



wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 07:31 AM EDT

PDB ID : 8UQ2
EMDB ID : EMD-42458
Title : Structure of human RyR2-S2808D in the subprimed state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-10-23
Resolution : 2.98 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

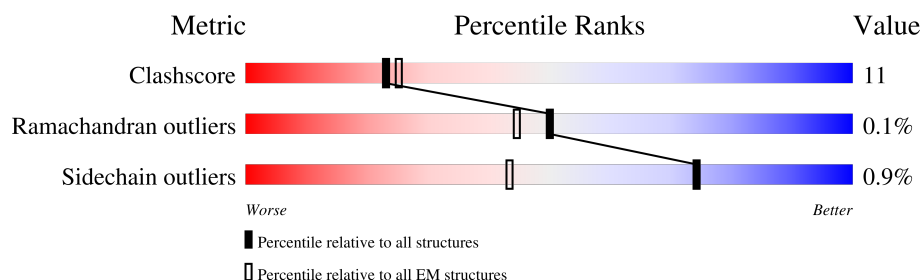
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.98 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	<div> <div>9%</div> <div>64%</div> <div>21%</div> <div>15%</div> </div>
1	B	4967	<div> <div>9%</div> <div>64%</div> <div>21%</div> <div>15%</div> </div>
1	C	4967	<div> <div>9%</div> <div>64%</div> <div>20%</div> <div>15%</div> </div>
1	D	4967	<div> <div>9%</div> <div>64%</div> <div>21%</div> <div>15%</div> </div>
2	E	108	<div> <div>66%</div> <div>32%</div> <div>..</div> </div>
2	F	108	<div> <div>69%</div> <div>30%</div> <div>..</div> </div>
2	G	108	<div> <div>66%</div> <div>32%</div> <div>..</div> </div>
2	H	108	<div> <div>66%</div> <div>32%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 138608 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	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	B	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	C	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		
1	D	4224	Total	C	N	O	S	2	0
			33771	21516	5745	6280	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2808	ASP	SER	engineered mutation	UNP Q92736
B	2808	ASP	SER	engineered mutation	UNP Q92736
C	2808	ASP	SER	engineered mutation	UNP Q92736
D	2808	ASP	SER	engineered mutation	UNP Q92736

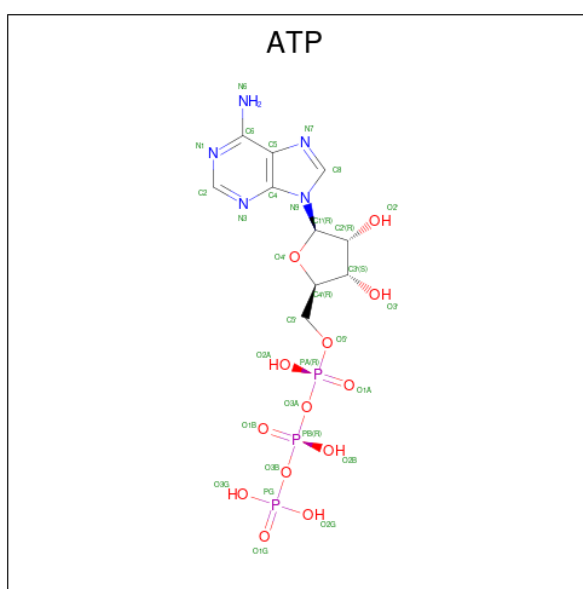
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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

- Molecule 3 is ZINC ION (three-letter code: 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 (three-letter code: 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	

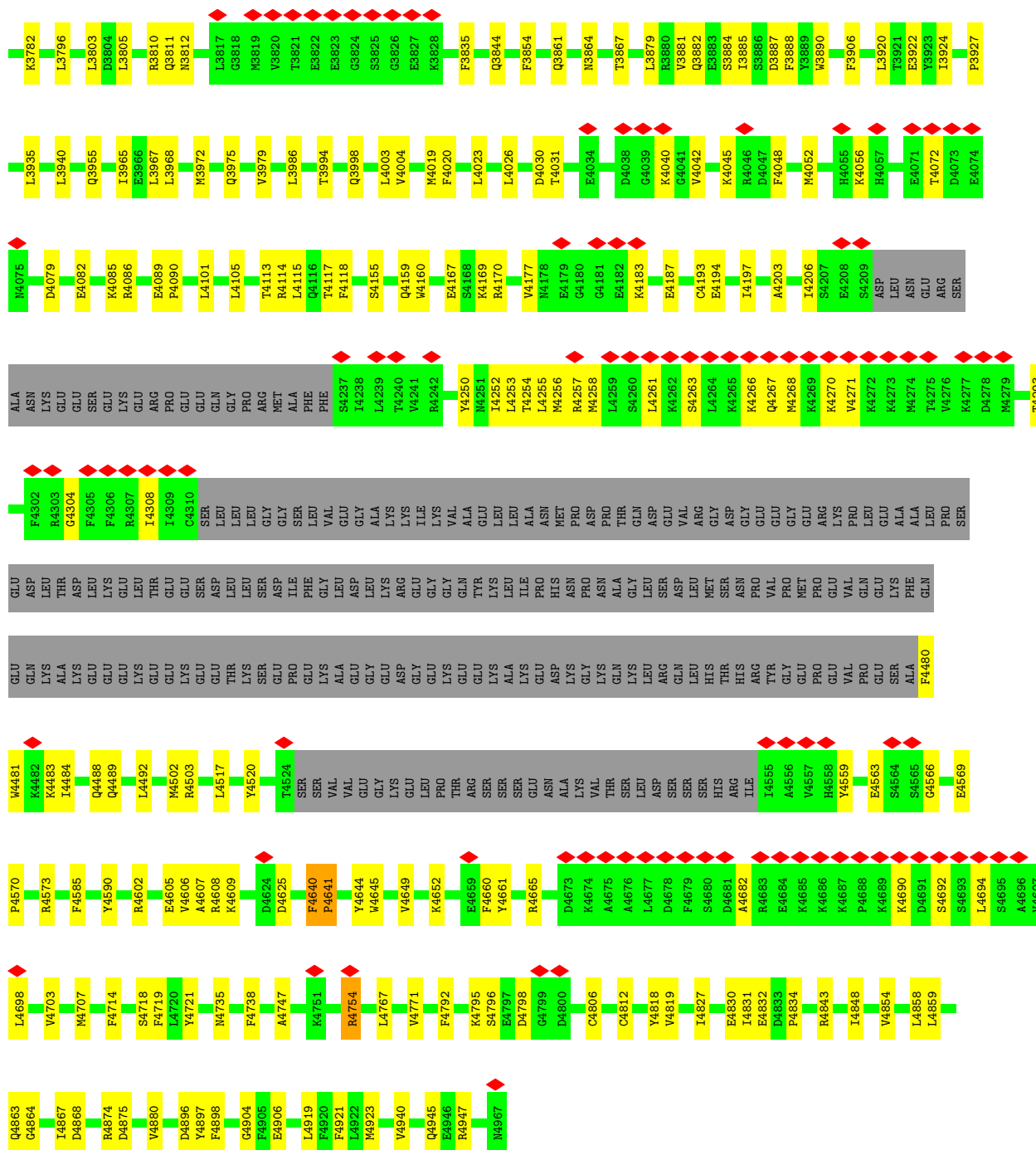
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	D	1	31	10	5	13	3	0

