



wwPDB EM Validation Summary Report ⓘ

Mar 25, 2026 – 09:19 AM UTC

PDB ID : 6JIU / pdb_00006jiu
EMDB ID : EMD-9836
Title : Structure of RyR2 (F/A/C/L-Ca²⁺/Ca²⁺+CaM dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-23
Resolution : 4.20 Å(reported)

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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

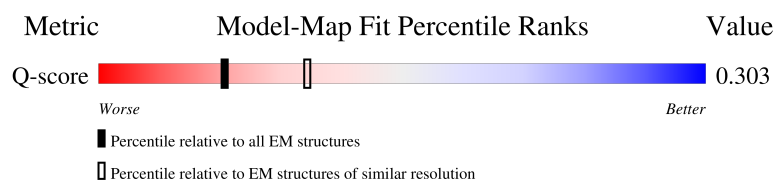
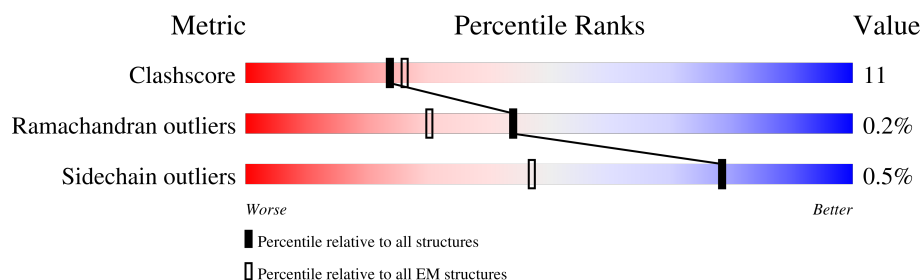
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 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	5410 (3.70 - 4.70)

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	4968	
1	D	4968	
1	G	4968	
1	J	4968	

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Mol	Chain	Length	Quality of chain
2	B	108	 77% 22%
2	E	108	 77% 22%
2	H	108	 78% 21%
2	K	108	 78% 21%
3	C	149	 42% 37% 9% 54%
3	F	149	 42% 38% 8% 54%
3	I	149	 42% 38% 8% 54%
3	L	149	 42% 38% 8% 54%

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
7	CFF	A	6003	-	X	-	-
7	CFF	D	6003	-	X	-	-
7	CFF	G	6003	-	X	-	-
7	CFF	J	6003	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 112212 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 RyR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	D	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	G	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		
1	J	3496	Total	C	N	O	S	0	0
			26661	16986	4571	4947	157		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	E	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	H	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
2	K	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	F	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	I	68	Total	C	N	O	S	0	0
			524	326	83	110	5		
3	L	68	Total	C	N	O	S	0	0
			524	326	83	110	5		

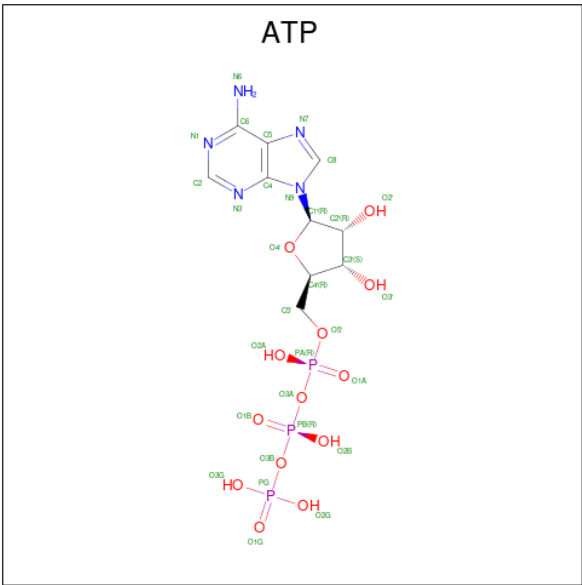
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	Zn 1	0
4	D	1	Total 1	Zn 1	0
4	G	1	Total 1	Zn 1	0
4	J	1	Total 1	Zn 1	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

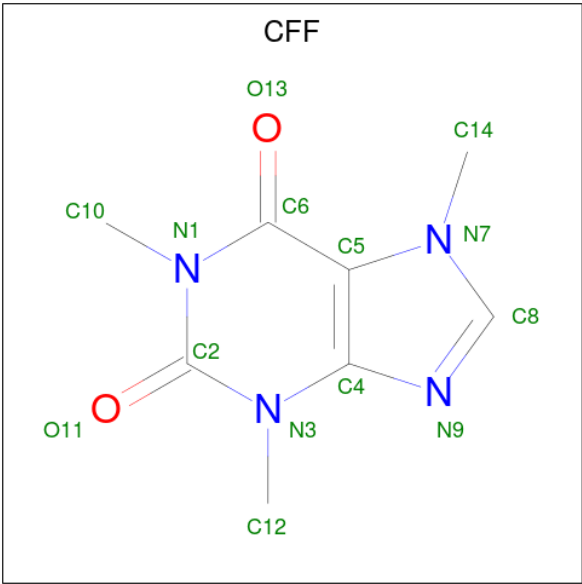
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total 1	Ca 1	0
5	C	2	Total 2	Ca 2	0
5	D	1	Total 1	Ca 1	0
5	F	2	Total 2	Ca 2	0
5	G	1	Total 1	Ca 1	0
5	I	2	Total 2	Ca 2	0
5	J	1	Total 1	Ca 1	0
5	L	2	Total 2	Ca 2	0

- Molecule 6 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- Molecule 7 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total 14	C 8	N 4	O 2	0
7	D	1	Total 14	C 8	N 4	O 2	0
7	G	1	Total 14	C 8	N 4	O 2	0
7	J	1	Total 14	C 8	N 4	O 2	0

