



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:40 PM UTC

PDB ID : 8UXI / pdb_00008uxi
EMDB ID : EMD-42765
Title : Structure of PKA phosphorylated human RyR2-R420W in the open state in the presence of calcium
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2023-11-09
Resolution : 3.29 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

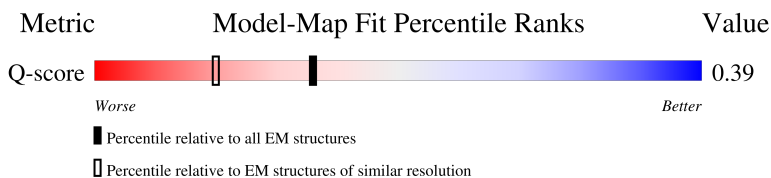
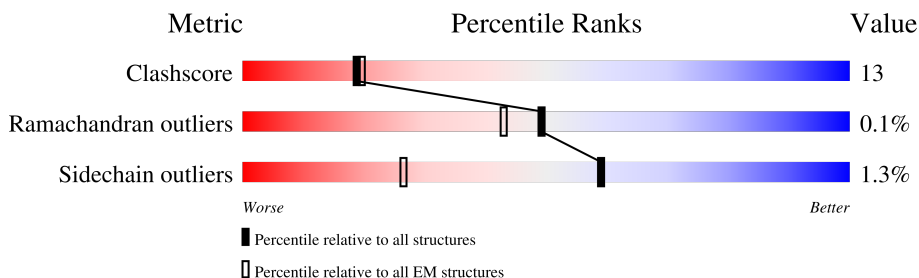
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.29 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% 57% 23% 19%
1	B	4967	11% 57% 23% 19%
1	C	4967	11% 57% 23% 19%
1	D	4967	11% 57% 22% 19%

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Mol	Chain	Length	Quality of chain
2	E	108	78% 19% ...
2	F	108	78% 19% ...
2	G	108	77% 19% ...
2	H	108	79% 18% ...

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 131656 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	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	B	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	C	4004	Total 32032	C 20411	N 5451	O 5955	S 215	2	0
1	D	4004	Total 32032	C 20411	N 5451	O 5955	S 215	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

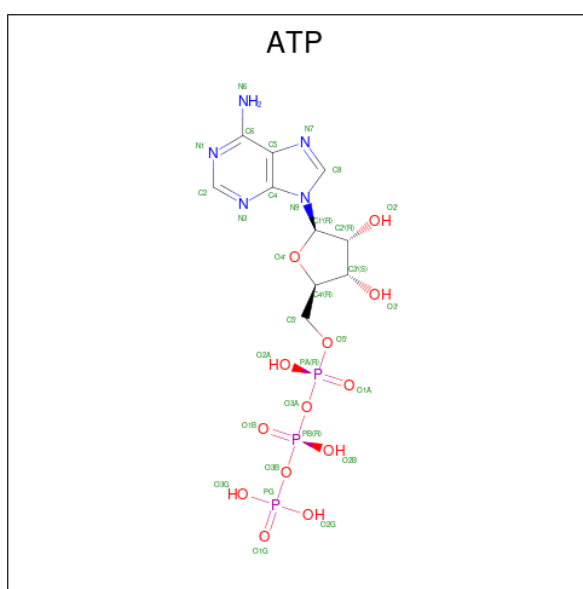
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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
4	D	1	Total	C	N	O	P	0
			31	10	5	13	3	

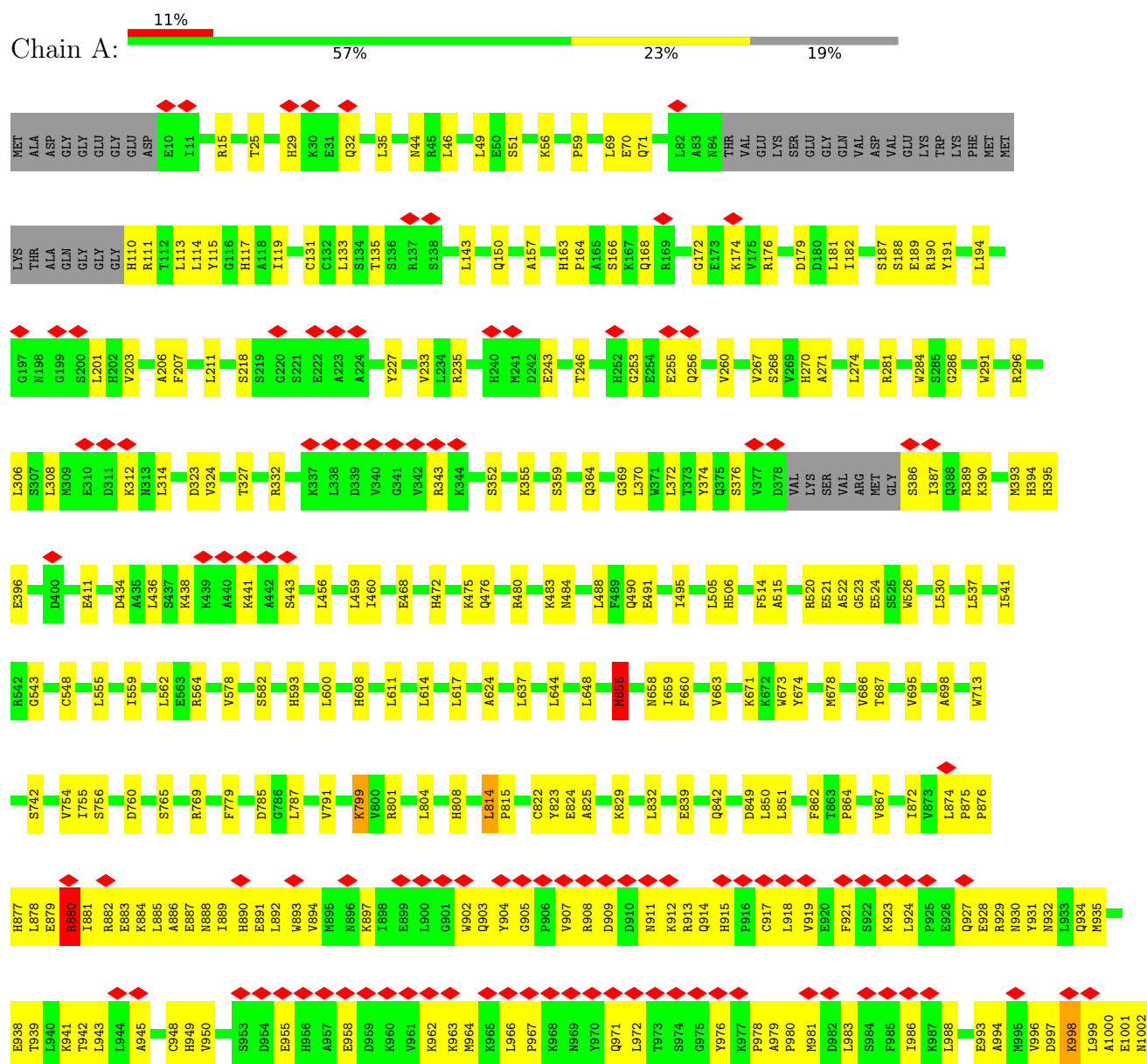
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

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	

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.