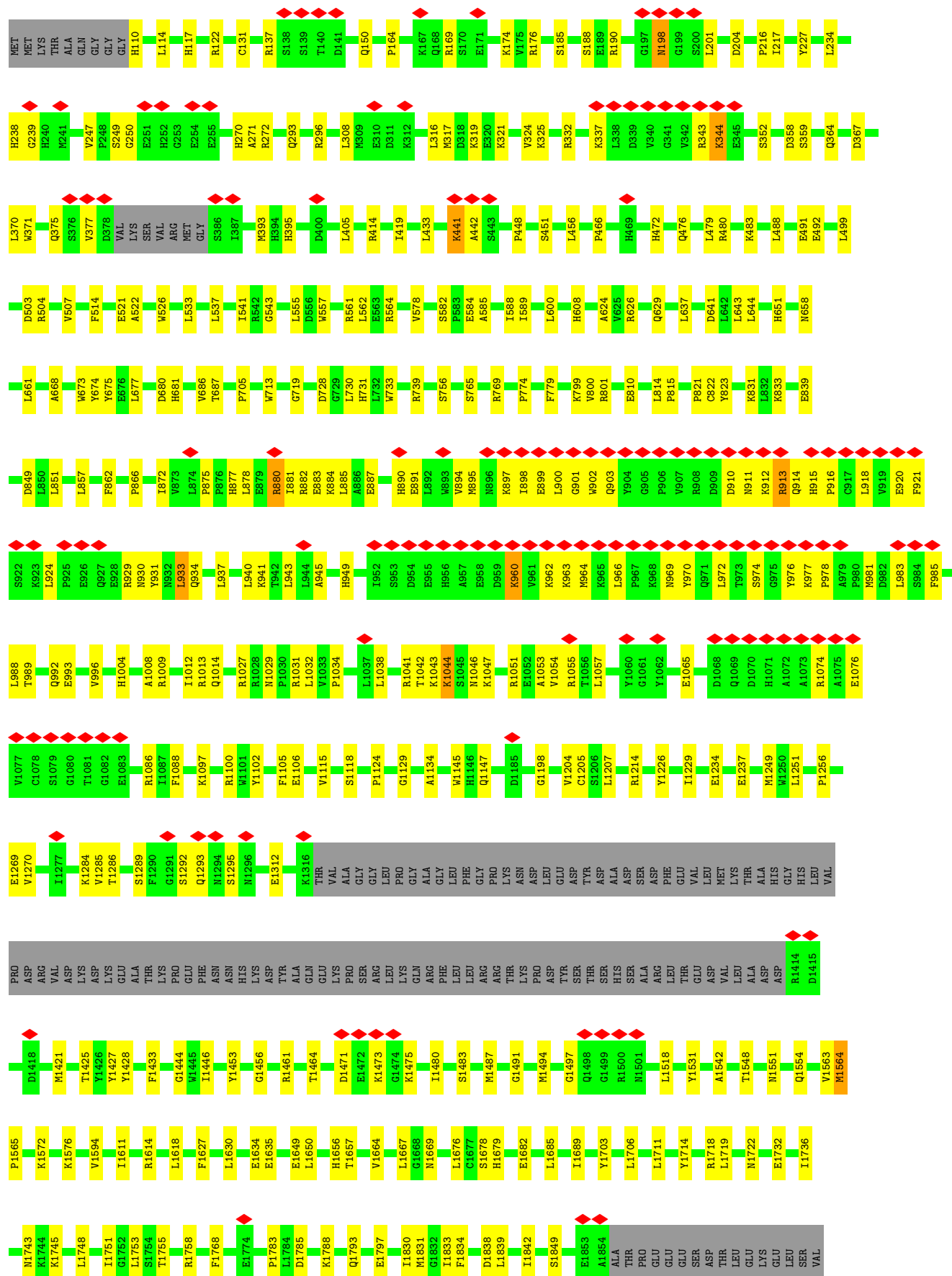






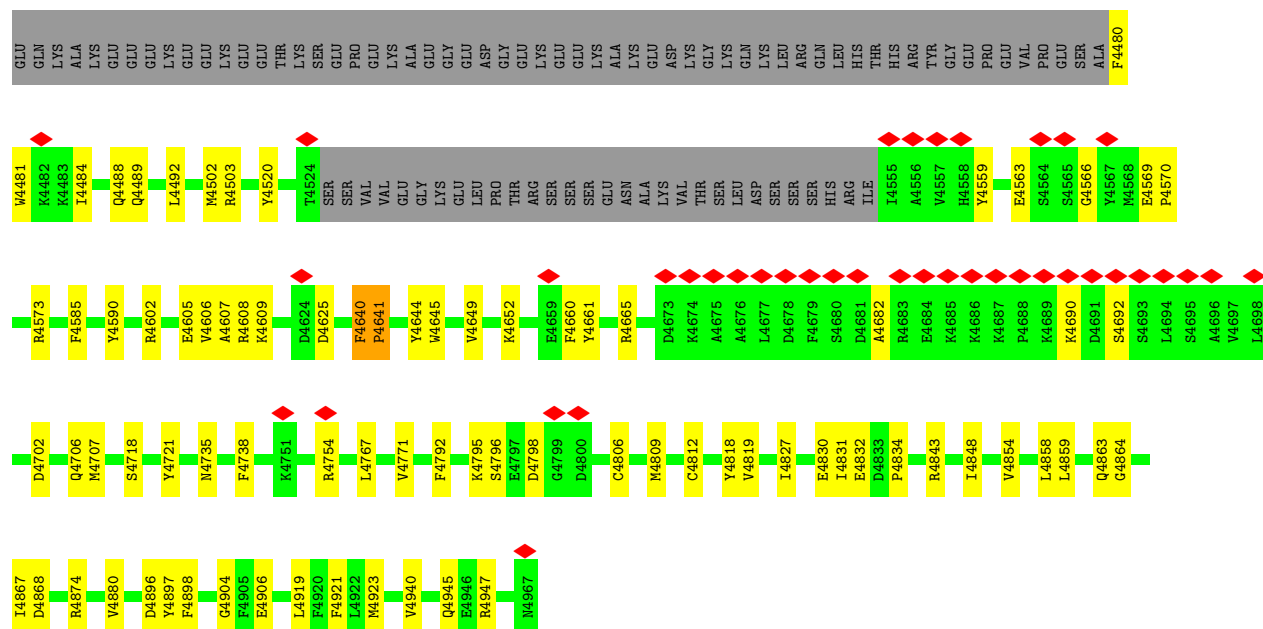
• Molecule 1: Ryanodine receptor 2



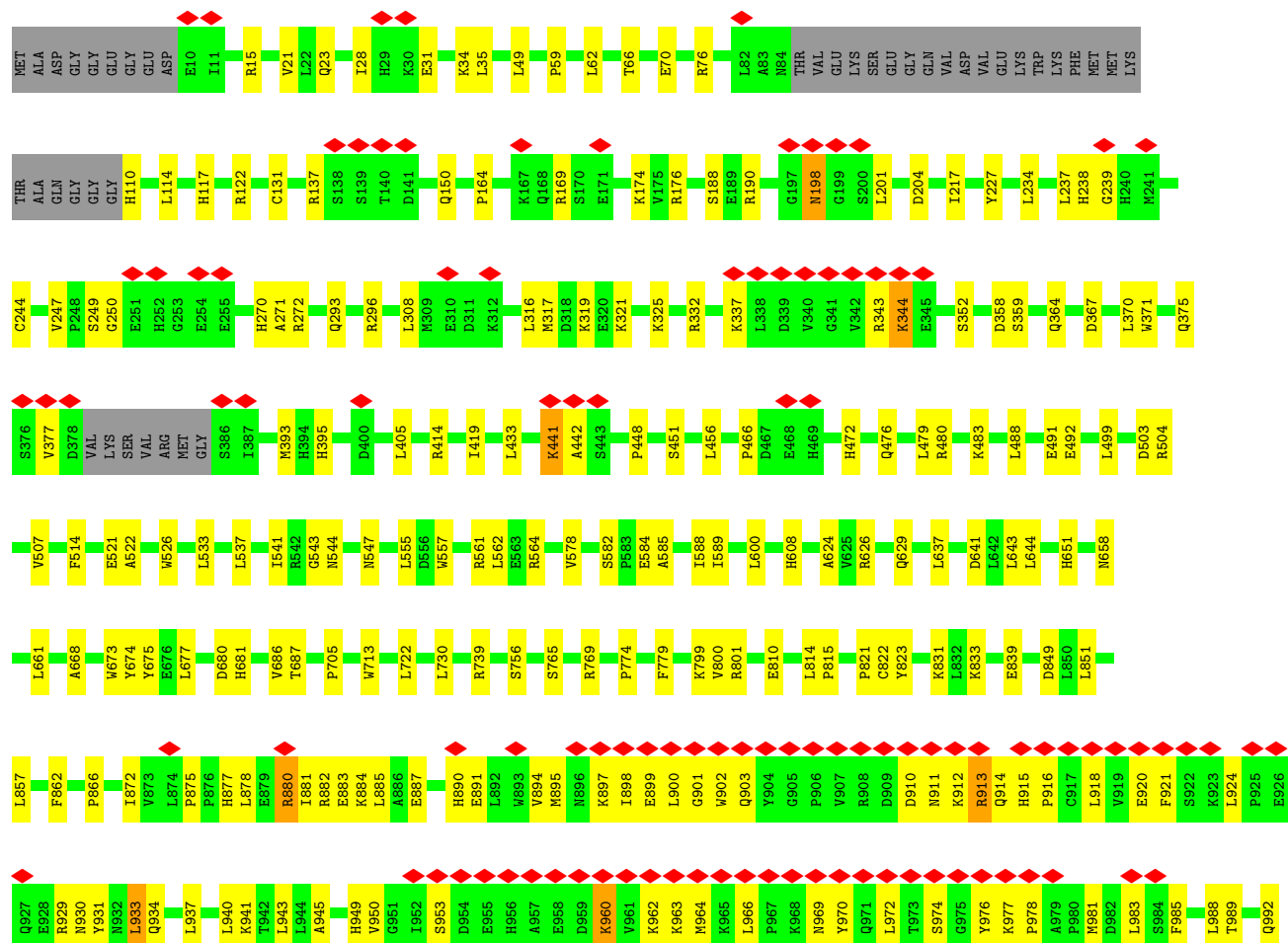






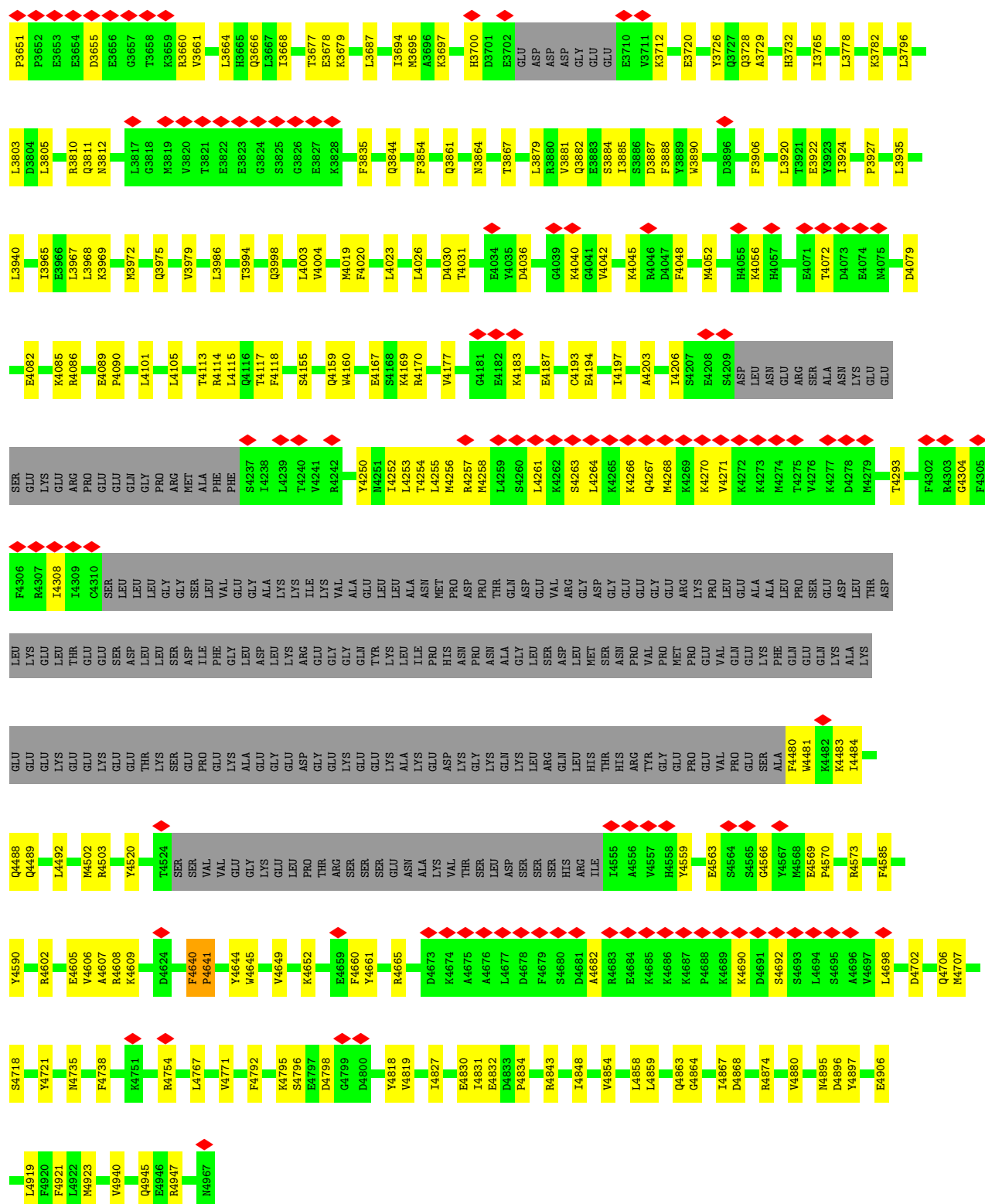


• Molecule 1: Ryanodine receptor 2



L2525	E2539	H2540	L2548	L2549	H2550	Q2565	R2566	D2567	S2568	L2569	E2570	V2571	R2581	M2584	L2589	R2590	R2591	L2592	V2593	M2605	P2606	C2617	Y2620	V2621	C2622	W2627	G2628	N2629	F2630	E2635	L2638	H2639	L2640	H2486	L2487	L2488	K2642	K2643	L2644	F2645	D2650	K2651	L2652	Q2654	E2658	Q2659		
LYS	THR	LEU	ASP	THR	GLU	E2377	E2378	D2379	D2380	A2403	K2413	G2414	E2415	A2416	L2429	G2430	D2431	V2435	I2436	A2446	K2447	V2452	M2456	K2465	V2469	V2475	Q2481	D2482	F2483	L2484	L2485	H2486	L2487	L2488	F2489	G2490	G2491	F2492	L2496	L2802	L2507	L2520						
E2183	S2184	K2185	E2186	T2187	M2192	Y2202	Y2202	T2206	Y2220	L2221	L2222	S2225	R2235	E2259	P2260	D2261	K2264	V2265	V2266	C2277	Q2278	M2279	L2280	K2283	R2287	D2300	F2301	L2302	R2303	L2323	G2332	P2333	R2336	P2364	ASN	SER	GLY	SER										
LYS	LYS	GLN	ALA	GLU	LYS	PRO	VAL	GLU	GLU	SER	ASP	SER	K2053	K2054	S2055	S2056	Q2059	T2065	L2075	E2076	D2077	V2081	R2082	L2087	R2090	Q2091	D2115	L2119	E2138	E2139	K2140	R2144	N2152	K2153	V2154	H2168	M2172	E2173	V2174	K2175	V2176	N2177	V2178	L2179	G2180	G2181	G2182	
E1083	I1086	I1087	F1088	K1097	R1100	W1101	Y1102	F1105	E1106	V1115	S1118	P1124	G1129	A1134	W1145	H1146	Q1147	D1185	G1198	V1204	C1205	V1054	L1207	R1214	Y1226	I1229	E1234	E1237	M1249	W1250	L1251	P1256	E1269	V1270	I1277	K1284												
E993	Y996	H1004	A1008	R1009	I1012	R1013	Q1014	R1027	R1031	P1034	L1037	L1038	R1041	T1042	K1043	S1045	N1046	K1047	D1048	R1051	E1052	A1053	V1054	R1055	T1056	L1057	Y1060	M1063	L1064	E1065	D1068	Q1069	D1070	H1071	A1072	A1073	R1074	A1075	E1076	V1077	C1078	S1079	G1080	T1081	G1082			
V1285	T1286	S1289	F1290	G1291	Q1293	M1294	S1295	M1296	E1312	K1316	THR	VAL	ALA	GLY	GLY	LEU	PRO	L1434	W1145	H1146	Q1147	D1185	G1198	V1204	C1205	V1054	L1207	R1214	Y1226	I1229	E1234	E1237	M1249	W1250	L1251	P1256	E1269	V1270	I1277	K1284								
ASP	LYS	GLU	ALA	LYS	PRO	GLU	PHE	ASN	GLN	HIS	LYS	ASP	TYR	ALA	GLN	LYS	PRO	ARG	ARG	THR	LYS	ASP	ASP	LEU	PRO	TYR	THR	SER	ALA	ARG	LEU	THR	GLU	VAL	ASP	LYS	THR	ALA	ASP	ASP	VAL	ARG	ASP	VAL	ASP	LYS		
Y1425	Y1427	Y1428	F1433	P1434	G1444	Y1445	I1446	Y1453	G1456	R1461	V1462	R1463	T1464	D1471	E1472	K1473	G1474	I1480	G1483	M1487	G1491	M1494	G1497	Q1498	G1499	R1500	N1501	L1518	Y1531	A1542	T1548	N1551	Q1554	V1563	M1564	P1565	K1572	K1576										
V1594	L1604	V1608	I1611	R1614	L1618	F1627	L1630	E1634	E1635	E1649	L1650	H1656	T1657	L1667	G1668	N1669	S1678	H1679	E1682	L1685	I1689	R1699	Y1703	L1706	L1711	Y1714	R1718	L1719	M1722	E1732	I1736	M1743	K1744															
K1745	L1748	I1751	G1752	L1753	S1754	T1755	R1758	F1768	E1774	P1783	L1784	D1785	K1788	L1829	I1830	M1831	G1832	I1833	F1834	D1838	L1839	I1842	E1853	A1854	ALA	THR	PRO	GLU	GLU	GLU	SER	ASP	THR	LEU	GLU	GLU	LYS	LEU	LEU	SER	VAL	ASP	ASP					
ALA	LYS	GLN	GLY	ALA	GLY	GLU	GLU	ALA	GLY	LYS	GLY	ARG	P1889	K1890	L1894	Q1895	M1896	K1897	L1898	V1902	Q1911	Y1912	L1913	C1914	V1918	R1919	I1922	V1926	D1931	F1932	L1936	Q1937	V1947	A1950	L1951	M1952	M1953	S1954	A1955	A1956	L1957	T1958	A1959	R1960	K1961	T1962		
F1965	R1966	S1967	P1968	Q1972	L1976	L1977	N1978	F1979	D1982	K1983	S1984	E1985	C1986	E1991	I1992	R1993	L1996	H2000	M2004	E2010	LEU	ASP	GLU	ASP	GLY	SER	LEU	ASP	GLY	ASN	SER	ASP	LEU	THR	ILE	ARG	GLY	ARG	LEU	SER	LEU	VAL	GLU	LYS	VAL	THR	LYS	
LYS	LYS	GLN	ALA	LYS	PRO	VAL	GLU	GLU	SER	ASP	SER	K2053	K2054	S2055	S2056	Q2059	T2065	L2075	E2076	D2077	V2081	R2082	L2087	R2090	Q2091	D2115	L2119	E2138	E2139	K2140	R2144	N2152	K2153	V2154	H2168	M2172	E2173	V2174	K2175	V2176	N2177	V2178	L2179	G2180	G2181	G2182		
E2183	S2184	K2185	E2186	T2187	M2192	Y2202	Y2202	T2206	Y2220	L2221	L2222	S2225	R2235	E2259	P2260	D2261	K2264	V2265	V2266	C2277	Q2278	M2279	L2280	K2283	R2287	D2300	F2301	L2302	R2303	L2323	G2332	P2333	R2336	P2364	ASN	SER	GLY	SER										
LYS	THR	LEU	ASP	THR	GLU	E2377	E2378	D2379	D2380	A2403	K2413	G2414	E2415	A2416	L2429	G2430	D2431	V2435	I2436	A2446	K2447	V2452	M2456	K2465	V2469	V2475	Q2481	D2482	F2483	L2484	L2485	H2486	L2487	L2488	F2489	G2490	G2491	F2492	L2496	L2802	L2507	L2520						

