



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 01:52 AM UTC

PDB ID : 9E18 / pdb_00009e18
EMDB ID : EMD-47385
Title : Structure of RyR1 in the primed state in the presence of pentoxifylline
Authors : Miotto, M.C.; Marks, A.R.
Deposited on : 2024-10-21
Resolution : 2.68 Å (reported)
Based on initial model : 7TZC

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:

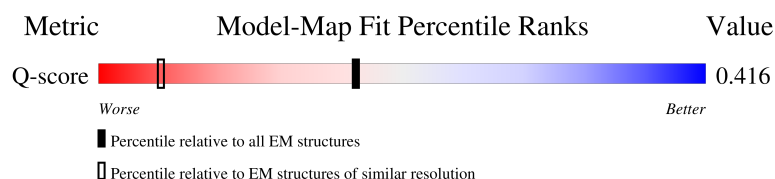
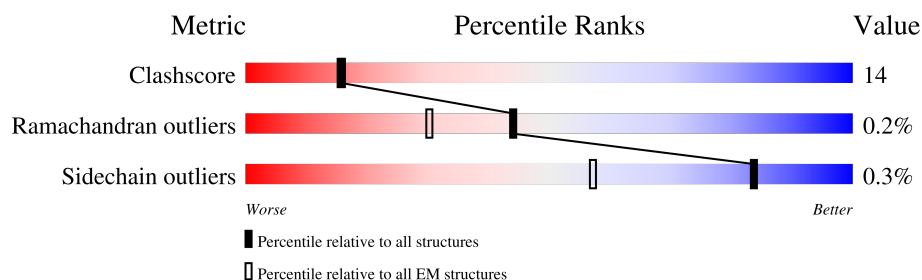
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.68 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	9255 (2.18 - 3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	21% 63% 23% • 13%
1	B	5037	21% 64% 23% • 13%
1	C	5037	21% 64% 23% • 13%
1	D	5037	21% 64% 23% • 13%

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Mol	Chain	Length	Quality of chain
2	E	108	5% 72% 20%
2	F	108	6% 72% 20%
2	G	108	5% 71% 21%
2	H	108	71% 21%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 144144 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	B	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	D	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		
1	C	4404	Total	C	N	O	S	9	0
			35150	22365	6063	6485	237		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	H	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	G	107	Total	C	N	O	S	0	0
			831	527	146	154	4		
2	F	107	Total	C	N	O	S	0	0
			831	527	146	154	4		

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

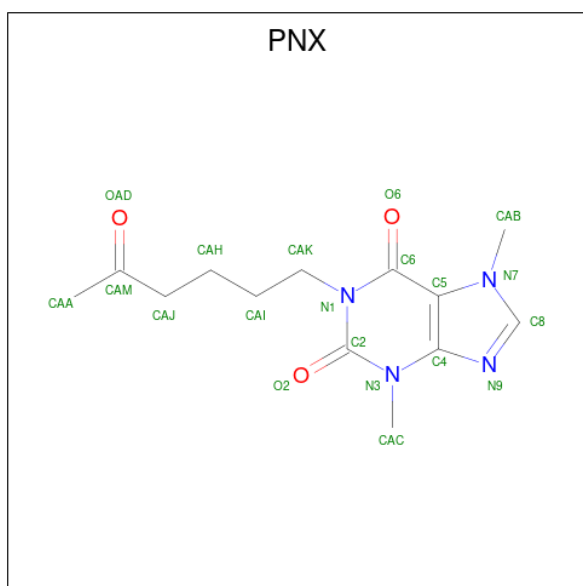
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total Zn 1 1	0

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

- Molecule 6 is 3,7-DIMETHYL-1-(5-OXOHEXYL)-3,7-DIHYDRO-1H-PURINE-2,6-DIONE (CCD ID: PNX) (formula: C₁₃H₁₈N₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			20	13	4	3	
6	B	1	Total	C	N	O	0
			20	13	4	3	
6	D	1	Total	C	N	O	0
			20	13	4	3	
6	C	1	Total	C	N	O	0
			20	13	4	3	

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	2	Total	O	0
			2	2	
7	B	2	Total	O	0
			2	2	

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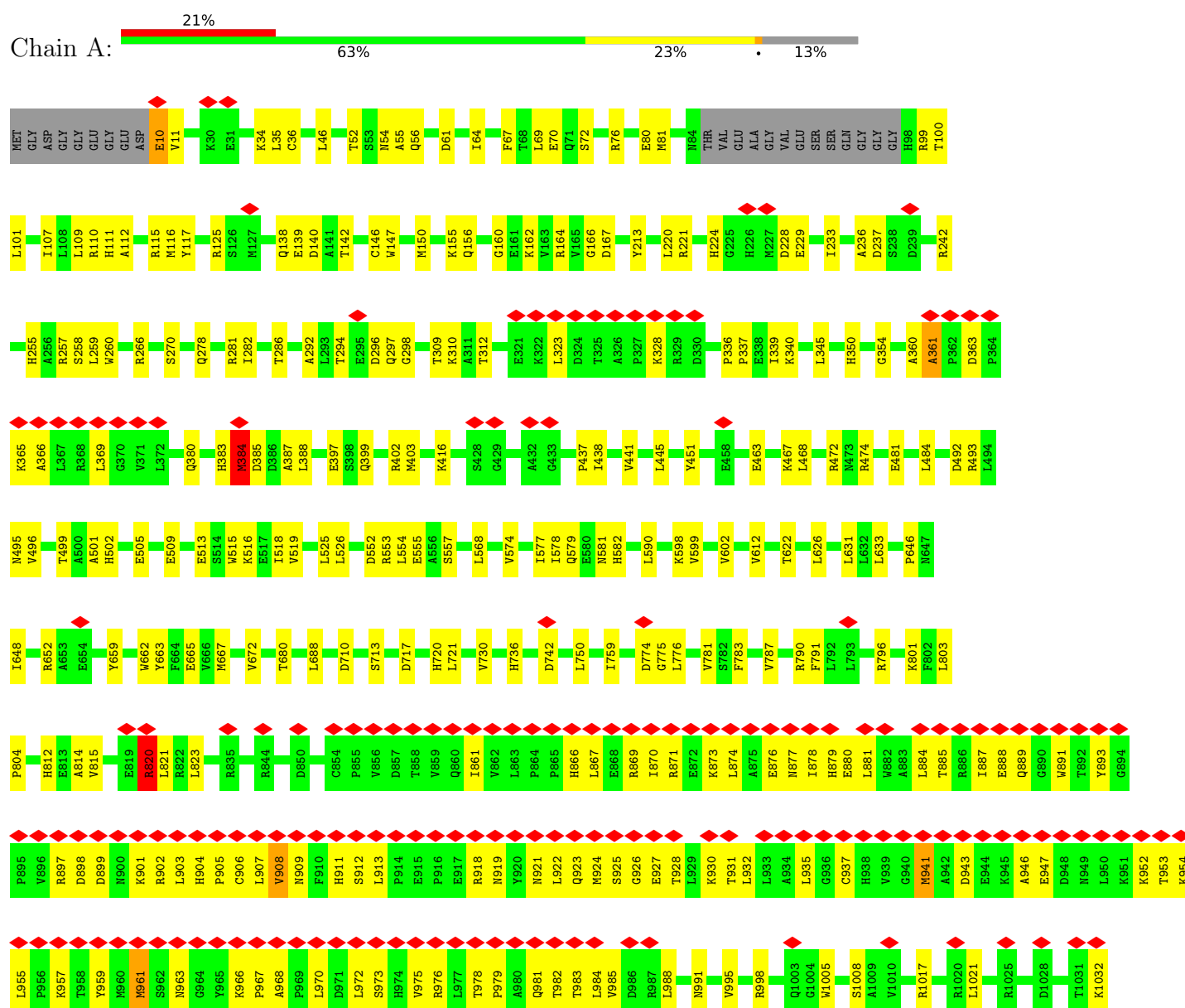
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Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	O	0
			2	2	
7	C	2	Total	O	0
			2	2	

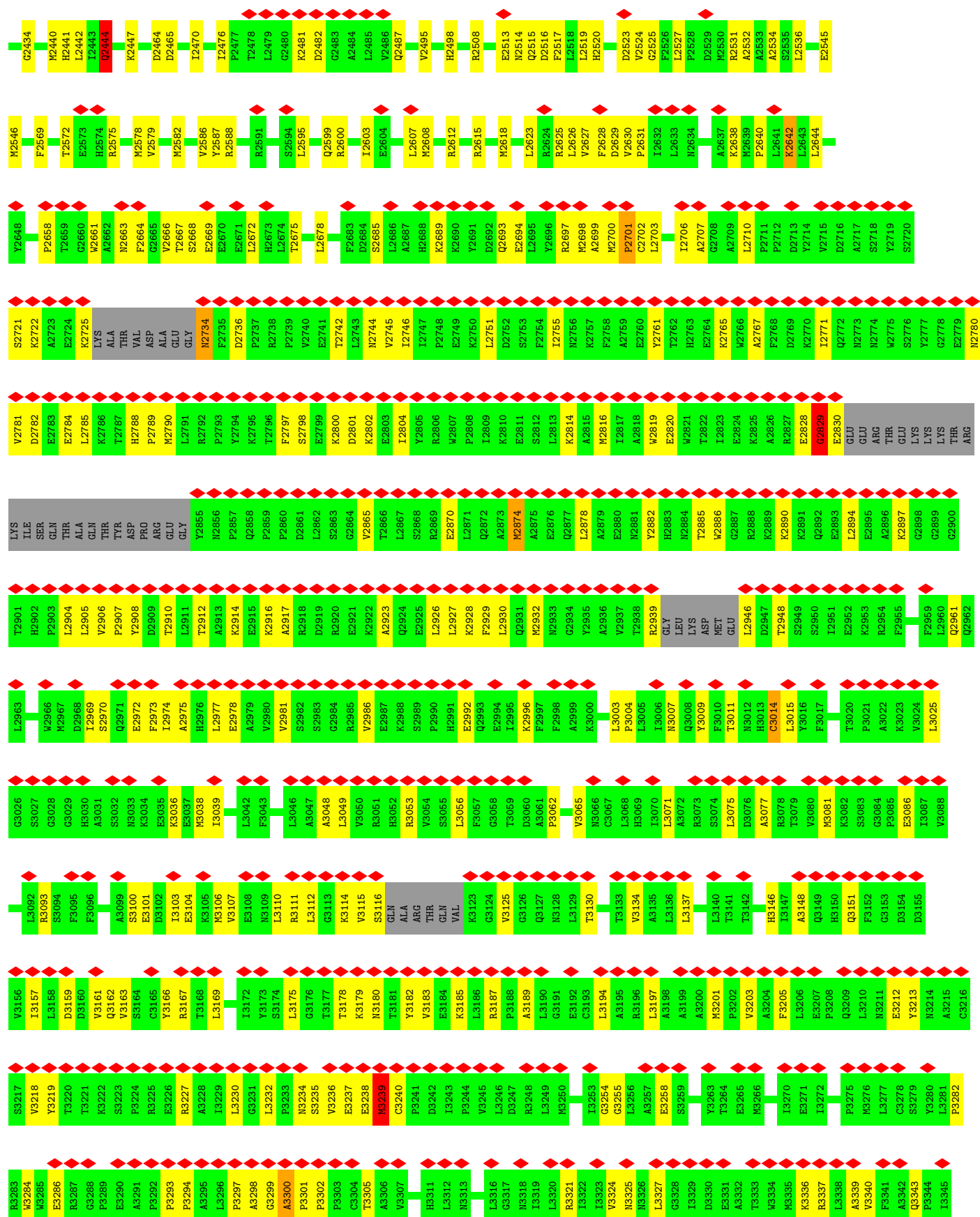
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