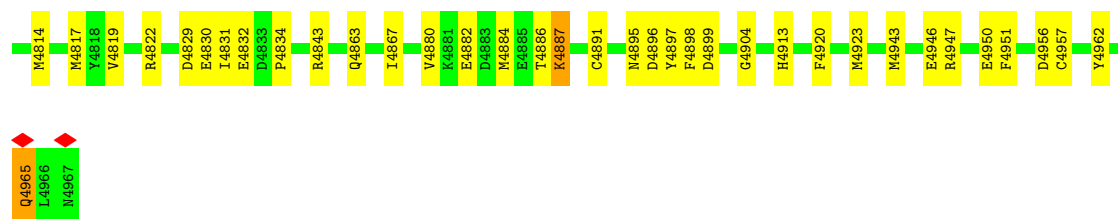
• Molecule 1: Ryanodine receptor 2



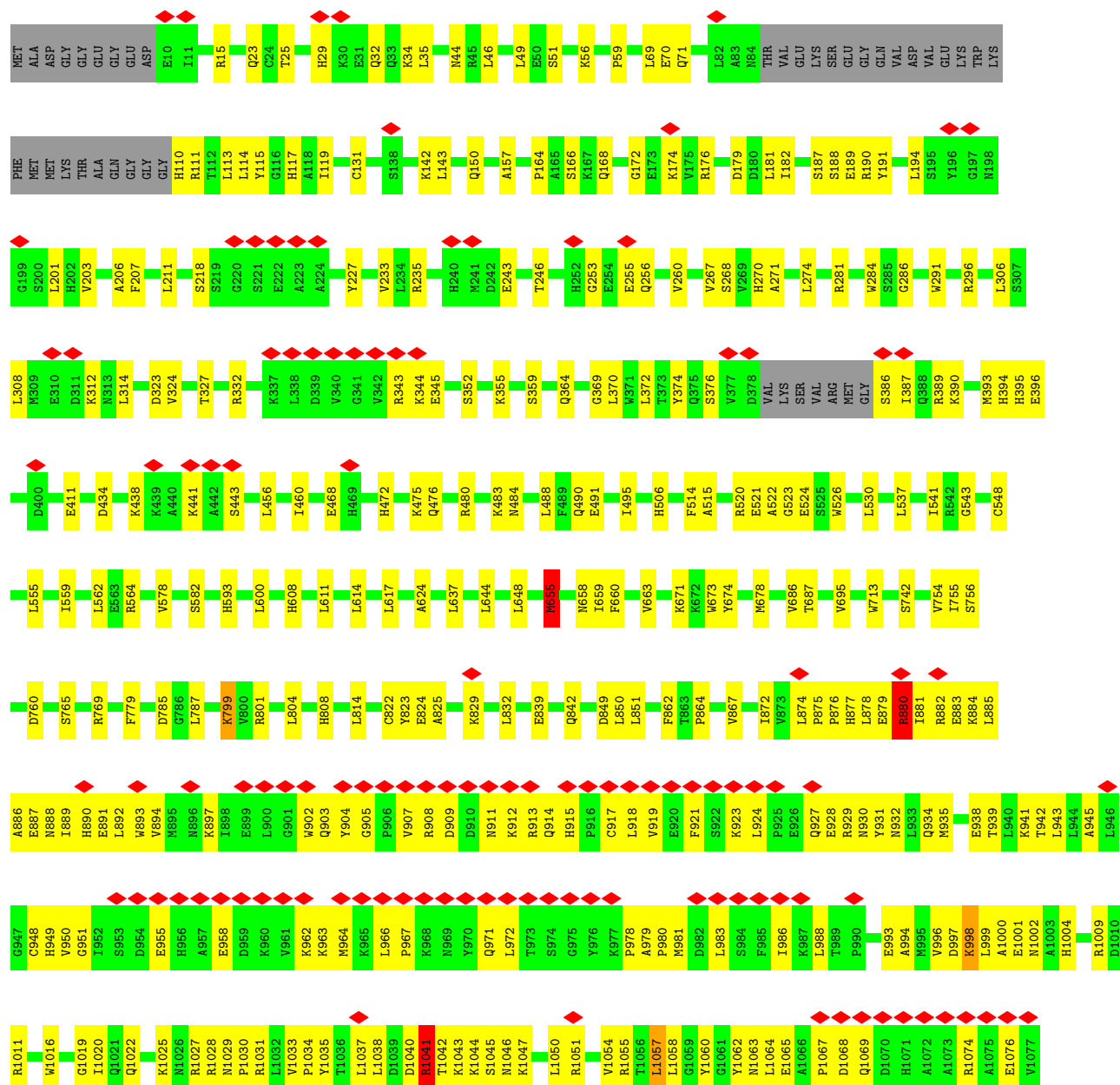








• Molecule 1: Ryanodine receptor 2



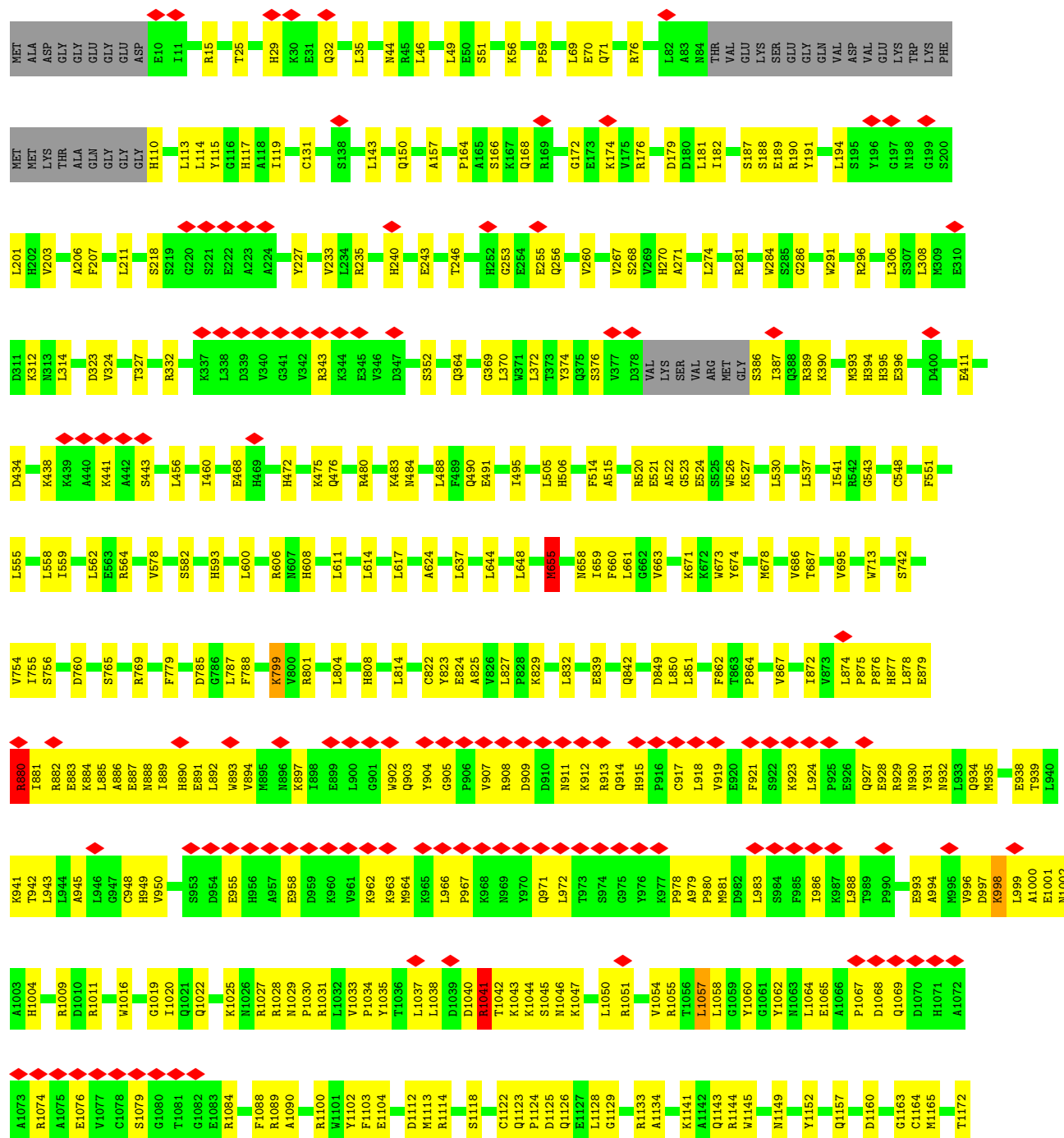
M2442	V2321	M2192	ASP	L1976	LYS	Q1620	D1471	ASP	L1177	C1078
I2445	R2322	V2193	SER	L1979	GLY	C1621	E1472	TTR	N1178	S1079
A2446	I2325	A2194	GLY	F1979	LYS	L1622	K1473	VAL	G1179	G1080
D2448	F2199	F2199	ARG	K1788	GLN	L1625	K1474	ALA	L1183	T1081
G2449	F2199	F2199	S1803	S1803	LYS	M1628	K1475	GLY	D1184	E1082
G2450	Y2202	Y2202	R1807	R1807	PRO	S1629	R1482	LEU	S1188	G1083
L2335	Y2206	Y2206	Q1895	Q1895	ARG	L1630	S1483	PRO	E1189	R1084
R2336	L2062	L2062	M1896	M1896	LYS	E1635	N1484	GLY	L1190	F1088
N2341	L2062	L2062	L1897	L1897	GLN	N1636	C1485	ALA	F1195	R1089
G2342	M2066	M2066	L1817	L1817	ARG	E1649	Y1486	GLY	A1090	A1090
G2459	V2074	V2074	F1825	F1825	PHE	L1650	M1487	LEU	Y1094	Y1094
R2359	V2074	V2074	I1830	I1830	LEU	H1656	M1494	GLY	P1203	P1203
S2363	V2086	V2086	M1831	M1831	ARG	H1656	S1495	PRO	V1204	R1100
P2364	L2087	L2087	I1832	I1832	THR	L1660	P1496	LYS	C1205	W1101
ASN	R2090	R2090	I1833	I1833	LYS	L1660	G1497	ASN	Y1102	Y1102
GLY	Q2091	Q2091	L1839	L1839	LYS	V1664	Q1498	ASP	F1103	F1103
SER	G2096	G2096	I1842	I1842	THR	L1667	G1499	ALA	E1104	E1104
GLY	V2099	V2099	E1847	E1847	THR	L1676	R1500	GLU	Q1211	Q1211
LEU	L2119	L2119	P1848	P1848	ASP	H1679	R1501	ASP	D1112	D1112
ASP	Q2125	Q2125	S1849	S1849	SER	L1685	M1502	ALA	M1113	M1113
THR	L2125	L2125	D1930	D1930	HIS	A1688	G1504	SER	R1214	R1214
GLU	L2129	L2129	F1932	F1932	ALA	T1689	L1505	ALA	M1215	M1215
E2377	L2130	L2130	A1854	A1854	LEU	K1692	T1537	GLU	K1226	K1226
E2378	E2137	E2137	THR	THR	THR	Y1693	K1538	VAL	I1229	I1229
D2379	E2138	E2138	GLU	GLU	GLU	M1694	Q1546	LEU	Y1236	Y1236
D2380	E2139	E2139	GLU	GLU	GLU	L1697	S1549	THR	F1239	F1239
H2383	M2142	M2142	ARG	ARG	ARG	Y1703	P1550	ASP	N1244	N1244
N2384	T2143	T2143	SER	SER	SER	L1706	N1551	LEU	R1245	R1245
N2386	G2144	G2144	THR	THR	THR	L1706	V1552	ALA	W1250	W1250
M2389	G2145	G2145	LEU	LEU	LEU	L1711	F1553	GLY	L1251	L1251
D2397	L2146	L2146	LYS	LYS	LYS	L1711	Q1554	HIS	A1134	A1134
R2401	M2150	M2150	GLU	GLU	GLU	Y1714	F1555	GLY	K1141	K1141
L2423	N2151	N2151	LEU	LEU	LEU	A1715	Q1556	LEU	N1142	N1142
L2426	N2152	N2152	LYS	LYS	LYS	T1716	N1560	VAL	Q1143	Q1143
L2426	R2154	R2154	VAL	VAL	VAL	A1717	V1563	PRO	R1144	R1144
L2426	T2170	T2170	THR	THR	THR	R1718	M1564	ARG	W1145	W1145
D2431	V2171	V2171	ALA	ALA	ALA	L1719	P1565	ASP	N1149	N1149
G2434	V2176	V2176	LYS	LYS	LYS	M1721	S1592	LYS	Y1152	Y1152
V2435	Q2181	Q2181	GLN	GLN	GLN	N1722	H1593	LYS	Q1157	Q1157
L2436	G2182	G2182	ALA	ALA	ALA	L1748	V1594	ALA	D1160	D1160
S2437	G2183	G2183	GLY	GLY	GLY	I1751	F1603	THR	T1297	T1297
I2438	E2183	E2183	GLY	GLY	GLY	P1759	N1604	LYS	D1298	D1298
A2439	N2184	N2184	GLU	GLU	GLU	I1751	Y1441	PRO	G1163	G1163
Q2441	K2185	K2185	GLU	GLU	GLU	P1759	Y1442	GLU	C1164	C1164
	E2186	E2186	ALA	ALA	ALA		G1444	ASN	M1165	M1165
								HIS	T1172	T1172
								LYS	M1173	M1173
									C1310	C1310







