



wwPDB EM Validation Summary Report ⓘ

Mar 17, 2026 – 09:38 PM UTC

PDB ID : 7U9Z / pdb_00007u9z
EMDB ID : EMD-26410
Title : Structure of PKA phosphorylated human RyR2-R2474S in the open state
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2022-03-11
Resolution : 3.29 Å (reported)
Based on initial model : 7U9X

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:

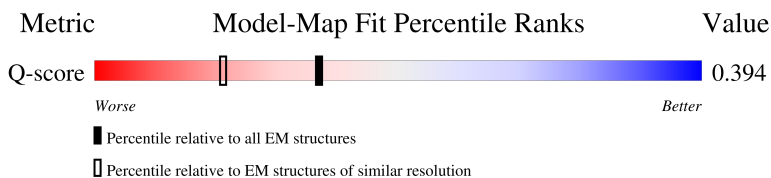
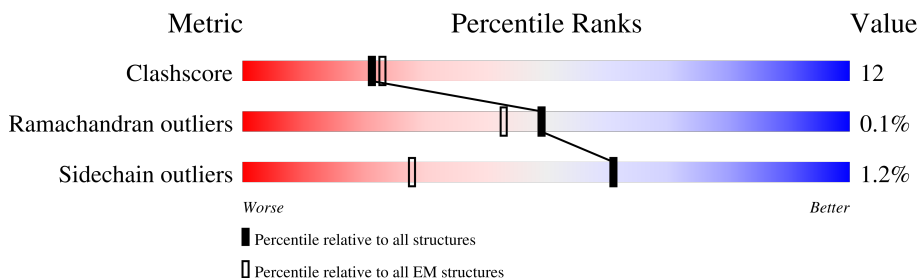
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.29 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	14466 (2.79 - 3.79)

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	11% 63% 22% 15%
1	B	4967	11% 63% 22% 15%
1	C	4967	11% 63% 21% 15%
1	D	4967	11% 63% 22% 15%

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Mol	Chain	Length	Quality of chain
2	E	108	 76%21%...
2	F	108	 77%20%...
2	G	108	 77%20%...
2	H	108	 77%20%...

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 138688 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	4226	Total	C	N	O	S	2	0
			33779	21520	5746	6283	230		
1	B	4226	Total	C	N	O	S	2	0
			33779	21520	5746	6283	230		
1	C	4226	Total	C	N	O	S	2	0
			33779	21520	5746	6283	230		
1	D	4226	Total	C	N	O	S	2	0
			33779	21520	5746	6283	230		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2474	SER	ARG	variant	UNP Q92736
B	2474	SER	ARG	variant	UNP Q92736
C	2474	SER	ARG	variant	UNP Q92736
D	2474	SER	ARG	variant	UNP Q92736

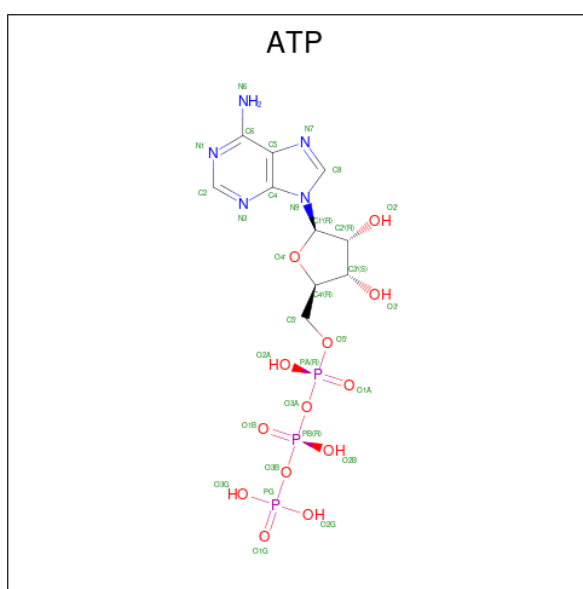
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	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 (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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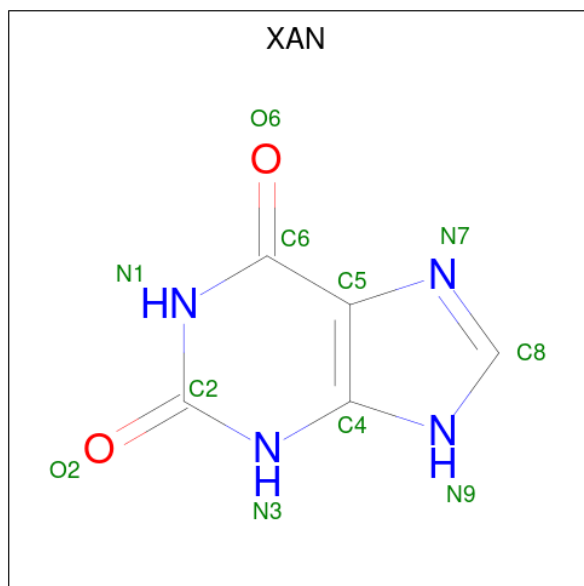
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Mol	Chain	Residues	Atoms					AltConf
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 6 is XANTHINE (CCD ID: XAN) (formula: C₅H₄N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			11	5	4	2	
6	B	1	Total	C	N	O	0
			11	5	4	2	
6	C	1	Total	C	N	O	0
			11	5	4	2	

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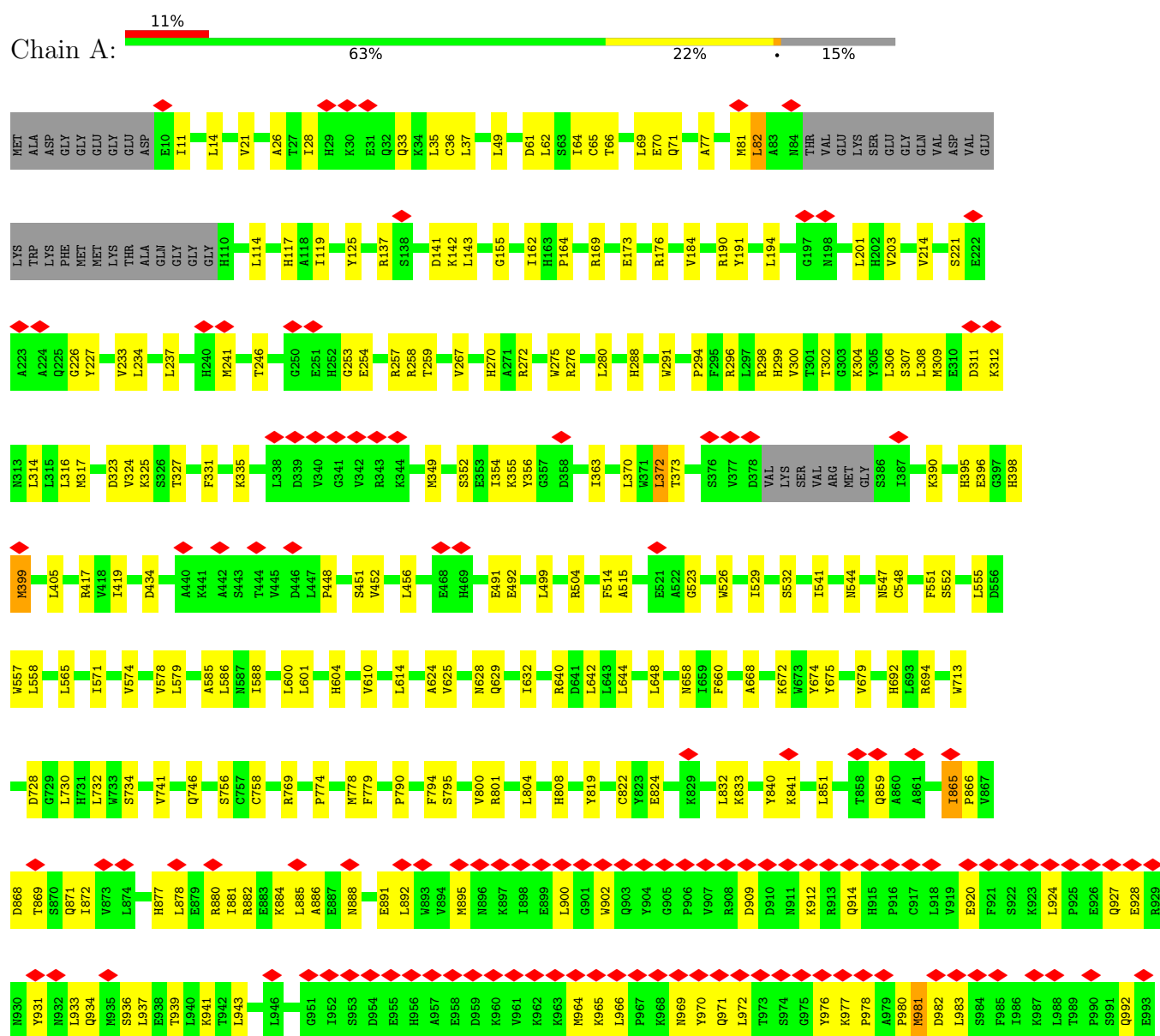
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	D	1	11	5	4	2	0

3 Residue-property plots

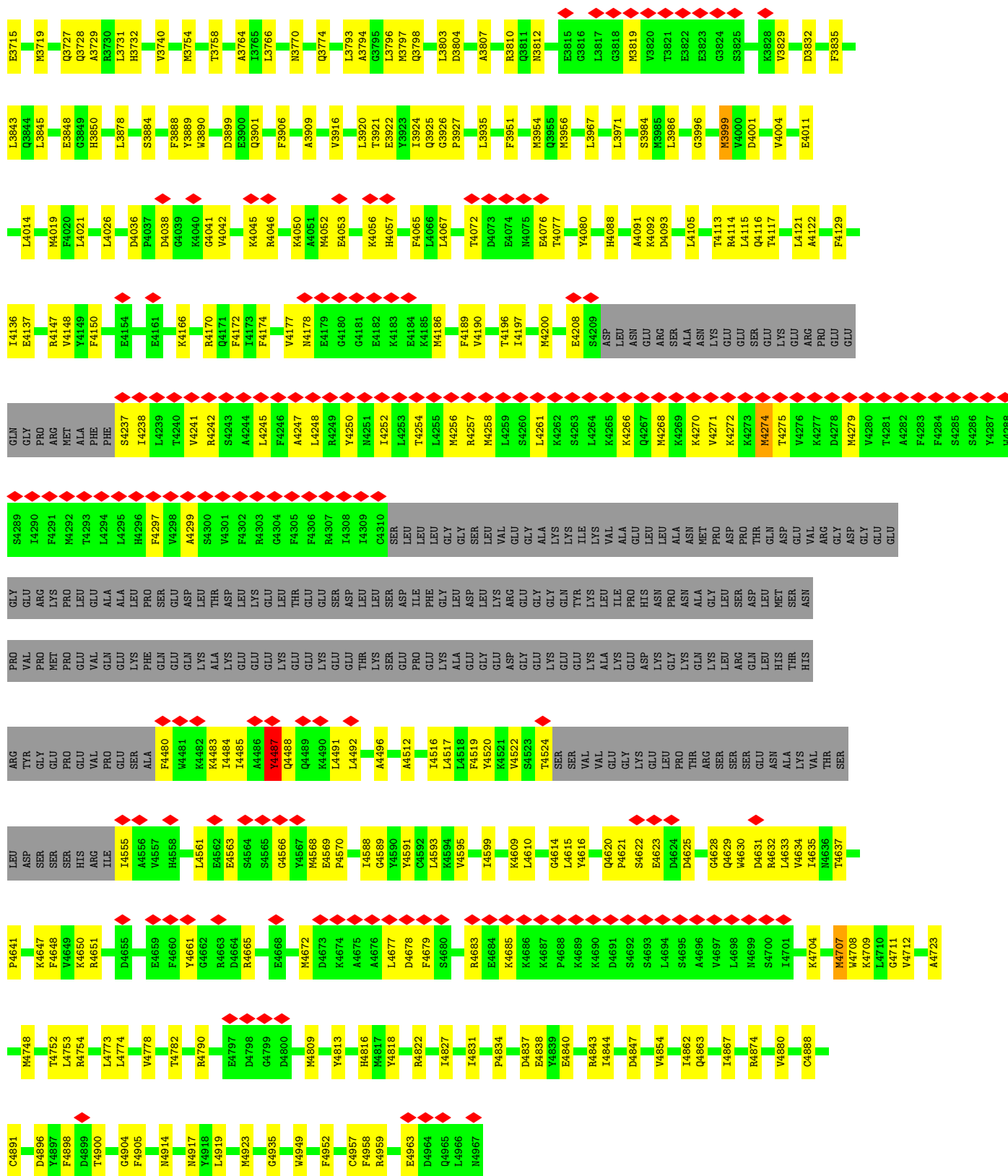
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



