



wwPDB EM Validation Summary Report ⓘ

Nov 9, 2024 – 11:19 pm GMT

PDB ID : 8RRT
EMDB ID : EMD-19464
Title : Structure of rabbit RyR1 reconstituted into lipid liposomes in open state in complex with FKBP and Nb9657
Authors : Li, C.; Efremov, R.G.
Deposited on : 2024-01-23
Resolution : 4.60 Å(reported)

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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

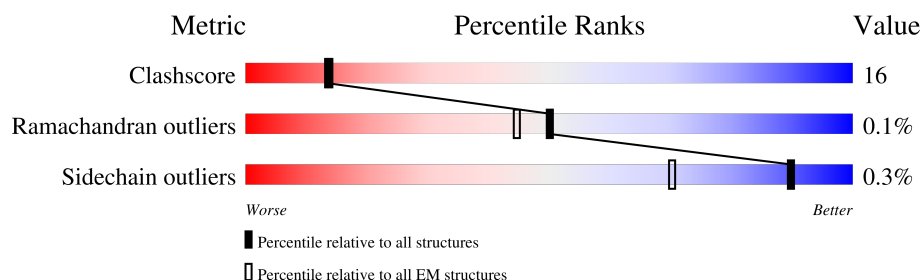
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	B	5027	58% 28% 14%
1	E	5027	57% 28% 14%
1	G	5027	57% 29% 14%
1	J	5027	57% 28% 14%
2	A	107	64% 36%
2	D	107	63% 37%
2	H	107	62% 37% .
2	I	107	61% 39%

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Mol	Chain	Length	Quality of chain
3	C	137	 51%40%8%
3	F	137	 51%40%8%
3	K	137	 53%38%8%
3	M	137	 57%34%8%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 143740 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	B	4319	Total	C	N	O	S	1	0
			34103	21737	5881	6261	224		
1	E	4319	Total	C	N	O	S	1	0
			34103	21737	5881	6261	224		
1	G	4319	Total	C	N	O	S	1	0
			34103	21737	5881	6261	224		
1	J	4319	Total	C	N	O	S	1	0
			34103	21737	5881	6261	224		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
2	I	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ASP	GLY	conflict	UNP Q8HYX6
D	100	ASP	GLY	conflict	UNP Q8HYX6
H	100	ASP	GLY	conflict	UNP Q8HYX6
I	100	ASP	GLY	conflict	UNP Q8HYX6

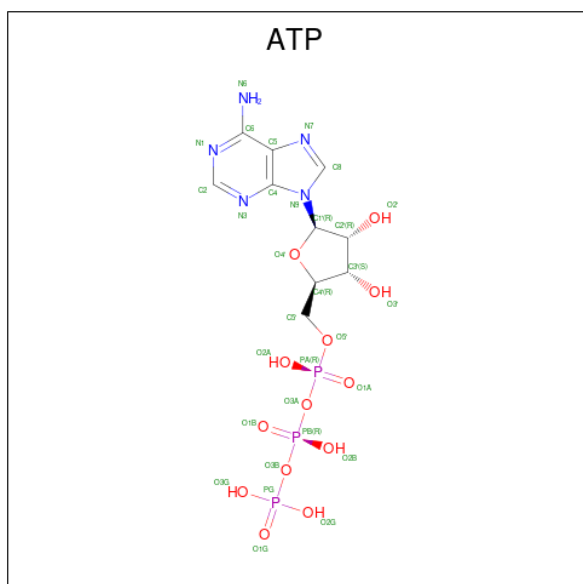
- Molecule 3 is a protein called Nanobody 9657.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	F	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	K	126	Total	C	N	O	S	0	0
			967	597	170	195	5		
3	M	126	Total	C	N	O	S	0	0
			967	597	170	195	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
4	B	1	Total	Zn	0
			1	1	
4	E	1	Total	Zn	0
			1	1	
4	G	1	Total	Zn	0
			1	1	
4	J	1	Total	Zn	0
			1	1	

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



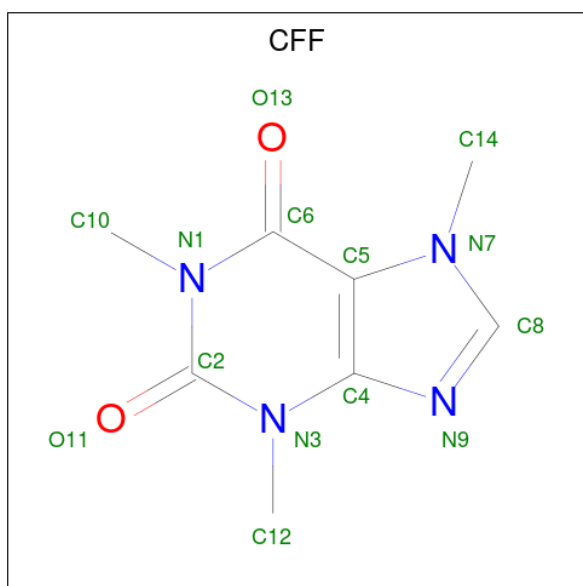
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

- Molecule 6 is CAFFEINE (three-letter code: CFF) (formula: $C_8H_{10}N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	G	1	Total	C	N	O	0
			14	8	4	2	
6	J	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Ca	0
			1	1	

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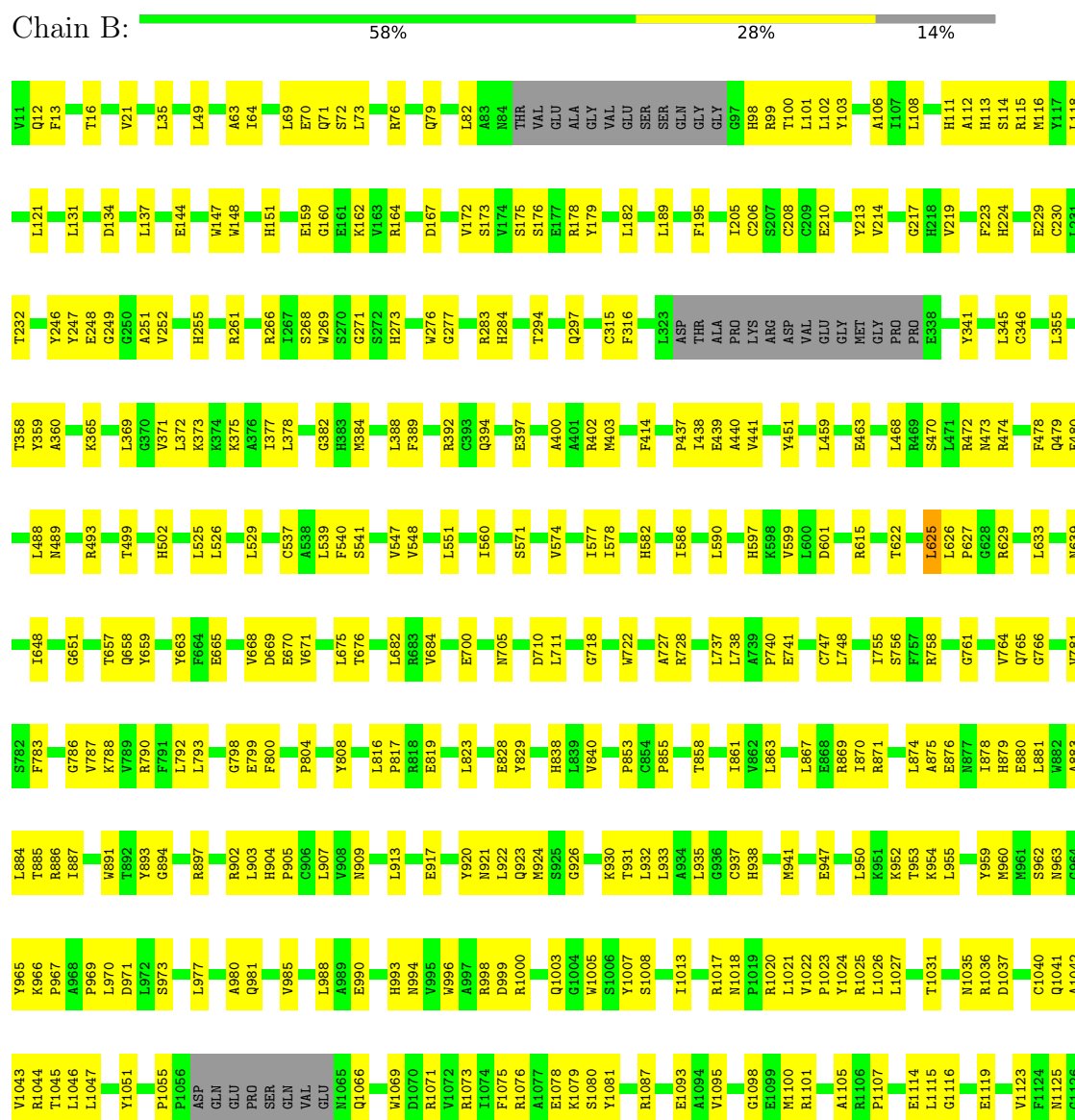
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Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total 1	Ca 1	0
7	G	1	Total 1	Ca 1	0
7	J	1	Total 1	Ca 1	0

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



S9581	R2454	F2364	Q2247	L2138	SER	GLU	M1494	LYS	TYR	R1232	H1127
H2582	R2458	G2365	F2251	A2141	SER	GLU	G1497	ALA	GLU	R1232	R1128
T2585	L2463	L2368	F2251	Y2142	LEU	GLU	G1498	LYS	ASN	G1129	Q1130
R2588	L2469	R2369	Y2256	M2153	ARG	ALA	D1499	ALA	ARG	R1131	W1132
R2591	L2472	G2372	L2257	R2163	SER	PRO	F1500	ALA	ARG	P1243	H1133
Q2592	L2472	L2376	L2263	R2163	LEU	GLU	S1502	MET	SER	Q1244	L1134
R2593	L2479	L2380	L2265	L2166	GLU	GLY	S1502	THR	ALA	F1245	P1138
S2594	L2479	I2380	Q2266	L2167	THR	LYS	W1502	GLN	GLY	P1248	W1143
L2595	L2489	E2381	Q2267	E2175	VAL	ASP	G1504	PRO	TRP	V1249	V1148
A2598	K2489	Q2268	Q2268	E2175	ARG	ASP	GLN	ALA	GLY	H1252	M1152
Q2599	K2490	Q2269	Q2269	E2175	LEU	ASP	R1508	THR	ALA	E1256	D1154
R2600	K2491	R2385	S2270	M2178	VAL	L1922	I1509	PRO	GLU	M1260	L1155
D2601	F2494	P2395	S2271	I2179	LYS	L1926	D1513	PRO	GLY	Q1269	T1159
I2603	V2495	GLY	P2272	I2182	LYS	L1931	L1514	ASP	LYS	H1274	I1161
E2604	P2496	VAL	L2273	V2190	GLU	M1939	G1547	VAL	GLY	R1275	T1177
D2605	D2497	ARG	S2279	V2190	LYS	L1942	M1548	PRO	THR	R1290	A1178
C2606	F2505	ASP	L2286	Q2193	PRO	L1945	L1518	GLY	THR	L1291	F1179
M2608	L2506	ARG	Q2292	H2194	GLU	Y1945	D1520	HIS	GLY	S1292	E1181
A2609	D2507	ARG	Q2293	L2197	LEU	Q1949	L1522	VAL	GLY	L1293	I1182
L2610	R2508	GLU	E2296	M2198	PRO	R1954	L1526	PRO	THR	F1297	T1184
I2614	V2509	HIS	E2296	G2202	ALA	R1964	M1527	ALA	THR	T1304	L1189
R2615	G2511	PHE	C2305	H2204	GLU	R1964	F1540	ASP	VAL	ALA	P1190
P2616	L2512	GLY	G2310	E2205	R2089	K1968	T1557	GLY	ALA	GLU	V1191
L2619	Q2515	PRO	C2310	T2206	L2094	GLU	Q1558	GLY	VAL	THR	C1192
Q2620	D2516	PRO	L2313	T2207	Q2095	GLU	Q1558	GLY	VAL	PRO	S1193
H2621	F2517	GLU	L2313	M2208	Q2096	GLU	Q1563	GLY	VAL	LEU	L1194
L2623	L2518	GLU	Y2318	E2209	L2097	P2001	I1562	ALA	ARG	PRO	G1195
R2624	L2519	N2414	L2321	V2210	H2100	Q2005	E1565	ALA	ALA	PRO	P1196
R2625	L2522	L2418	L2321	M2211	H2100	Q2005	Q1569	GLY	GLY	GLY	V1199
L2626	F2526	I2422	N2324	V2212	Q2107	F2012	Q1569	GLN	ASN	LEU	G1200
V2630	F2541	L2429	P2325	R2213	Q2107	K2013	T1557	PRO	GLN	GLN	H1201
P2631	L2550	I2430	F2329	L2215	Y2110	L2031	Q1557	LYS	LYS	PRO	V1208
L2633	L2550	D2431	R2330	G2216	V2111	L2031	Q1557	ALA	THR	ALA	A1215
F2636	V2558	R2435	D2333	GLY	Q2112	D2037	Q1569	GLY	THR	GLU	L1219
P2640	L2562	E2439	F2334	GLY	S2113	Q2045	L1703	GLY	GLY	ALA	Q1220
L2641	T2563	M2440	L2335	THR	V2117	LEU	P1704	LYS	ASN	ARG	E1221
L2643	K2564	H2441	R2336	GLU	M2120	GLY	P1574	ALA	ALA	ALA	G1222
L2644	C2565	L2442	V2352	I2223	S2122	GLY	L1575	THR	THR	ASP	F1224
T2645	T2572	K2447	V2353	V2229	L2123	GLY	L1581	GLY	GLY	GLU	L1228
N2646	T2573	R2355	R2355	T2230	R2126	GLU	R1584	LYS	LYS	ALA	Q1229
H2647	H2574	L2357	L2357	C2233	Q2127	GLU	R1594	ALA	LYS	ARG	E1221
Y2648	R2575	R2358	R2359	R2234	Y2128	GLY	L1595	GLY	GLY	PRO	F1224
C2651	V2579	L2451	E2362	I2242	L2131	THR	E1596	PHE	PHE	ASP	I1228
W2652	D2580	R2452	C2363	I2242	L2134	LEU	Q1597	LEU	LEU	PRO	N1229
		I2453					M1599	ASP	PHE	ASP	



