



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:13 PM UTC

PDB ID : 9CGQ / pdb_00009cgq
EMDB ID : EMD-45585
Title : Rabbit RyR1 disease mutant Y523S in complex with FKBP12.6, nanodisc and inhibitor dantrolene in the presence of activating calcium
Authors : Iyer, K.A.; Samso, M.
Deposited on : 2024-06-30
Resolution : 3.23 Å(reported)
Based on initial model : 7T65

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

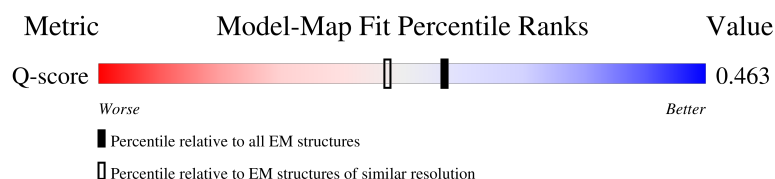
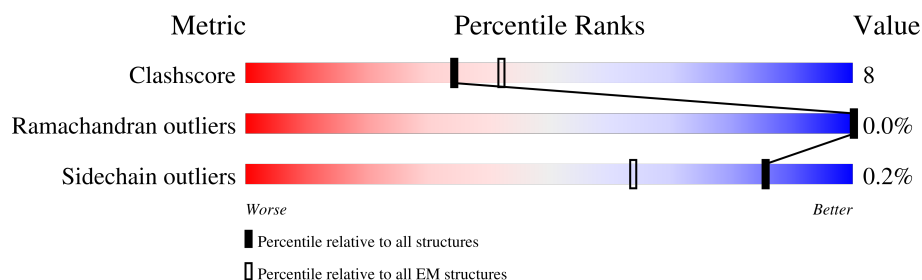
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.23 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.



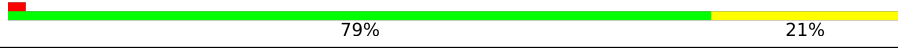
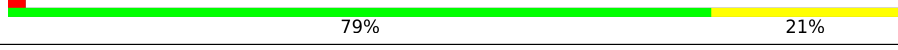
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.73 - 3.73)

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	 6% 68% 14% 18%
1	B	5037	 6% 67% 15% 18%
1	C	5037	 6% 68% 14% 18%
1	D	5037	 6% 68% 15% 18%

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Mol	Chain	Length	Quality of chain
2	E	107	 81% 18%
2	F	107	 72% 28%
2	G	107	 79% 21%
2	H	107	 79% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	U1C	A	5103	-	X	-	-
6	U1C	C	5103	-	X	-	-
6	U1C	D	5103	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 129760 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	4155	Total	C	N	O	S	0	0
			31570	20075	5432	5865	198		
1	B	4155	Total	C	N	O	S	0	0
			31570	20075	5432	5865	198		
1	C	4155	Total	C	N	O	S	0	0
			31570	20075	5432	5865	198		
1	D	4155	Total	C	N	O	S	0	0
			31570	20075	5432	5865	198		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	523	SER	TYR	engineered mutation	UNP P11716
B	523	SER	TYR	engineered mutation	UNP P11716
C	523	SER	TYR	engineered mutation	UNP P11716
D	523	SER	TYR	engineered mutation	UNP P11716

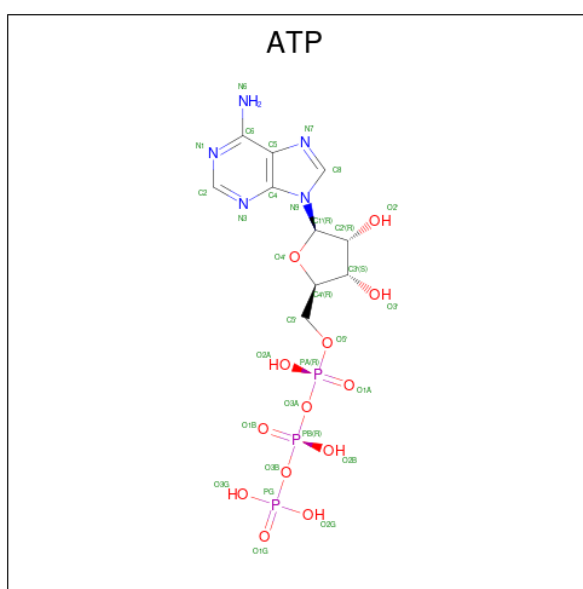
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	107	Total	C	N	O	S	0	0
			814	513	143	154	4		
2	F	107	Total	C	N	O	S	0	0
			814	513	143	154	4		
2	G	107	Total	C	N	O	S	0	0
			814	513	143	154	4		
2	H	107	Total	C	N	O	S	0	0
			814	513	143	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	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	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).

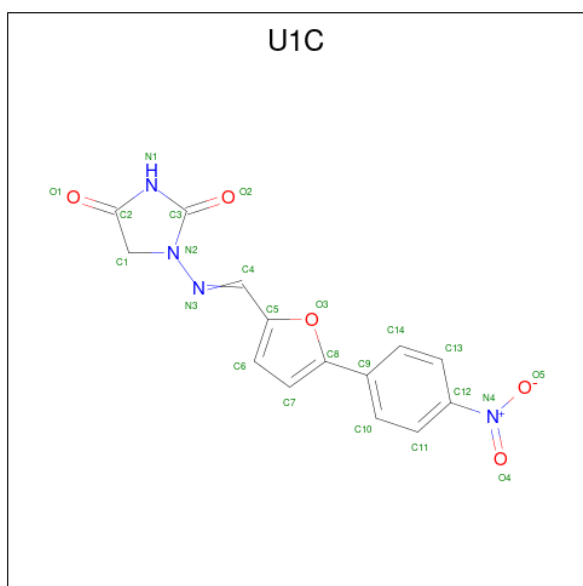
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
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 Dantrolene (CCD ID: U1C) (formula: $C_{14}H_{10}N_4O_5$) (labeled as "Ligand of Interest" by depositor).

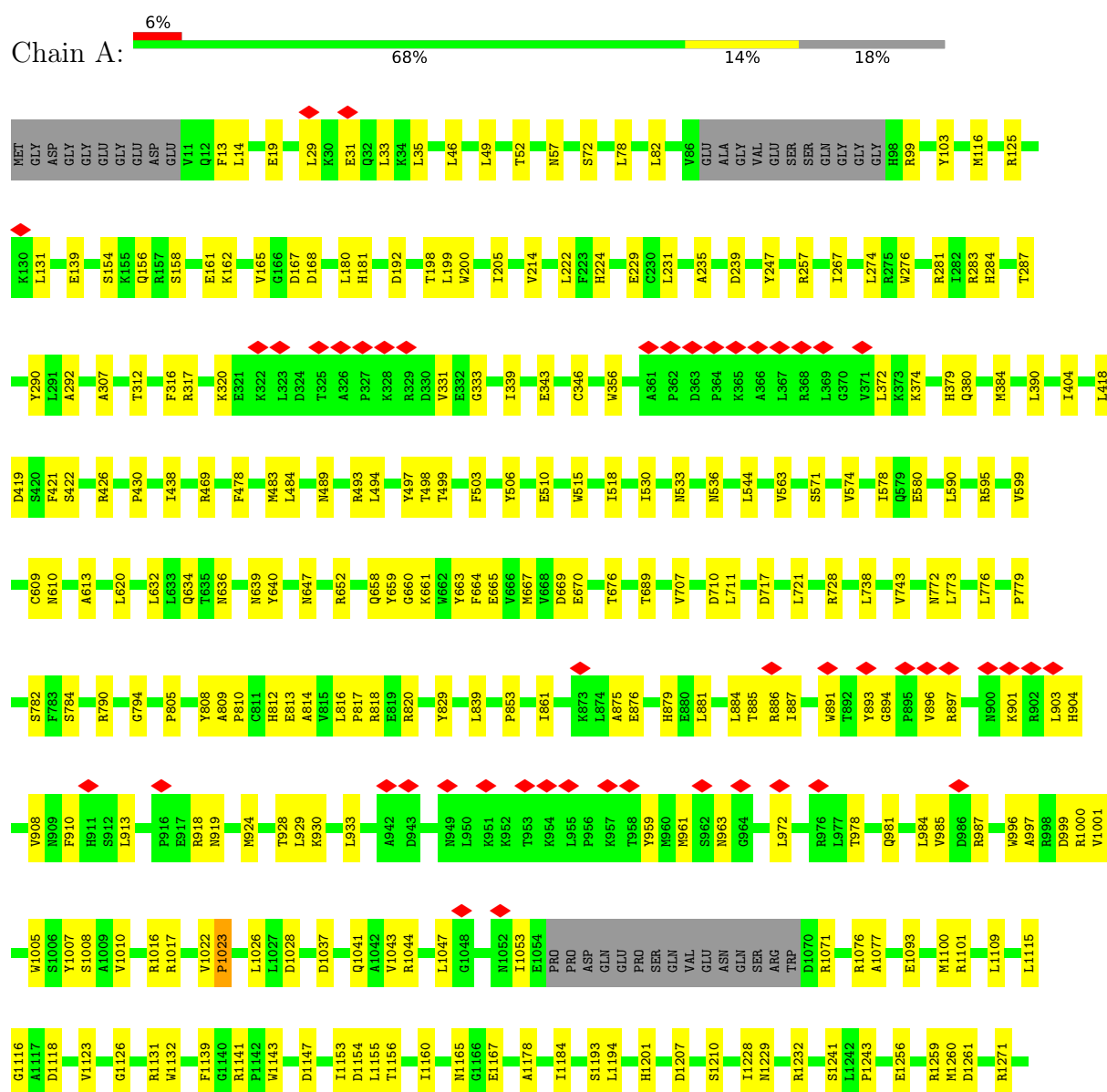


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			23	14	4	5	
6	B	1	Total	C	N	O	0
			23	14	4	5	
6	C	1	Total	C	N	O	0
			23	14	4	5	
6	D	1	Total	C	N	O	0
			23	14	4	5	