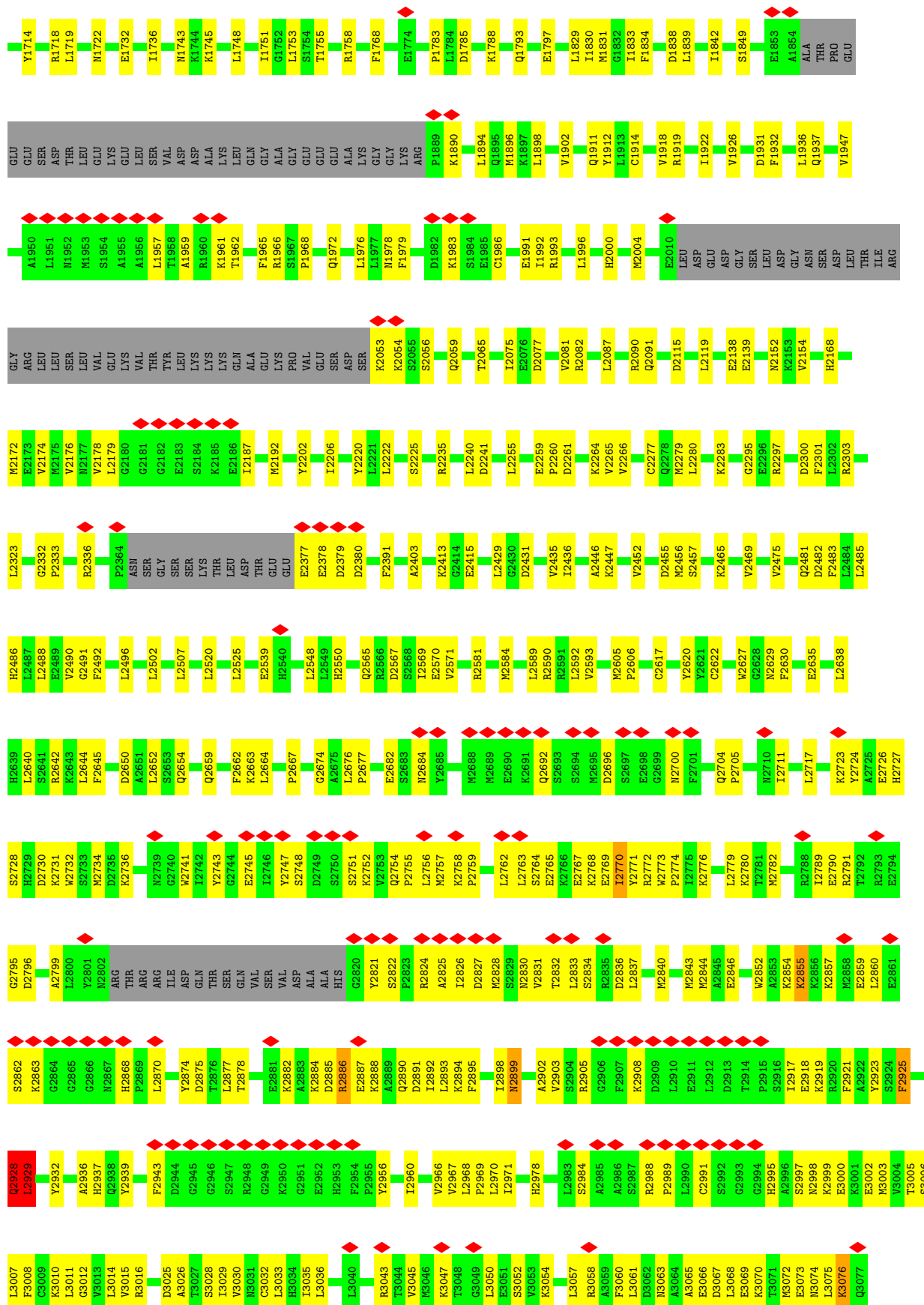




• Molecule 1: Ryanodine receptor 2







G3078	G3156	M3235	V3301	ALA	ASN	PRO	ASP	F3603	E3720	F3888	K4045	I4197	K4269
Q3079	G3159	E3236	F3302	ARG	GLU	GLY	PRO	R3604	E3726	T3889	R4046	A4203	K4270
F3080	L3159	I3237	S3303	ASP	ILE	ASP	GLU	M3605	Y3726	W3890	D4047	A4206	V4271
T3081	F3162	L3239	Q3304	TYR	ASN	GLU	THR	P3607	Q3727	D3896	F4048	S4207	K4272
HIS	A3163	M3240	P3305	ALA	MET	ILE	VAL	L3608	A3728	F3906	M4052	E4208	K4273
THR	G3164	M3241	T3307	PHE	SER	ALA	GLU	A3729	A3729	L3906	H4052	S4209	M4274
ARG	F3165	L3242	N3308	PRO	PHE	ALA	ARG	Q3622	Q3622	L3920	H4055	ASP	T4275
ASN	F3167		K3309	LEU	ILE	ALA	VAL	K3626	L3765	T3921	K4056	LEU	V4276
PRO	P3167		Q3312	LEU	THR	ASN	ASP	E3637	L3778	E3922	H4057	ASN	K4277
K3088	V3168		Q3313	ILE	ASP	ARG	ALA	E3642	K3782	L3935	E4071	ARG	D4278
G3089	G3089		L3314	ARG	THR	THR	ASN	K3646	L3803	L3940	T4072	ALA	M4279
V3090	A3169		L3315	VAL	LYS	GLU	VAL	E3650	D3884	L3965	D4073	LYS	L4294
T3091	F3170		K3316	SER	SER	ASP	GLN	P3651	R3810	E3966	E4074	GLU	F4302
G3092	L3171			ASP	LEU	ASP	VAL	E3653	Q3811	L3967	D4075	SER	R4303
I3093			F3319	TYR	MET	LYS	ARG	E3654	N3812	L3968	M4079	GLY	G4304
I3094	H3174		L3320	ASN	SER	THR	GLY	D3655	L3817	M3972	D4082	PRO	F4305
K3095	L3175		P3321	LYS	LYS	GLU	ILE	E3656	G3818	Q3975	E4086	GLU	F4306
Y3096	L3176		L3322	TRP	ARG	VAL	GLU	T3658	V3820	V3979	R4086	GLU	R4307
T3097	K3177		M3323	LEU	GLY	ASP	VAL	E3659	T3821	L3986	E4089	GLN	I4308
L3101	H3178		E3324	LYS	ASN	ILE	VAL	D3660	E3822	L3986	P4090	ARG	T4309
M3104	D3176		K3325	PRO	GLU	ILE	GLY	V3661	E3823	T3994	L4101	ALA	G4310
L3105	N3179		L3326	GLU	GLU	ARG	GLU	L3664	G3824	M4012	L4105	PHE	LEU
F3109	Y3184		K3327	PRO	ASN	ARG	THR	Q3665	S3825	M4019	T4113	PHE	LEU
	K3187		K3328	ALA	LYS	THR	LYS	L3666	E3826	F4020	R4114	ALA	GLY
	S3188		K3329	ALA	GLY	GLN	VAL	Q3667	G3827	L4023	L4115	ALA	GLY
G3113	R3189		A3330	VAL	GLN	ASP	GLU	E3677	K3828	F4026	R4116	ALA	GLY
G3114	S3190		A3331	THR	ASN	ASP	GLU	E3678	F3835	M4030	V4177	ALA	GLY
H3115	E3191		T3332	LEU	GLY	PRO	GLN	K3679	Q3844	T4031	G4181	ALA	GLY
Q3116	S3192		V3333	PHE	ASP	THR	ALA	L3687	F3854	E4034	E4182	ALA	GLY
F3117	A3193		V3334	VAL	THR	ILE	VAL	T3694	Q3861	G4039	K4183	ALA	GLY
G3118	A3194		E3336	ALA	SER	TRP	TRP	A3695	N3864	K4040	E4187	ALA	GLY
E3119			E3337	ALA	MET	GLN	GLN	K3697	T3867	G4041	C4193	ALA	GLY
D3120	L3197		ASP	GLU	GLN	ASP	GLU	H3700	L3879	V4042	E4194	ALA	GLY
L3121	P3198		HIS	VAL	ASN	THR	ALA	D3701	R3880			ALA	GLY
I3122	T3199		LEU	PHE	LEU	THR	LYS	E3702	V3881			ALA	GLY
L3123	D3203		LYS	ILE	SER	ILE	LYS	ASP	Q3882			ALA	GLY
E3124			ALA	TRP	LEU	TRP	VAL	ASP	E3883			ALA	GLY
D3125	N3207		GLU	SER	VAL	GLN	TRP	GLY	S3884			ALA	GLY
V3126			ALA	LYS	ALA	MET	ALA	H3700	T3867			ALA	GLY
Q3127	L3211		ARG	LYS	ALA	GLN	ALA	D3701	L3879			ALA	GLY
V3128	E3212		GLY	ASP	ALA	VAL	LYS	ASP	R3880			ALA	GLY
S3129	K3213		ASP	ASN	LEU	VAL	LEU	ASP	V3881			ALA	GLY
C3130	L3214		SER	PHE	ARG	TRP	SER	GLY	E3883			ALA	GLY
Y3131	M3215		GLU	LYS	LEU	LYS	LYS	GLU	S3884			ALA	GLY
R3132	G3216		ALA	ARG	LEU	ASP	GLN	E3710	L3879			ALA	GLY
I3133	E3217		ALA	GLU	PRO	PRO	ARG	V3701	T3867			ALA	GLY
L3134	I3218		LEU	GLU	ASN	ASN	VAL	E3702	L3879			ALA	GLY
	A3222		LEU	GLN	LEU	THR	ARG	ASP	R3880			ALA	GLY
L3137	G3225		ILE	ASN	LEU	ASP	ALA	ASP	V3881			ALA	GLY
V3138	I3226		LEU	PHE	ASN	ASP	ALA	GLY	E3883			ALA	GLY
A3139	Y3228		LEU	VAL	ILE	THR	VAL	GLU	S3884			ALA	GLY
	H3233		THR	GLN	THR	SER	SER	E3710	L3879			ALA	GLY
	V3234		LEU					V3711	D3887			ALA	GLY

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	191898	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	0.628	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/34511	0.51	7/46614 (0.0%)
1	B	0.26	0/34511	0.51	7/46614 (0.0%)
1	C	0.26	0/34511	0.51	7/46614 (0.0%)
1	D	0.26	0/34511	0.51	7/46614 (0.0%)
2	E	0.30	0/834	0.54	0/1123
2	F	0.30	0/834	0.54	0/1123
2	G	0.30	0/834	0.54	0/1123
2	H	0.30	0/834	0.54	0/1123
All	All	0.26	0/141380	0.51	28/190948 (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	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2928	GLN	CA-CB-CG	6.25	127.15	113.40
1	B	2928	GLN	CA-CB-CG	6.25	127.15	113.40
1	C	2928	GLN	CA-CB-CG	6.23	127.11	113.40
1	D	2928	GLN	CA-CB-CG	6.23	127.11	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	933	LEU	CA-CB-CG	5.72	128.47	115.30

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3227	ARG	Sidechain
1	A	3606	ALA	Peptide
1	A	4640	PHE	Peptide
1	B	3227	ARG	Sidechain
1	B	3606	ALA	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	33771	0	33455	752	0
1	B	33771	0	33455	745	0
1	C	33771	0	33455	741	0
1	D	33771	0	33455	752	0
2	E	818	0	821	24	0
2	F	818	0	821	21	0
2	G	818	0	821	23	0
2	H	818	0	821	25	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	0	0
4	B	62	0	24	0	0
4	C	62	0	24	0	0
4	D	62	0	24	0	0
All	All	138608	0	137200	3013	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 11.