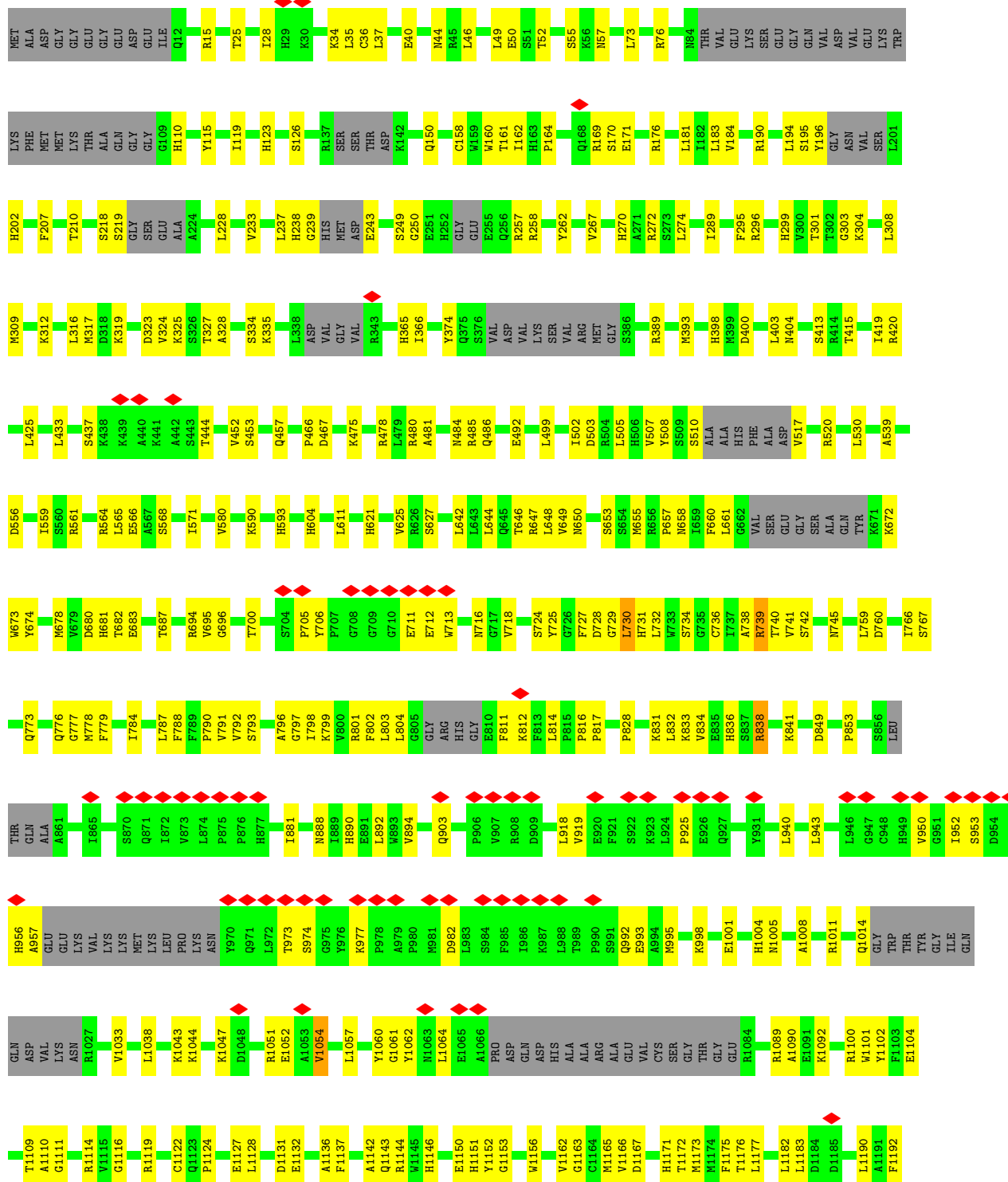








• Molecule 1: RyR2



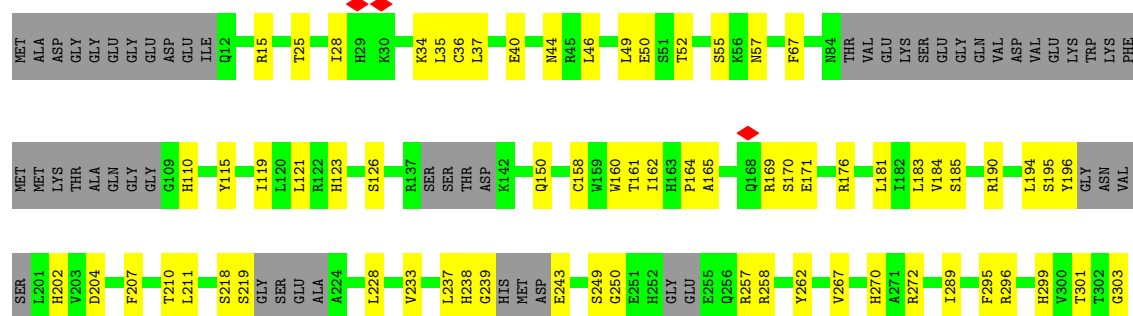
A2514	L2418	R2327	K2195	H2090	L1993	P1900	L1817	S1713	S1609	ASN	ASP	ARG	CYS	K1193
L2515	R2421	E2330	N2196	L2099	D2013	K1904	L1821	Y1714	R1610	N1502	TYR	VAL	LEU	D1194
N2518	S2422	C2304	P2204	Y2107	GLU	L1905	I1822	A1715	E1506	E1507	MET	LYS	GLN	F1196
L2528	L2423	G2312	N2211	D2116	ASP	Q1948	Y1826	R1719	S1612	I1507	THR	ASP	GLN	D1196
L2529	P2429	P2313	K2213	N2119	SER	Q1948	L1839	N1722	R1614	Y1510	THR	LYS	GLU	P1203
ARG	L2433	L2222	L2222	A2122	LEU	H1921	I1842	P1728	W1617	Y1511	ASP	ALA	GLU	S1206
CYS	V2434	G2343	G2343	Q2126	ASP	R1922	I1846	M1728	L1618	ALA	GLY	LYS	PRO	V1209
PRO	G2435	GLY	GLY	Q2126	ASN	A1925	E1847	T1730	Q1620	GLY	GLN	PRO	ALA	A1210
L2535	V2436	GLY	LEU	Q2126	ASP	A1928	P1843	T1733	C1621	G1516	PRO	PHE	GLU	Q1211
F2536	L2437	ASN	ALA	V2133	L2024	Q1938	S1849	T1734	L1622	Y1521	ALA	ASN	GLU	V1212
A2537	Q2442	G2343	ALA	Q2133	T2025	Q1938	VAL	S1735	Q1626	A1522	ALA	ASN	GLU	G1213
H2541	H2542	L2354	PRO	GLY	R2029	Y1945	PHE	T1736	F1627	Y1441	LYS	HIS	VAL	R1214
A2543	A2543	ALA	ALA	LYS	R2029	Y1945	LYS	T1737	M1628	Y1531	ASP	LYS	PHE	K1219
T2546	GLY	GLY	ARG	E2138	V2037	V1948	GLY	T1738	S1629	P1535	TVR	LYS	ALA	V1221
L2550	LYS	T2239	T2239	K2141	Y2039	M1949	ALA	F1739	L1630	Y1539	ALA	GLN	THR	L1224
L2550	ASP	P2240	P2240	L2142	LEU	L2142	PRO	D1741	E1634	F1540	GLY	LYS	ALA	F1227
V2553	GLY	L2241	L2241	L2142	LYS	MET	GLY	ASN	E1635	P1541	GLY	PRO	GLY	T1228
TYR	ASN	L2241	LYS	L2142	LYS	LYS	GLY	LYS	S1638	T1548	LYS	ARG	ILE	L1232
ARG	VAL	L2254	ALA	L2147	GLN	ALA	SER	HIS	I1641	E1556	LEU	LEU	GLY	Y1236
LEU	VAL	L2258	ALA	T2150	ALA	LEU	ASP	G1747	T1645	E1556	ASP	GLN	LYS	E1237
K2558	THR	L2263	LYS	L2150	LYS	THR	THR	I1751	Y1655	GLY	ARG	ARG	LEU	P1238
L2562	GLY	L2263	GLY	N2153	VAL	ALA	GLY	G1752	R1659	ILE	VAL	PHE	GLY	F1239
Q2566	SER	L2275	GLN	K2154	GLU	THR	LYS	L1753	Y1661	LYS	ARG	LEU	PRO	A1240
R2567	ALA	L2275	LYS	V2156	ASP	LYS	PRO	S1756	Y1661	ASN	VAL	ARG	LYS	V1241
D2568	GLY	L2275	GLY	F2156	SER	GLY	CYS	L1757	Y1661	MET	THR	THR	ASP	R1245
S2576	GLY	L2275	GLY	Q2158	LYS	PHE	ALA	R1758	Y1661	LEU	LEU	LYS	ASP	D1246
ILE	GLY	L2275	GLY	H2159	LYS	ARG	GLY	P1759	H1670	PRO	PRO	LYS	GLU	M1249
CYS	GLY	L2275	GLY	P2160	LYS	SER	GLY	P1766	L1676	SER	ASP	PRO	ASP	W1250
GLY	GLY	L2275	GLY	N2161	SER	PRO	ASP	S1767	E1682	A1568	TYR	TYR	ASP	R1254
LEU	GLY	L2275	GLY	L2162	SER	PRO	ARG	F1768	E1682	G1569	THR	THR	ALA	L1255
ARG	GLY	L2275	GLY	A2165	GLY	GLN	LEU	V1769	L1685	L1570	THR	THR	ALA	P1256
P2583	GLY	L2275	GLY	L2166	Q2060	GLN	GLY	G1775	L1685	S1573	SER	HIS	SER	Q1257
N2601	GLY	L2275	GLY	M2176	S2064	ILE	PRO	Y1776	A1688	Y1579	CYS	SER	ASP	F1258
ALA	GLY	L2275	GLY	G2181	M2067	ASN	ALA	Q1777	I1689	P1580	GLY	ALA	PHE	H1265
K2605	THR	L2275	GLY	GLY	M2070	LEU	GLY	Y1778	E1690	M1487	VAL	LEU	VAL	E1266
M2606	ALA	L2275	GLY	GLY	W2070	ASN	GLY	D1785	N1691	H1567	GLY	THR	LEU	H1267
P2607	ALA	L2275	GLY	GLY	S2074	PHE	LYS	K1790	Y1693	Q1569	ASP	GLY	LYS	R1272
L2611	ALA	L2275	GLY	GLY	V2075	LYS	GLY	M1794	P1695	L1595	GLY	VAL	THR	I1273
G2627	ALA	L2275	GLY	GLY	I2076	ASP	GLY	V1799	R1699	S1597	LEU	ALA	HIS	D1274
THR	ALA	L2275	GLY	GLY	P2079	LYS	LYS	R1807	Y1703	R1598	THR	ALA	GLY	GLY
ALA	ALA	L2275	GLY	GLY	P2080	SER	ARG	D1808	I1709	G1599	ASP	ASP	HIS	THR
LEU	LEU	L2275	GLY	GLY	L2081	GLY	PRO	P1809	I1709	M1599	PRO	ARG	GLY	ASP
SER	SER	L2275	GLY	GLY	M2085	C1987	LYS	R1807	I1709	P1600	GLY	ASP	VAL	SER
ALA	ALA	L2275	GLY	GLY	M2085	C1988	GLY	D1809	I1709	P1600	GLY	ASP	PRO	SER
ASN	ASN	L2275	GLY	GLY	M2085	P1990	L1894	S1712	I1712	K1605	GLY	TVR	ASP	PRO





D2708	HIS	VAL	V1488	P1580	E1690	Y1778	PRO	GLN	S2064	E2170	ASP	ILE	GLU	HIS	D2708
T2709	ALA	LEU	C1489	H1587	M1691	D1785	ALA	ILE	M2067	M2176	ILE	GLY	Q2481	K2605	T2709
S2710	M2606	ASP	GLY	V1588	Y1693	D1785	GLU	MET	M2067	M2176	GLY	GLY	L2485	M2606	S2710
N2711	P2607	GLU	GLU	Q1589	M1694	K1790	GLU	LEU	W2070	G2181	ASN	ASN	L2485	P2607	N2711
I2712	L2611	ASP	SER	L1595	P1695	M1794	SER	LEU	W2070	G2181	GLY	GLY	L2503	L2611	I2712
T2713	G2627	ASP	MET	W1596	R1699	M1794	LYS	ASN	S2074	GLY	P2293	GLY	L2503	G2627	T2713
P2715	GLY	TYR	PRO	S1597	Y1703	V1799	GLY	PHE	V2075	GLU	F2308	GLU	L2503	P2715	P2715
E2716	ASN	GLY	GLY	R1598	Y1703	V1799	LYS	ASP	L2076	GLY	S2313	LYS	L2503	E2716	E2716
K2717	PHE	LEU	GLN	M1599	D1704	R1807	ARG	ASP	P2079	GLU	R2323	ILE	L2409	K2717	K2717
L2718	GLY	ARG	GLY	P1600	L1705	D1808	PRO	LYS	E2080	ILE	R2323	THR	L2410	L2718	L2718
E2719	ALA	MET	ASN	K1605	I1709	P1809	LYS	GLY	L2081	PHE	I2326	THR	H2411	E2719	E2719
Y2720	L2634	THR	N1502	L1605	GLU	G1812	GLY	C1987	M2085	P2191	R2327	GLY	A2412	Y2720	Y2720
F2721	L2639	SER	E1506	S1609	S1712	G1812	GLY	C1988	H2080	K2193	E2330	GLY	I2418	F2721	F2721
I2722	R2643	ALA	I1507	R1610	S1713	L1817	GLY	C1989	L2090	M2192	E2330	GLY	I2418	I2722	I2722
N2723	K2644	GLN	V1510	S1612	A1715	L1821	GLY	P1990	L2099	V2194	PHE	GLY	R2421	N2723	N2723
K2724	G2648	GLN	V1511	R1614	R1718	I1822	GLY	D2013	Y2107	M2196	PRO	PRO	I2423	K2724	K2724
Y2725	L2653	GLY	ASP	W1617	L1719	Y1826	ASN	GLU	D2116	F2204	ALA	LEU	P2429	Y2725	Y2725
A2726	SER	ALA	ALA	L1618	M1722	L1839	GLY	GLY	D2116	M2211	GLY	GLY	P2429	A2726	A2726
E2727	GLN	ALA	ALA	L1618	M1722	L1839	SER	SER	N2119	Q2212	ARG	ARG	L2433	E2727	E2727
H2728	GLN	SER	G1516	V1619	R1922	I1842	ASP	ASP	M2119	K2213	GLY	GLY	V2434	H2728	H2728
S2729	LYS	GLU	T1521	Q1621	M1729	I1846	GLY	GLY	A2122	A2122	GLY	GLY	V2435	S2729	S2729
H2730	LYS	GLU	T1521	L1622	T1730	I1846	ASN	ASN	Q2126	V2228	ASN	ASN	V2437	H2730	H2730
D2731	Y2658	GLY	ASP	L1622	T1730	I1846	SER	SER	Q2126	V2228	GLY	GLY	S2438	D2731	D2731
K2732	P2679	ALA	ALA	L1622	T1730	I1846	LEU	ASP	V2133	L2024	ALA	ALA	Q2442	K2732	K2732
W2733	TYR	ASP	ASP	L1622	T1730	I1846	LEU	ASP	V2133	L2024	ALA	ALA	Q2442	W2733	W2733
S2734	MET	GLY	ASP	L1622	T1730	I1846	PRO	SER	ARG	SER	PRO	PRO	GLU	S2734	S2734
M2735	GLY	ASP	ASP	L1622	T1730	I1846	GLY	GLY	GLY	GLY	ALA	ALA	THR	M2735	M2735
D2736	SER	ASN	F1540	L1630	F1739	PHE	LYS	VAL	E2138	E2138	PRO	PRO	ILE	D2736	D2736
K2737	ASN	GLY	P1541	L1630	F1739	PHE	LYS	GLY	E2138	E2138	ASP	ASP	LYS	K2737	K2737
L2738	VAL	GLY	L1539	L1630	F1739	PHE	LYS	LEU	E2138	E2138	GLY	GLY	ASN	L2738	L2738
A2739	SER	GLY	L1539	L1630	F1739	PHE	LYS	LEU	E2138	E2138	GLY	GLY	ASN	A2739	A2739
N2740	MET	ASP	L1459	L1641	HIS	GLU	GLY	LYS	M2143	L2254	PRO	PRO	VAL	N2740	N2740
W2741	GLY	ARG	E1556	L1641	GLU	GLU	MET	LYS	M2143	L2254	SER	SER	VAL	W2741	W2741
G2742	LYS	ARG	GLY	L1645	I1751	GLU	ALA	GLN	L2147	L2258	PRO	PRO	GLU	G2742	G2742
I2743	GLN	ARG	ILE	L1655	L1753	THR	ALA	LYS	L2150	D2262	SER	SER	PRO	I2743	I2743
S2744	SER	ASN	VAL	L1655	L1753	THR	ALA	LYS	L2150	D2262	GLY	GLY	ASP	S2744	S2744
G2745	MET	VAL	VAL	L1655	L1753	THR	ALA	LYS	L2150	D2262	SER	SER	GLY	G2745	G2745
E2746	ASP	MET	ASN	L1655	L1753	THR	ALA	LYS	L2150	D2262	SER	SER	GLY	E2746	E2746
I2747	PRO	PRO	PRO	L1670	P1759	CYS	THR	ASP	F2156	Y2157	MET	MET	ILE	I2747	I2747
Y2748	LEU	LEU	LEU	L1670	P1759	CYS	THR	ASP	F2156	Y2157	ASP	ASP	CYS	Y2748	Y2748
S2749	SER	SER	SER	L1676	P1766	ALA	LYS	SER	Q2158	H2169	THR	THR	GLY	S2749	S2749
D2750	ASP	ASP	A1568	L1676	P1766	ALA	LYS	SER	Q2158	H2169	THR	THR	GLY	D2750	D2750
S2751	GLY	ASP	A1568	L1676	P1766	ALA	LYS	SER	Q2158	H2169	THR	THR	GLY	S2751	S2751
S2752	ARG	ASP	E1682	L1685	S1770	ARG	SER	SER	L2162	N2161	GLY	GLY	R2475	S2752	S2752
K2753	GLY	ARG	L1570	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	K2753	K2753
V2754	CYS	GLY	S1573	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	V2754	V2754
Q2755	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	Q2755	Q2755
P2756	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	P2756	P2756
L2757	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	L2757	L2757
M2758	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	M2758	M2758
K2759	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	K2759	K2759
P2760	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	P2760	P2760
Y2761	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	Y2761	Y2761
K2762	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	K2762	K2762
L2763	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	L2763	L2763
L2764	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	L2764	L2764
S2765	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	S2765	S2765
E2766	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	E2766	E2766
V2767	GLY	GLY	V1579	L1685	S1770	ARG	PRO	PRO	L2162	N2161	GLY	GLY	R2475	V2767	V2767