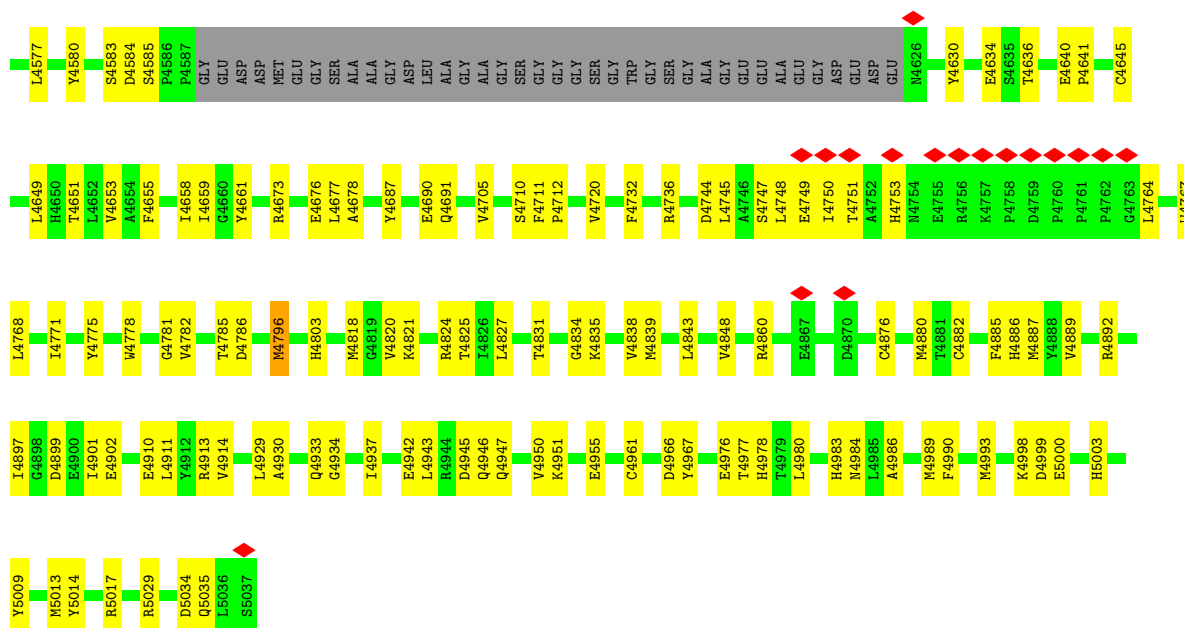
• Molecule 1: Ryanodine receptor 1



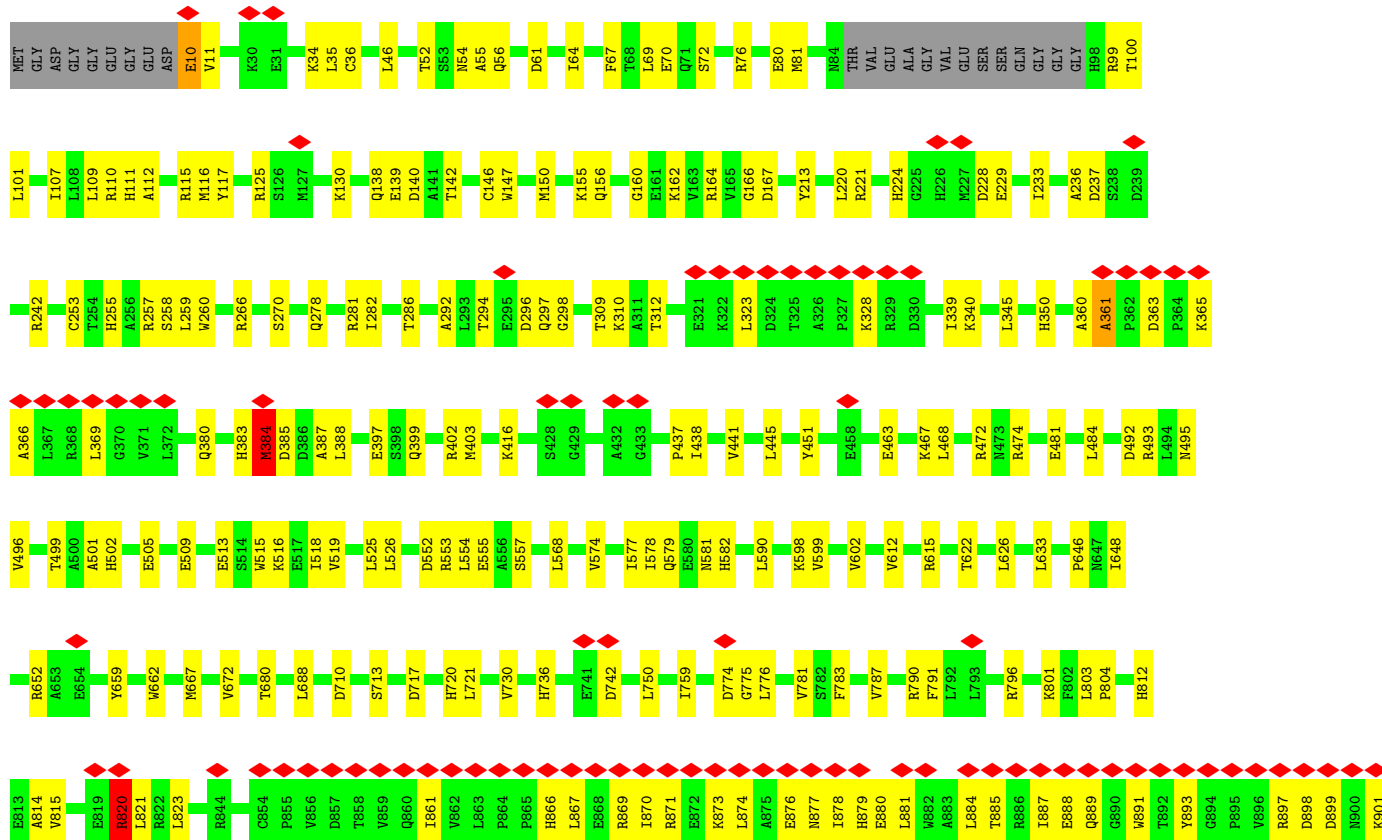
Q2308	M2101	D2017	L1926	G1855	R1727	D1513	ASP	LYS	M1286	H1127	M1035
M2312	Q2107	E2018	L1927	D1858	R1728	L1514	VAL	GLU	R1128	R1127	M1036
L2313	Q2107	E2019	Q1928	V1859	M1729	V1515	VAL	THR	W1132		D1037
Y2318	V2117	D2020	M1929	I1866	L1731	A1531	ALA	PRO	P1142		S1038
P2319	M2120	C2021	L1931	E1873	S1732	E1535	D1419	GLY	W1143		L1039
D2320	F2121	R2028	V1935	E1874	E1733	S1536	M1420	THR	D1147		C1040
E2329	S2122	A2040	M1939		T1742	M1537	R1421	GLN			Q1041
R2330	L2123	Q2045	L1943	GLU	R1743	V1552	D1423	PRO	M1152		A1042
D2333	L2135	L2046	E1944	GLU	F1748	F1553	P1424	VAL	I1153		V1043
A2350	P2146	GLY	A1960	GLU	F1749	V1554	T1427	GLU	L1154		R1044
R2351	V2149	GLU	F1961	GLU	P1750	Q1559	L1428	ALA	L1155		T1045
V2352	V2149	GLU	A1962	GLU	G1751	M1560	M1429	GLN	T1156		L1046
V2353	E2157	GLU	Y1965	GLU	R1752	V1561	T1430	VAL	E1157		L1047
V2354	E2157	GLU	V1966	GLU	K1753	Q1562	Y1434	ARG	M1170		G1048
V2355	Q2161	GLU	D1967	GLU	G1754	Q1563	Y1435	ALA	S1171		Y1049
R2369	L2165	GLU	K1968	GLU	F1755	F1564	S1436	PRO	D1172		G1050
C2373	L2167	THR	L1969	GLU	N1756	E1565	F1440	GLY	S1173		Y1051
S2374	I2167	GLU	Q1973	GLU	A1757	K1568	A1441	ASN	G1174		N1052
G2375	R1974	GLU	R1974	GLU	P1787	Q1569	T1454	LYS	S1175		I1053
L2376	S1975	ASP	S1975	ASP	A1788	K1570	T1454	ALA	E1176		E1054
L2377	L2170	GLU	L1979	GLU	A1789	N1571	D1456	THR	E1181		P1055
L2377	L2177	GLU	L1980	GLU	A1789	I1572	D1456	GLU	I1182		P1056
A2378	L2182	GLU	M1981	LYS	G1790	A1577	D1461	LYS	D1186		D1057
E2382	I2182	GLU	R1982	GLU	V1791	R1584	F1464	ARG	Q1058		Q1058
R2385	I2185	LEU	A1983	ASP	A1792	P1593	K1468	ALA	E1059		E1059
R2392	M2186	GLU	F1984	GLU	E1793	M1599	V1469	GLY	P1060		P1060
D2393	V2190	THR	T1985	GLU	A1794	M1599	R1470	PRO	S1061		S1061
G2396	F2191	VAL	T1985	GLU	L1804	P1602	M1476	PRO	Q1062		Q1062
V2397	Y2192	ARG	M1986	GLU	A1806	V1603	G1477	ASP	V1063		V1063
G2396	Q2193	LEU	S1987	GLU	L1807	V1603	M1476	ASP	E1064		E1064
V2397	H2194	VAL	A1988	LYS	A1806	R1619	D1478	TYR	N1065		N1065
ARG	P2195	LYS	A1989	ASP	R1808	R1619	E1479	GLU	Q1066		Q1066
ASP	L2197	LYS	E1990	ALA	D1809	V1626	E1479	ASN	S1067		S1067
ASP	L2197	LYS	E1990	ALA	K1810	L1639	G1481	LEU	R1068		R1068
ARG	N2198	GLU	T1991	LYS	A1811	L1639	M1482	ARG	W1069		W1069
ARG	R2199	LYS	A1992	GLU	L1812	L1676	H1484	SER	D1070		D1070
GLU	A2200	PRO	R1993	GLU	R1813	L1676	H1484	ALA	R1071		R1071
HIS	L2201	GLU	R1994	GLU	M1814	R1680	G1497	GLY	V1072		V1072
PHE	G2202	GLU	T1995	ALA	V1819	R1680	G1497	TRP	A1077		A1077
GLY	H2204	LEU	R1996	PRO	R1820	A1684	V1501	GLY	Q1084		Q1084
GLU	E2205	ALA	E1997	GLY	D1821	L1694	S1502	ALA	D1263		D1263
GLU	M2208	ALA	R1999	GLU	G1822	L1694	P1503	GLY	V1264		V1264
F2410	M2211	GLU	S2000	LYS	D1828	L1698	G1504	LEU	D1265		D1265
P2411	V2212	E2088	P2001	ASP	S1833	G1705	Q1505	ARG	T1266		T1266
P2411	V2212	K2089	Q2005	L1922	F1836	Y1712	Q1506	LYS	L1272		L1272
E2412	N2213	K2090	Q2006	E1923	Q1837	Y1712	G1507	GLY	R1275		R1275
E2413	V2214	P2091	I2006	E1924	P1840	S1726	R1508	LEU	Q1280		Q1280
N2414	G2216	Q2092	H2011	E1925	I1853		T1509	THR	D1281		D1281
L2418		V2098	D2014		E2015		H1511	ALA	V1112		V1112
Y2426			A2016		F1854		T1512		E1113		E1113
									L1115		L1115
									V1123		V1123
									G1126		G1126