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



L2809	E2749	K2690	M2530	Q2247	M2101	A2016	GLU	P1774	I1572	ALA	ALA	GLY	R1276
K2810	K2750	TYR	M2537	Y2256	V2102	D2017	GLU	H1775	R1573	LEU	LEU	GLY	S1279
E2811	L2751	ASP	T2538	M2260	W2105	E2018	GLU	H1776	P1574	ARG	ARG	GLU	Q1280
S2812	D2752	GLN	T2538	N2261	A2106	E2019	GLU	F1777	M1579	LEU	LEU	THR	N1281
L2813	S2753	LEU	L2556	G2261	Q2107	L2023	ASP	S1778	R1594	PRO	PRO	THR	S1282
K2814	F2754	TYR	L2556	ILE	Q2107	L2026	GLU	A1784	L1595	HIS	ALA	ALA	L1283
A2815	I2755	ARG	P2560	GLY	L2116	D2026	GLU	F1787	L1600	ASP	VAL	GLY	F1288
M2816	N2756	MET	L2561	GLY	M2120	R2028	GLU	ALA	L1600	VAL	VAL	THR	Q1296
L2817	K2757	MET	L2561	MET	R2126	L2031	GLU	VAL	V1603	ALA	ALA	PRO	Q1299
A2818	T2758	PRO	P2567	Q2268	Q2127	E2047	GLU	ALA	M1608	D1419	HIS	GLY	H1289
W2819	A2759	CYS	L2568	A2278	Y2128	GLY	ASP	GLU	M1608	N1420	PHE	GLY	PHE
E2820	E2760	LEU	F2569	R2458	Q2127	GLU	ALA	A1794	L1613	R1421	THR	THR	ARG
W2821	T2761	ALA	A2570	N2283	L2131	GLU	GLU	L1798	Q1614	PRO	PRO	GLN	CYS
H2763	H2763	ILE	R2575	L2286	G2132	GLU	GLU	E1806	V1615	P1424	PRO	THR	THR
E2764	K2765	ALA	V2579	Q2293	V2149	PRO	GLU	E1806	T1617	I1427	VAL	GLY	ALA
K2765	W2766	GLY	D2580	E2296	D2151	GLU	GLU	R1808	L1624	C1447	ALA	GLY	ALA
W2766	A2767	PRO	S2581	E2297	T2152	THR	GLU	L1812	D1632	V1448	PRO	GLN	PRO
A2767	F2768	ASP	T2585	V2298	T2152	THR	GLU	L1815	T1634	V1453	VAL	VAL	LEU
F2768	D2769	TYR	R2588	L2313	T2182	GLY	GLY	L1815	L1634	P1455	ARG	ARG	PRO
K2770	K2770	ASP	K2597	F2334	M2178	SER	GLU	R1827	D1465	D1465	ALA	GLY	PRO
L2771	L2771	ALA	L2597	E2388	T2185	SER	GLU	D1828	E1643	E1479	GLY	GLY	GLY
Q2772	Q2772	TYR	A2609	L2377	M2186	ARG	GLU	P1829	E1644	Q1480	ASN	LEU	LEU
N2773	N2773	SER	L2610	L2377	W2187	LEU	GLU	V1830	H1646	R1470	GLN	GLN	GLN
N2774	N2774	SER	C2611	T2384	M2188	SER	GLU	Q1837	L1653	E1479	PRO	PRO	PRO
W2775	W2775	LYS	T2614	ASP	M2203	LEU	GLU	V1845	L1667	Q1480	ALA	ALA	ALA
S2776	S2776	ALA	G2493	S2387	M2203	LEU	GLU	L1942	L1667	C1489	THR	THR	THR
L2777	L2777	LYS	K2499	E2388	V2207	THR	GLU	H1953	R1671	C1489	GLU	GLU	GLU
G2778	G2778	LYS	S2493	A2391	M2208	VAL	VAL	M1851	Q1504	G1504	LYS	ALA	ALA
E2779	E2779	ALA	F2494	ARG	M2211	ARG	ARG	F1854	Q1505	Q1505	ASN	ARG	ARG
N2780	N2780	THR	V2495	ASP	M2211	LEU	LEU	F1854	Q1506	Q1506	LYS	ALA	ALA
S2781	S2781	VAL	P2496	GLY	V2212	VAL	VAL	I1866	G1507	G1507	ARG	GLU	GLU
GLN	W2781	ASP	D2497	PRO	N2213	LYS	LYS	I1866	L1676	L1676	GLY	PRO	PRO
THR	D2782	ALA	F2628	GLY	V2214	LYS	LYS	E1874	V1681	V1681	PHE	PHE	PHE
ALA	E2783	GLU	L2633	VAL	L2215	LYS	GLU	GLU	L1707	L1707	LEU	LEU	LEU
ALA	E2784	GLY	L2633	ARG	G2216	GLU	GLU	GLU	L1738	L1738	PRO	PRO	PRO
THR	E2784	ARG	C2651	ARG	GLY	LYS	LYS	GLU	F1549	F1549	LYS	LYS	LYS
ASP	L2785	ASP	W2652	ASP	THR	PRO	PRO	GLU	P1550	P1550	ALA	ALA	ALA
PRO	K2786	ARG	G2511	ARG	LYS	GLU	GLU	GLU	A1551	A1551	LYS	LYS	LYS
ARG	T2787	ARG	T2659	ARG	GLU	LEU	LEU	GLU	T1746	T1746	ALA	ALA	ALA
GLU	H2788	GLU	G2660	GLU	L2223	LEU	LEU	GLU	L1747	L1747	ALA	ALA	ALA
GLY	P2789	GLY	N2663	HIS	T2223	PRO	PRO	GLU	F1748	F1748	MET	MET	MET
M2790	M2790	TYR	N2663	PHE	T1995	ALA	ALA	GLU	P1749	P1749	THR	THR	THR
L2791	L2791	TYR	H2519	GLY	T1995	GLU	GLU	GLU	R1752	R1752	GLN	GLN	GLN
R2792	R2792	GLY	H2520	GLY	T1995	GLU	GLU	GLU	K1753	K1753	PRO	PRO	PRO
P2793	P2793	GLY	V2521	GLU	T2230	GLU	GLU	GLU	G1754	G1754	ALA	ALA	ALA
Q2858	Q2793	GLY	E2669	PRO	T2230	GLU	GLU	GLU	Q1559	Q1559	THR	THR	THR
P2859	Y2794	GLY	E2670	PRO	F2235	GLU	GLU	GLU	I1562	I1562	GLY	GLY	GLY
P2860	K2795	GLY	E2671	GLU	L2236	GLU	GLU	GLU	R1758	R1758	ALA	ALA	ALA
L2861	T2796	GLY	L2672	GLU	F2236	GLU	GLU	GLU	Q1569	Q1569	THR	THR	THR
L2862	T2796	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	PRO	PRO	PRO
S2863	F2797	GLY	L2674	GLU	F2236	GLU	GLU	GLU	Q1569	Q1569	ALA	ALA	ALA
G2864	S2798	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	THR	THR	THR
V2865	E2799	GLY	L2674	GLU	F2236	GLU	GLU	GLU	Q1569	Q1569	PRO	PRO	PRO
T2866	K2800	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	ALA	ALA	ALA
L2867	D2801	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	THR	THR	THR
S2868	K2802	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	PRO	PRO	PRO
	E2803	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	ALA	ALA	ALA
	I2804	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	THR	THR	THR
	Y2805	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	PRO	PRO	PRO
	R2806	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	ALA	ALA	ALA
	W2807	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	THR	THR	THR
	P2808	GLY	L2674	GLU	F2236	GLU	GLU	GLU	K1568	K1568	PRO	PRO	PRO