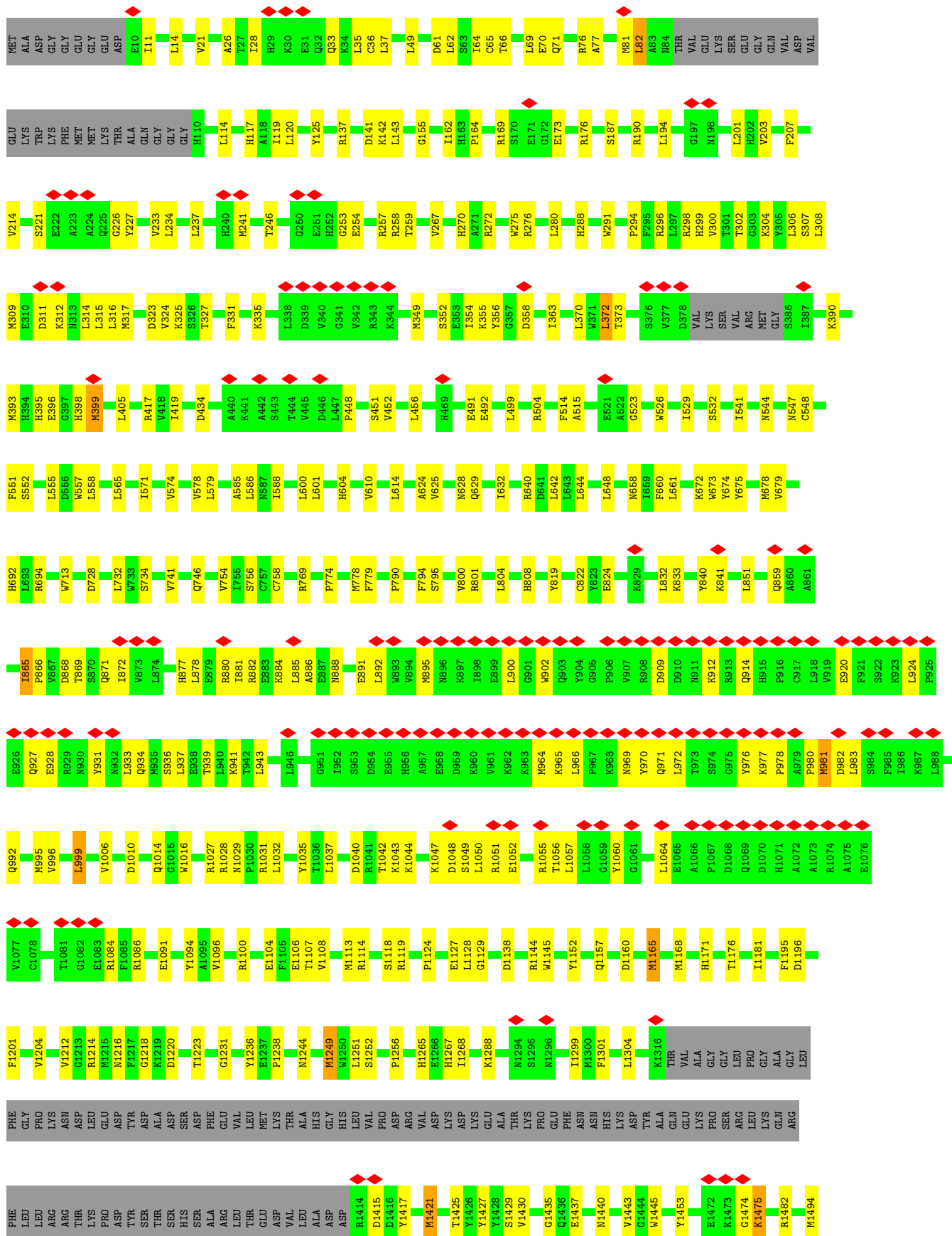
R2566	L2432	L2288	L2130	V1902	T1813	T1645	M1494	G1200	E1076	A994
T2569	V2433	G2289	L2141	L1910	T1814	T1650	S1495	F1201	V1077	M995
C2572	M2442	R2297	M2142	Q1912	F1825	L1667	P1496	V1204	C1078	Y996
I2576	Y2447	R2322	L2143	L1913	L1829	G1667	G1499	V1212	T1081	D997
L2580	M2456	T2325	C2144	C1914	L1830	G1668	R1500	R1213	G1082	R998
M2584	S2457	R2326	D2145	D1915	M1831	N1669	N1502	R1214	E1083	L999
M2585	I2149	L2338	L2146	R1919	D1838	S1678	M1503	M1215	R1084	V1006
M2586	M2150	L2344	M2157	F1932	I1842	D1681	L1505	F1217	F1085	D1010
H2587	Q2157	L2344	L2165	N1939	E1853	F1683	V1511	G1218	R1086	Q1014
L2588	L2166	L2344	M2167	V1947	A1854	Q1684	L1518	K1219	E1091	G1015
R2590	G2166	A2354	Q1948	M1948	ALA	L1685	A1522	S1223	Y1094	W1016
R2591	T2167	P2357	A1950	Q1949	THR	L1689	A1523	T1223	Y1096	T1017
L2592	M2172	S2358	L1951	L1948	PRO	P1695	M1524	G1231	R1100	R1027
V2593	V2176	R2359	N1952	N1953	GLU	L1706	G1524	Y1236	E1104	R1028
F2594	L2177	L2364	M1953	M1953	GLU	I1707	K1525	E1237	F1105	N1029
L2599	L2179	ASN	S1954	S1954	GLU	D1708	L1539	P1238	E1106	P1030
H2602	G2180	THR	A1955	A1955	THR	L1711	F1544	M1244	T1107	R1031
A2603	G2181	GLU	A1956	A1956	LEU	S1712	A1545	W1250	V1108	L1032
P2606	G2182	LYS	L1957	L1957	GLU	L1719	Q1546	L1251	M1113	G1035
L2607	E2183	LYS	T1958	T1958	LYS	M1720	S1549	S1252	R1114	T1036
P2607	S2184	VAL	A1959	A1959	LEU	M1721	E1556	P1256	R1041	D1040
H2613	K2185	ASP	K1960	K1960	LEU	N1722	E1556	P1266	S1118	T1042
Y2614	E2186	ASP	K1961	K1961	VAL	L1726	R1559	H1265	R1119	K1043
R2616	T2187	THR	R1966	R1966	GLN	V1727	R1584	H1266	P1124	K1044
Y2621	F2199	Q2059	R1975	R1975	GLY	P1728	L1586	H1267	Q1126	K1047
C2622	L2200	Q2059	L1976	L1976	ALA	M1729	V1583	I1268	E1127	D1048
L2623	M2214	T2065	D1982	D1982	LEU	K1744	K1576	S1429	L1128	S1049
G2625	H2217	T2065	K1983	K1983	GLY	R1757	P1584	K1288	G1129	L1050
E2635	Y2220	V2067	S1984	S1984	ALA	L1758	L1586	M1294	D1138	R1051
E2636	Y2220	Q2071	E1985	E1985	GLU	P1765	H1593	S1295	R1055	E1052
E2637	L2229	L2080	C1986	C1986	GLU	S1767	V1594	M1300	T1056	R1055
H2639	R2285	L2087	C1987	C1987	LYS	P1768	R1598	F1301	L1057	L1057
L2640	A2245	R2090	R1993	R1993	GLY	P1780	M1599	Y1152	Y1152	G1059
S2641	S2246	Q2091	L1996	L1996	GLY	E1781	P1600	Q1157	Q1157	G1060
L2644	V2247	Y2092	L1996	L1996	LYS	F1782	M1601	D1160	D1160	G1061
R2643	M2248	R2100	D2002	D2002	ARG	D1785	V1608	K1316	M1185	L1064
R2644	N2248	R2117	E2010	E2010	THR	L1786	M1617	THR	M1185	E1065
R2645	L2257	L2117	L2010	L2010	ALA	L1787	L1618	VAL	M1168	A1065
V2646	R2258	L2120	ASP	ASP	GLY	K1788	V1619	ALA	P1067	L1066
V2646	P2260	L2126	GLU	GLU	GLY	L1795	L1630	GLY	T1176	P1067
D2650	E2259	R2127	ASP	ASP	ASP	E1801	L1630	LEU	I1181	D1068
Q2654	R2259	L2127	GLY	GLY	GLY	E1801	L1630	PRO	D1196	Q1069
A2665	M2279	R2127	LYS	LYS	LYS	E1801	L1630	GLY	D1199	D1070
	Y2285	R2127	ASP	ASP	ASP	E1801	L1630	ALA		A1072
		R2418	GLY	GLY	GLY	E1801	L1630	GLY		A1073
			ASP	ASP	ASP	E1801	L1630	GLY		A1074
			GLY	GLY	GLY	E1801	L1630	GLY		A1075