W5019	R4913	K4774	L4648	Y4573	GLY	VAL	LEU	GLU	D4118	L4019	Y3937
D5020	V4914	Y4775	L4652	Y4577	ALA	ASP	ALA	ALA	ASP	Q4020	
P5023	I4918	Q4776	W653		ASP	GLY	PRO	GLY	M4122	K4021	D3941
S5037		K4779	A4654	Y4580	GLU	GLY	MET	THR	I4123	D4022	V3942
	I4927	F4655	L4656	K4581	GLU	PRO	ASP	ALA	N4124	M4023	L3943
	I4931	V4782	E4657	V4582	ASN	PHE	PRO	ARG	F4125	V4024	E3944
	L4935	I4783	I4658	S4583	GLY	ARG	THR	GLY	E4126	E3945	E3944
			I4659	D4584	GLY	PRO	SER	ALA	E4127	M4026	Q3946
					LYS	GLU	ASP	ALA	F4128	G3947	G3947
						GLU	ASP	ALA	N4129	K3948	K3948
						GLY	GLU	THR	L4130	R3949	R3949
						VAL	VAL	ALA	R4131		
						PRO	HIS	LEU	F4132	M3955	M3955
						GLY	GLY	ALA	Q4133	I4040	
						LEU	GLY	ALA	E4134		A3958
						GLY	LEU	LEU	P4135	Q4043	X3959
						ASP	PRO	LEU	GLY	M4044	Q3960
						MET	ALA	TRP	N4142	V4045	V3961
						GLY	GLY	ALA	D4046	F3962	F3962
						ALA	PRO	VAL	T4148	M4047	
						PRO	GLY	VAL	N4149	L4048	L3965
						LYS	GLY	ALA	L4150	V4049	T3986
						ASP	GLY	ALA	S4151		E3967
						ALA	ASP	ARG	E4152	F4061	Y3968
						PRO	ASP	GLY	F4062	F3969	
						GLY	GLY	ALA	Y4177	D4063	Q3970
						ALA	ALA	ALA			
						THR	GLY	GLY	R4180	K4067	C3973
						PRO	GLY	ALA	THR	T3974	T3974
						GLY	GLY	GLY	M4184	V4072	G3975
						LYS	GLU	ALA	N3976	Q3977	N3976
						LYS	GLY	ALA	R4192	F4077	Q3977
						PRO	GLY	ALA		Q4078	Q3978
						ILE	GLY	GLY	E4199	D4079	
						ALA	ASP	ALA			
						LYS	LEU	LEU	R4202	V4081	A3981
						ALA	ALA	ARG	ALA		H3982
						LYS	GLU	LEU	E4206	S3983	S3983
						GLY	GLY	LEU	L4088	R3984	R3984
						LEU	GLY	THR	S4089	L3985	L3985
						GLY	ASP	TRP	A4090	W3986	W3986
						VAL	GLY	GLY	F4219	D3987	D3987
						GLY	ASP	SER	ALA		
						GLY	GLU	LEU	E4229	F4093	H3994
						GLU	VAL	PHE	ARG	V3995	V3995
						GLY	GLY	GLY	E4232	A4096	F3996
						GLU	ALA	GLY	M4037	M4037	A3997
						GLY	GLY	ARG	D4098	D4098	H3998
						LEU	HIS	LEU	S4099	M3999	M3999
						VAL	GLU	VAL	F4243	Q4100	M4000
						PRO	ALA	GLU	SER		
						GLY	GLY	TYR	I4247	F4103	L4003
						PRO	GLY	ALA	ARG	T4104	
						GLY	LYS	SER	I4251	Q4105	Q4009
						PRO	GLY	LEU	S4252		
						GLU	ALA	VAL	E4253	I4108	L4013
						PRO	GLY	THR	PRO		K4014
						GLY	GLY	ARG	GLY	L4112	E4015
						PRO	VAL	THR	GLY		L4016
						GLU	GLY	VAL	GLY	S4115	L4017
						PRO	VAL	ARG	PRO		D4018
						GLY	GLY	LEU	ARG		

● Molecule 1: Ryanodine receptor 1

Chain E: 57% 28% 14%

V11	Q12	F13	T16	V21	L35	L49	A63	I64	L69	E70	Q71	S72	L73	R76	Q79	L82	A83	H84	THR	VAL	GLU	ALA	GLY	GLY	VAL	GLU	SER	SER	GLN	GLY	G97	H98	R99	T100	L101	L102	Y103	A106	T107	L108	H111	A112	H113	S114	R115	L116	Y117	L118
L121	L131	D134	L137	E144	W147	W148	T149	H150	E159	C160	E161	K162	R164	D167	V172	S173	V174	S175	S176	S177	R178	Y179	L180	H181	L182	L189	F195	I205	C206	S207	C208	E210	Y213	V214	G217	H218	V219	F223	H224	D228								

L1703	L1574	V1483	ASN	E1221	G1116	M1035	L955	A875	G761	R629	R474	L345	E229
P1704	L1575	H1484	LYS	G1222	E1119	R1036	Y959	T878	V764	R629	Q479	C346	C230
R1708	L1581	S1485	ARG	E1224	V1123	D1037	M960	T879	Q765	L633	Q480	L355	T231
Y1712	R1584	S1486	GLY		F1124	C1040	N961	E880	G766	Q634	L488	L355	V245
I1716	P1587	L1487	PHE	I1228	N1125	Q1041	N963	A882	V761	N639	M489	T358	Y246
R1594		K1488	LEU	M1229	G1126	A1042	G964	A883	S762	L648	Y359	Y359	Y247
L1595		C1489	ASP	R1232	H1127	V1043	N965	T885	F763	R493	A360	E248	E248
E1721	R1596	G1497	TYR	K1240	G1129	R1044	K966	T886	G786	G651	K365	G249	G249
S1722	E1596	G1498	ALA	S1241	Q1130	T1045	P967	T887	V787	T499	A251	G250	G250
A1723	V1597	G1499	ARG	L1242	R1131	L1046	A968	I887	K788	H502	V252	A251	A251
G1724	E1598	P1243	ARG	P1243	H1132	L1047	P969	T887	Q658	L369			
R1725	M1599	Q1244	SER	Q1244	L1134	Y1051	L370	T889	Q658				
R1727	L1613	F1245	ALA	F1245	L1134	D971	D971	T892	Y659				
M1730	Q1614	V1248	GLY	V1248	P1138	P1055	S973	T893	Y659				
L1731	V1615	P1249	TRP	P1249	W1143	ASP	L977	G894	Y659				
Y1734	GLN	GLN	GLY	H1262	V1148	GLN		G897					
E1741	R1508	GLY	GLY	H1262	V1148	GLN	A980	R902	V668				
T1742	I1509	ALA	ALA	E1256	M1152	SER	Q981	H904	D669				
R1743	I1509	ALA	ALA	M1260	I1153	VAL	V985	P905	E670				
A1744	D1513	LEU	LEU	M1260	D1154	GLU	L988	P906	P804				
I1745	L1514	PRO	PRO	C1269	L1155	GLU	A989	L907	Y808				
C1630	C1518	PRO	GLY	L1270	T1159	GLY	E990	P908	L816				
P1749	V1520	ASP	GLY	R1271	I1160	GLY	N994	H904	P817				
R1759	D1521	VAL	GLY	H1274	I1161	GLY	N995	P905	L682				
P1763	L1522	VAL	GLY	R1275	T1177	R1071	W996	E917	L682				
R1772	L1526	PRO	THR	R1290	A1178	D1070	A997	Y920	L821				
P1773	M1527	ALA	THR	L1291	F1179	R1073	R998	N921	R822				
H1775	F1540	ASP	GLY	S1292	R1180	F1075	D999	L922	L823				
S1778	K1547	ASP	THR	L1293	E1181	R1076	R1000	Q923	E828				
P1779	L1548	GLY	THR	F1297	I1182	A1077	Q1003	M924	Y829				
P1780	F1549	GLY	GLN	T1304	E1183	E1078	Q1004	S925	G718				
P1780	F1550	VAL	GLN	ALA	I1184	K1079	W1005	G926	W722				
A1784	P1550	GLY	GLY	GLY	L1189	S1080	Y1007	K930	H582				
L1785	R1438	GLY	VAL	ALA	P1190	Y1081	S1006	T931	L586				
P1787	V1439	GLY	VAL	ALA	C1192	R1087	S1008	L932	A727				
ALA	V1442	ALA	ALA	ALA	S1193	E1093	L935	L932	R728				
ALA	Q1443	VAL	PRO	PRO	L1194	A1094	R1017	L935	L737				
ALA	E1444	ARG	VAL	ALA	G1195	V1095	M1018	G937	L738				
ALA	P1445	ALA	ALA	PRO	P1196	G1098	P1019	H938	A739				
ALA	W1449	ASN	GLY	GLY	V1199	E1099	R1020	P740	H597				
ALA	V1450	ASN	GLY	GLY	G1200	M1100	L1021	E741	L599				
E1793	P1455	LYS	LYS	PRO	H1201	R1101	P1022	C747	L600				
R1797	H1458	ASP	ASP	ALA	V1208	A1105	Y1024	L748	D601				
L1799	M1476	THR	THR	GLU	A1215	R1025	R1025	R615	L468				
I1802	G1477	GLY	GLY	ALA	Q1220	P1107	L1026	T622	L468				
						E1114	L1027	L625	L468				
						L1115	T1031	L626	L468				

K3023	L2946	M2874	K2802	V2630	F2541	L2429	E2329	G2216	Y2110	L2031	P1803
A3031	S2950	L2878	R2806	P2631	L2550	I2430	R2330	GLY	V2111	ASP	L1804
S3032	R2954	A2879	R2810	L2632	L2559	D2431	D2333	GLY	Q2112	GLU	R1808
E3035	R2954	E2880	K2813	F2636	L2559	R2435	L2335	THR	V2117	LYS	M1814
K3036	G2958	N2881	L2814	P2640	I2562	E2439	R2336	GLY	M2120	GLU	L1815
E3037	G2958	Y2882	K2815	L2641	T2563	H2440	V2352	GLY	F2121	GLU	G1816
M3038	Q2961	H2883	L2816	K2642	K2564	I2442	V2353	V2229	G2127	ASP	R1820
	Q2962	N2884	L2817	L2643	C2565	L2443	V2354	T2230	L2123	GLU	L1821
	L2963	T2885	L2818	L2644	T2572	K2447	R2355	V2239	GLU	GLU	G1822
	L2964	W2886	V2819	T2645	T2573	G2448	L2356	C2233	R2126	GLU	R1827
K3045	R2965	R2888	E2820	N2646	E2575	G2448	L2357	R2234	Q2127	GLU	D1828
L3046	W2966	Q2892	T2822	H2647	R2575	E2449	R2359	Y2238	Y2128	LYS	
A3047	W2966	T2742	T2822	Y2648	R2575	E2449	R2359	Y2238	GLU	GLU	
A3048	R2968	L2746	L2823	H2648	T2579	L2451	E2362	I2242	L2131	ASP	F1836
L3049	L2969	I2747	R2827	C2651	V2579	R2452	E2362	I2242	L2134	ALA	Q1837
V3050	S2970	P2748	R2827	W2652	D2580	I2453	C2363	THR	L2134	GLU	F1838
R3051	S2970	E2749	L2827	K2653	S2581	R2454	F2364	LEU	L2166	LYS	V1839
R3052	F2973	K2750	E2830	Y2654	M2582	R2458	G2365	GLU	L2138	GLU	K1843
R3053	A2975	L2751	GLU	C2656	T2585	L2463	L2368	ARG	A2141	GLU	L1844
V3054	A2975	F2754	THR	W2651	R2588	L2463	R2369	LEU	Y2142	GLU	V1845
F3057	L2977	L2755	GLU	S2658	R2588	I2469	G2372	ARG	M2153	ALA	
	E2978	A2759	LYS	E2671	R2591	L2472	L2376	LEU	R2163	GLU	M1851
D3060	W2980	E2760	LYS	E2671	G2592	L2472	L2376	LEU	L2166	GLY	G1852
V3065	V2986	E2764	LYS	H2673	S2594	L2479	I2380	GLU	L2166	GLU	F1854
C3067	S2989	K2765	THR	L2674	L2595	K2489	E2381	VAL	E2175	LYS	
L3068	S2989	W2766	LYS	L2674	L2595	M2490	I2384	ARG	E2175	ASP	E1857
H3069	Q2992	A2767	GLU	K2677	L2595	S2491	R2385	LEU	L1922	GLU	D1858
I3070	Q2993	F2768	GLN	L2678	R2600	F2494	R2385	VAL	L1926	VAL	V1859
	Q2994	D2769	THR	L2682	K2601	F2494	P2395	LYS	L1926	LYS	K1860
S3074	L2995	K2770	ALA	F2683	V2602	V2495	GLY	LYS	L1931	LYS	I1862
L3075	K2996	I2771	GLN	D2684	L2603	P2496	VAL	GLU	L1931	LYS	L1863
D3076	F2997	Q2772	THR	H2688	E2604	D2497	ARG	GLU	M1939	GLU	K1864
A3077	F2998	N2773	TYR	K2688	D2605	H2498	ARG	LYS	L1942	LYS	M1866
R3078	A2999	E2779	ASP	K2689	C2606	F2505	ASP	PRO	L1942	PRO	
T3079	K3000	N2780	PRO	K2690	C2606	F2505	ARG	GLU	Y1945	GLU	V1870
V3080	L3002	E2783	ARG	Y2691	M2608	L2506	ARG	GLU	Y1945	GLU	F1871
M3081	L3003	E2784	GLU	D2692	A2609	D2507	ARG	GLU	Q1949	GLU	
K3082	P3004	L2785	GLY	Q2693	L2610	R2508	GLU	LEU	Q1949	LEU	F1874
P3085	L3005	E2784	Y2855	L2694	E2614	V2509	HIS	PRO	GLU	PRO	GLU
E3086	L3006	E2784	P2857	L2695	R2615	Y2510	PHE	ALA	R1954	GLU	GLU
K3089	L3008	K2785	Q2858	Y2696	P2616	I2512	GLY	GLU	R1964	GLU	GLU
	L3009	T2787	P2859	R2697	P2616	I2512	GLU	GLU	R1964	GLU	GLU
L3092	F3010	H2788	P2860	H2698	L2619	Q2515	PRO	K1968	K1968	GLU	GLU
R3093	T3011	P2789	P2861	C2702	Q2620	D2516	PRO	L2094	L2094	GLU	GLU
S3094	N3012	L2790	L2862	L2706	H2621	F2517	GLU	Q2095	Q2095	GLU	GLU
F3095	L3018	R2792	S2863	L2706	L2622	L2518	GLU	E2209	E2209	GLU	GLU
C3096	S3019	P2793	L2866	L2710	L2623	L2519	N2414	V2210	V2210	GLU	GLU
E3097	T3020	F2797	T2866	P2711	R2624	L2522	L2418	V2212	V2212	GLU	GLU
S3098	P3021	S2798	S2868	D2716	R2625	L2522	L2418	R2213	R2213	GLU	GLU
A3099	A3022	E2799	L2871		L2625	F2526	I2422	P2325	P2325	GLU	GLU
S3100		K2800			V2627				L2215	K2013	