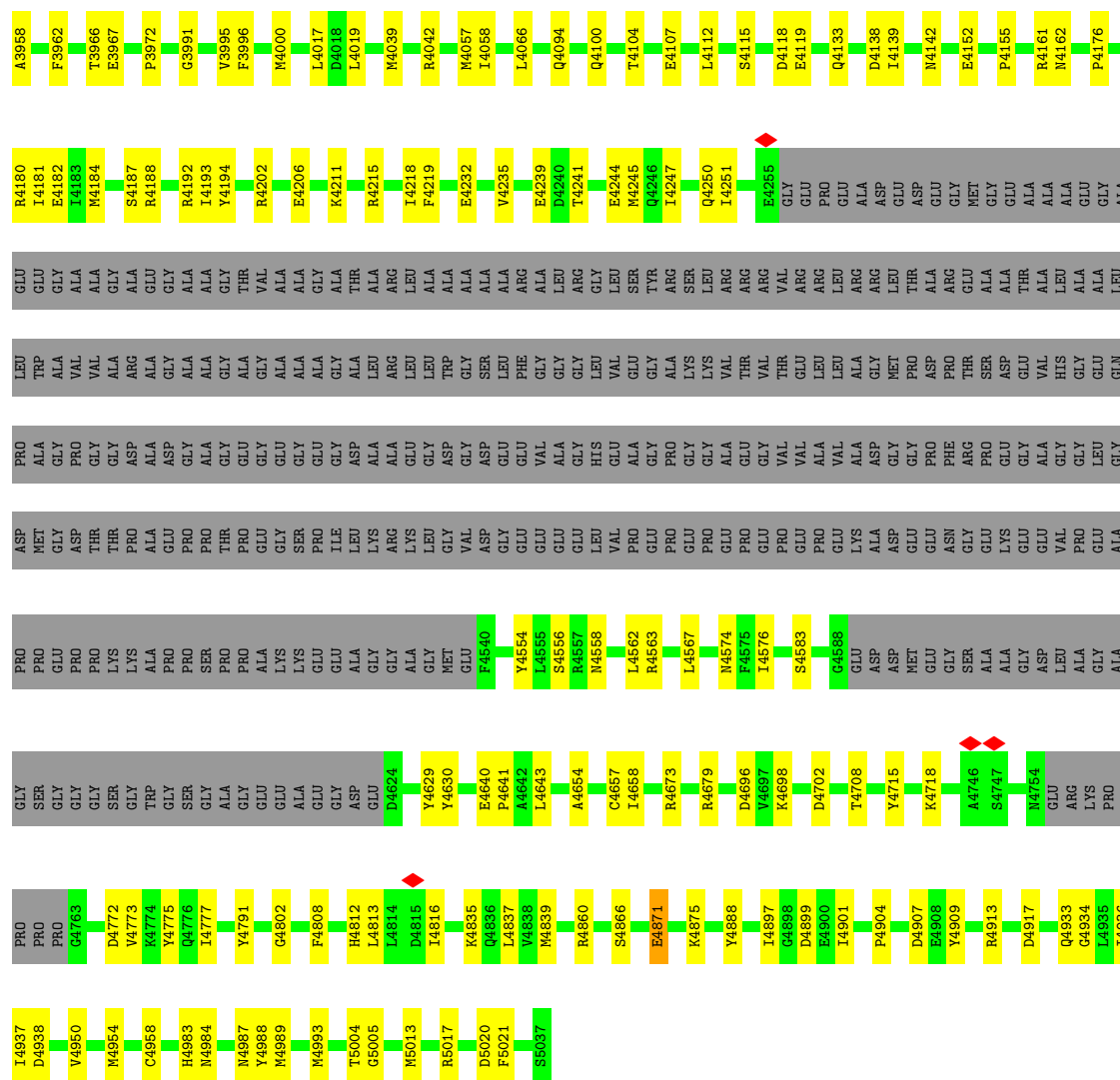




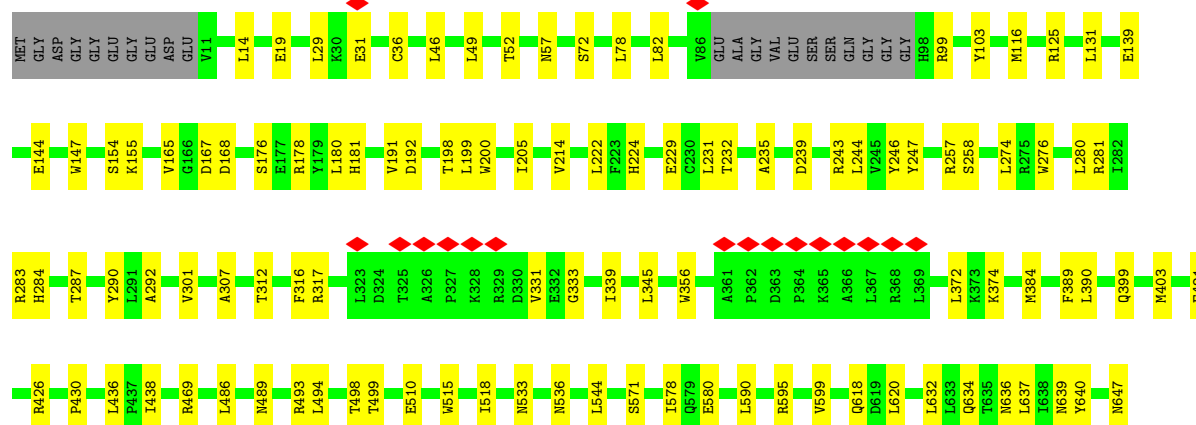


GLU	ASN	ARG	V2416	H2420	A2421	I2422	M2423	I2430	A2445	V2460	P2462	L2463	D2464	D2465	L2466	I2470	T2476	THR	LEU	GLY	LYS	ASP	G2483	K2489	S2493	F2494	V2495	P2496	D2497	N2502	F2505	L2506	V2509	Y2510	G2511	I2512	D2516	L2519	H2520	V2521	G2524	V2525	F2526					
Y2256	S2261	ILE	GLY	LEU	GLY	MET	Q2268	A2278	N2283	L2286	D2294	V2298	L2313	P2325	V2339	V2353	L2357	L2377	I2384	S2387	E2388	A2391	ARG	ASP	GLY	PRO	GLY	VAL	ARG	ARG	ASP	ASP	ARG	ARG	ARG	HIS	PHE	GLY	GLU	PRO	PRO	GLU						
Q2095	E2096	M2101	Q2107	L2116	R2126	Q2127	Y2128	E2133	L2138	V2149	E2150	D2151	T2152	I2162	M2178	M2186	N2187	N2188	M2203	V2207	M2211	V2212	N2213	V2214	L2215	G2216	GLY	GLY	GLU	THR	LYS	GLU	I2223	P2226	K2227	M2228	T2230	S2231	C2232	F2235	Q2247							
S2000	Q2005	L2010	E2019	L2023	D2026	I2027	R2028	E2047	GLY	GLU	GLU	GLU	PRO	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU					
GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU					
F1748	P1749	R1752	K1753	G1754	R1758	R1759	P1763	L1771	F1777	S1778	P1787	ALA	ALA	VAL	ALA	A1794	L1798	E1805	R1808	D1809	K1810	A1811	L1812	L1813	M1814	L1815	R1827	D1828	P1829	V1830	Q1837	V1845	M1851	F1854	E1874	GLU	GLU	E1989	E1990	T1991	T1995	R1996						
R1594	L1595	M1599	L1600	V1603	Q1614	V1615	E1616	T1617	R1618	R1619	L1624	Q1629	L1634	T1635	M1636	E1643	L1653	L1659	L1667	R1671	A1672	V1673	N1678	V1681	L1694	L1698	L1707	R1708	Y1712	L1715	I1716	S1717	E1721	P1737	L1738	T1746	L1747											
C1447	V1448	G1451	W1452	V1453	T1454	D1456	L1466	R1470	Q1480	C1489	M1494	G1504	Q1505	Q1506	G1507	R1508	S1510	H1511	V1520	D1521	V1524	M1527	E1535	F1540	F1549	P1550	A1551	V1552	F1553	V1554	L1555	I1562	K1568	T1572	M1573	P1574	M1579	P1589										
ALA	GLN	PRO	VAL	ARG	ALA	GLU	ASN	GLU	GLU	GLU	THR	THR	GLU	LYS	ASN	ARG	LYS	LYS	GLY	PHE	LEU	PHE	LYS	ALA	LYS	GLN	LEU	PRO	ALA	ALA	VAL	VAL	PRO	ALA	D1419	N1420	R1421	D1422	D1423	I1426	Y1434							
THR	PRO	LEU	ALA	PRO	PRO	GLY	LEU	PRO	ALA	ALA	ASP	GLU	GLU	GLU	GLU	PRO	PRO	ASP	GLY	ASP	PRO	TYR	GLU	ASN	LEU	ARG	GLY	TRP	PRO	GLY	GLU	ALA	GLY	THR	GLY	THR	PRO	GLN	PRO	GLY	VAL	GLU						
L1155	L1164	N1165	G1166	E1167	R1180	E1181	I1184	C1192	S1193	L1194	Q1198	H1201	L1204	I1228	M1229	S1241	L1242	P1243	E1256	R1259	M1260	D1261	P1268	R1275	T1276	N1281	S1282	L1283	F1288	L1291	S1292	L1293	Q1299	HIS	PHE	ARG	CYS	THR	ALA	ALA								
N1052	I1053	E1054	PRO	ASP	GLN	PRO	GLN	VAL	GLU	ASN	GLN	GLN	ASP	ARG	TRP	F1075	R1076	A1077	F1090	E1093	E1099	M1100	R1101	L1109	D1112	L1115	G1116	A1117	D1118	V1123	F1124	N1125	G1126	Q1130	R1131	W1132	S1136	R1141	P1142	W1143	D1147	M1152						
K957	T958	Y959	H960	N961	S962	N963	G964	Y965	K966	P967	A968	L972	S973	H974	Y975	R976	L977	T978	Q981	R987	N991	G992	H993	N994	Y995	W996	R1000	Y1007	S1008	R1017	V1022	P1023	Y1024	R1025	L1026	L1027	D1028	K1032	R1033	R1036	D1037	Q1041	R1044	T1045	L1046	Y1049		
H879	E880	L881	W882	A883	L884	T885	R886	I887	E888	Q889	G890	W891	T892	Y893	G894	P895	V896	R897	N900	K901	R902	L903	H904	P905	C906	F910	H911	S912	L913	R918	N919	L922	E927	T928	L929	K930	L933	A934	L935	H938	A942	D943	N949	L950	K951	T953	K954	L955



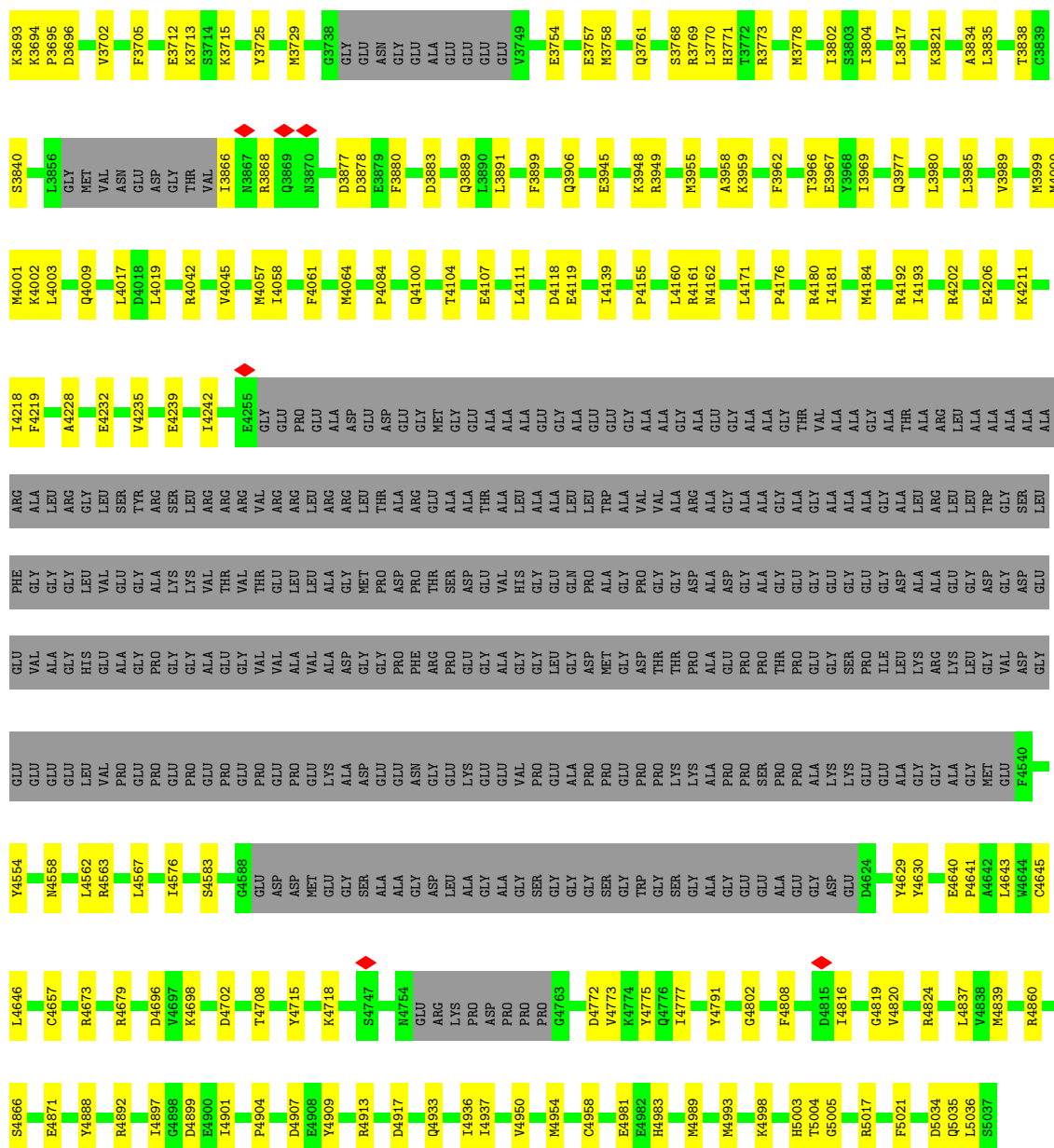


• Molecule 1: Ryanodine receptor 1









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

Chain E: 81% 18%



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

Chain F: 72% 28%



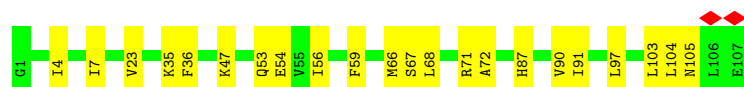
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G:  79% 21%



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

Chain H:  79% 21%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	189847	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.512	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.088	Depositor
Recommended contour level	0.307	Depositor
Map size ($\text{\AA}$)	501.12003, 501.12003, 501.12003	wwPDB
Map dimensions	464, 464, 464	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, ATP, CA, U1C

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	0.11	0/32230	0.31	2/43818 (0.0%)
1	B	0.12	1/32230 (0.0%)	0.31	6/43818 (0.0%)
1	C	0.21	3/32230 (0.0%)	0.34	6/43818 (0.0%)
1	D	0.10	0/32230	0.30	2/43818 (0.0%)
2	E	0.11	0/830	0.41	0/1119
2	F	0.13	0/830	0.45	0/1119
2	G	0.13	0/830	0.45	0/1119
2	H	0.12	0/830	0.40	0/1119
All	All	0.14	4/132240 (0.0%)	0.32	16/179748 (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	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2640	PRO	CG-CD	-30.84	0.45	1.50
1	B	1294	PRO	N-CD	-8.22	1.36	1.47
1	C	2640	PRO	CB-CG	7.24	1.85	1.49
1	C	2640	PRO	N-CD	6.93	1.57	1.47

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	2640	PRO	N-CD-CG	-30.79	57.02	103.20
1	B	1294	PRO	CA-N-CD	-18.22	86.49	112.00
1	C	2640	PRO	CA-CB-CG	-12.18	81.37	104.50
1	C	2640	PRO	CA-N-CD	-8.33	100.34	112.00
1	C	2640	PRO	N-CA-CB	-8.01	94.52	103.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	658	GLN	Peptide
1	C	4871	GLU	Peptide

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	31570	0	30212	490	0
1	B	31570	0	30212	515	0
1	C	31570	0	30212	489	0
1	D	31570	0	30212	499	0
2	E	814	0	813	15	0
2	F	814	0	813	27	0
2	G	814	0	813	23	0
2	H	814	0	813	18	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	31	0	12	1	0
4	B	31	0	12	2	0
4	C	31	0	12	3	0
4	D	31	0	12	2	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	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	23	0	0	0	0
6	C	23	0	0	0	0
6	D	23	0	0	0	0
All	All	129760	0	124148	2050	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 8.