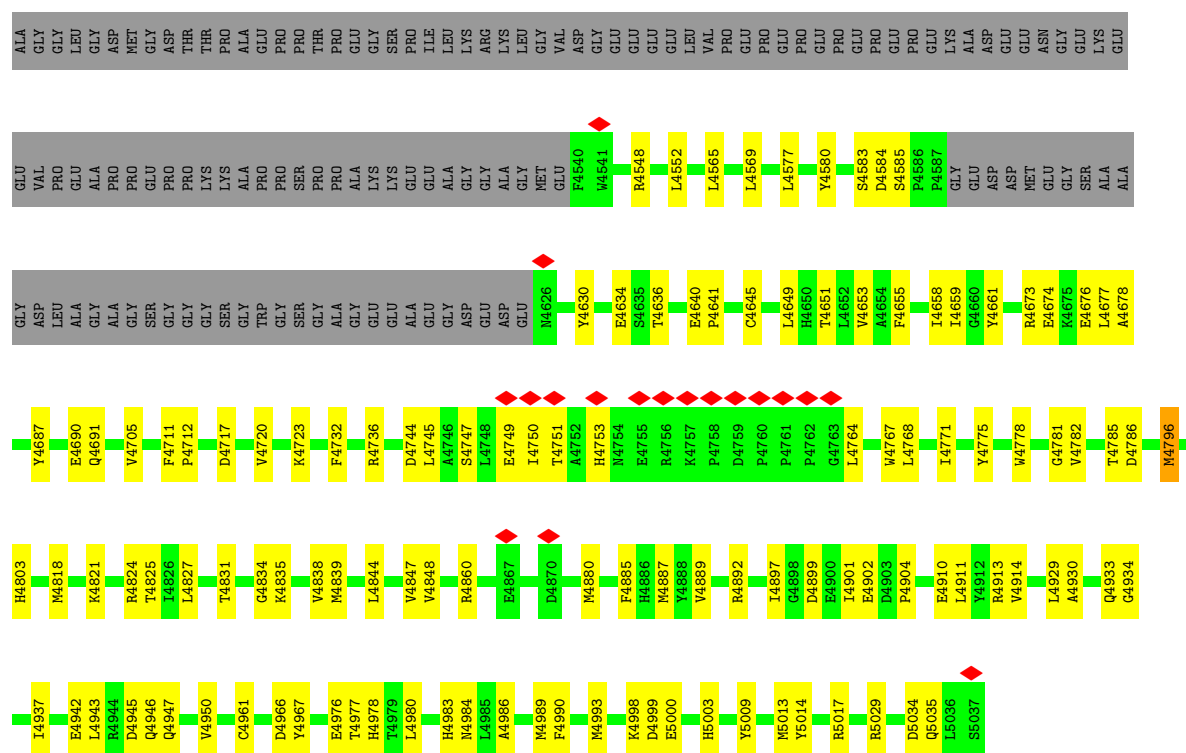
• Molecule 1: Ryanodine receptor 1



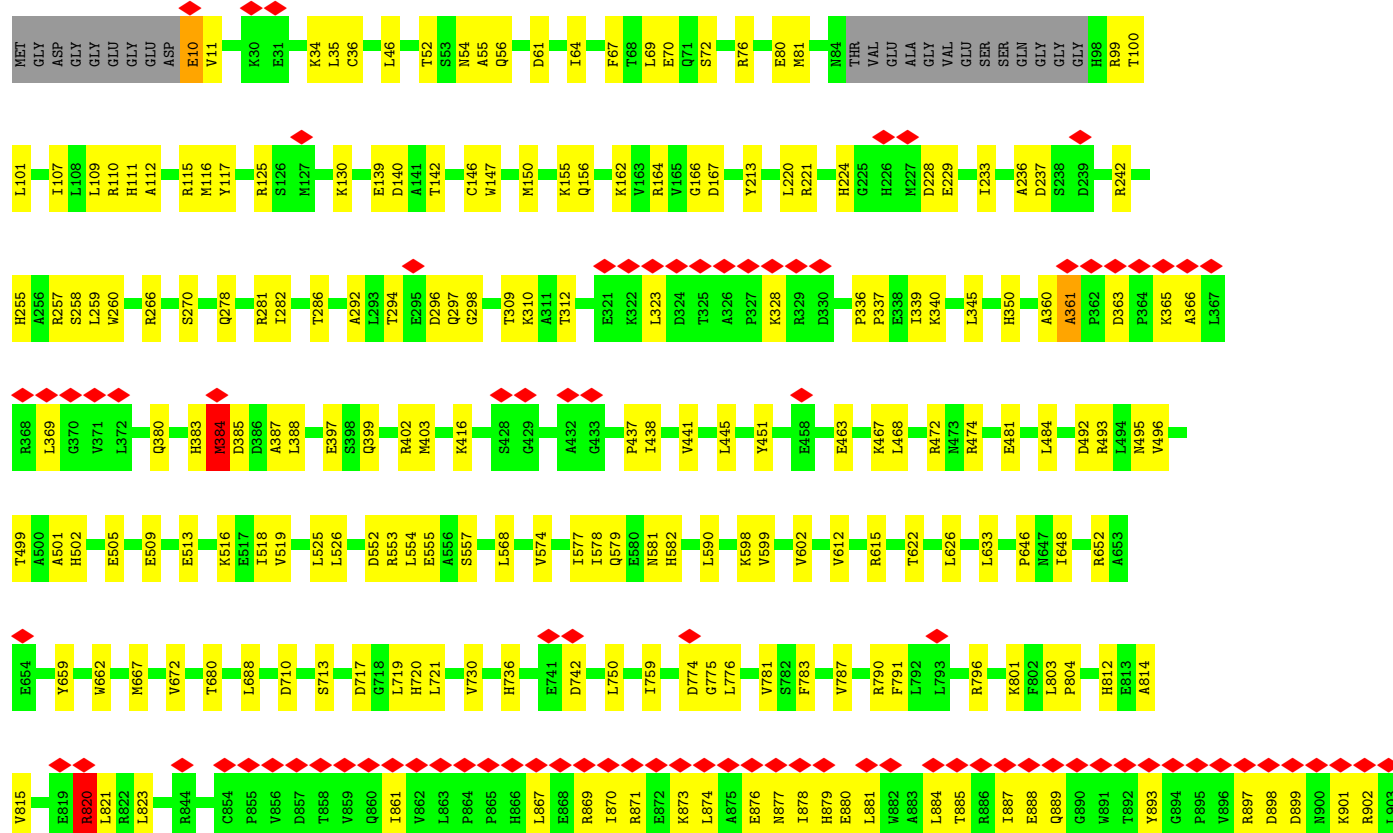








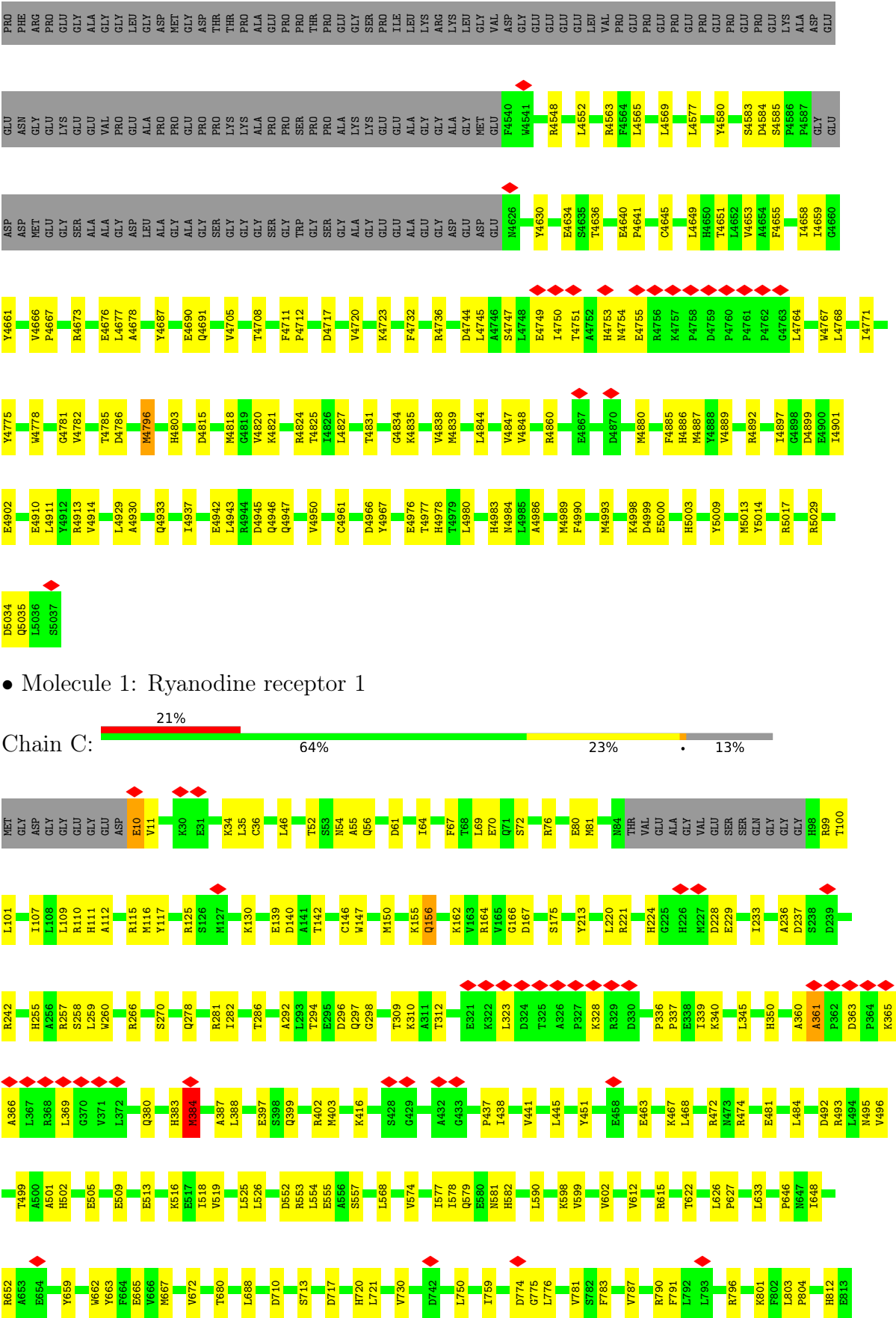
• Molecule 1: Ryanodine receptor 1







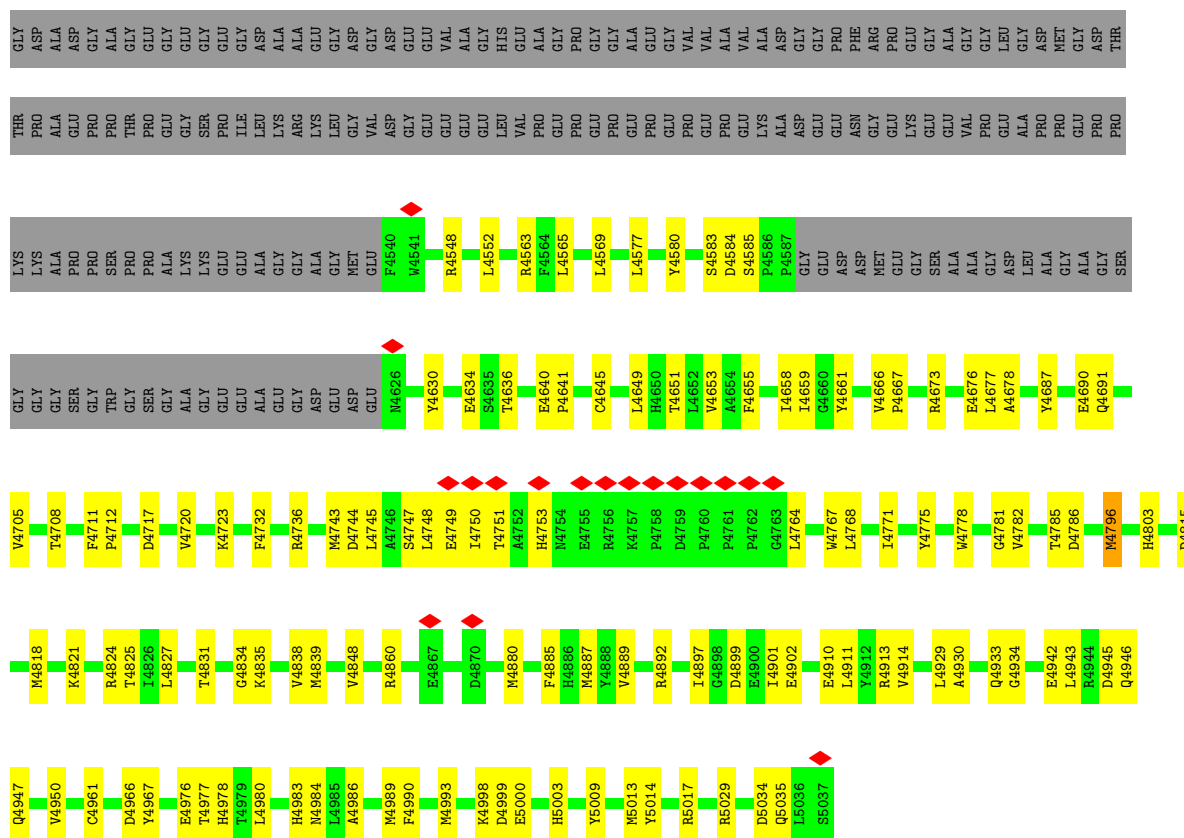




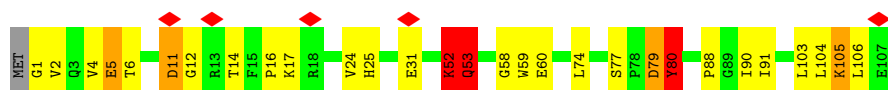




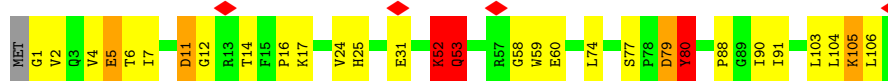




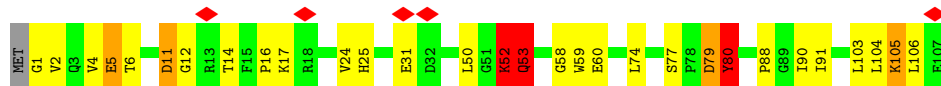
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1A



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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	64353	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.555	Depositor
Minimum map value	-0.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.022	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	428.544, 428.544, 428.544	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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, PNx, CA, 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	0.48	61/35977 (0.2%)	0.57	65/48726 (0.1%)
1	B	0.48	61/35977 (0.2%)	0.57	65/48726 (0.1%)
1	C	0.48	61/35977 (0.2%)	0.57	66/48726 (0.1%)
1	D	0.48	61/35977 (0.2%)	0.57	65/48726 (0.1%)
2	E	1.69	18/850 (2.1%)	2.45	24/1146 (2.1%)
2	F	1.69	18/850 (2.1%)	2.45	24/1146 (2.1%)
2	G	1.69	18/850 (2.1%)	2.45	24/1146 (2.1%)
2	H	1.69	18/850 (2.1%)	2.45	24/1146 (2.1%)
All	All	0.54	316/147308 (0.2%)	0.67	357/199488 (0.2%)

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	14
1	B	0	14
1	C	0	14
1	D	0	14
2	E	0	5
2	F	0	5
2	G	0	5
2	H	0	5
All	All	0	76

The worst 5 of 316 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	80	TYR	CD1-CE1	23.90	2.10	1.38
2	F	80	TYR	CD1-CE1	23.89	2.10	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	80	TYR	CD1-CE1	23.88	2.10	1.38
2	G	80	TYR	CD1-CE1	23.86	2.10	1.38
1	D	1036	ARG	CZ-NH1	-20.77	1.03	1.32

The worst 5 of 357 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	80	TYR	CE1-CZ-CE2	-44.72	30.86	120.30
2	F	80	TYR	CE1-CZ-CE2	-44.71	30.88	120.30
2	G	80	TYR	CE1-CZ-CE2	-44.71	30.89	120.30
2	E	80	TYR	CE1-CZ-CE2	-44.70	30.90	120.30
2	H	80	TYR	CD1-CG-CD2	-32.83	68.86	118.10

There are no chirality outliers.

5 of 76 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1035	ASN	Peptide
1	A	1036	ARG	Sidechain,Mainchain
1	A	1051	TYR	Sidechain
1	A	1128	ARG	Sidechain
1	A	820	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	35150	0	34792	1042	0
1	B	35150	0	34792	1033	0
1	C	35150	0	34792	1024	0
1	D	35150	0	34792	1035	0
2	E	831	0	831	24	0
2	F	831	0	831	25	0
2	G	831	0	831	25	0
2	H	831	0	831	24	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	20	0	18	3	0
6	B	20	0	18	3	0
6	C	20	0	18	3	0
6	D	20	0	18	3	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	144144	0	142612	4151	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 14.

The worst 5 of 4151 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:941:MET:HE1	1:D:1051:TYR:CD1	1.45	1.52
1:B:941:MET:HE1	1:B:1051:TYR:CD1	1.45	1.50
1:C:941:MET:HE1	1:C:1051:TYR:CD1	1.45	1.50
1:A:941:MET:HE1	1:A:1051:TYR:CD1	1.45	1.49
1:D:3239:MET:CG	1:D:3239:MET:SD	2.09	1.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	43	65
1	B	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	43	65
1	C	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	43	65
1	D	4385/5037 (87%)	4268 (97%)	109 (2%)	8 (0%)	43	65
2	E	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	F	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	G	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
2	H	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	17960/20580 (87%)	17480 (97%)	448 (2%)	32 (0%)	44	65

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	908	VAL
1	A	2829	GLY
1	A	3239	MET
1	A	3300	ALA
1	B	908	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	3836/4276 (90%)	3825 (100%)	11 (0%)	86	94
1	B	3836/4276 (90%)	3825 (100%)	11 (0%)	86	94
1	C	3836/4276 (90%)	3824 (100%)	12 (0%)	86	94
1	D	3836/4276 (90%)	3824 (100%)	12 (0%)	86	94
2	E	89/90 (99%)	89 (100%)	0	100	100
2	F	89/90 (99%)	89 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	89/90 (99%)	89 (100%)	0	100	100
2	H	89/90 (99%)	89 (100%)	0	100	100
All	All	15700/17464 (90%)	15654 (100%)	46 (0%)	84	94

5 of 46 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2444	GLN
1	C	820	ARG
1	D	2870[A]	GLU
1	D	3239	MET
1	C	1559	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 141 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1130	GLN
1	C	1824	GLN
1	C	3605	HIS
1	B	1938	GLN
1	B	1824	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 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	$\# Z > 2$
6	PNX	A	5304	-	21,21,21	0.38	0	30,30,30	0.53	0
3	ATP	D	5301	-	32,33,33	0.30	0	48,52,52	0.77	2 (4%)
3	ATP	C	5301	-	32,33,33	0.30	0	48,52,52	0.77	2 (4%)
6	PNX	C	5304	-	21,21,21	0.39	0	30,30,30	0.52	0
3	ATP	A	5301	-	32,33,33	0.30	0	48,52,52	0.77	2 (4%)
3	ATP	B	5301	-	32,33,33	0.30	0	48,52,52	0.77	2 (4%)
6	PNX	D	5304	-	21,21,21	0.38	0	30,30,30	0.53	0
6	PNX	B	5304	-	21,21,21	0.38	0	30,30,30	0.53	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
6	PNX	A	5304	-	-	5/7/7/7	0/2/2/2
3	ATP	D	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	C	5301	-	-	6/22/38/38	0/3/3/3
6	PNX	C	5304	-	-	5/7/7/7	0/2/2/2
3	ATP	A	5301	-	-	6/22/38/38	0/3/3/3
3	ATP	B	5301	-	-	6/22/38/38	0/3/3/3
6	PNX	D	5304	-	-	5/7/7/7	0/2/2/2
6	PNX	B	5304	-	-	5/7/7/7	0/2/2/2