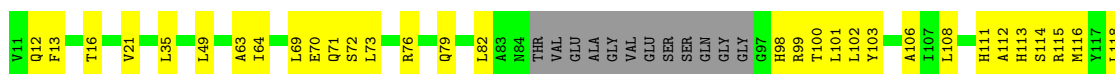




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C2606	L2607	M2608	A2609	L2610	L2614	L2615	P2616	L2619	Q2620	H2621	L2622	L2623	R2624	R2625	F2627	F2628	D2629	V2630	P2631	V2632	L2633	P2636	P2640	L2641	K2642	L2643	L2644	A2645	D2646	H2647	Y2648	C2651	W2652	K2653	Y2654	Y2655	C2656	W2661	S2668	E2671	L2672	H2673	L2674	A2676	K2677	R2678	V2679	I2682	F2683	D2684																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
H2688	K2689	K2690	Y2691	D2692	L2693	E2694	E2697	Y2698	H2699	L2700	C2702	L2706	L2710	P2711	D2716	K2725	LYS	ALA	THR	VAL	ASP	ALA	GLU	GLY	N2734	N2735	D2736	P2739	T2742	L2746	L2747	P2748	E2749	K2750	L2751	F2754	L2755	A2759	E2760	E2764	K2765	H2766	A2767	F2768	D2769	L2770	L2771																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
Q2772	N2773	E2779	E2783	E2784	L2785	K2786	H2788	P2789	M2790	L2791	R2792	P2793	F2797	S2798	E2799	K2800	D2801	K2802	R2806	K2810	E2811	L2812	L2813	N2814	A2815	M2816	L2817	A2818	W2819	E2820	T2821	L2823	R2827	E2830	GLU	GLU	ARG	THR	GLU	LYS	LYS	THR	ARG	LYS	ILE	F2768	D2769	GLN	THR	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
GLN	THR	TYR	ASP	PRO	ARG	GLY	GLY	L2985	L2986	P2987	Q2988	P2989	P2990	D2991	L2992	S2993	T2994	L2995	M2996	A2997	L2998	L2999	L3000	P3001	L3002	L3003	L3004	L3005	L3006	L3007	Q3008	Y3009	S3010	P3011	N3012	L3013	L3014	E3015	M3016	V3017	K3018	S3019	M3020	P3021	A3022	K3023	S3032	N3033	K3034	E3035	K3036	E3037	L3042	K3045	L3046	A3047	A3048	V3049	R3050	L3051	H3052	K3053	V3054	F3057	D3060	V3065	C3067	H3068	L3069	L3070	R3073	S3074	L3075	L2911																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
K2914	E2915	Q2924	E2925	L2926	L2927	K2928	L2930	N2933	G2934	Y2935	A2936	L2937	R2938	L2939	GLY	LEU	L3018	L3019	S3020	P3021	A3022	K3023	S3032	N3033	K3034	E3035	K3036	E3037	L3042	K3045	L3046	A3047	A3048	V3049	R3050	L3051	H3052	K3053	V3054	F3057	D3060	V3065	C3067	H3068	L3069	L3070	R3073	S3074	L3075	L2911																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
L2995	K2996	F2997	F2998	A2999	K3000	L3001	L3002	L3003	P3004	L3005	L3006	L3007	Q3008	Y3009	S3010	P3011	N3012	L3013	L3014	E3015	M3016	V3017	K3018	S3019	M3020	P3021	A3022	K3023	S3032	N3033	K3034	E3035	K3036	E3037	L3042	K3045	L3046	A3047	A3048	V3049	R3050	L3051	H3052	K3053	V3054	F3057	D3060	V3065	C3067	H3068	L3069	L3070	R3073	S3074	L3075	L2911																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
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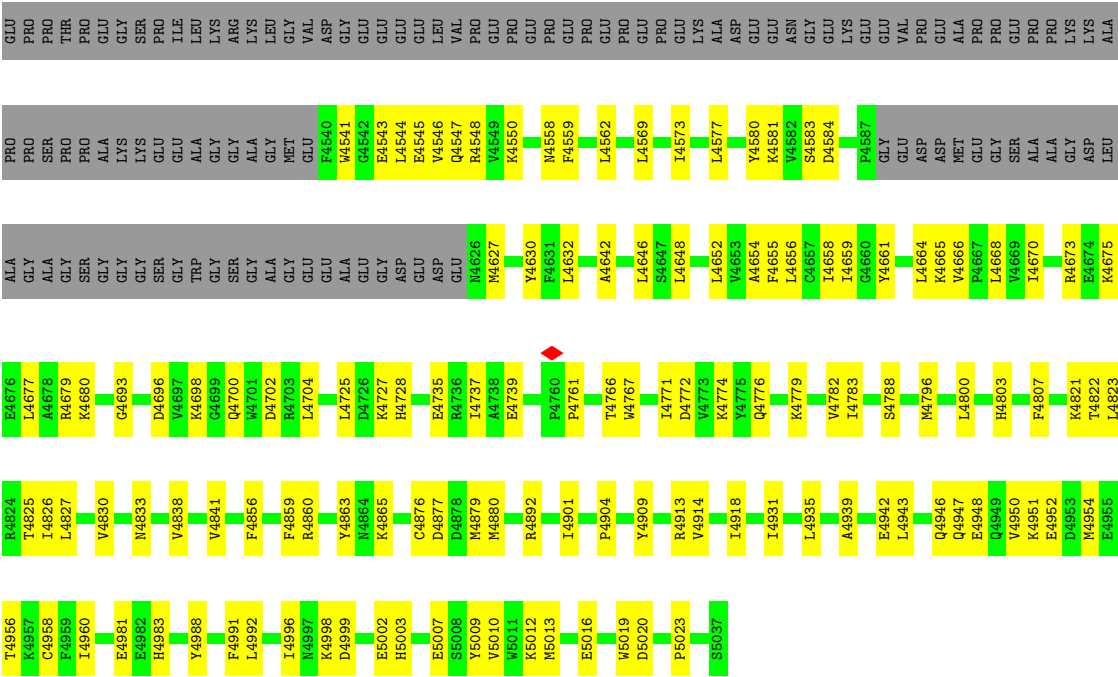
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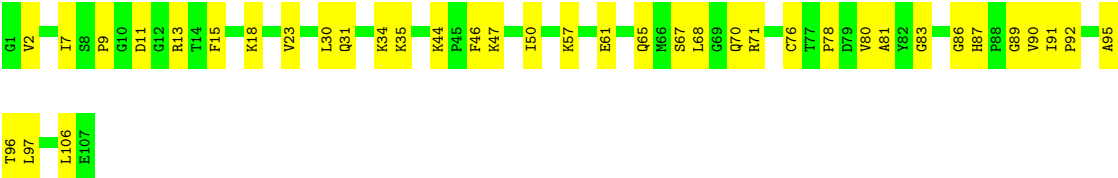
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Q1559	E1444	PRO	P1196	G1098	P1019	H938	V862	L748	D601	L471	L345	L231	L137
N1560	P1445	ALA	GLU	E1099	R1020	H938	L863	P753	R615	R472	C346	T232	E144
V1561	W1449	ASN	V1199	M1100	L1021	M941	L867	P754	R622	R474	L355	A235	D134
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Q1569	GLU	ASP	GLU	E1114	L1027	T1031	L874	G761	R629	N489	D363	G249	W147
T1572	M1476	GLU	L1219	L1115	GLU	K954	A875	V764	L633	N489	F384	G250	W148
M1573	G1477	ALA	G1220	G1116	ALA	L955	S876	W764	Q634	C490	F384	A251	T149
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R1584	S1486	PRO	E1224	E1119	D1037	M960	H879	L773	I648	T499	L369	H255	E159
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F1500	F1500	ARG	P1243	W1132	L1047	P969	H891	W788	Y659	I518	I377	I267	D167
M1501	M1501	SER	Q1244	H1133	L1047	L970	H892	V789	Y659	I518	I377	I267	D167
S1502	S1502	ALA	F1245	H1134	Y1051	D971	H893	F791	Y659	I518	I377	I267	D167
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G1504	G1504	GLY	P1249	P1138	P1055	S973	G894	L792	Y659	I518	I377	I267	D167
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L1519	L1519	THR	L1270	L1155	Q1066	E990	N909	Y808	Y659	I518	I377	I267	D167
V1520	V1520	ALA	R1271	T1159	Q1066	E990	N909	Y808	Y659	I518	I377	I267	D167
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M1527	M1527	GLY	R1290	T1177	V1072	V995	E818	E819	Y659	I518	I377	I267	D167
F1540	F1540	THR	L1291	A1178	R1073	A997	Y920	L823	Y659	I518	I377	I267	D167
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S1664	S1664	PRO	T1297	I1183	E1078	G1004	S925	H838	Y659	I518	I377	I267	D167
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H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
H1665	H1665	ALA	ALA	V1191	Y1007	S1066	K930	V840	Y659	I518	I377	I267	D167
S1664	S1664	ALA	ALA	V1191	Y1007	S1066	K930						



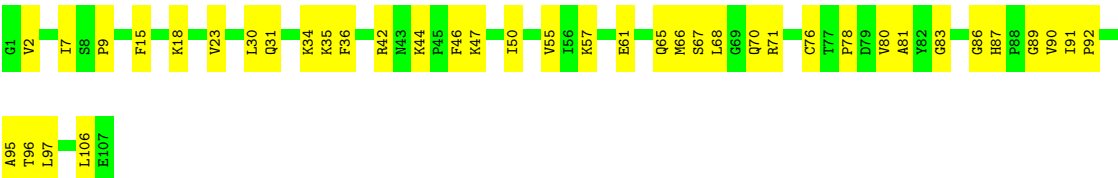




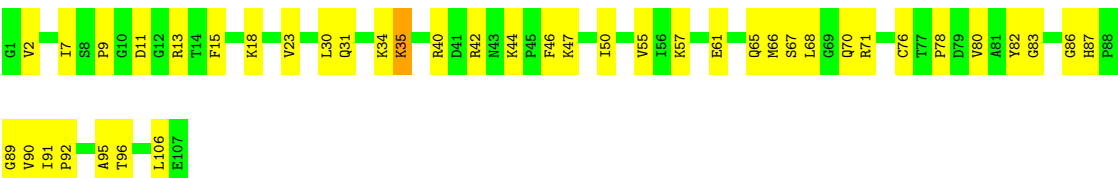
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



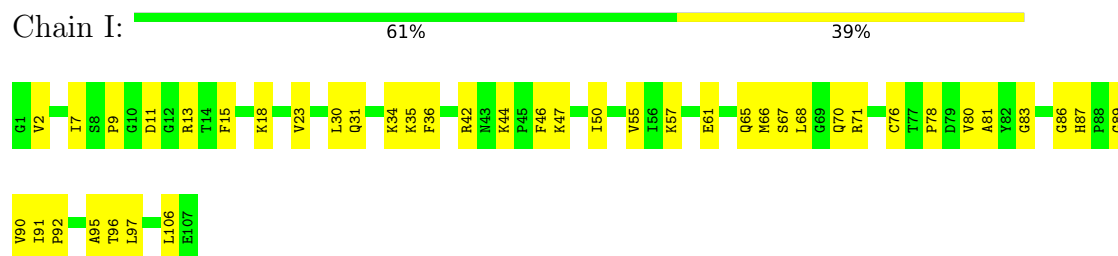
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



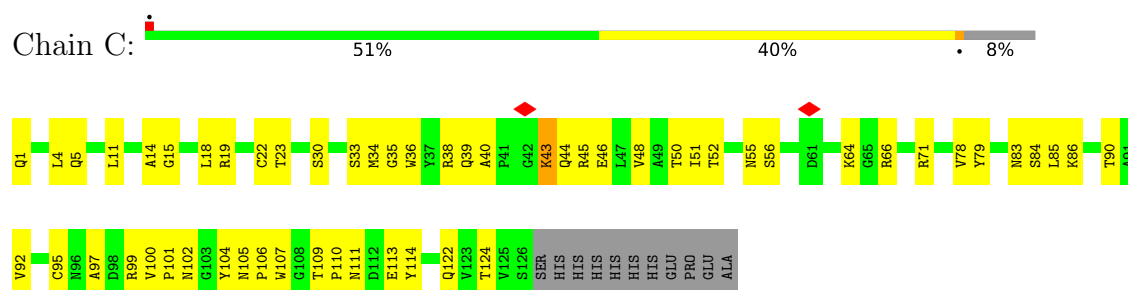
● Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



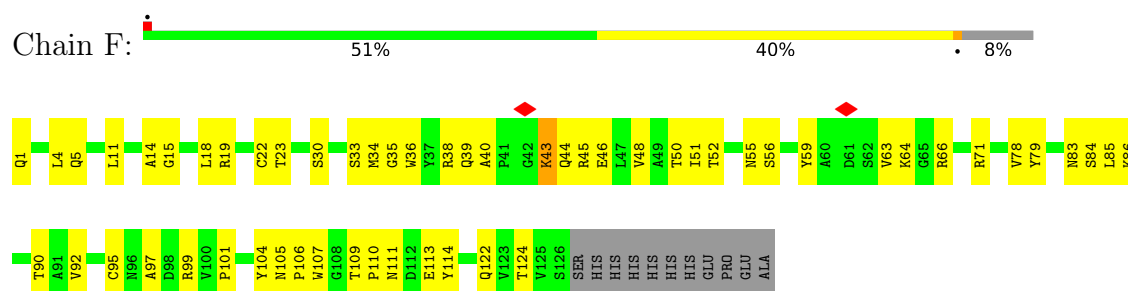
- Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