The worst 5 of 2050 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:LEU:HD22	1:A:1470:ARG:HB3	1.59	0.85
2:G:90:VAL:HG12	2:G:91:ILE:HD12	1.60	0.81
1:B:3836:MET:HG3	1:B:3884:LEU:HD21	1.64	0.80
1:D:3694:LYS:HD3	1:D:3695:PRO:HD2	1.63	0.80
2:G:23:VAL:H	2:G:105:ASN:HB2	1.47	0.79

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	4097/5037 (81%)	3828 (93%)	268 (6%)	1 (0%)	100	100
1	B	4097/5037 (81%)	3829 (94%)	267 (6%)	1 (0%)	100	100
1	C	4097/5037 (81%)	3835 (94%)	261 (6%)	1 (0%)	100	100
1	D	4097/5037 (81%)	3846 (94%)	250 (6%)	1 (0%)	100	100
2	E	105/107 (98%)	91 (87%)	14 (13%)	0	100	100
2	F	105/107 (98%)	90 (86%)	15 (14%)	0	100	100
2	G	105/107 (98%)	90 (86%)	15 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	105/107 (98%)	91 (87%)	14 (13%)	0	100	100
All	All	16808/20576 (82%)	15700 (93%)	1104 (7%)	4 (0%)	100	100

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1023	PRO
1	B	1023	PRO
1	D	1023	PRO
1	C	1023	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	3254/4276 (76%)	3248 (100%)	6 (0%)	87	88
1	B	3254/4276 (76%)	3248 (100%)	6 (0%)	87	88
1	C	3254/4276 (76%)	3251 (100%)	3 (0%)	88	90
1	D	3254/4276 (76%)	3250 (100%)	4 (0%)	88	90
2	E	87/88 (99%)	85 (98%)	2 (2%)	44	68
2	F	87/88 (99%)	86 (99%)	1 (1%)	65	77
2	G	87/88 (99%)	87 (100%)	0	100	100
2	H	87/88 (99%)	87 (100%)	0	100	100
All	All	13364/17456 (77%)	13342 (100%)	22 (0%)	85	88

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	3462	ASN
1	D	2241	ARG
1	D	919	ASN
1	D	3357	HIS
1	B	343	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 186 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2646	ASN
1	D	624	ASN
1	C	3449	HIS
1	C	4133	GLN
1	D	963	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	C	5101	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	A	5101	-	32,33,33	0.25	0	48,52,52	0.27	0
6	U1C	D	5103	-	25,25,25	6.17	16 (64%)	33,35,35	3.39	15 (45%)
6	U1C	C	5103	-	25,25,25	6.18	16 (64%)	33,35,35	3.38	15 (45%)
4	ATP	B	5101	-	32,33,33	0.25	0	48,52,52	0.27	0
6	U1C	B	5103	-	25,25,25	6.18	15 (60%)	33,35,35	3.40	15 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	U1C	A	5103	-	25,25,25	6.17	15 (60%)	33,35,35	3.43	15 (45%)
4	ATP	D	5101	-	32,33,33	0.26	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	C	5101	-	-	9/22/38/38	0/3/3/3
4	ATP	A	5101	-	-	7/22/38/38	0/3/3/3
6	U1C	D	5103	-	-	7/11/25/25	0/3/3/3
6	U1C	C	5103	-	-	7/11/25/25	0/3/3/3
4	ATP	B	5101	-	-	7/22/38/38	0/3/3/3
6	U1C	B	5103	-	-	5/11/25/25	0/3/3/3
6	U1C	A	5103	-	-	11/11/25/25	0/3/3/3
4	ATP	D	5101	-	-	6/22/38/38	0/3/3/3

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	5103	U1C	C1-N2	-18.76	1.32	1.45
6	B	5103	U1C	C1-N2	-18.73	1.32	1.45
6	A	5103	U1C	C1-N2	-18.64	1.32	1.45
6	D	5103	U1C	C1-N2	-18.61	1.32	1.45
6	A	5103	U1C	C1-C2	-10.69	1.38	1.51

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5103	U1C	C2-C1-N2	8.43	106.94	101.45
6	C	5103	U1C	C2-C1-N2	8.39	106.91	101.45
6	A	5103	U1C	C2-C1-N2	8.35	106.89	101.45
6	D	5103	U1C	C2-C1-N2	8.33	106.88	101.45
6	A	5103	U1C	O3-C8-C9	7.80	125.97	116.73

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

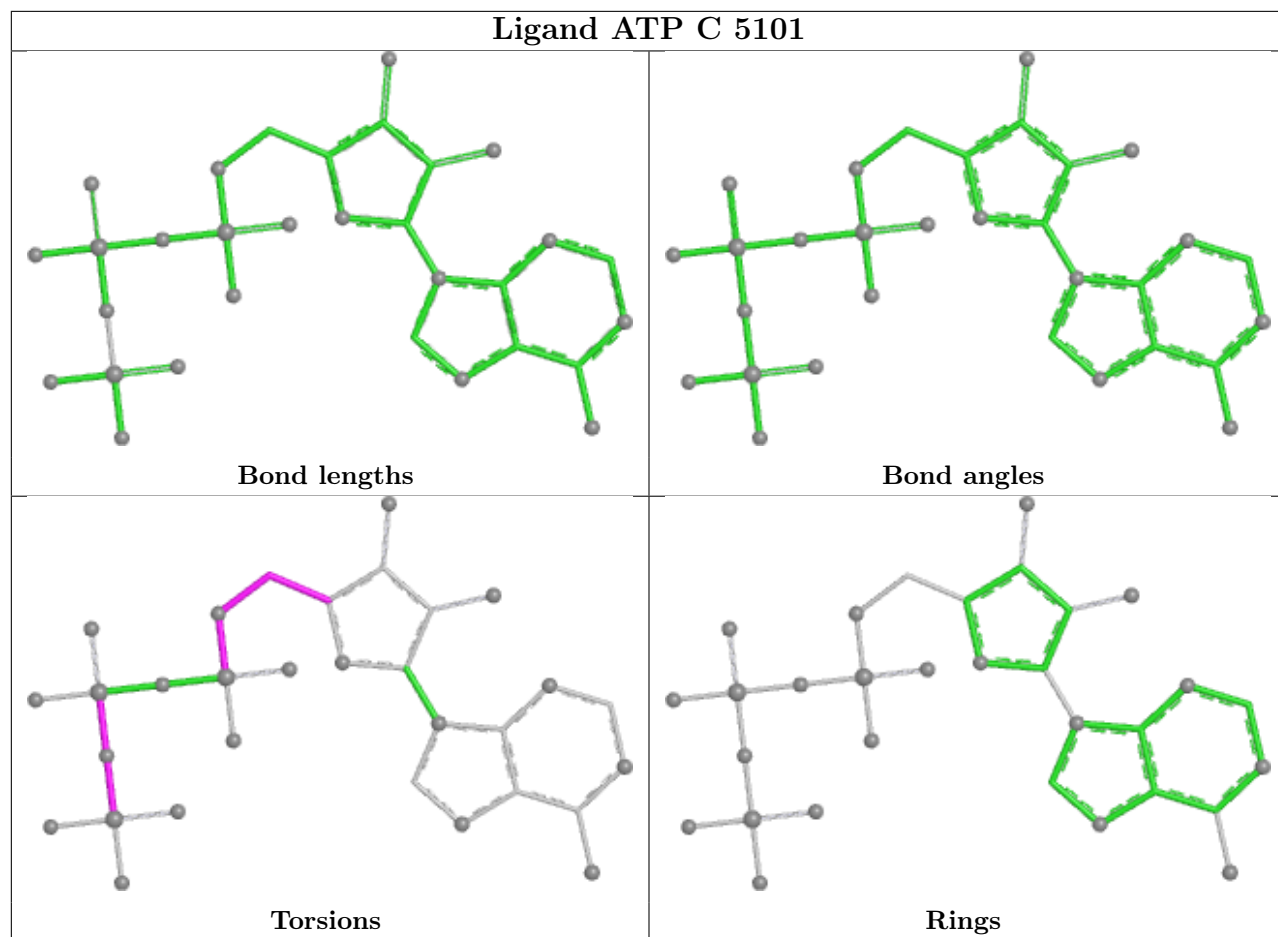
Mol	Chain	Res	Type	Atoms
4	A	5101	ATP	PB-O3B-PG-O2G
4	A	5101	ATP	C5'-O5'-PA-O1A
4	A	5101	ATP	O4'-C4'-C5'-O5'
4	B	5101	ATP	PB-O3B-PG-O2G
4	B	5101	ATP	C5'-O5'-PA-O1A

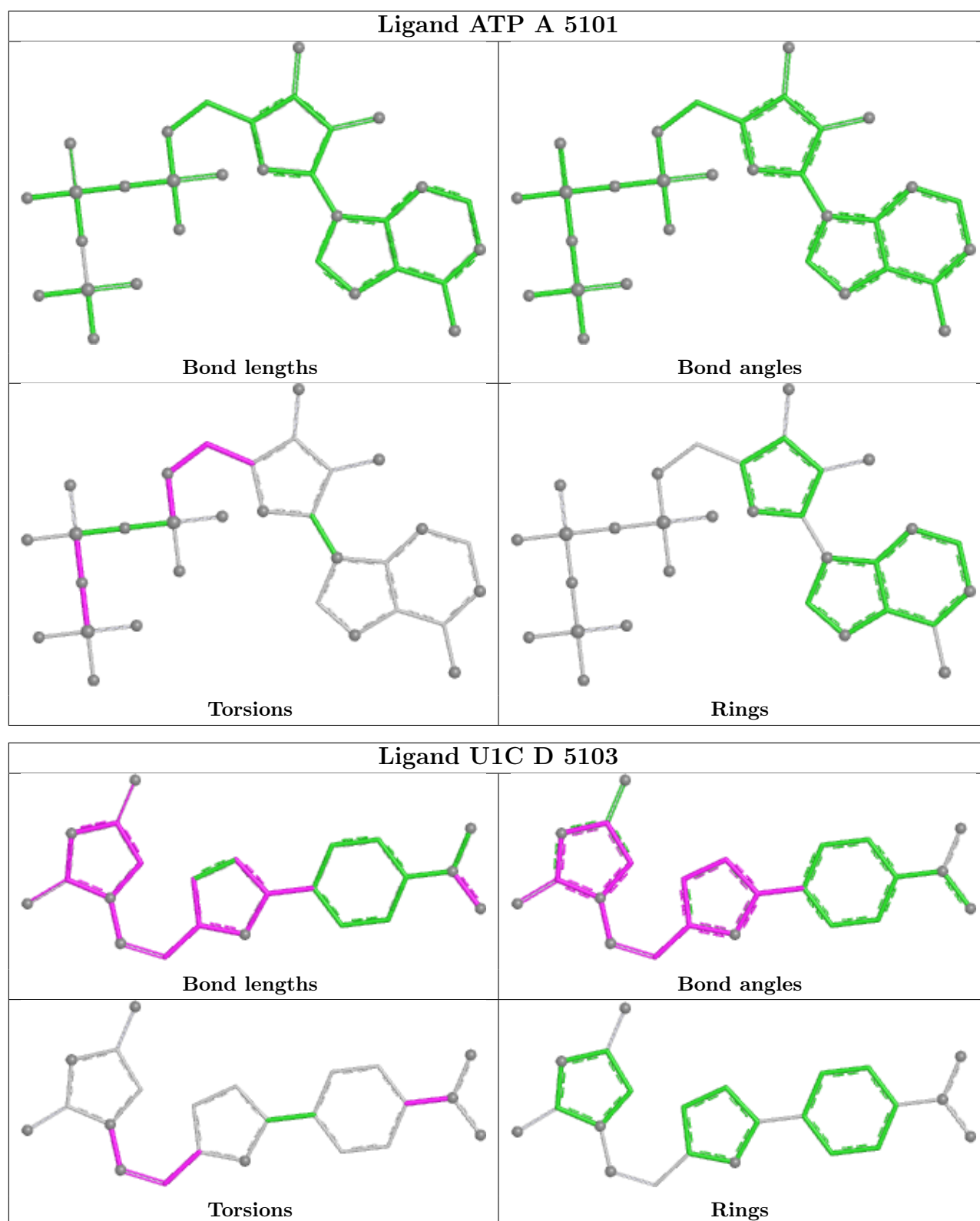
There are no ring outliers.

