



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 03:37 PM EDT

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.dev133
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) : 2.50

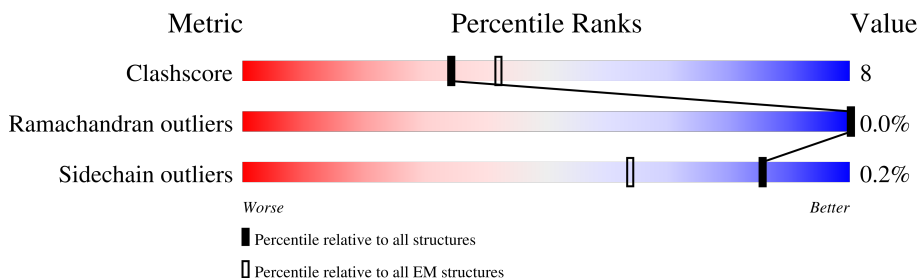
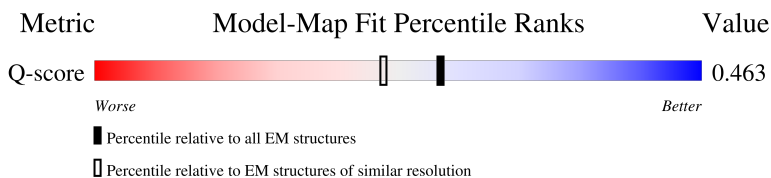
1 Overall quality at a glance

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.



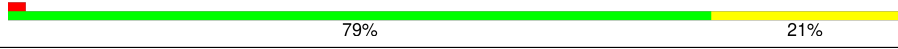
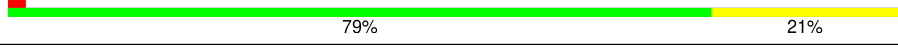
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14612 (2.73 - 3.73)

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%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	107	
2	F	107	
2	G	107	
2	H	107	

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

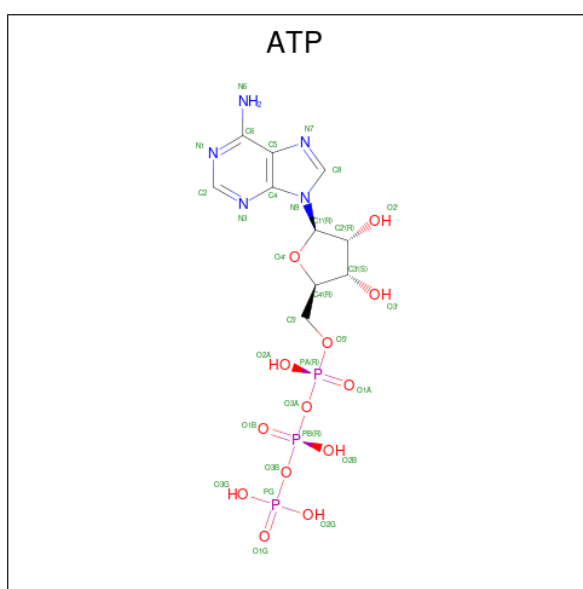
- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

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).

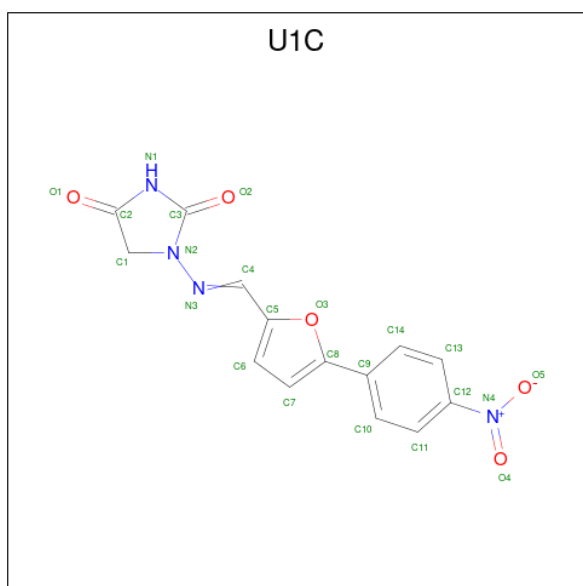
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	

Continued on next page...

Continued from previous page...

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).

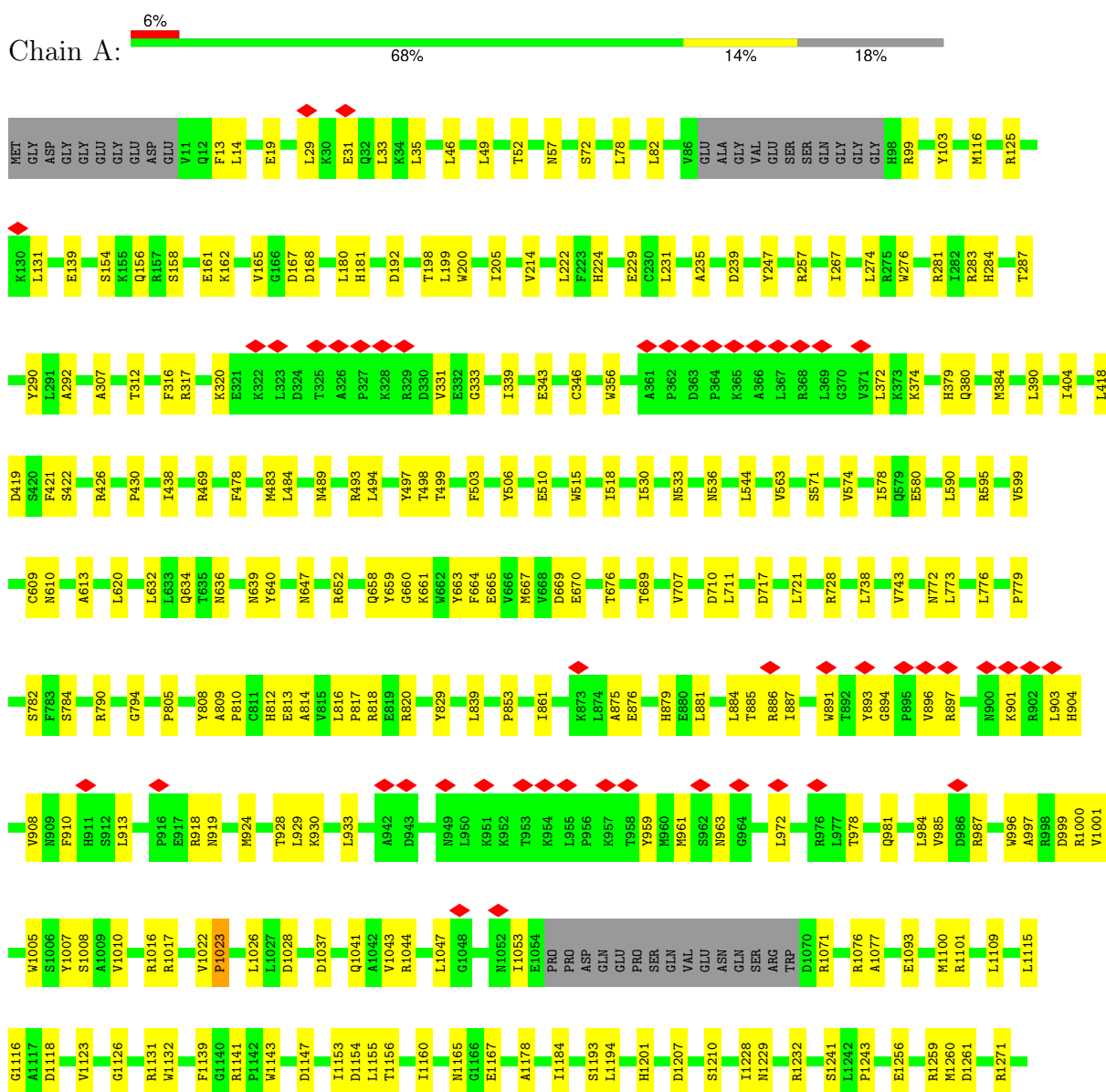


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			23	14	4	5	
6	B	1	Total	C	N	O	0
			23	14	4	5	
6	C	1	Total	C	N	O	0
			23	14	4	5	
6	D	1	Total	C	N	O	0
			23	14	4	5	