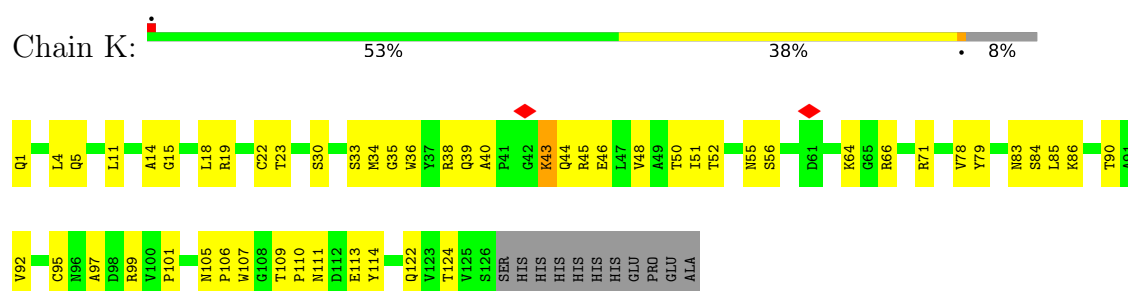
- Molecule 3: Nanobody 9657



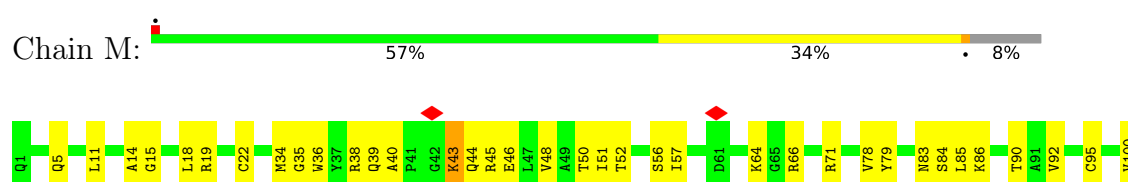
- Molecule 3: Nanobody 9657



- Molecule 3: Nanobody 9657



- Molecule 3: Nanobody 9657



P101	M102	G103	N105	P106	W107	G108	T109	P110	N111	Y114	Q122	V123	T124	V125	S126	SER	HIS	HIS	HIS	HIS	HIS	HIS	HIS	GLU	PRO	GLU	ALA
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	26815	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.503	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.053	Depositor
Map value standard deviation	0.121	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	504.0, 504.0, 504.0	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.5, 1.5, 1.5	Depositor

5 Model quality

5.1 Standard geometry

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

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	B	0.25	0/34879	0.51	3/47280 (0.0%)
1	E	0.25	0/34879	0.51	3/47280 (0.0%)
1	G	0.25	0/34879	0.51	3/47280 (0.0%)
1	J	0.25	0/34879	0.51	3/47280 (0.0%)
2	A	0.29	0/834	0.57	0/1123
2	D	0.29	0/834	0.57	0/1123
2	H	0.29	0/834	0.57	0/1123
2	I	0.29	0/834	0.57	0/1123
3	C	0.25	0/987	0.54	0/1340
3	F	0.25	0/987	0.54	0/1340
3	K	0.25	0/987	0.54	0/1340
3	M	0.25	0/987	0.54	0/1340
All	All	0.25	0/146800	0.51	12/198972 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2905	LEU	CA-CB-CG	6.09	129.32	115.30
1	J	2905	LEU	CA-CB-CG	6.09	129.32	115.30
1	E	2905	LEU	CA-CB-CG	6.09	129.31	115.30
1	G	2905	LEU	CA-CB-CG	6.08	129.28	115.30
1	E	1503	PRO	N-CA-CB	5.66	110.09	103.30

There are no chirality outliers.

There are no planarity outliers.

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	B	34103	0	33491	1051	0
1	E	34103	0	33491	1054	0
1	G	34103	0	33491	1068	0
1	J	34103	0	33491	1061	0
2	A	818	0	824	25	0
2	D	818	0	824	29	0
2	H	818	0	824	33	0
2	I	818	0	824	30	0
3	C	967	0	916	51	0
3	F	967	0	916	53	0
3	K	967	0	916	48	0
3	M	967	0	916	44	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	B	31	0	12	2	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
5	J	31	0	12	2	0
6	B	14	0	10	1	0
6	E	14	0	10	1	0
6	G	14	0	10	1	0
6	J	14	0	10	1	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	G	1	0	0	0	0
7	J	1	0	0	0	0
All	All	143740	0	141012	4460	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 16.

The worst 5 of 4460 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:G:1616:GLU:HG3	1:G:1629:GLN:HG3	1.58	0.86
1:E:1008:SER:HB2	1:E:1017:ARG:HE	1.41	0.85
1:J:1616:GLU:HG3	1:J:1629:GLN:HG3	1.58	0.85
1:E:2214:VAL:HG13	1:E:2215:LEU:HD12	1.58	0.85
1:J:2214:VAL:HG13	1:J:2215:LEU:HD12	1.58	0.85

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	B	4280/5027 (85%)	4189 (98%)	89 (2%)	2 (0%)	100	100
1	E	4280/5027 (85%)	4190 (98%)	88 (2%)	2 (0%)	100	100
1	G	4280/5027 (85%)	4190 (98%)	88 (2%)	2 (0%)	100	100
1	J	4280/5027 (85%)	4190 (98%)	88 (2%)	2 (0%)	100	100
2	A	105/107 (98%)	96 (91%)	8 (8%)	1 (1%)	13	48
2	D	105/107 (98%)	96 (91%)	8 (8%)	1 (1%)	13	48
2	H	105/107 (98%)	96 (91%)	8 (8%)	1 (1%)	13	48
2	I	105/107 (98%)	96 (91%)	8 (8%)	1 (1%)	13	48
3	C	124/137 (90%)	113 (91%)	11 (9%)	0	100	100
3	F	124/137 (90%)	113 (91%)	11 (9%)	0	100	100
3	K	124/137 (90%)	113 (91%)	11 (9%)	0	100	100
3	M	124/137 (90%)	111 (90%)	13 (10%)	0	100	100
All	All	18036/21084 (86%)	17593 (98%)	431 (2%)	12 (0%)	50	83

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	86	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	86	GLY
2	H	86	GLY
2	I	86	GLY
1	B	2909	ASP

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	B	3659/4270 (86%)	3650 (100%)	9 (0%)	92	93
1	E	3659/4270 (86%)	3650 (100%)	9 (0%)	92	93
1	G	3659/4270 (86%)	3650 (100%)	9 (0%)	92	93
1	J	3659/4270 (86%)	3649 (100%)	10 (0%)	91	91
2	A	88/88 (100%)	86 (98%)	2 (2%)	45	64
2	D	88/88 (100%)	86 (98%)	2 (2%)	45	64
2	H	88/88 (100%)	86 (98%)	2 (2%)	45	64
2	I	88/88 (100%)	86 (98%)	2 (2%)	45	64
3	C	104/114 (91%)	103 (99%)	1 (1%)	73	81
3	F	104/114 (91%)	103 (99%)	1 (1%)	73	81
3	K	104/114 (91%)	103 (99%)	1 (1%)	73	81
3	M	104/114 (91%)	103 (99%)	1 (1%)	73	81
All	All	15404/17888 (86%)	15355 (100%)	49 (0%)	90	91

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	1954	ARG
1	J	3694	LYS
1	J	2268	GLN
1	J	2827	ARG
2	A	35	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	1691	GLN
3	K	44	GLN
1	G	3813	GLN
3	F	122	GLN
1	J	3960	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	ATP	G	5102	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
5	ATP	E	5102	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
5	ATP	B	5102	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
5	ATP	J	5102	-	26,33,33	0.60	0	31,52,52	0.77	2 (6%)
6	CFF	B	5103	-	8,15,15	1.03	0	8,23,23	2.46	2 (25%)
6	CFF	G	5103	-	8,15,15	1.02	0	8,23,23	2.45	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	CFF	J	5103	-	8,15,15	1.03	0	8,23,23	2.44	2 (25%)
6	CFF	E	5103	-	8,15,15	1.01	0	8,23,23	2.45	2 (25%)

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
5	ATP	G	5102	-	-	5/18/38/38	0/3/3/3
5	ATP	E	5102	-	-	5/18/38/38	0/3/3/3
5	ATP	B	5102	-	-	5/18/38/38	0/3/3/3
5	ATP	J	5102	-	-	5/18/38/38	0/3/3/3
6	CFF	B	5103	-	-	-	0/2/2/2
6	CFF	G	5103	-	-	-	0/2/2/2
6	CFF	J	5103	-	-	-	0/2/2/2
6	CFF	E	5103	-	-	-	0/2/2/2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	5103	CFF	C5-C6-N1	-5.83	111.98	118.20
6	E	5103	CFF	C5-C6-N1	-5.82	111.99	118.20
6	G	5103	CFF	C5-C6-N1	-5.82	111.99	118.20
6	J	5103	CFF	C5-C6-N1	-5.82	112.00	118.20
6	E	5103	CFF	C4-C5-C6	3.47	122.19	119.96

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

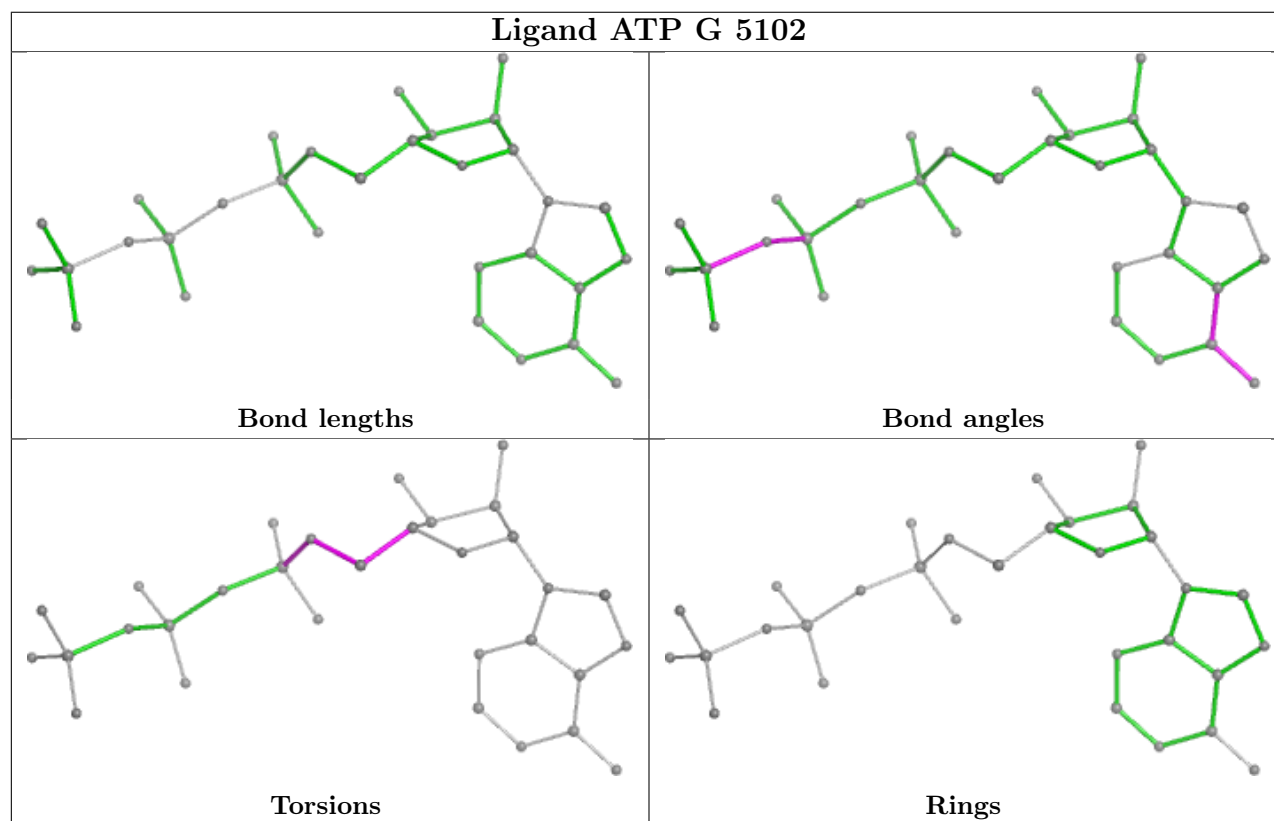
Mol	Chain	Res	Type	Atoms
5	B	5102	ATP	C5'-O5'-PA-O1A
5	B	5102	ATP	C5'-O5'-PA-O2A
5	E	5102	ATP	C5'-O5'-PA-O1A
5	E	5102	ATP	C5'-O5'-PA-O2A
5	G	5102	ATP	C5'-O5'-PA-O1A