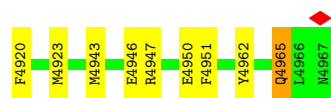
● Molecule 1: Ryanodine receptor 2



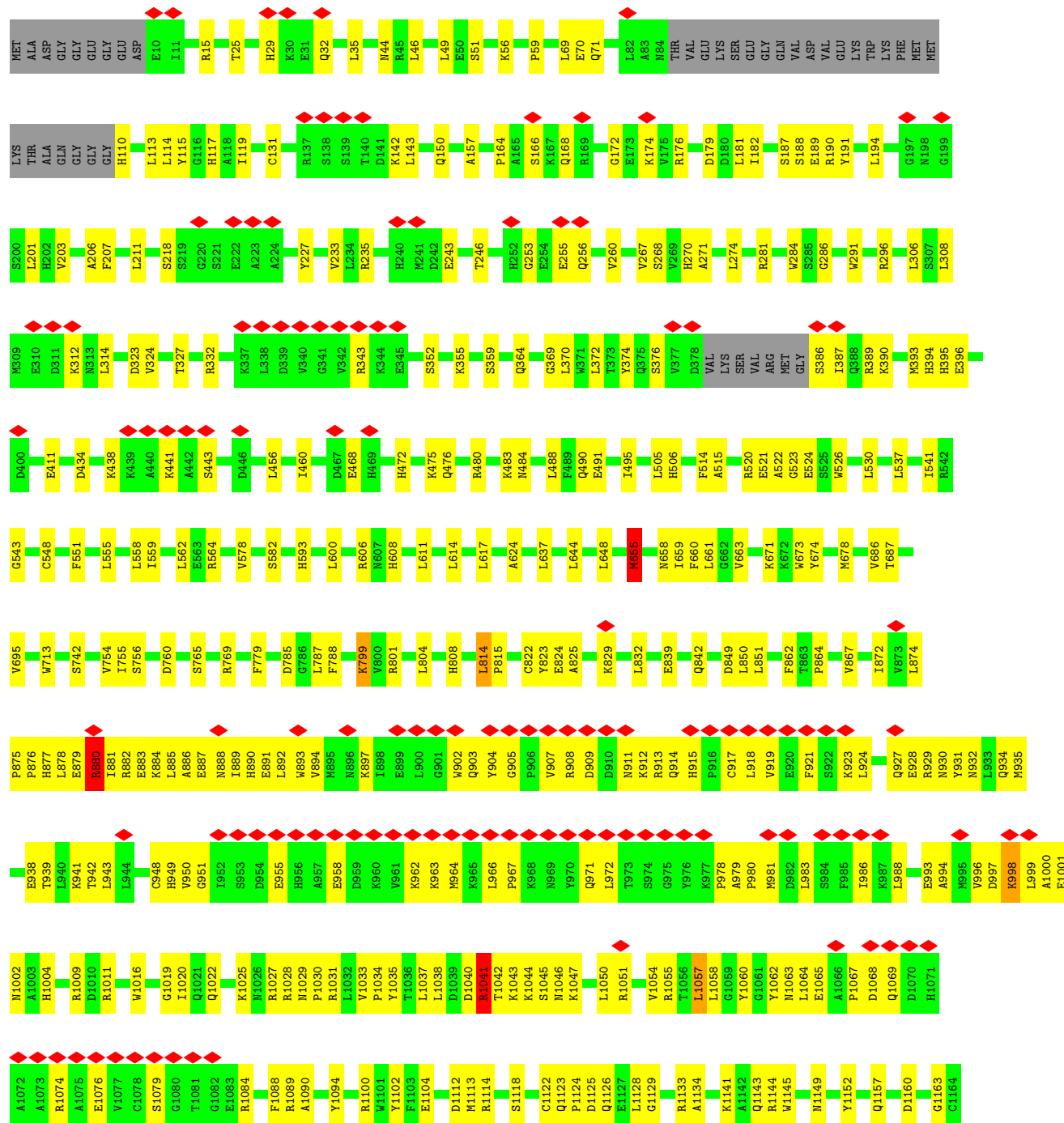
R2581	F2440	N2309	K2185	Q1972	LYS	Q1620	D1471	ASP	H1173
N2584	Q2441	N2316	E2186	M1975	GLY	L1625	E1472	TYR	T1176
N2585	M2442	A2317	F2186	L1976	GLY	M1628	K1473	ALA	L1177
Q2586	I2445	V2321	V2192	F1979	GLY	S1629	G1474	GLN	M1178
N2587	A2446	A2317	A2194	D1982	ARG	L1630	K1475	GLY	G1179
L2588	K2447	F2331	F2199	E1983	P1889	H1631	R1482	PRO	L1183
R2589	D2448	G2332	F2202	S1984	K1890	I1632	S1483	LEU	D1184
R2590	N2450	L2335	Y2202	E1985	L1894	H1633	G1484	ARG	L1188
R2591	L2449	R2336	T2206	L2081	M1896	I1632	C1485	LEU	E1189
L2592	V2451	G2337	F2215	C1988	K1897	H1632	Y1486	GLY	L1190
V2593	S2457	G2337	F2215	E1989	L1898	H1632	M1487	LEU	F1195
H2602	A2458	N2341	Y2220	P1989	V1902	H1650	M1494	GLY	F1195
A2603	G2459	G2342	Y2220	E1991	L1829	L1850	M1494	LEU	F1195
N2605	L2460	V2074	L2221	I1992	I1830	H1656	S1495	PRO	I1202
P2606	K2465	R2369	L2222	T1992	M1831	H1656	P1496	LYS	P1203
L2607	L2478	V2086	L2222	R1993	G1832	L1660	G1497	ASN	P1204
K2608	I2478	L2087	V2227	Q1994	I1833	V1664	Q1498	LEU	C1205
L2609	Q2481	P2364	S2237	Q1995	L1839	L1667	G1499	PRO	G1208
Y2614	D2482	GLY	D2241	E2010	V1918	L1667	R1500	TYR	Q1211
K2619	F2483	SER	D2241	LEU	R1919	L1676	N1501	ASP	Q1211
Y2620	L2484	GLY	A2245	ASP	I1922	L1676	N1502	ALA	R1214
L2623	L2485	LYS	S2246	GLU	V1926	H1679	N1503	ASP	M1215
P2624	L2488	THR	V2247	GLY	S1929	H1679	N1504	ASP	K1225
G2625	F2492	LEU	M2248	ASP	D1930	L1685	G1504	ALA	Y1226
G2626	R2497	THR	N2251	SER	I1932	A1688	T1537	LEU	I1229
W2627	GLU	GLU	L2252	LEU	F1932	I1689	K1538	THR	I1229
A2632	C2521	GLU	L2253	ASN	V1933	I1689	Q1546	GLY	Y1236
E2635	L2525	THR	L2254	ASP	L1936	K1692	S1549	VAL	F1239
L2638	L2527	THR	L2255	THR	Q1937	M1694	P1550	LEU	Y1239
S2641	L2534	H2383	L2257	ILE	Y1944	Y1703	N1551	GLY	M1244
R2642	E2539	P2384	L2257	ARG	Y1944	L1706	N1552	HIS	R1245
K2643	H2540	G2385	L2258	GLY	V1947	L1711	F1553	LEU	W1250
L2644	H2541	N2386	L2259	ARG	M1948	L1711	I1559	VAL	L1251
F2649	A2542	M2389	C2272	LEU	Q1949	Y1714	I1560	PRO	E1266
D2650	S2543	D2397	C2273	SER	A1950	A1715	K1561	ASP	E1266
A2651	L2544	R2401	C2273	VAL	L1951	A1716	N1562	ARG	H1267
Q2654	L2545	R2401	Y2285	VAL	M1952	A1717	V1563	VAL	I1277
Y2657	L2548	L2423	P2286	LYS	S1954	R1718	M1564	LYS	I1277
E2658	L2555	L2426	Y2290	THR	A1955	M1720	P1578	ASP	N1294
Q2659	K2557	D2431	N2291	TYR	A1956	H1721	I1578	LYS	N1294
F2662	L2561	G2434	P2292	LEU	L1957	M1722	S1592	ALA	T1297
K2663	L2566	V2435	R2297	LYS	T1958	L1748	H1593	THR	D1298
L2664	I2576	R2301	F2301	LYS	A1959	L1748	V1594	LYS	I1299
A2665	L2576	L2302	G2181	GLN	R1960	I1751	F1603	PRO	M1300
L2666	L2576	R2303	G2182	ALA	K1961	P1759	L1604	PHE	R1303
P2667	L2580	C2308	E2183	GLU	T1962	F1768	V1608	ASN	C1310
			S2184	PRO	F1965		Q1615	HIS	H1312
				VAL	R1966		V1619	LYS	





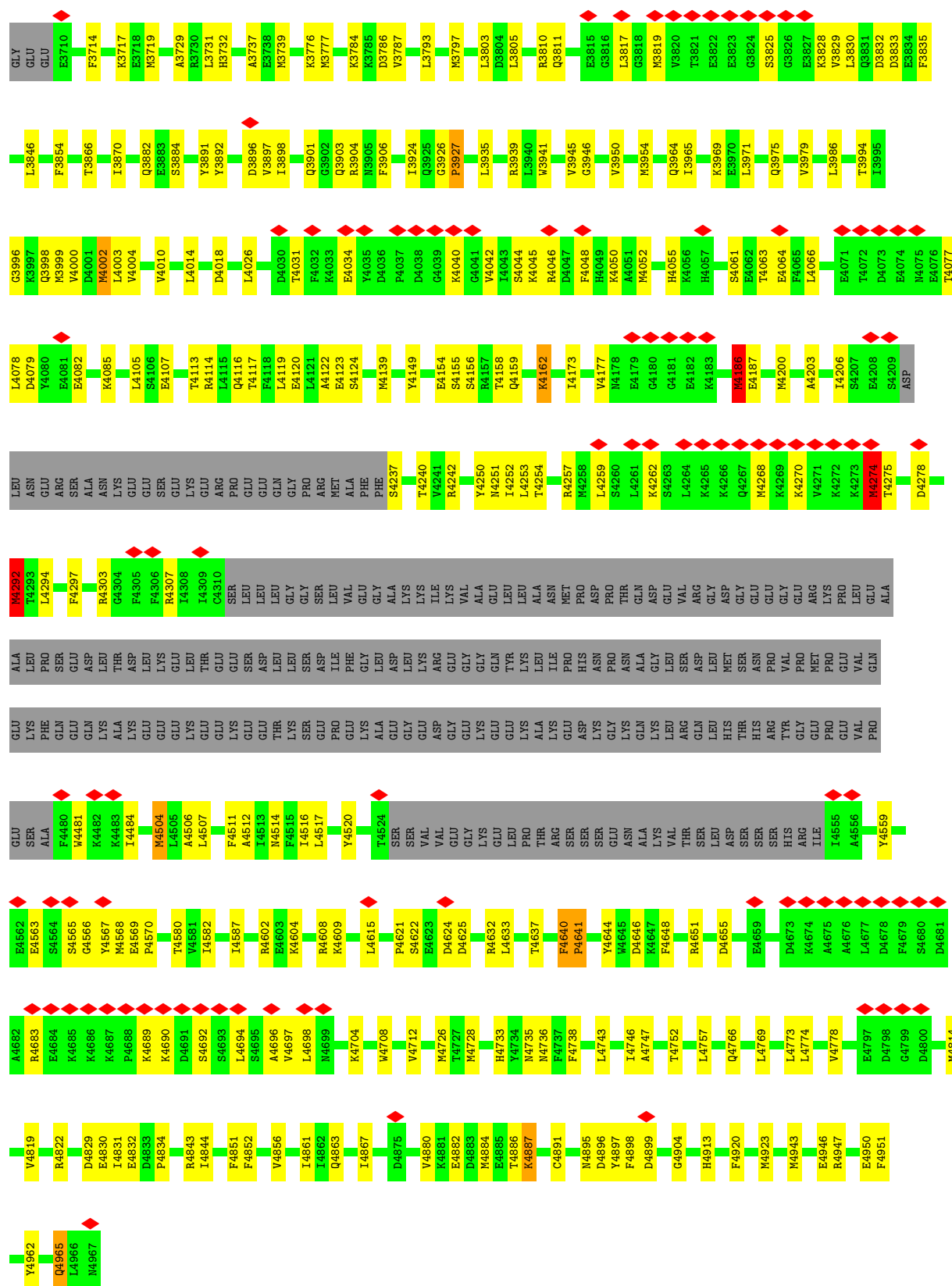


● Molecule 1: Ryanodine receptor 2









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

Chain E:  78% 19% ...



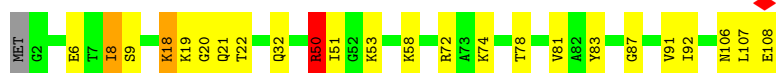
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F:  78% 19% ...



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

Chain G:  77% 19% ...



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

Chain H:  79% 18% ...



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149448	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	0.599	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	431.36, 431.36, 431.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8425, 0.8425, 0.8425	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.16	0/32738	0.46	15/44213 (0.0%)
1	B	0.16	0/32738	0.46	15/44213 (0.0%)
1	C	0.16	0/32738	0.46	14/44213 (0.0%)
1	D	0.16	0/32738	0.46	15/44213 (0.0%)
2	E	0.18	0/834	0.56	3/1123 (0.3%)
2	F	0.18	0/834	0.56	3/1123 (0.3%)
2	G	0.18	0/834	0.56	3/1123 (0.3%)
2	H	0.18	0/834	0.56	3/1123 (0.3%)
All	All	0.16	0/134288	0.47	71/181344 (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	4
1	B	0	4
1	C	0	4
1	D	0	4
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	2
All	All	0	24

There are no bond length outliers.

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1563	VAL	CA-C-N	8.82	132.48	120.67
1	A	1563	VAL	C-N-CA	8.82	132.48	120.67
1	C	1563	VAL	CA-C-N	8.82	132.48	120.67
1	C	1563	VAL	C-N-CA	8.82	132.48	120.67
1	D	1563	VAL	CA-C-N	8.78	132.43	120.67

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2827	ASP	Peptide
1	A	4640	PHE	Peptide
1	A	880	ARG	Peptide,Sidechain
2	E	50	ARG	Peptide,Sidechain
2	F	50	ARG	Sidechain

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	32032	0	31689	837	0
1	B	32032	0	31689	841	0
1	C	32032	0	31689	860	0
1	D	32032	0	31689	844	0
2	E	818	0	821	19	0
2	F	818	0	821	17	0
2	G	818	0	821	18	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	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
All	All	131656	0	130136	3382	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 13.