The worst 5 of 3013 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:2736:LYS:NZ	1:A:2757:MET:SD	2.38	0.97
1:D:2736:LYS:NZ	1:D:2757:MET:SD	2.38	0.97
1:C:2736:LYS:NZ	1:C:2757:MET:SD	2.38	0.97
1:B:2736:LYS:NZ	1:B:2757:MET:SD	2.38	0.96
1:A:901:GLY:HA3	1:A:913:ARG:HH22	1.36	0.90

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%)	4080 (97%)	115 (3%)	3 (0%)	48	79
1	B	4198/4967 (84%)	4081 (97%)	114 (3%)	3 (0%)	48	79
1	C	4198/4967 (84%)	4082 (97%)	113 (3%)	3 (0%)	48	79
1	D	4198/4967 (84%)	4081 (97%)	114 (3%)	3 (0%)	48	79
2	E	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	F	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	G	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
2	H	105/108 (97%)	100 (95%)	5 (5%)	0	100	100
All	All	17212/20300 (85%)	16724 (97%)	476 (3%)	12 (0%)	50	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3927	PRO
1	A	4641	PRO
1	B	3927	PRO
1	B	4641	PRO

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Mol	Chain	Res	Type
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%)	3674 (99%)	34 (1%)	75	88
1	B	3708/4358 (85%)	3674 (99%)	34 (1%)	75	88
1	C	3708/4358 (85%)	3674 (99%)	34 (1%)	75	88
1	D	3708/4358 (85%)	3674 (99%)	34 (1%)	75	88
2	E	88/89 (99%)	87 (99%)	1 (1%)	70	86
2	F	88/89 (99%)	87 (99%)	1 (1%)	70	86
2	G	88/89 (99%)	87 (99%)	1 (1%)	70	86
2	H	88/89 (99%)	87 (99%)	1 (1%)	70	86
All	All	15184/17788 (85%)	15044 (99%)	140 (1%)	74	88

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	1013	ARG
1	D	2053	LYS
1	D	3076	LYS
1	B	1044	LYS
1	B	1013	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1593	HIS
1	D	261	HIS
1	C	2654	GLN
1	C	2978	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1046	ASN

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 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	B	5002	-	28,33,33	0.62	0	34,52,52	0.60	1 (2%)
4	ATP	C	5003	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
4	ATP	A	5002	-	28,33,33	0.62	0	34,52,52	0.59	1 (2%)
4	ATP	C	5002	-	28,33,33	0.63	0	34,52,52	0.61	1 (2%)
4	ATP	D	5003	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
4	ATP	B	5003	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
4	ATP	A	5003	-	28,33,33	0.64	0	34,52,52	0.58	1 (2%)
4	ATP	D	5002	-	28,33,33	0.63	0	34,52,52	0.60	1 (2%)

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	-	-	6/18/38/38	0/3/3/3
4	ATP	C	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5002	-	-	6/18/38/38	0/3/3/3
4	ATP	C	5002	-	-	6/18/38/38	0/3/3/3
4	ATP	D	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	B	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	A	5003	-	-	7/18/38/38	0/3/3/3
4	ATP	D	5002	-	-	6/18/38/38	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(°)
4	C	5002	ATP	C5-C6-N6	2.35	123.89	120.31
4	A	5003	ATP	C5-C6-N6	2.34	123.87	120.31
4	D	5003	ATP	C5-C6-N6	2.33	123.86	120.31
4	B	5003	ATP	C5-C6-N6	2.32	123.84	120.31
4	C	5003	ATP	C5-C6-N6	2.32	123.84	120.31

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

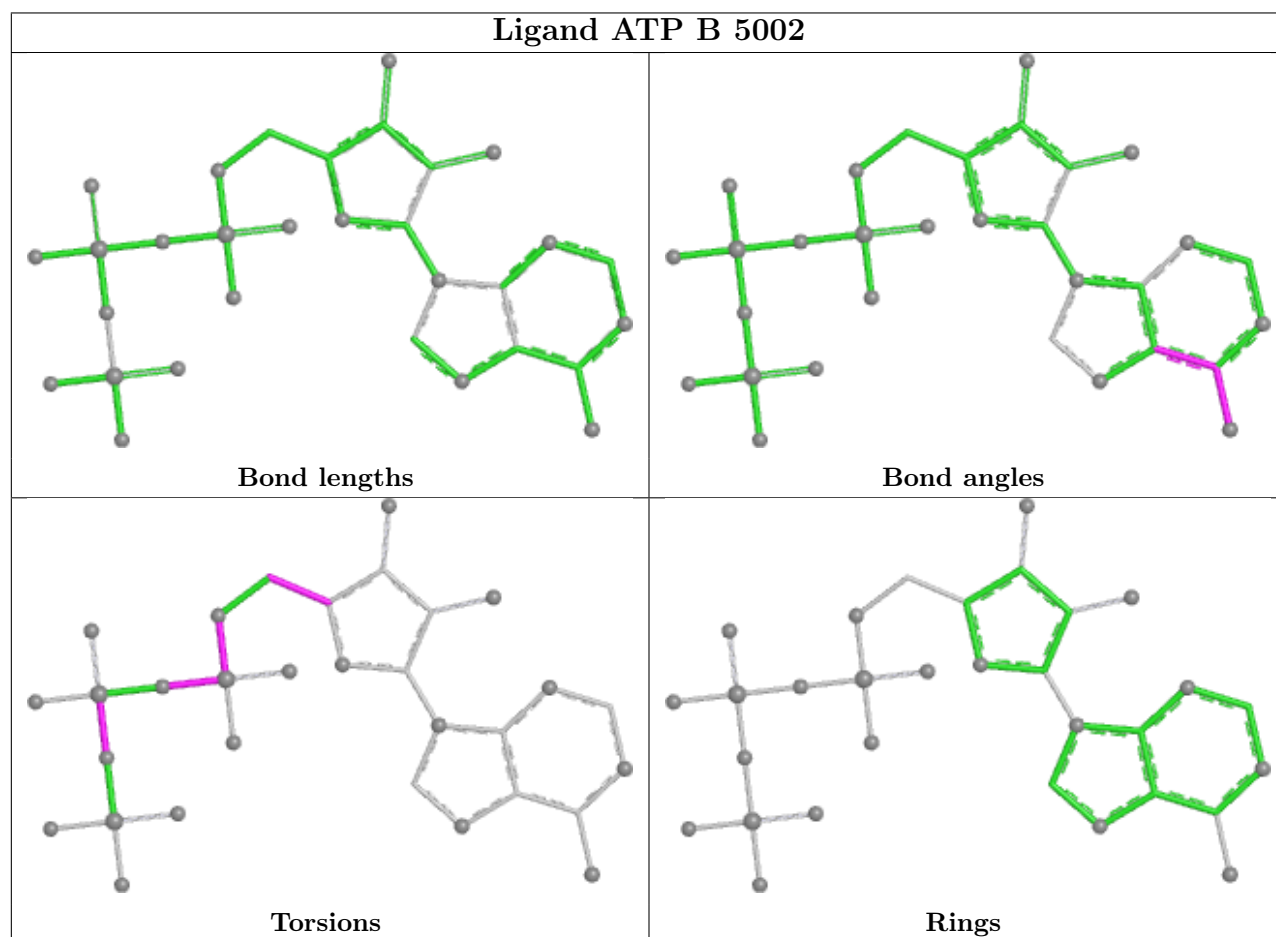
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5003	ATP	PB-O3B-PG-O3G
4	A	5003	ATP	C5'-O5'-PA-O1A
4	A	5003	ATP	C5'-O5'-PA-O2A

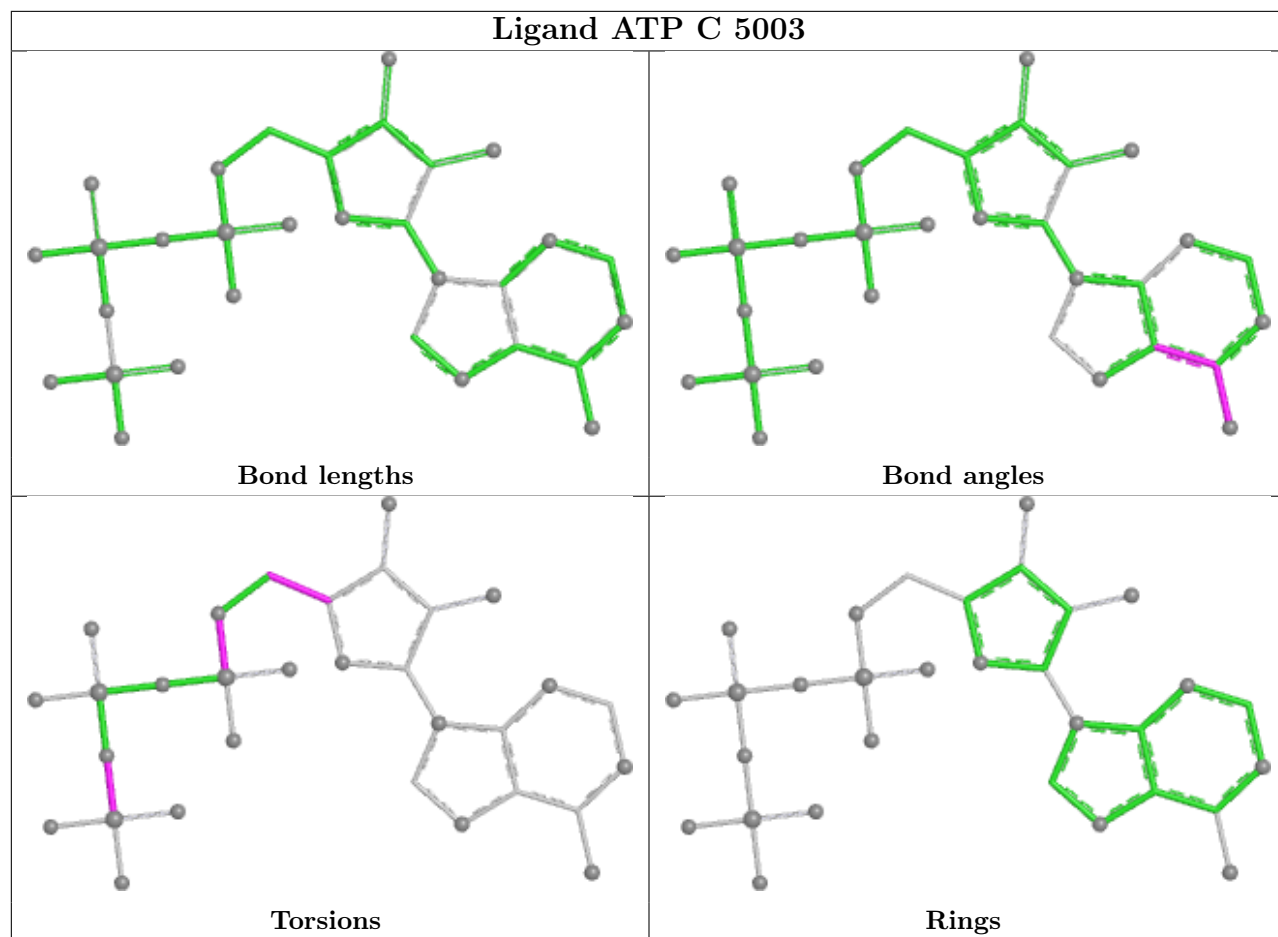
There are no ring outliers.