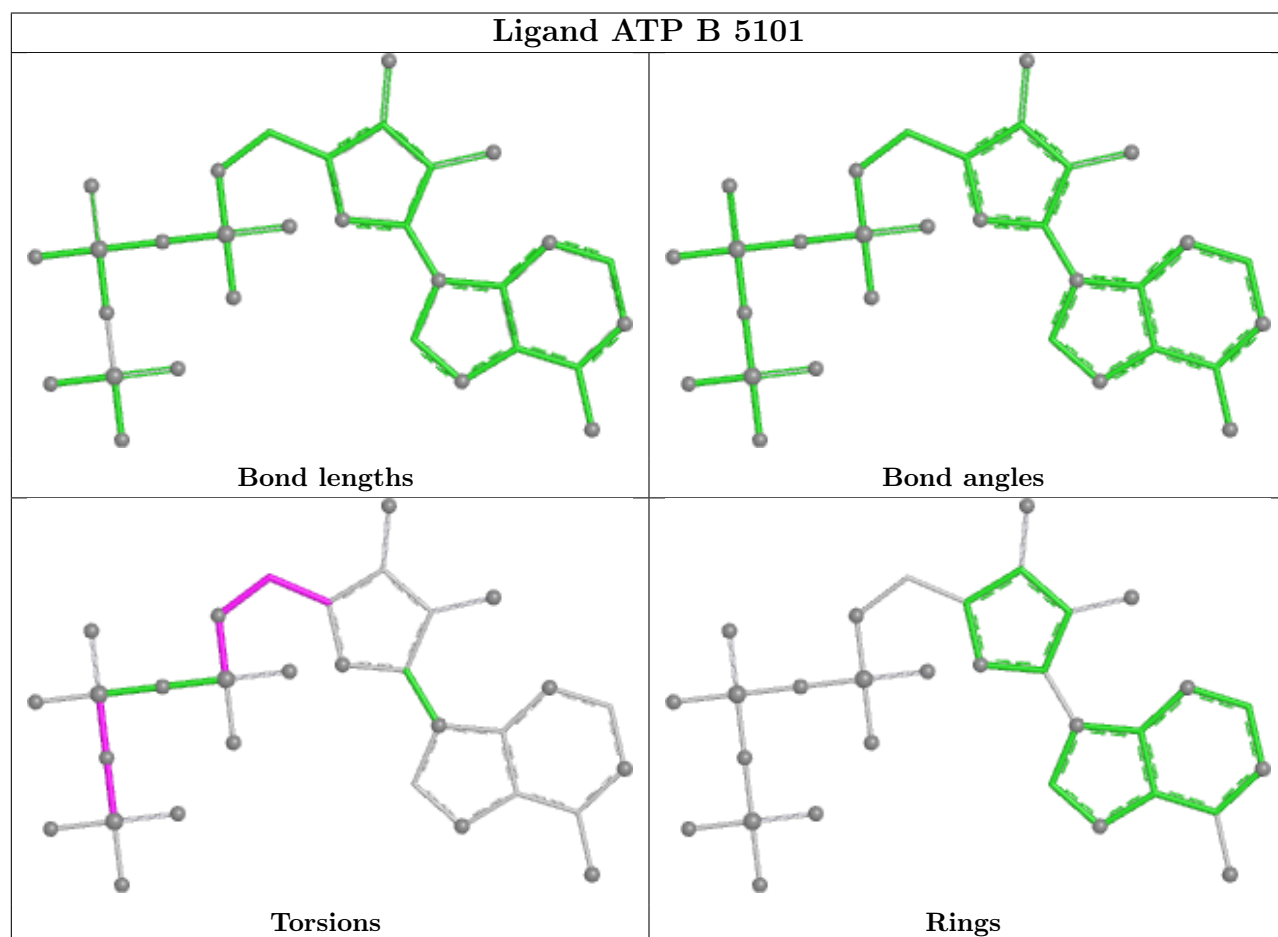
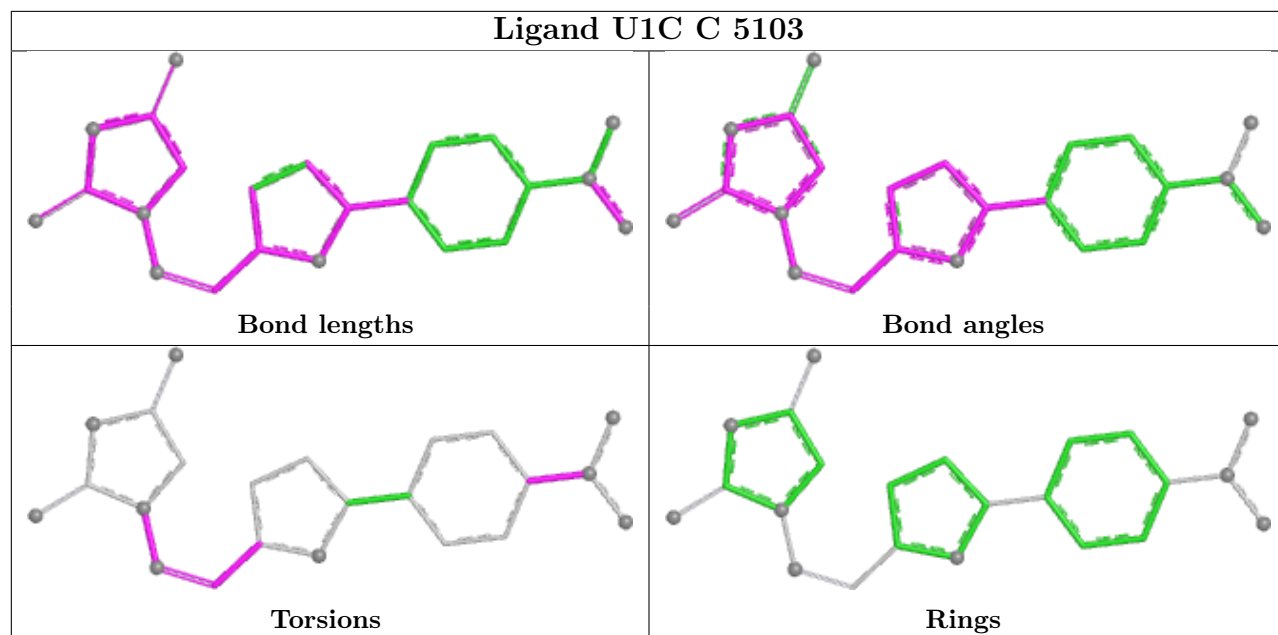
4 monomers are involved in 8 short contacts:

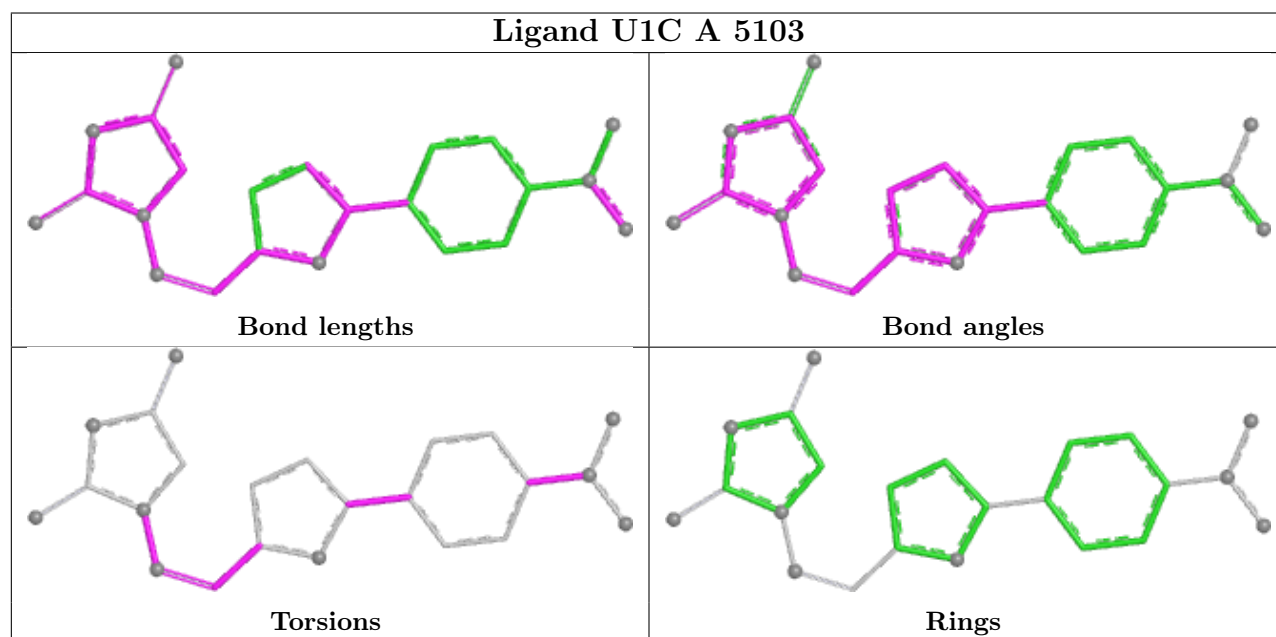
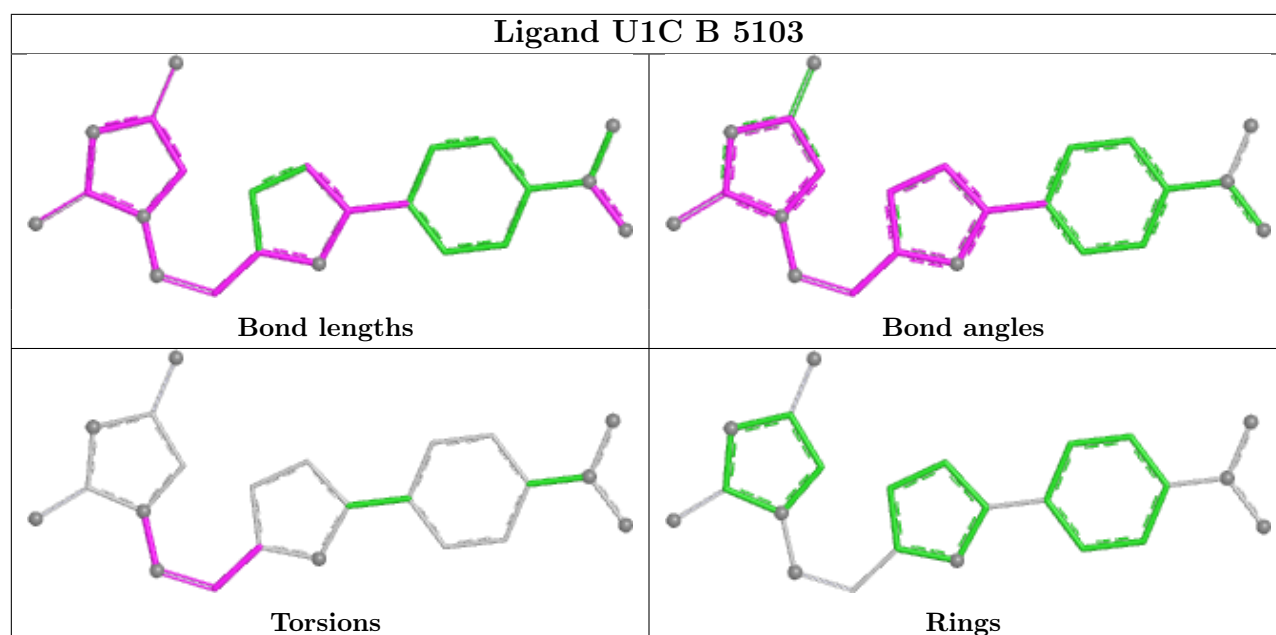
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	5101	ATP	3	0
4	A	5101	ATP	1	0
4	B	5101	ATP	2	0
4	D	5101	ATP	2	0