The worst 5 of 3382 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:4237:SER:N	1:B:4240:THR:HG1	1.59	1.01
1:A:4237:SER:N	1:A:4240:THR:HG1	1.59	1.00
1:D:4237:SER:N	1:D:4240:THR:HG1	1.58	1.00
1:C:4237:SER:N	1:C:4240:THR:HG1	1.61	0.95
1:B:4259:LEU:HD21	1:C:4701:ILE:HG21	1.51	0.91

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	3978/4967 (80%)	3852 (97%)	123 (3%)	3 (0%)	48	75
1	B	3978/4967 (80%)	3852 (97%)	123 (3%)	3 (0%)	48	75
1	C	3978/4967 (80%)	3851 (97%)	124 (3%)	3 (0%)	48	75
1	D	3978/4967 (80%)	3850 (97%)	125 (3%)	3 (0%)	48	75
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	16332/20300 (80%)	15805 (97%)	515 (3%)	12 (0%)	49	75

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2988	ARG
1	A	3927	PRO
1	A	4641	PRO
1	B	2988	ARG
1	B	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	3513/4358 (81%)	3469 (99%)	44 (1%)	61	74
1	B	3513/4358 (81%)	3469 (99%)	44 (1%)	61	74
1	C	3513/4358 (81%)	3469 (99%)	44 (1%)	61	74
1	D	3513/4358 (81%)	3469 (99%)	44 (1%)	61	74
2	E	88/89 (99%)	86 (98%)	2 (2%)	44	66
2	F	88/89 (99%)	86 (98%)	2 (2%)	44	66
2	G	88/89 (99%)	86 (98%)	2 (2%)	44	66
2	H	88/89 (99%)	86 (98%)	2 (2%)	44	66
All	All	14404/17788 (81%)	14220 (99%)	184 (1%)	59	74

5 of 184 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2765	GLU
1	D	799	LYS
1	C	2836	ASP
1	C	4002	MET
1	D	1057	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 173 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2639	HIS
1	D	1005	ASN
1	C	3767	ASN
1	C	4108	HIS
1	D	1710	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 16 ligands modelled in this entry, 8 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	D	5004	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	D	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	B	5004	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	B	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	A	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	A	5004	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	C	5002	-	32,33,33	0.25	0	48,52,52	0.28	0
4	ATP	C	5004	-	32,33,33	0.25	0	48,52,52	0.27	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	D	5004	-	-	6/22/38/38	0/3/3/3
4	ATP	D	5002	-	-	12/22/38/38	0/3/3/3
4	ATP	B	5004	-	-	6/22/38/38	0/3/3/3
4	ATP	B	5002	-	-	12/22/38/38	0/3/3/3
4	ATP	A	5002	-	-	12/22/38/38	0/3/3/3
4	ATP	A	5004	-	-	6/22/38/38	0/3/3/3
4	ATP	C	5002	-	-	12/22/38/38	0/3/3/3
4	ATP	C	5004	-	-	6/22/38/38	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5002	ATP	PB-O3A-PA-O5'
4	A	5002	ATP	C5'-O5'-PA-O1A
4	A	5002	ATP	C5'-O5'-PA-O2A
4	A	5002	ATP	C5'-O5'-PA-O3A
4	B	5002	ATP	PB-O3A-PA-O5'

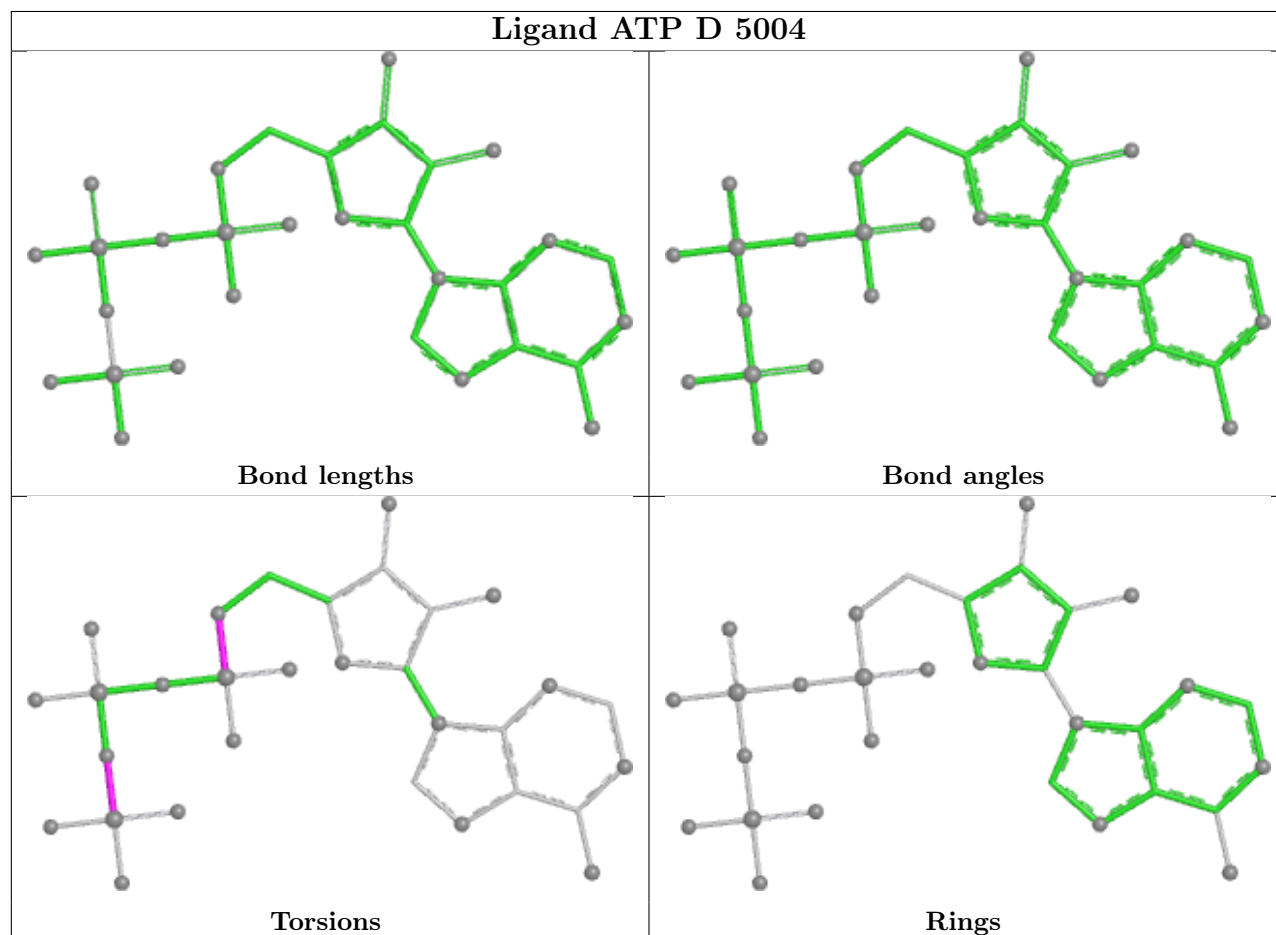
There are no ring outliers.

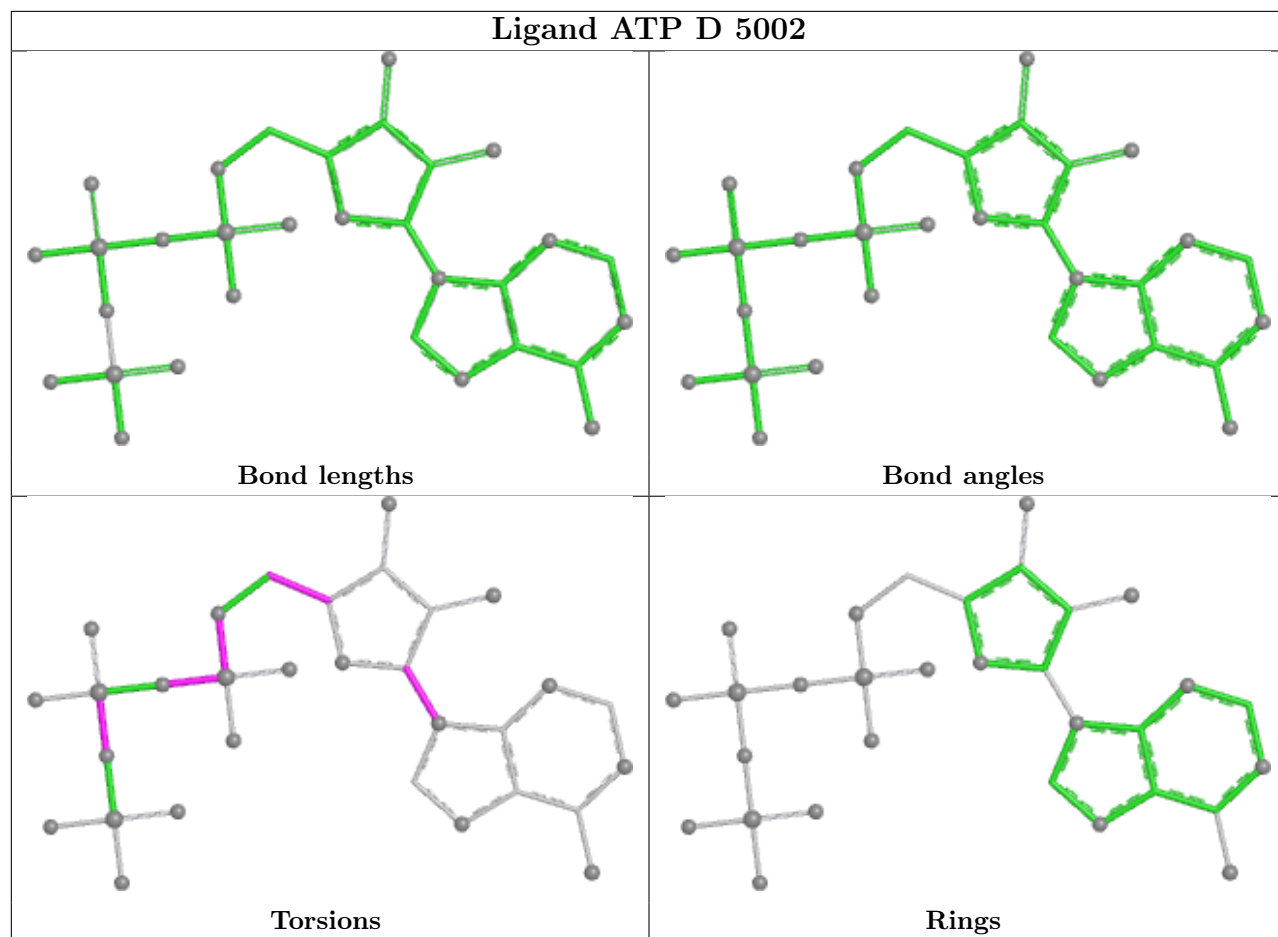
4 monomers are involved in 8 short contacts:

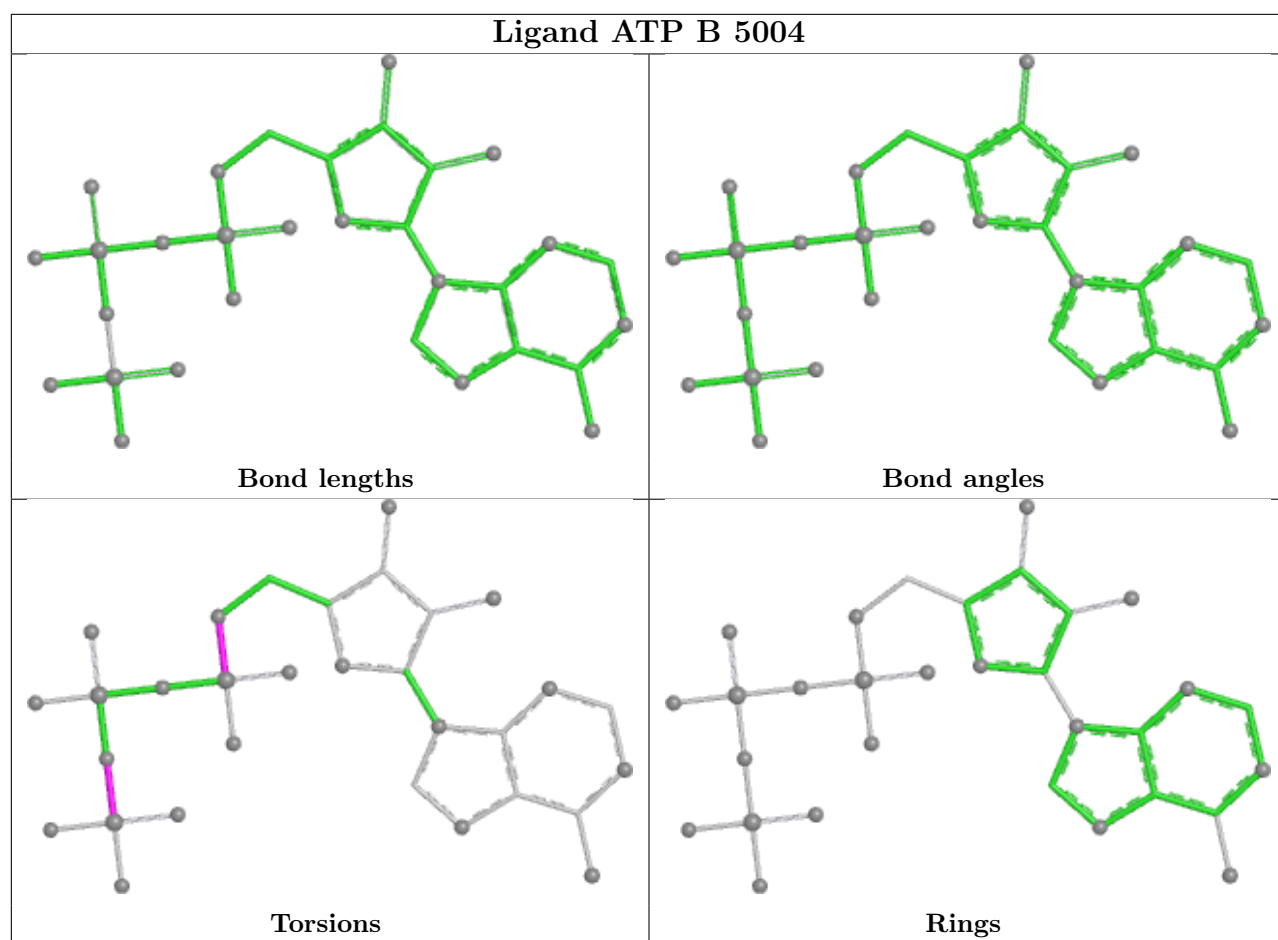
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5004	ATP	2	0
4	B	5004	ATP	2	0
4	A	5004	ATP	2	0
4	C	5004	ATP	2	0

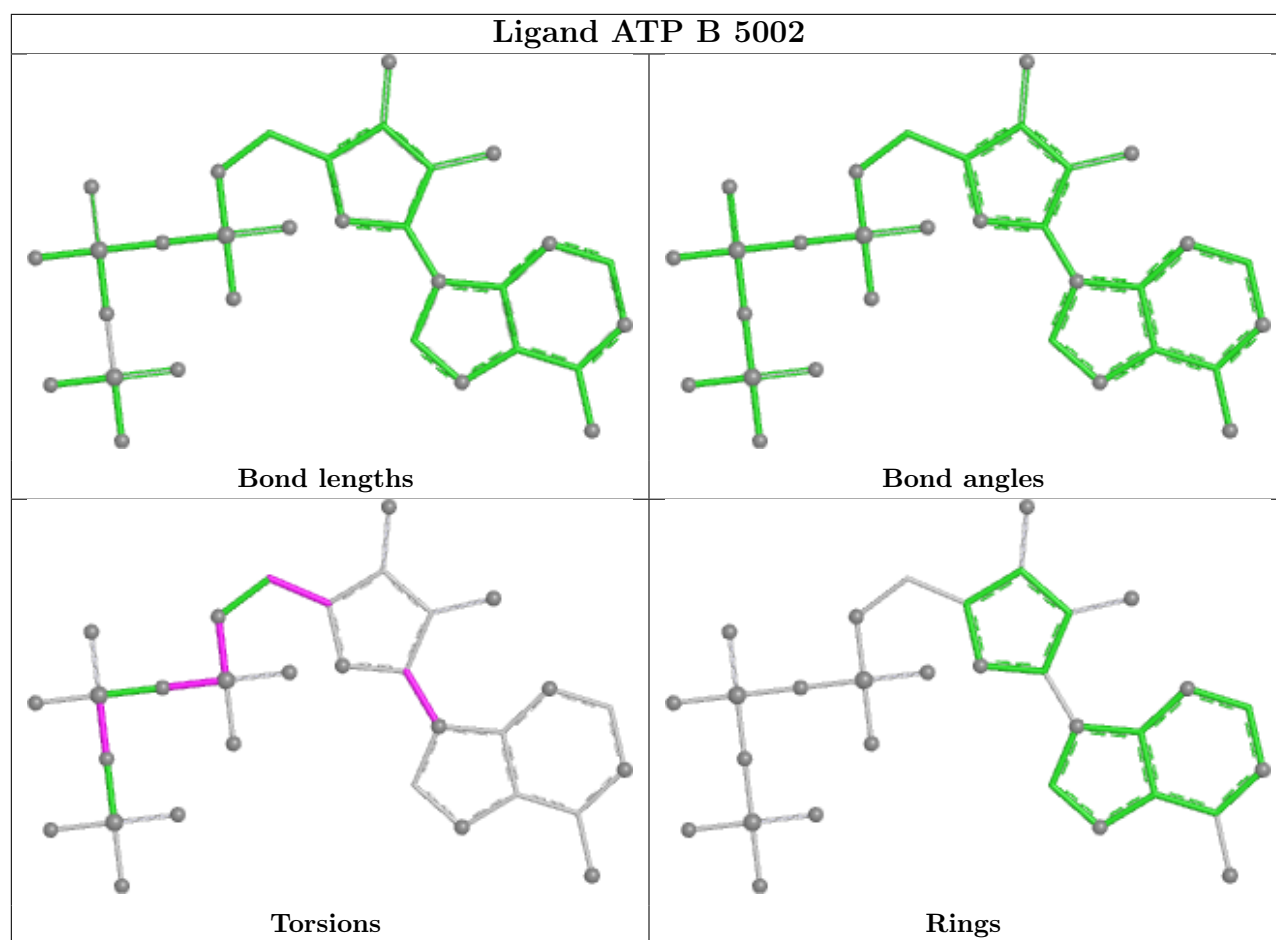
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

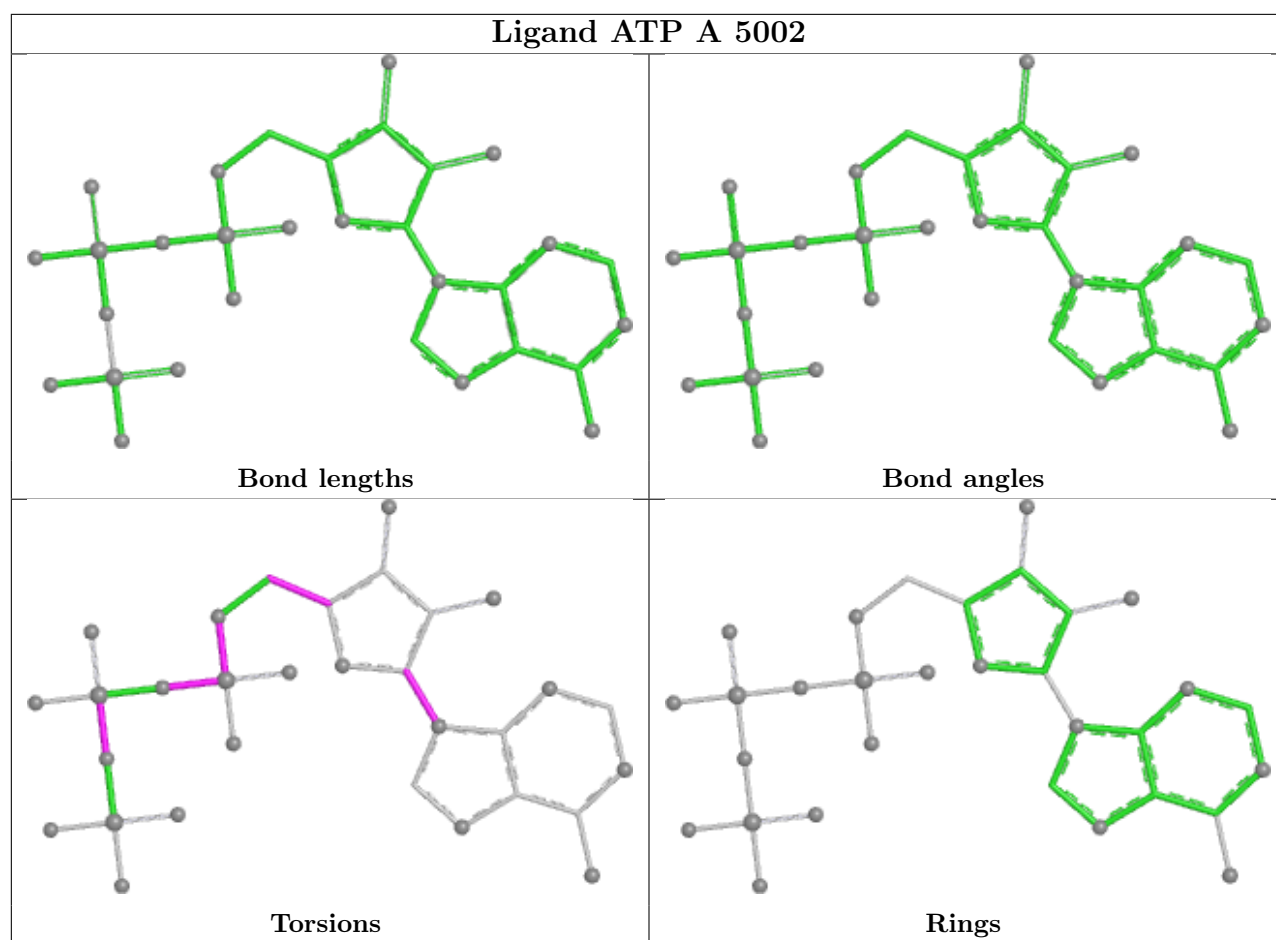
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