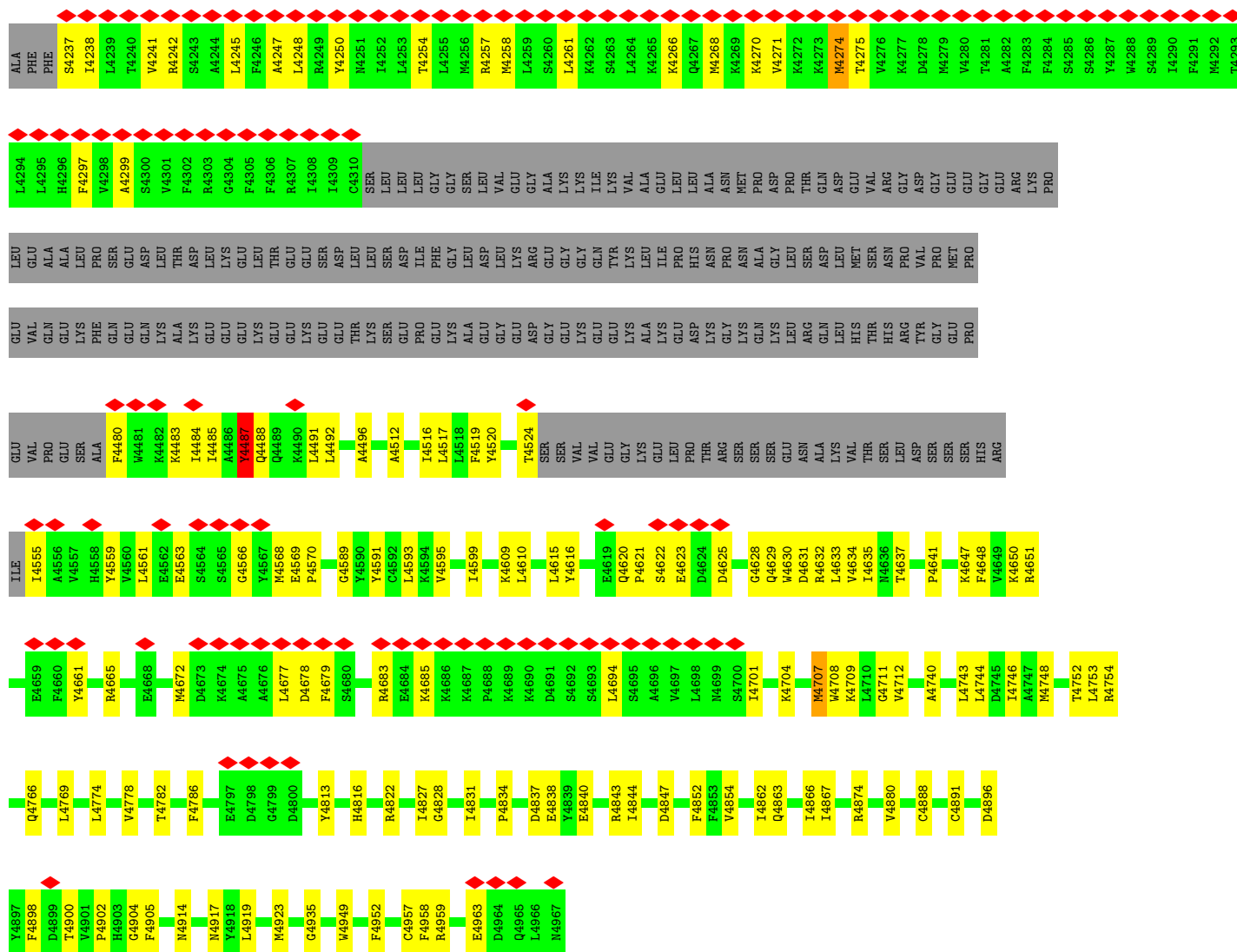
• Molecule 1: Ryanodine receptor 2



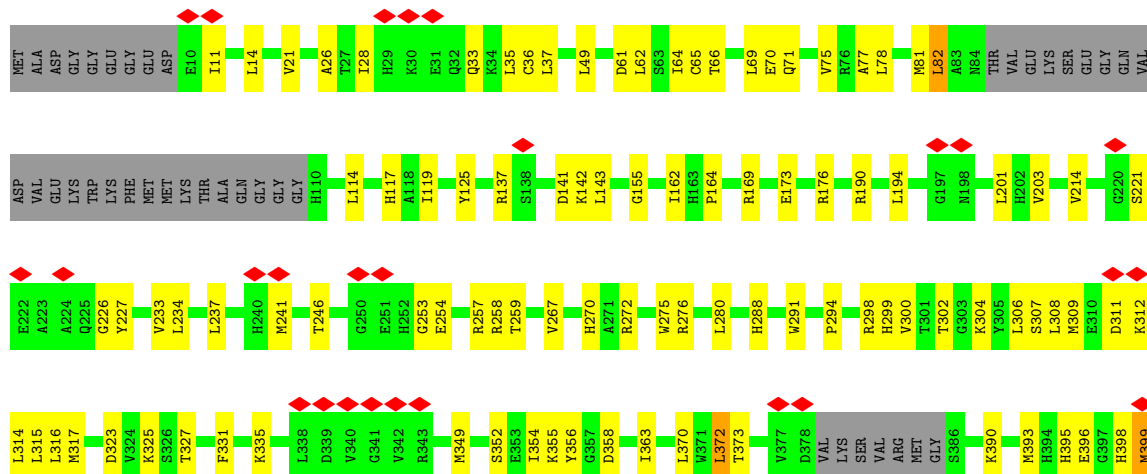




F4150	L4026	G3849	E3715	LYS	ASN	ILE	GLU	LEU	E3292	T3226	L3169	THR	A2996
E4154	D4036	H3850	M3719	ARG	ARG	GLY	GLN	ASP	G3293	R3227	L3162	ARG	S2997
E4161	D4037	L3878		ALA	THR	LEU	ASN	PHE	A3294		F3162	ASN	N2998
V4165	D4038	S3884	Q3727	VAL	ASP	ILE	VAL	THR	M3296	Q3231	A3163	GLN	K2999
K4166	G4039	F3888	Q3728	SER	THR	ALA	GLN	LEU	L3299	P3232	F3166	PRO	E3000
K4170	K4040	Y3889	Q3729	ASP	ASP	PRO	ASN	ALA	A3300	H3233	V3167		K3001
F4171	G4041	L3731	R3730	GLU	PRO	GLY	ILE	ARG	S3303	V3234	V3168		E3002
F4172	V4042	H3732	L3731	ASN	GLY	ASN	ILE	ASP	S3304	E3236	A3169		K3003
F4173	K4045	D3899	H3732	LEU	LYS	GLN	ASN	LEU	S3305	M3235	F3170		V3004
F4174	R4046	E3900	M3754	VAL	THR	LEU	ASN	TVR	P3306	E3237	L3171		L3007
V4177	K4050	Q3901	M3754	GLU	VAL	ILE	SER	PHE	L3306	V3238	L3171		F3008
N4178	F3906	L3608	A3764	ARG	GLU	ALA	ILE	ALA	V3310	L3239	E3172		C3009
E4179	A4051	L3611	I3765	VAL	ARG	ALA	PHE	THR	K3311	L3242	T3173		K3010
G4180	M4052	L3614	L3766	LEU	ASP	ALA	ILE	PRO	K3312		H3174		L3011
G4181	E4053	R3615	N3770	LYS	ILE	LYS	THR	LEU	P3312	Y3245	L3175		V3013
E4182	K4056	R3615	Q3774	ASN	ALA	ASN	ASP	ILE	Q3313	M3246	D3176		L3014
K4183	H4057	S3627	L3793	PHE	VAL	PHE	THR	ARG	L3314	R3247	K3177		V3015
E4184	F4065	T3631	L3796	LEU	VAL	SER	SER	VAL	L3315	R3248	K3177		R3016
K4185	G3926	L3640	M3797	THR	LEU	LEU	LYS	ASP	K3316	K3249	H3178		H3017
M4186	P3927	A3649	L3803	ASN	LEU	LYS	LYS	THR	T3317	V3250	N3179		R3018
F4189	D4073	E3650	D3804	HIS	LEU	ASP	SER	ASN	H3318	E3251	S3182		I3019
V4190	A4075	P3651	A3807	LEU	LEU	THR	LYS	ARG	F3319	H3252	T3183		S3020
E4196	E4076	E3652	R3810	GLN	GLN	GLU	ALA	ALA	L3320	Y3184	Y3184		L3021
I4197	T4077	E3653	Q3811	LYS	ASN	GLU	VAL	TRP	P3321	G3253	N3185		C3032
M4200	Y4080	E3654	N3812	SER	GLN	GLU	VAL	VAL	L3322	P3254	T3186		L3033
E4208	H4088	E3656	E3815	LYS	LYS	ASP	ASP	GLY	E3324	K3187	Q3038		Q3038
S4209	A4091	G3657	G3818	ARG	ARG	ILE	GLN	GLU	K3325	N3256			
LEU	K4092	L3971	M3819	VAL	VAL	ILE	GLU	PRO	L3326	E3259	S3188		B3041
ASN	D4093	M3981	V3820	GLY	GLY	ILE	LYS	ASN	K3327	R3260	R3190		A3042
GLU	L4105	S3984	T3821	ASN	ASN	ILE	LYS	GLY	K3328	R3261	E3191		K3046
ARG	T4113	G3996	E3822	HIS	TYR	ILE	LYS	ALA	K3329	E3262	R3192		
ALA	R4114	M3999	E3824	PRO	CYS	HIS	GLY	VAL	A3330	M3263	A3194		K3064
LYS	Q4116	M3999	G3824	GLN	LEU	LEU	GLY	ALA	A3331	C3264	L3195		S3055
GLU	T4117	V4000	S3825	VAL	LEU	LEU	ASP	PHE	T3332	T3266	S3196		L3057
GLU	L4121	D4001	K3826	THR	GLY	LEU	THR	MET	V3334	A3267	P3198		R3058
SER	A4122	V4004	V3829	LEU	PRO	GLU	SER	VAL	S3335	L3268	T3199		F3060
LYS	E4011	F3835	L3830	GLY	ARG	ASP	MET	GLY	E3336	N3269	N3200		L3061
ARG	F4129	L4014	Q3831	ILE	LYS	ILE	THR	ILE	E3337	S3270	V3201		
PRO	I4136	M4019	D3832	ALA	LYS	ALA	LEU	TVR	ASP	E3271	D3203		L3068
GLU	E4137	F4020	F3835	VAL	VAL	TRP	ILE	TRP	ASP	H3272	V3204		E3069
GLY	R4147	L3843	K3836	TRP	TRP	GLN	ILE	TRP	LEU	K3273	L3208		K3070
PRO	V4148	L3845	H3700	LYS	LYS	ALA	LEU	SER	LEU	T3274	K3144		N3072
ARG	Y4149	E3948	D3701	LEU	LEU	ALA	VAL	GLY	ALA	T3275	K3144		N3074
MET			E3702	GLY	GLY	ALA	VAL	GLY	ALA	L3276	L3211		L3075
			ASP	ASP	ASP	TRP	VAL	THR	ALA	L3277	E3212		K3076
			ASP	ASP	ASP	LYS	VAL	ASN	ALA	E3278	K3213		Q3077
			GLY	GLY	GLY	LEU	ARG	PHE	GLY	G3278	L3214		G3078
			GLU	GLU	GLU	LEU	LEU	LYS	ASP	N3279	K3215		Q3079
			E3710	GLY	GLY	LEU	LEU	LEU	MET	K3282	E3220		F3080
			V3711	GLU	GLU	LEU	PRO	ARG	GLU	V3225	L3221		T3081
									ALA	N3285	A3222		
									GLU	N3286	G3224		
									LEU	N3287	E3223		
									LEU	G3269	S3224		
									ILE	D3291	G3225		



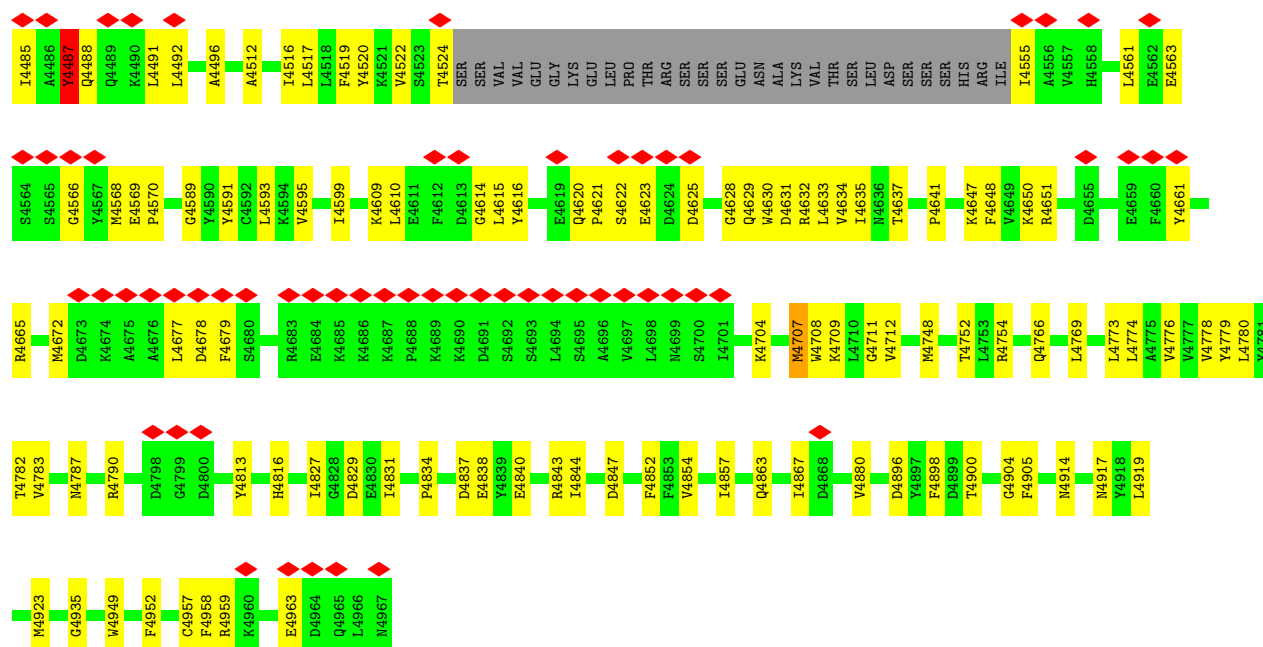
• Molecule 1: Ryanodine receptor 2



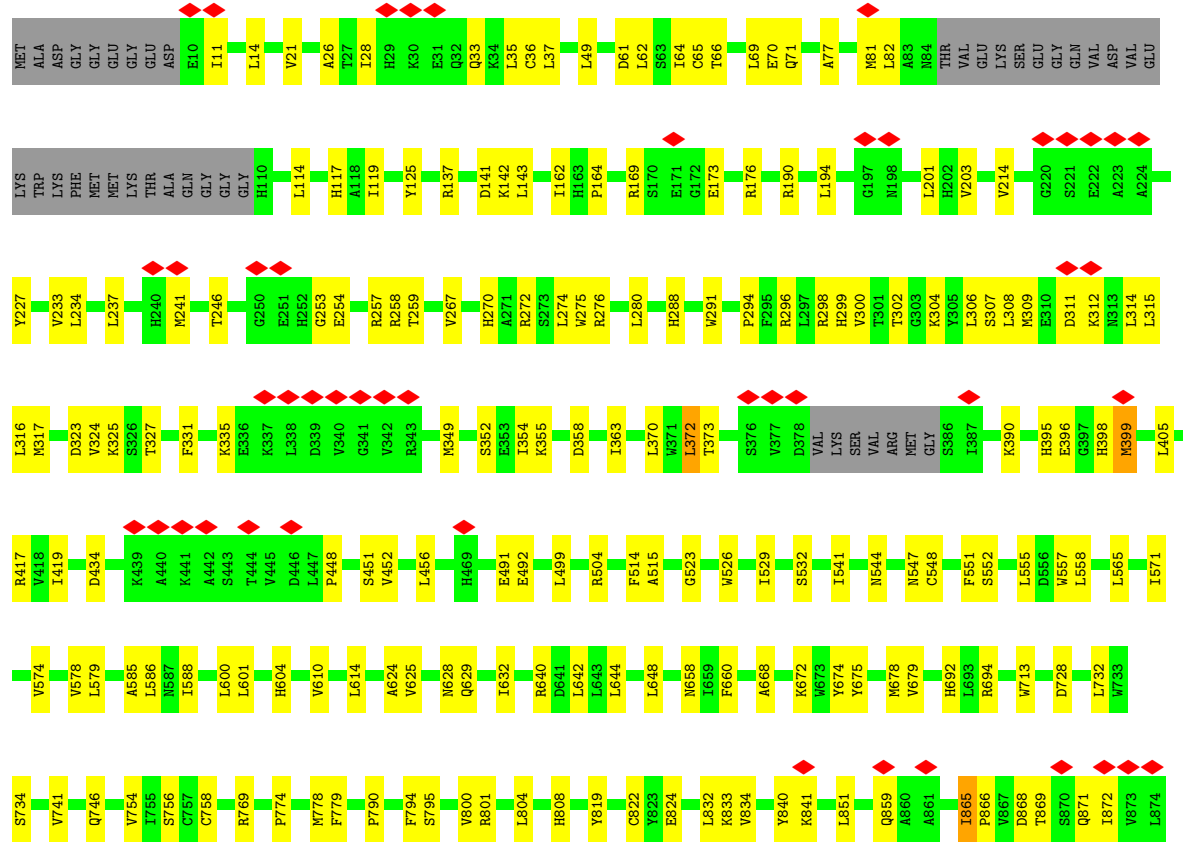








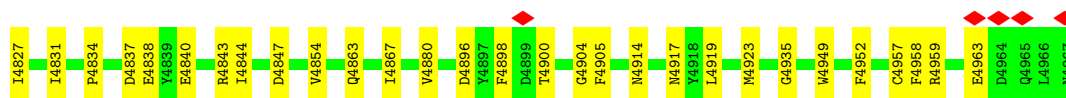
• Molecule 1: Ryanodine receptor 2





[illegible]





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

Chain E: 76% 21% ...



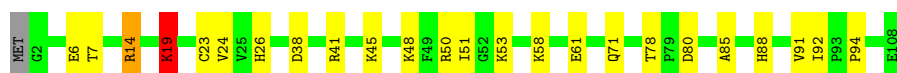
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 77% 20% ...



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

Chain G: 77% 20% ...



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

Chain H: 77% 20% ...



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41126	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)	400	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.643	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	425.984, 425.984, 425.984	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.15	1/34520 (0.0%)	0.41	17/46627 (0.0%)
1	B	0.15	1/34520 (0.0%)	0.41	17/46627 (0.0%)
1	C	0.15	1/34520 (0.0%)	0.41	17/46627 (0.0%)
1	D	0.15	1/34520 (0.0%)	0.41	17/46627 (0.0%)
2	E	0.22	0/834	0.54	1/1123 (0.1%)
2	F	0.22	0/834	0.54	1/1123 (0.1%)
2	G	0.22	0/834	0.54	1/1123 (0.1%)
2	H	0.22	0/834	0.54	1/1123 (0.1%)
All	All	0.15	4/141416 (0.0%)	0.41	72/191000 (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	6
1	B	0	6
1	C	0	6
1	D	0	6
All	All	0	24

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3254	PRO	CG-CD	-5.94	1.30	1.50
1	B	3254	PRO	CG-CD	-5.94	1.30	1.50
1	D	3254	PRO	CG-CD	-5.93	1.30	1.50
1	A	3254	PRO	CG-CD	-5.93	1.30	1.50

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2793	ARG	CB-CG-CD	7.97	129.63	111.30
1	B	2793	ARG	CB-CG-CD	7.95	129.59	111.30
1	A	2793	ARG	CB-CG-CD	7.95	129.58	111.30
1	D	2793	ARG	CB-CG-CD	7.95	129.57	111.30
1	A	3254	PRO	N-CD-CG	-7.48	91.98	103.20

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2793	ARG	Sidechain
1	A	2835	ARG	Sidechain
1	A	2905	ARG	Sidechain
1	A	3248	ARG	Sidechain
1	A	3252	HIS	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	33779	0	33454	822	0
1	B	33779	0	33454	825	0
1	C	33779	0	33454	800	0
1	D	33779	0	33454	803	0
2	E	818	0	821	22	0
2	F	818	0	821	20	0
2	G	818	0	821	18	0
2	H	818	0	821	20	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	3	0
4	D	62	0	24	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	11	0	4	0	0
6	B	11	0	4	0	0
6	C	11	0	4	0	0
6	D	11	0	4	0	0
All	All	138688	0	137212	3255	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 12.