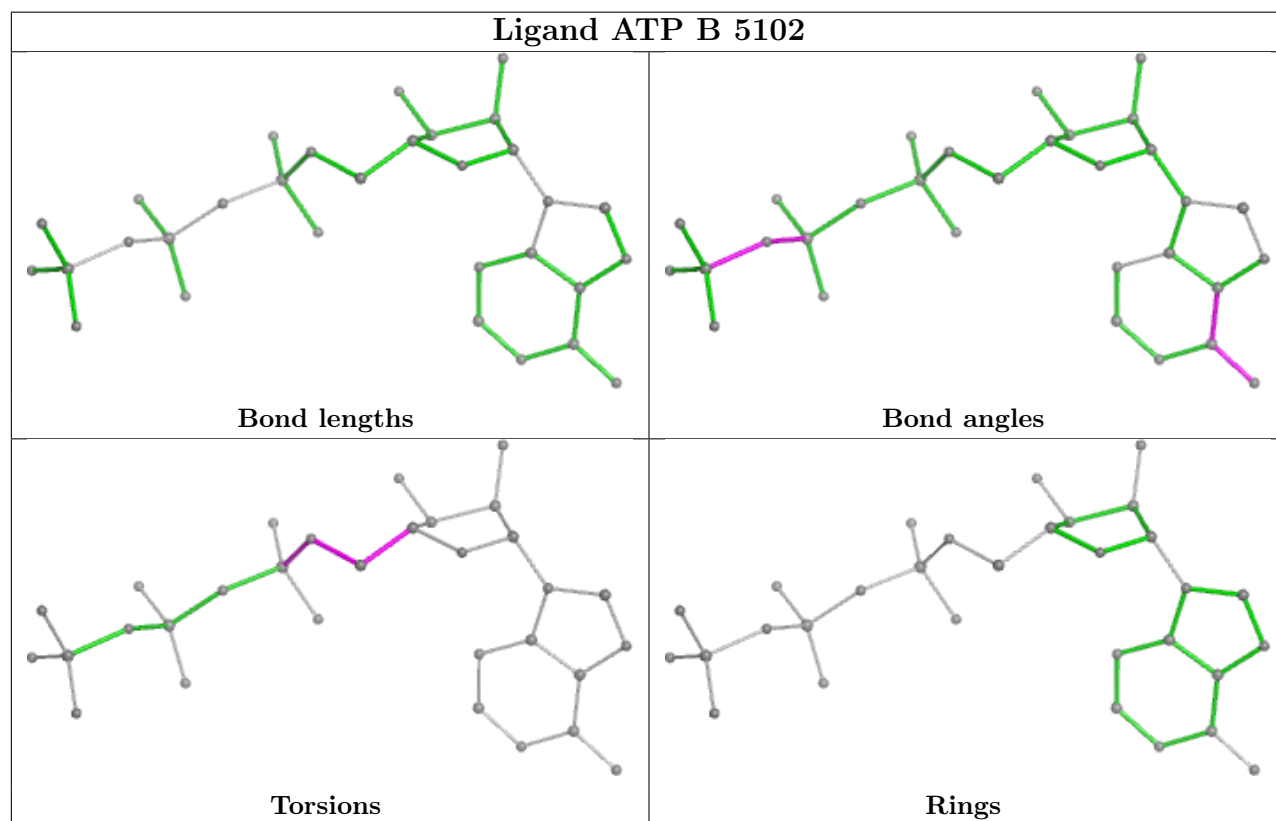
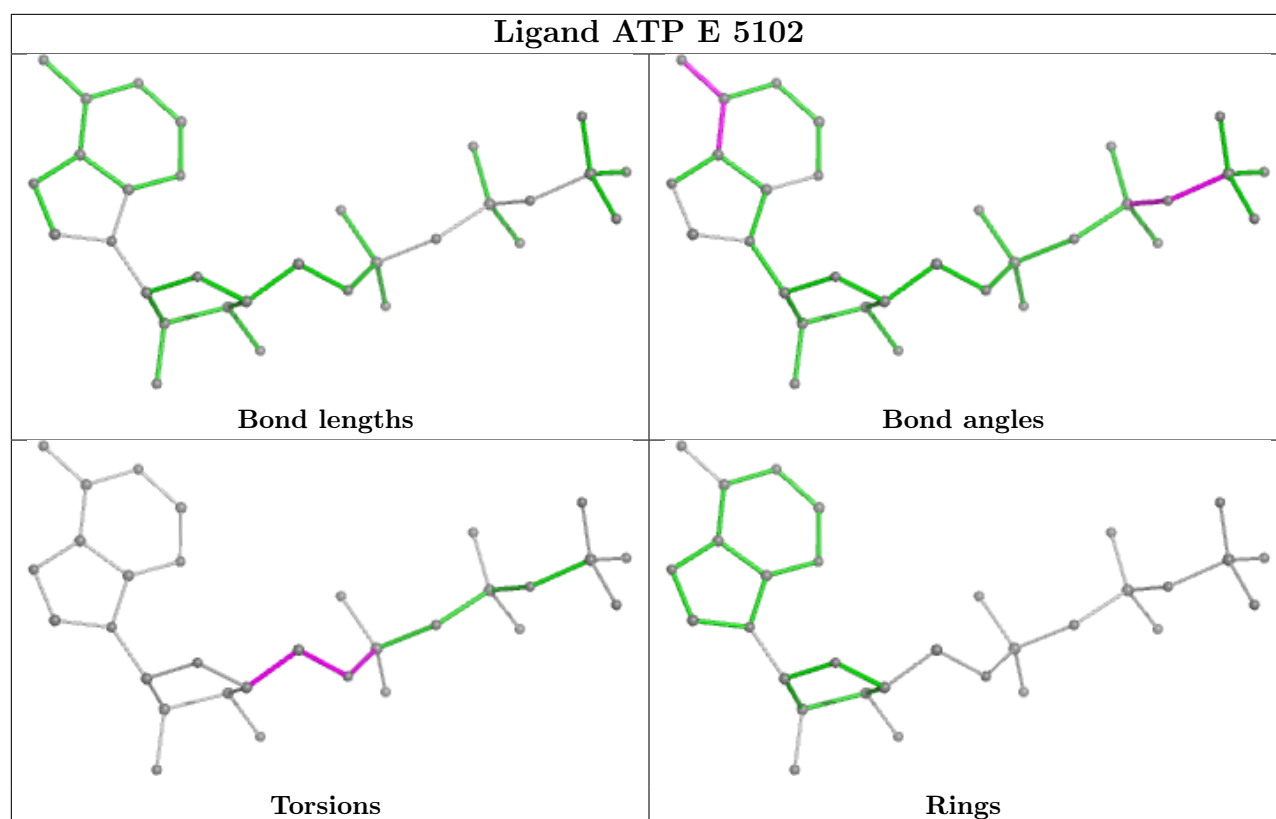
There are no ring outliers.

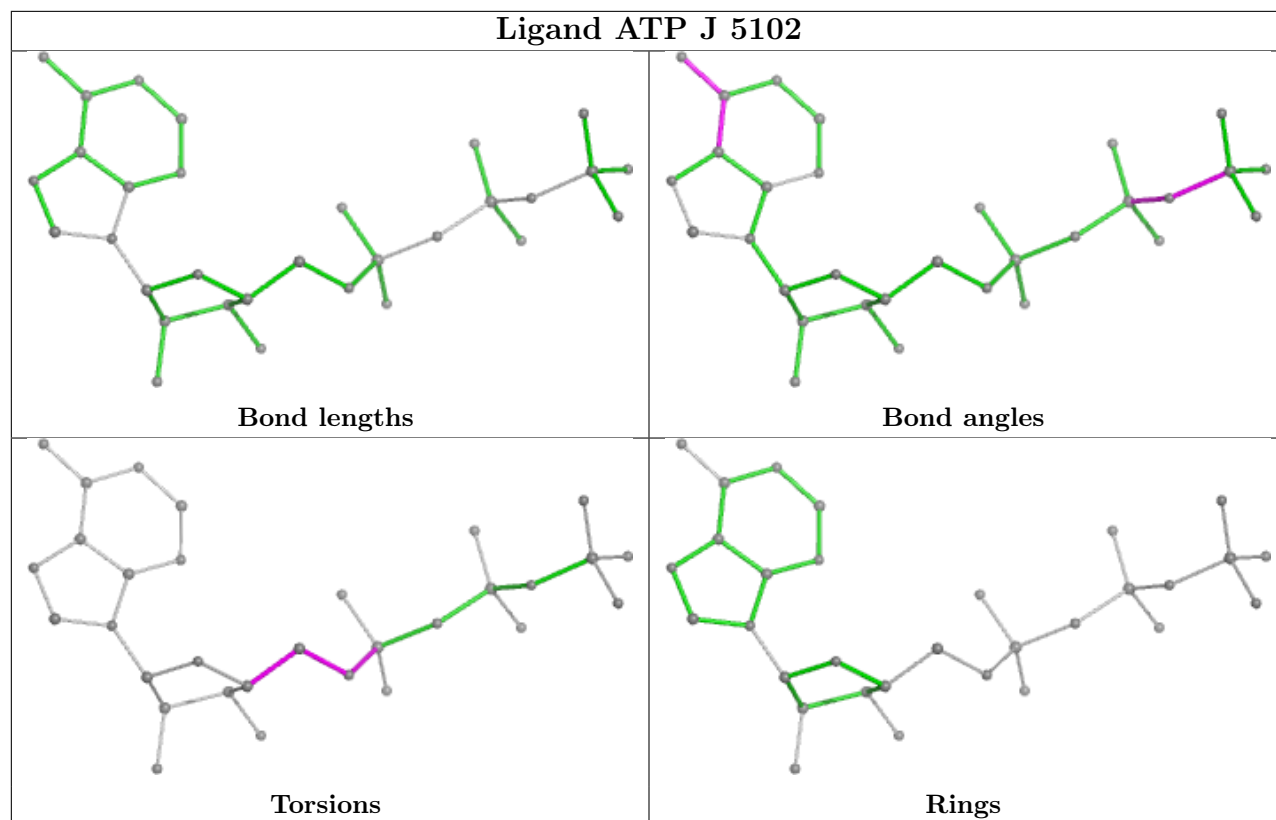
8 monomers are involved in 10 short contacts:

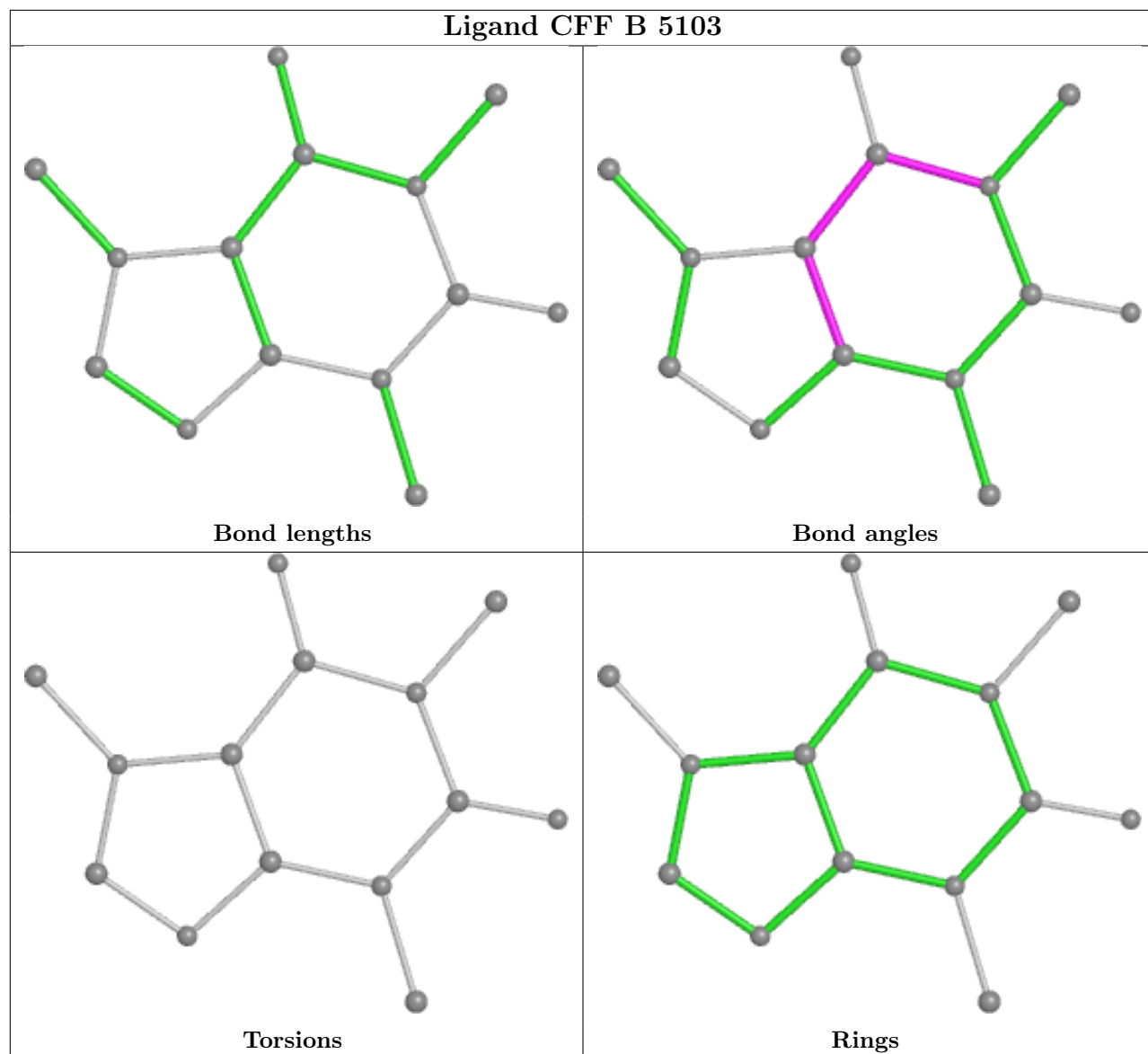
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	5102	ATP	1	0
5	E	5102	ATP	1	0
5	B	5102	ATP	2	0
5	J	5102	ATP	2	0
6	B	5103	CFF	1	0
6	G	5103	CFF	1	0
6	J	5103	CFF	1	0
6	E	5103	CFF	1	0

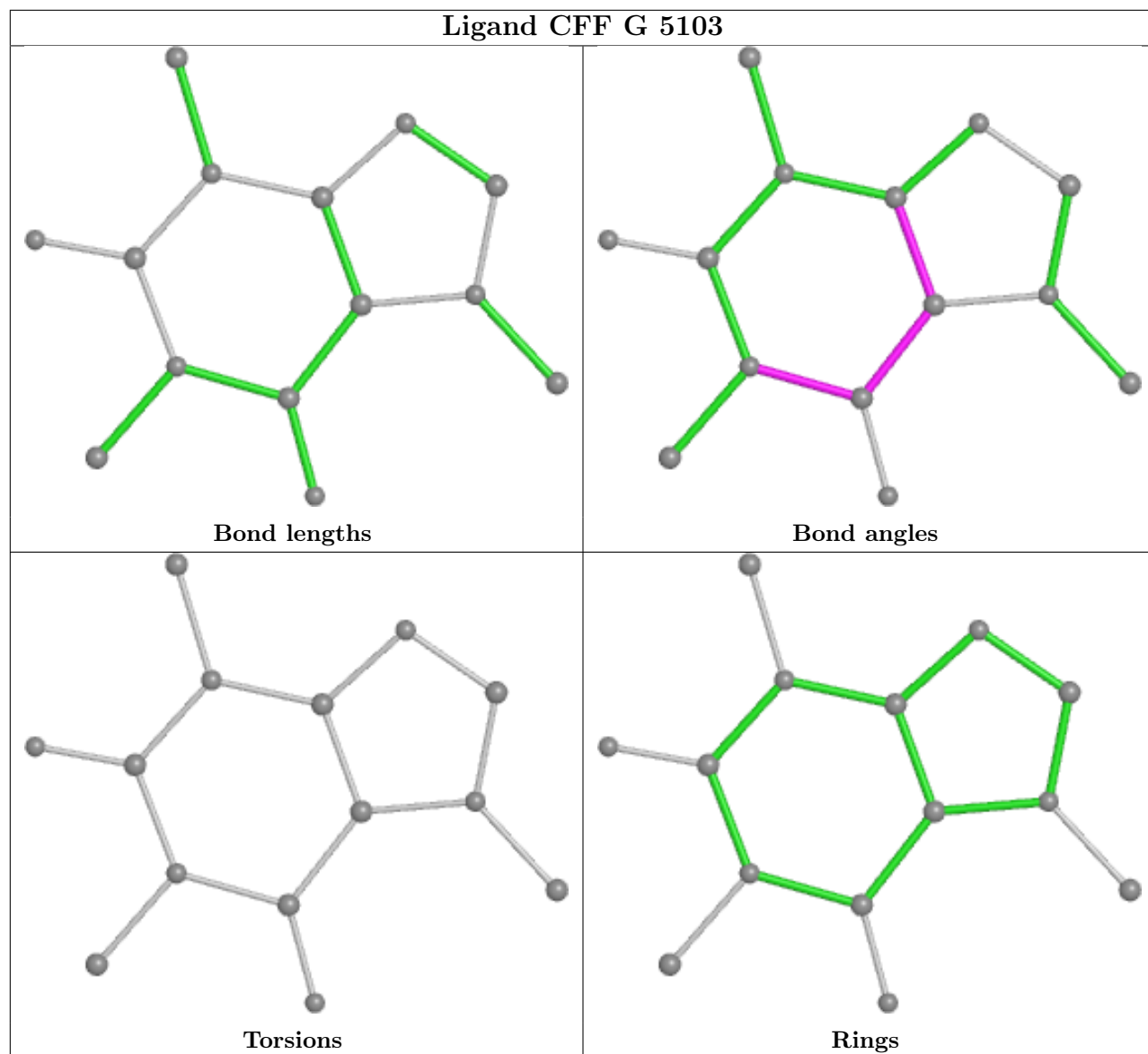
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