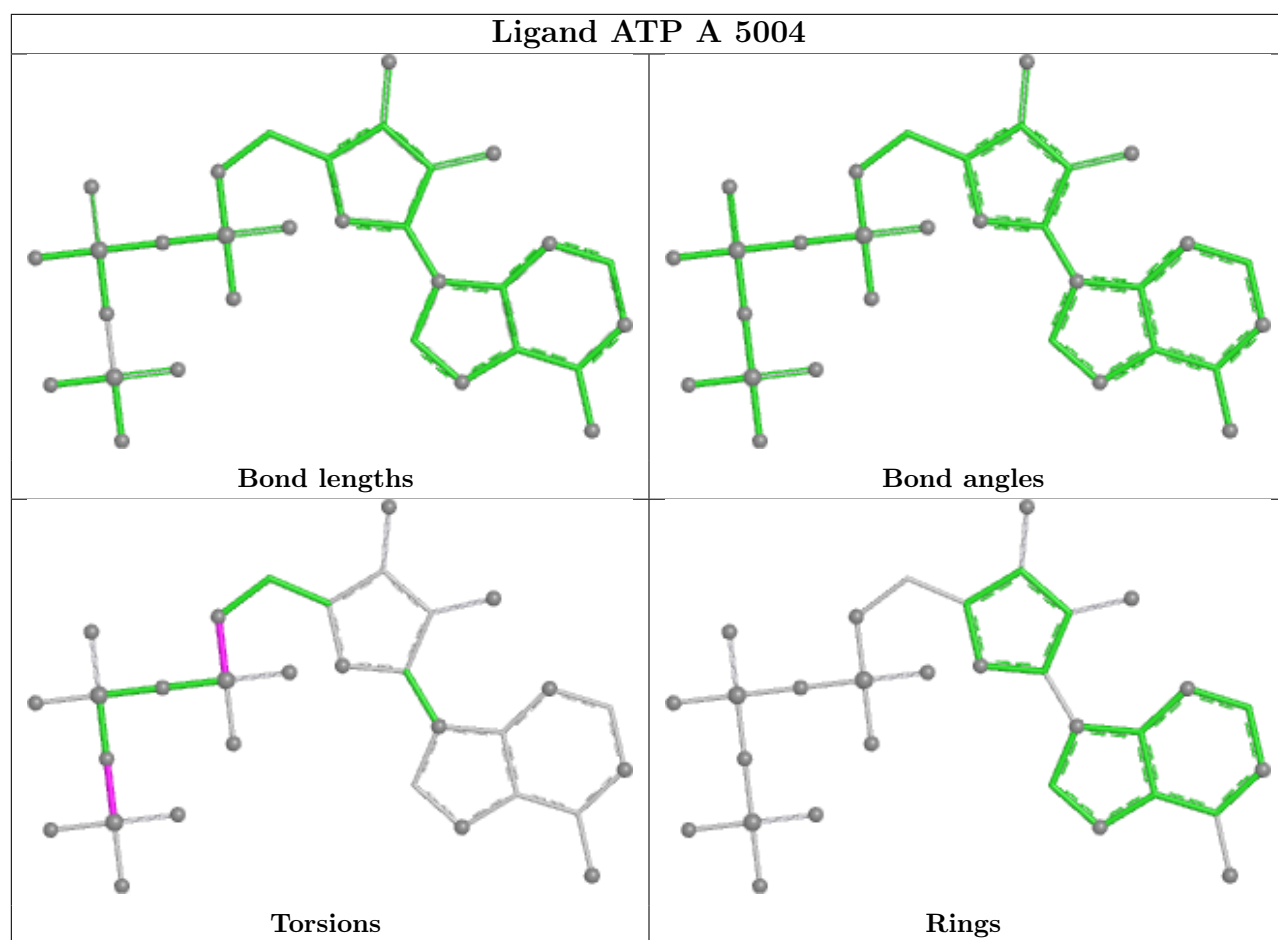


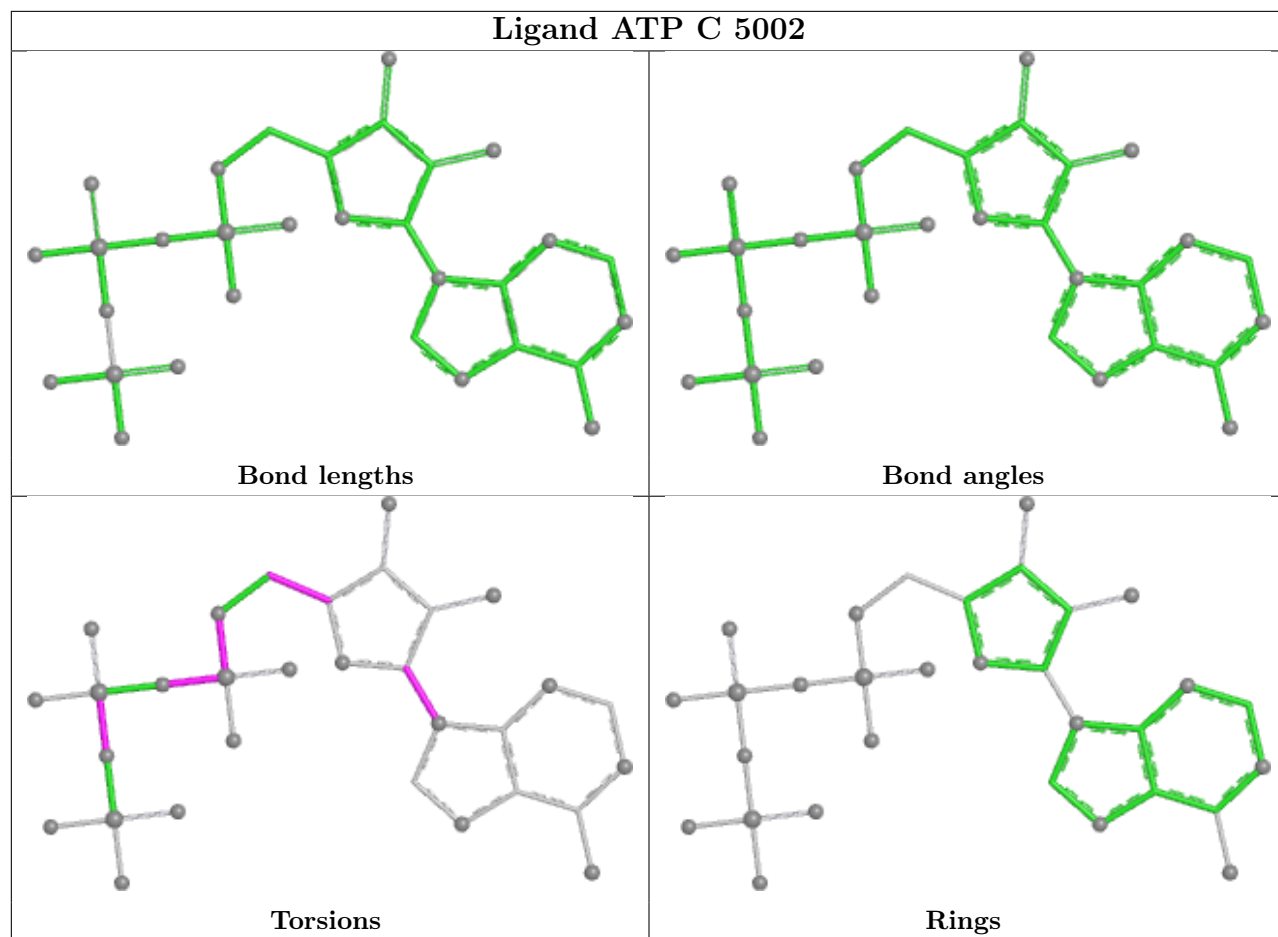


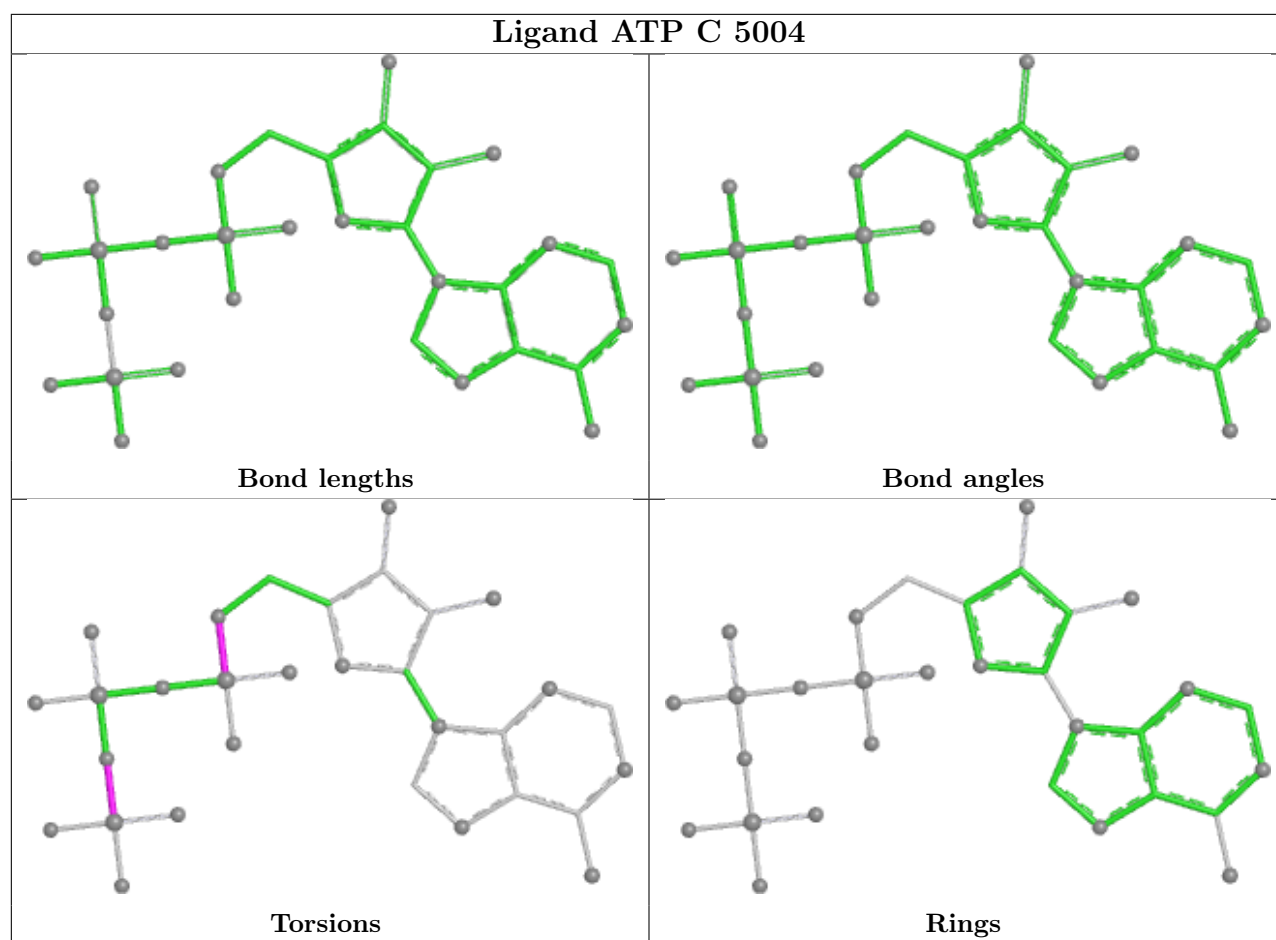












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

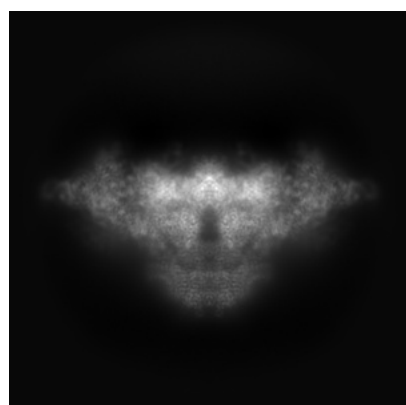
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42765. These allow visual inspection of the internal detail of the map and identification of artifacts.

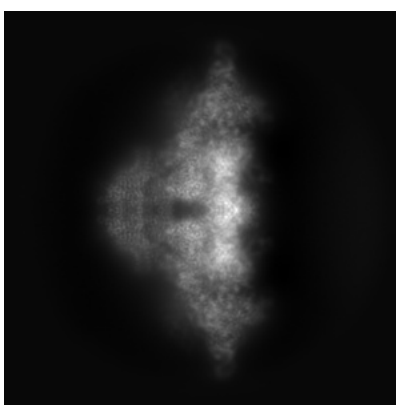
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

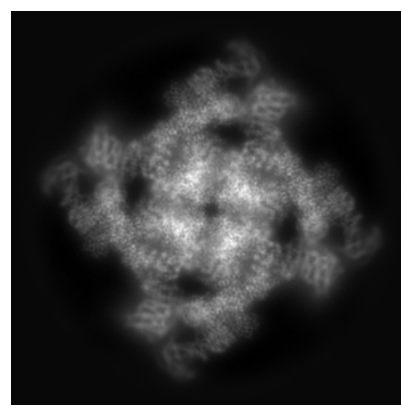
6.1.1 Primary map



X



Y

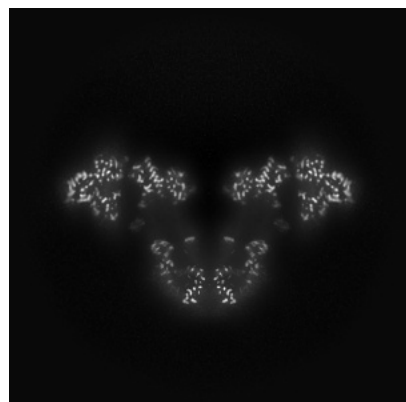


Z

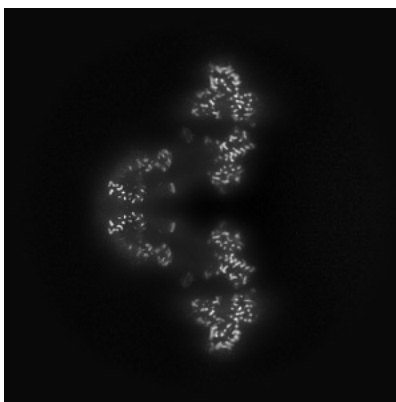
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