The worst 5 of 3255 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:B:3166:PHE:O	1:B:3248:ARG:NH1	1.94	1.00
1:D:3166:PHE:O	1:D:3248:ARG:NH1	1.94	1.00
1:A:3166:PHE:O	1:A:3248:ARG:NH1	1.94	1.00
1:C:3166:PHE:O	1:C:3248:ARG:NH1	1.94	1.00
1:A:2741:TRP:HB3	1:A:2754:GLN:HB2	1.50	0.93

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	4200/4967 (85%)	4001 (95%)	193 (5%)	6 (0%)	48	75
1	B	4200/4967 (85%)	4000 (95%)	194 (5%)	6 (0%)	48	75
1	C	4200/4967 (85%)	4000 (95%)	194 (5%)	6 (0%)	48	75
1	D	4200/4967 (85%)	4000 (95%)	194 (5%)	6 (0%)	48	75
2	E	105/108 (97%)	101 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	G	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
2	H	105/108 (97%)	101 (96%)	4 (4%)	0	100	100
All	All	17220/20300 (85%)	16405 (95%)	791 (5%)	24 (0%)	49	75

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2681	MET
1	A	2686	VAL
1	A	2915	PRO
1	B	2681	MET
1	B	2686	VAL

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%)	3666 (99%)	42 (1%)	65	76
1	B	3708/4358 (85%)	3666 (99%)	42 (1%)	65	76
1	C	3708/4358 (85%)	3666 (99%)	42 (1%)	65	76
1	D	3708/4358 (85%)	3666 (99%)	42 (1%)	65	76
2	E	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	F	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	G	88/89 (99%)	85 (97%)	3 (3%)	32	59
2	H	88/89 (99%)	85 (97%)	3 (3%)	32	59
All	All	15184/17788 (85%)	15004 (99%)	180 (1%)	61	75

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2715	GLU

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Mol	Chain	Res	Type
1	D	981	MET
1	C	2835	ARG
1	C	3689	MET
1	D	1729	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2849	HIS
1	D	3252	HIS
1	D	4766	GLN
1	B	1257	GLN
1	B	1146	HIS

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 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ATP	B	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
4	ATP	C	5005	-	32,33,33	0.26	0	48,52,52	0.28	0
4	ATP	D	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	C	5002	-	32,33,33	0.26	0	48,52,52	0.31	0
6	XAN	B	5004	-	12,12,12	1.79	5 (41%)	14,17,17	2.31	6 (42%)
6	XAN	D	5004	-	12,12,12	1.79	5 (41%)	14,17,17	2.31	6 (42%)
4	ATP	A	5002	-	32,33,33	0.26	0	48,52,52	0.30	0
4	ATP	B	5005	-	32,33,33	0.26	0	48,52,52	0.28	0
6	XAN	C	5004	-	12,12,12	1.78	5 (41%)	14,17,17	2.32	6 (42%)
4	ATP	D	5005	-	32,33,33	0.26	0	48,52,52	0.28	0
6	XAN	A	5004	-	12,12,12	1.79	5 (41%)	14,17,17	2.31	6 (42%)
4	ATP	A	5005	-	32,33,33	0.26	0	48,52,52	0.28	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	-	-	7/22/38/38	0/3/3/3
4	ATP	C	5005	-	-	9/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	7/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	7/22/38/38	0/3/3/3
6	XAN	B	5004	-	-	-	0/2/2/2
6	XAN	D	5004	-	-	-	0/2/2/2
4	ATP	A	5002	-	-	7/22/38/38	0/3/3/3
4	ATP	B	5005	-	-	9/22/38/38	0/3/3/3
6	XAN	C	5004	-	-	-	0/2/2/2
4	ATP	D	5005	-	-	9/22/38/38	0/3/3/3
6	XAN	A	5004	-	-	-	0/2/2/2
4	ATP	A	5005	-	-	9/22/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	5004	XAN	C6-N1	-3.29	1.32	1.38
6	D	5004	XAN	C6-N1	-3.28	1.32	1.38
6	C	5004	XAN	C6-N1	-3.27	1.32	1.38
6	A	5004	XAN	C6-N1	-3.26	1.32	1.38
6	A	5004	XAN	O6-C6	-2.44	1.18	1.23

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	5004	XAN	C6-N1-C2	-4.62	120.00	126.37
6	B	5004	XAN	C6-N1-C2	-4.61	120.02	126.37
6	D	5004	XAN	C6-N1-C2	-4.61	120.03	126.37
6	A	5004	XAN	C6-N1-C2	-4.60	120.03	126.37
6	C	5004	XAN	N9-C8-N7	-4.27	108.02	112.98

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

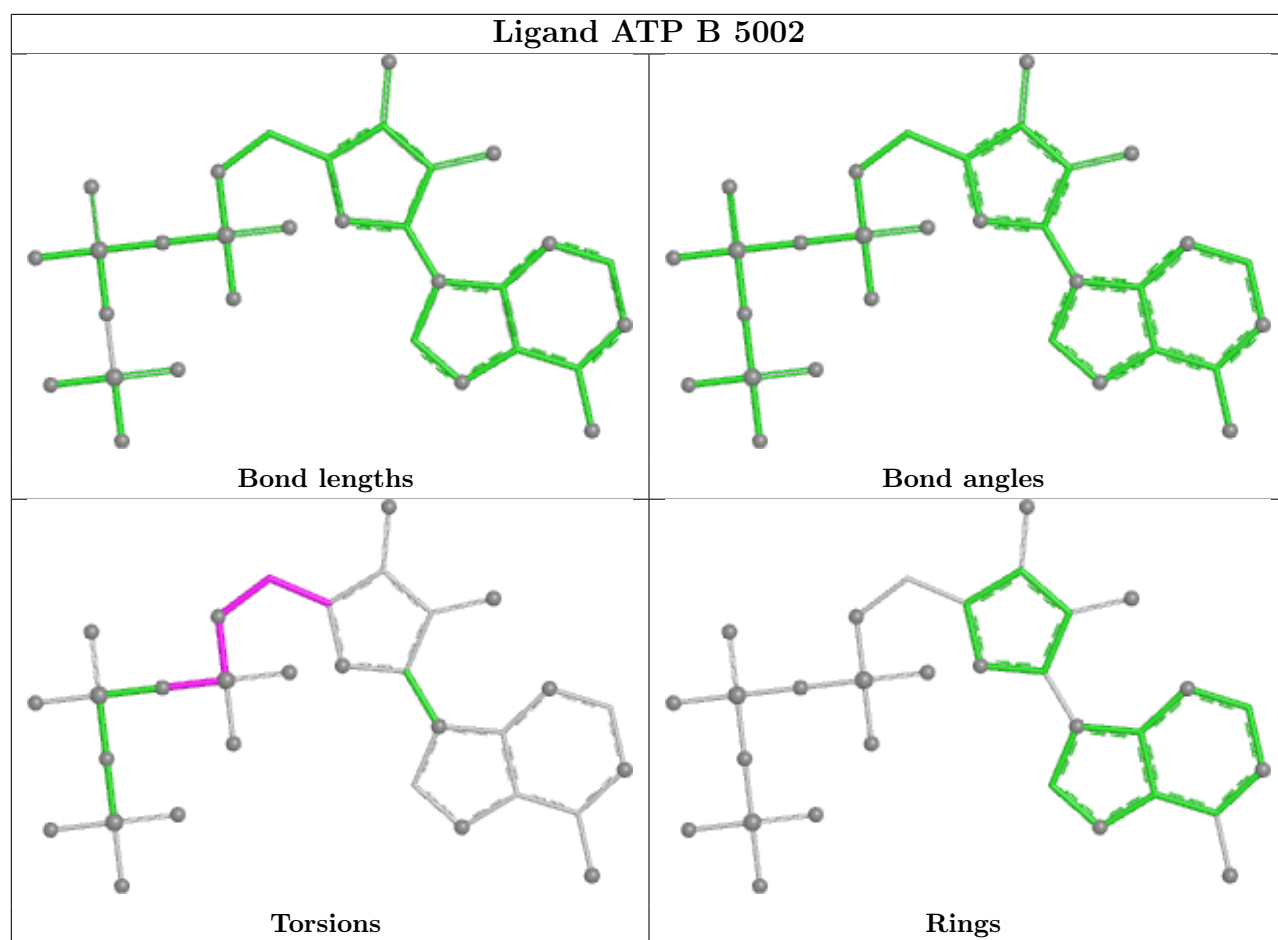
Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	A	5005	ATP	O4'-C4'-C5'-O5'
4	B	5002	ATP	C5'-O5'-PA-O1A
4	B	5002	ATP	C5'-O5'-PA-O3A

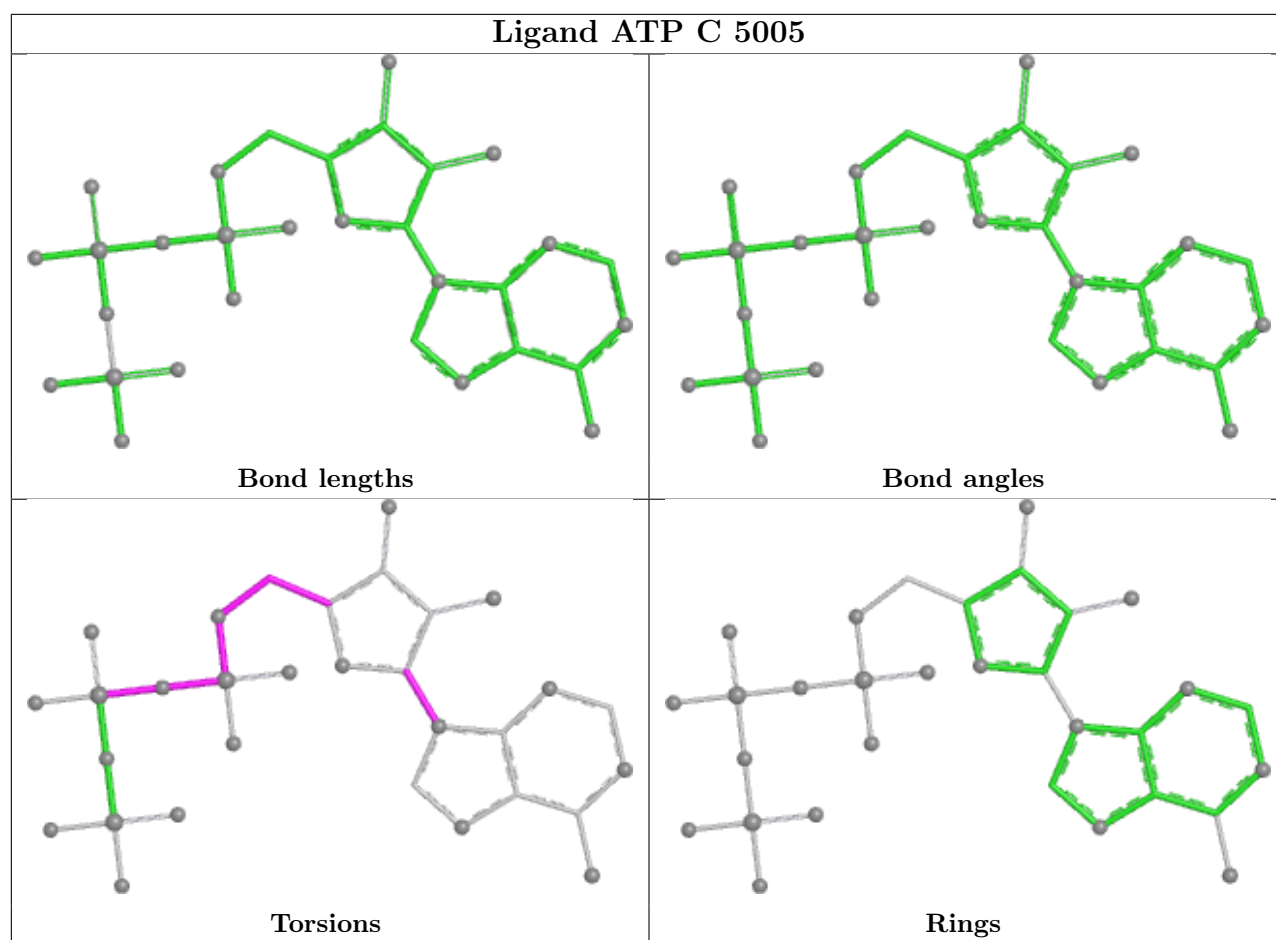
There are no ring outliers.