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(°)
3	D	5301	ATP	O3'-C3'-C4'	-2.09	105.09	111.08
3	C	5301	ATP	O3'-C3'-C4'	-2.07	105.12	111.08
3	A	5301	ATP	O3'-C3'-C4'	-2.07	105.13	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	5301	ATP	O3'-C3'-C4'	-2.06	105.15	111.08
3	C	5301	ATP	O3'-C3'-C2'	-2.05	105.25	111.82

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

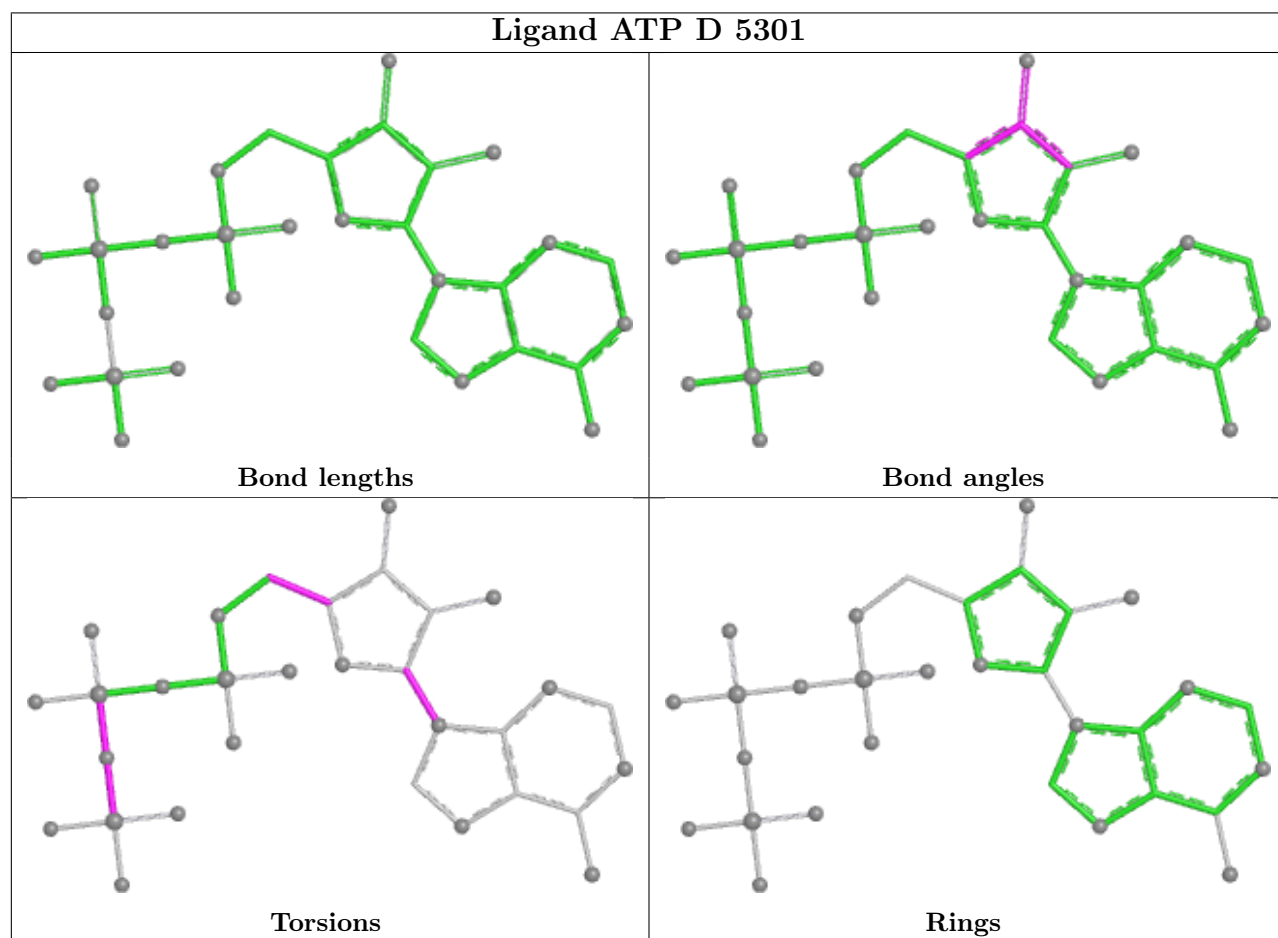
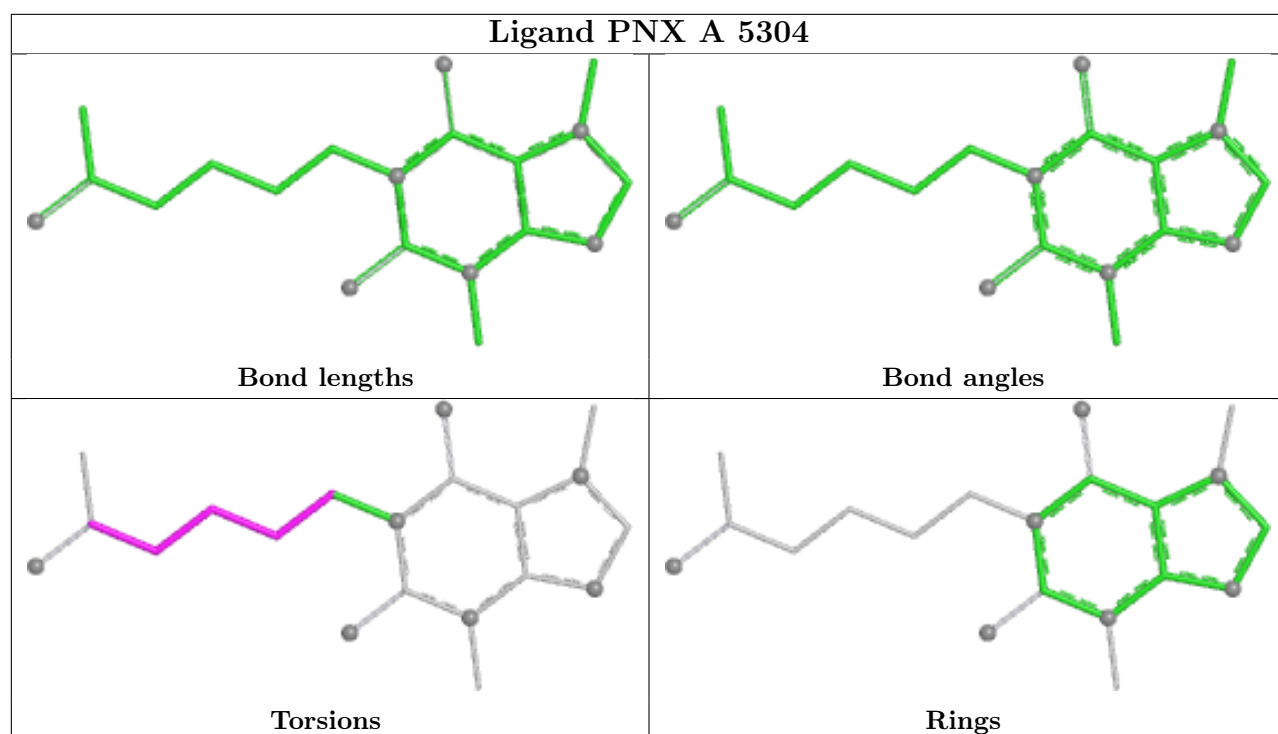
Mol	Chain	Res	Type	Atoms
3	A	5301	ATP	PB-O3B-PG-O3G
3	B	5301	ATP	PB-O3B-PG-O3G
3	D	5301	ATP	PB-O3B-PG-O3G
3	C	5301	ATP	PB-O3B-PG-O3G
6	B	5304	PNX	CAH-CAI-CAK-N1

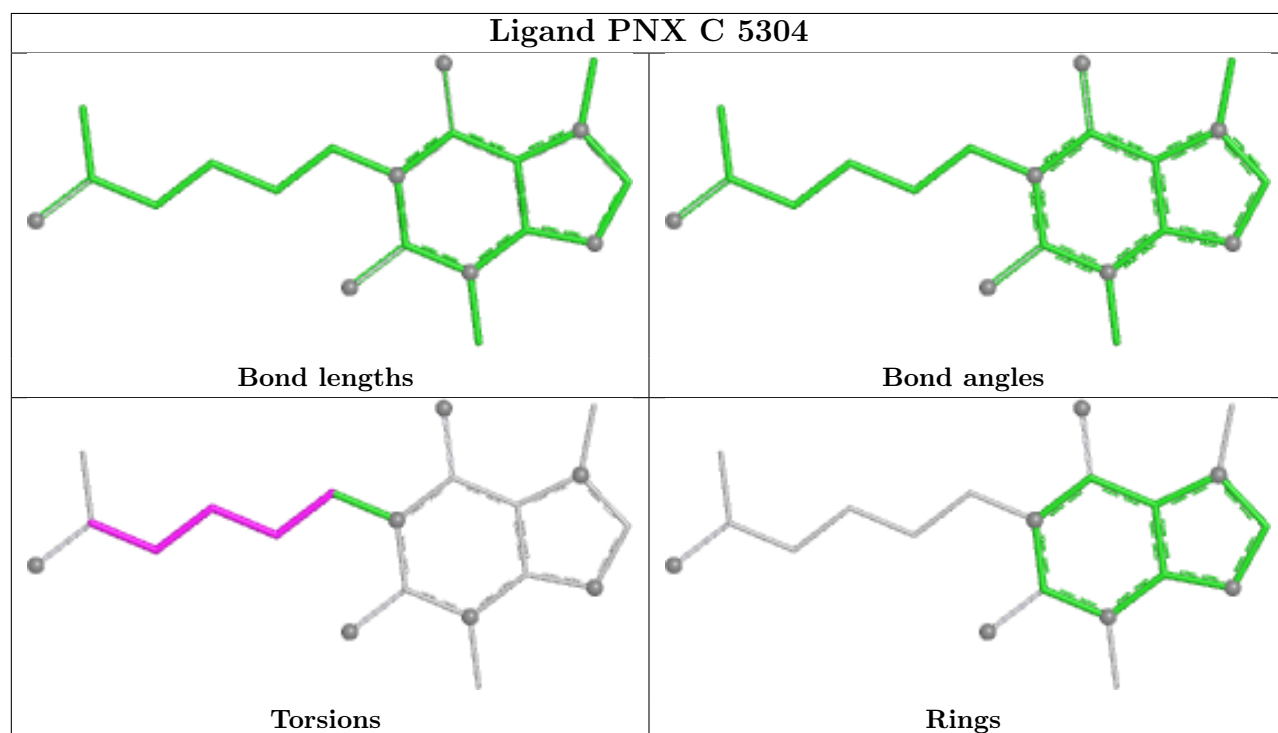
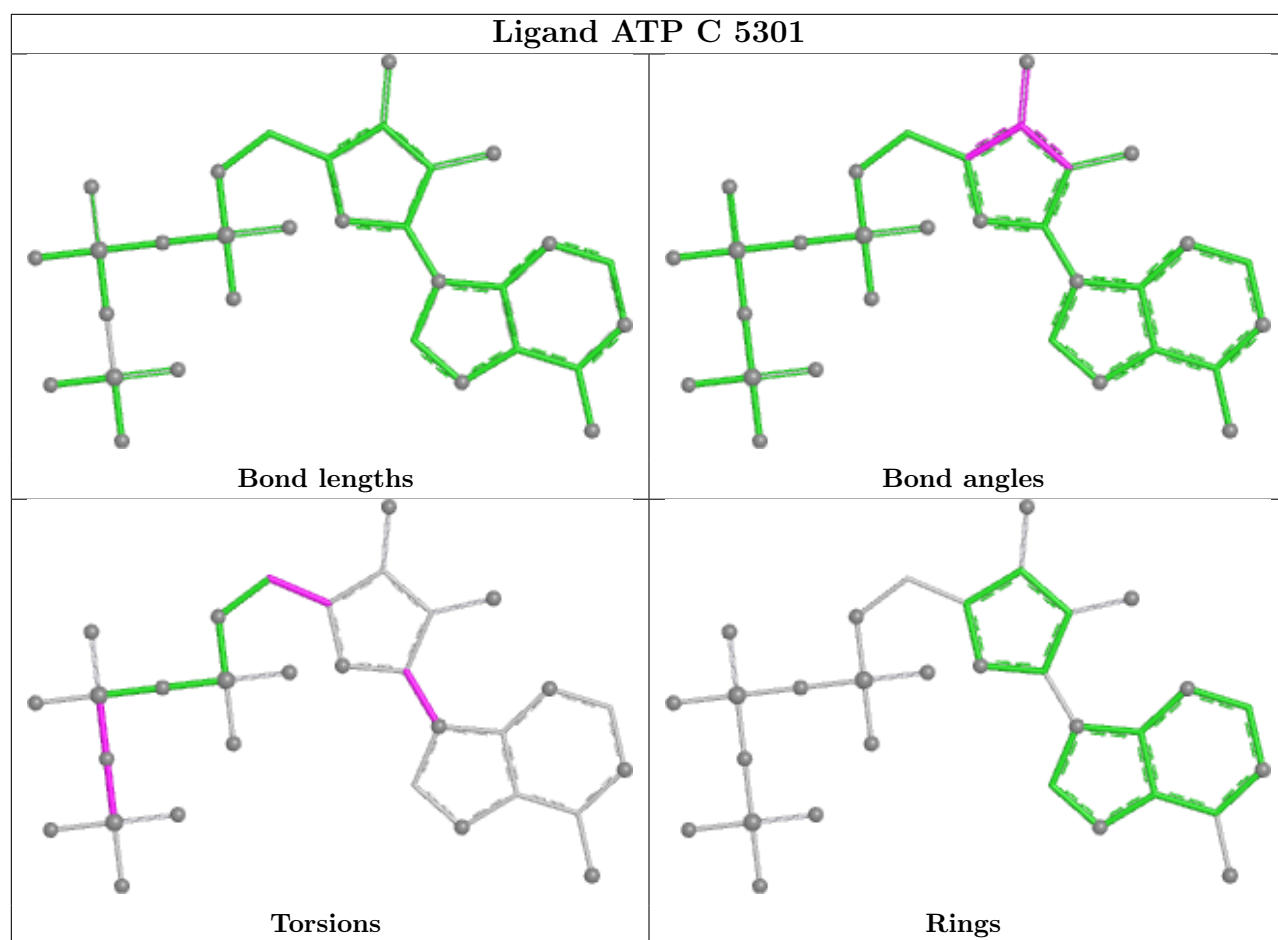
There are no ring outliers.