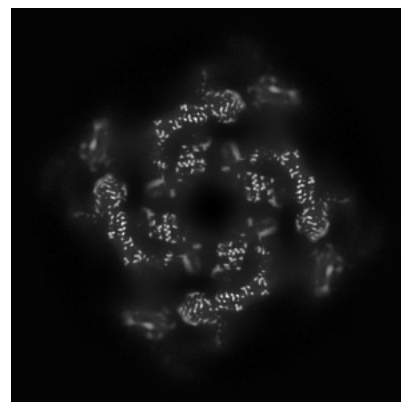
6.2.1 Primary map



X Index: 256



Y Index: 256

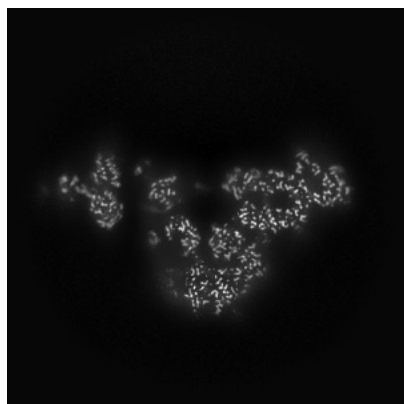


Z Index: 256

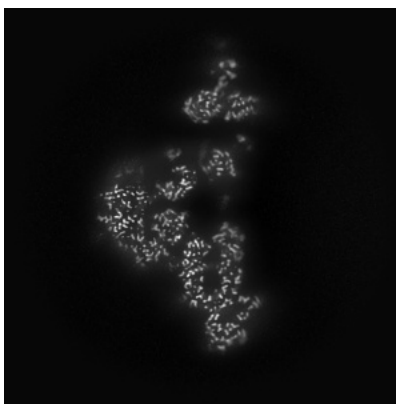
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

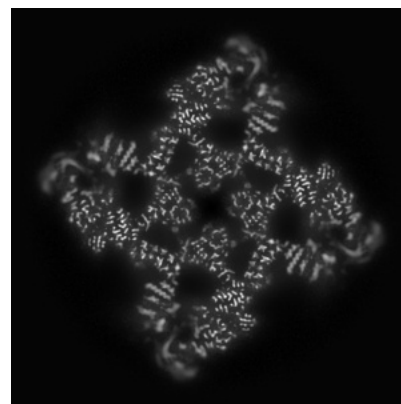
6.3.1 Primary map



X Index: 239



Y Index: 239

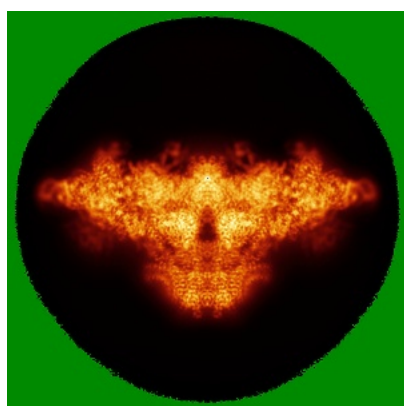


Z Index: 277

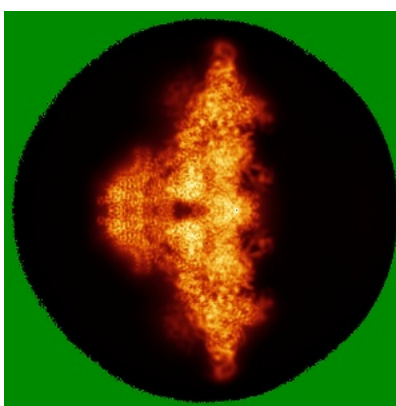
The images above show the largest variance slices of the map in three orthogonal directions.

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

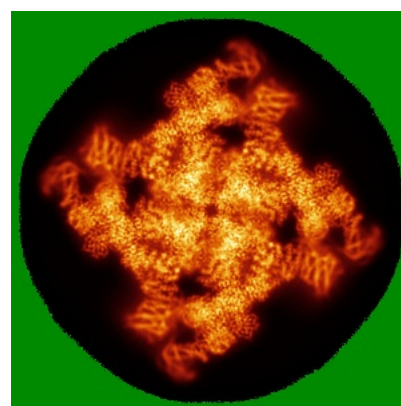
6.4.1 Primary map



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

This section was not generated.

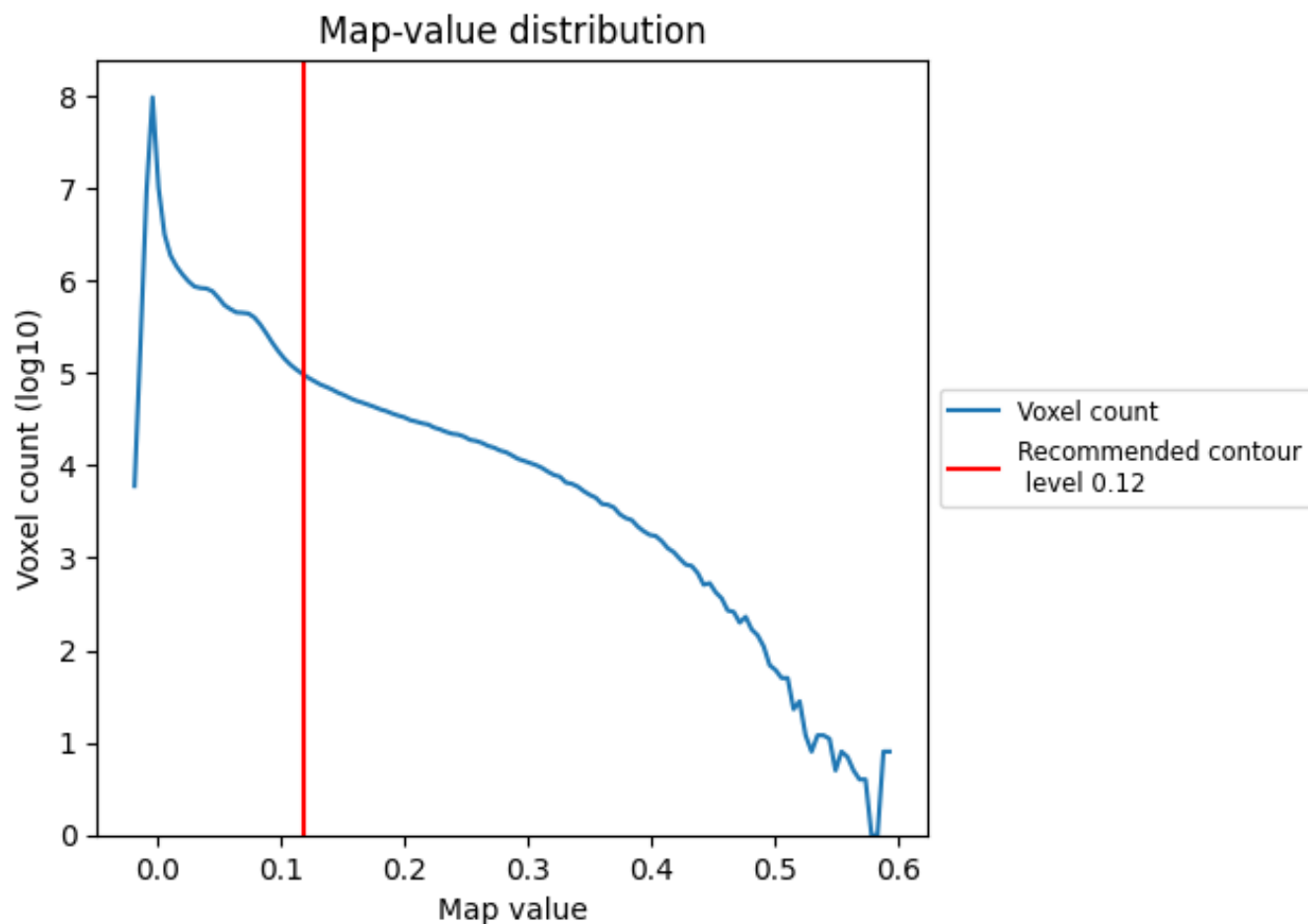
6.6 Mask visualisation

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

7 Map analysis [i](#)

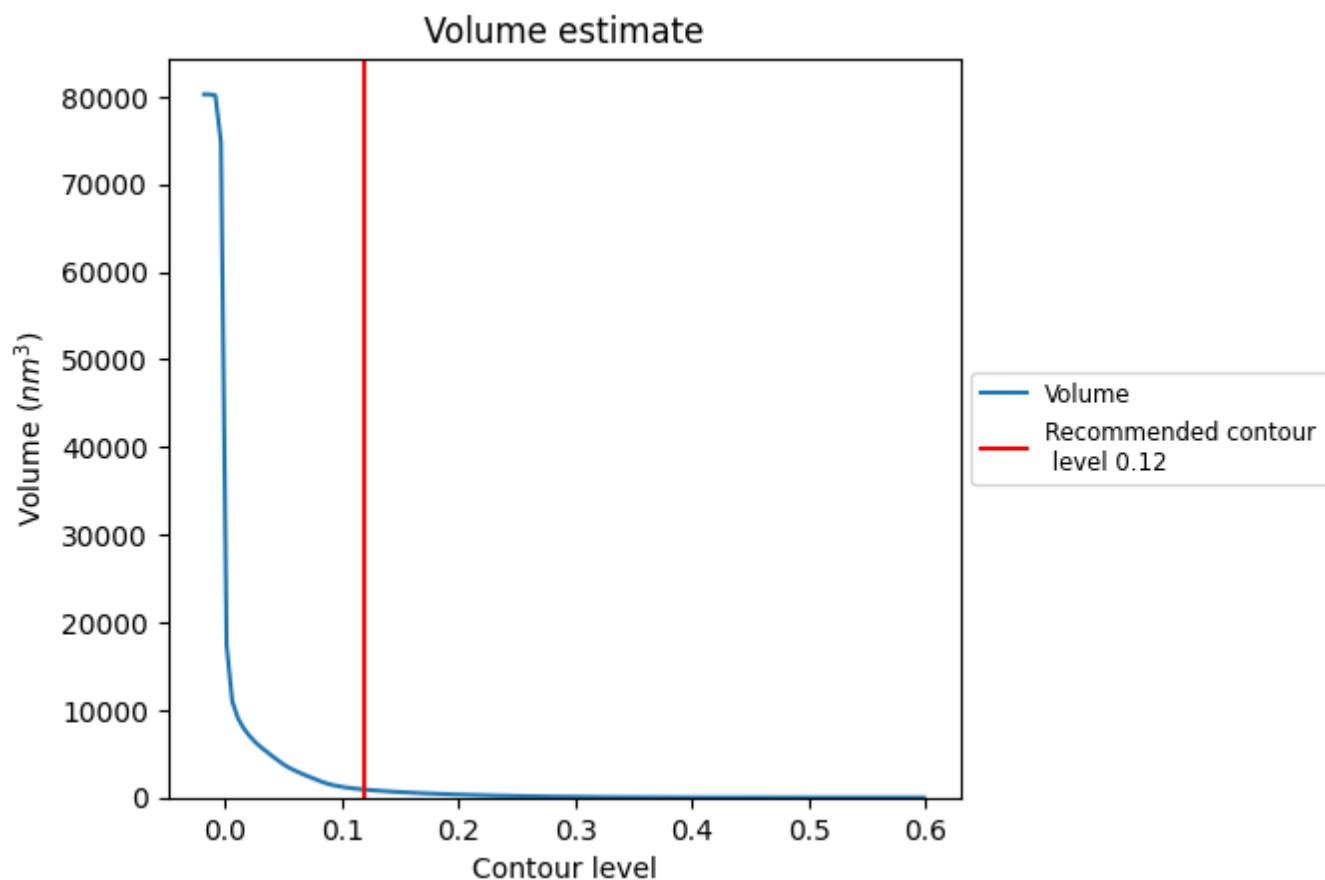
This section contains the results of statistical analysis of the map.