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	T2537	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	G2268	Q2107	L2023	ASP	S1778	R1594	PRO	PRO	THR	S1282
K2814	F2754	TYR	L2556	Q2268	Q2107	L2023	ASP	A1784	HIS	ALA	ALA	ALA	L1283
A2815	L2755	ARG	P2560	Q2268	L2116	D2026	GLU	F1787	ASP	VAL	VAL	GLY	F1288
M2816	N2756	MET	L2561	Q2268	M2120	R2028	GLU	ALA	VAL	VAL	VAL	THR	Q1296
L2817	K2757	MET	L2561	Q2268	R2126	L2031	GLU	VAL	GLY	ALA	ALA	PRO	Q1299
A2818	F2758	PRO	P2567	Q2268	Q2127	E2047	GLU	ALA	M1608	D1419	D1420	GLY	HIS
W2819	A2759	CYS	L2568	A2278	Y2128	GLY	ASP	A1794	M1608	R1421	R1421	THR	PHE
E2820	E2760	LEU	F2569	Q2283	L2131	GLU	ALA	L1798	L1613	PRO	PRO	ARG	THR
W2821	Y2761	ALA	A2570	M2283	G2132	GLU	LYS	L1798	Q1614	PRO	PRO	GLN	CYS
T2822	T2762	ILE	R2575	L2286	E2133	GLU	GLU	E1806	V1615	VAL	VAL	GLY	THR
H2763	H2763	ALA	V2579	Q2293	V2149	PRO	GLU	E1806	T1617	I1427	I1427	GLY	ALA
E2764	K2765	ALA	D2580	Q2293	E2150	GLU	GLU	R1808	L1624	C1447	C1447	ALA	ALA
K2825	W2766	PRO	S2581	E2296	D2151	GLU	ALA	L1812	V1448	Y1448	Y1448	THR	ALA
A2826	A2767	LEU	T2585	Q2297	T2152	THR	PRO	L1812	D1632	V1453	V1453	VAL	LEU
R2827	F2768	ASP	T2585	W2298	Y2182	SER	GLY	L1815	L1634	T1454	T1454	ARG	PRO
E2828	D2769	TYR	R2588	L2313	M2178	SER	GLU	R1827	E1643	D1465	D1465	ALA	PRO
G2829	K2770	VAL	K2597	F2334	T2185	SER	LYS	D1828	E1644	GLY	GLY	GLY	GLY
E2830	L2771	ALA	L2597	L2377	M2186	ARG	GLU	P1829	H1645	R1470	R1470	GLN	LEU
GLU	Q2772	ALA	A2609	L2377	W2187	LEU	GLU	V1830	R1646	E1479	E1479	LYS	PRO
ARG	N2773	LYS	L2610	L2384	M2188	SER	GLU	Q1837	L1653	ALA	ALA	ASP	PRO
THR	N2774	THR	C2611	Y2384	M2203	LEU	GLU	V1845	L1667	THR	THR	THR	GLU
GLU	W2775	LYS	T2614	E2387	M2203	LEU	GLU	L1942	L1667	C1489	C1489	ASP	GLU
LYS	S2776	ALA	L2614	E2388	Y2207	THR	THR	H1953	L1671	ALA	ALA	LYS	ALA
LYS	Y2777	LYS	H2621	A2391	N2207	VAL	VAL	M1851	R1672	G1504	G1504	ASN	ARG
THR	G2778	LYS	L2622	ARG	M2208	ARG	ARG	S1957	V1673	Q1505	Q1505	LYS	ALA
ALA	E2779	ALA	L2623	ASP	M2211	LEU	LEU	F1864	V1673	Q1506	Q1506	LYS	ALA
THR	N2780	THR	L2623	GLY	M2212	VAL	VAL	I1866	L1676	G1507	G1507	ARG	GLU
VAL	W2781	VAL	F2628	PRO	N2213	LYS	LYS	I1866	L1676	R1508	R1508	GLY	PRO
ASP	Y2781	ASP	L2628	GLY	Y2214	LYS	LYS	E1874	V1681	P1509	P1509	PHE	ASP
GLN	D2782	ALA	L2633	VAL	L2215	LYS	LYS	GLU	V1681	I1509	I1509	LEU	PRO
THR	E2783	GLY	L2633	ARG	G2216	GLU	GLU	GLU	L1707	S1510	S1510	PRO	ASP
ALA	E2784	GLY	L2633	ARG	G2216	GLU	GLU	GLU	L1707	H1511	H1511	PHE	ASP
GLN	L2784	THR	C2651	ARG	GLY	LYS	LYS	GLU	L1738	F1549	F1549	LYS	TYR
THR	L2785	ASP	W2652	ASP	GLU	PRO	PRO	GLU	L1738	P1550	P1550	LYS	GLY
ASP	K2786	ASP	W2652	ARG	THR	GLU	GLU	GLU	T1746	A1551	A1551	LYS	ASN
PRO	T2787	PRO	T2659	ARG	LYS	GLU	GLU	GLU	L1746	V1552	V1552	ALA	LEU
ARG	H2788	ARG	G2660	GLU	GLU	LEU	LEU	GLU	F1748	F1553	F1553	ALA	ARG
GLY	P2789	GLY	G2660	HIS	T2223	PRO	PRO	GLU	P1749	V1554	V1554	SER	ARG
GLY	M2790	GLY	N2663	PHE	T1995	ALA	ALA	GLU	R1752	L1555	L1555	THR	ALA
N2855	N2790	GLY	L2519	GLY	T1995	GLU	GLU	GLU	K1753	Q1559	Q1559	GLN	GLY
N2856	E2791	GLY	H2520	GLY	T1995	GLU	GLU	GLU	G1754	I1562	I1562	PRO	THR
P2857	E2792	GLY	V2521	P2226	T2230	S2000	GLU	GLU	G1754	I1562	I1562	ALA	ALA
Q2858	R2792	GLY	V2521	T2230	T2230	Q2005	GLU	GLU	R1758	K1568	K1568	THR	PRO
Q2859	P2793	GLY	E2669	F2235	F2235	Q2005	GLU	GLU	R1758	Q1569	Q1569	ALA	GLY
Y2794	T2793	GLY	E2670	L2236	L2236	E2092	GLU	ASP	R1758	Q1569	Q1569	ALA	GLY
K2795	K2795	GLY	E2671	F2236	F2236	S2093	GLU		R1758	Q1569	Q1569	ALA	GLY
K2796	K2796	GLY	L2672	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY
T2796	T2796	GLY	L2672	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY
F2797	F2797	GLY	L2674	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY
S2798	S2798	GLY	L2674	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY
G2864	G2864	GLY	L2674	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY
V2865	V2865	GLY	L2674	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY
T2866	T2866	GLY	L2674	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY
L2867	L2867	GLY	L2674	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY
S2868	S2868	GLY	L2674	L2236	L2236	E2096	GLU		R1758	Q1569	Q1569	ALA	GLY



V2524	I2422	S2281	M2101	Q2005	GLU	P1763	L1613	V1448	PRO	L1184	ARG	G964
G2525	M2423	ILE	W2105	A2016	GLU	P1773	Q1614	W1449	VAL	G1185	TRP	P967
F2526	A2106	GLY	W2106	D2017	GLU	P1773	E1616	V1450	ALA	D1070		L972
W2530	Q2107	LEU	Q2107	E2018	GLU	F1777	T1617	V1453	ASN	C1192		R1076
T2538	L2116	GLY	E2018	E2019	GLU	S1778	R1619	P1455	GLN	L1194		A1077
E2545	M2120	GLY	L2116	L2023	ASP	A1784	R1623	D1456	LYS	Q1198		R976
L2556	R2126	GLU	GLU	D2026	GLU	P1787	L1624	D1465	PRO	W1088		L977
A2445	S2279	GLY	GLU	L2027	GLU	ALA	Q1629	Y1089	ALA	F1090		Q981
G2448	V2280	VAL	GLY	R2028	GLU	GLY	C1630	Y1090	ASP	F1090		L984
L2451	E2133	GLU	ALA	E2047	ASP	GLU	Q1631	Y1090	GLU	E1093		R987
L2460	L2138	GLU	GLU	GLY	GLU	ALA	L1634	C1489	ALA	D1207		W996
D2465	V2149	GLU	L1798	GLU	GLU	A1794	L1638	M1494	PRO	L1211		A997
L2466	E2150	GLU	L1798	GLU	GLU	GLU	A1643	G1504	ASP	E1224		R1000
V2467	D2151	PRO	E1805	GLU	GLU	GLU	L1653	Q1505	ASP	L1115		V1001
G2468	T2152	GLU	E1805	GLU	GLU	GLU	L1659	Q1506	TYR	G1116		Y1007
I2469	M2153	GLU	R1808	ALA	ALA	GLU	L1667	G1507	ALA	D1118		R1017
I2470	L2156	GLU	K1810	GLU	GLU	GLU	L1671	R1508	ASN	V1123		L1021
L2476	L2162	GLU	A1811	GLU	GLU	GLU	R1673	I1509	LEU	F1124		V1022
PRO	L2178	GLU	R1812	GLU	GLU	GLU	A1672	S1510	ARG	N1125		P1023
THR	M2188	GLU	R1814	GLU	GLU	GLU	V1673	H1511	SER	G1126		L1026
LEU	M2188	GLU	L1815	ALA	ALA	GLU	V1681	D1521	ALA	R1131		L1027
GLY	V2207	GLU	R1827	PRO	PRO	GLU	L1694	T1524	GLY	W1132		D1028
ASP	M2208	GLU	D1828	GLU	GLU	GLU	L1698	F1549	TRP	G1140		R1033
G2483	L2211	GLU	R1829	GLU	GLU	GLU	L1698	P1556	GLU	F1141		R1036
K2489	V2212	GLU	V1830	GLU	GLU	GLU	L1707	A1551	GLY	P1142		D1037
S2493	V2213	GLU	Q1837	GLU	GLU	GLU	R1708	V1552	LYS	W1143		Q1041
P2494	L2214	GLU	V1845	GLU	GLU	GLU	Y1712	F1553	GLY	D1147		R1044
V2495	G2216	GLU	M1851	GLU	GLU	GLU	L1715	V1554	GLY	M1152		G1048
P2496	L2215	GLU	F1854	GLU	GLU	GLU	I1716	L1555	THR	I1153		Y1051
L2626	GLY	GLU	L1862	GLU	GLU	GLU	S1717	H1558	GLY	D1154		E1054
D2497	GLY	GLU	L1863	GLU	GLU	GLU	E1721	Q1559	GLY	L1156		T1159
H2498	THR	GLU	F1871	GLU	GLU	GLU	M1730	I1562	PRO	T1159		I1161
P2628	L2223	GLU	E1874	GLU	GLU	GLU	L1738	K1568	GLY	I1161		L1164
P2631	P2226	GLU	GLU	GLU	GLU	GLU	T1746	P1574	THR	L1164		G1166
A2637	T2230	GLU	GLU	GLU	GLU	GLU	T1747	M1579	PRO	G1166		N1165
L2641	F2235	PRO	GLU	GLU	GLU	GLU	F1748	R1594	GLN	C1166		Y1167
C2651	L2236	PRO	GLU	GLU	GLU	GLU	P1749	L1595	PRO	V1168		L1169
W2652	Q2247	GLU	GLU	GLU	GLU	GLU	R1752	L1600	VAL	GLY		GLU
T2659	Y2256	ASN	GLU	GLU	GLU	GLU	R1758	V1603	GLU	ALA		ASN
G2660		ARG	GLU	GLU	GLU	GLU		V1603	GLN	THR		GLN
V2663								M1608	PRO	PRO		SER
E2669												