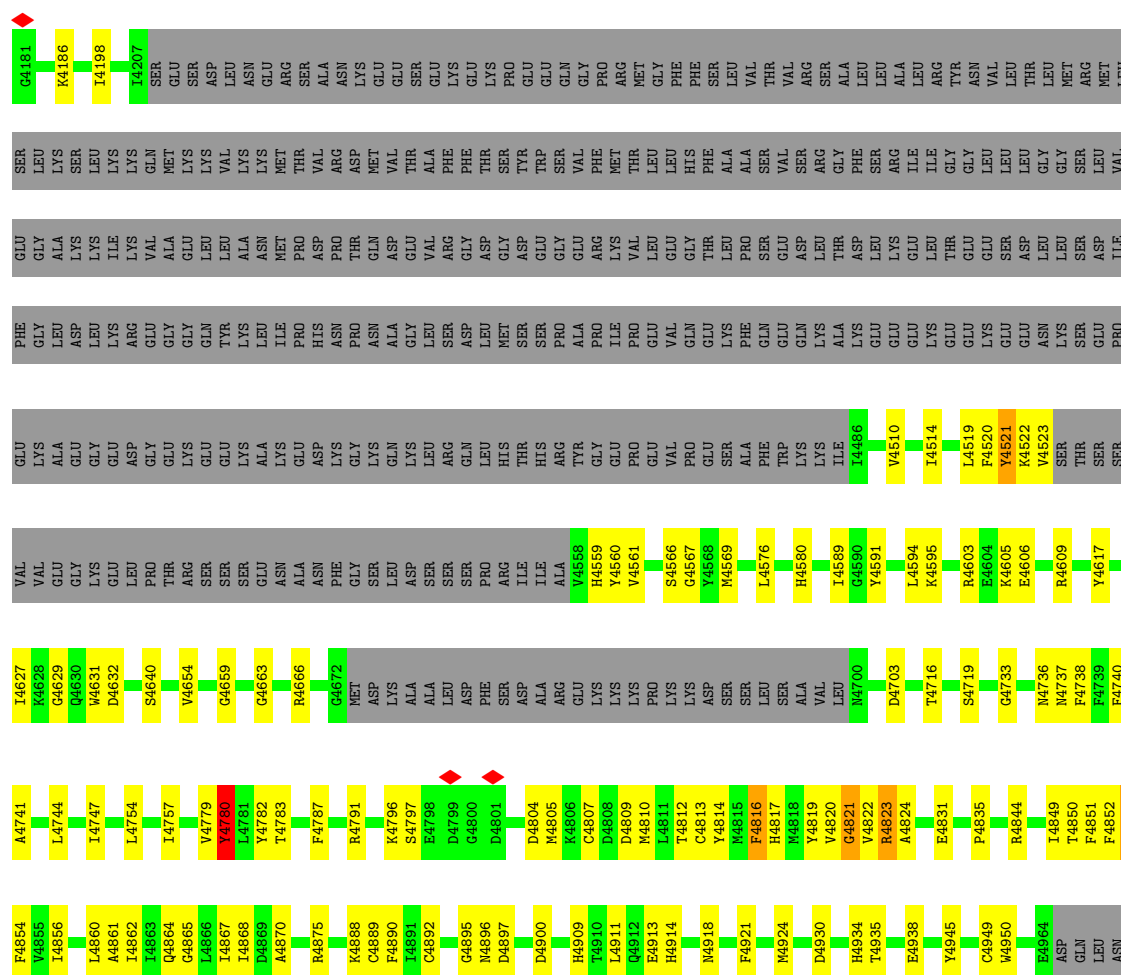
K3783	E2768	D2828	E2888	THR	LEU	THR	ASN	VAL	ASP	ARG	HIS	SER	K3783
E3784	K2769	M2829	K2889	LYS	ARG	V3149	THR	SER	LEU	MET	LEU	LEU	E3784
K3785	E2770	S2830	A2890	GLU	SER	E3150	GLU	LYS	ASP	GLU	GLY	ASP	K3785
K3786	D2771	N2831	Q2891	LYS	GLY	L3062	ILE	ASN	VAL	ASP	VAL	ASP	K3786
D3787	E2772	V2832	D2892	THR	HIS	E3158	THR	GLN	GLY	ILE	GLY	ASP	D3787
F3790	D2773	T2833	T2893	PRO	PHE	A3161	ASN	LEU	ASP	LEU	LEU	ASP	F3790
S3800	E2774	L2834	L2894	LYS	THR	A3162	LYS	ALA	ASP	ALA	LEU	ASP	S3800
C3801	P2775	S2835	K2895	ILE	THR	F3163	ILE	SER	VAL	ILE	GLY	ASP	C3801
L3804	D2776	R2836	F2896	GLY	ASN	A3164	GLY	THR	ARG	GLY	GLY	ASP	L3804
F3809	K2777	L2837	T2897	THR	GLN	G3165	THR	ASN	GLY	ILE	ILE	ASP	F3809
E3810	E2778	L2838	Q2898	PRO	ILE	A3166	PHE	PRO	ASP	THR	VAL	ASP	E3810
R3811	S2779	H2839	T2899	LYS	PHE	PRO	PRO	THR	SER	THR	VAL	ASP	R3811
Q3812	L2780	A2840	N2900	GLY	GLY	VAL	ASN	GLN	GLY	GLN	ASP	ASP	Q3812
K3819	K2781	M2841	G2901	ALA	ALA	A3170	ASN	MET	ALA	ASP	THR	ASP	K3819
VAL	T2782	A2842	Y2902	LYS	LYS	F3171	PRO	PRO	THR	PRO	GLY	ASP	VAL
THR	M2783	E2843	A2903	VAL	VAL	L3172	THR	THR	VAL	HIS	VAL	ASP	THR
THR	L2784	M2844	V2904	LEU	LEU	E3173	ILE	ILE	ILE	ILE	ILE	ASP	THR
GLU	E2785	A2845	S2905	PRO	PRO	T3174	ASN	ASN	VAL	VAL	VAL	ASP	GLU
GLU	E2786	A2846	R2906	LEU	LEU	H3175	GLY	GLY	ASP	GLY	GLY	ASP	GLU
G3825	G2787	E2847	T3097	ASP	ASP	D3177	LEU	LEU	PHE	ASN	THR	THR	G3825
K3829	E2788	N2848	PHE	LYS	GLN	T3098	PRO	PRO	THR	ILE	GLU	ASP	K3829
D3834	E2789	Y2849	ASP	ASP	THR	V3100	VAL	VAL	THR	THR	THR	ASP	D3834
L3879	L2790	H2850	LEU	LEU	PHE	P3104	ASN	ASN	GLY	GLY	GLY	ASP	L3879
L3880	E2791	N2851	GLU	GLU	LYS	M3105	CYS	SER	ALA	ALA	GLY	ASP	L3880
R3881	D2792	L2852	LEU	LEU	ASN	L3106	THR	THR	ARG	ARG	ALA	ASP	R3881
V3882	T2793	W2853	THR	THR	ARG	G3114	ILE	ASN	ASN	ASN	ASN	ASP	V3882
S3885	E2794	A2854	PRO	PRO	LYS	Q3115	TRP	TRP	TRP	TRP	TRP	ASP	S3885
D3888	E2795	K2855	SER	SER	ILE	H3116	ASN	ASN	ASN	ASN	ASN	ASP	D3888
F3889	G2796	K2856	ILE	ILE	F2983	Q3117	THR	THR	THR	THR	THR	ASP	F3889
W3891	D2797	K2857	GLY	GLY	K3002	F3118	LYS	LYS	LYS	LYS	LYS	ASP	W3891
A3910	SER	K2858	ARG	ARG	V3005	GLY	SER	SER	SER	SER	SER	ASP	A3910
I3911	ALA	L2859	PHE	PHE	THR	GLU	ARG	ARG	ARG	ARG	ARG	ASP	I3911
N3919	LEU	E2860	TYR	TYR	SER	ASP	GLY	GLY	GLY	GLY	GLY	ASP	N3919
T3922	TYR	L2861	SER	SER	LEU	ILE	ALA	ALA	ALA	ALA	ALA	ASP	T3922
I3925	ASN	E2862	PHE	PHE	LEU	L3124	PRO	PRO	PRO	PRO	PRO	ASP	I3925
Q3926	ARG	S2863	GLN	GLN	THR	S3130	ASN	ASN	ASN	ASN	ASN	ASP	Q3926
Q3934	ARG	K2864	GLN	GLN	ARG	C3131	LEU	LEU	LEU	LEU	LEU	ASP	Q3934
S3935	ILE	G2865	ILE	ILE	ILE	Y3132	PRO	PRO	PRO	PRO	PRO	ASP	S3935
L3936	SER	G2866	ARG	ARG	T3028	R3133	THR	THR	THR	THR	THR	ASP	L3936
L3937	THR	G2867	TYR	TYR	SER	I3134	ASN	ASN	ASN	ASN	ASN	ASP	L3937
H3938	THR	N2868	VAL	VAL	ILE	S3137	VAL	VAL	VAL	VAL	VAL	ASP	H3938
S3939	GLN	H2869	ASP	ASP	VAL	L3138	ASP	ASP	ASP	ASP	ASP	ASP	S3939
R3940	VAL	P2870	ALA	ALA	CYS	L3141	CYS	CYS	CYS	CYS	CYS	ASP	R3940
	SER	L2871	HIS	HIS	THR	G3142	ASN	ASN	ASN	ASN	ASN	ASP	
	ASP	L2872	TYR	TYR	SER	T3143	PRO	PRO	PRO	PRO	PRO	ASP	
A2818	ASP	V2873	ILE	ILE	ALA	S3144	LEU	LEU	LEU	LEU	LEU	GLY	A2818
A2819	ASP	P2874	LEU	LEU	SER	L3144	GLY	GLY	GLY	GLY	GLY	GLY	A2819
H2820	ASP	Y2875	PHE	PHE	ALA	LYS	SER	SER	SER	SER	SER	GLY	H2820
G2821	ASP	D2876	GLY	GLY	ALA	LYS	GLY	GLY	GLY	GLY	GLY	GLY	G2821
Y2822	ASP	T2877	GLY	GLY	ALA	LYS	GLY	GLY	GLY	GLY	GLY	GLY	Y2822
F2824	ASP	L2878	ILE	ILE	SER	L3141	THR	THR	THR	THR	THR	GLY	F2824
R2825	ASP	T2879	SER	SER	ALA	G3142	ASN	ASN	ASN	ASN	ASN	GLY	R2825
A2826	ASP	S2880	GLY	GLY	ALA	S3144	PRO	PRO	PRO	PRO	PRO	GLY	A2826
	ASP	K2881	GLY	GLY	ALA	LYS	LEU	LEU	LEU	LEU	LEU	GLY	
	ASP	E2882	GLY	GLY	ALA	LYS	GLY	GLY	GLY	GLY	GLY	GLY	
	ASP	K2883	GLY	GLY	ALA	LYS	GLY	GLY	GLY	GLY	GLY	GLY	
	ASP	A2884	GLY	GLY	ALA	LYS	GLY	GLY	GLY	GLY	GLY	GLY	
	ASP	K2885	GLY	GLY	ALA	LYS	GLY	GLY	GLY	GLY	GLY	GLY	
	ASP	D2886	GLY	GLY	ALA	LYS	GLY	GLY	GLY	GLY	GLY	GLY	
	ASP	R2887	GLY	GLY	ALA	LYS	GLY	GLY	GLY	GLY	GLY	GLY	