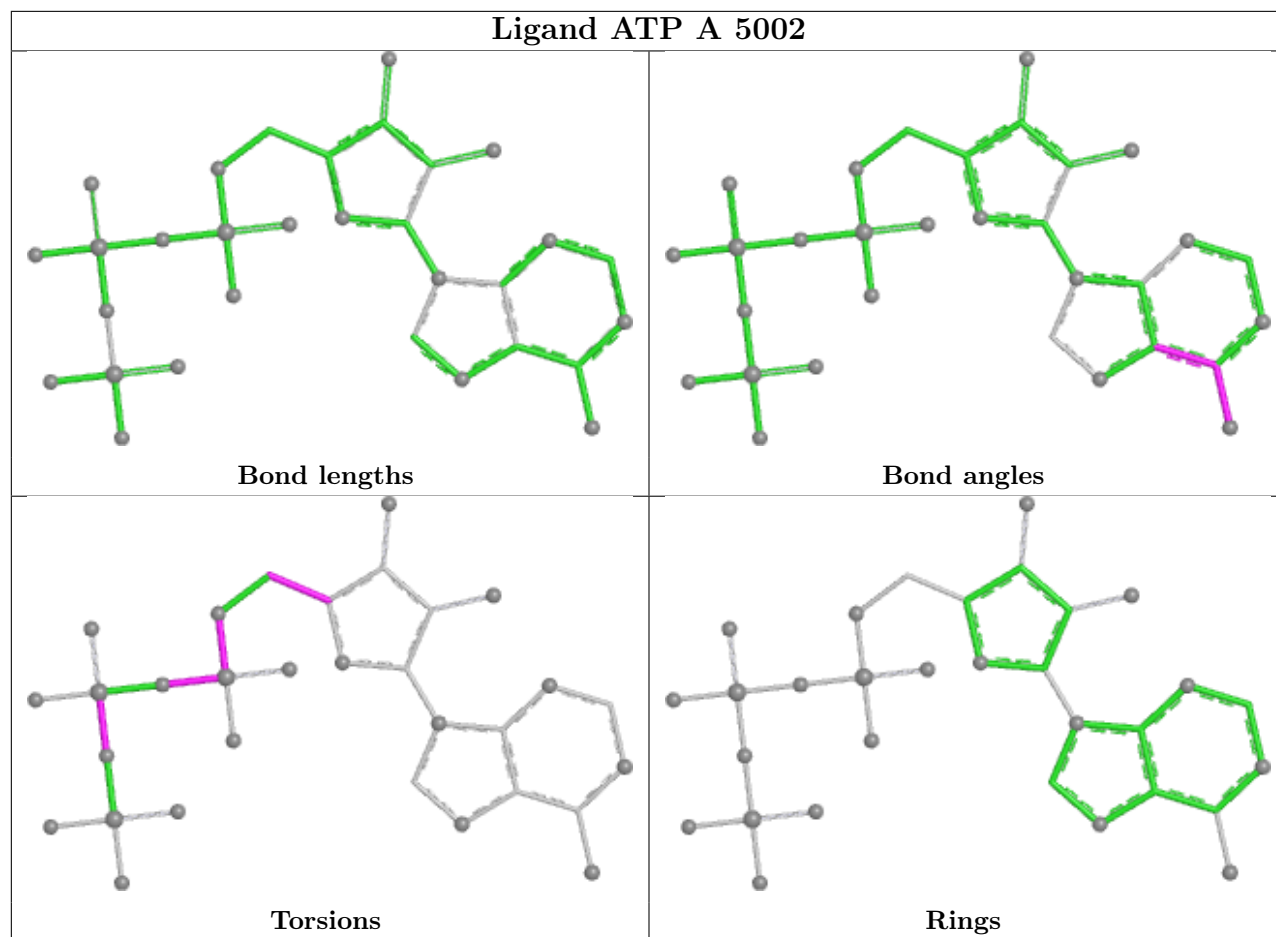
No monomer is involved in short contacts.

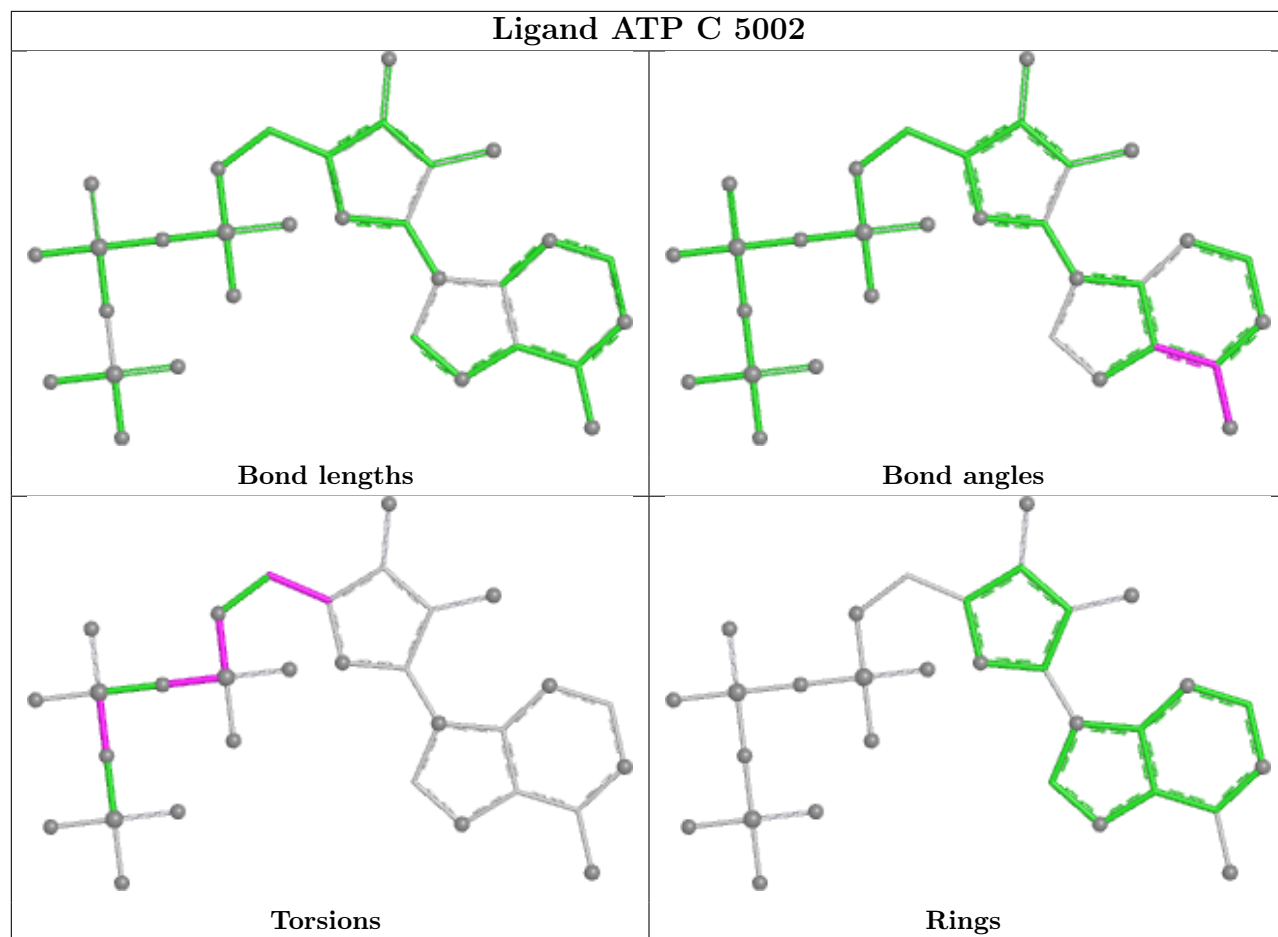
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

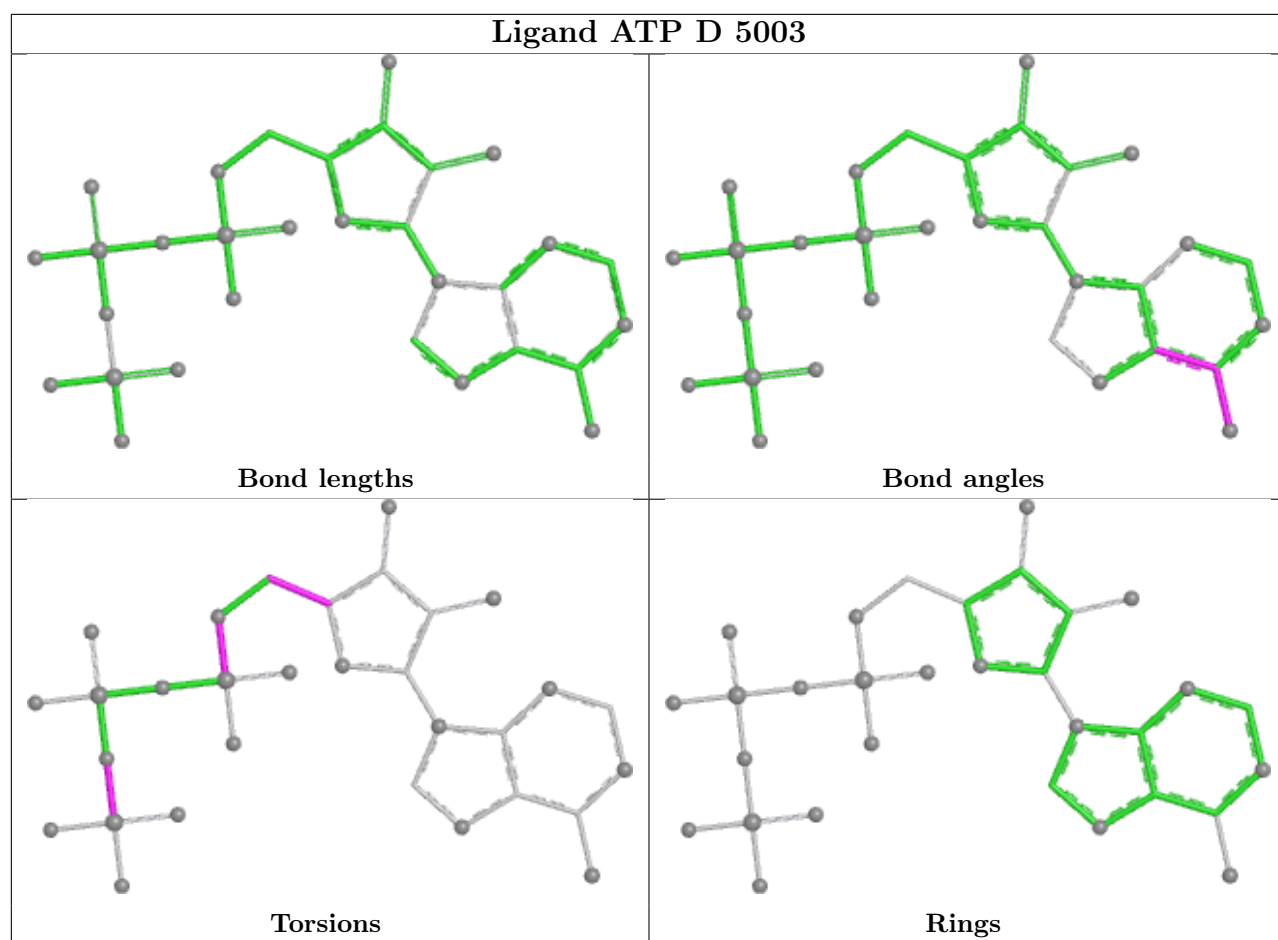
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