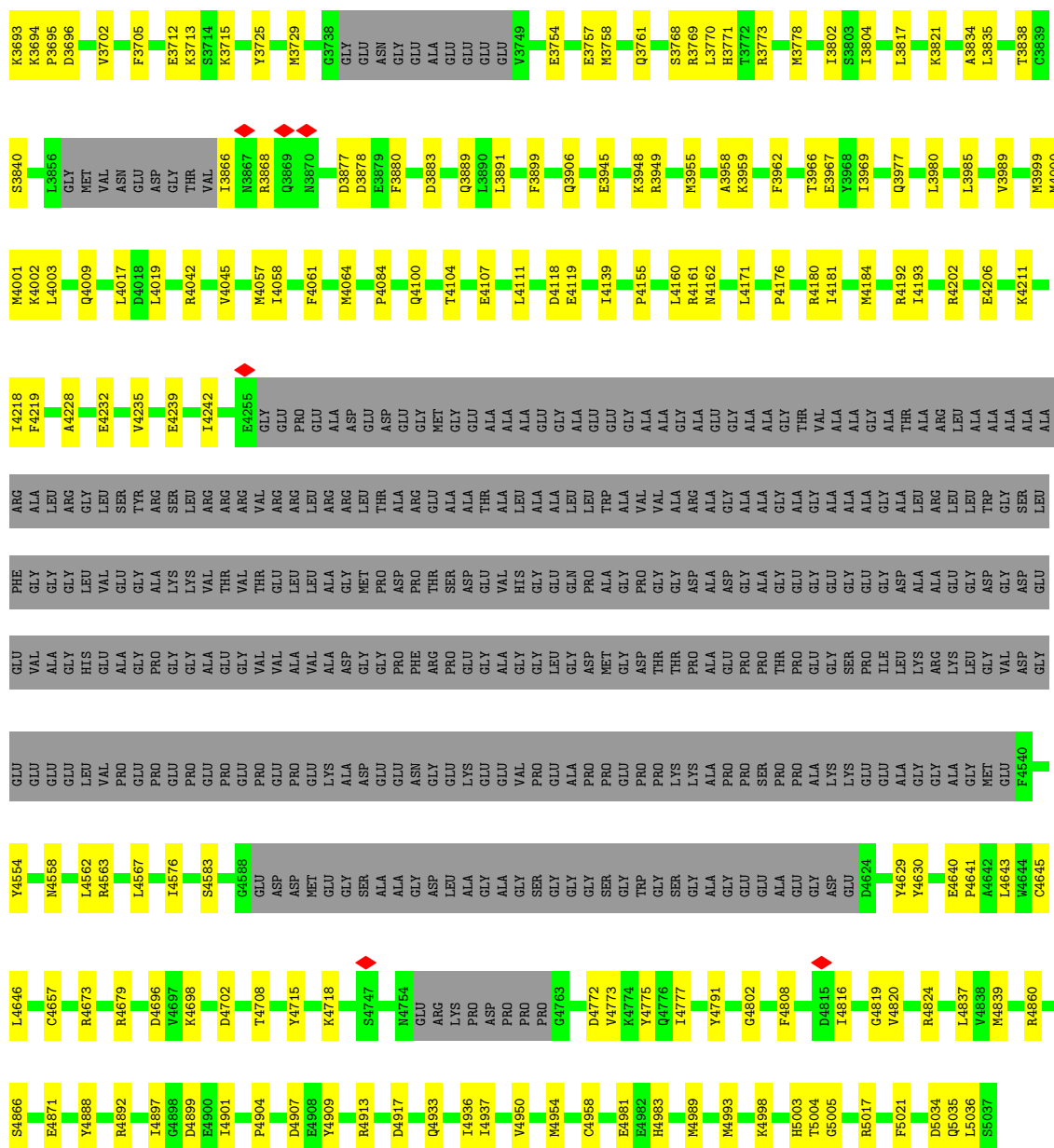


GLU	ASN	ARG	V2416	H2420	A2421	I2422	M2423	I2430	A2445	L2460	V2461	P2462	L2463	D2464	D2465	L2466	I2470	I2476	THR	LEU	GLY	LYS	ASP	G2483	K2489	S2493	F2494	V2495	P2496	D2497	N2502	F2505	L2506	V2509	Y2510	G2511	I2512	D2516	L2519	H2520	V2521	G2524	V2525	F2526					
Y2256	S2261	ILE	GLY	GLY	LEU	GLY	MET	Q2268	A2278	N2283	L2286	D2294	E2150	D2161	T2152	L2162	M2178	V2207	M2211	V2212	N2213	V2214	L2215	G2216	GLY	GLY	THR	LYS	GLY	ARG	ASP	GLY	PRO	ARG	ARG	ARG	ARG	GLY	HIS	PHE	GLY	GLU	PRO	PRO	GLU				
Q2095	E2096	M2101	Q2107	L2116	R2126	Q2127	Y2128	E2133	L2138	V2149	E2150	D2161	T2152	L2162	M2178	V2207	M2211	V2212	N2213	V2214	L2215	G2216	GLY	GLY	GLY	THR	LYS	GLY	ARG	ASP	GLY	PRO	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG	ARG					
S2000	Q2005	L2010	E2019	L2023	D2026	I2027	R2028	E2047	GLY	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	R1813	M1814	L1815	R1827	D1828	P1829	V1830	Q1837	V1845	M1851	F1854	E1874	GLU	GLU	E1989	E1990	T1991	T1995	R1996							
GLU	GLU	GLU	GLU	GLU	GLU	GLU	ASP	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	GLU	PRO	GLY	LYS	GLU	GLU	GLU	GLU	D1921	K1936	L1943	H1953	S1957	E1963	M1985	M1986	A1989	E1990	T1991	T1995	R1996									
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					
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	T1524	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	THR	PRO	ALA	ALA	D1419	N1420	R1421	D1422	D1423	T1426	Y1434											
THR	PRO	LEU	ALA	PRO	PRO	GLY	LEU	PRO	GLU	ALA	ASP	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					
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	K952	T953	K954	L955
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			
N1052	I1053	E1054	PRO	ASP	GLN	GLU	PRO	GLU	GLU	GLN	VAL	GLU	ASN	GLN	SER	ARG	TRP	D1070	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				



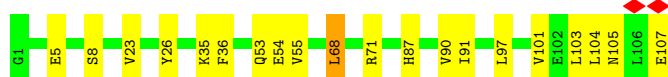
R52	R20	R18	D108	R141	THR	PRO	Y148	L160	G154	G174	L203	R216	S261
R59	Y829	N919	R1033	D1154	GLY	GLY	S1436	L1608	R1758	Q2127	L2026	Q2128	Q2127
P842	P842	L922	R1036	L1155	ALA	ALA	V1437	L1613	R1759	D2027	R2028	E2047	Q2128
I861	I861	G926	D1037	T1156	THR	THR	C1447	Q1614	P1763	L1771	E2047	L2138	Q2128
V862	V862	K930	C1040	E1167	PRO	PRO	T1454	V1615	L1771	S1778	E2047	V2149	E2150
P863	P863	L933	Q1041	D1456	ALA	ALA	P1455	E1616	P1778	Q2127	E2047	D2151	E2150
P865	P865	A934	R1044	S1171	GLY	GLY	D1456	T1617	P1787	Q2127	E2047	M2163	E2150
V866	V866	G937	G1048	S1175	LEU	LEU	R1470	R1618	Q2127	Q2127	E2047	I2162	E2150
H867	H867	A942	E1054	I1182	GLN	GLN	Q1480	R1619	Q2127	Q2127	E2047	L2166	E2150
L867	L867	D942	PRO	E1183	PRO	PRO	C1489	L1624	Q2127	Q2127	E2047	M2178	E2150
E868	E868	P943	ASP	I1184	ALA	ALA	C1489	Q1629	Q2127	Q2127	E2047	P2325	E2150
R869	R869	E944	GLN	S1193	ASP	ASP	S1502	D1632	Q2127	Q2127	E2047	L2166	E2150
T870	T870	K945	GLU	G1197	ALA	ALA	P1503	L1634	Q2127	Q2127	E2047	Q2165	E2150
G708	G708	D946	PRO	H1201	ARG	ARG	Q1504	E1643	Q2127	Q2127	E2047	L2166	E2150
D709	D709	N949	SER	H1201	ALA	ALA	Q1506	E1644	Q2127	Q2127	E2047	M2186	E2150
D710	D710	T953	GLN	L1204	ALA	ALA	G1507	R1646	Q2127	Q2127	E2047	N2188	E2150
S713	S713	K964	ASN	L1207	PRO	PRO	T1509	L1653	Q2127	Q2127	E2047	M2203	E2150
R728	R728	L881	SER	D1207	ASP	ASP	S1510	L1667	Q2127	Q2127	E2047	V2207	E2150
L737	L737	L884	ARG	S1210	PRO	PRO	H1511	L1671	Q2127	Q2127	E2047	M2210	E2150
V743	V743	T885	TRP	L1211	THR	THR	S1510	R1678	Q2127	Q2127	E2047	M2211	E2150
N772	N772	I887	GLY	T1228	GLY	GLY	H1511	M1678	Q2127	Q2127	E2047	M2212	E2150
L773	L773	E888	GLY	N1229	TRP	TRP	D1521	V1681	Q2127	Q2127	E2047	M2214	E2150
L776	L776	Q889	ASP	R1232	ALA	ALA	T1524	D1690	Q2127	Q2127	E2047	M2215	E2150
W891	W891	N961	Y1089	P1243	ALA	ALA	E1535	Q1693	Q2127	Q2127	E2047	M2216	E2150
T892	T892	N963	F1090	Q1244	GLY	GLY	F1539	L1707	Q2127	Q2127	E2047	M2217	E2150
Y893	Y893	G964	E1093	F1245	TRP	TRP	F1549	R1708	Q2127	Q2127	E2047	M2218	E2150
F763	F763	L972	E1099	E1256	GLY	GLY	V1552	Y1712	Q2127	Q2127	E2047	M2219	E2150
S784	S784	S973	M1100	R1101	GLY	GLY	F1553	S1717	Q2127	Q2127	E2047	M2220	E2150
R790	R790	N991	L1109	R1271	LYS	LYS	L1555	E1721	Q2127	Q2127	E2047	M2221	E2150
G794	G794	W995	L1115	R1275	GLY	GLY	Q1559	L1738	Q2127	Q2127	E2047	M2222	E2150
K801	K801	W996	G1116	F1288	THR	THR	T1562	T1746	Q2127	Q2127	E2047	M2223	E2150
F802	F802	A997	V1123	F1288	ALA	ALA	Q1563	L1747	Q2127	Q2127	E2047	M2224	E2150
P805	P805	D999	N1125	F1288	LYS	LYS	K1568	F1748	Q2127	Q2127	E2047	M2225	E2150
Y808	Y808	R1000	Q1130	S1292	GLY	GLY	Q1570	P1749	Q2127	Q2127	E2047	M2226	E2150
A809	A809	C906	R1131	L1293	THR	THR	N1571	R1752	Q2127	Q2127	E2047	M2227	E2150
P810	P810	N907	W1132	HIS	PRO	PRO	T1572	K1752	Q2127	Q2127	E2047	M2228	E2150
C811	C811	N909	S1136	PHE	GLY	GLY	M1573	L1594	Q2127	Q2127	E2047	M2229	E2150
H812	H812	F910	F1139	ARG	THR	THR	P1574	L1595	Q2127	Q2127	E2047	M2230	E2150
L816	L816	N917	G1140	CYS	GLM	GLM	M1579		Q2127	Q2127	E2047	M2231	E2150
P817	P817	V1022							Q2127	Q2127	E2047	M2232	E2150
R818	R818	P1023							Q2127	Q2127	E2047	M2233	E2150
E819	E819	L1026							Q2127	Q2127	E2047	M2234	E2150
		E915							Q2127	Q2127	E2047	M2235	E2150
		P916							Q2127	Q2127	E2047	M2236	E2150
		E917							Q2127	Q2127	E2047	M2237	E2150
									Q2127	Q2127	E2047	M2238	E2150
									Q2127	Q2127	E2047	M2239	E2150
									Q2127	Q2127	E2047	M2240	E2150
									Q2127	Q2127	E2047	M2241	E2150
									Q2127	Q2127	E2047	M2242	E2150
									Q2127	Q2127	E2047	M2243	E2150
									Q2127	Q2127	E2047	M2244	E2150
									Q2127	Q2127	E2047	M2245	E2150
									Q2127	Q2127	E2047	M2246	E2150
									Q2127	Q2127	E2047	M2247	E2150
									Q2127	Q2127	E2047	M2248	E2150
									Q2127	Q2127	E2047	M2249	E2150
									Q2127	Q2127	E2047	M2250	E2150
									Q2127	Q2127	E2047	M2251	E2150
									Q2127	Q2127	E2047	M2252	E2150
									Q2127	Q2127	E2047	M2253	E2150
									Q2127	Q2127	E2047	M2254	E2150
									Q2127	Q2127	E2047	M2255	E2150
									Q2127	Q2127	E2047	M2256	E2150
									Q2127	Q2127	E2047	M2257	E2150
									Q2127	Q2127	E2047	M2258	E2150
									Q2127	Q2127	E2047	M2259	E2150
									Q2127	Q2127	E2047	M2260	E2150
									Q2127	Q2127	E2047	M2261	E2150
									Q2127	Q2127	E2047	M2262	E2150
									Q2127	Q2127	E2047	M2263	E2150
									Q2127	Q2127	E2047	M2264	E2150
									Q2127	Q2127	E2047	M2265	E2150
									Q2127	Q2127	E2047	M2266	E2150
									Q2127	Q2127	E2047	M2267	E2150
									Q2127	Q2127	E2047	M2268	E2150
									Q2127	Q2127	E2047	M2269	E2150
									Q2127	Q2127	E2047	M2270	E2150
									Q2127	Q2127	E2047	M2271	E2150
									Q2127	Q2127	E2047	M2272	E2150
									Q2127	Q2127	E2047	M2273	E2150
									Q2127	Q2127	E2047	M2274	E2150
									Q2127	Q2127	E2047	M2275	E2150
									Q2127	Q2127	E2047	M2276	E2150
									Q2127	Q2127	E2047	M2277	E2150
									Q2127	Q2127	E2047	M2278	E2150
									Q2127	Q2127	E2047	M2279	E2150
									Q2127	Q2127	E2047	M2280	E2150
									Q2127	Q2127	E2047	M2281	E2150
									Q2127	Q2127	E2047	M2282	E2150
									Q2127	Q2127	E2047	M2283	E2150
									Q2127	Q2127	E2047	M2284	E2150
									Q2127	Q2127	E2047	M2285	E2150
									Q2127	Q2127	E2047	M2286	E2150
									Q2127	Q2127	E2047	M2287	E2150
									Q2127	Q2127	E2047	M2288	E2150
									Q2127	Q2127	E2047	M2289	E2150
									Q2127	Q2127	E2047	M2290	E2150
									Q2127	Q2127	E2047	M2291	E2150
									Q2127	Q2127	E2047	M2292	E2150
									Q2127	Q2127	E2047	M2293	E2150
									Q2127	Q2127	E2047	M2294	E2150
									Q2127	Q2127	E2047	M2295	E2150
									Q2127	Q2127	E2047	M2296	E2150
									Q2127	Q2127	E2047	M2297	E2150
									Q2127	Q2127	E2047	M2298	E2150
									Q2127	Q2127	E2047	M2299	E2150
									Q2127	Q2127	E2047	M2300	E2150
									Q2127	Q2127	E2047	M2301	E2150
									Q2127	Q2127	E2047	M2302	E2150
									Q2127	Q2127	E2047	M2303	E2150
									Q2127	Q2127	E2047	M2304	E2150
									Q2127	Q2127	E2047	M2305	E2150
									Q2127	Q2127	E2047	M2306	E2150
									Q2127	Q2127	E2047	M2307	E2150
									Q2127	Q2127	E2047	M2308	E2150
									Q2127	Q2127	E2047	M2309	E2150
									Q2127	Q2127	E2047	M2310	E2150
									Q2127	Q2127	E2047	M2311	E2150
									Q2127	Q2127	E2047	M2312	E2150
									Q2127	Q2127	E2047	M2313	E2150
									Q2127	Q2127	E2047	M2314	E2150
									Q2127	Q2127	E2047	M2315	E2150
									Q2127	Q2127	E2047	M2316	E2150