Y4046	I3925	A3737	GLY	LYS	GLY	VAL	TRP	GLU	LYS	CYS	VAL	S3137	CYS	LEU	E2882
R4047	Q3926	M3740	ALA	SER	VAL	ASP	LEU	VAL	LYS	CYS	SER	L3138	L3034	GLU	K2883
D4048	Q3934	F4049	PRO	THR	ARG	GLN	GLY	ASP	LYS	THR	ASN		K3055	PHE	A2884
H4050	S3935	S3748	PRO	CYS	ILE	GLU	PRO	ILE	LYS	ALA	PRO	G3141	SER	GLY	K2885
K4051	L3936		GLU	MET	ARG	ILE	ASN	ARG	LYS	SER	SER	G3142	ALA	GLY	D2886
A4052	A3937	K3777	GLU	ARG	ARG	ARG	LYS	LYS	ALA	GLU	PRO	T3143	LEU	SER	D2887
H4053	H3938	Y3781	ASP	ARG	SER	SER	GLU	GLU	ALA	ALA	SER	LYS	ARG	ARG	E2888
S3939	S3939	K3785	GLY	THR	ASN	ILE	VAL	VAL	MET	GLU	GLU	SER	ALA	SER	K2889
S4055	R3940	K3786	THR	SER	HIS	ARG	ASP	ASP	VAL	ASN	LEU	LYS	F3061	LYS	A2890
H4056	D3943	D3787	LYS	LEU	LEU	LYS	PHE	GLU	SER	THR	GLU	ILE	L3062	GLY	Q2891
H4058	Y3946		R3661	VAL	GLY	ASP	ARG	GLU	GLU	LEU	GLU	V3149	D3068	HIS	Q2892
Y4059	T4060	F3790	V3662	GLU	HIS	ARG	THR	GLY	ASP	GLY	ILE	T3072	T3072	PHE	D2893
Q4061	L3949		D3663	PRO	LYS	THR	VAL	VAL	ASP	ASN	VAL			PRO	T2894
S4062	H3950	S3800	L3665	GLN	LEU	TRP	ALA	GLU	LEU	ILE	ASP	E3150		GLU	L2894
E4063	G3955	C3801	H3666	SER	ASP	ILE	VAL	VAL	LYS	LEU	LEU	E3158	G3079	GLN	K2895
C4070	Q3956	L3804	L3668	LYS	PRO	ALA	THR	PHE	SER	LYS	ALA	A3161	T3082	GLU	F2896
A4071	M3957		I3669	LYS	ILE	SER	ILE	ILE	GLU	ILE	GLU	A3162	HIS	ILE	L2897
E4072	K3958	F3809	R3674	ALA	ARG	LEU	TRP	TRP	ARG	THR	GLY	F3163	THR	PHE	Q2898
T4073	L3959	E3810	R3677	VAL	TRP	ILE	TRP	GLY	ASN	ARG	ILE	A3164	ARG	PHE	T2899
D4074	S3960	R3811	L3677	TRP	GLN	VAL	SER	ASP	ASN	ASN	ARG	G3165	ASN	ALA	A2900
T4078	M3973	Q3812		HIS	ALA	ALA	SER	LYS	MET	LEU	THR	A3166	PRO	VAL	Q2901
L4079	Q3976	G3819	K3682	LYS	LEU	LEU	HIS	GLY	SER	GLY	THR		LYS	VAL	T2902
Y4081	K3977	MET	L3683	THR	TYR	LYS	ASN	ALA	GLU	ILE	GLY		GLY	VAL	A2903
P4091	V3981	GLU	Y3689	THR	ASP	ASP	PHE	LEU	LEU	GLY	VAL		VAL	LEU	V2904
D4094	L3984	GLU	Y3692	GLU	LEU	LEU	ARG	LEU	ASP	ILE	THR		THR	ILE	K2905
F4097	M3986	G3825	I3695	ASN	ASN	ILE	GLY	GLY	ASP	GLY	GLN		ILE	GLN	R2906
M4110	L3987	K3829	C3700	ARG	THR	GLU	ASN	GLN	VAL	VAL	VAL		TYR	PHE	Q2907
D4113	N3993	D3834	HIS	R3605	ASP	ASP	THR	ASP	PHE	ALA	PRO		T3098	LYS	PHE
T4114		L3844	ASP	Y3610	GLU	GLU	SER	GLU	LEU	THR	MET		T3099	ASN	LYS
R4115	I3996		GLU	N3611	ASP	PRO	ASP	ASN	LEU	LEU	LEU		V3100	ASN	LEU
L4116	S4007	L3879	ASP	L3612	ASP	GLY	GLU	GLU	ALA	THR	LEU		P3104	ARG	GLU
Q4117	M4010	L3880	ASP	R3616	ASP	GLY	ILE	ILE	ASP	SER	CYS		M3105	LEU	LEU
T4118		R3881	GLY		LYS	GLN	ASN	ASN	ASP	PRO	TYR		L3106	ASP	THR
F4119	L4015	V3882	GLY	F3621	THR	GLU	ASN	THR	TYR	ILE	MET		G3114	PRO	PRO
L4122	D3885	S3885	GLU	L3622	VAL	LEU	MET	ALA	ALA	ASN	SER		Q3115	ILE	GLU
A4123	D4031	D3888	GLU	Q3623	GLU	ILE	SER	PHE	TYR	LYS	TRP		Q3116	ARG	LYS
F4130	F4032	F3889	VAL	G3624	ARG	ALA	PHE	THR	VAL	VAL	TRP		Q3117	THR	ARG
L4134	F4033	Y3890	LYS	E3626	VAL	LEU	LEU	ILE	PRO	LYS	HIS		Q3118	PHE	ARG
M4140	K4034	M3891	S3714	K3627	LEU	ALA	THR	LEU	LEU	GLN	GLY		GLY	ALA	ALA
R4148	E4035	D3900			ASP	ASN	ASP	ILE	ILE	LEU	PRO		ASP	SER	TYR
S4154	Y4036	A3910	K3724	E3633	ILE	ARG	THR	ARG	ARG	LEU	GLU		ASP	PHE	GLU
E4155	D4039	A3910	R3731	E3634	ASN	ALA	SER	VAL	VAL	LYS	ASN		ASP	LEU	LEU
	G4042	N3919	L3732	H3635	LEU	LEU	LYS	LYS	ASP	HIS	PRO		ILE	GLN	GLN
	V4043	H3733	H3733	E3643	HIS	ASP	SER	PHE	TYR	PHE	GLY		L3124	ASN	ASN
	I4044	D3735	D3735	L3644	LEU	THR	LYS	THR	ARG	LEU	ARG		S3130	ILE	LEU
	S4045	T3922	G3736	L3645	GLN	GLU	ALA	ALA	ALA	PRO	ALA		C3131	VAL	ILE
													Y3132	VAL	ARG
													R3133	VAL	TYR
													I3134	ASP	GLN
														HIS	ALA
														GLY	ALA
														ASP	ILE



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

Chain B: 77% 22%

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

Chain E: 77% 22%

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

Chain H: 78% 21%

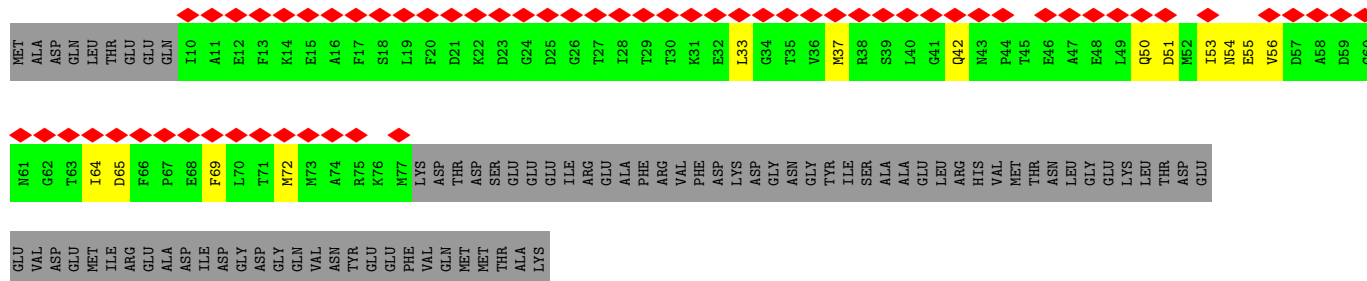
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain K:  78% 21%



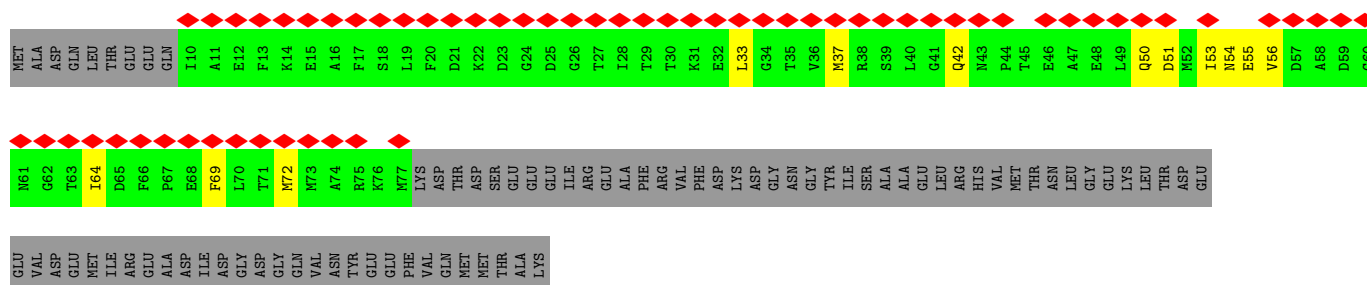
- Molecule 3: Calmodulin-1

Chain C:  42% 37% 9% 54%



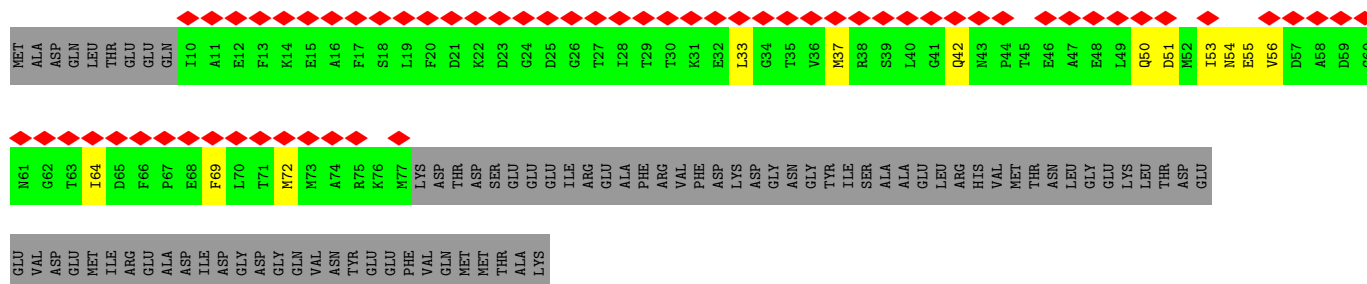
- Molecule 3: Calmodulin-1

Chain F:  42% 38% 8% 54%



- Molecule 3: Calmodulin-1

Chain I:  42% 38% 8% 54%



- Molecule 3: Calmodulin-1

Chain L:  42% 38% 8% 54%



GLU	VAL	ASP	GLU	MET	ILE	ARG	GLU	ALA	ASP	ILE	ASP	GLY	ASP	GLN	VAL	VAL	GLN	MET	MET	THR	ALA	LYS																																				
N61	G62	T63	I64	D65	F66	P67	E68	F69	L70	T71	M72	M73	A74	R75	K76	M77	LYS	ASP	THR	ASP	SER	GLU	GLU	ILE	ARG	GLU	ALA	PHE	ARG	VAL	PHE	ASP	LYS	ASP	GLY	ASN	GLY	TYR	SER	ILE	ALA	GLU	LEU	ARG	HIS	VAL	MET	THR	ASN	LEU	GLY	GLU	LYS	LEU	THR	ASP	GLU	
ALA	ASP	GLN	LEU	THR	GLU	GLU	GLN	I10	A11	E12	F13	K14	E15	A16	F17	S18	L19	F20	D21	K22	D23	G24	D25	G26	T27	I28	T29	T30	K31	E32	L33	G34	T35	V36	M37	R38	S39	L40	G41	Q42	M43	P44	T45	E46	A47	E48	L49	Q50	D51	M52	I53	N54	E55	V56	D57	A58	D59	C60

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	77092	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.046	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	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, ZN, CA, CFF

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	0.31	3/27161 (0.0%)	0.59	9/36737 (0.0%)
1	D	0.29	0/27161	0.60	12/36737 (0.0%)
1	G	0.29	0/27161	0.59	7/36737 (0.0%)
1	J	0.29	0/27161	0.59	10/36737 (0.0%)
2	B	0.25	0/835	0.54	0/1123
2	E	0.26	0/835	0.54	0/1123
2	H	0.25	0/835	0.54	0/1123
2	K	0.25	0/835	0.54	0/1123
3	C	0.18	0/530	0.53	0/711
3	F	0.18	0/530	0.53	0/711
3	I	0.18	0/530	0.53	0/711
3	L	0.18	0/530	0.53	0/711
All	All	0.29	3/114104 (0.0%)	0.59	38/154284 (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	23
1	D	0	23
1	G	0	23
1	J	0	23
All	All	0	92

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4522	LYS	CA-C	-13.08	1.36	1.52
1	A	4521	TYR	N-CA	12.78	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4522	LYS	N-CA	5.60	1.53	1.45

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4823	ARG	N-CA-C	19.57	139.02	113.97
1	J	2326	ILE	N-CA-C	-8.74	103.32	111.45
1	D	4823	ARG	CB-CA-C	-8.71	94.43	109.07
1	J	2326	ILE	CB-CA-C	7.26	121.44	111.92
1	A	4522	LYS	N-CA-CB	-6.97	98.69	111.37

There are no chirality outliers.

5 of 92 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	295	PHE	Peptide
1	A	728	ASP	Peptide
1	A	729	GLY	Peptide
1	A	739	ARG	Peptide
1	A	816	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	26661	0	25136	624	0
1	D	26661	0	25136	615	0
1	G	26661	0	25136	624	0
1	J	26661	0	25136	622	0
2	B	819	0	824	16	0
2	E	819	0	824	16	0
2	H	819	0	824	15	0
2	K	819	0	824	15	0
3	C	524	0	504	9	0
3	F	524	0	504	8	0
3	I	524	0	504	8	0
3	L	524	0	504	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
5	I	2	0	0	0	0
5	J	1	0	0	0	0
5	L	2	0	0	0	0
6	A	31	0	12	0	0
6	D	31	0	12	0	0
6	G	31	0	12	0	0
6	J	31	0	12	0	0
7	A	14	0	10	2	0
7	D	14	0	10	2	0
7	G	14	0	10	2	0
7	J	14	0	10	2	0
All	All	112212	0	105944	2381	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 11.