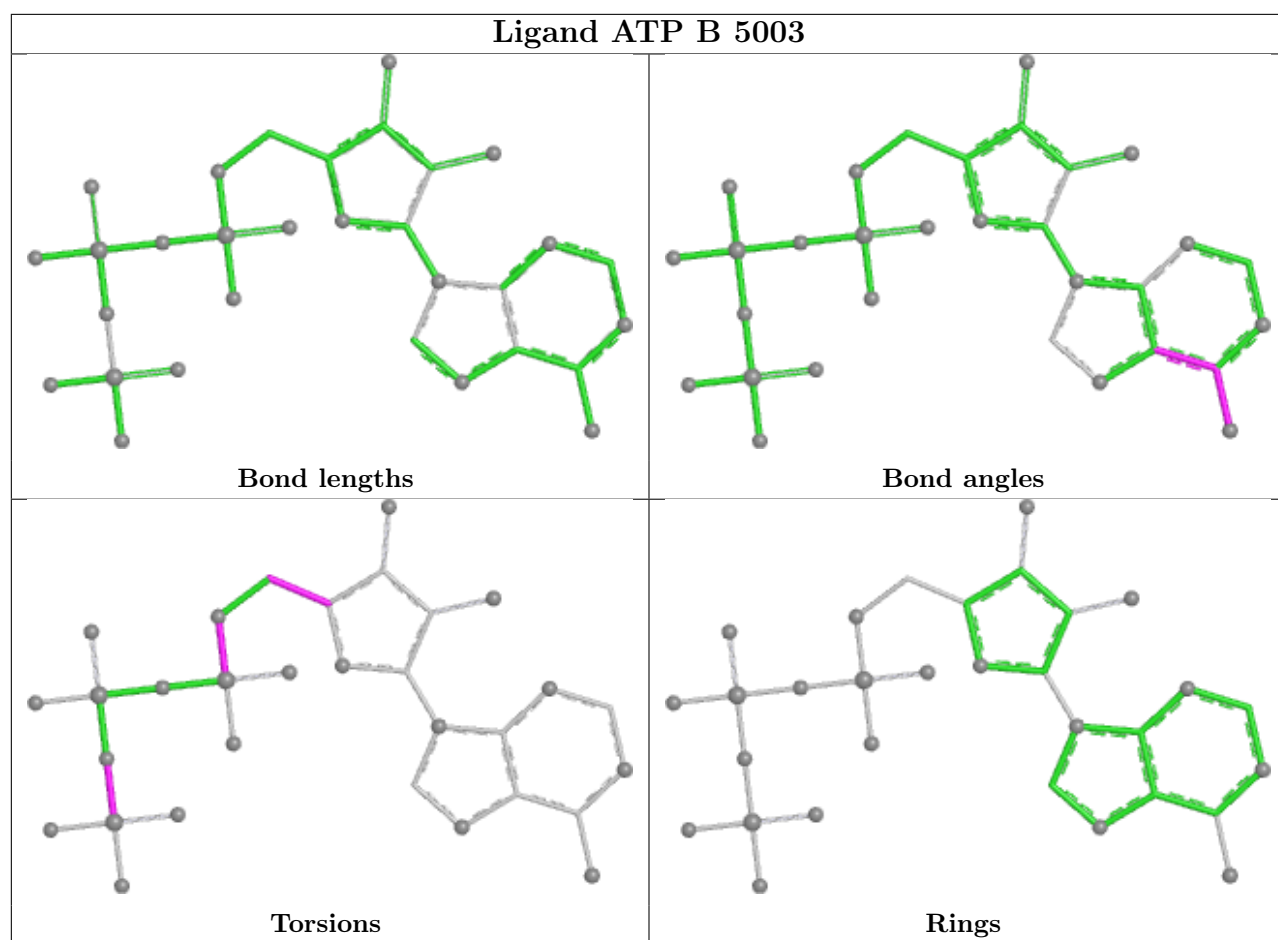


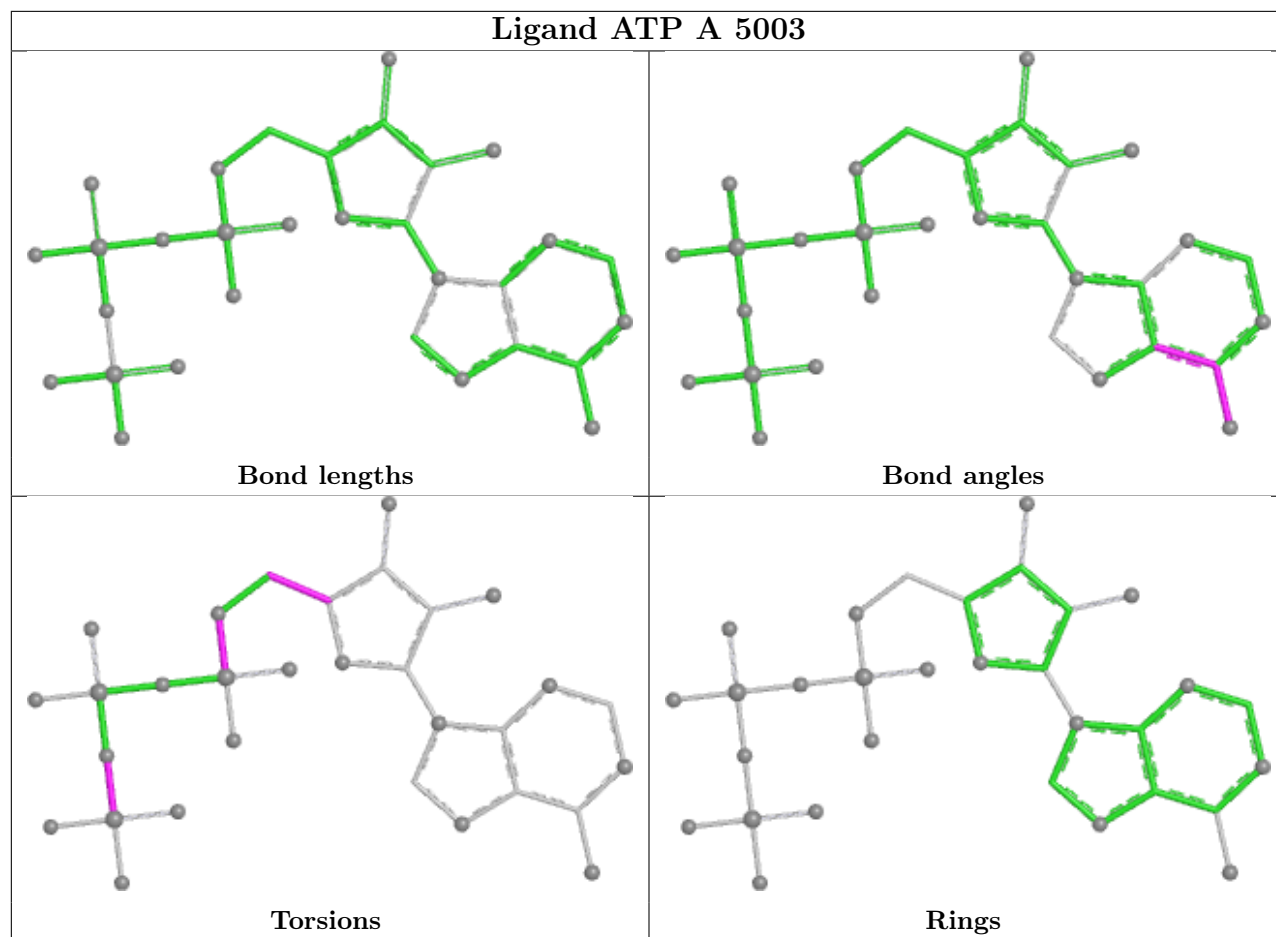


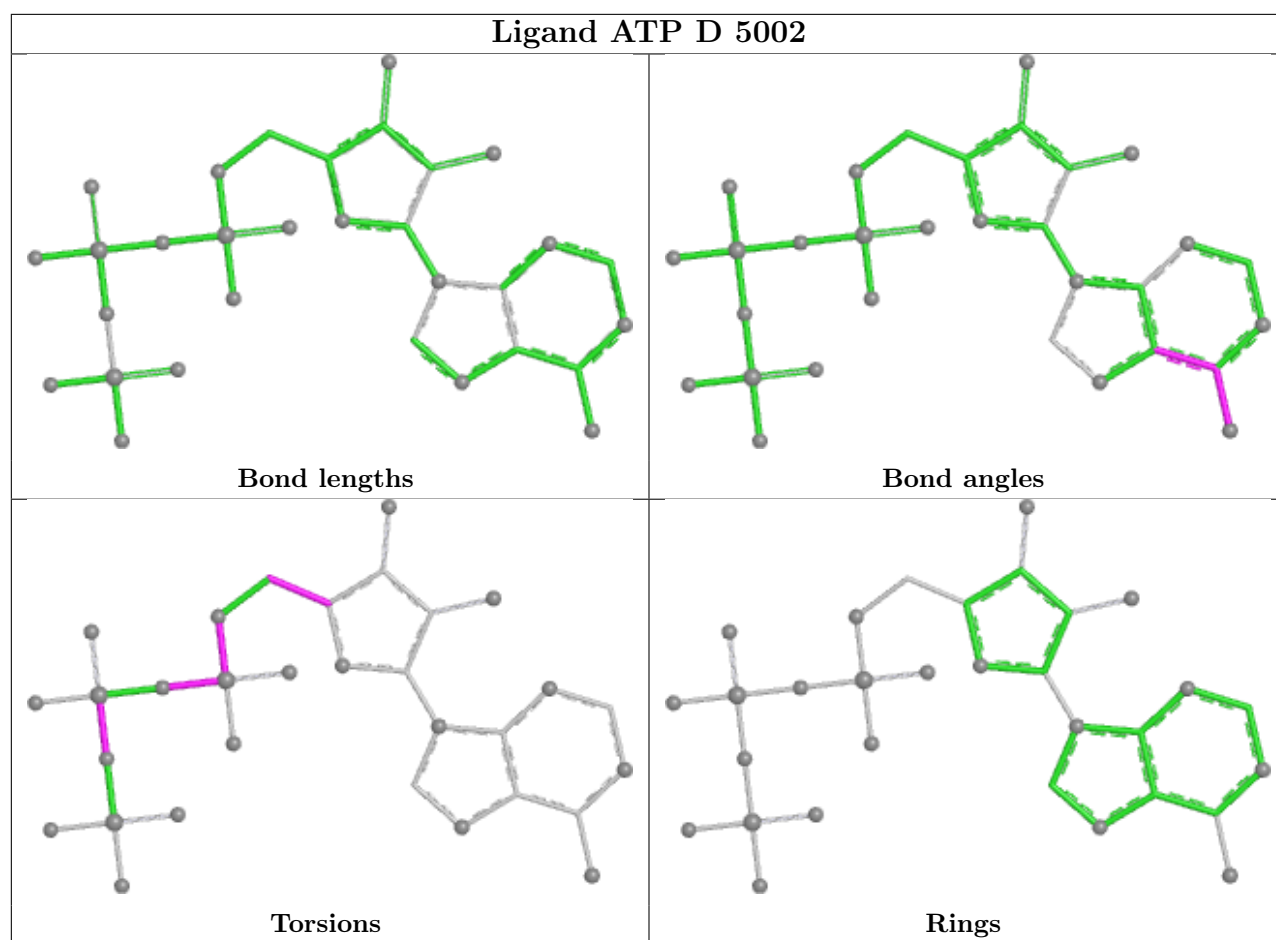












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42458. These allow visual inspection of the internal detail of the map and identification of artifacts.

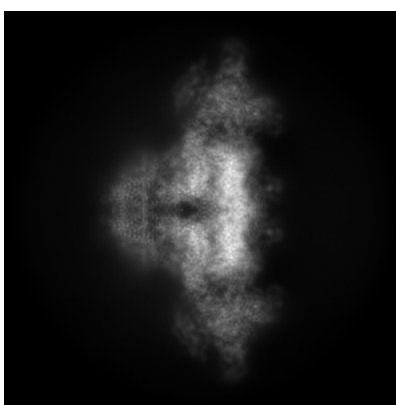
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

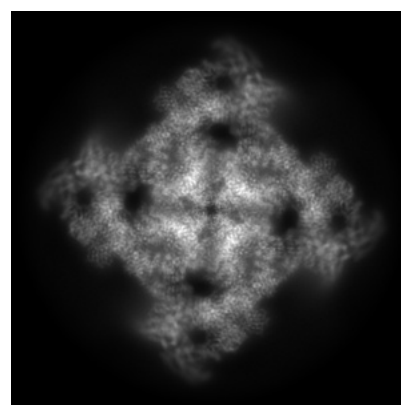
6.1.1 Primary map



X



Y

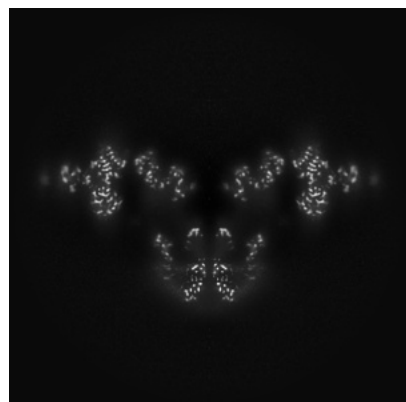


Z

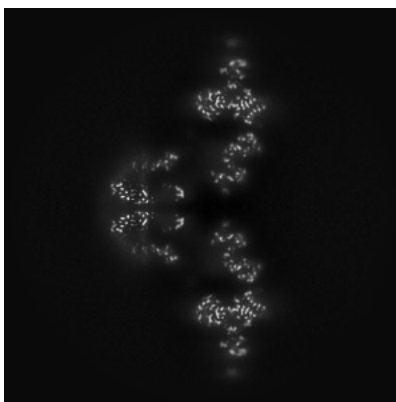
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

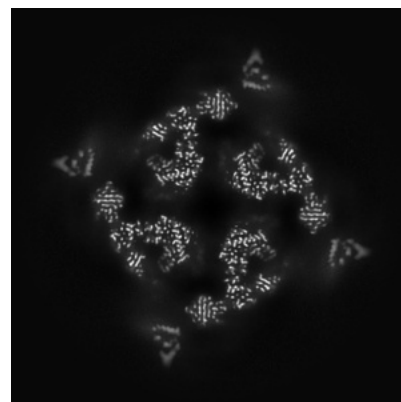
6.2.1 Primary map



X Index: 256



Y Index: 256

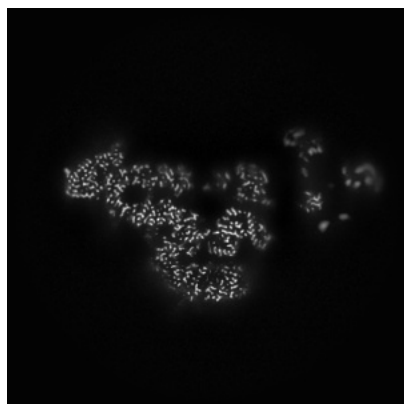


Z Index: 256

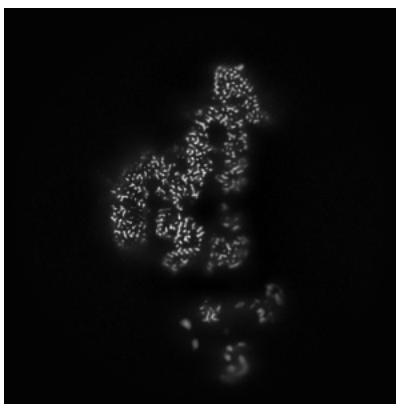
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