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.

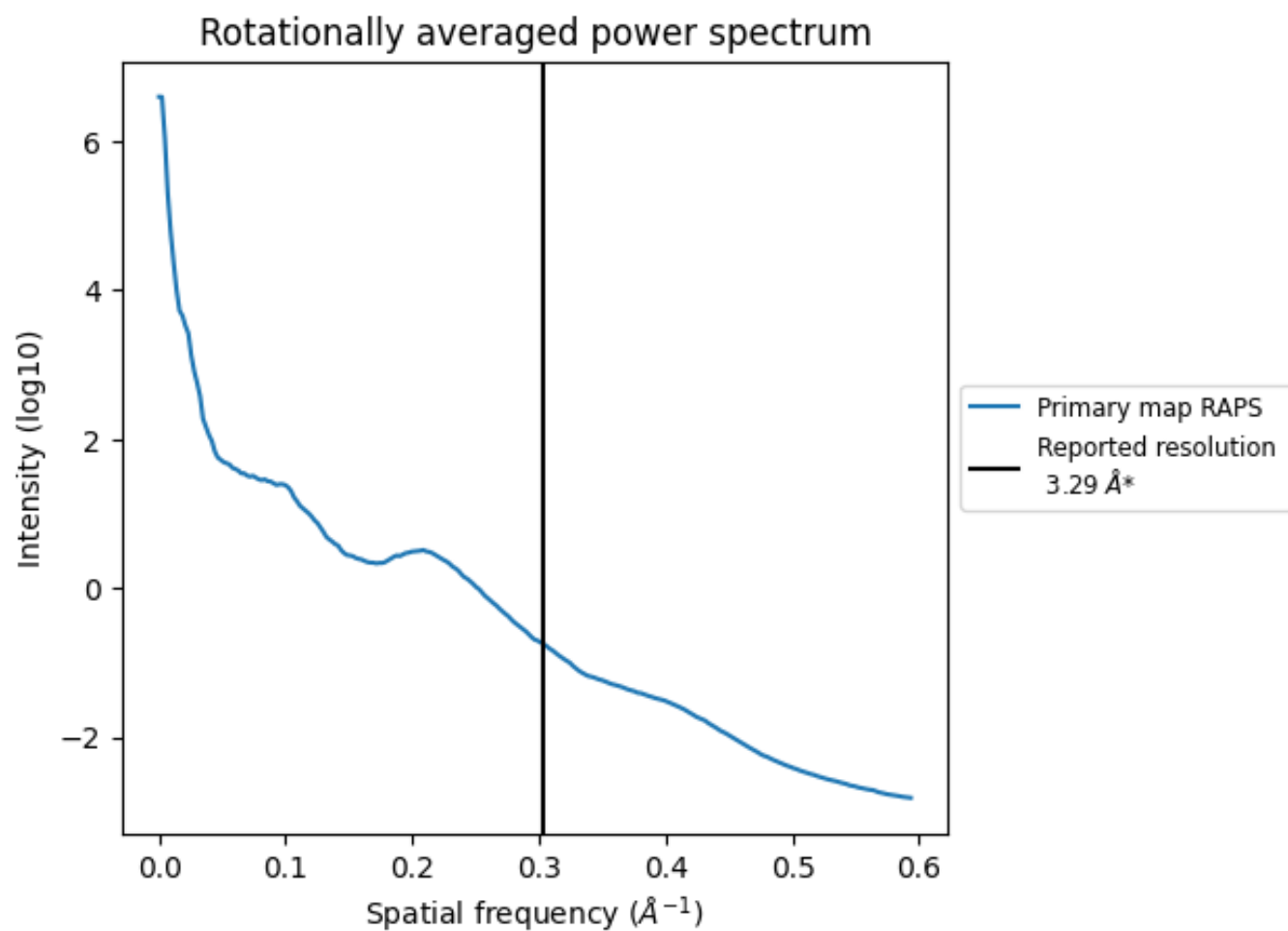
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 906 nm³; this corresponds to an approximate mass of 818 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

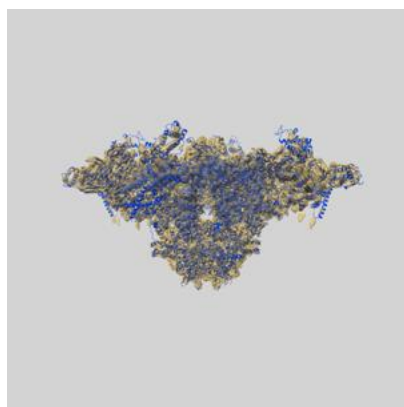
8 Fourier-Shell correlation

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

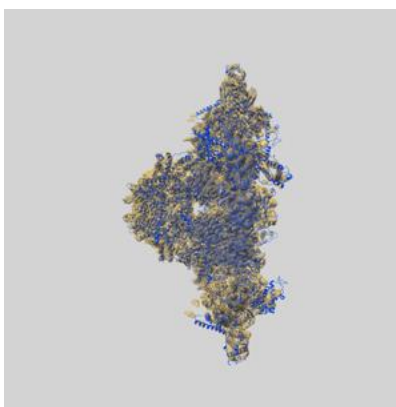
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42765 and PDB model 8UXI. Per-residue inclusion information can be found in section [3](#) on page [7](#).

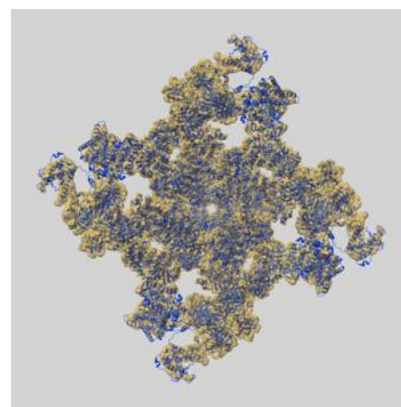
9.1 Map-model overlay [i](#)



X



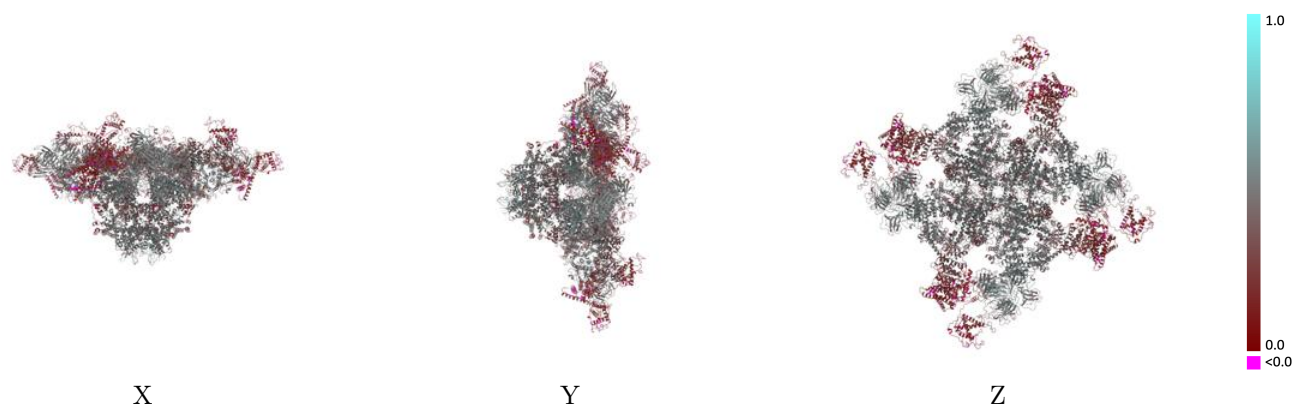
Y



Z

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](#)

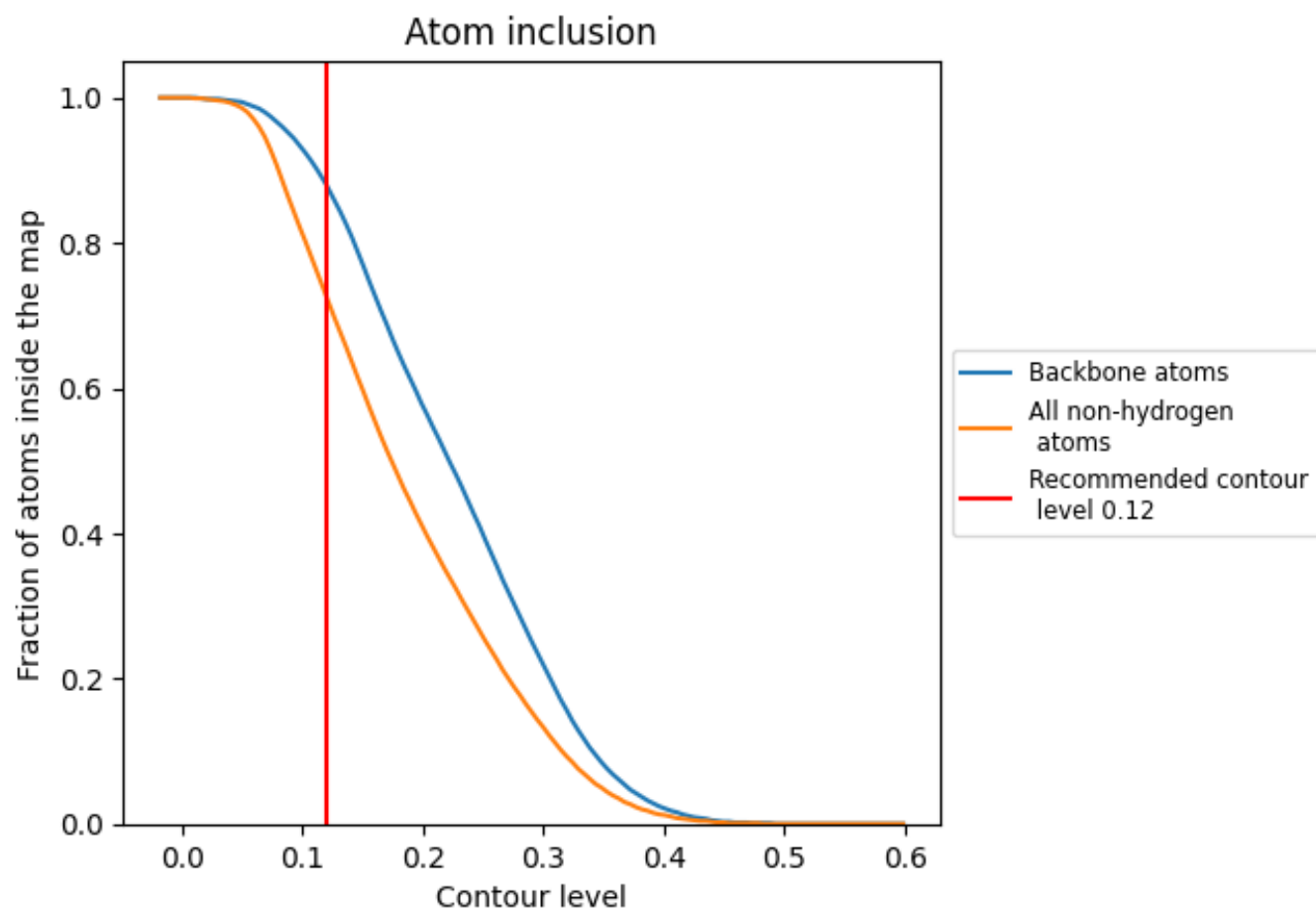


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 88% of all backbone atoms, 73% 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	0.7260	0.3900
A	0.7250	0.3900
B	0.7210	0.3840
C	0.7290	0.3950
D	0.7170	0.3790
E	0.8420	0.4870
F	0.8340	0.4830
G	0.8420	0.4880
H	0.8510	0.4860

1.0

0.0

<0.0