The worst 5 of 2381 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:4852:PHE:CZ	1:D:4823:ARG:HA	1.59	1.37
1:G:4861:ALA:CB	1:J:4864:GLN:HE21	1.53	1.22
1:D:4861:ALA:CB	1:G:4864:GLN:HE21	1.52	1.22
1:A:4861:ALA:CB	1:D:4864:GLN:HE21	1.52	1.21
1:A:4782:TYR:CD2	1:A:4851:PHE:CD1	2.30	1.20

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	3374/4968 (68%)	3009 (89%)	357 (11%)	8 (0%)	43	77
1	D	3374/4968 (68%)	3012 (89%)	355 (10%)	7 (0%)	43	77
1	G	3374/4968 (68%)	3012 (89%)	354 (10%)	8 (0%)	43	77
1	J	3374/4968 (68%)	3010 (89%)	355 (10%)	9 (0%)	36	71
2	B	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	E	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	H	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
2	K	105/108 (97%)	99 (94%)	6 (6%)	0	100	100
3	C	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
3	F	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
3	I	66/149 (44%)	63 (96%)	3 (4%)	0	100	100
3	L	66/149 (44%)	64 (97%)	2 (3%)	0	100	100
All	All	14180/20900 (68%)	12694 (90%)	1454 (10%)	32 (0%)	44	77

5 of 32 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4823	ARG
1	J	4823	ARG
1	G	4823	ARG
1	A	730	LEU
1	A	853	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	2672/4355 (61%)	2656 (99%)	16 (1%)	78	80
1	D	2671/4355 (61%)	2656 (99%)	15 (1%)	78	80
1	G	2671/4355 (61%)	2655 (99%)	16 (1%)	78	80
1	J	2671/4355 (61%)	2657 (100%)	14 (0%)	81	81
2	B	88/89 (99%)	88 (100%)	0	100	100
2	E	88/89 (99%)	88 (100%)	0	100	100
2	H	88/89 (99%)	88 (100%)	0	100	100
2	K	88/89 (99%)	88 (100%)	0	100	100
3	C	57/127 (45%)	57 (100%)	0	100	100
3	F	57/127 (45%)	57 (100%)	0	100	100
3	I	57/127 (45%)	57 (100%)	0	100	100
3	L	57/127 (45%)	57 (100%)	0	100	100
All	All	11265/18284 (62%)	11204 (100%)	61 (0%)	78	81

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	4817	HIS
1	J	2876	ASP
1	G	950	VAL
1	J	2793	THR
1	J	4816	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 214 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	783	ASN
1	G	3902	GLN
1	J	3916	GLN
1	G	1157	GLN
1	G	2196	ASN

5.3.3 RNA ⓘ

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 24 ligands modelled in this entry, 16 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	ATP	D	6002	-	32,33,33	1.32	4 (12%)	48,52,52	1.85	10 (20%)
6	ATP	G	6002	-	32,33,33	1.32	4 (12%)	48,52,52	1.85	10 (20%)
7	CFF	A	6003	-	15,15,15	2.01	7 (46%)	23,23,23	2.75	9 (39%)
6	ATP	J	6002	-	32,33,33	1.32	4 (12%)	48,52,52	1.85	10 (20%)
7	CFF	G	6003	-	15,15,15	2.02	8 (53%)	23,23,23	2.75	9 (39%)
7	CFF	J	6003	-	15,15,15	2.01	7 (46%)	23,23,23	2.75	9 (39%)
6	ATP	A	6002	-	32,33,33	1.32	4 (12%)	48,52,52	1.85	10 (20%)
7	CFF	D	6003	-	15,15,15	2.01	8 (53%)	23,23,23	2.75	9 (39%)

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	ATP	D	6002	-	-	9/22/38/38	0/3/3/3
6	ATP	G	6002	-	-	9/22/38/38	0/3/3/3
7	CFF	A	6003	-	-	-	0/2/2/2
6	ATP	J	6002	-	-	9/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CFF	G	6003	-	-	-	0/2/2/2
7	CFF	J	6003	-	-	-	0/2/2/2
6	ATP	A	6002	-	-	9/22/38/38	0/3/3/3
7	CFF	D	6003	-	-	-	0/2/2/2

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	J	6002	ATP	C5-C4	4.41	1.47	1.39
6	A	6002	ATP	C5-C4	4.41	1.47	1.39
6	D	6002	ATP	C5-C4	4.41	1.47	1.39
6	G	6002	ATP	C5-C4	4.41	1.47	1.39
7	A	6003	CFF	C6-N1	-4.00	1.32	1.40

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	6003	CFF	C14-N7-C8	-7.58	112.09	126.28
7	D	6003	CFF	C14-N7-C8	-7.58	112.09	126.28
7	G	6003	CFF	C14-N7-C8	-7.58	112.09	126.28
7	J	6003	CFF	C14-N7-C8	-7.58	112.09	126.28
6	A	6002	ATP	C5-C4-N3	-6.17	118.23	126.72

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

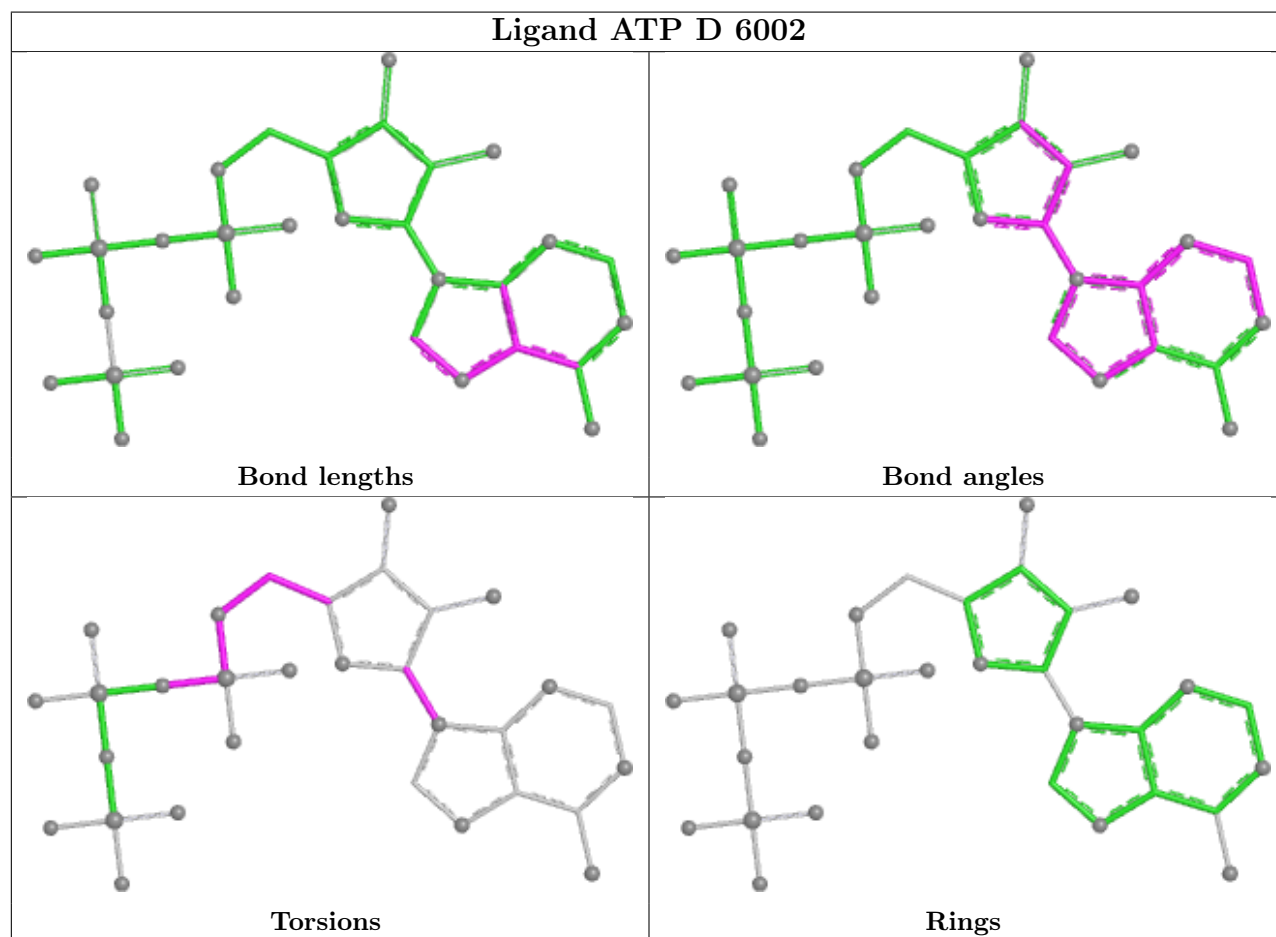
Mol	Chain	Res	Type	Atoms
6	A	6002	ATP	C5'-O5'-PA-O2A
6	A	6002	ATP	C5'-O5'-PA-O3A
6	A	6002	ATP	O4'-C1'-N9-C8
6	A	6002	ATP	O4'-C1'-N9-C4
6	D	6002	ATP	C5'-O5'-PA-O2A

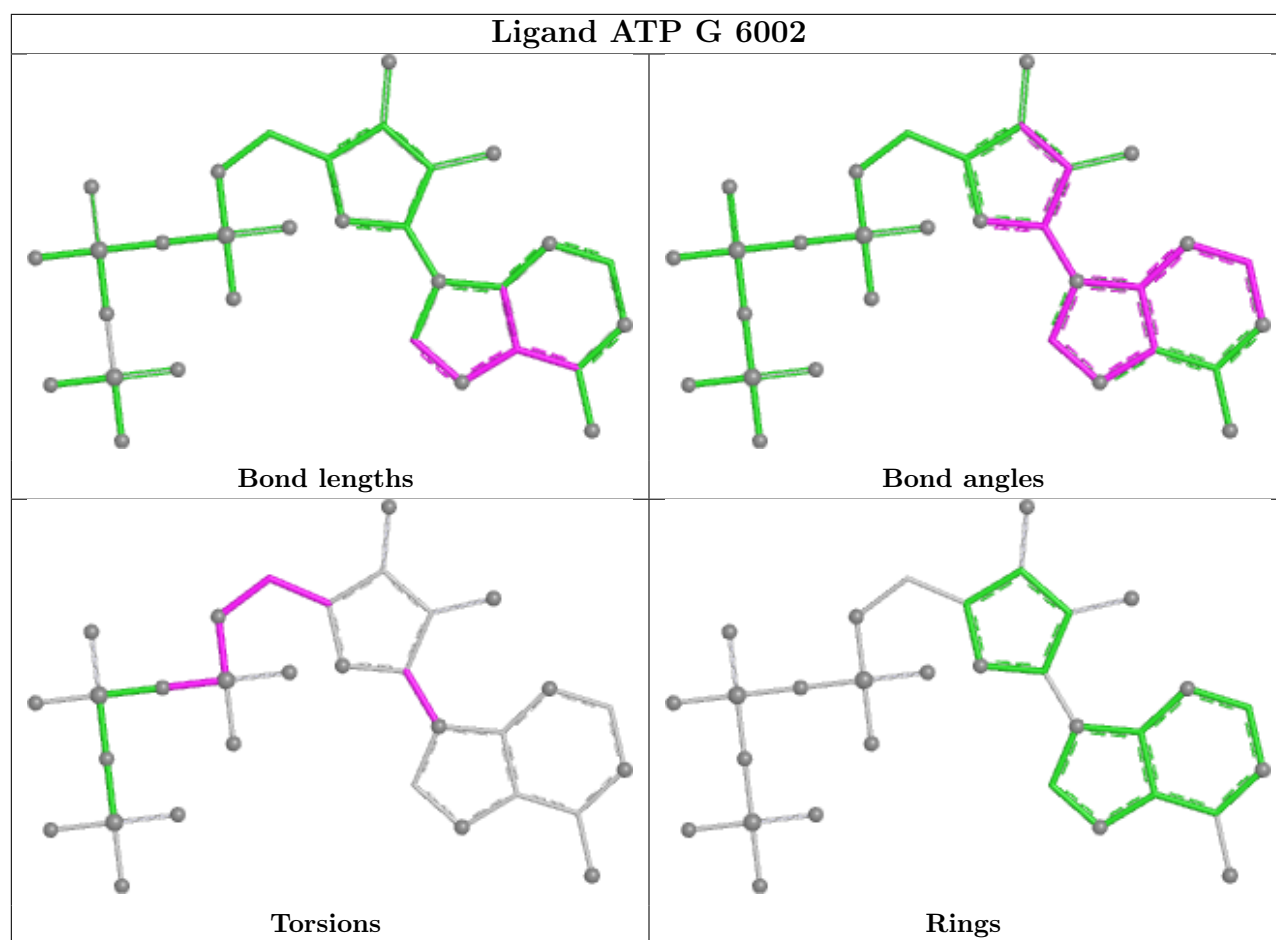
There are no ring outliers.