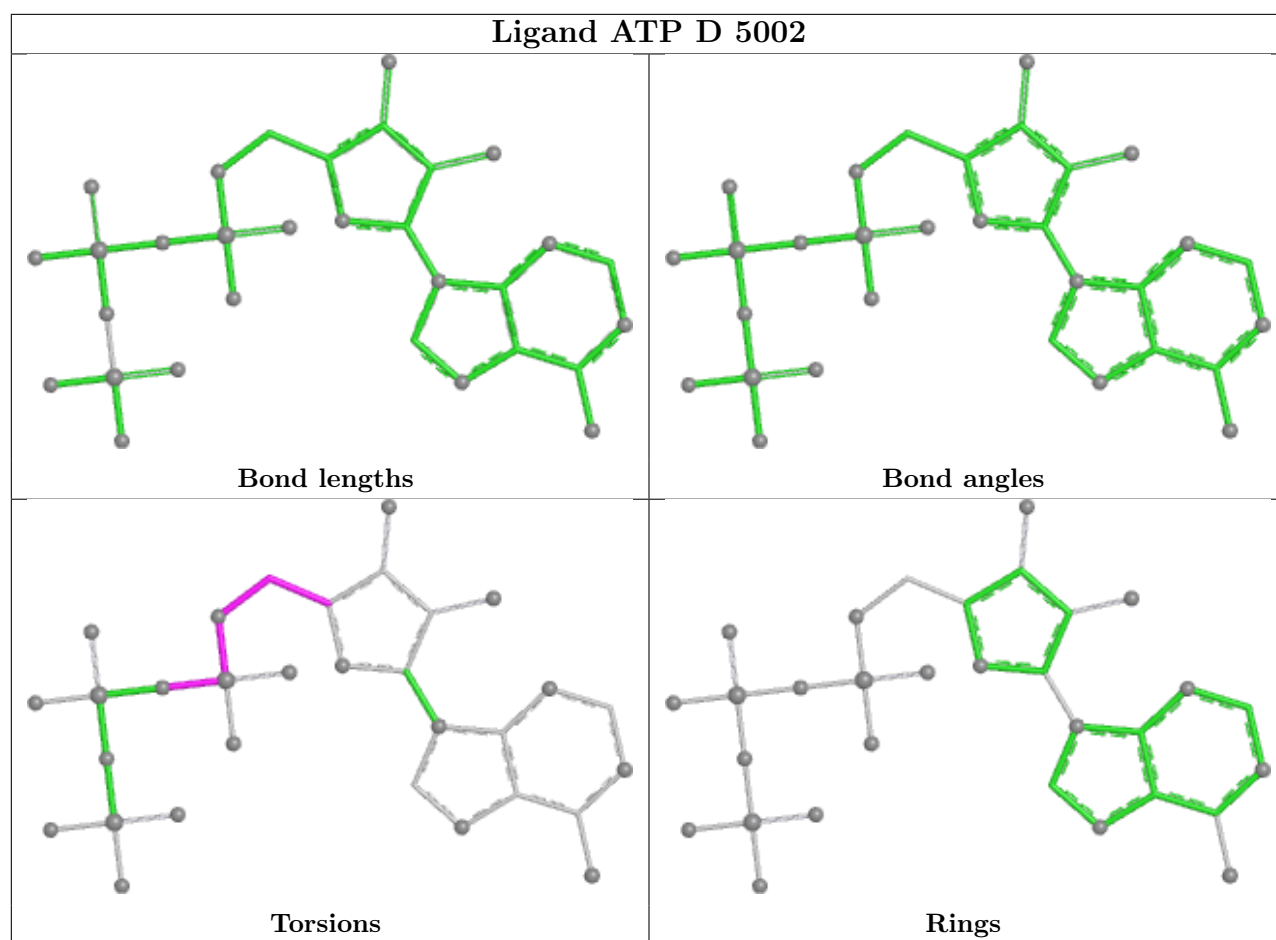
8 monomers are involved in 10 short contacts:

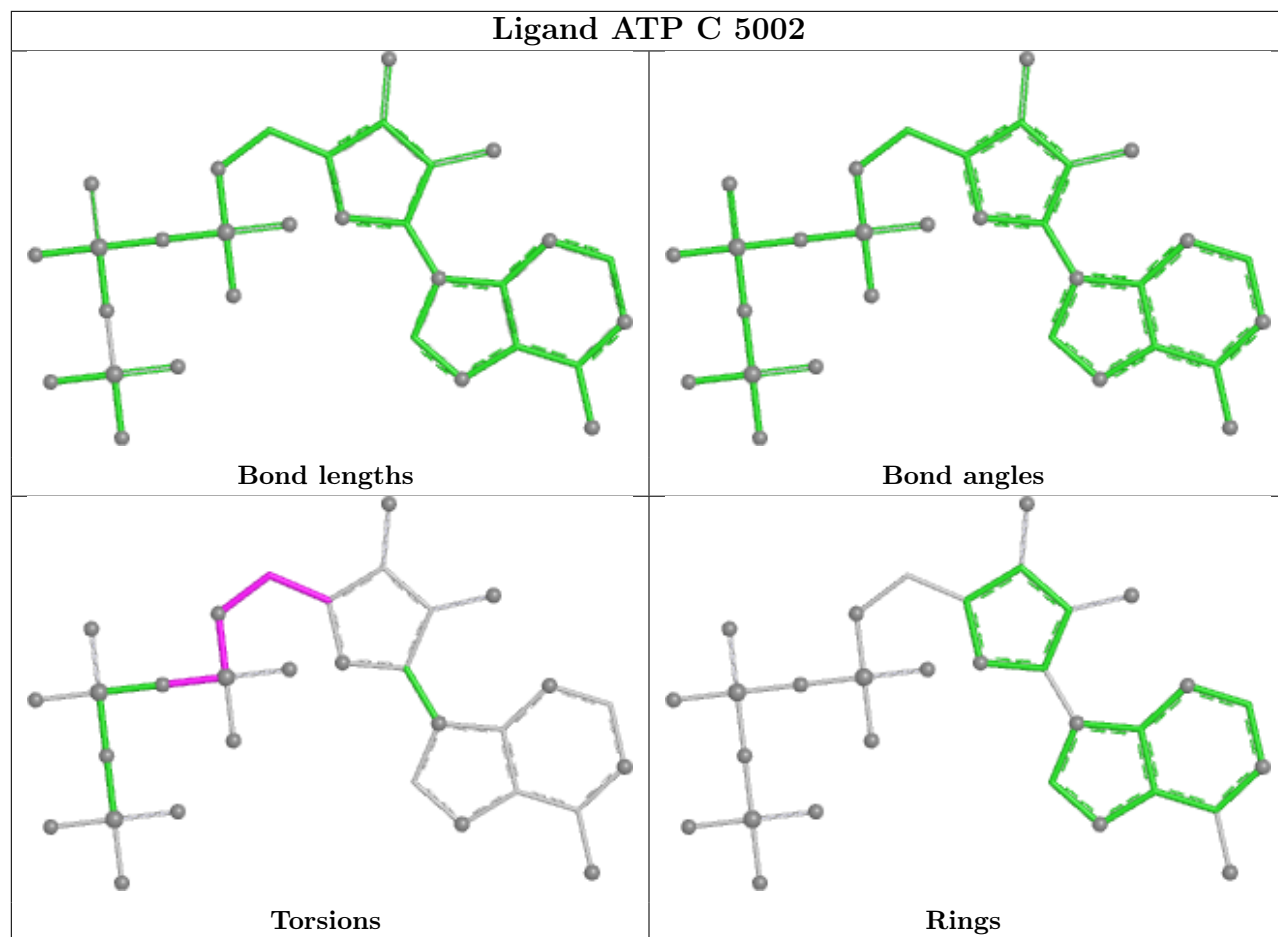
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	5002	ATP	1	0
4	C	5005	ATP	2	0
4	D	5002	ATP	1	0
4	C	5002	ATP	1	0
4	A	5002	ATP	1	0
4	B	5005	ATP	1	0
4	D	5005	ATP	2	0
4	A	5005	ATP	1	0

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.







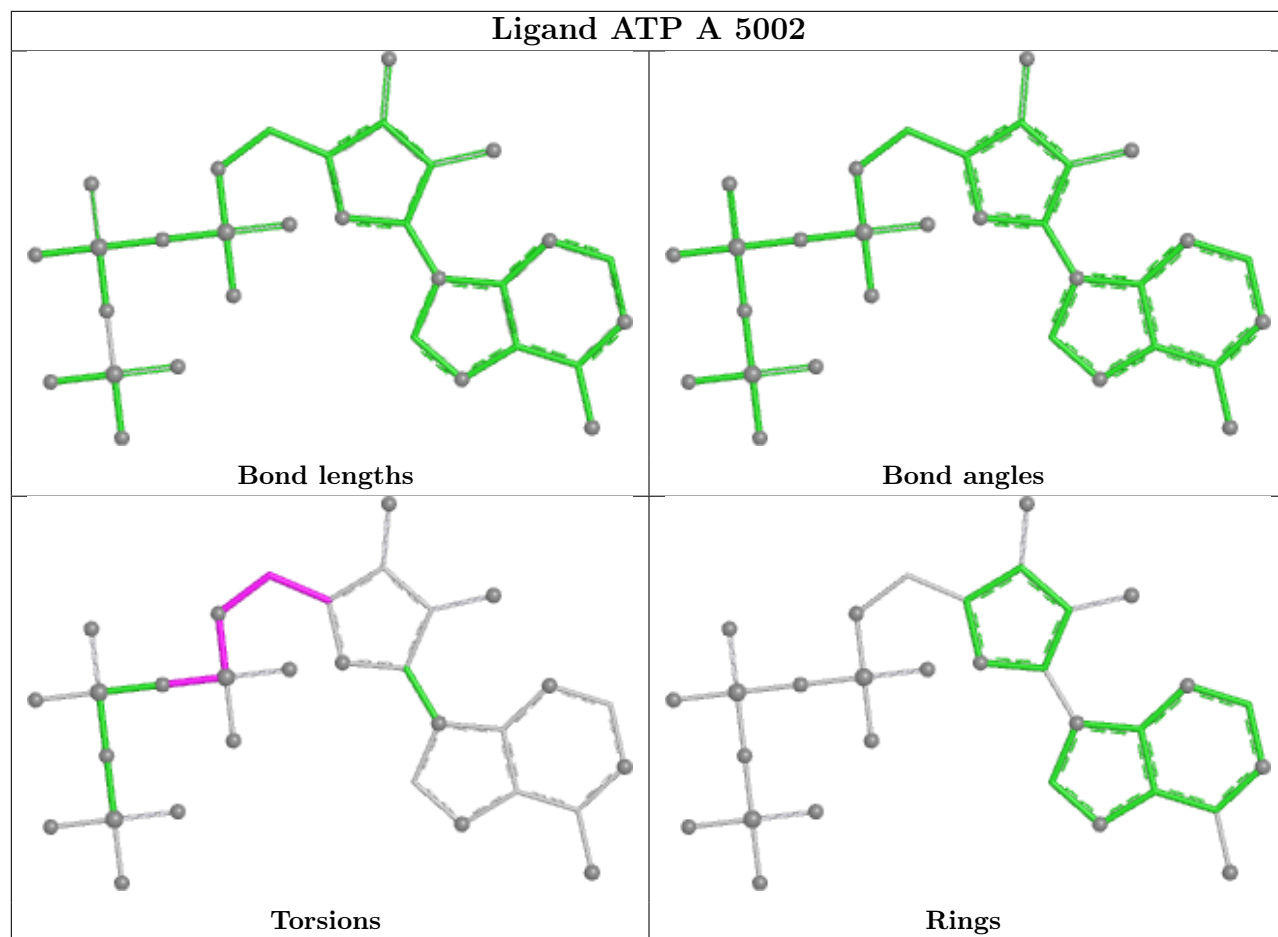


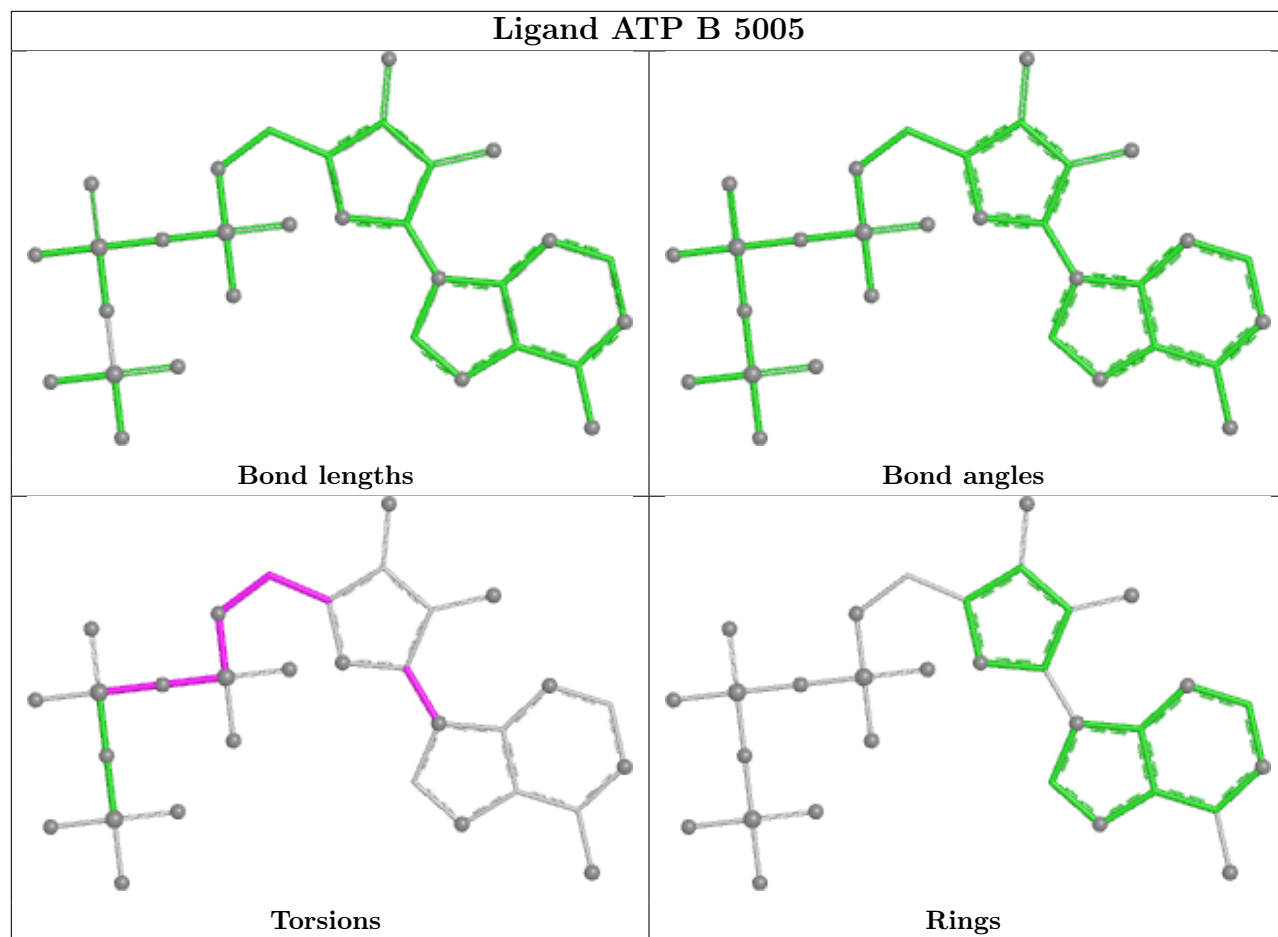
The figure displays four panels illustrating different types of bond analysis for a bicyclic molecule. The molecule consists of two fused rings, one six-membered and one five-membered, with three substituents. The panels are labeled as follows:

- Bond lengths:** Shows the molecule with magenta and green bonds, indicating different bond length categories.
- Bond angles:** Shows the molecule with magenta and green bonds, indicating different bond angle categories.
- Torsions:** Shows the molecule with grey bonds, indicating different torsion categories.
- Rings:** Shows the molecule with green bonds, indicating different ring categories.