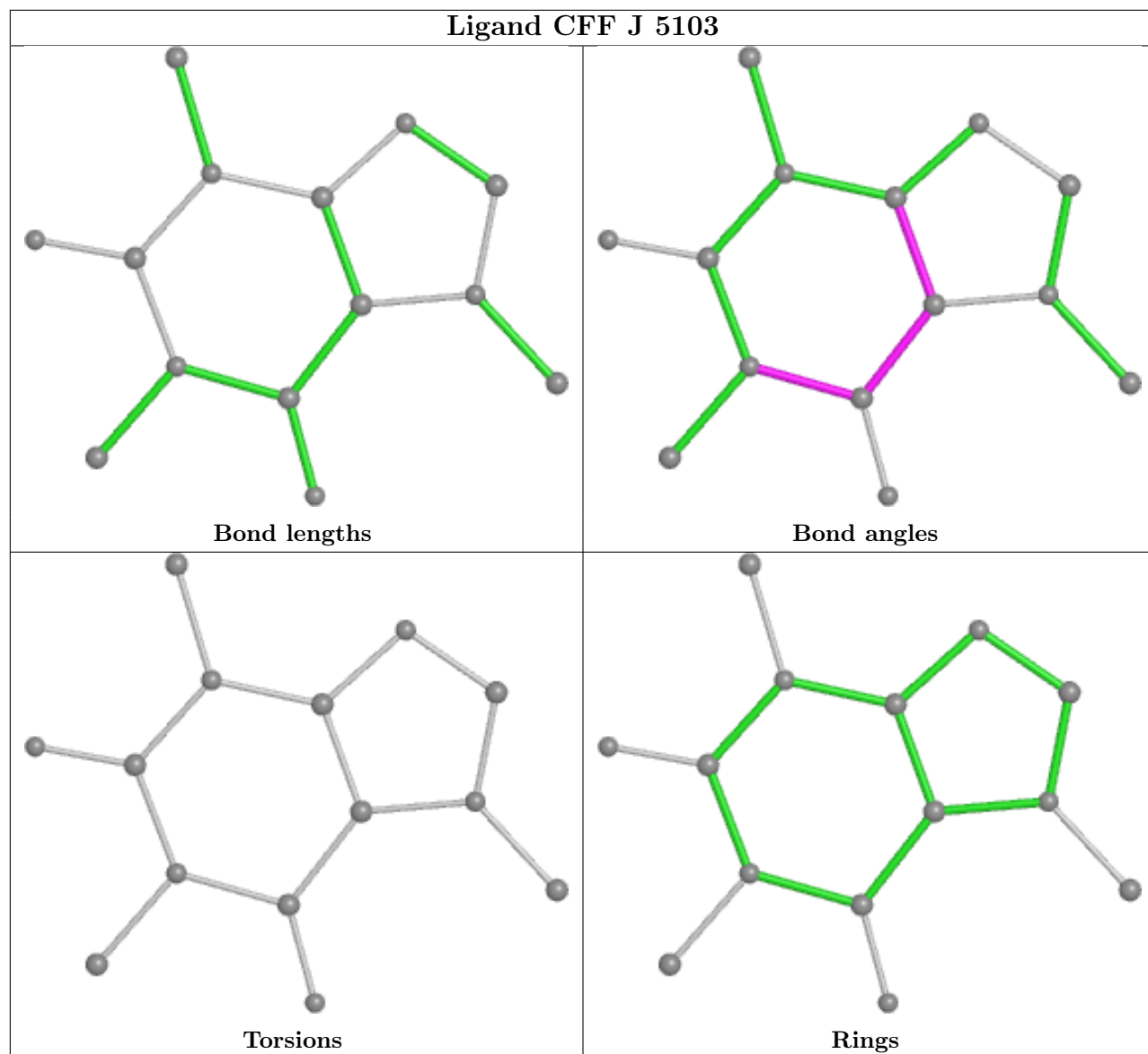


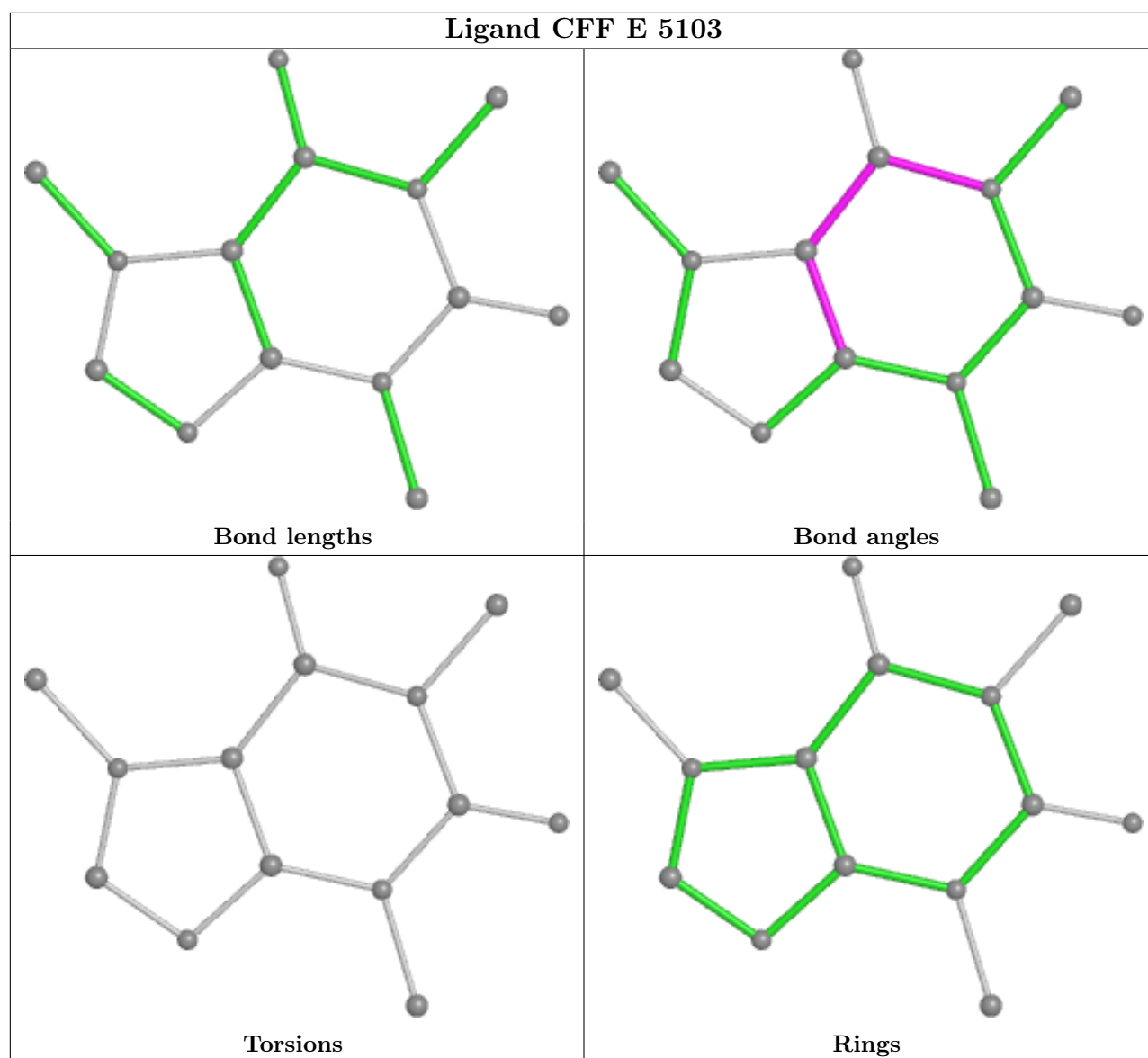












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

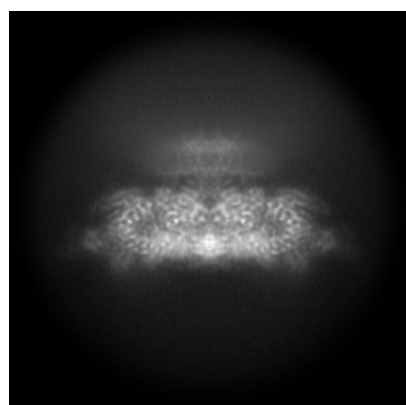
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19464. These allow visual inspection of the internal detail of the map and identification of artifacts.

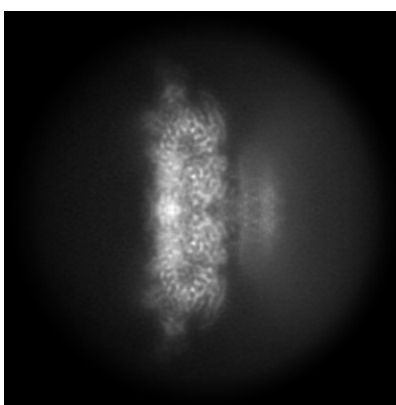
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

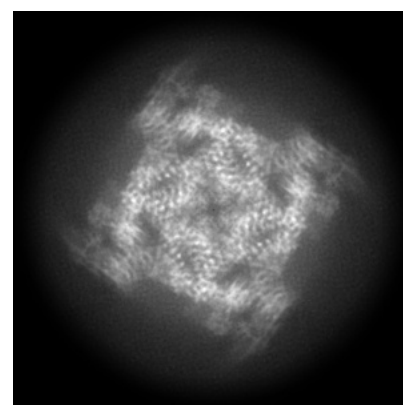
6.1.1 Primary map



X



Y

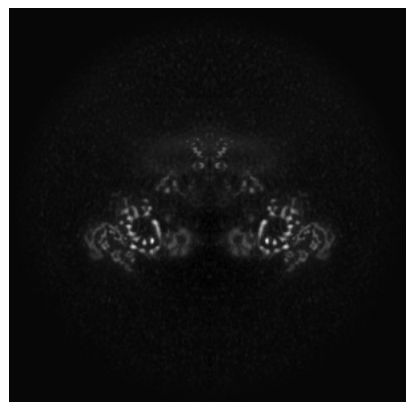


Z

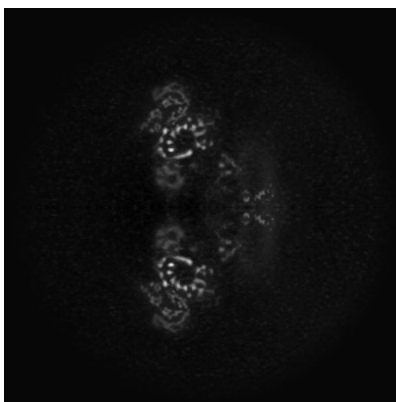
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

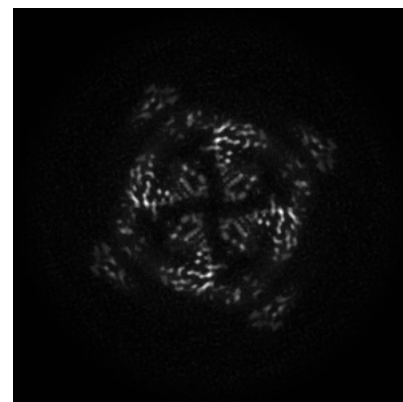
6.2.1 Primary map



X Index: 168



Y Index: 168

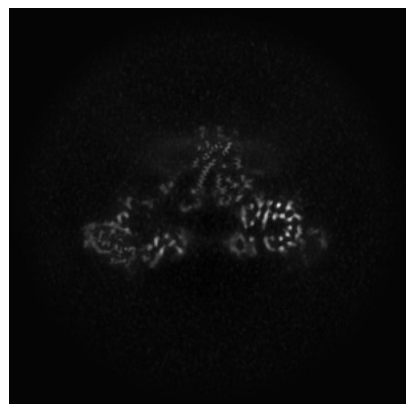


Z Index: 168

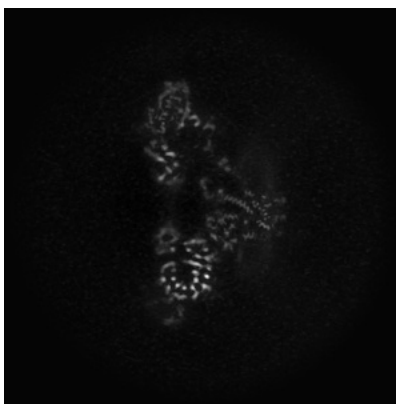
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

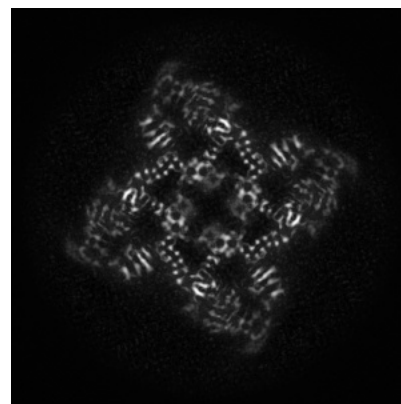
6.3.1 Primary map



X Index: 175



Y Index: 175

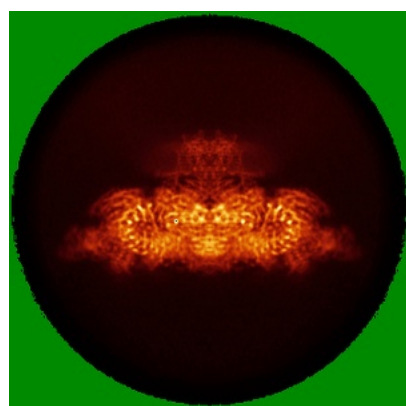


Z Index: 144

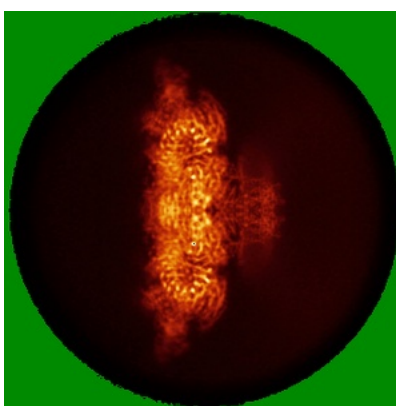
The images above show the largest variance slices of the map in three orthogonal directions.