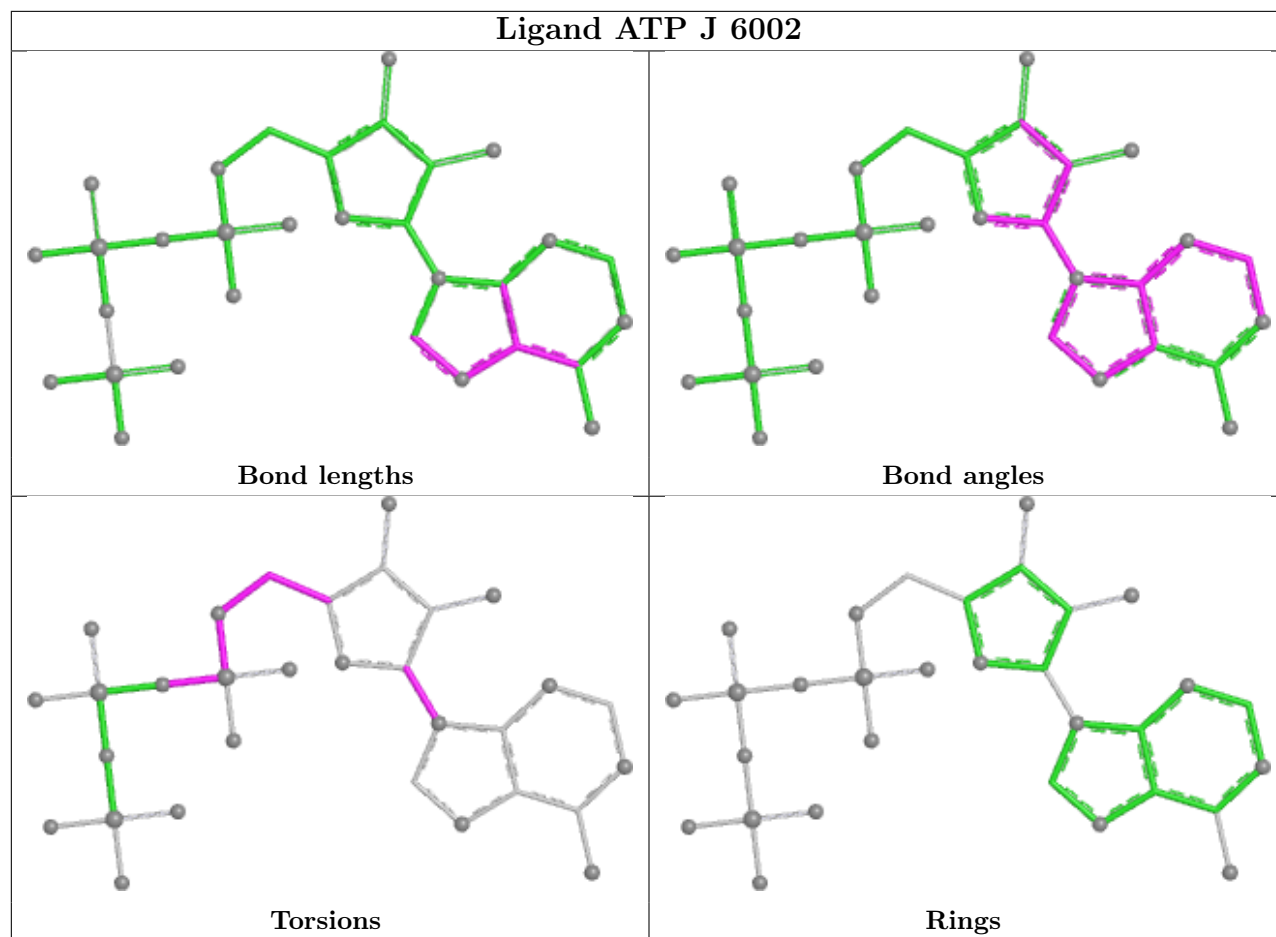
4 monomers are involved in 8 short contacts:

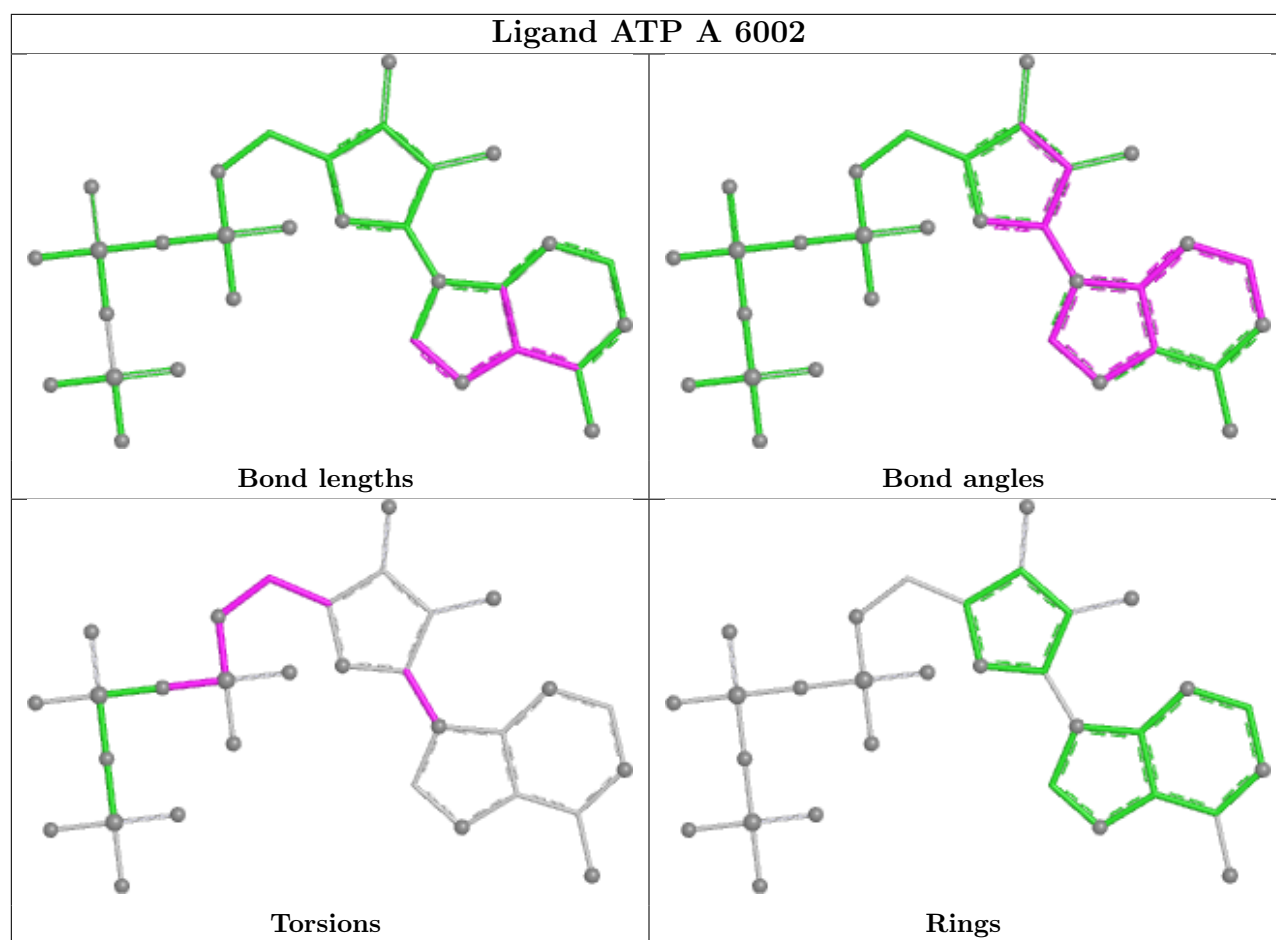
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	6003	CFF	2	0
7	G	6003	CFF	2	0
7	J	6003	CFF	2	0
7	D	6003	CFF	2	0

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.

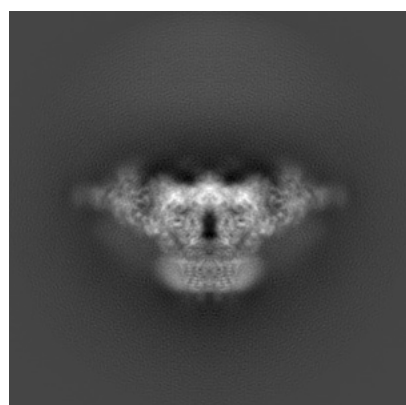
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9836. These allow visual inspection of the internal detail of the map and identification of artifacts.

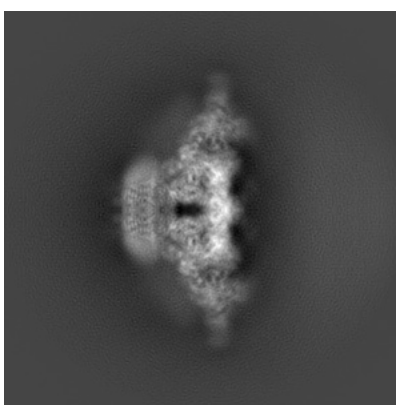
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

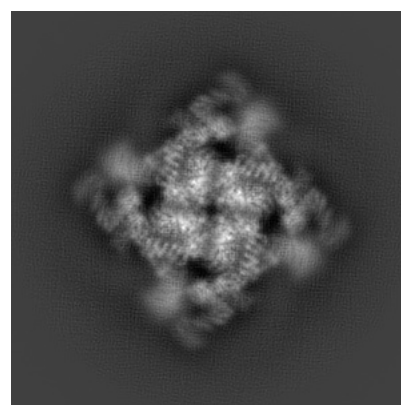
6.1.1 Primary map



X



Y

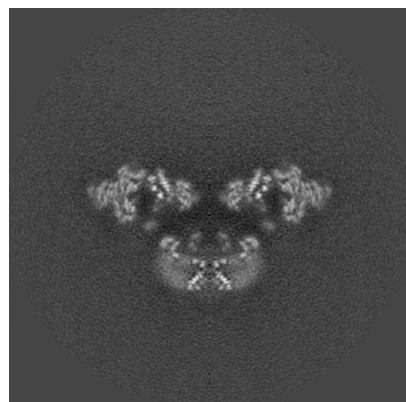


Z

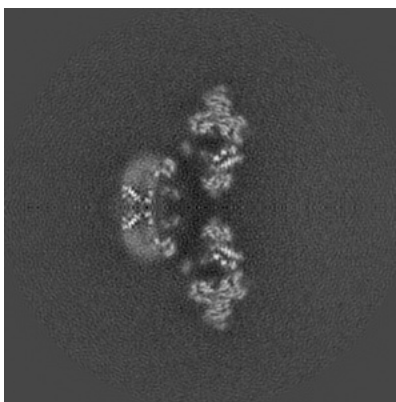
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

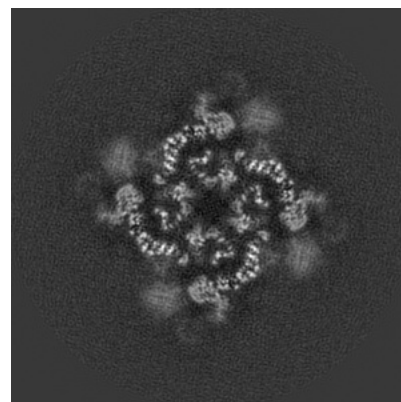
6.2.1 Primary map



X Index: 200



Y Index: 200

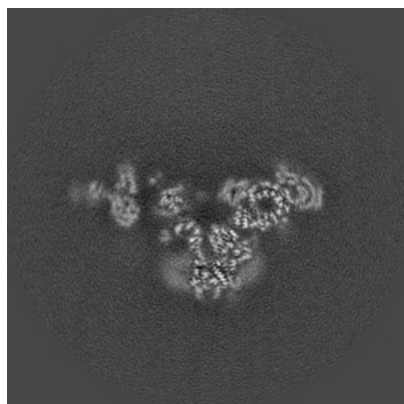


Z Index: 200

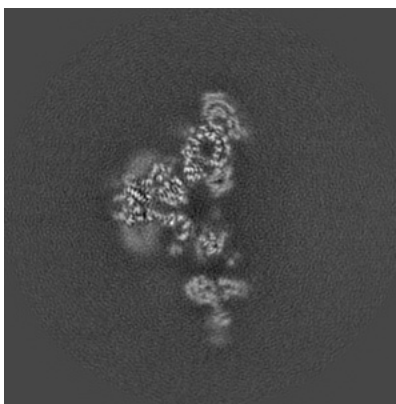
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

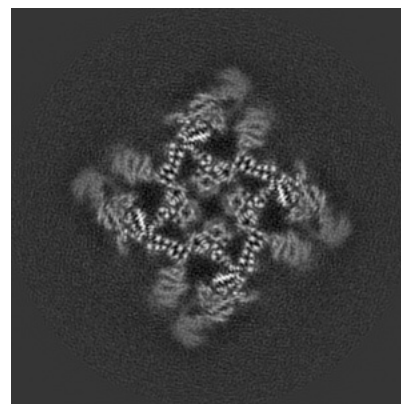
6.3.1 Primary map



X Index: 190



Y Index: 210

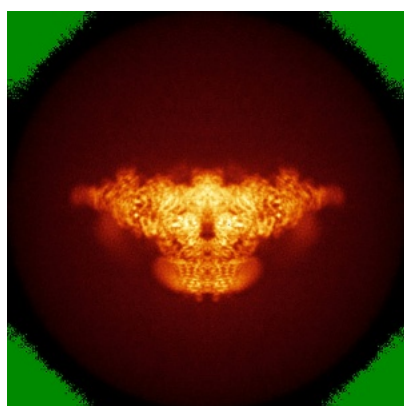


Z Index: 209

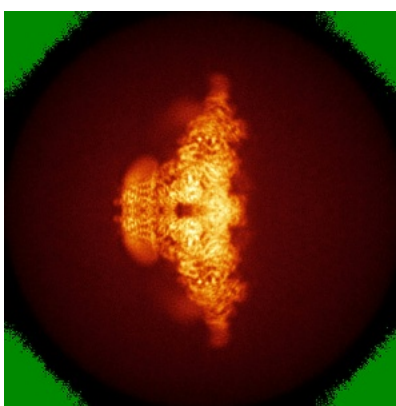
The images above show the largest variance slices of the map in three orthogonal directions.