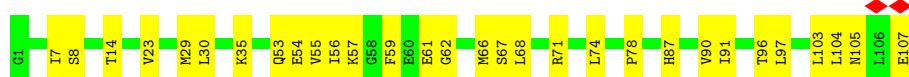
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain E:



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

Chain F:



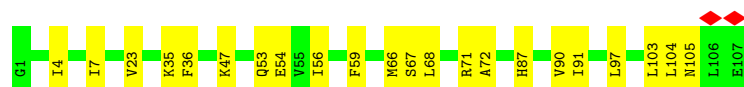
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

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 [i](#)

5.1 Standard geometry [i](#)

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	D	5101	-	32,33,33	0.26	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%)
4	ATP	B	5101	-	32,33,33	0.25	0	48,52,52	0.27	0
4	ATP	C	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%)
4	ATP	A	5101	-	32,33,33	0.25	0	48,52,52	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	U1C	C	5103	-	25,25,25	6.18	16 (64%)	33,35,35	3.38	15 (45%)
6	U1C	A	5103	-	25,25,25	6.17	15 (60%)	33,35,35	3.43	15 (45%)

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	5101	-	-	6/22/38/38	0/3/3/3
6	U1C	D	5103	-	-	7/11/25/25	0/3/3/3
4	ATP	B	5101	-	-	7/22/38/38	0/3/3/3
4	ATP	C	5101	-	-	9/22/38/38	0/3/3/3
6	U1C	B	5103	-	-	5/11/25/25	0/3/3/3
4	ATP	A	5101	-	-	7/22/38/38	0/3/3/3
6	U1C	C	5103	-	-	7/11/25/25	0/3/3/3
6	U1C	A	5103	-	-	11/11/25/25	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:

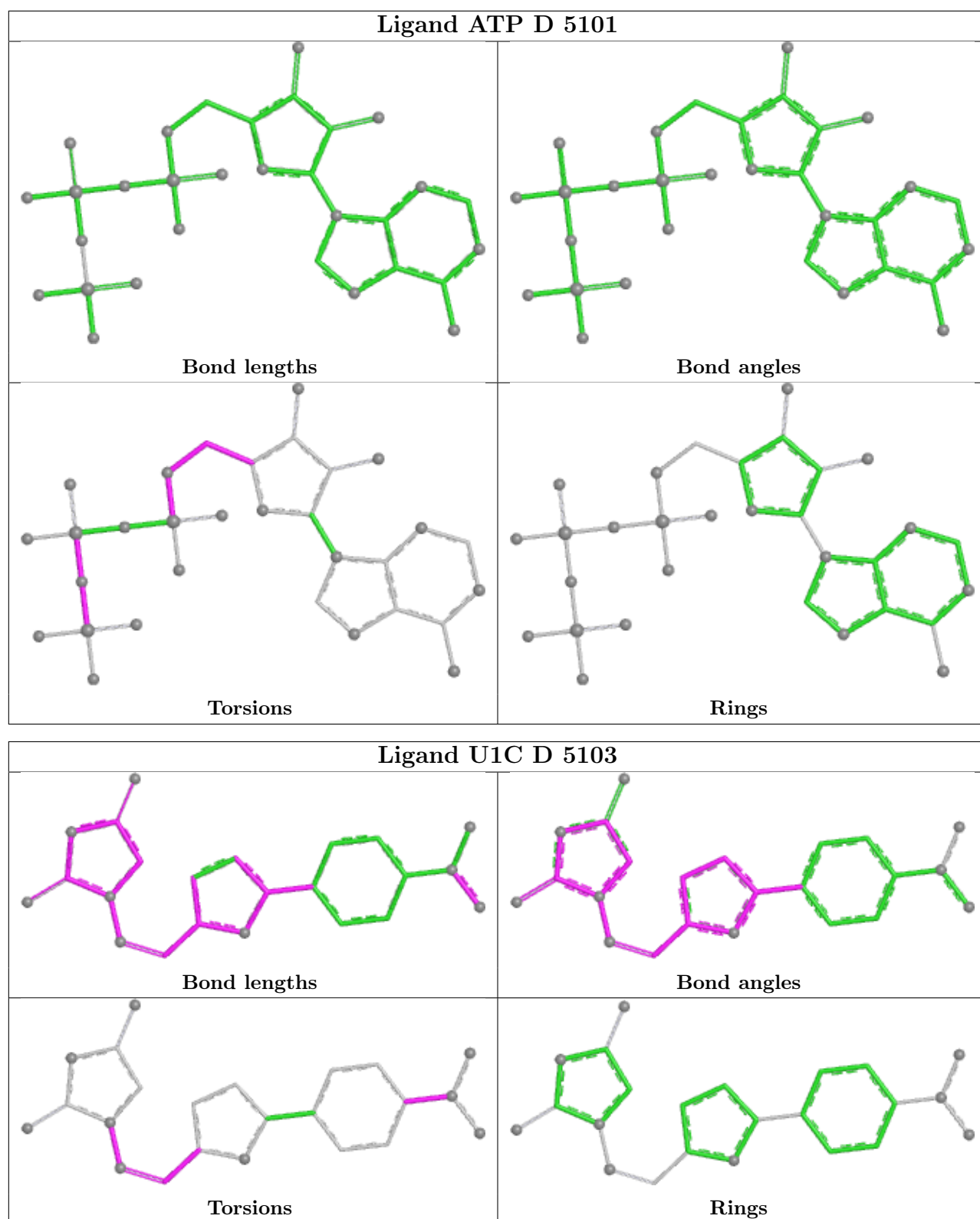
Mol	Chain	Res	Type	Atoms
4	A	5101	ATP	PB-O3B-PG-O2G
4	A	5101	ATP	C5'-O5'-PA-O1A
4	A	5101	ATP	O4'-C4'-C5'-O5'
4	B	5101	ATP	PB-O3B-PG-O2G
4	B	5101	ATP	C5'-O5'-PA-O1A

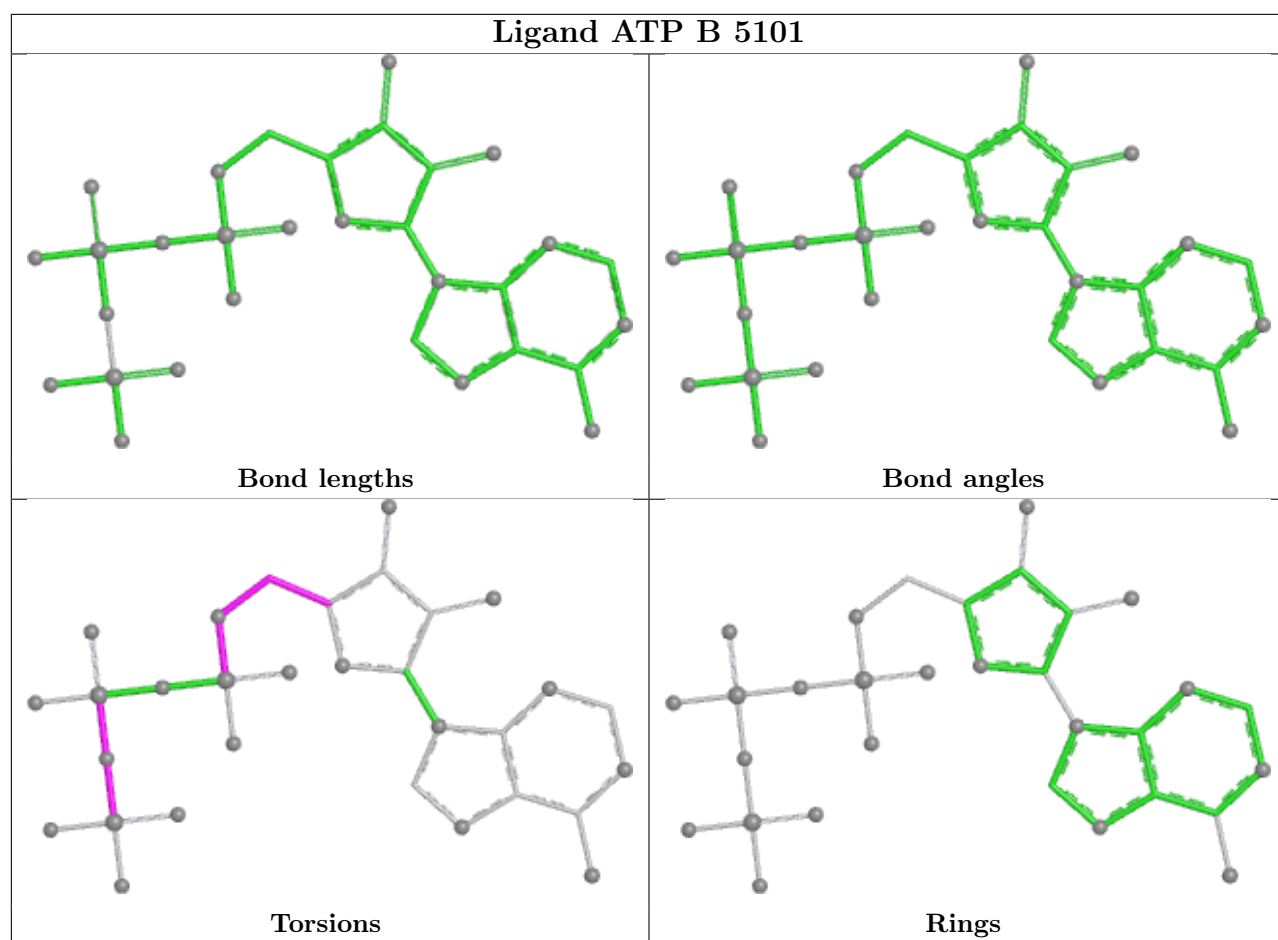
There are no ring outliers.