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

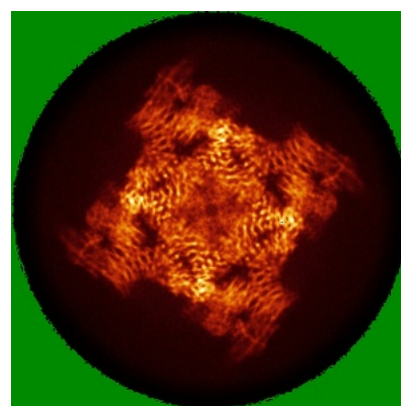
6.4.1 Primary map



X



Y

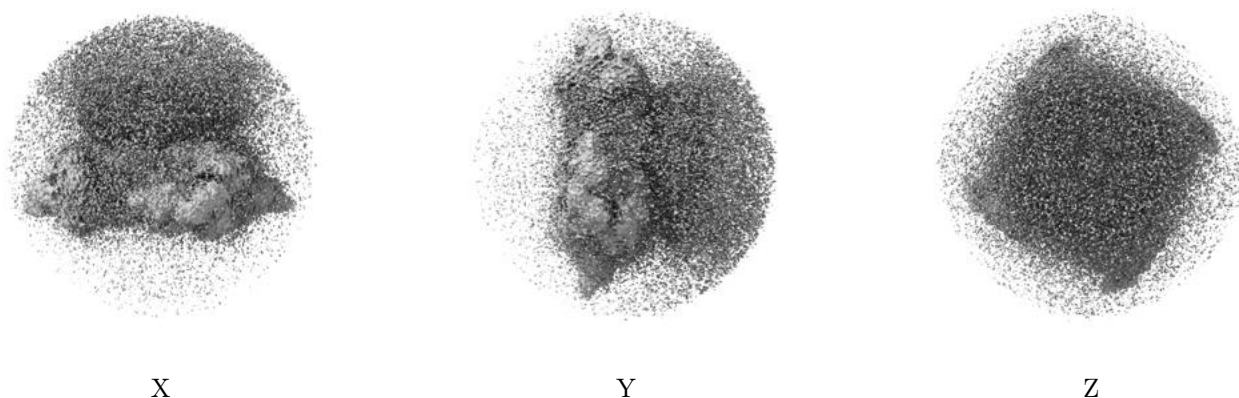


Z

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

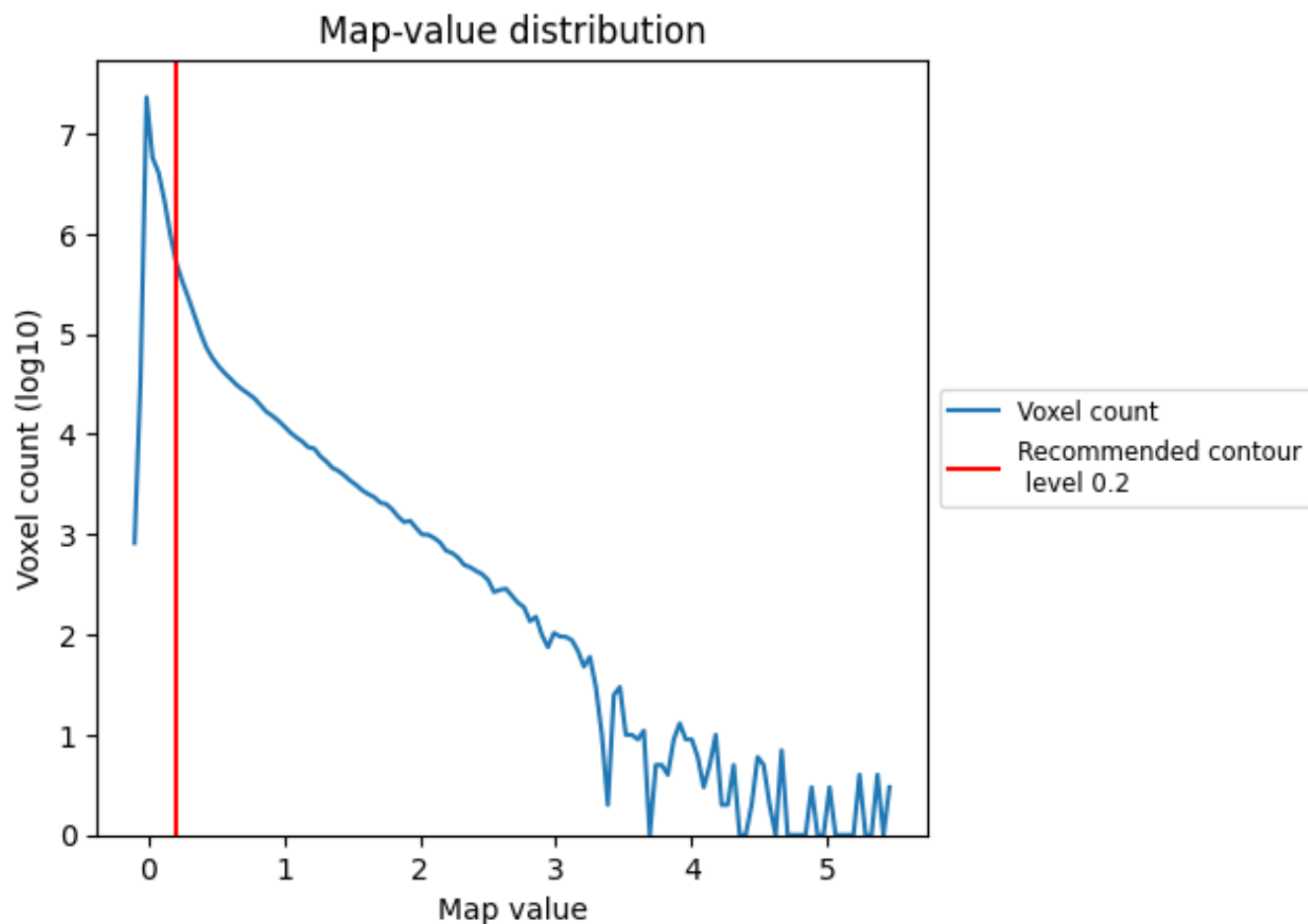
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

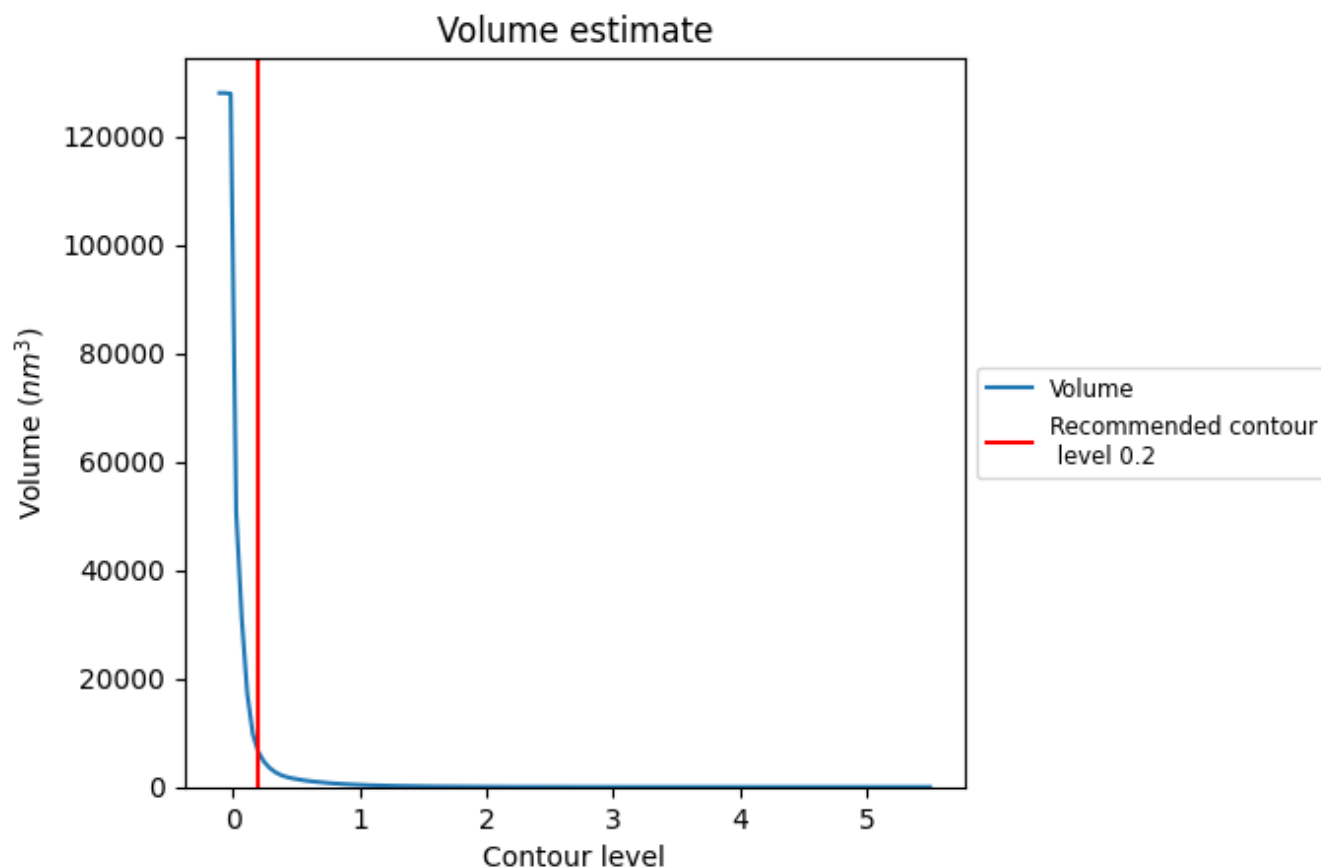
This section contains the results of statistical analysis of the map.

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.

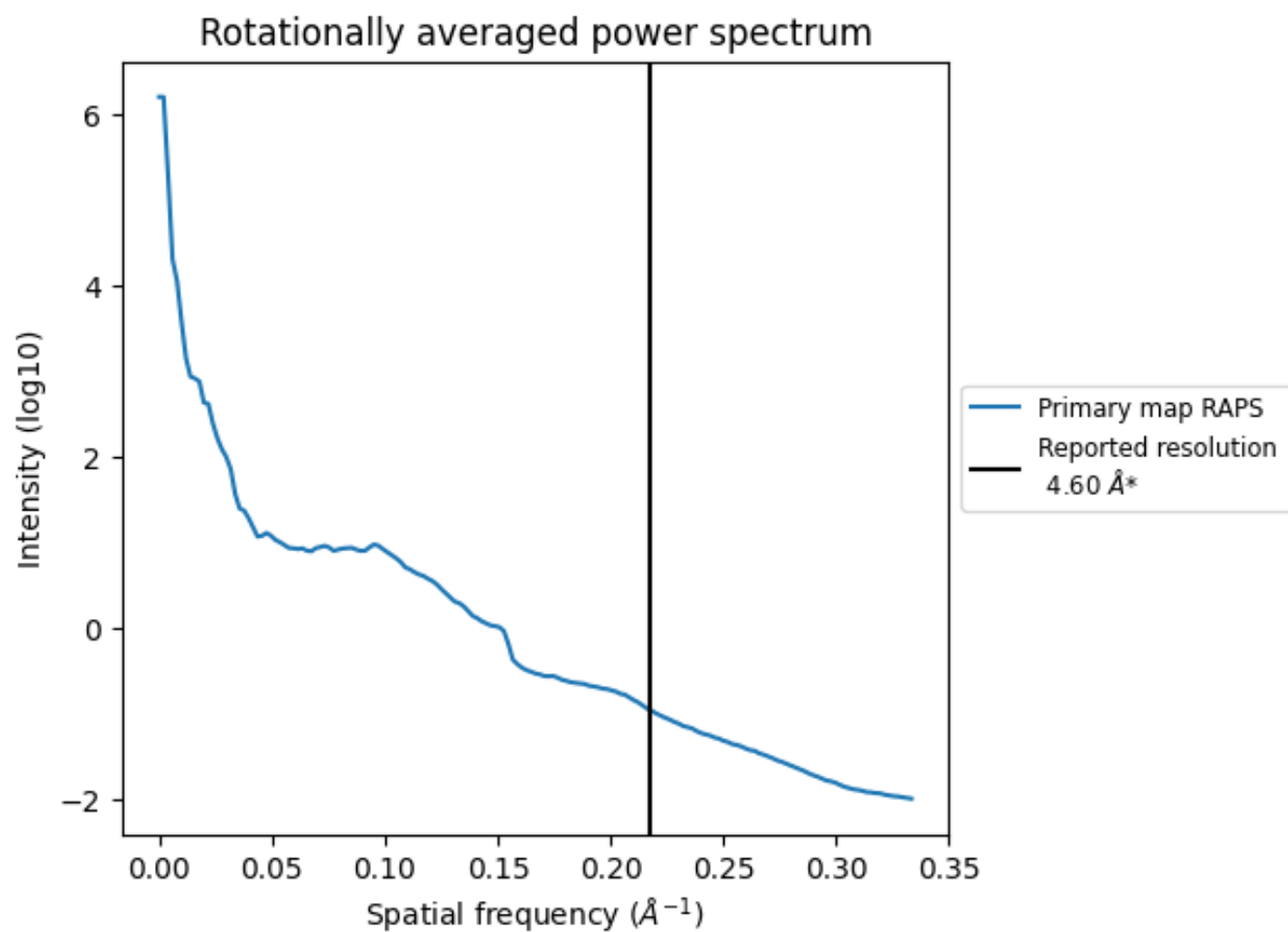
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6569 nm^3 ; this corresponds to an approximate mass of 5934 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 ⓘ