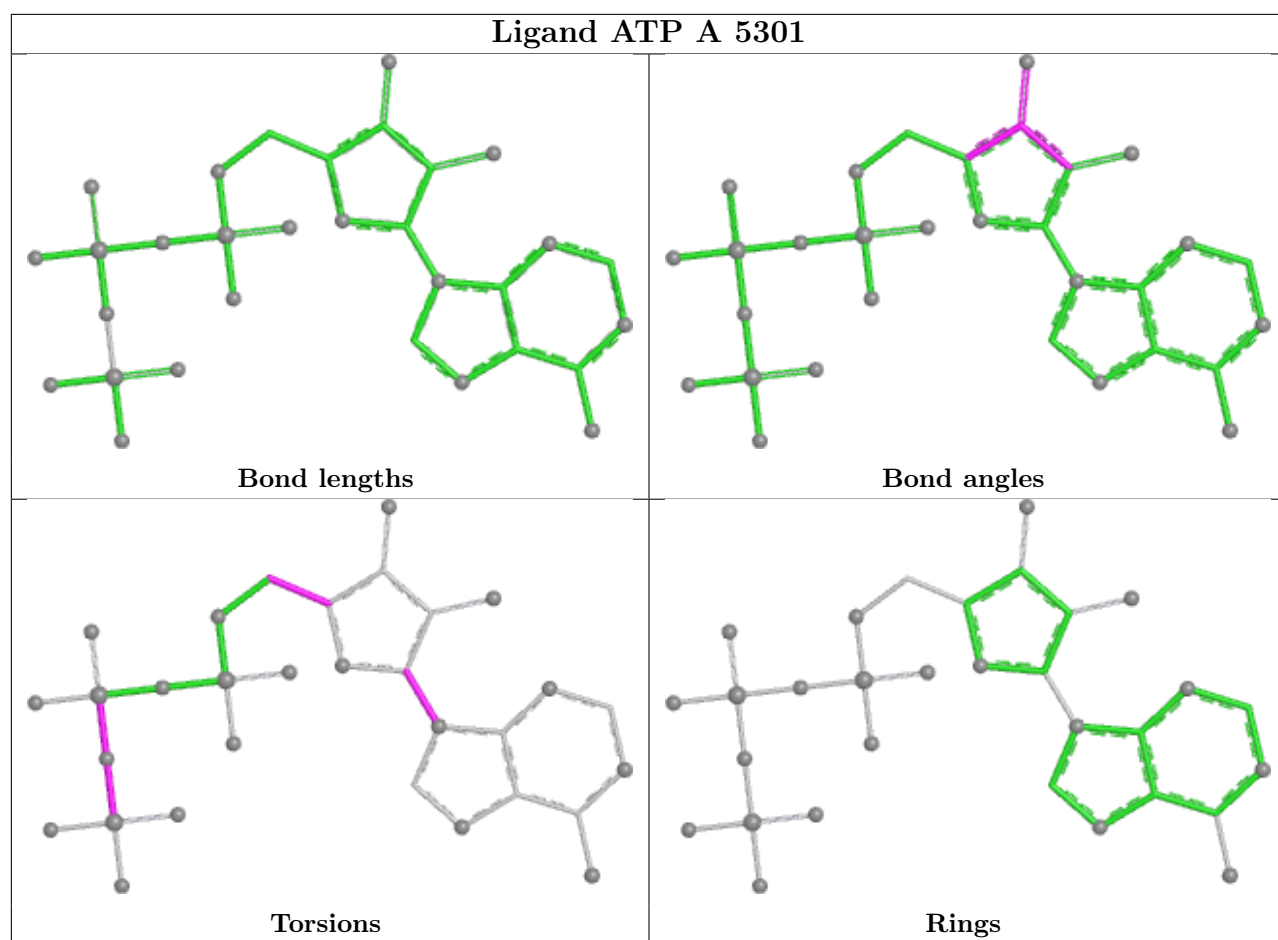
4 monomers are involved in 12 short contacts:

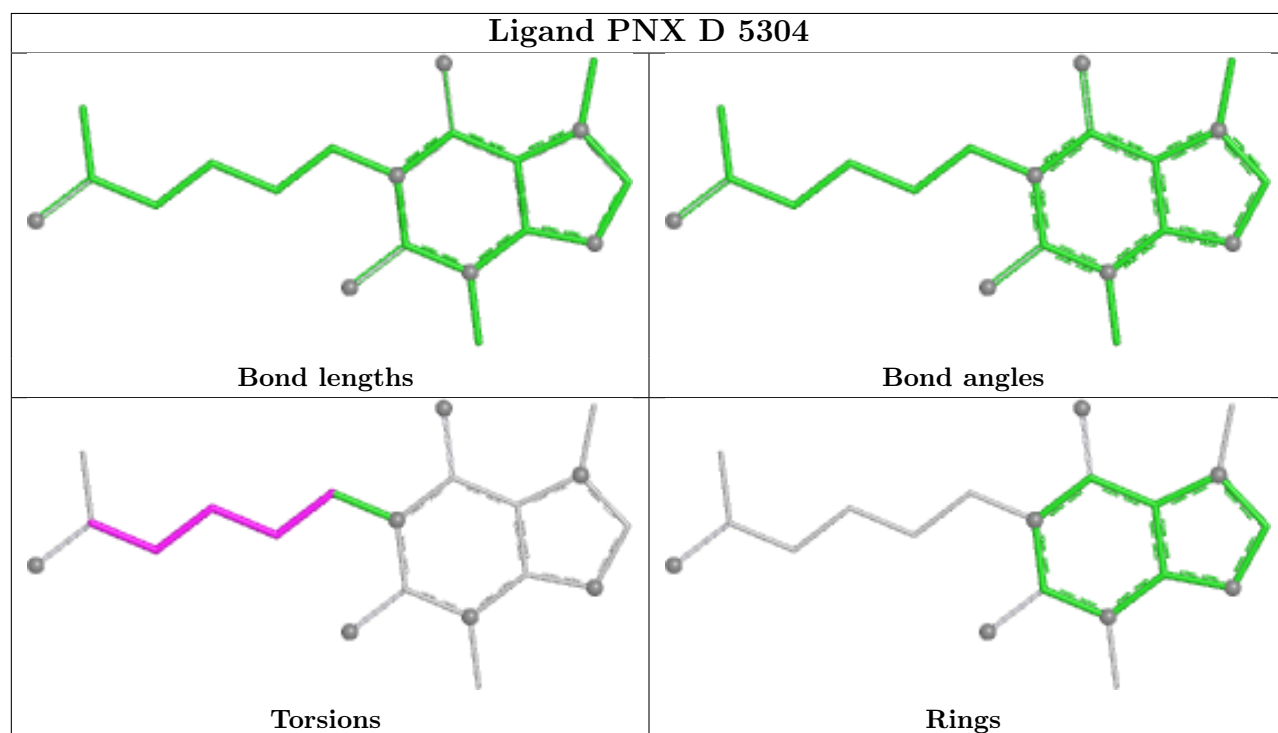
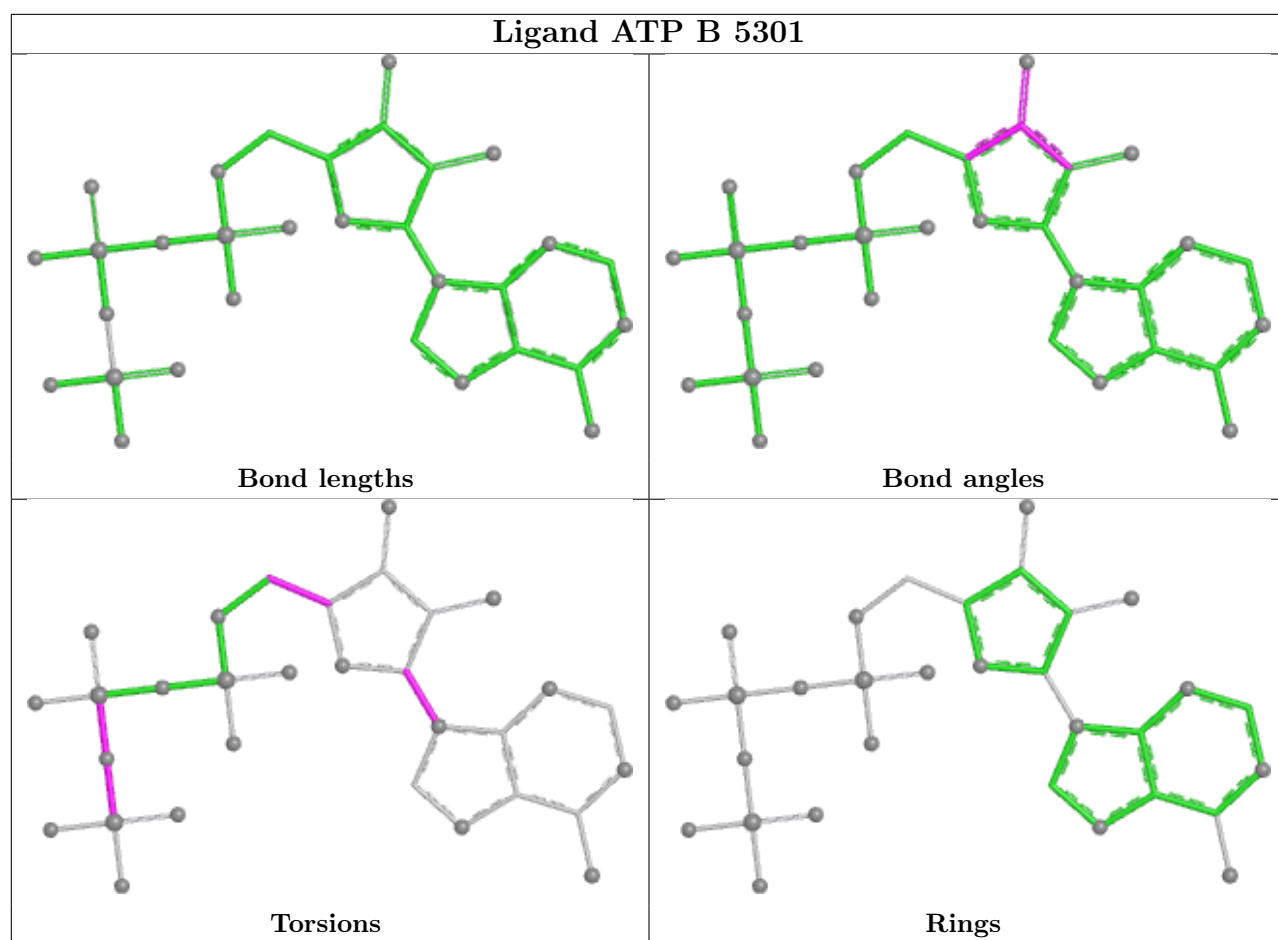
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	5304	PNX	3	0
6	C	5304	PNX	3	0
6	D	5304	PNX	3	0
6	B	5304	PNX	3	0

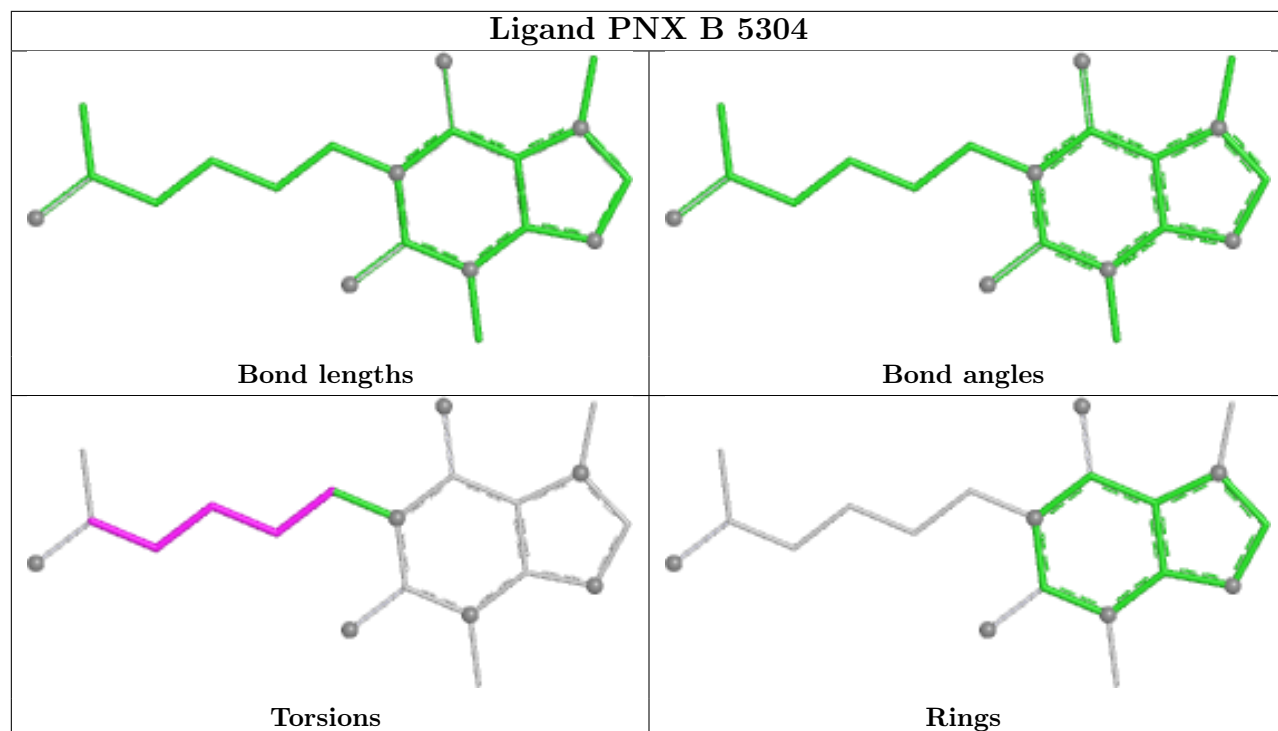
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

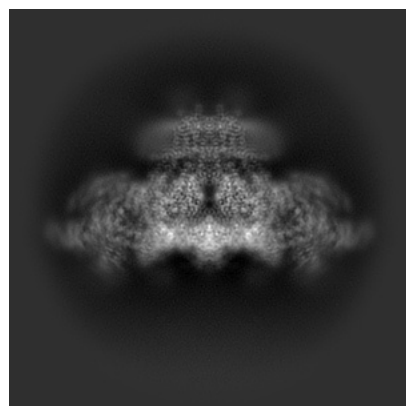
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47385. These allow visual inspection of the internal detail of the map and identification of artifacts.