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

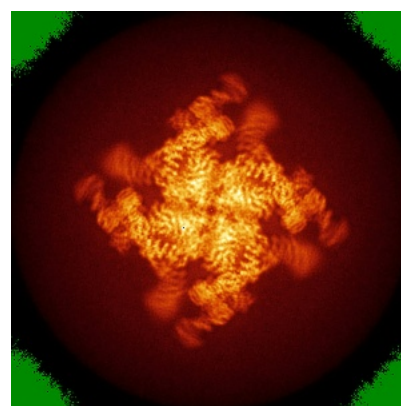
6.4.1 Primary map



X



Y

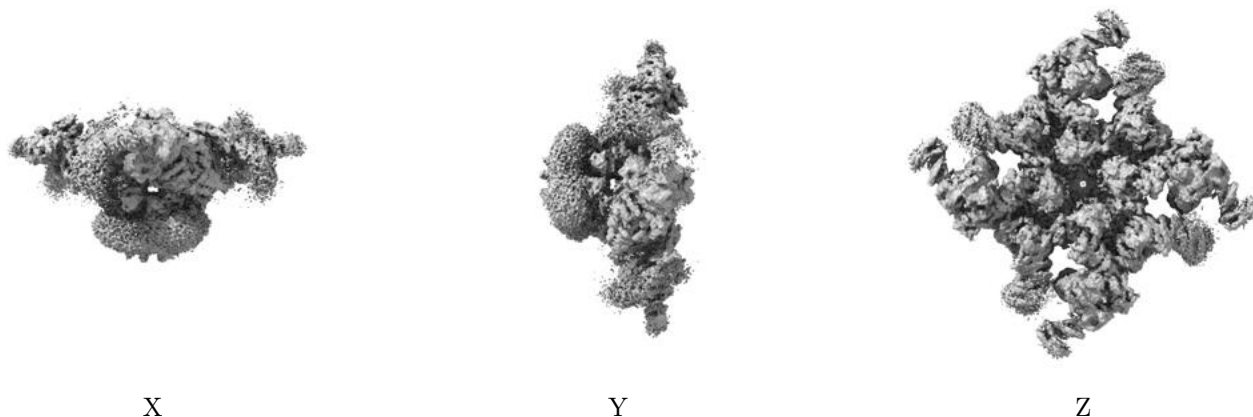


Z

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

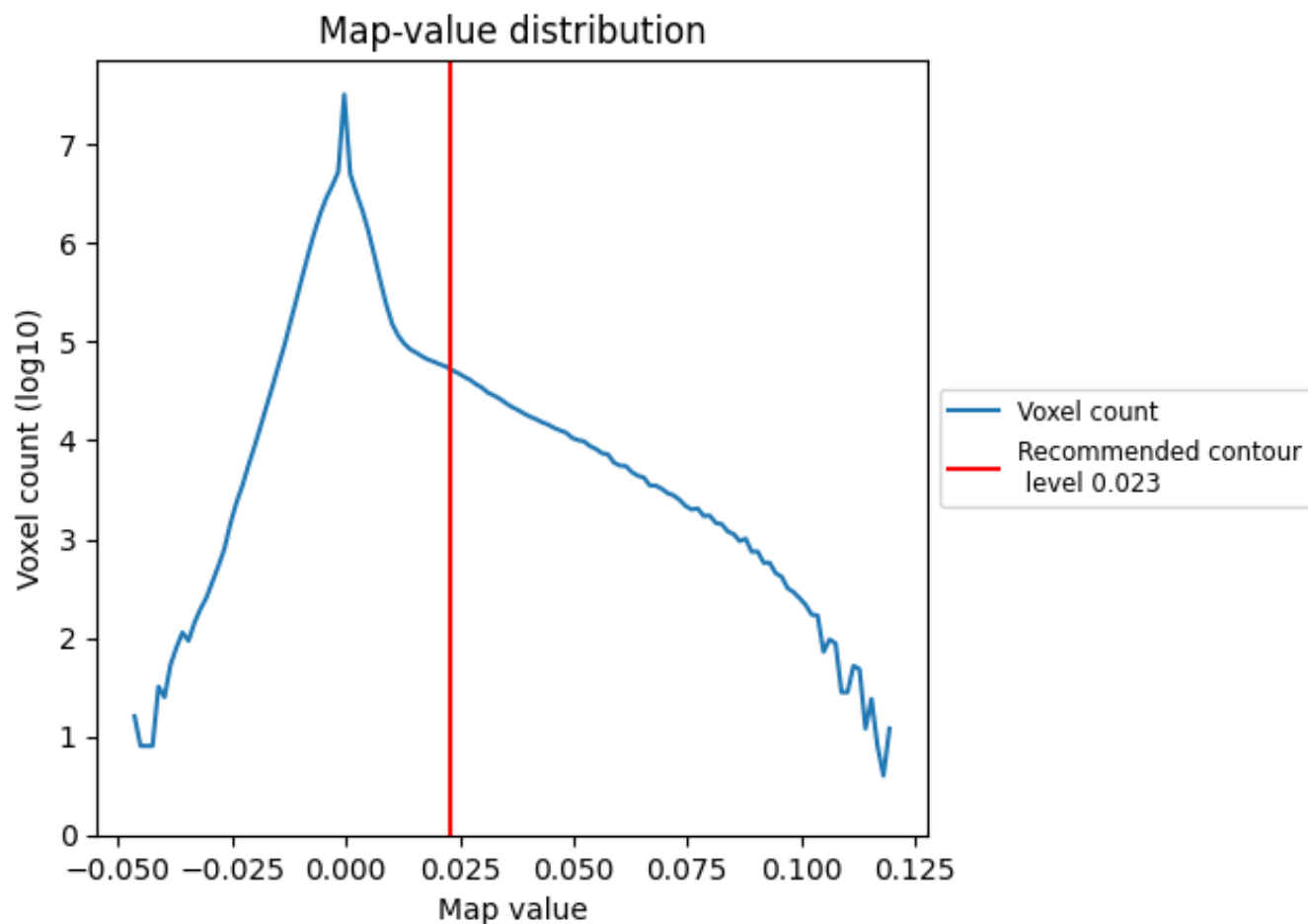
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

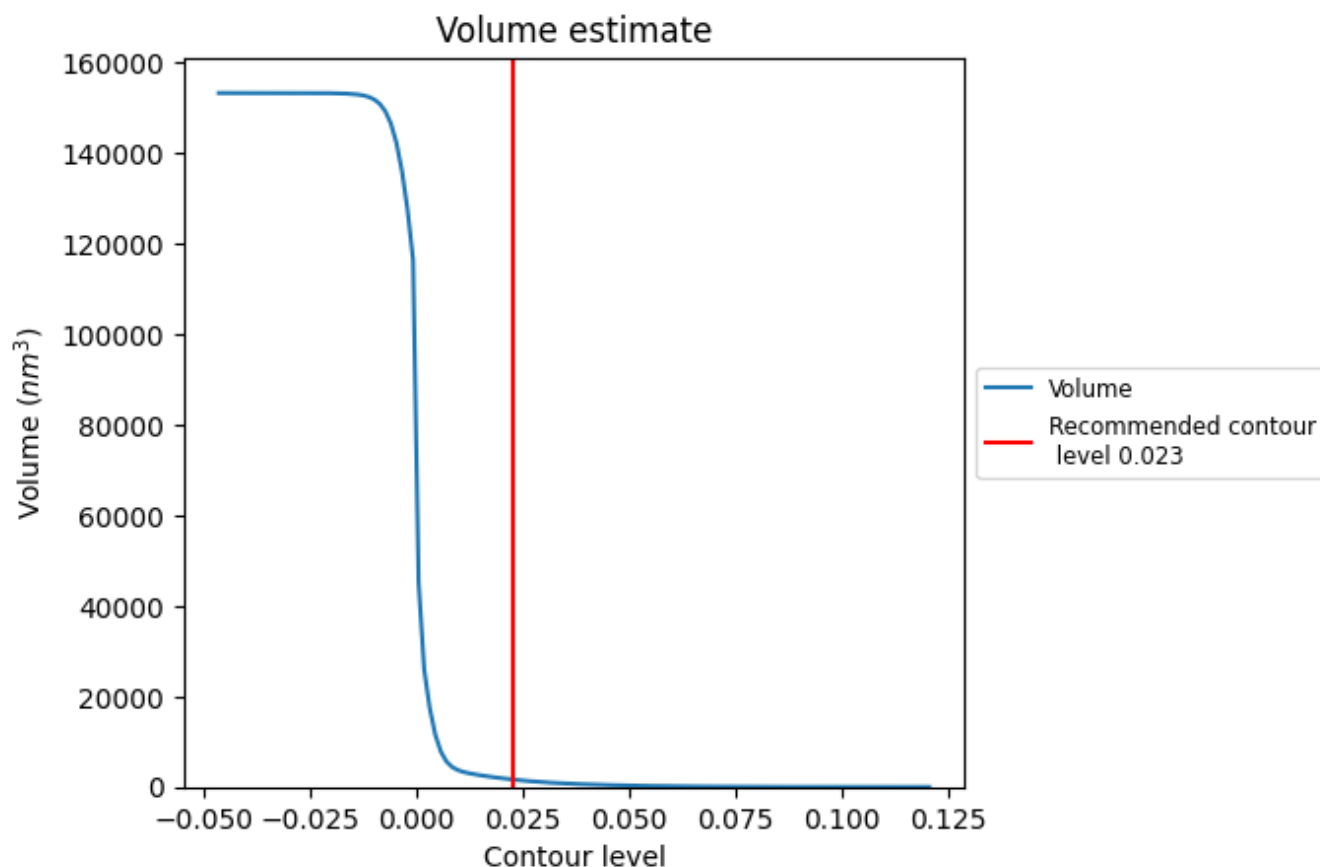
This section contains the results of statistical analysis of the map.

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.

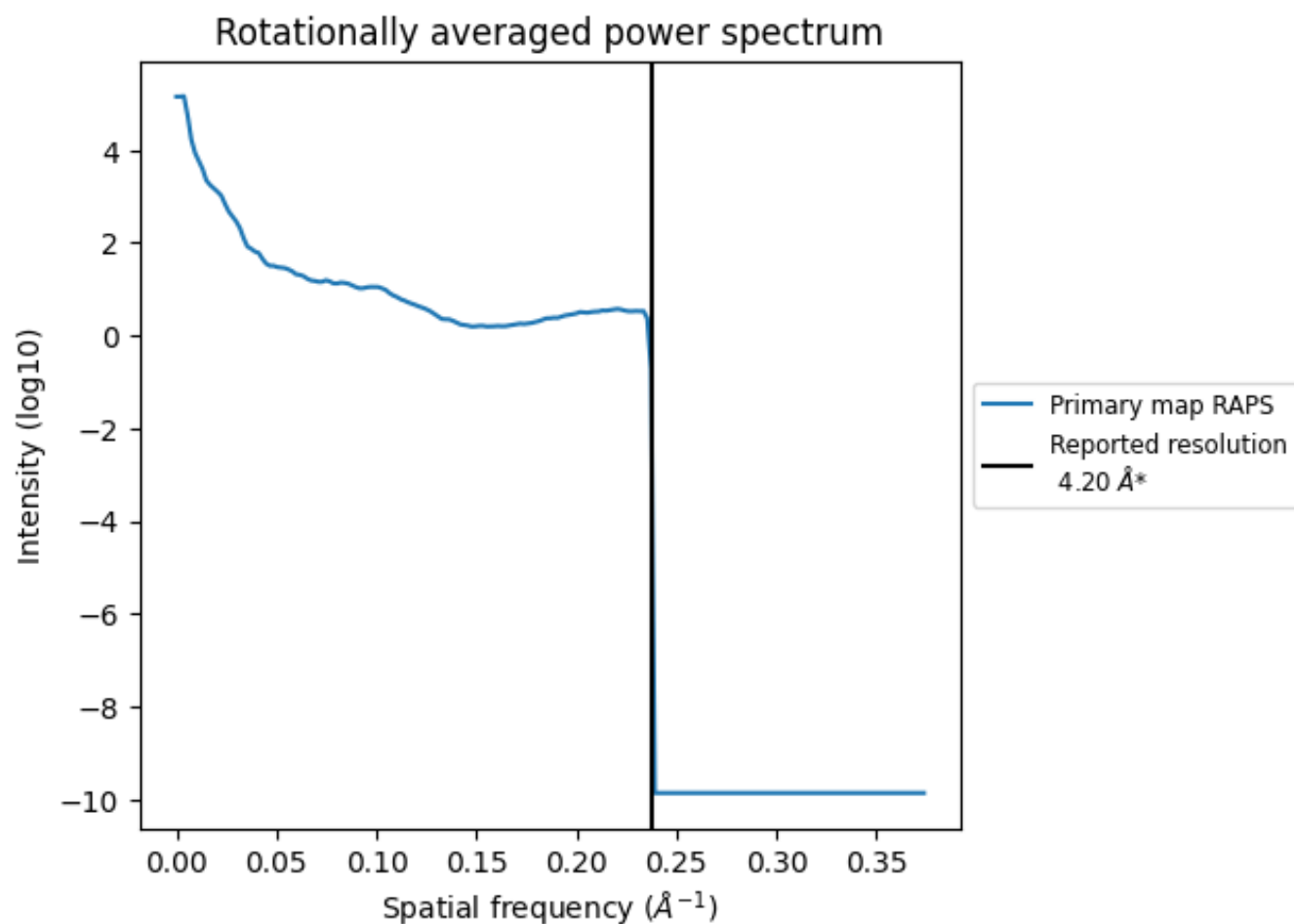
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1619 nm³; this corresponds to an approximate mass of 1462 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 ⓘ