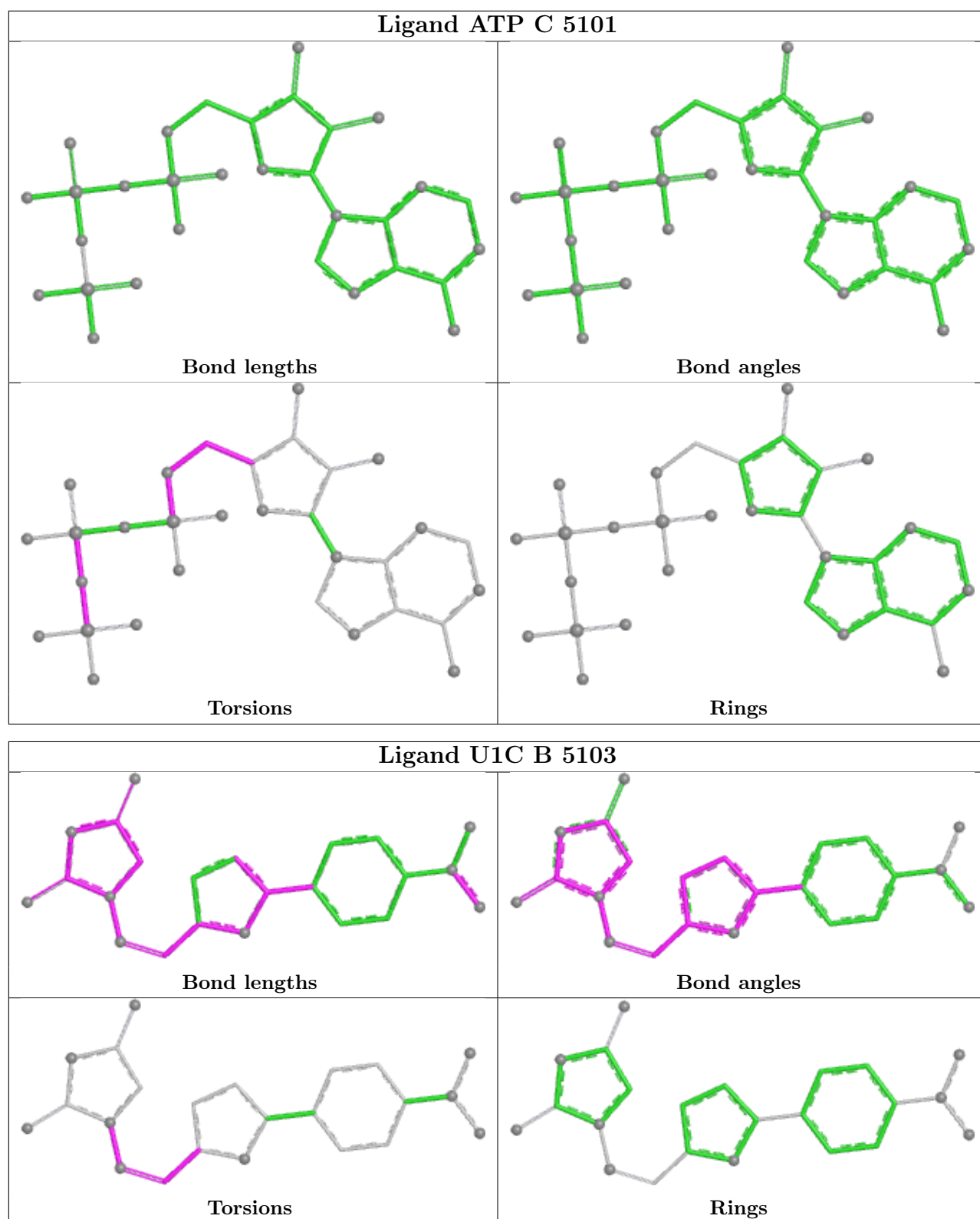
4 monomers are involved in 8 short contacts:

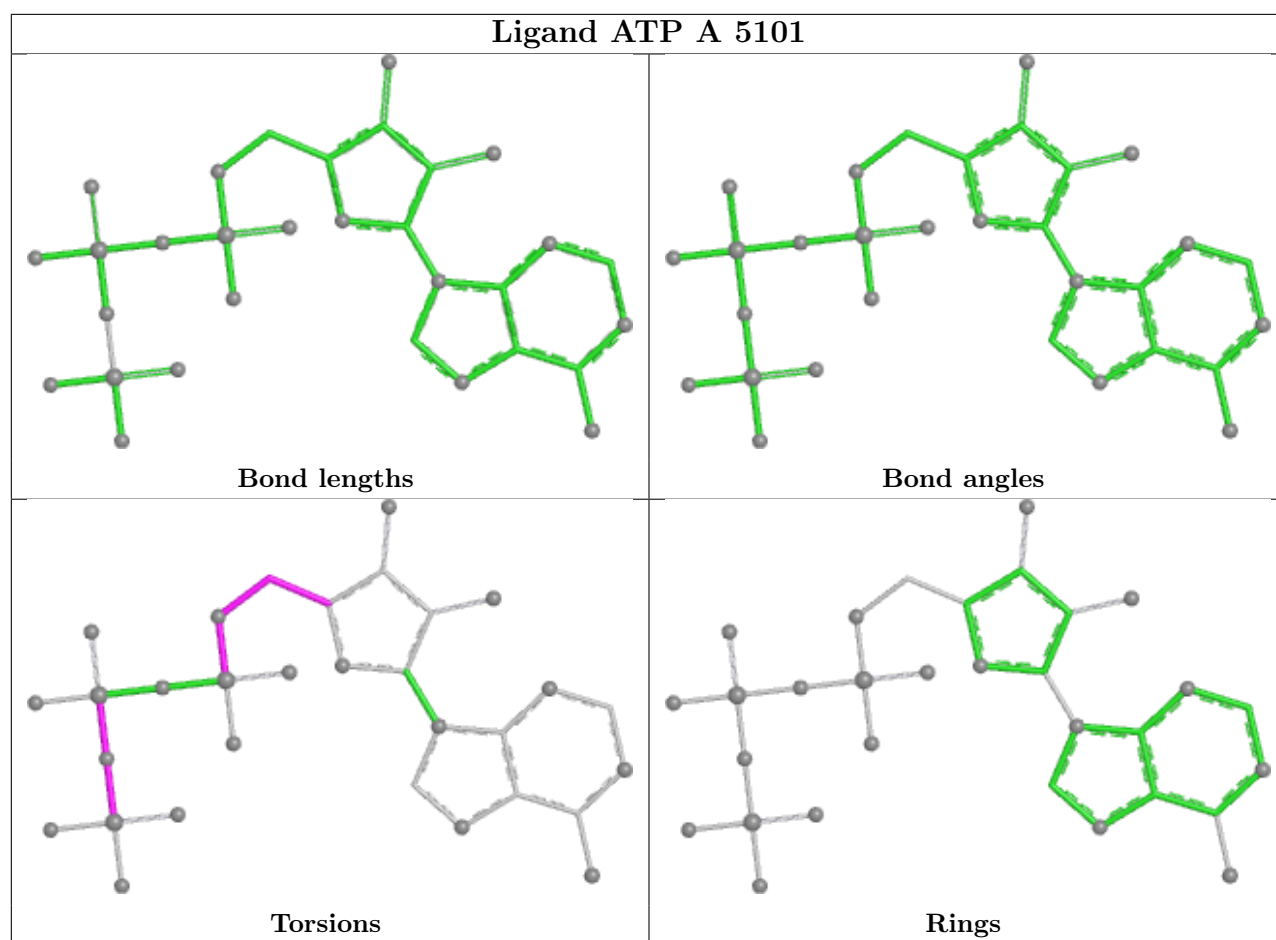
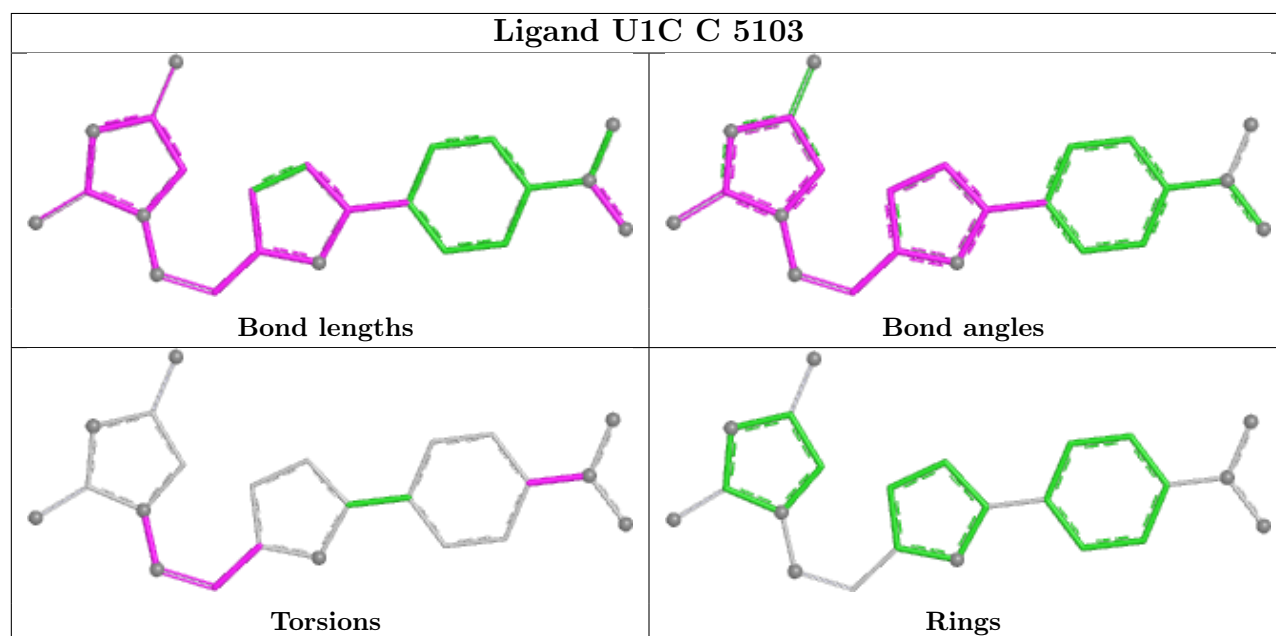
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	5101	ATP	2	0
4	B	5101	ATP	2	0
4	C	5101	ATP	3	0
4	A	5101	ATP	1	0