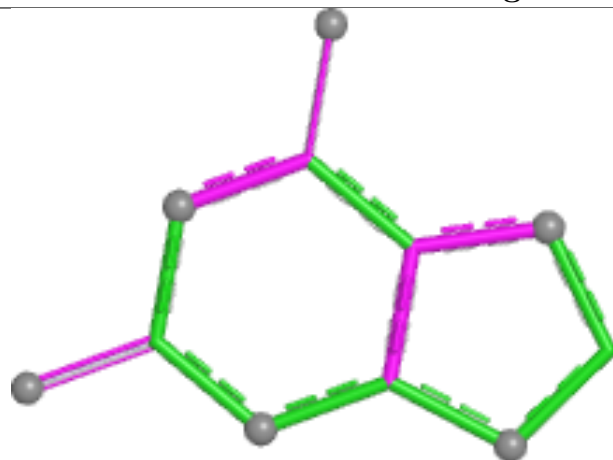
The figure displays four panels illustrating different types of bond analysis for a bicyclic molecule. The molecule consists of two fused rings, one six-membered and one five-membered, with three substituents. The panels are labeled as follows:

- Bond lengths:** Shows the molecule with magenta and green bonds, representing different bond length categories.
- Bond angles:** Shows the molecule with magenta and green bonds, representing different bond angle categories.
- Torsions:** Shows the molecule with grey bonds, representing different torsion categories.
- Rings:** Shows the molecule with green bonds, representing different ring categories.

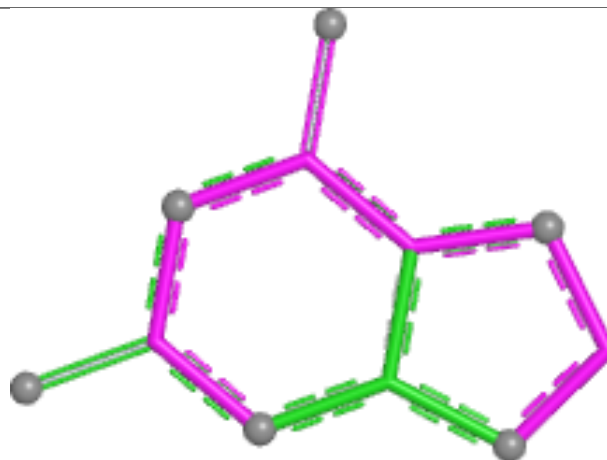




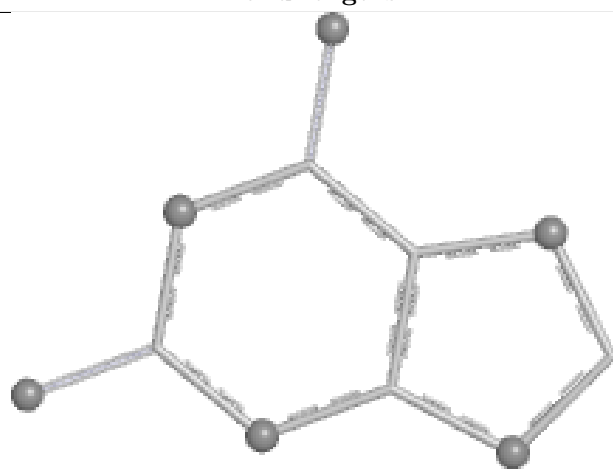
Ligand XAN C 5004



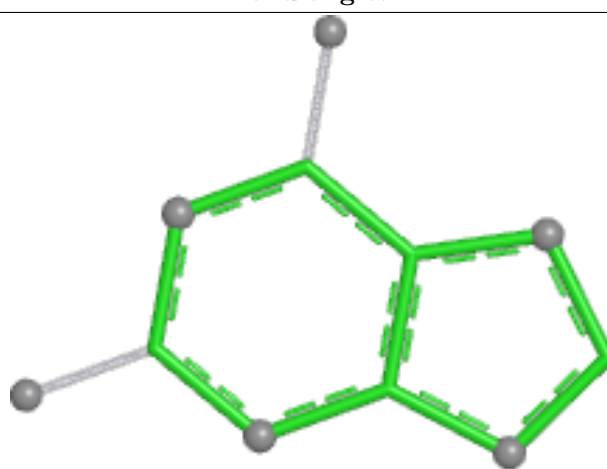
Bond lengths



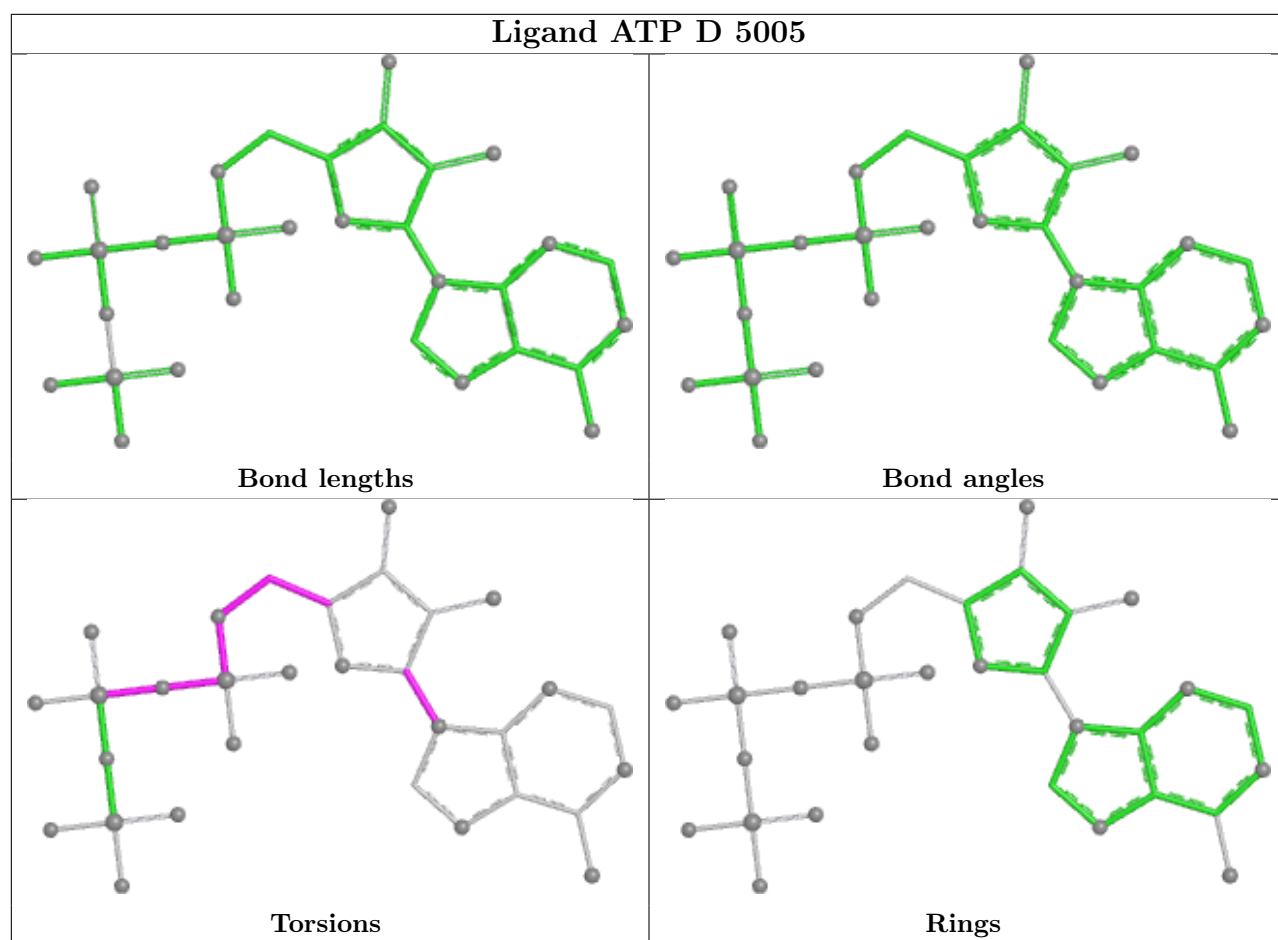
Bond angles



Torsions



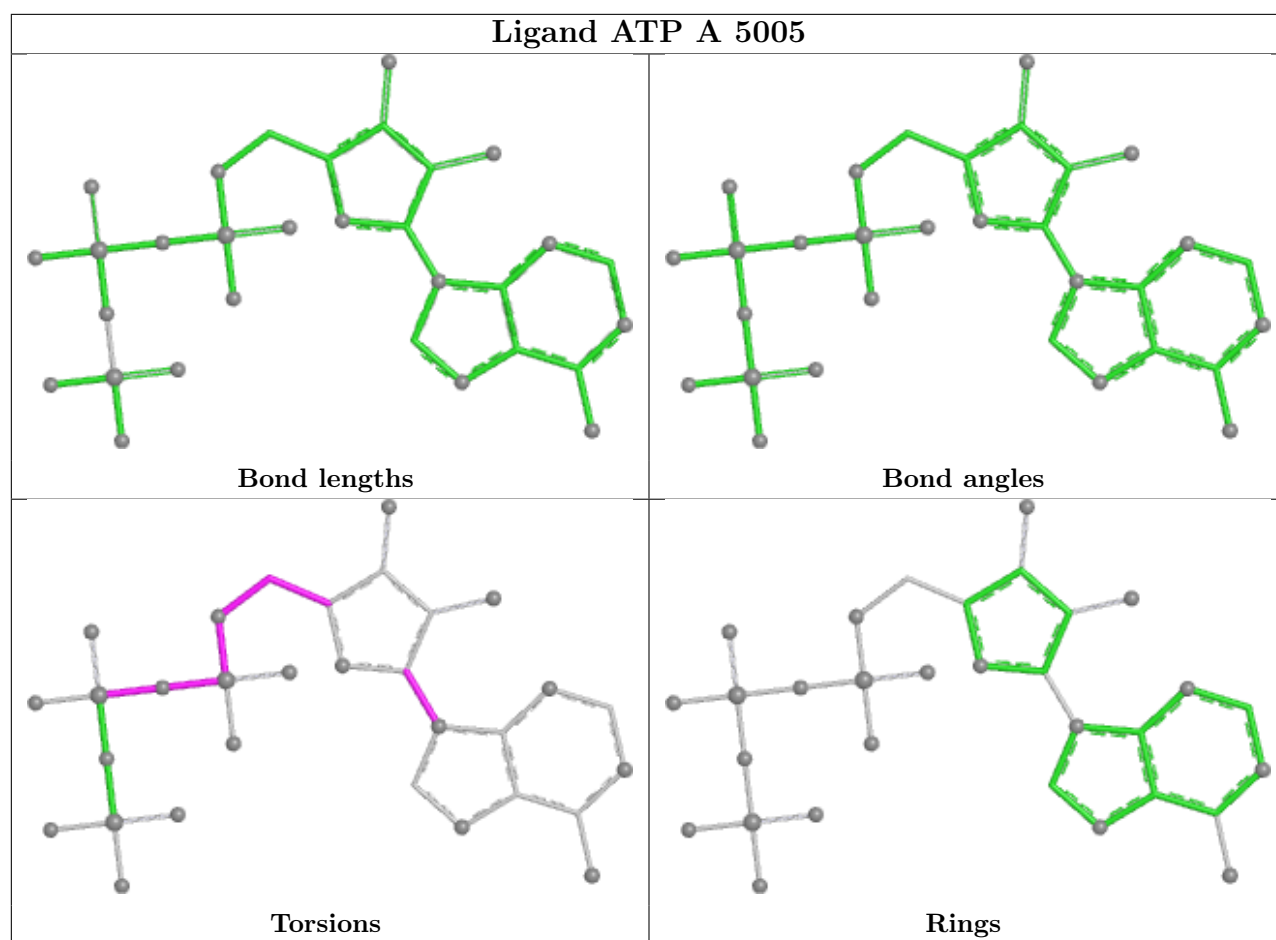
Rings



Ligand XAN A 5004

The figure displays four panels of structural analysis for Ligand XAN A 5004, which is a tricyclic molecule consisting of a benzene ring fused to a five-membered ring, which is further fused to another five-membered ring. The molecule has three substituents: a methyl group, a methoxy group, and a trifluoromethyl group.

- Bond lengths:** This panel shows the bond lengths for the molecule. The bonds are color-coded: green for C-C bonds, magenta for C-O bonds, and grey for C-F bonds. The bond lengths are labeled with values in Ångströms (Å).
- Bond angles:** This panel shows the bond angles for the molecule. The bonds are color-coded: green for C-C bonds, magenta for C-O bonds, and grey for C-F bonds. The bond angles are labeled with values in degrees.
- Torsions:** This panel shows the torsion angles for the molecule. The bonds are color-coded: green for C-C bonds, magenta for C-O bonds, and grey for C-F bonds. The torsion angles are labeled with values in degrees.
- Rings:** This panel shows the ring closure for the molecule. The bonds are color-coded: green for C-C bonds, magenta for C-O bonds, and grey for C-F bonds. The ring closure is labeled with values in degrees.



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.

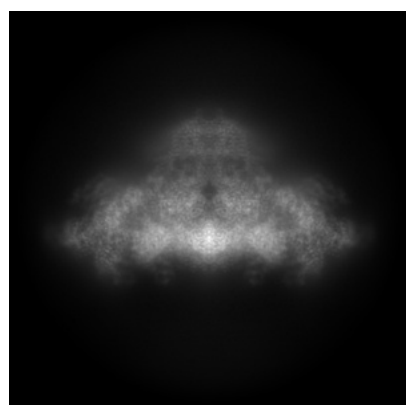
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26410. These allow visual inspection of the internal detail of the map and identification of artifacts.