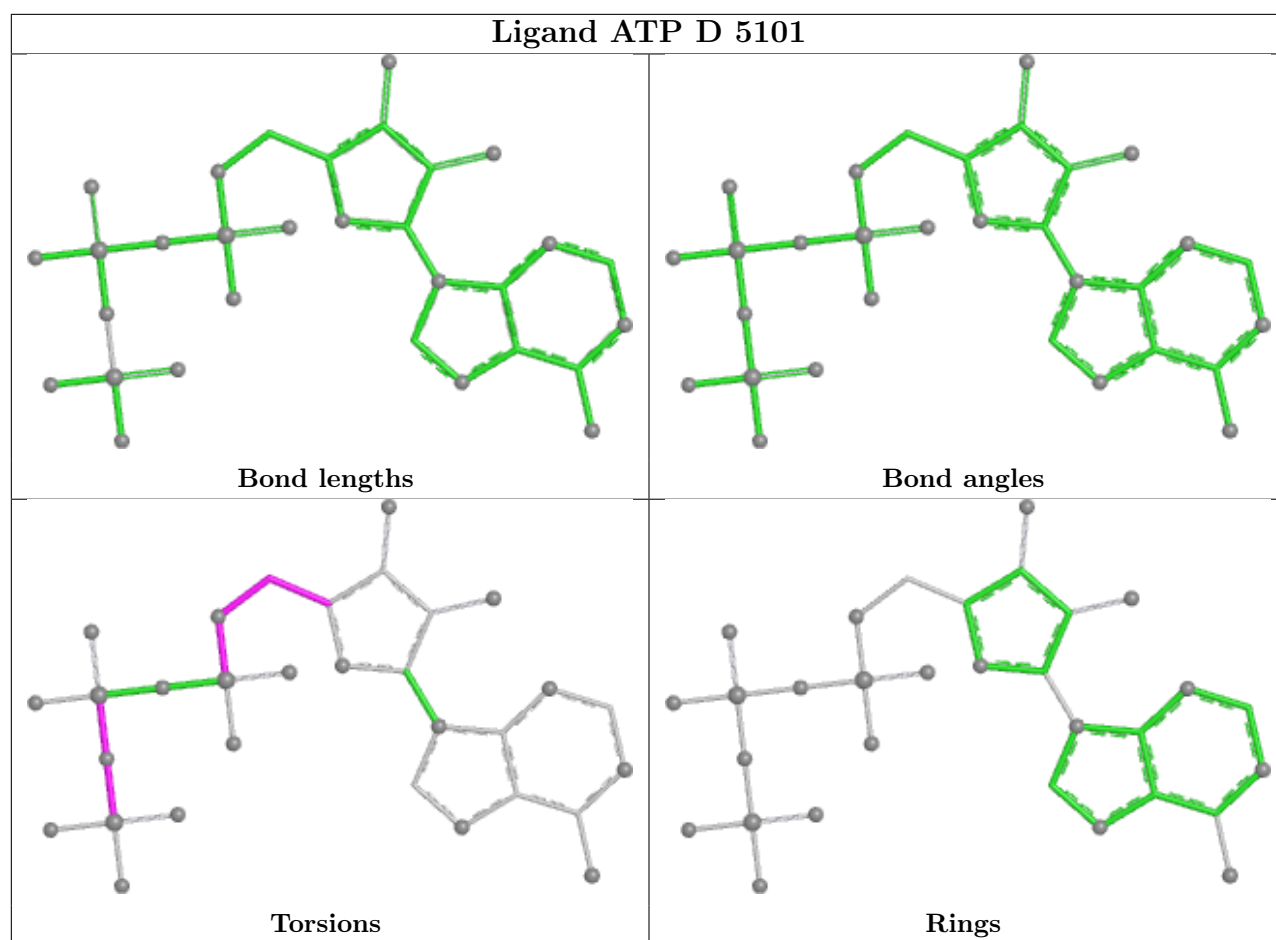
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

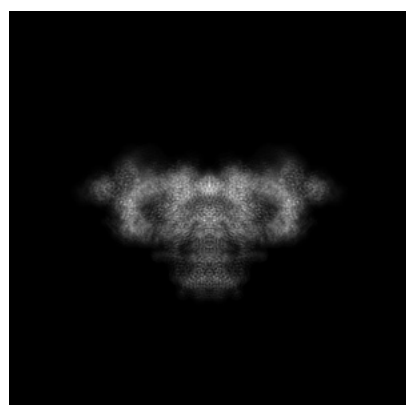
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45585. These allow visual inspection of the internal detail of the map and identification of artifacts.

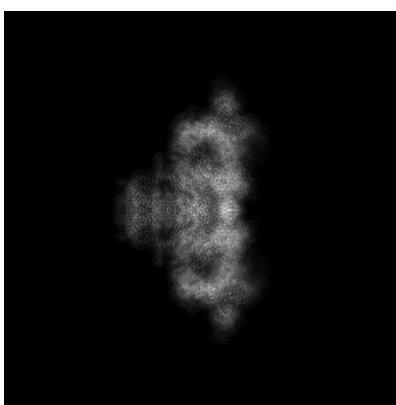
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

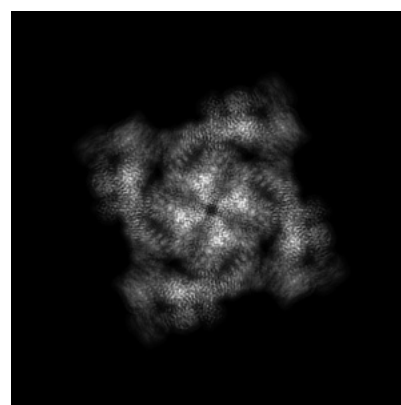
6.1.1 Primary map



X



Y

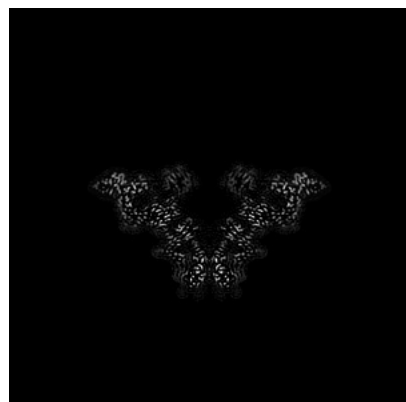


Z

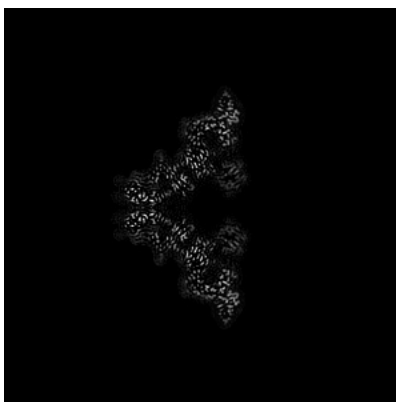
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

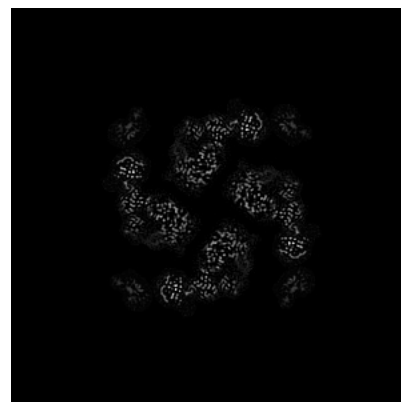
6.2.1 Primary map



X Index: 232



Y Index: 232

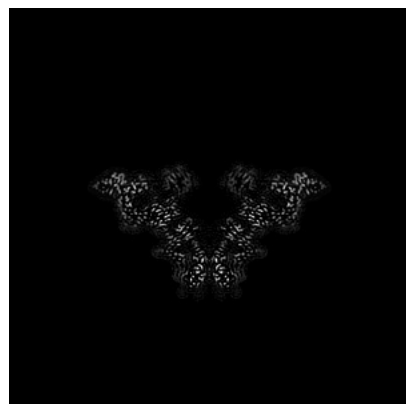


Z Index: 232

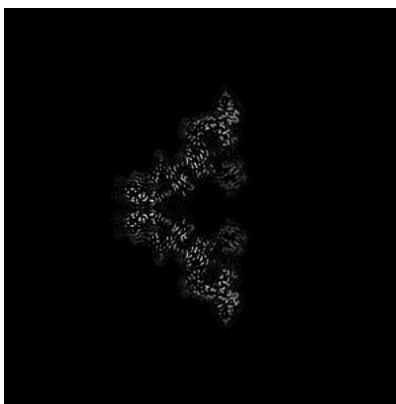
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

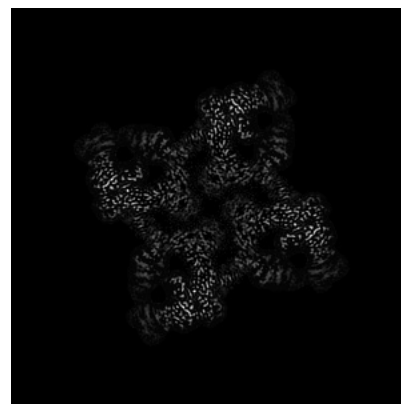
6.3.1 Primary map



X Index: 232



Y Index: 232

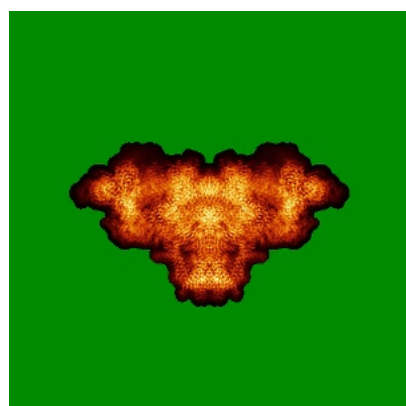


Z Index: 260

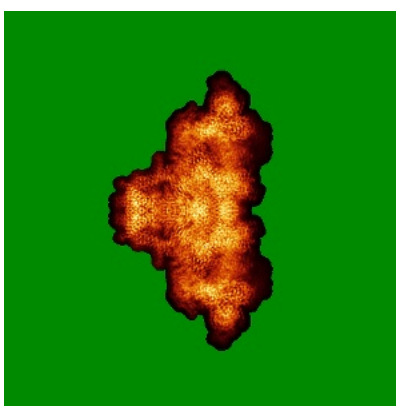
The images above show the largest variance slices of the map in three orthogonal directions.