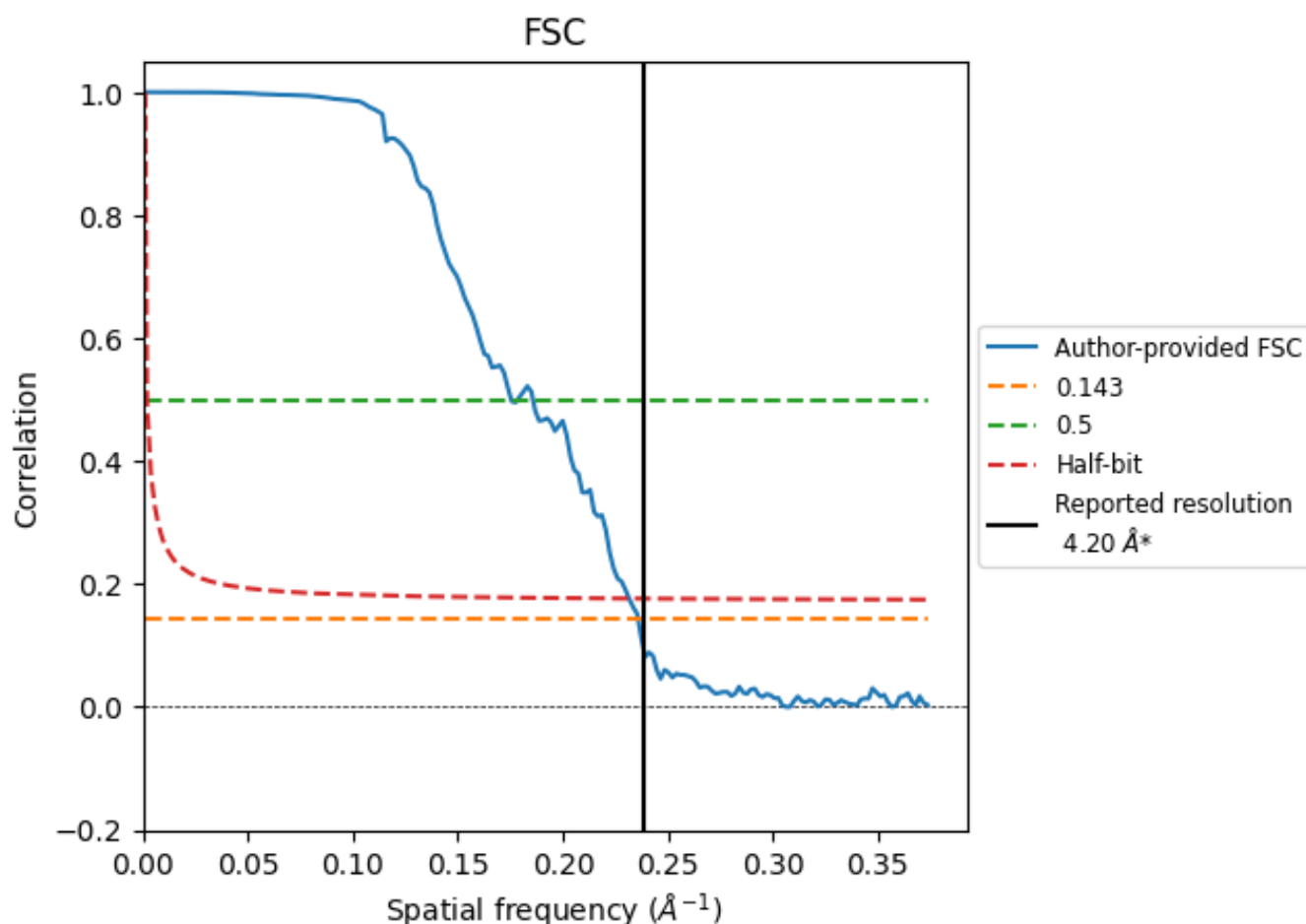


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

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 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

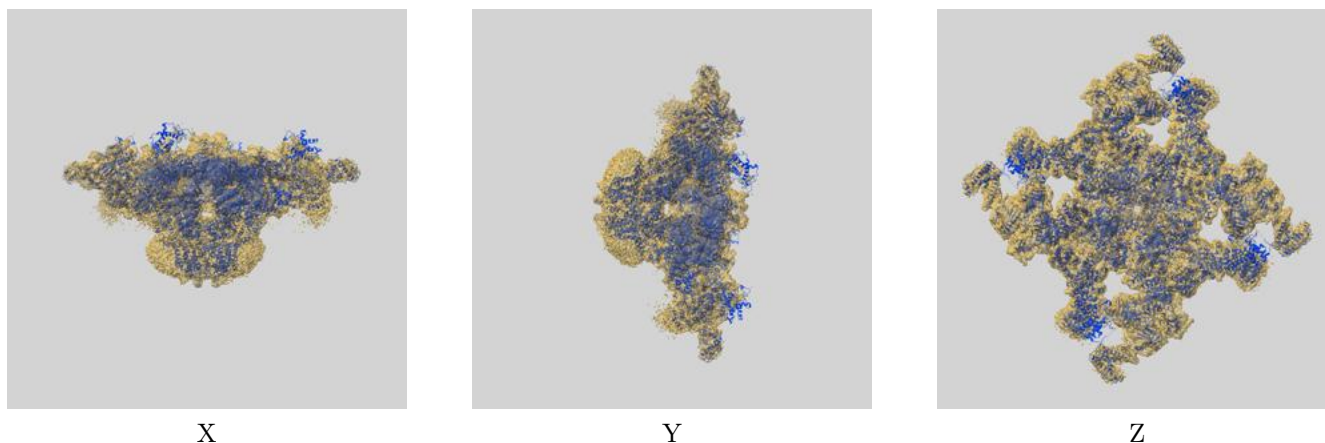
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.24	5.70	4.32
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

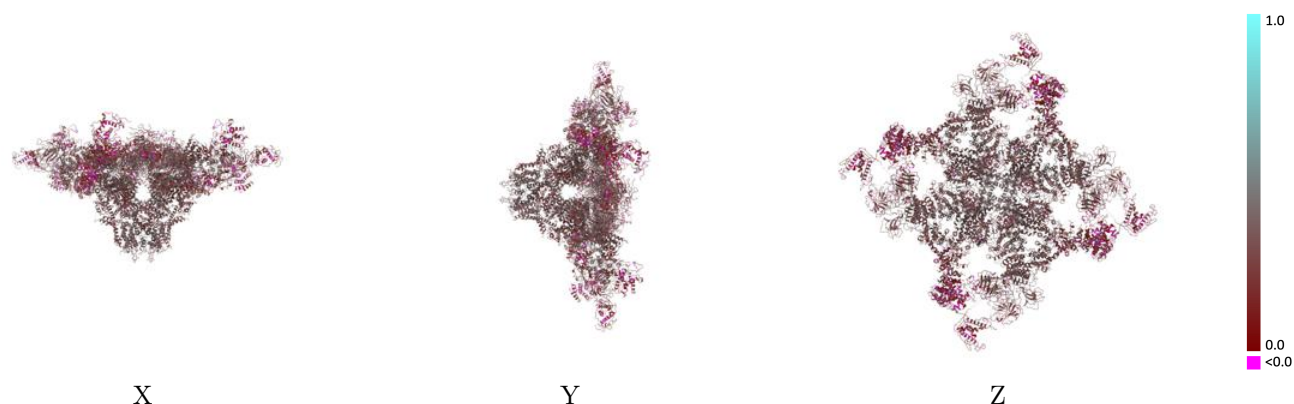
This section contains information regarding the fit between EMDB map EMD-9836 and PDB model 6JIU. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



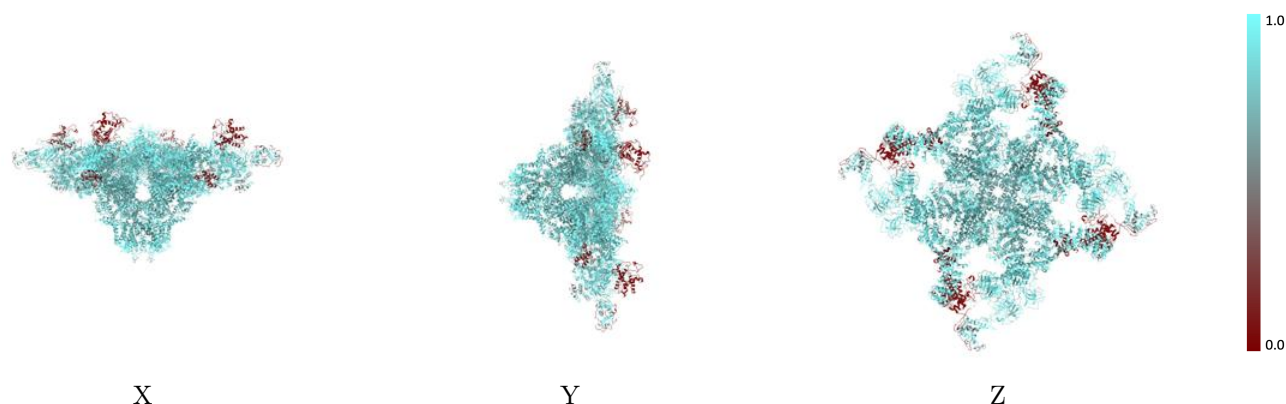
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



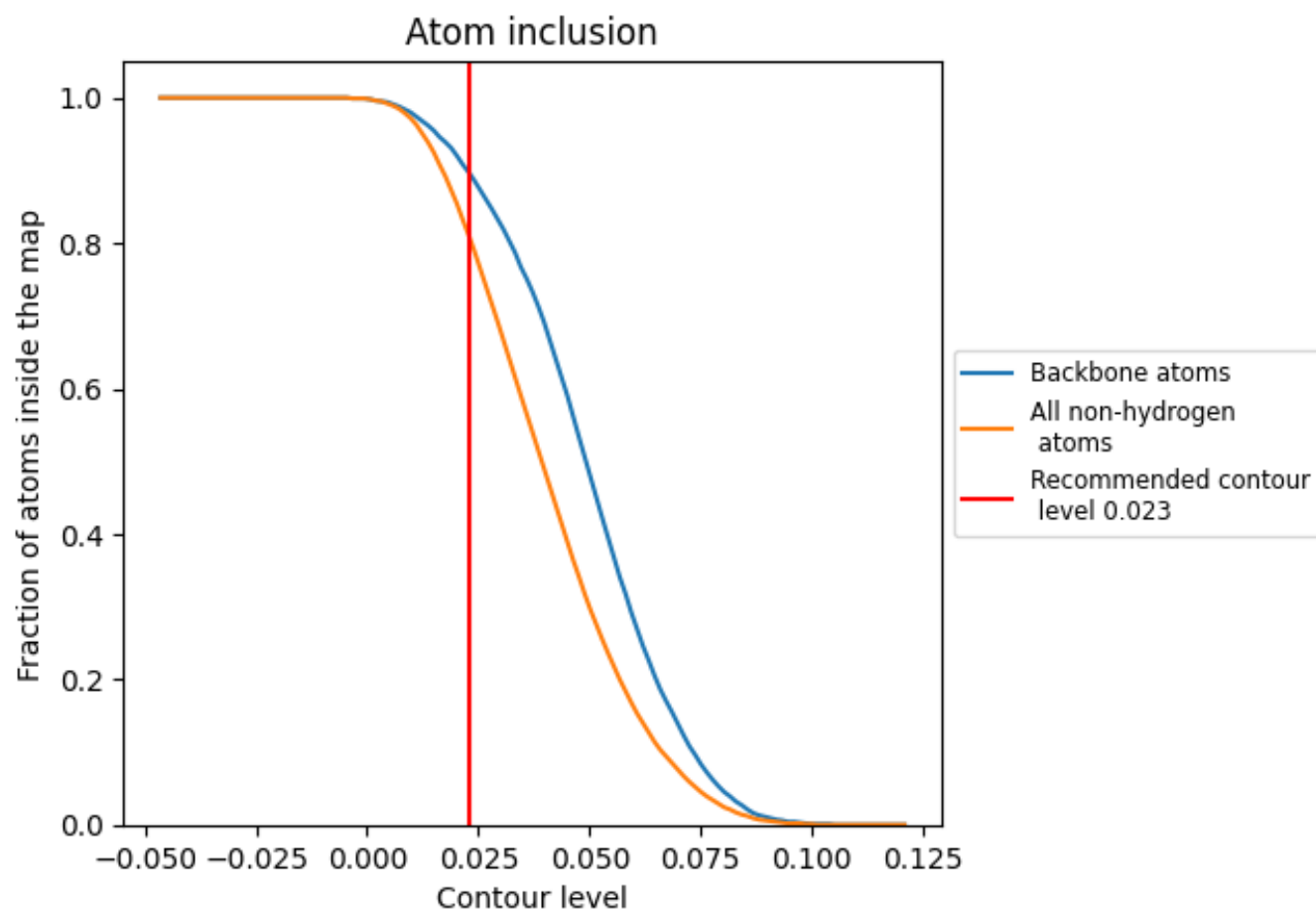
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 81% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8080	0.3030
A	0.8200	0.3050
B	0.8710	0.3450
C	0.1110	0.1780
D	0.8200	0.3050
E	0.8700	0.3430
F	0.1110	0.1750
G	0.8200	0.3040
H	0.8720	0.3420
I	0.1110	0.1790
J	0.8210	0.3040
K	0.8720	0.3420
L	0.1110	0.1800

1.0

0.0

<0.0