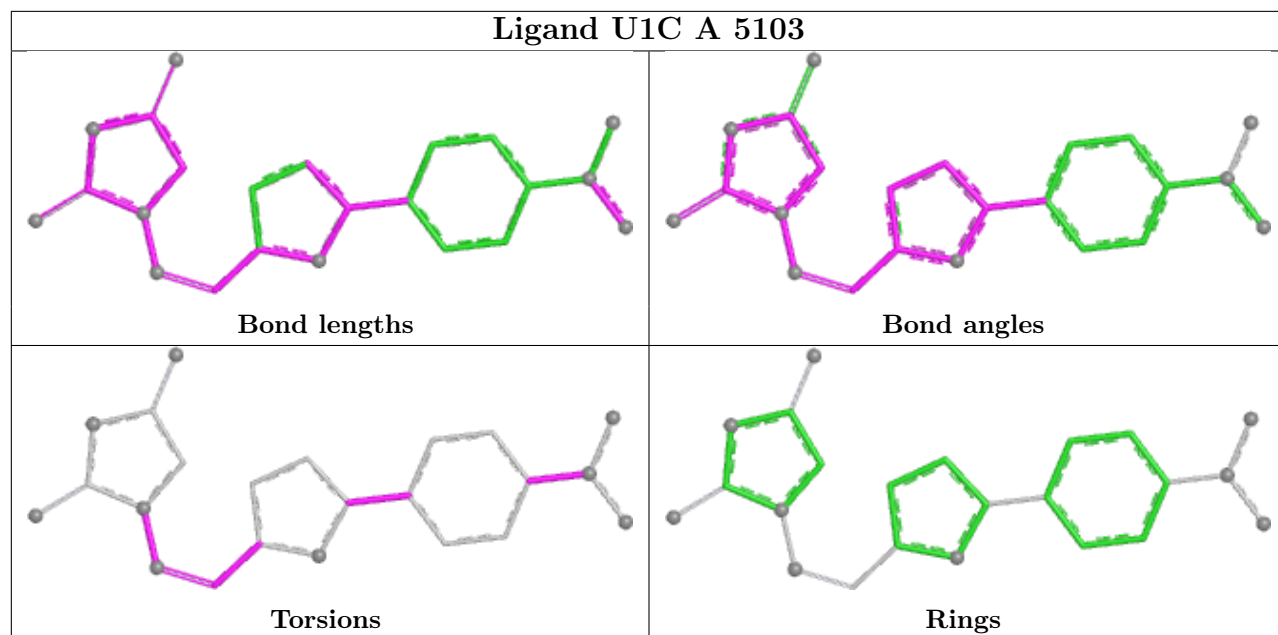
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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.

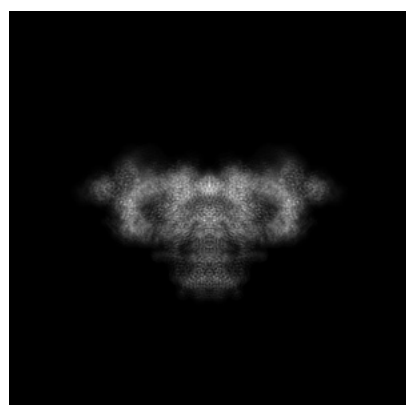
6 Map visualisation [i](#)

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.

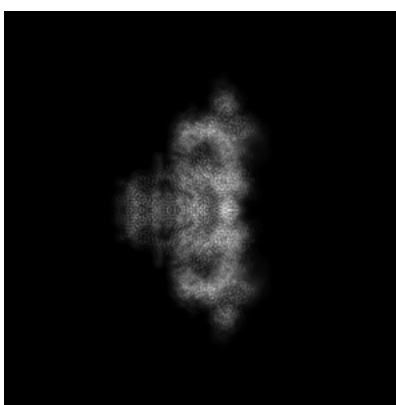
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

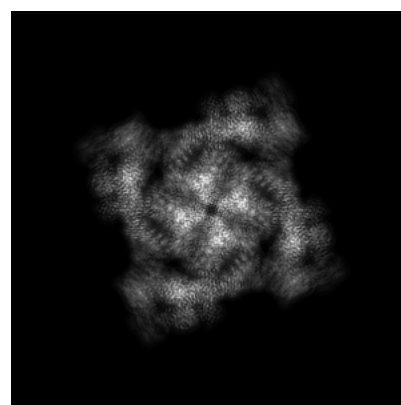
6.1.1 Primary map



X



Y

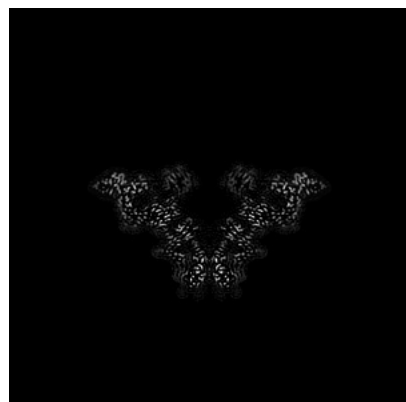


Z

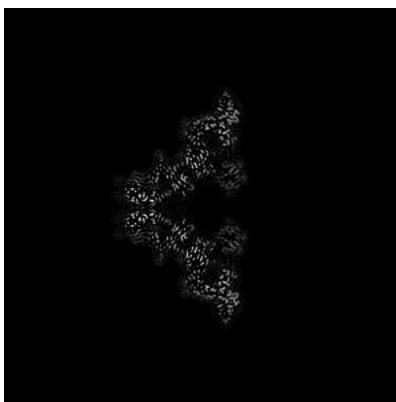
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

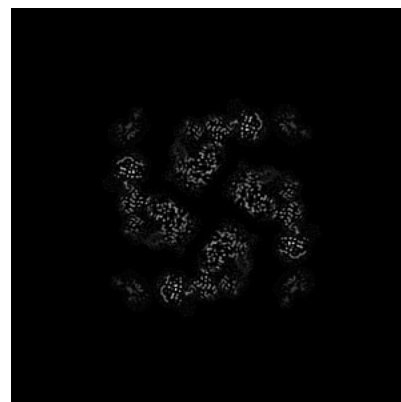
6.2.1 Primary map



X Index: 232



Y Index: 232

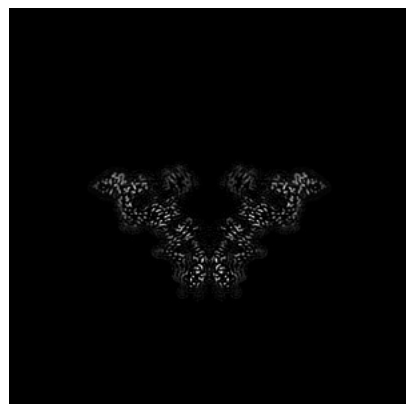


Z Index: 232

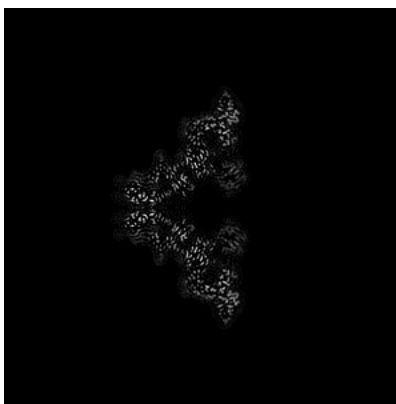
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

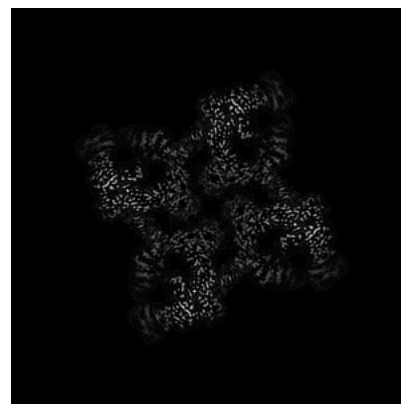
6.3.1 Primary map



X Index: 232



Y Index: 232

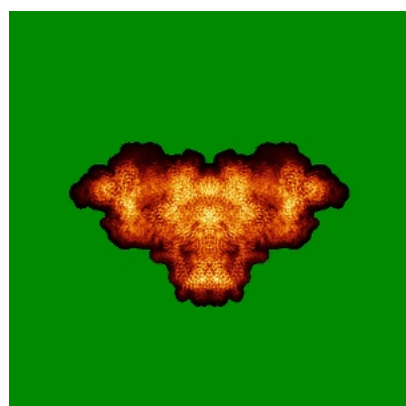


Z Index: 260

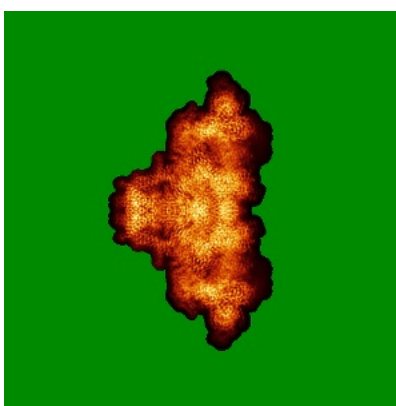
The images above show the largest variance slices of the map in three orthogonal directions.

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

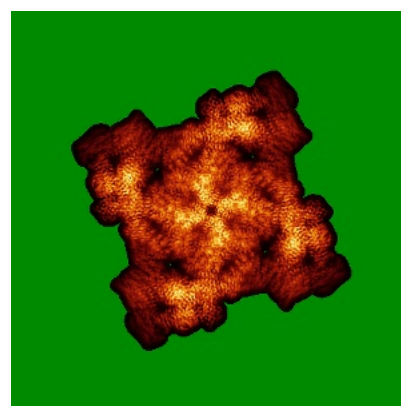
6.4.1 Primary map



X



Y

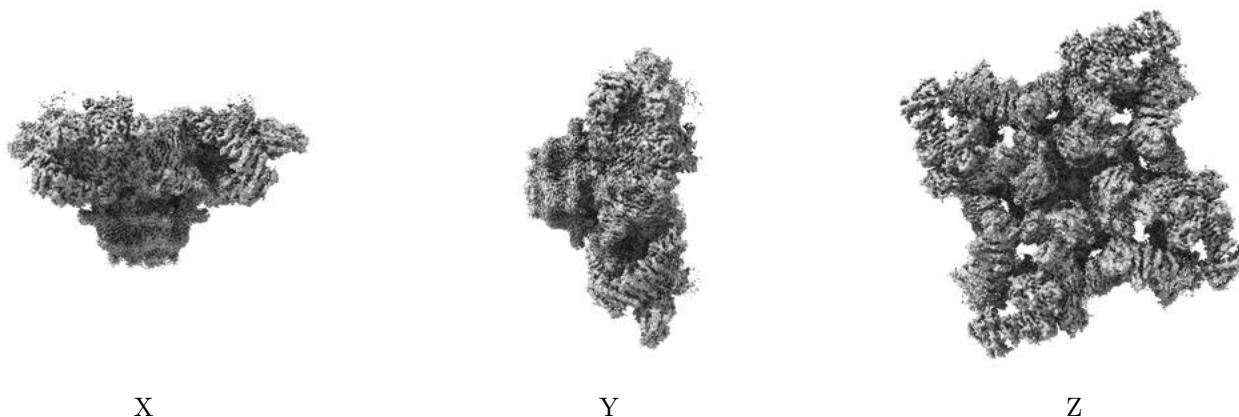


Z

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.