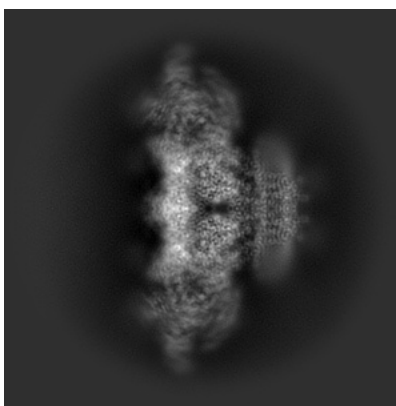
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

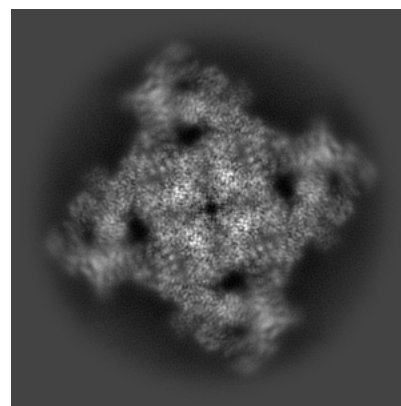
6.1.1 Primary map



X

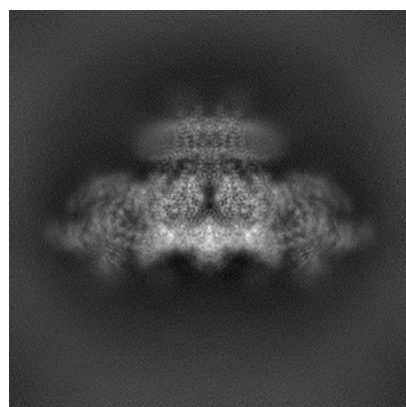


Y

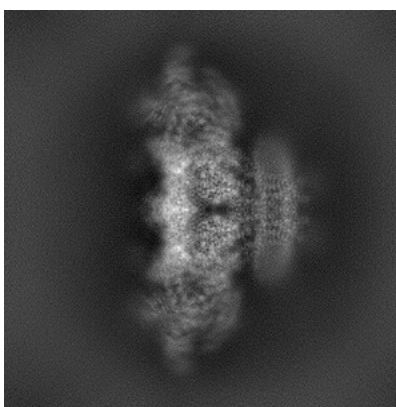


Z

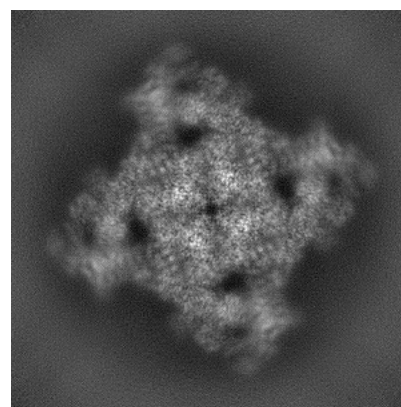
6.1.2 Raw map



X



Y

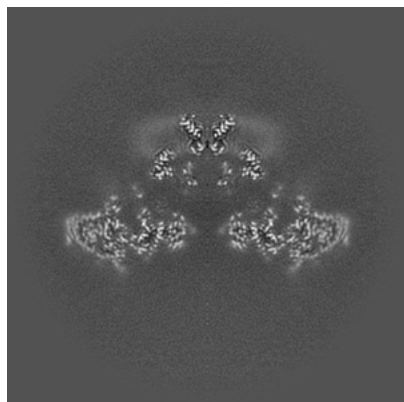


Z

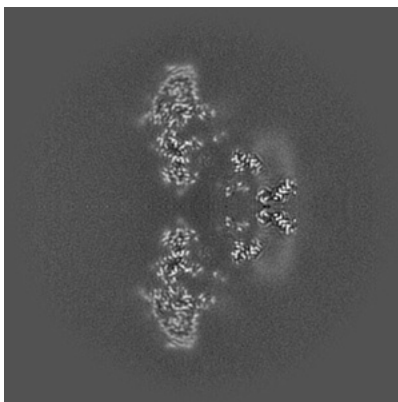
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

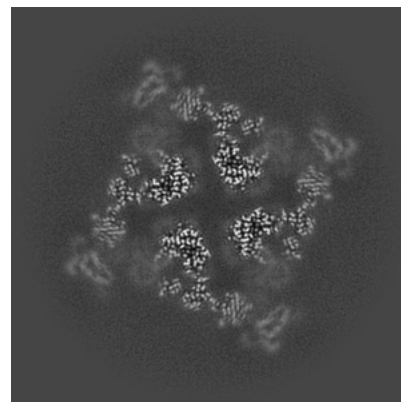
6.2.1 Primary map



X Index: 256

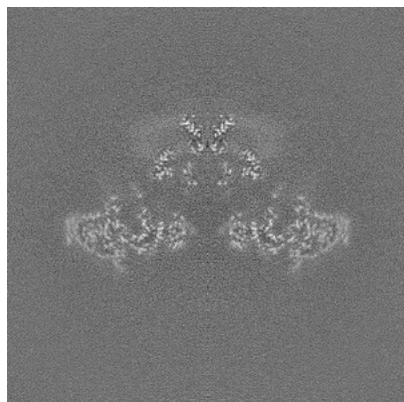


Y Index: 256

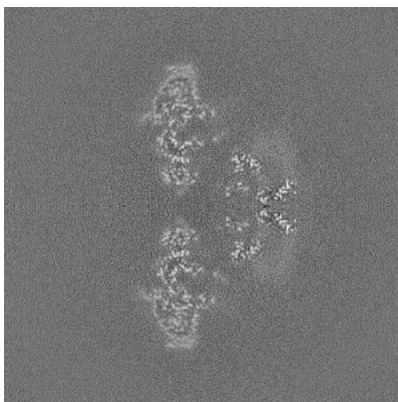


Z Index: 256

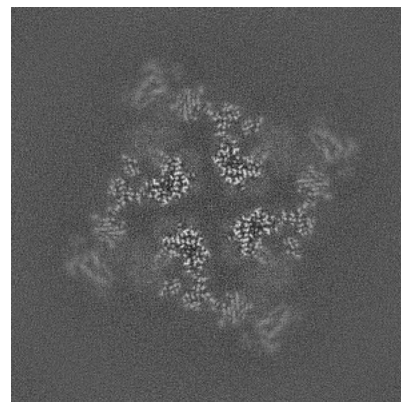
6.2.2 Raw map



X Index: 256



Y Index: 256

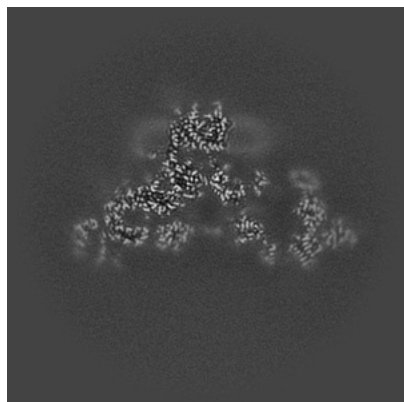


Z Index: 256

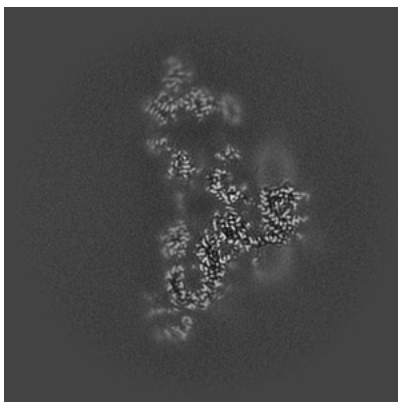
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

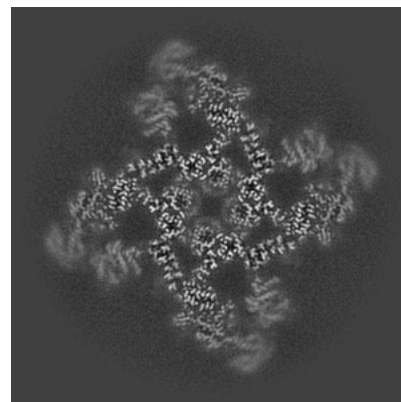
6.3.1 Primary map



X Index: 239

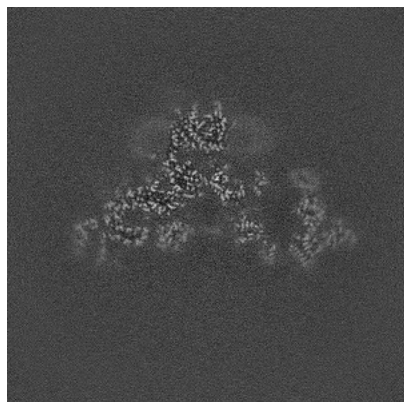


Y Index: 273



Z Index: 229

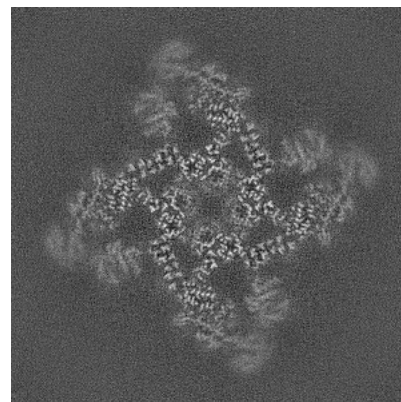
6.3.2 Raw map



X Index: 239



Y Index: 239

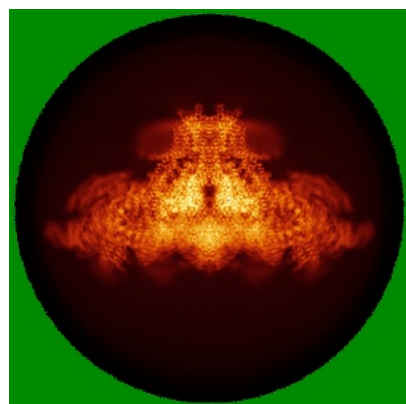


Z Index: 229

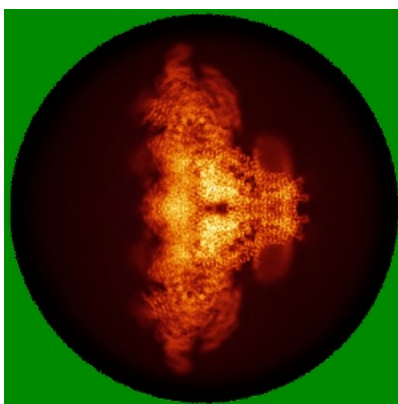
The images above show the largest variance slices of the map in three orthogonal directions.

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

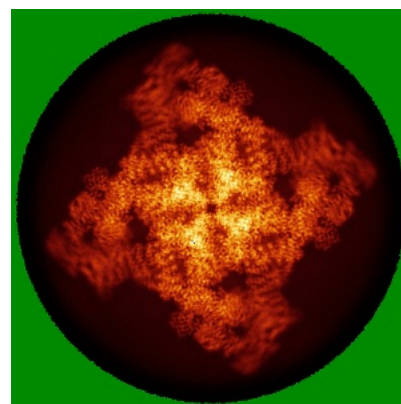
6.4.1 Primary map



X

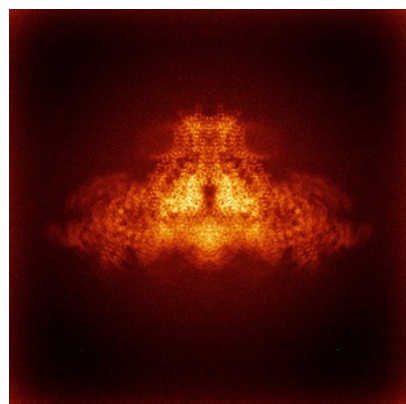


Y

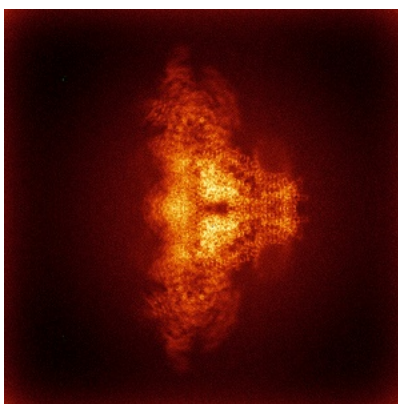


Z

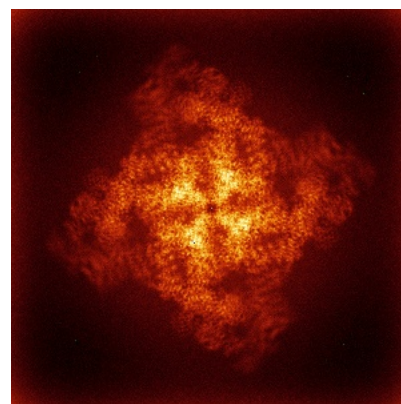
6.4.2 Raw map



X



Y

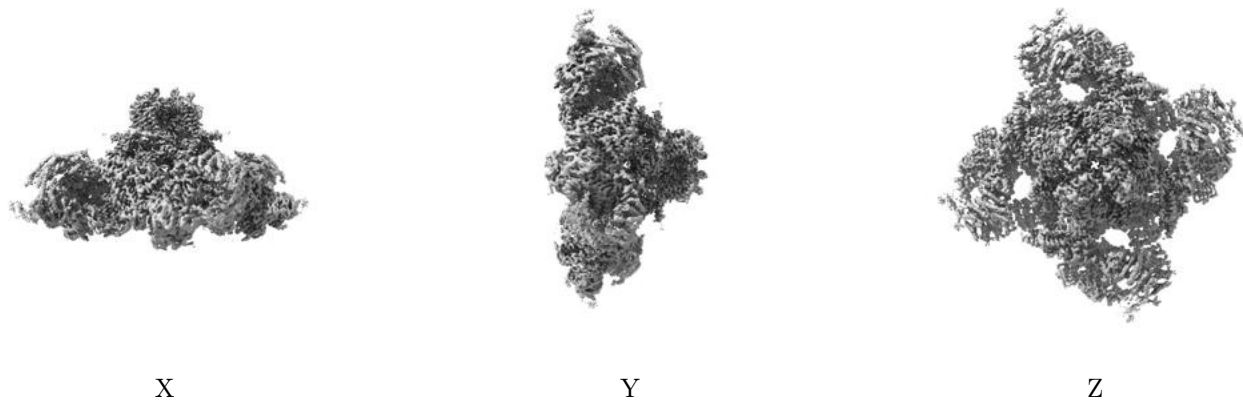


Z

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.