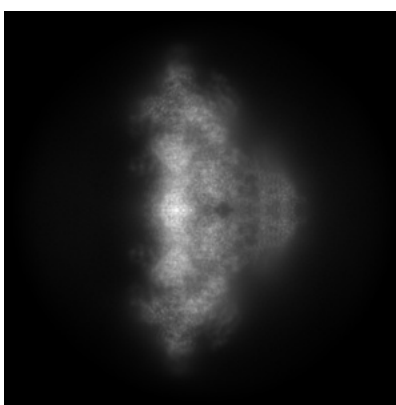
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

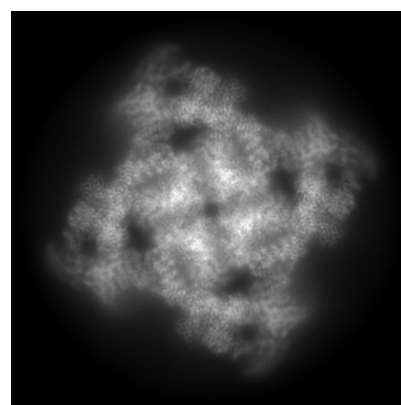
6.1.1 Primary map



X



Y

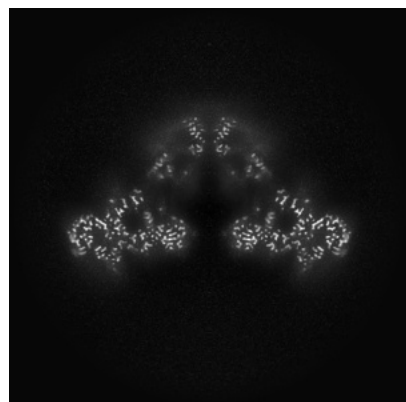


Z

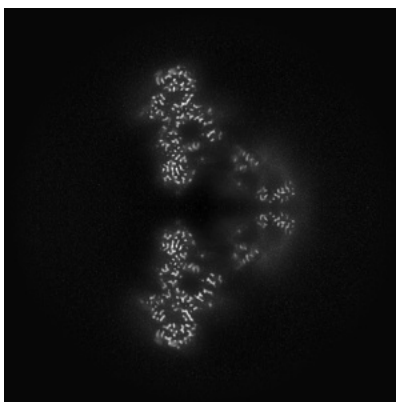
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

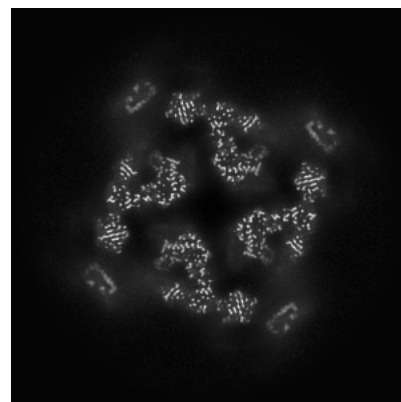
6.2.1 Primary map



X Index: 256



Y Index: 256

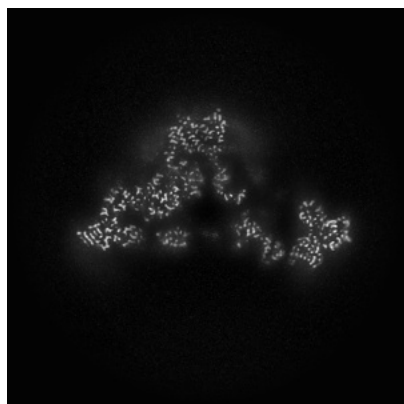


Z Index: 256

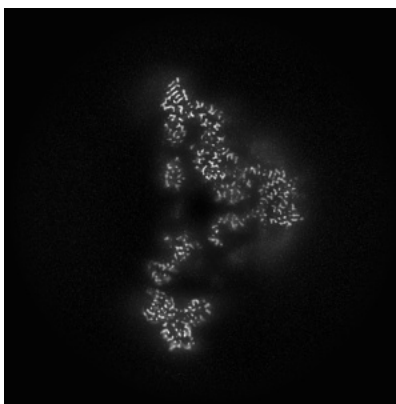
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

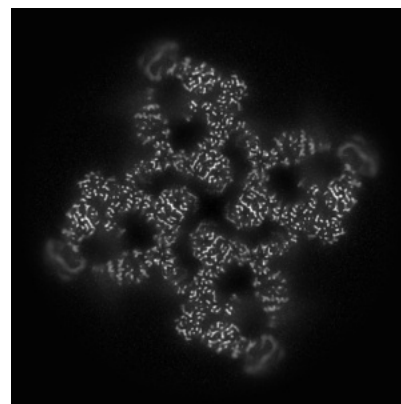
6.3.1 Primary map



X Index: 238



Y Index: 238

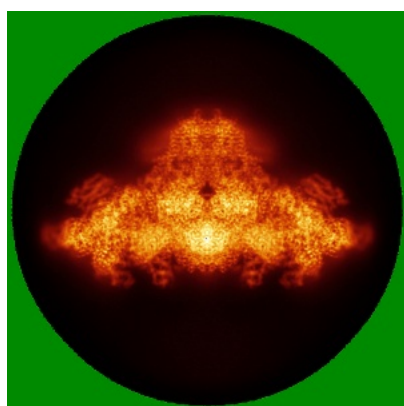


Z Index: 220

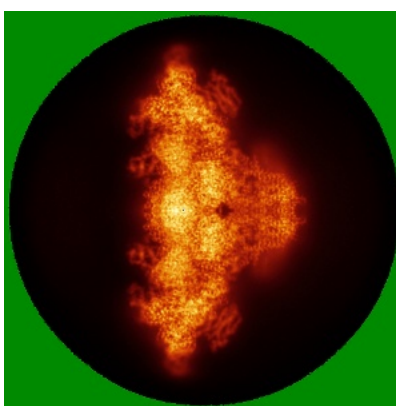
The images above show the largest variance slices of the map in three orthogonal directions.

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

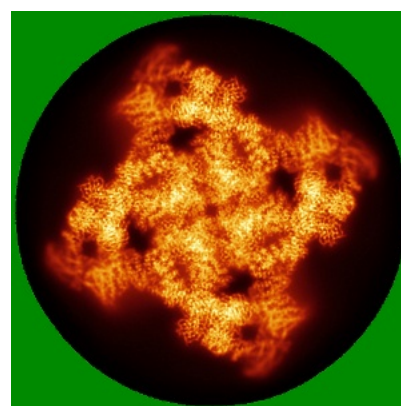
6.4.1 Primary map



X



Y

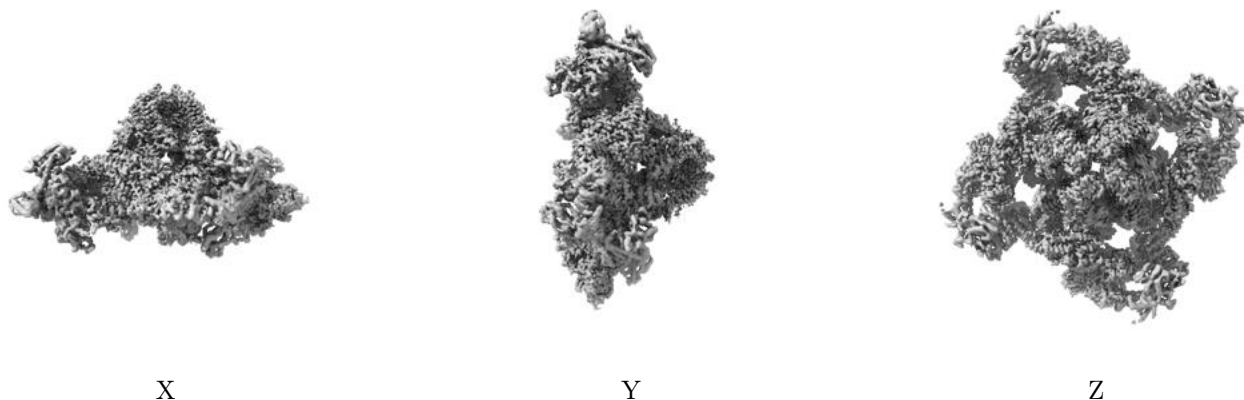


Z

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

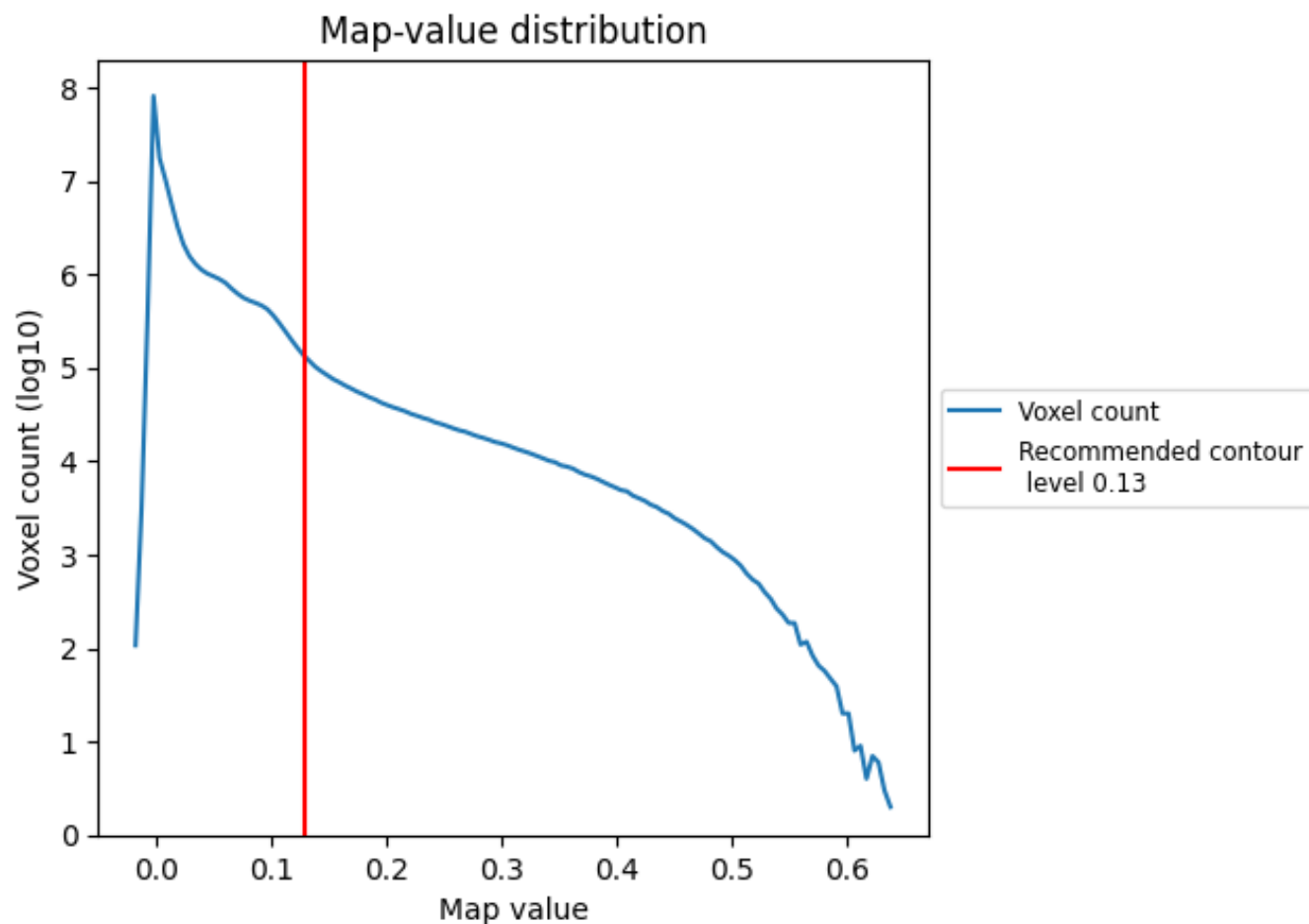
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

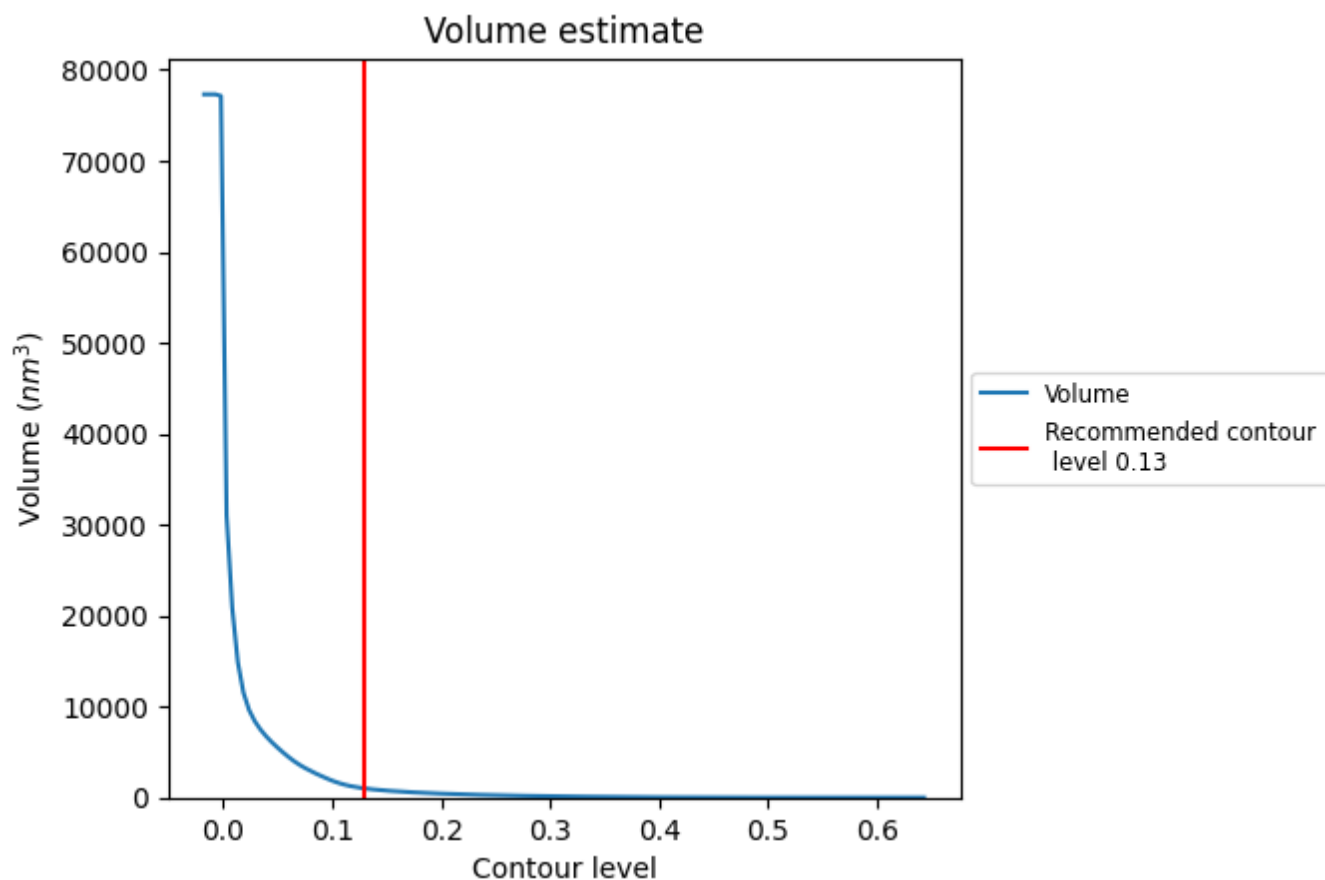
This section contains the results of statistical analysis of the map.