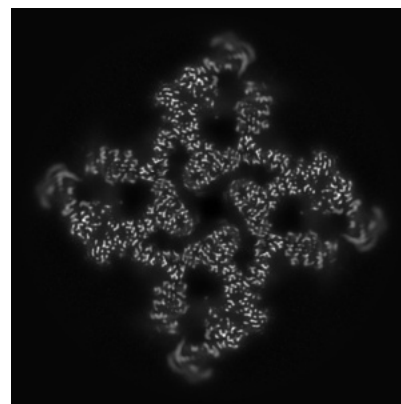
6.3.1 Primary map



X Index: 279



Y Index: 279

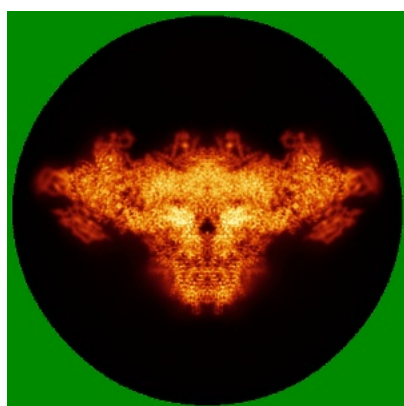


Z Index: 290

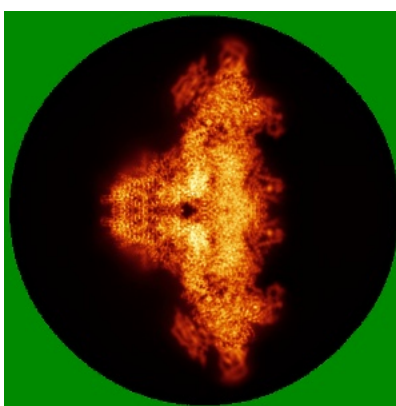
The images above show the largest variance slices of the map in three orthogonal directions.

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

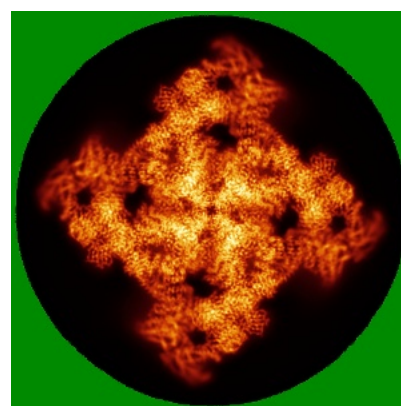
6.4.1 Primary map



X



Y

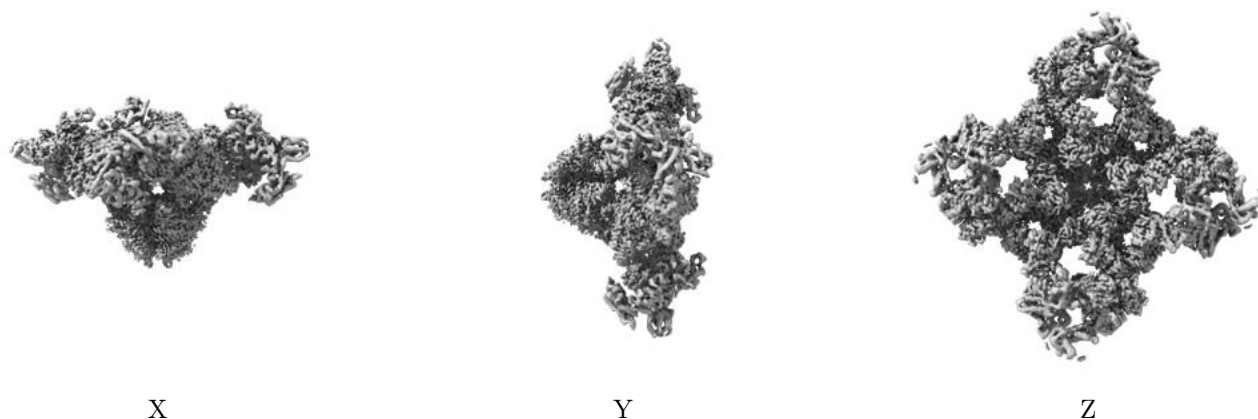


Z

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.

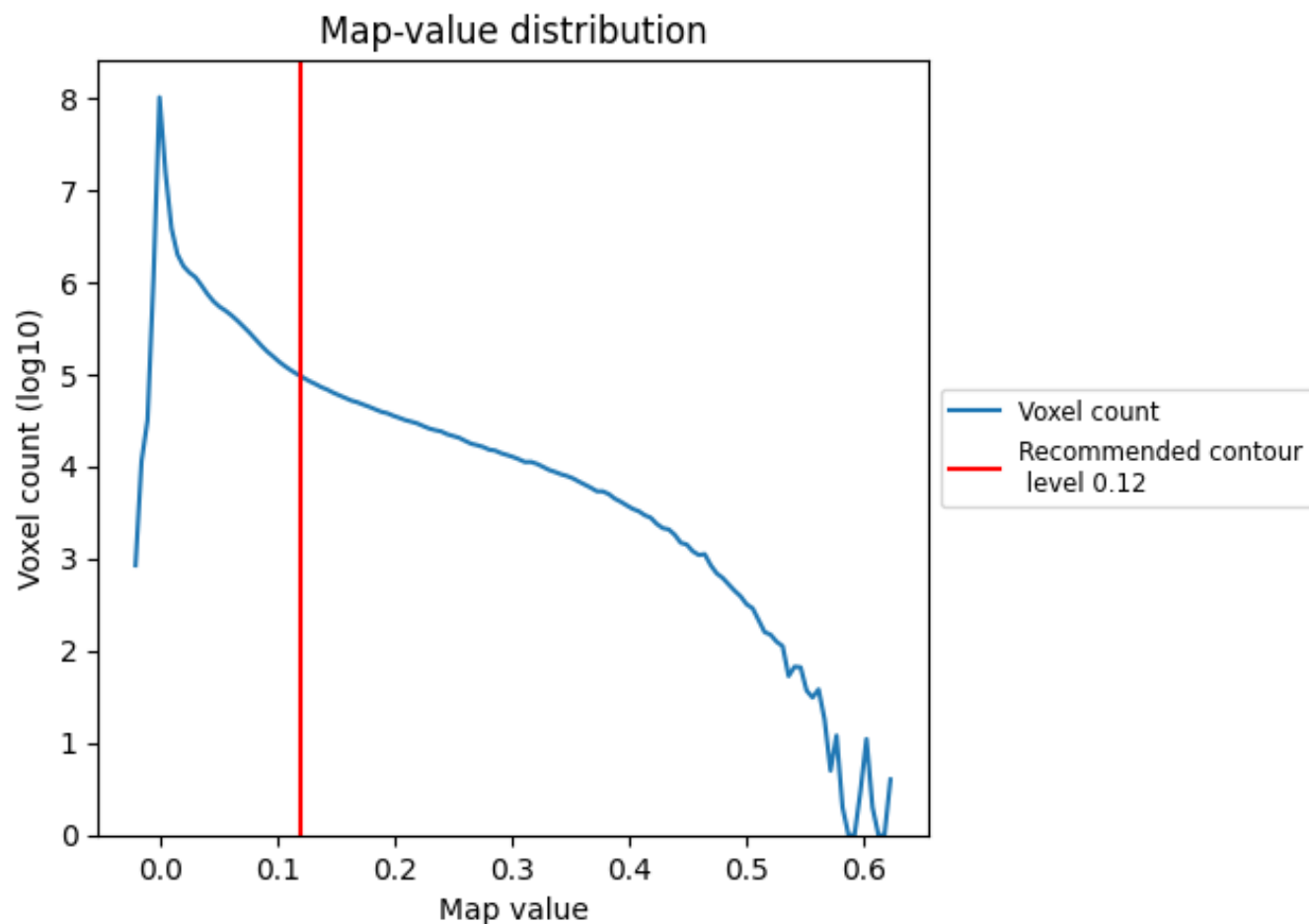
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

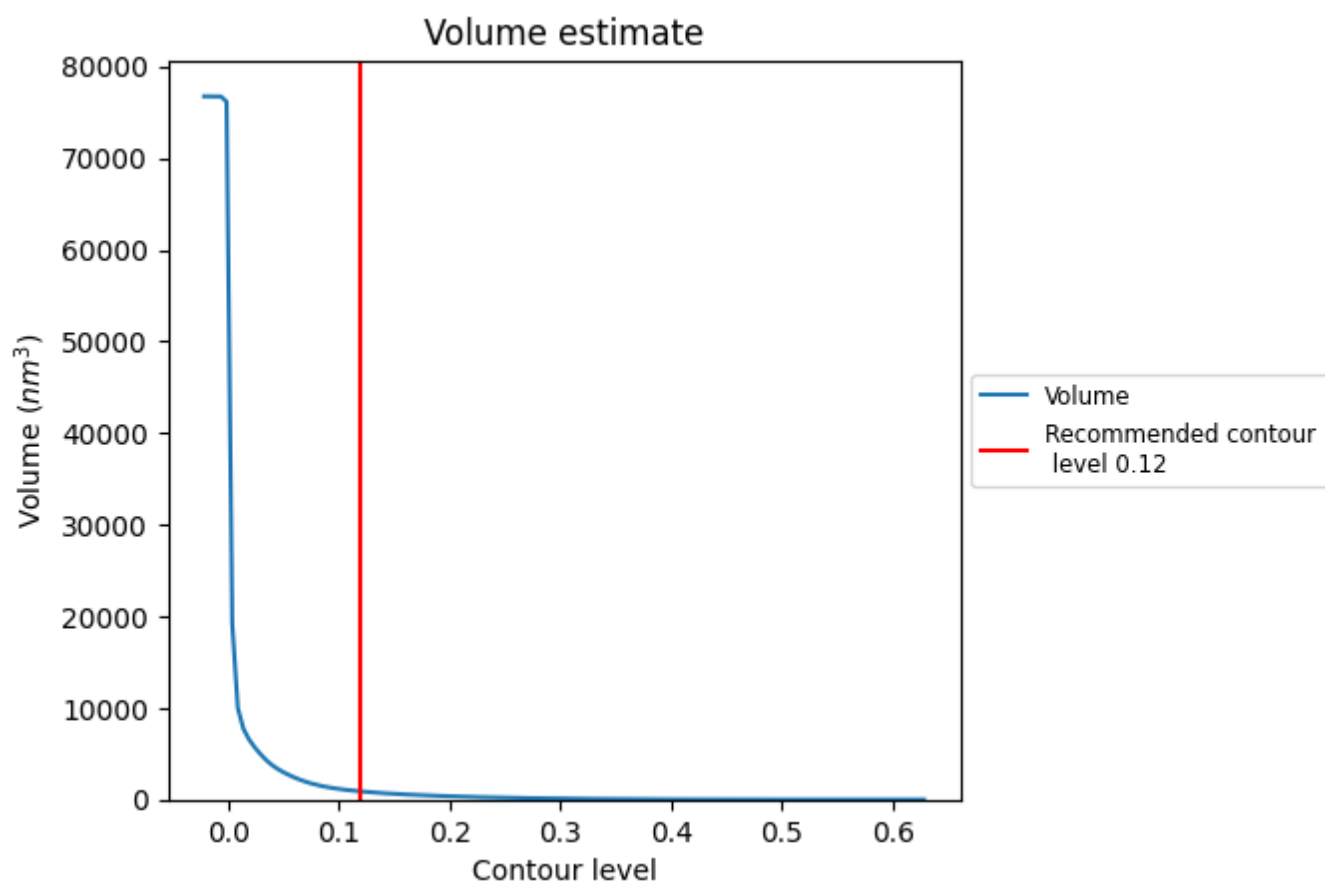
This section contains the results of statistical analysis of the map.

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.