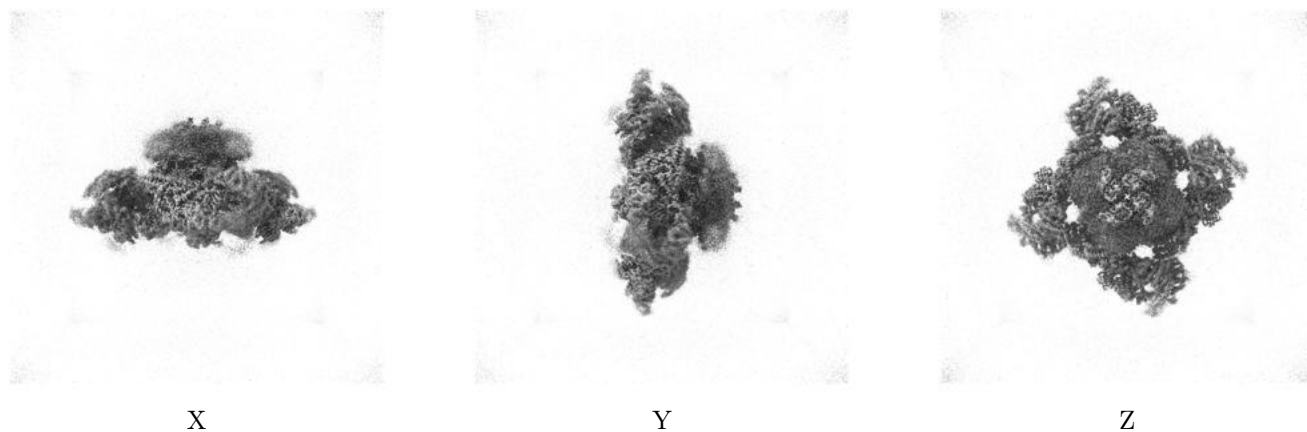
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

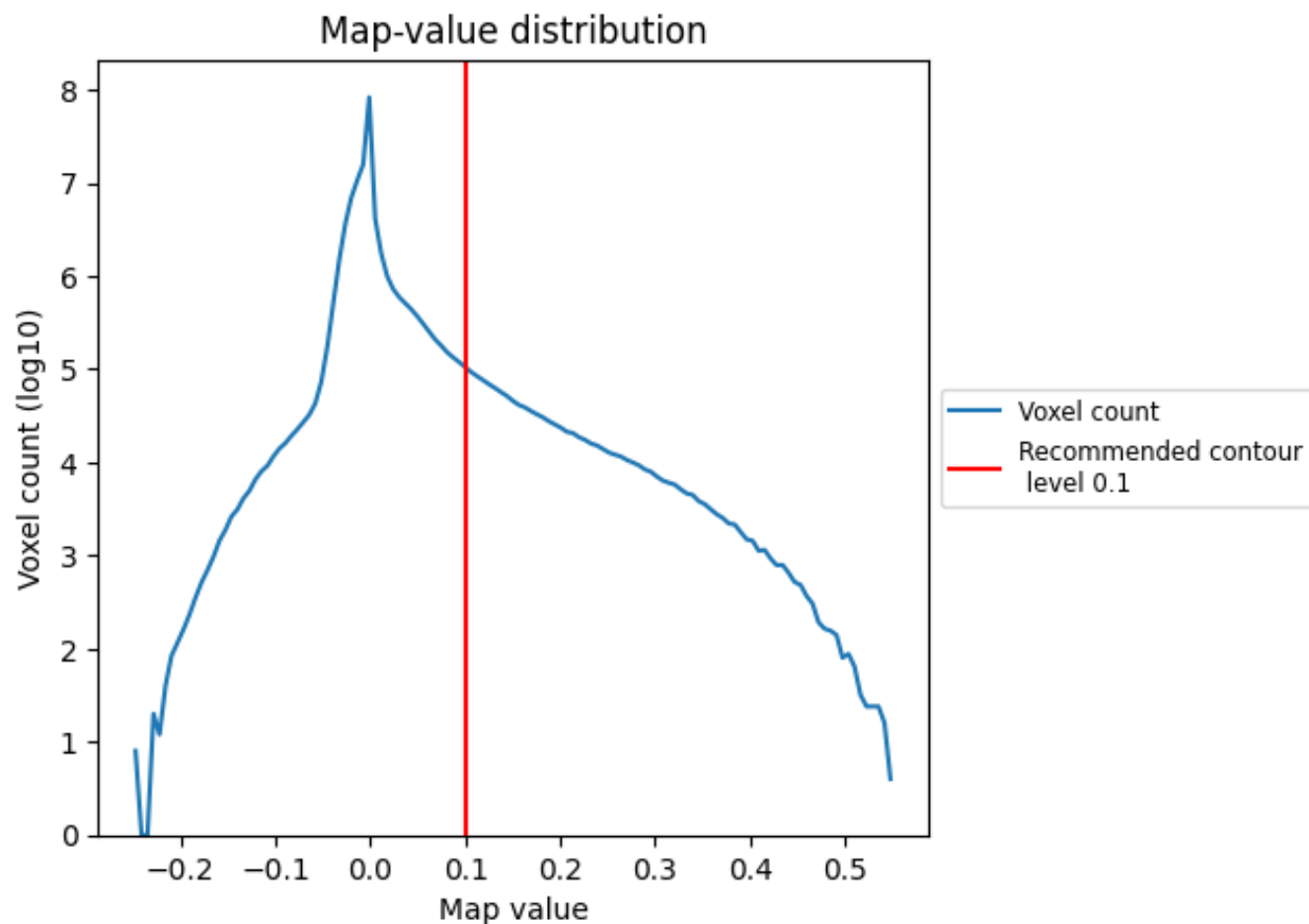
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

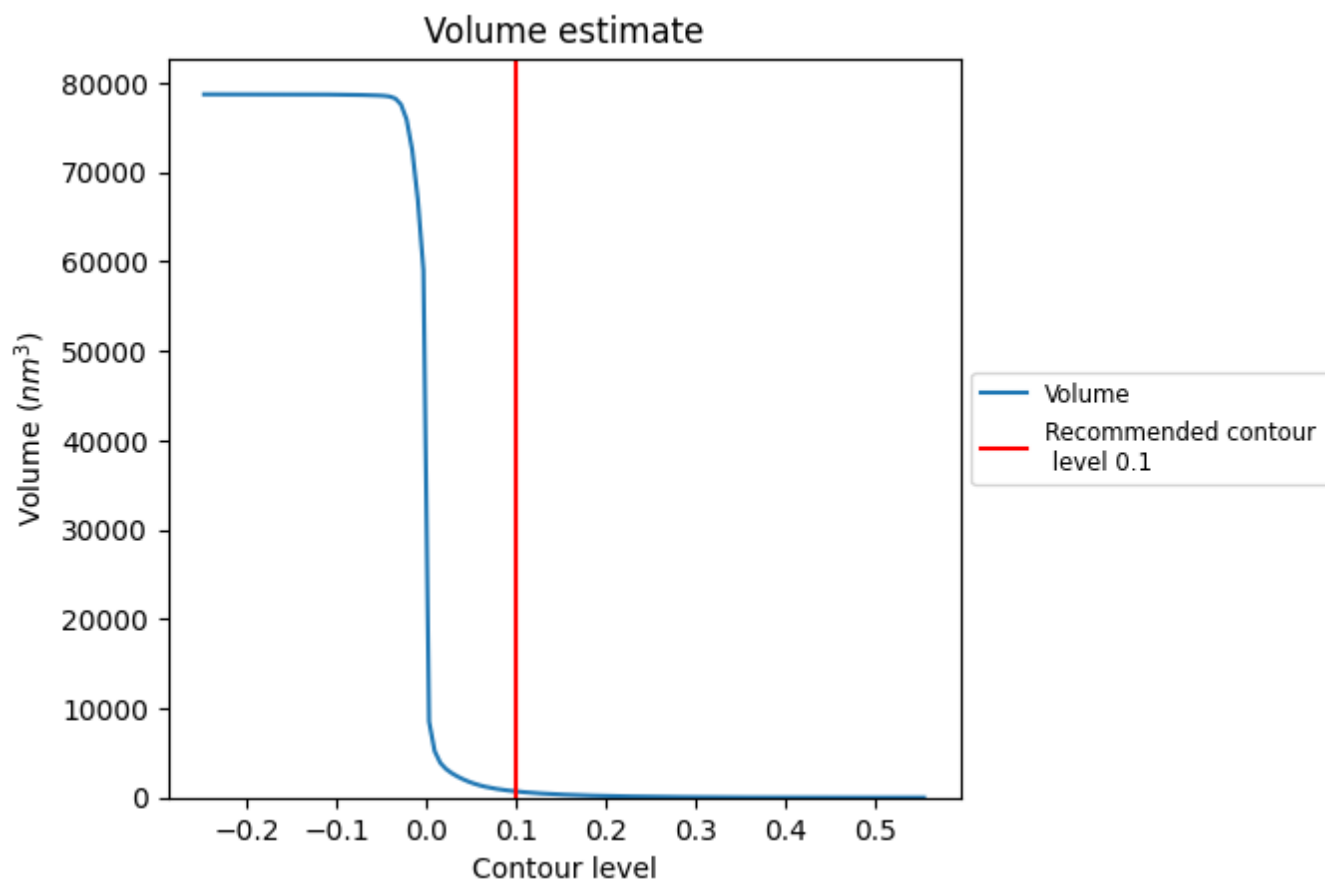
This section contains the results of statistical analysis of the map.

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.

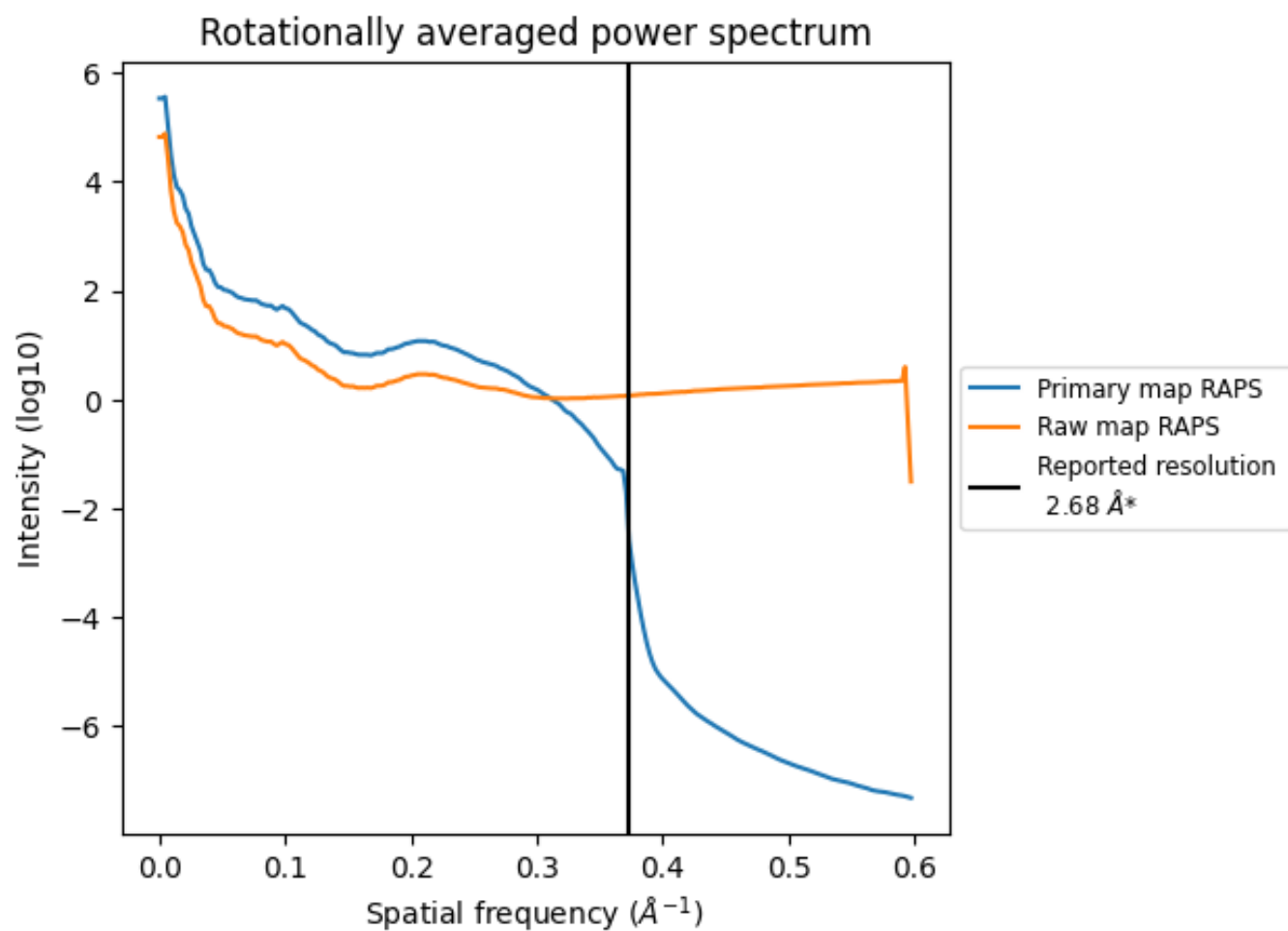
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 692 nm³; this corresponds to an approximate mass of 625 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 ⓘ