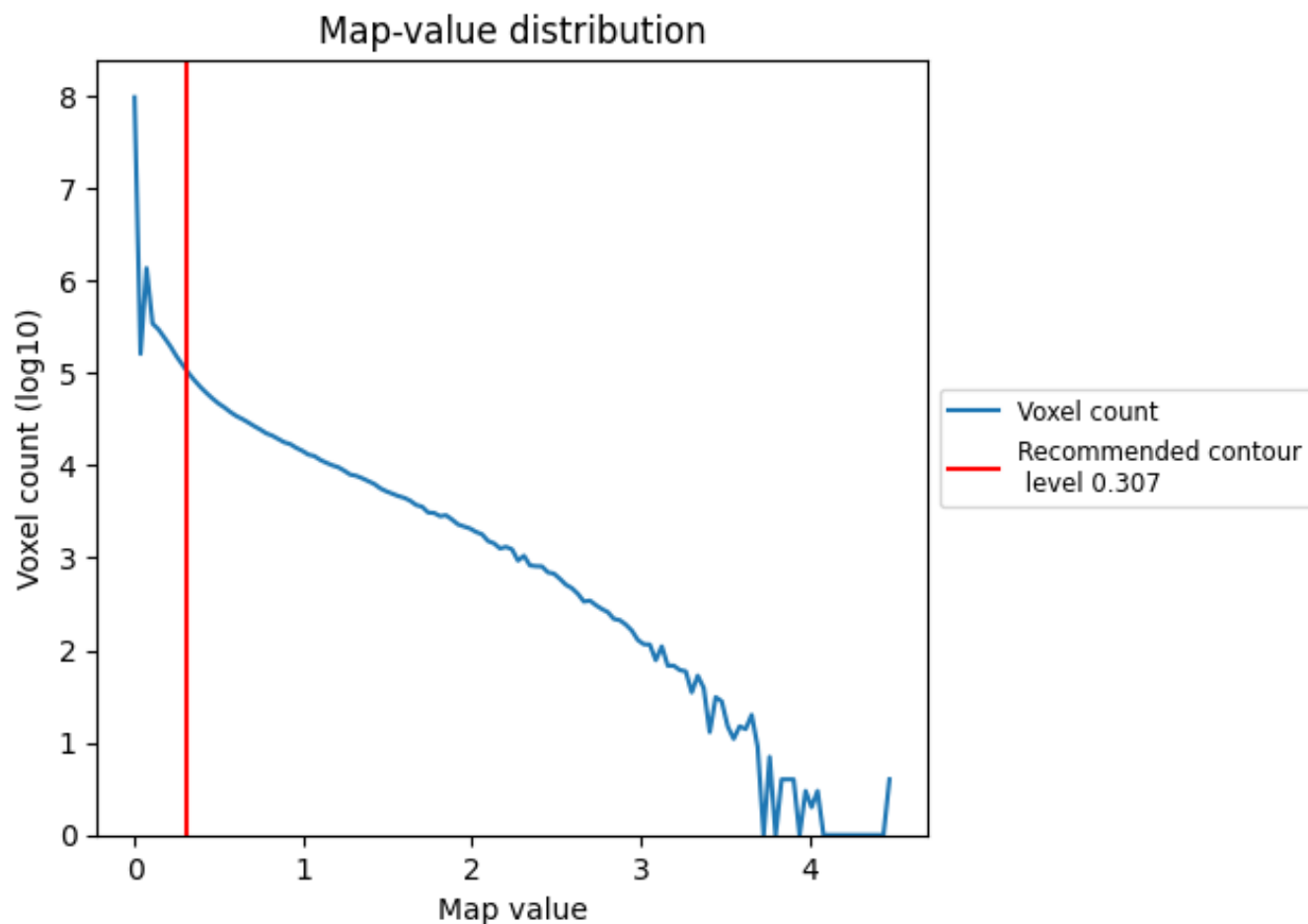
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

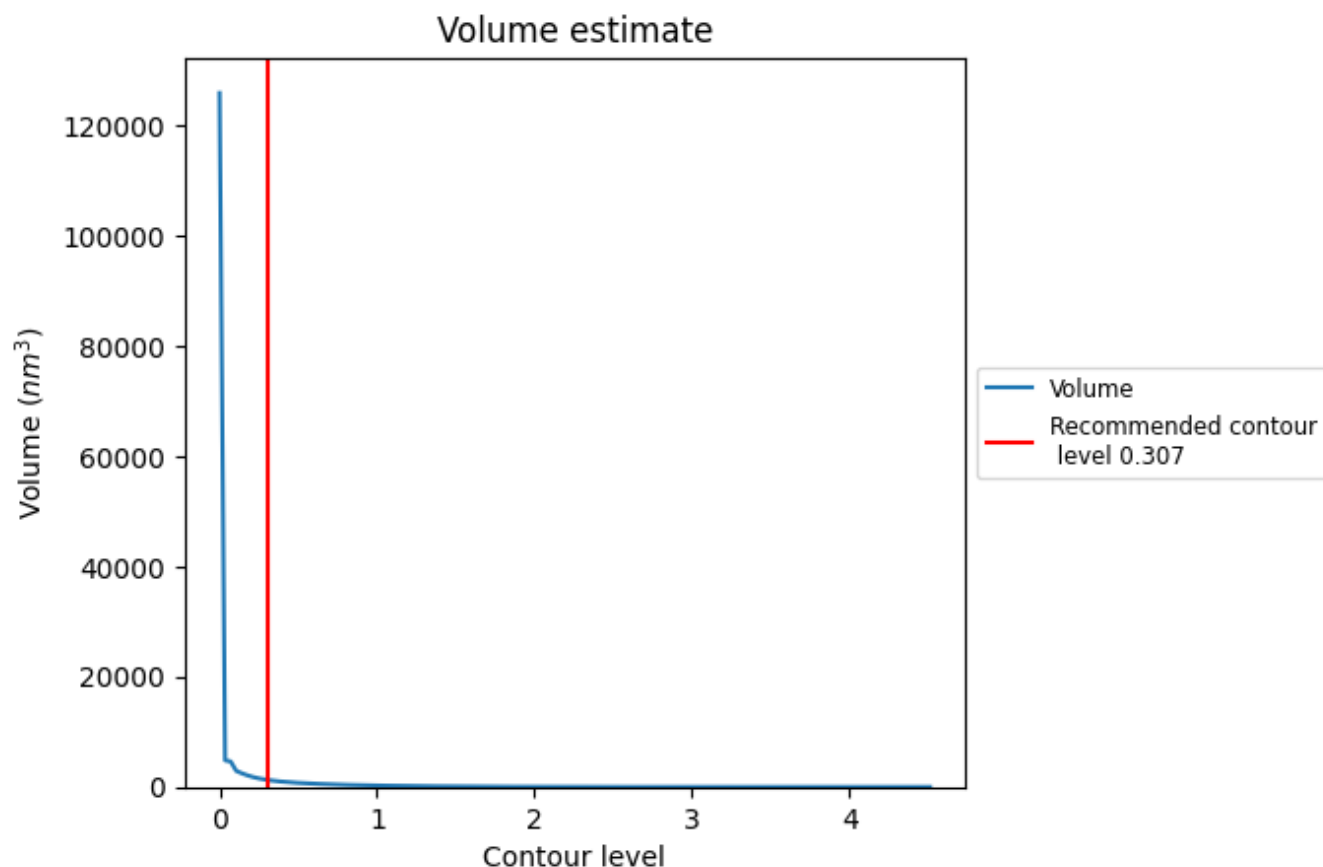
This section contains the results of statistical analysis of the map.

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.

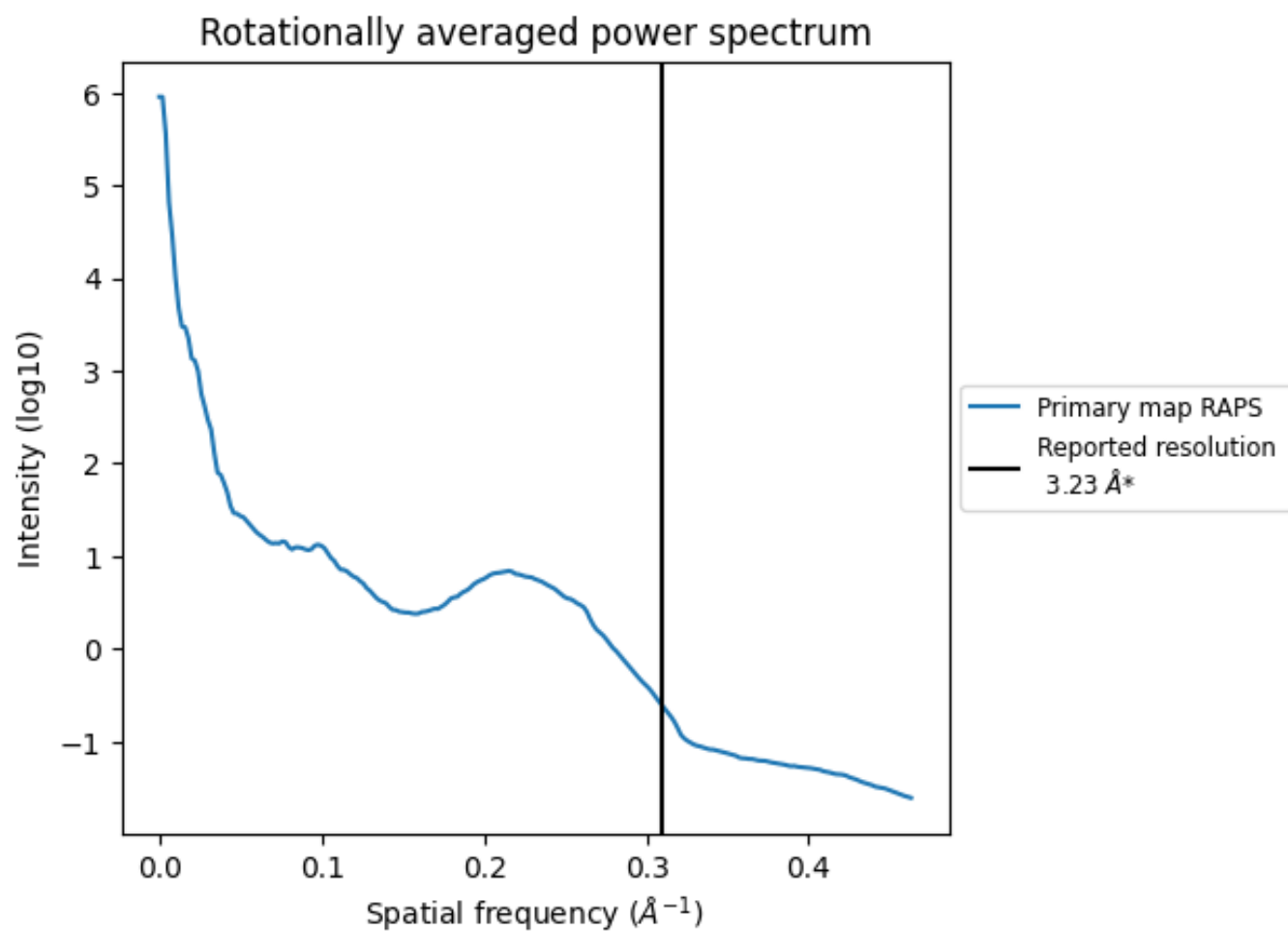
7.2 Volume estimate [i](#)