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

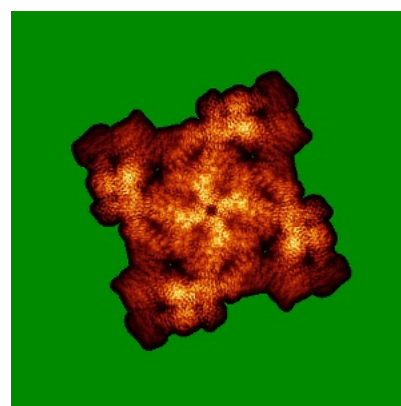
6.4.1 Primary map



X



Y

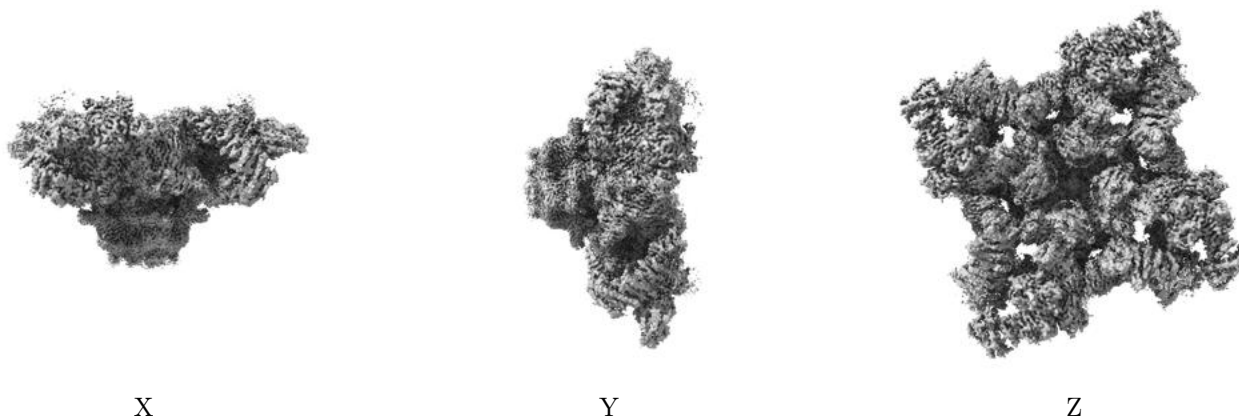


Z

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

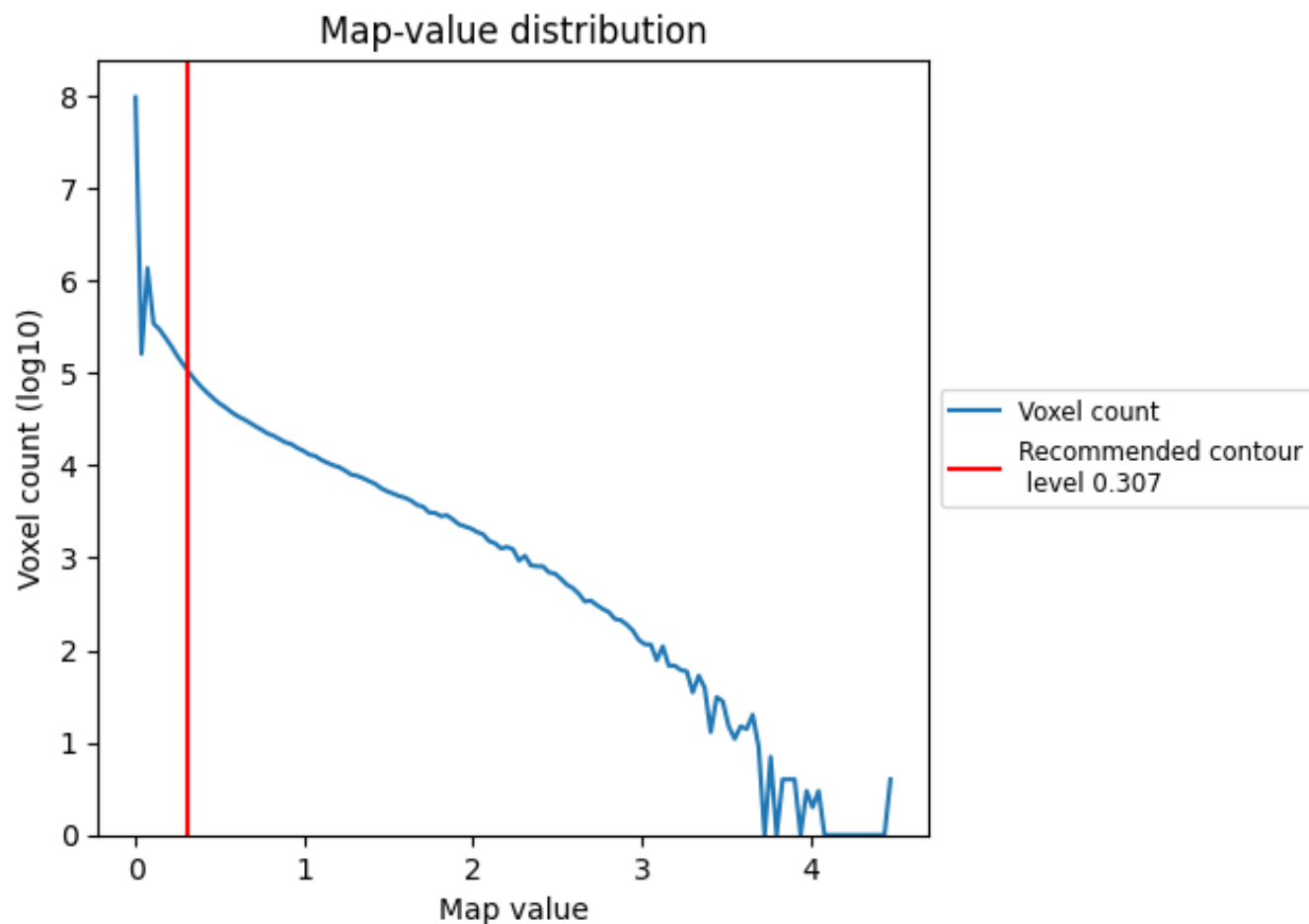
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

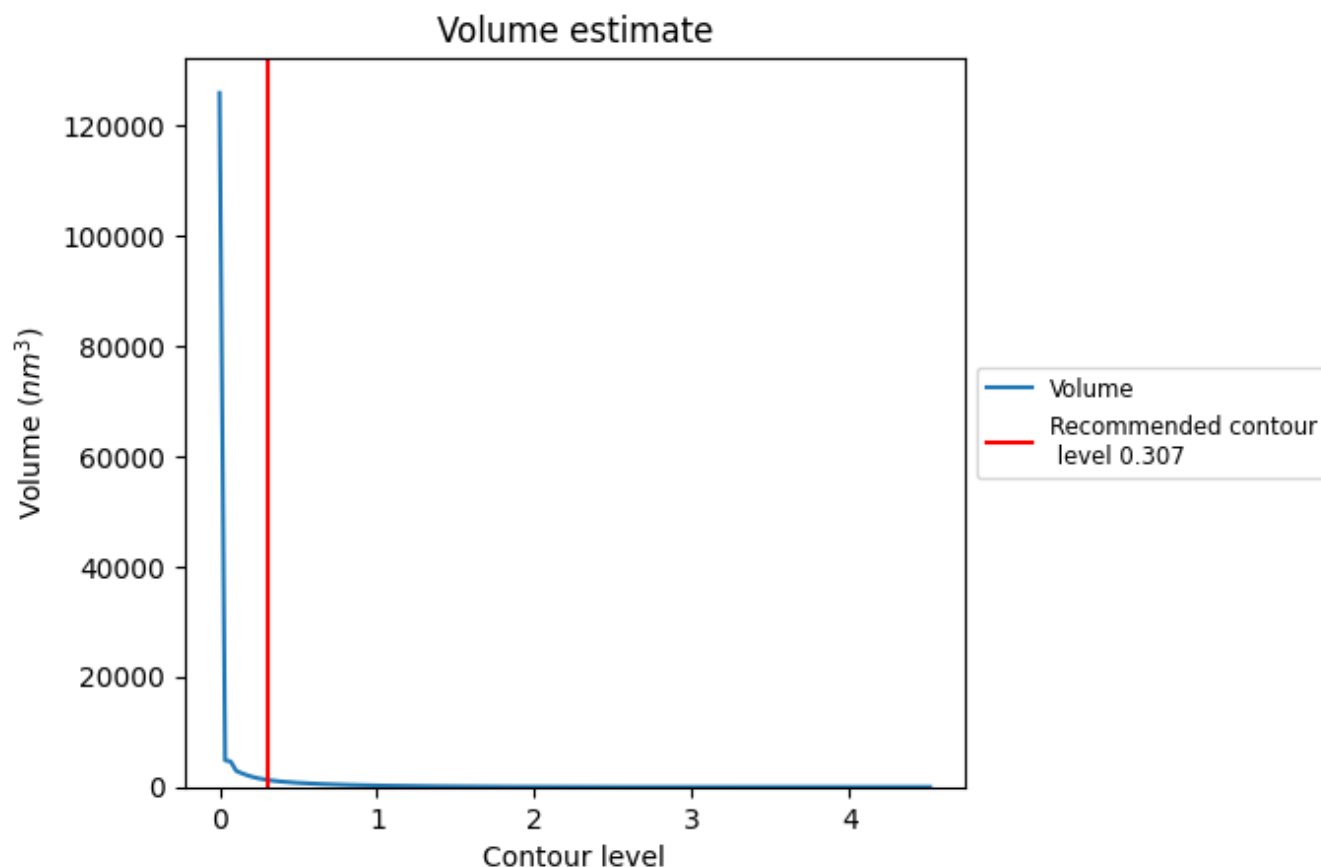
This section contains the results of statistical analysis of the map.

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.