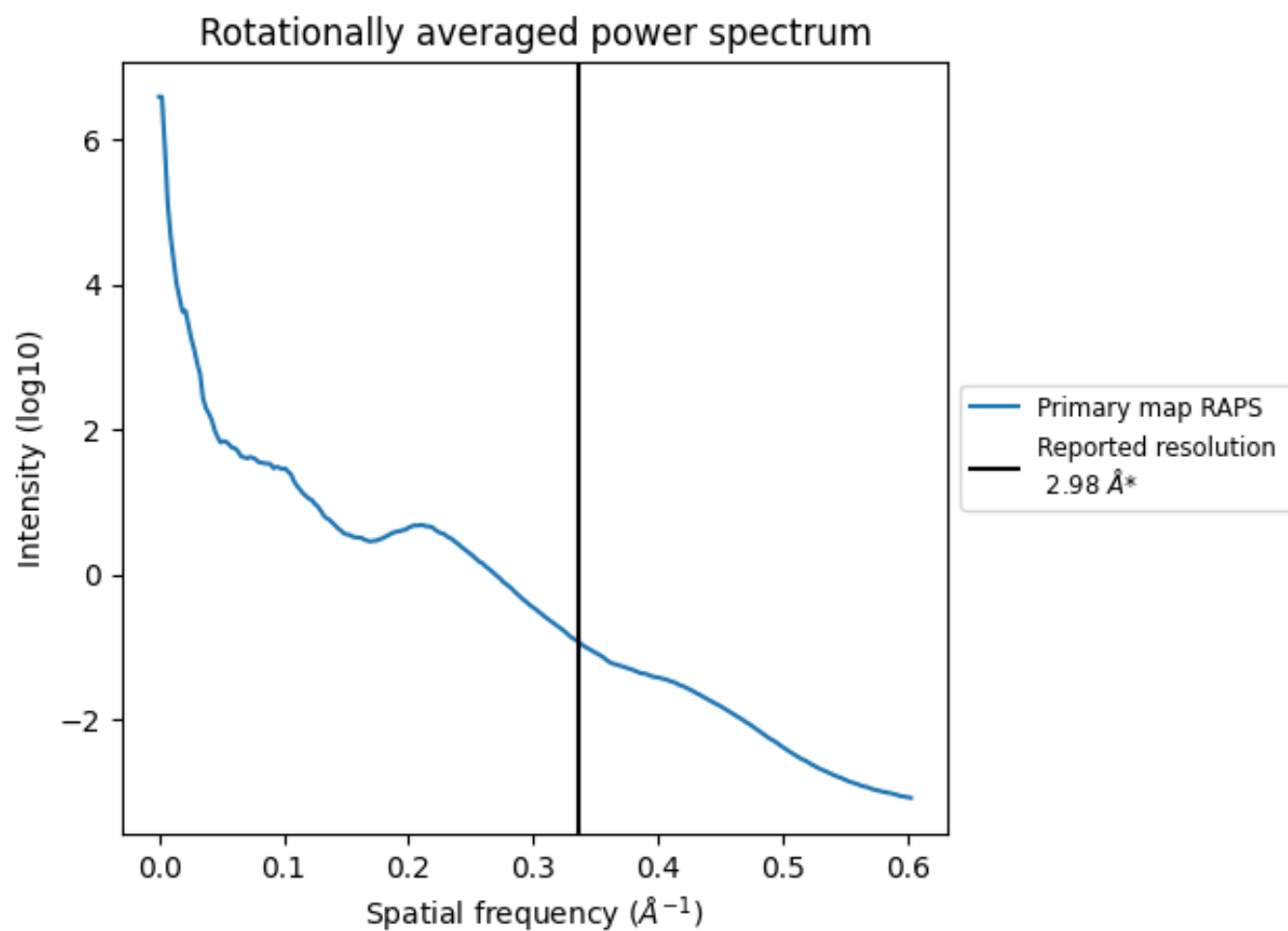
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 891 nm³; this corresponds to an approximate mass of 805 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 0.336 Å⁻¹

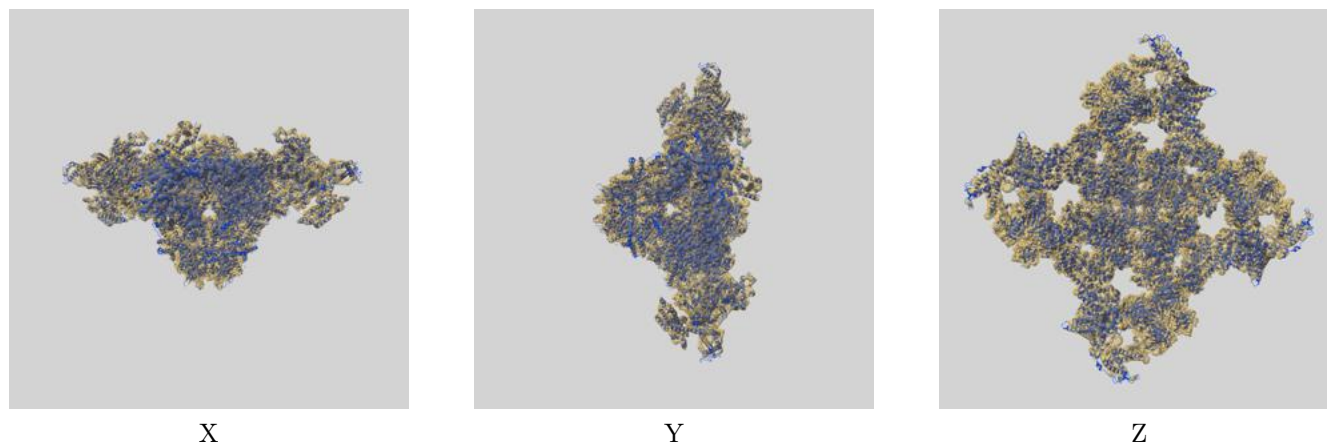
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

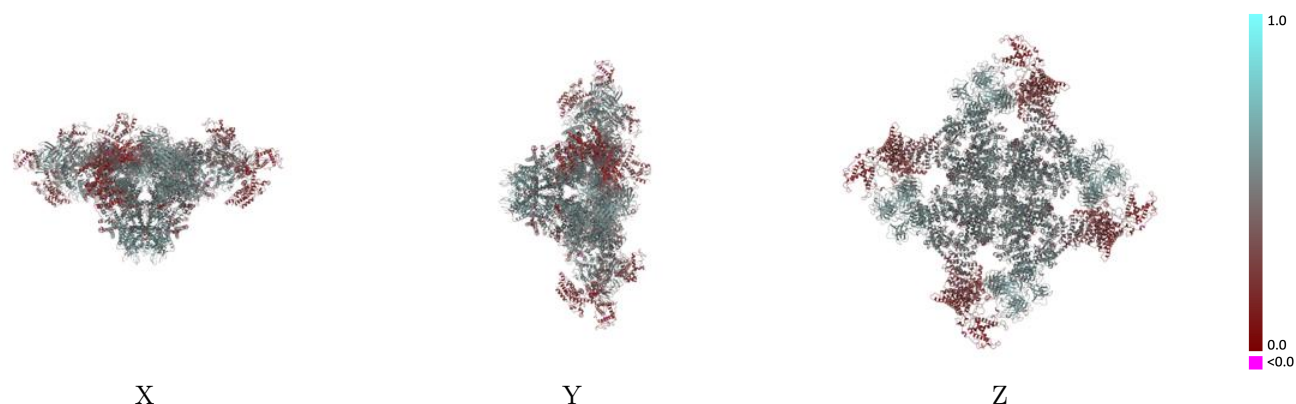
This section contains information regarding the fit between EMDB map EMD-42458 and PDB model 8UQ2. Per-residue inclusion information can be found in section [3](#) on page [6](#).

9.1 Map-model overlay [i](#)



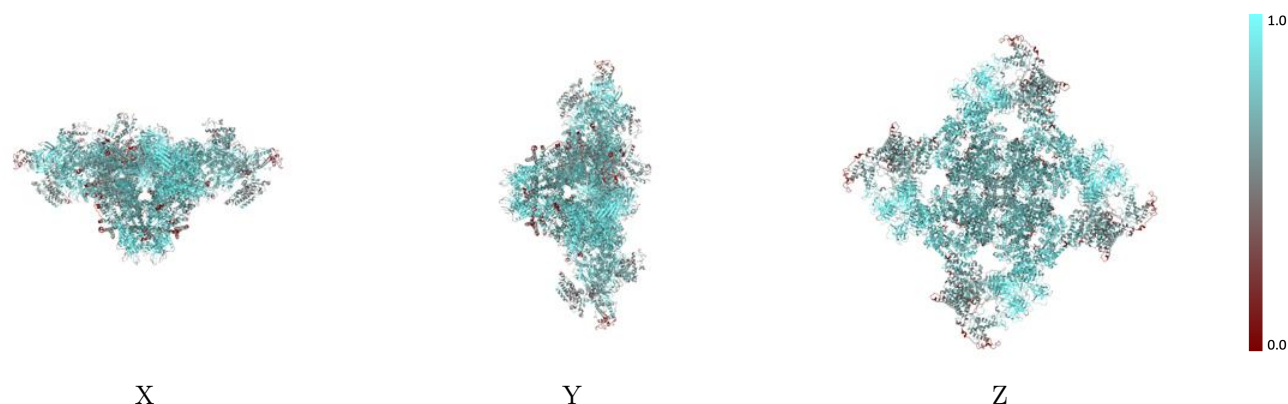
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



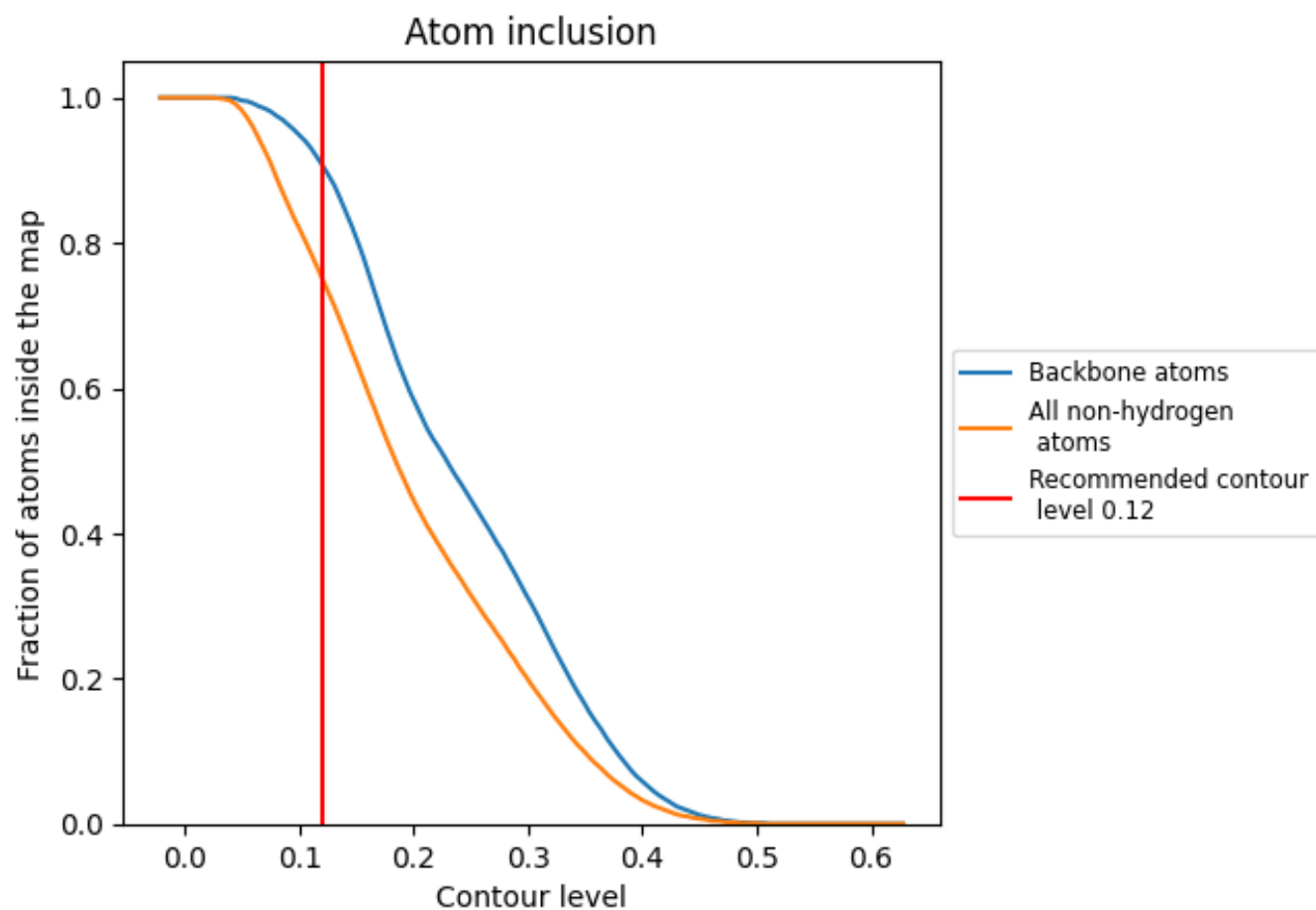
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 91% of all backbone atoms, 75% 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	<div></div> 0.7510	<div></div> 0.4430
A	<div></div> 0.7490	<div></div> 0.4400
B	<div></div> 0.7480	<div></div> 0.4410
C	<div></div> 0.7480	<div></div> 0.4410
D	<div></div> 0.7490	<div></div> 0.4410
E	<div></div> 0.8710	<div></div> 0.5380
F	<div></div> 0.8730	<div></div> 0.5370
G	<div></div> 0.8730	<div></div> 0.5370
H	<div></div> 0.8730	<div></div> 0.5370

1.0

0.0

<0.0