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

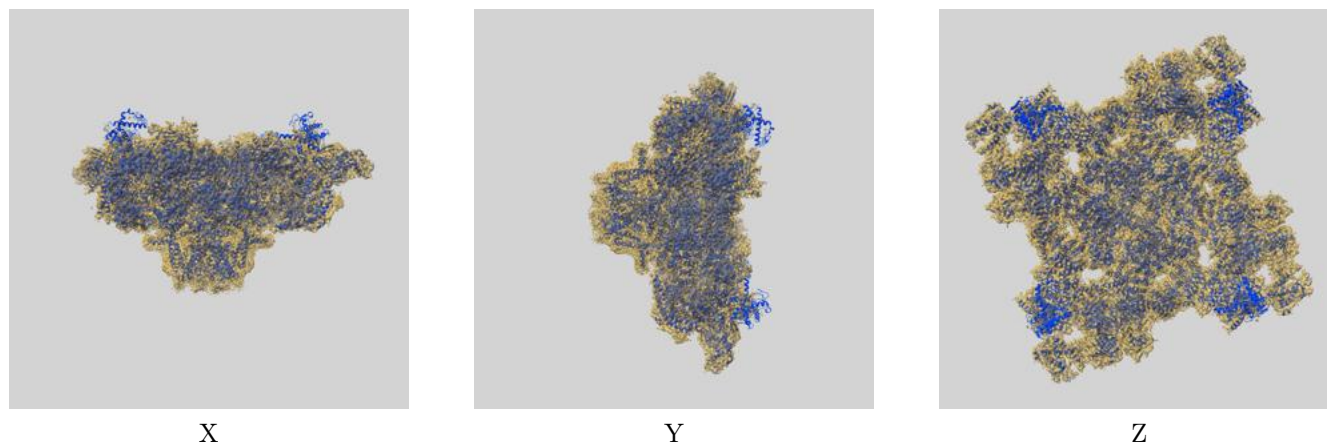
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

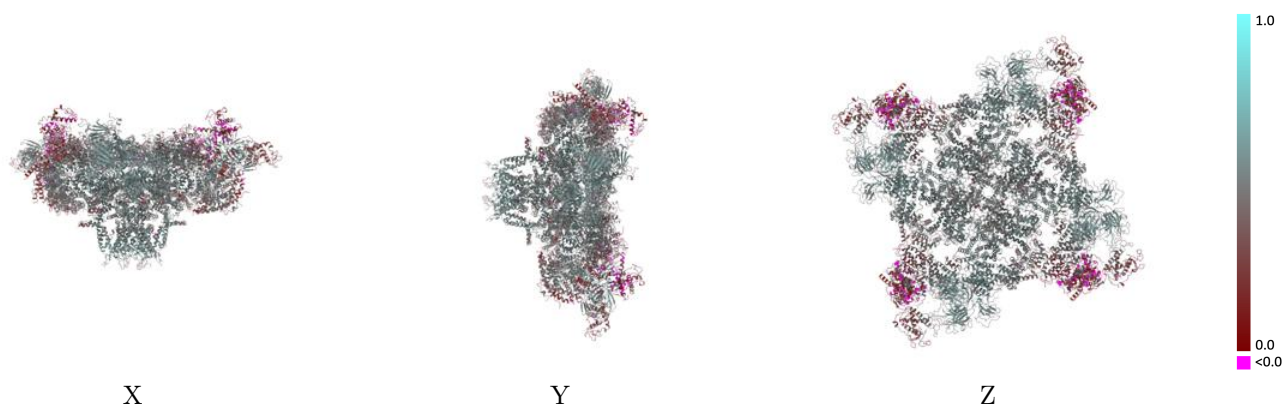
This section contains information regarding the fit between EMDB map EMD-45585 and PDB model 9CGQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



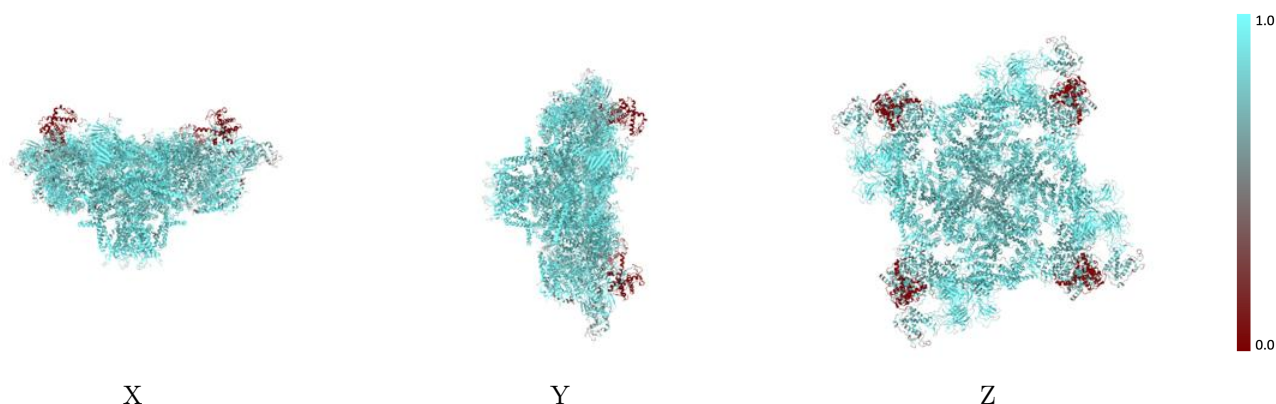
The images above show the 3D surface view of the map at the recommended contour level 0.307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



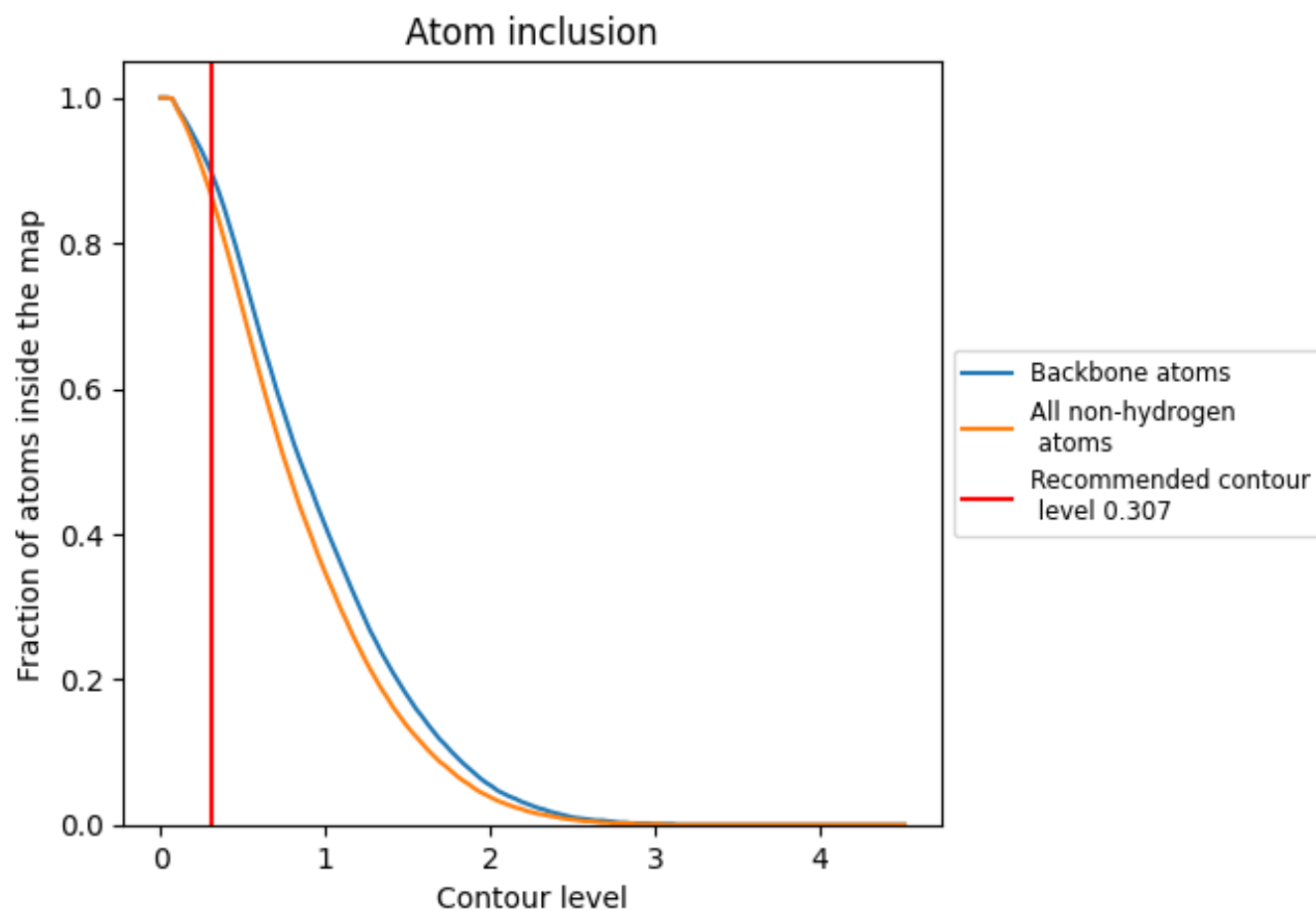
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	<div></div> 0.8660	<div></div> 0.4630
A	<div></div> 0.8640	<div></div> 0.4620
B	<div></div> 0.8640	<div></div> 0.4630
C	<div></div> 0.8650	<div></div> 0.4610
D	<div></div> 0.8650	<div></div> 0.4610
E	<div></div> 0.9250	<div></div> 0.5060
F	<div></div> 0.9180	<div></div> 0.5040
G	<div></div> 0.9180	<div></div> 0.5040
H	<div></div> 0.9190	<div></div> 0.5020