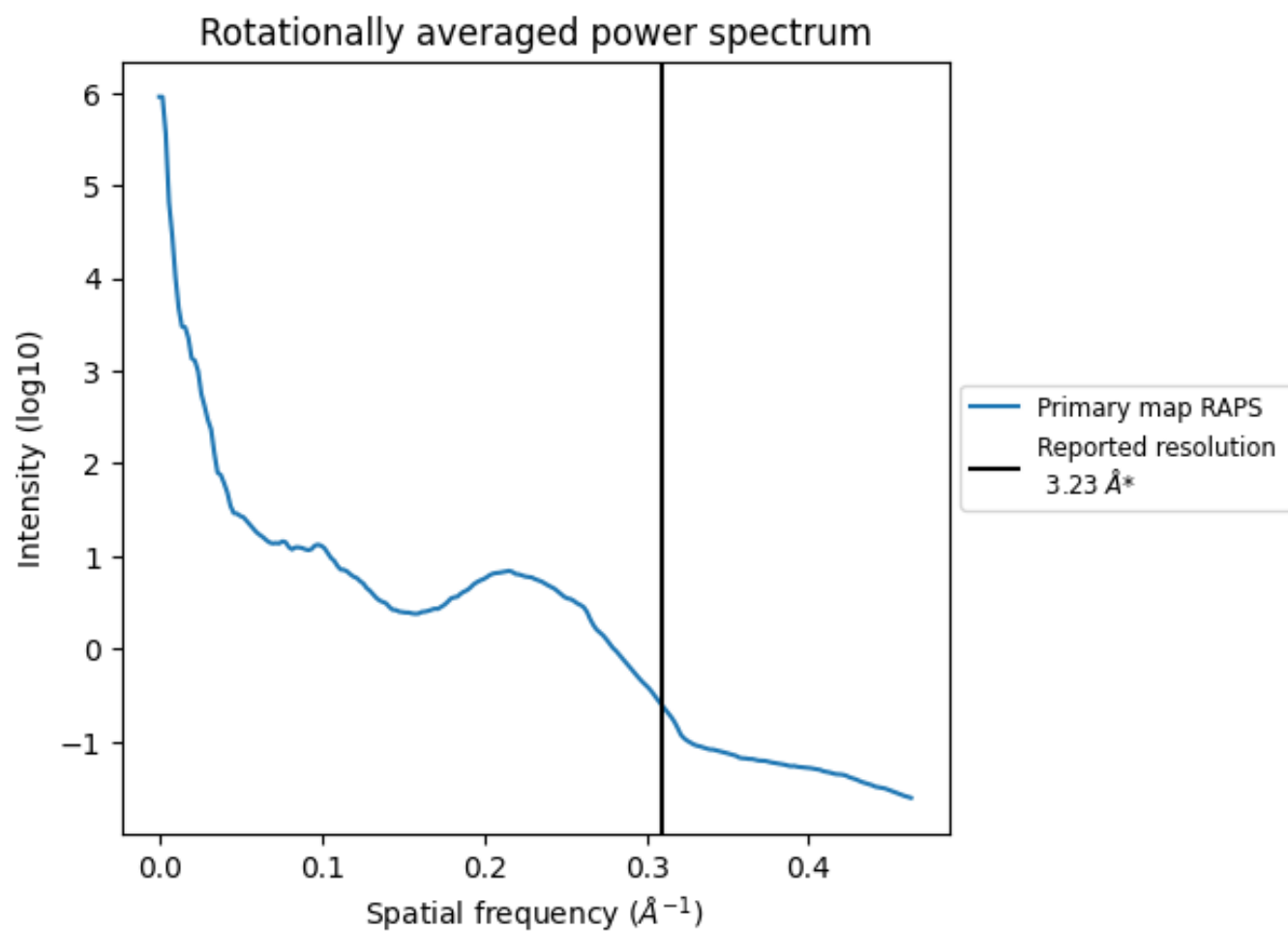
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1262 nm^3 ; this corresponds to an approximate mass of 1140 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 0.310 Å⁻¹

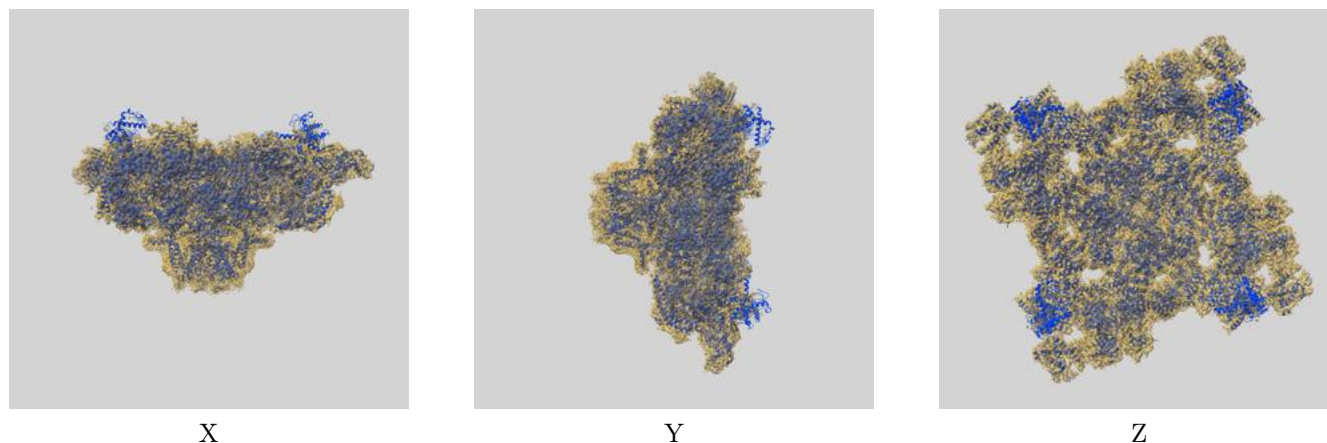
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

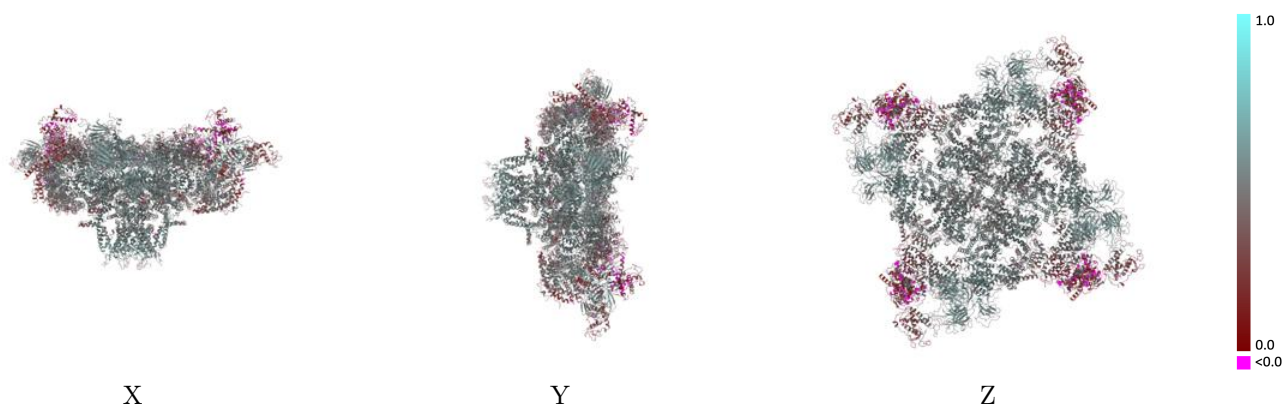
This section contains information regarding the fit between EMDB map EMD-45585 and PDB model 9CGQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



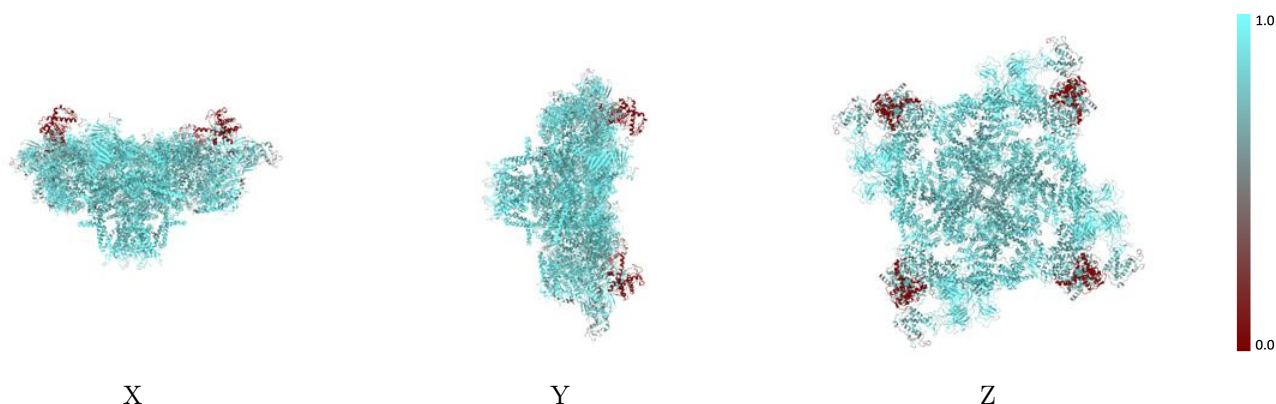
The images above show the 3D surface view of the map at the recommended contour level 0.307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



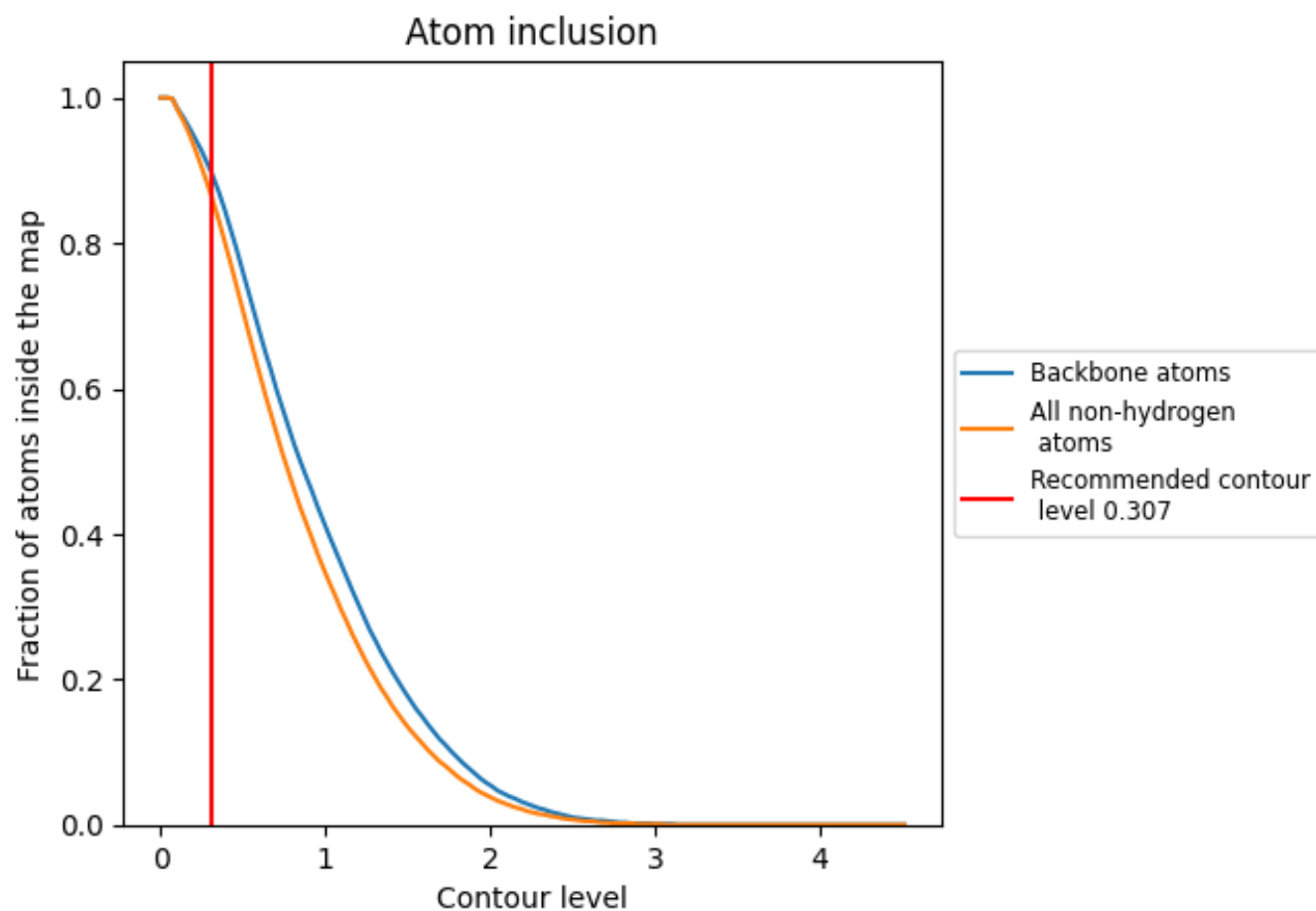
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.307).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% 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 (0.307) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8660	0.4630
A	0.8640	0.4620
B	0.8640	0.4630
C	0.8650	0.4610
D	0.8650	0.4610
E	0.9250	0.5060
F	0.9180	0.5040
G	0.9180	0.5040
H	0.9190	0.5020