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.

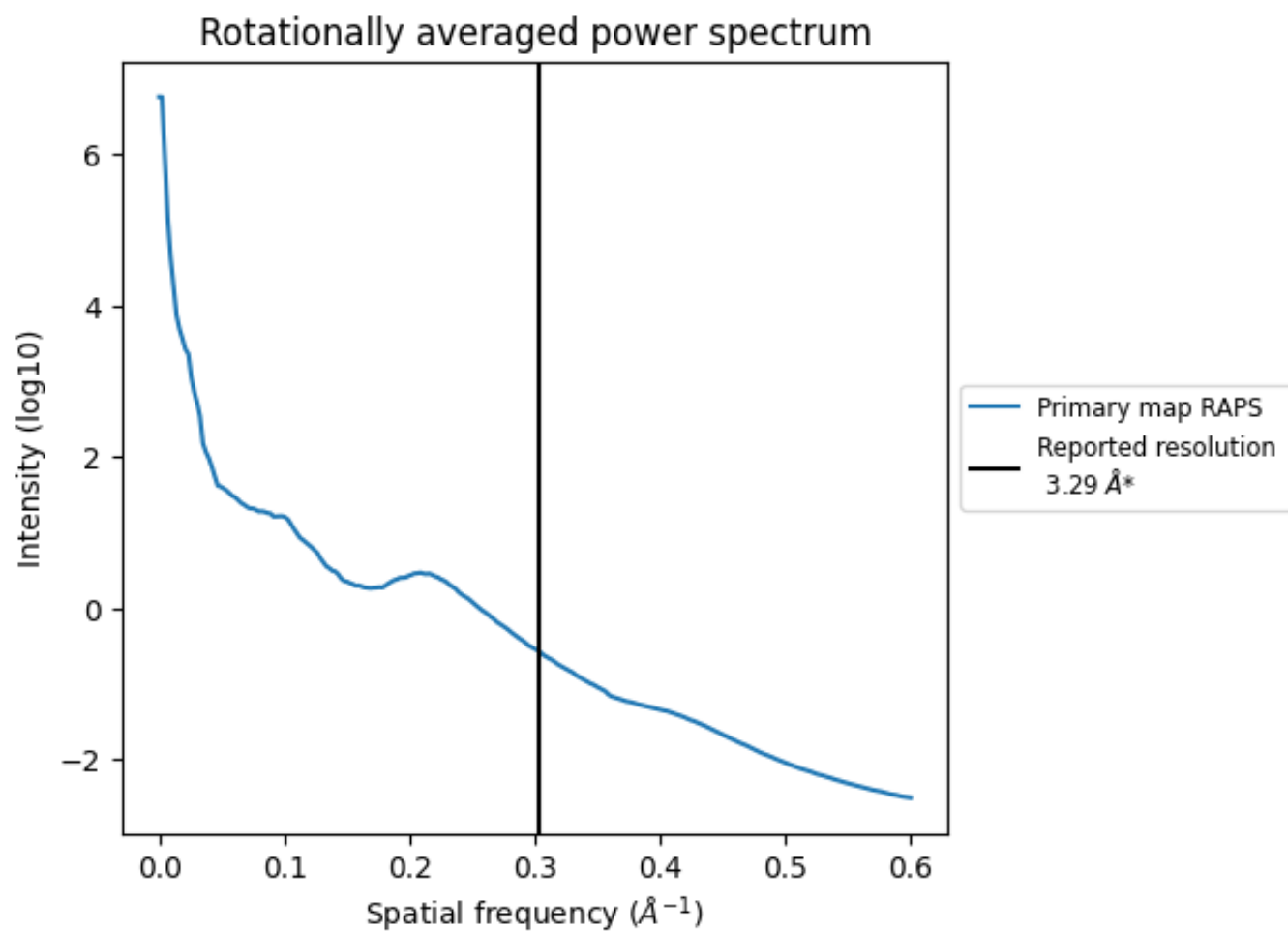
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1001 nm³; this corresponds to an approximate mass of 904 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 0.304 Å⁻¹

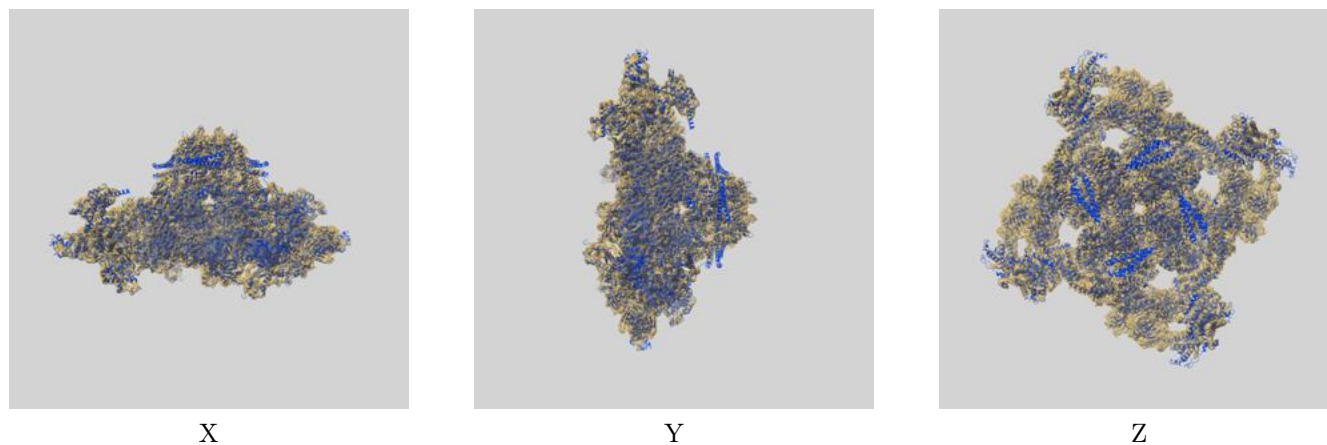
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

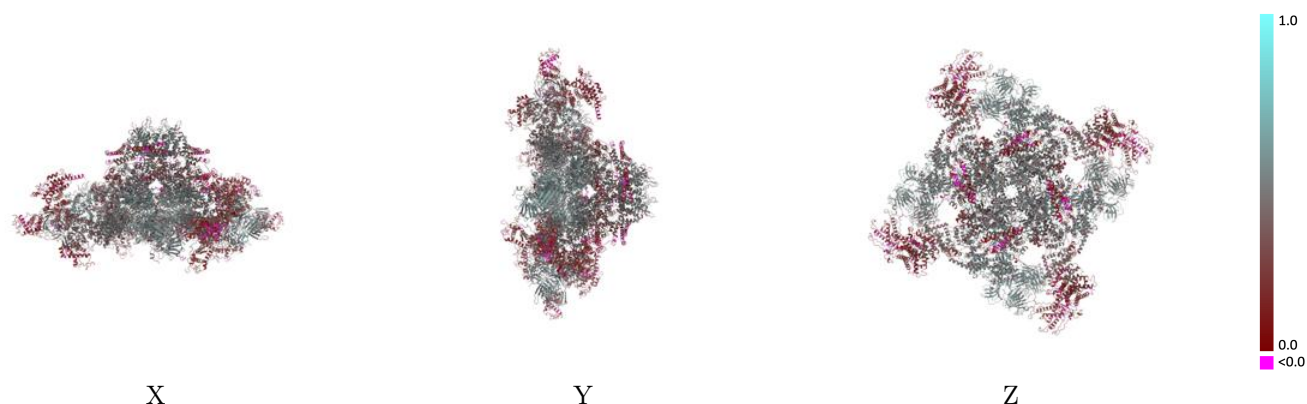
This section contains information regarding the fit between EMDB map EMD-26410 and PDB model 7U9Z. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



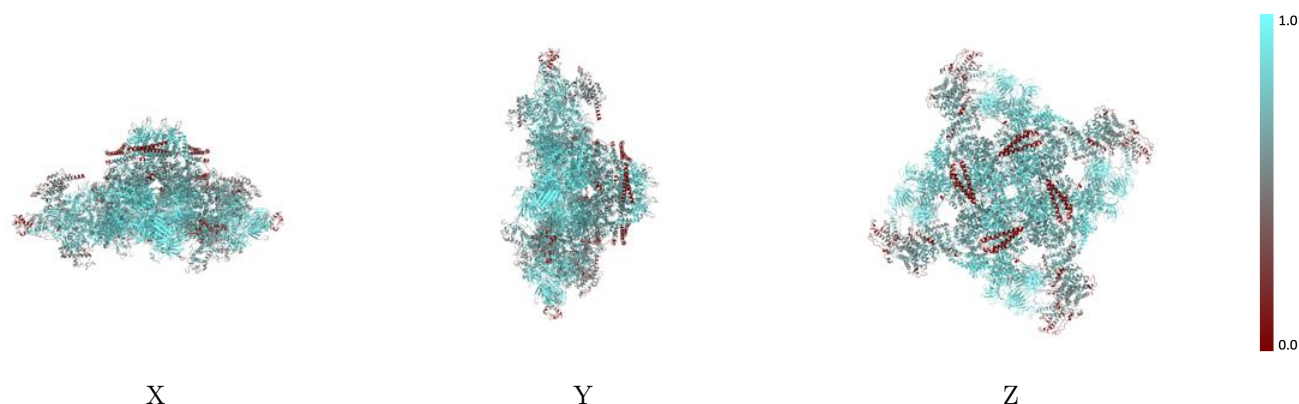
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



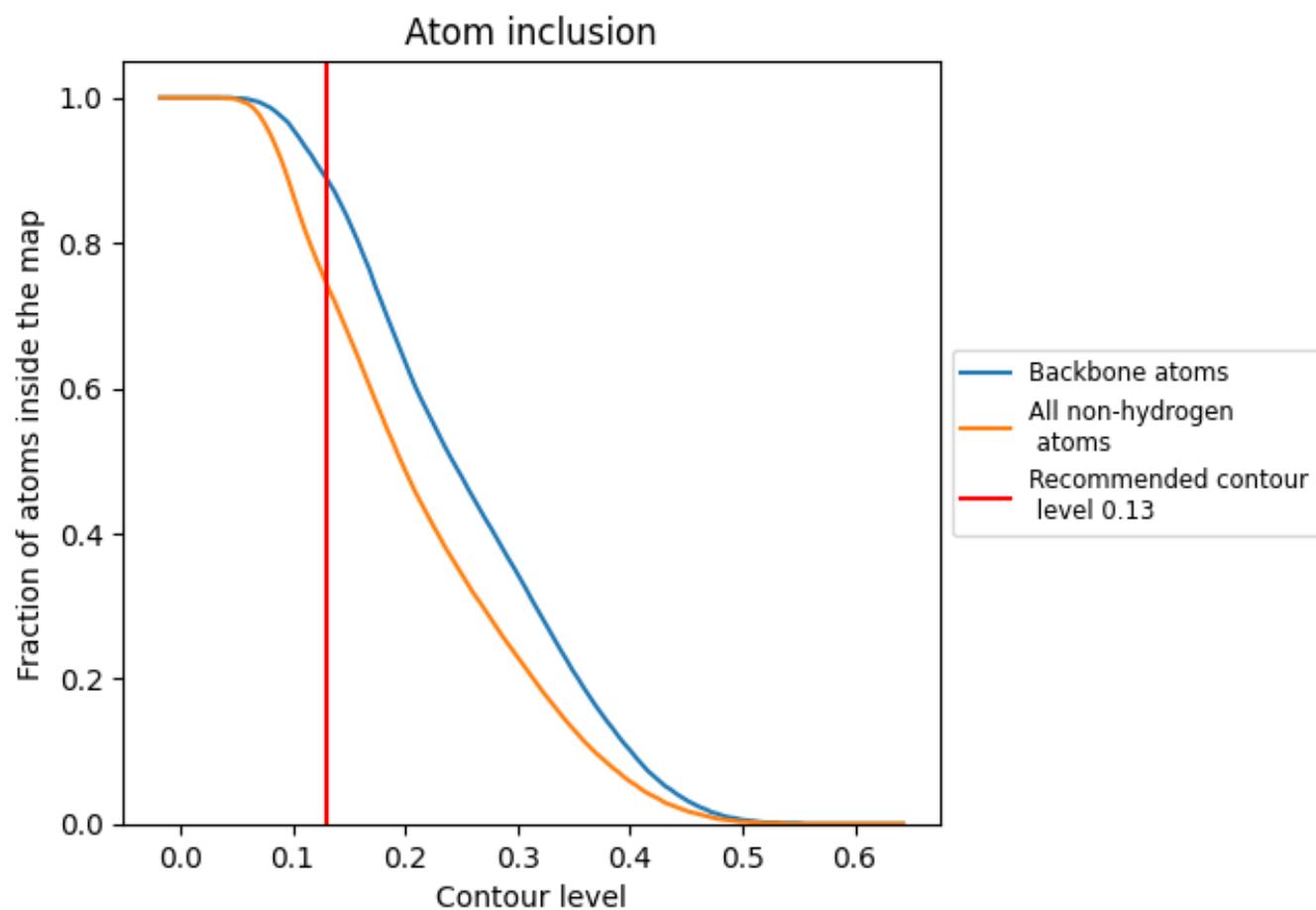
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 74% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.3940
A	0.7370	0.3860
B	0.7430	0.3980
C	0.7380	0.3850
D	0.7420	0.3940
E	0.9180	0.5420
F	0.9130	0.5260
G	0.9160	0.5250
H	0.9210	0.5450

1.0

0.0

<0.0