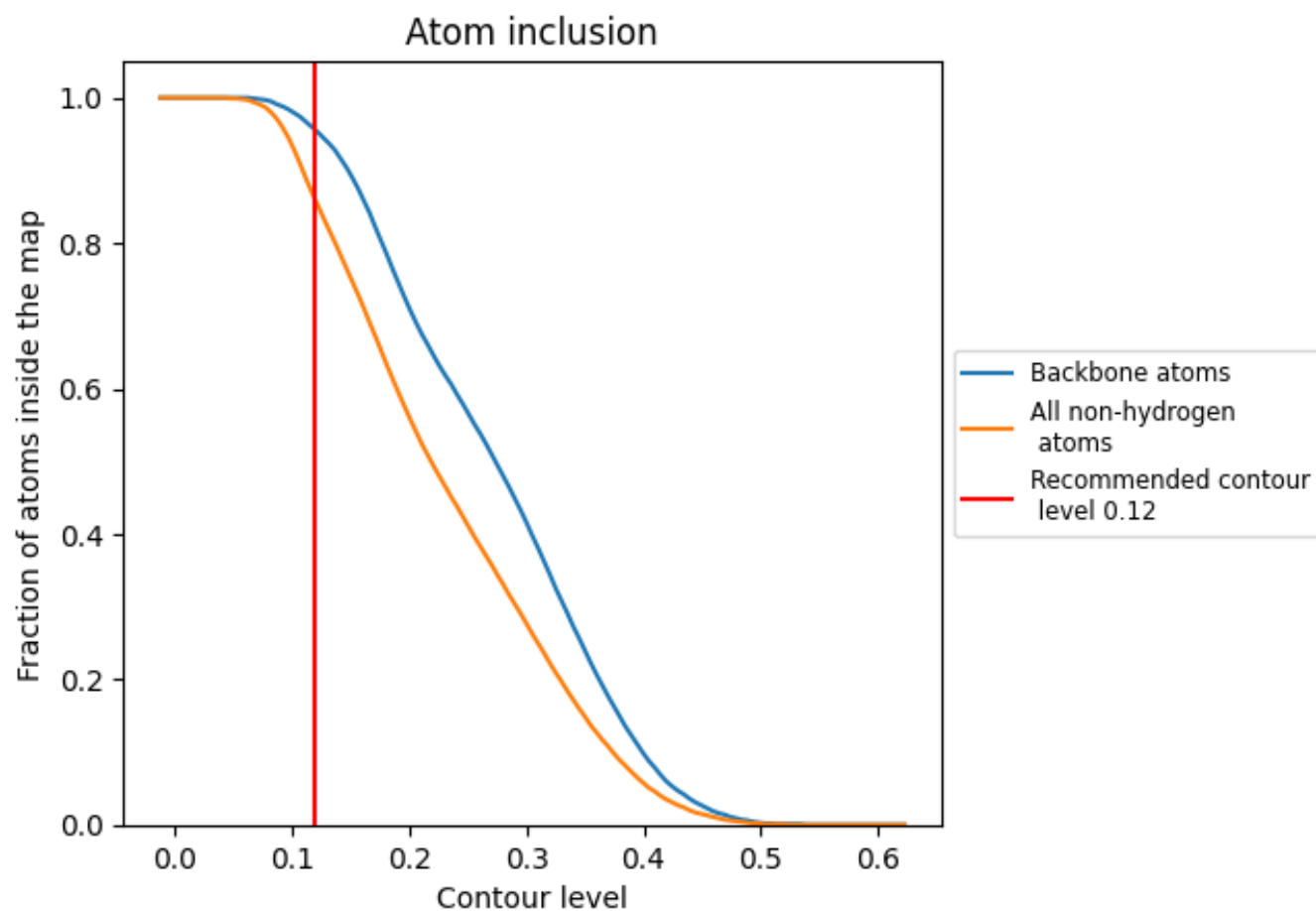
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 86% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8590	0.4340
A	0.8580	0.4310
B	0.8580	0.4300
C	0.8590	0.4340
D	0.8560	0.4300
E	0.9330	0.5340
F	0.9290	0.5330
G	0.9340	0.5350
H	0.9340	0.5360

1.0

0.0

<0.0