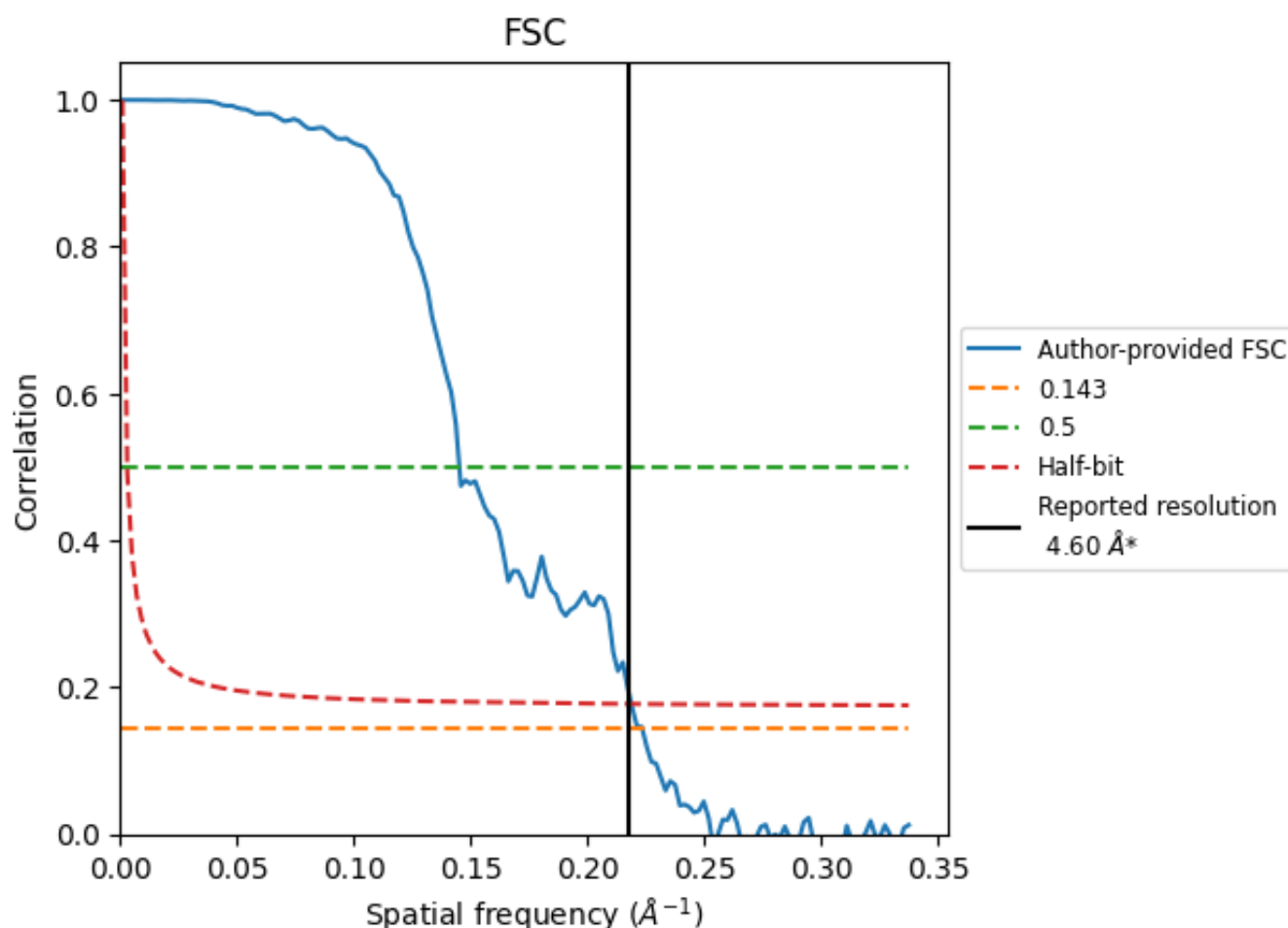


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

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 0.217 Å⁻¹

8.2 Resolution estimates [i](#)

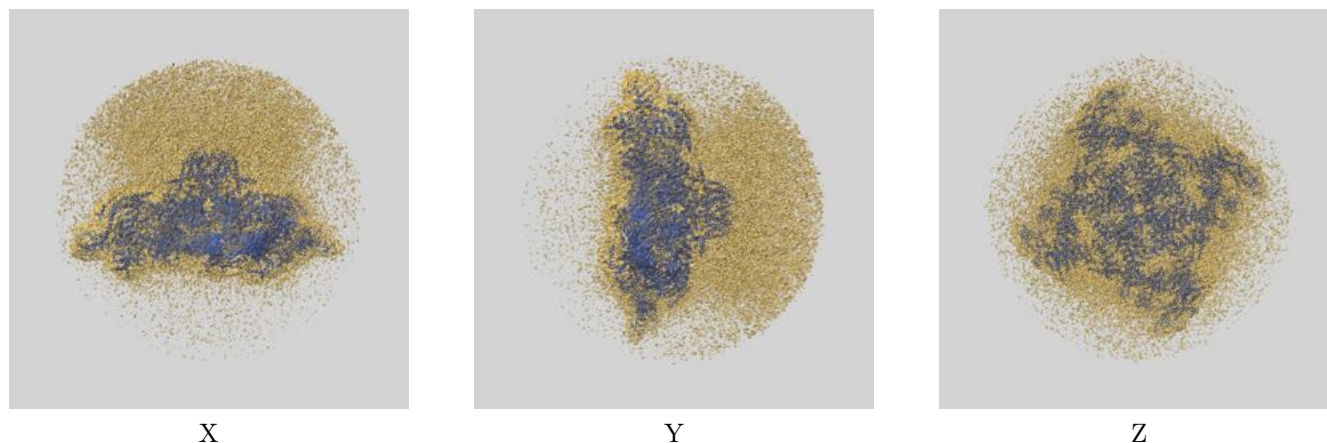
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	4.48	6.89	4.57
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

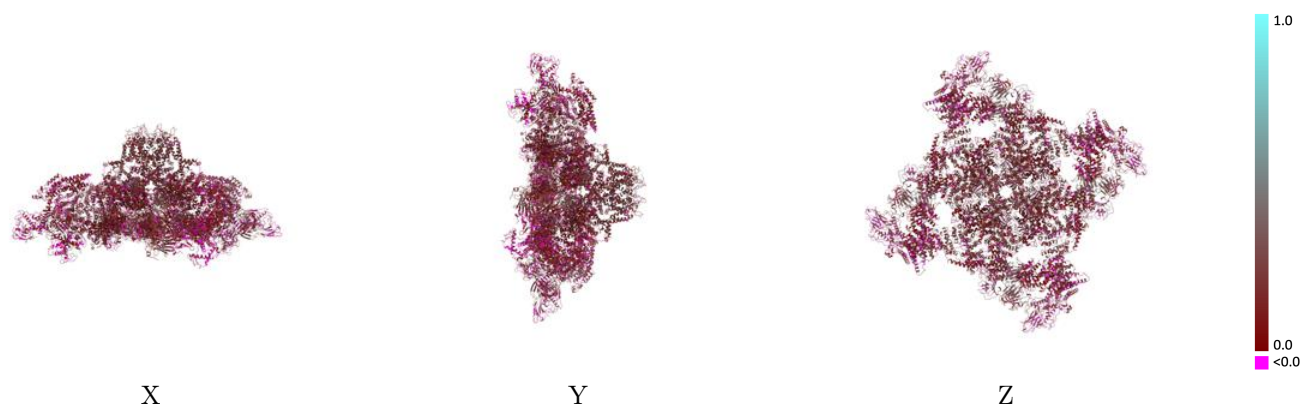
This section contains information regarding the fit between EMDB map EMD-19464 and PDB model 8RRT. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



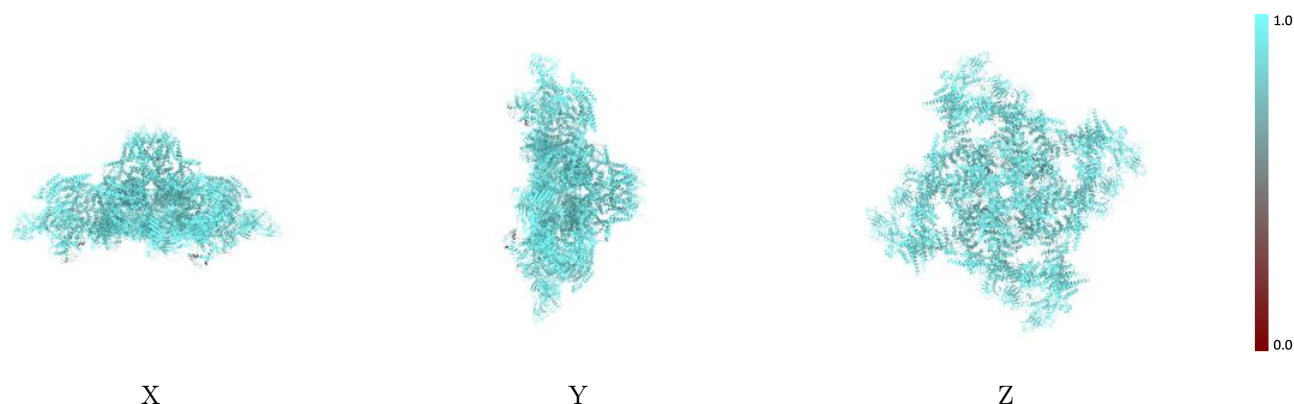
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



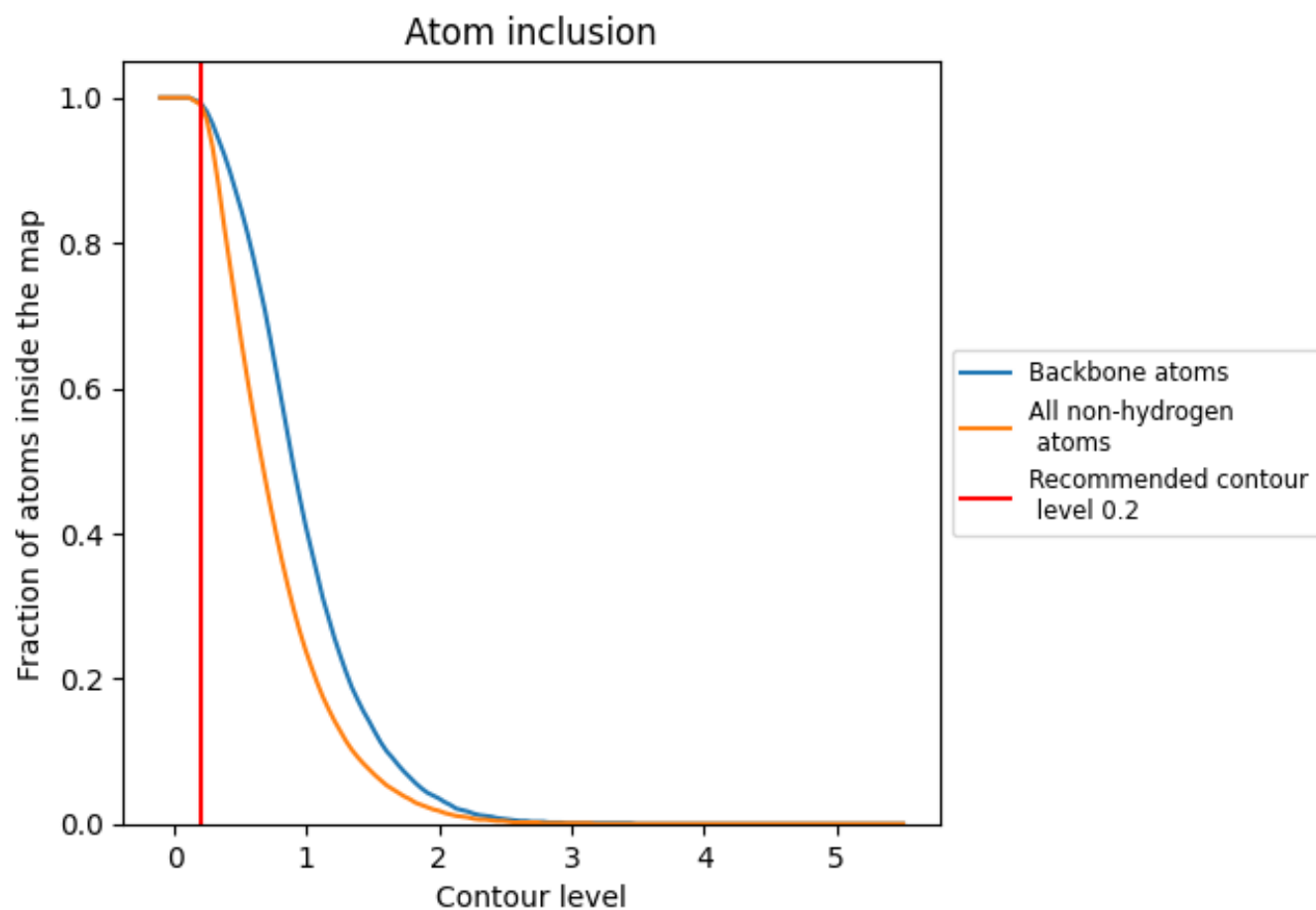
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.9900</div>	<div><div></div>0.1540</div>
A	<div><div></div>0.9980</div>	<div><div></div>0.1450</div>
B	<div><div></div>0.9910</div>	<div><div></div>0.1570</div>
C	<div><div></div>0.9680</div>	<div><div></div>0.0830</div>
D	<div><div></div>0.9980</div>	<div><div></div>0.1380</div>
E	<div><div></div>0.9910</div>	<div><div></div>0.1560</div>
F	<div><div></div>0.9680</div>	<div><div></div>0.0820</div>
G	<div><div></div>0.9910</div>	<div><div></div>0.1570</div>
H	<div><div></div>0.9980</div>	<div><div></div>0.1350</div>
I	<div><div></div>0.9980</div>	<div><div></div>0.1380</div>
J	<div><div></div>0.9910</div>	<div><div></div>0.1560</div>
K	<div><div></div>0.9680</div>	<div><div></div>0.0800</div>
M	<div><div></div>0.9670</div>	<div><div></div>0.0810</div>

1.0

0.0

<0.0