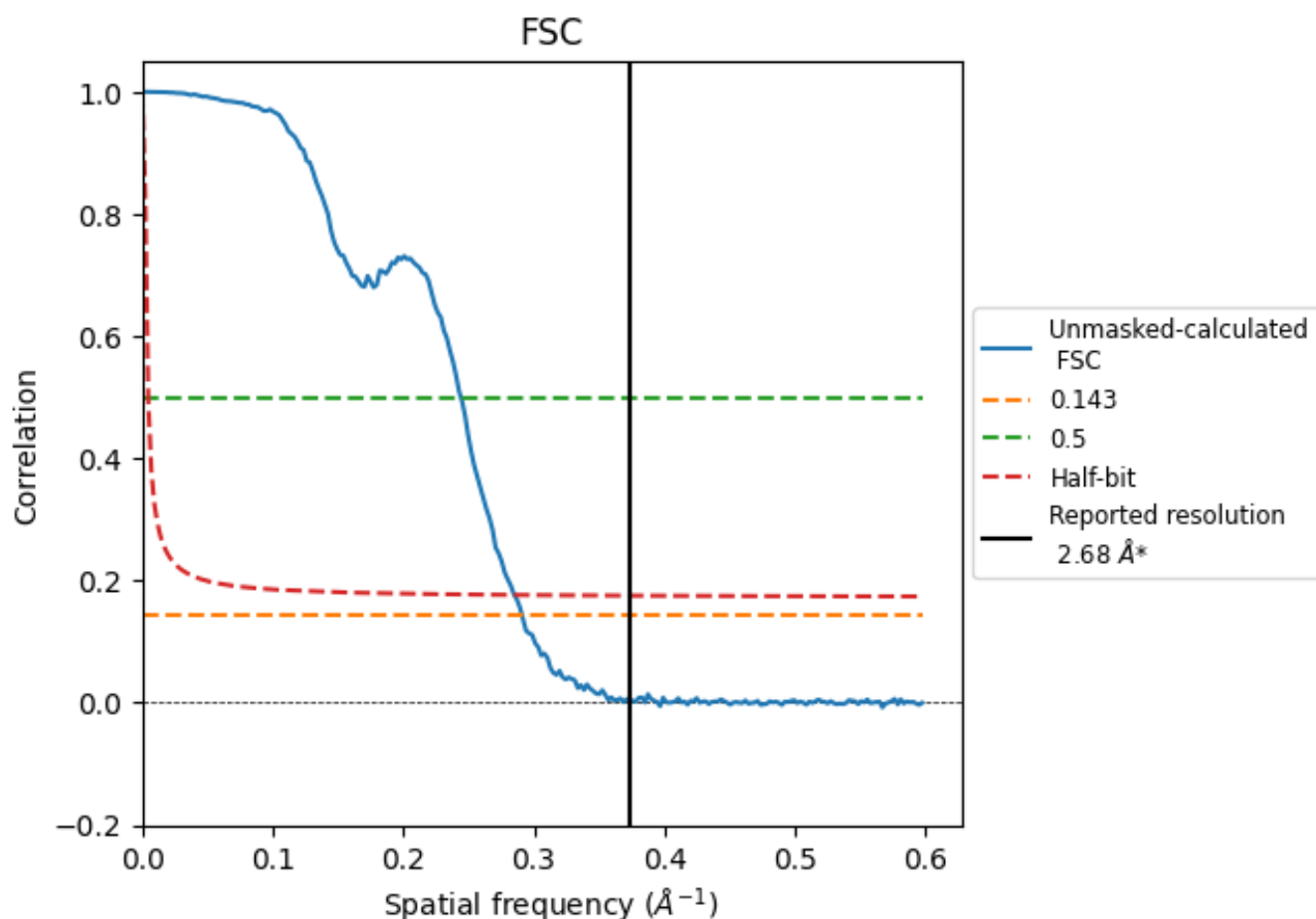


*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8.2 Resolution estimates [i](#)

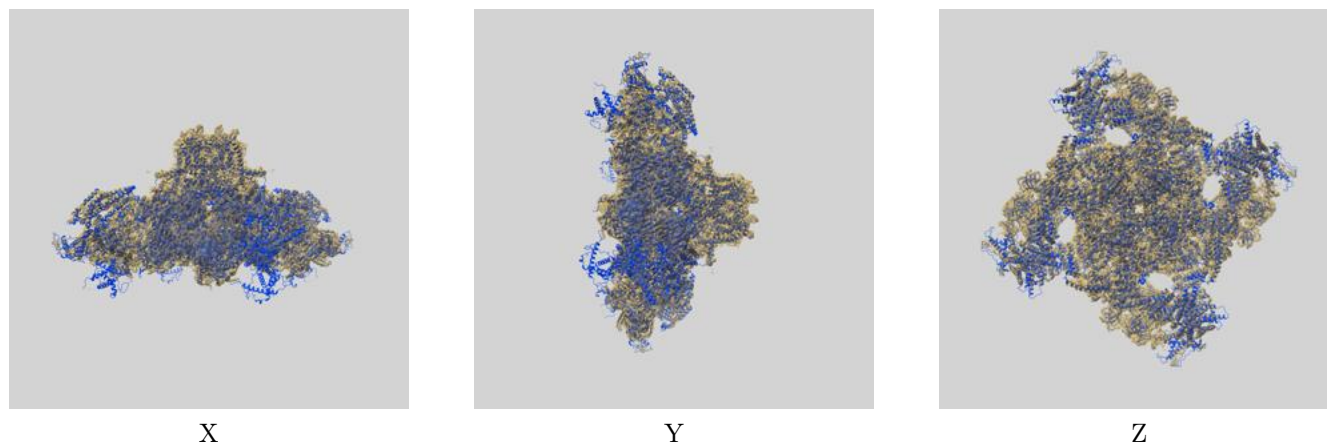
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.44	4.10	3.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 2.68 by more than 10 %

9 Map-model fit [i](#)

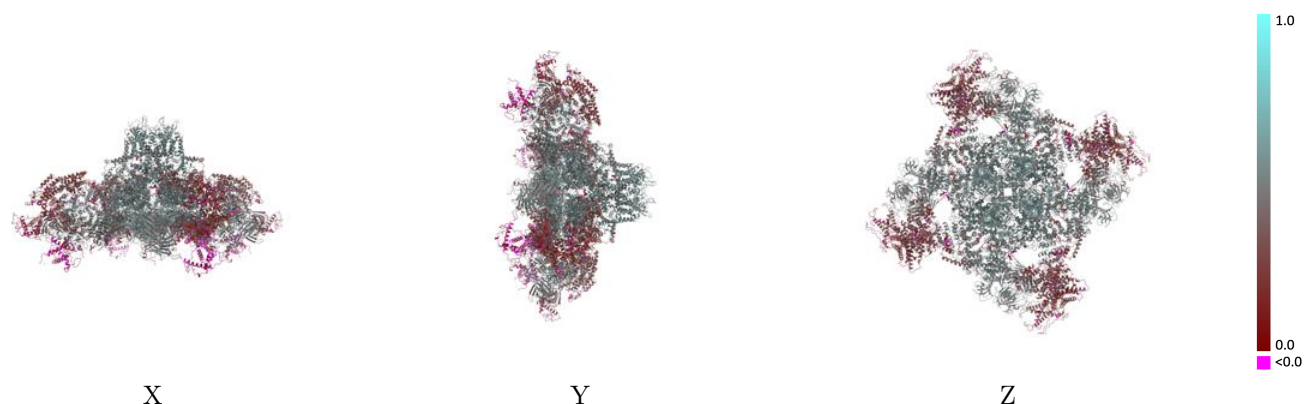
This section contains information regarding the fit between EMDB map EMD-47385 and PDB model 9E18. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



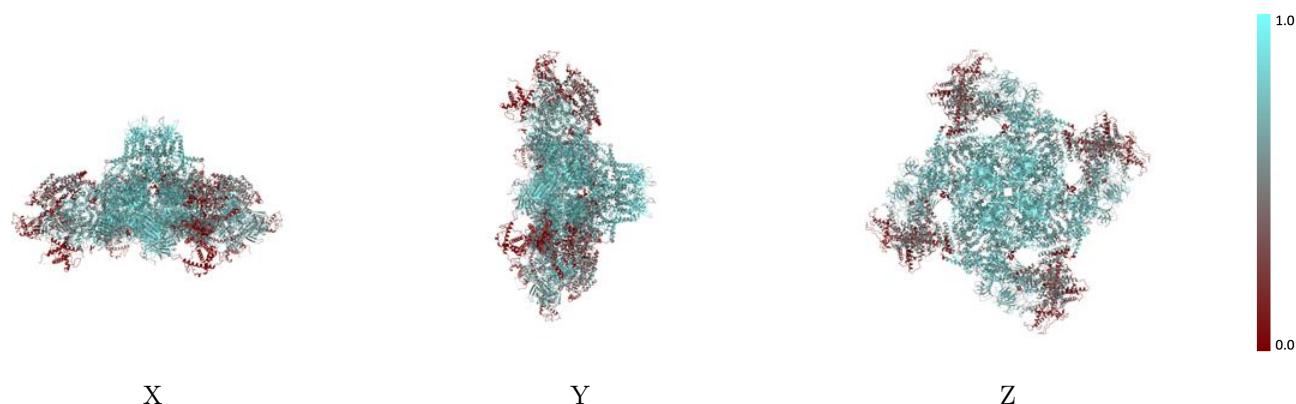
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



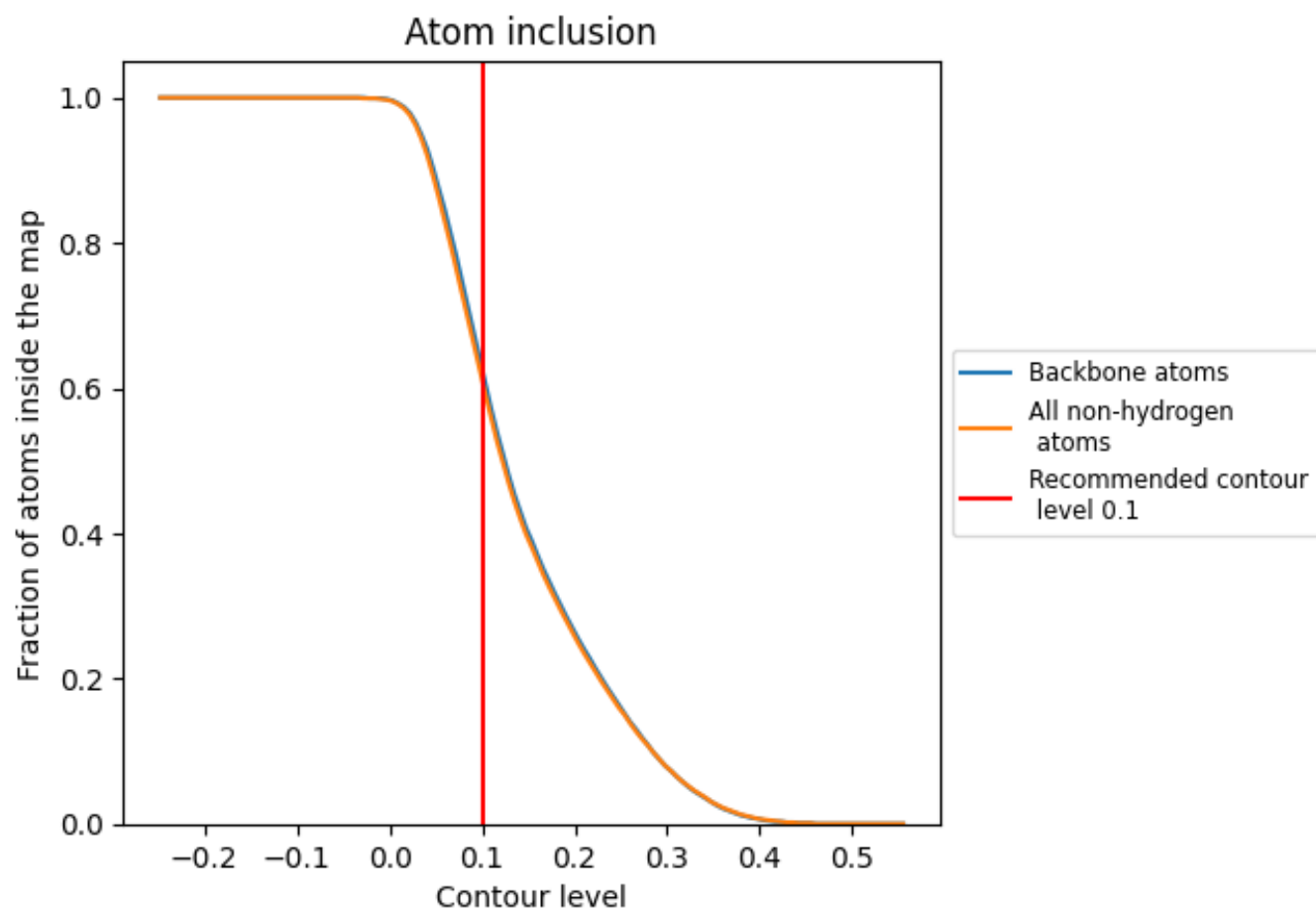
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 61% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6110	0.4160
A	0.6180	0.4140
B	0.6180	0.4150
C	0.6180	0.4140
D	0.6180	0.4140
E	0.6470	0.5000
F	0.6500	0.4970
G	0.6430	0.4940
H	0.6470	0.4960

