



wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 03:01 PM UTC

PDB ID : 8RRU / pdb_00008rru
EMDB ID : EMD-19465
Title : Structure of RyR1 reconstituted into lipid liposomes in primed state in complex with FKBP and Nb9657.
Authors : Li, C.; Efremov, R.G.
Deposited on : 2024-01-23
Resolution : 4.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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

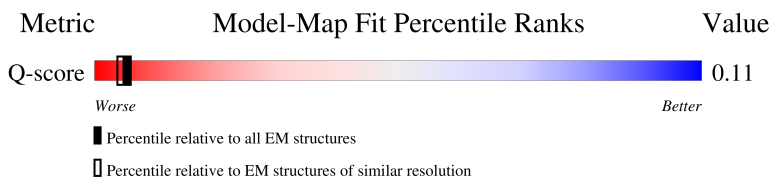
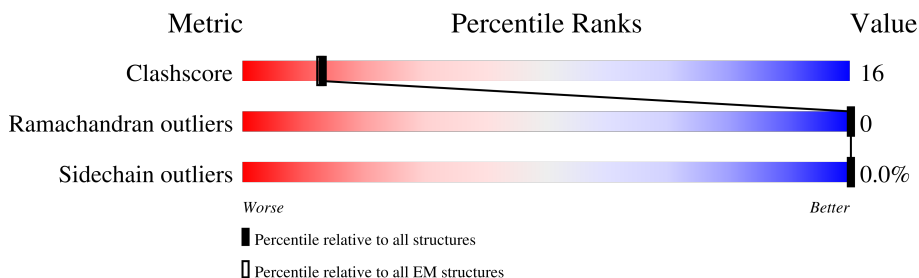
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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.



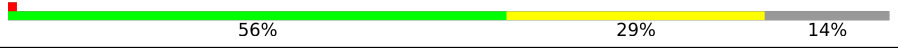
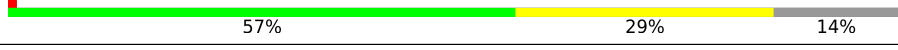
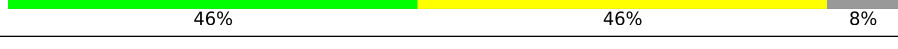
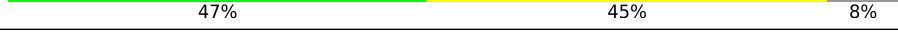
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1989 (4.20 - 5.20)

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	107	
1	D	107	
1	H	107	
1	I	107	

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Mol	Chain	Length	Quality of chain
2	B	5027	
2	E	5027	
2	G	5027	
2	J	5027	
3	C	137	
3	F	137	
3	K	137	
3	M	137	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 143907 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	D	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	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 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4319	Total	C	N	O	S	1	0
			34143	21748	5888	6283	224		
2	E	4319	Total	C	N	O	S	1	0
			34143	21748	5888	6283	224		
2	G	4319	Total	C	N	O	S	1	0
			34150	21752	5888	6285	225		
2	J	4319	Total	C	N	O	S	1	0
			34143	21748	5888	6283	224		

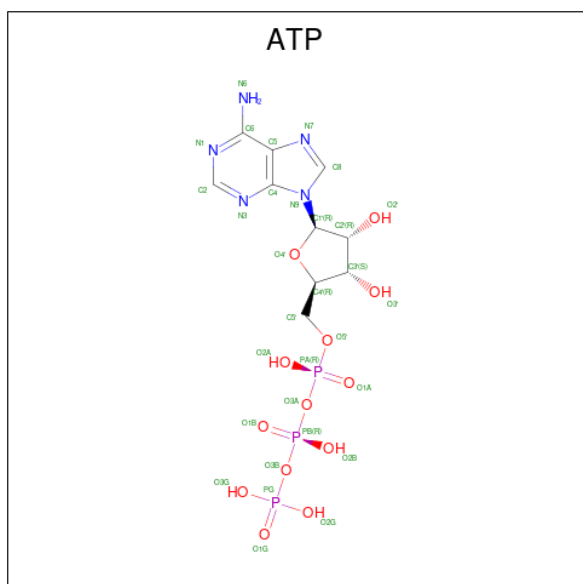
- Molecule 3 is a protein called Nanobody 9657.

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 (CCD ID: 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 (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



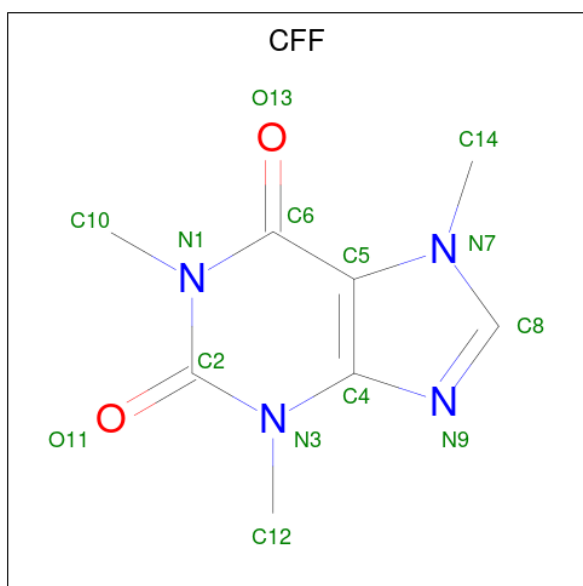
Mol	Chain	Residues	Atoms					AltConf
5	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

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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 (CCD ID: 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 (CCD ID: 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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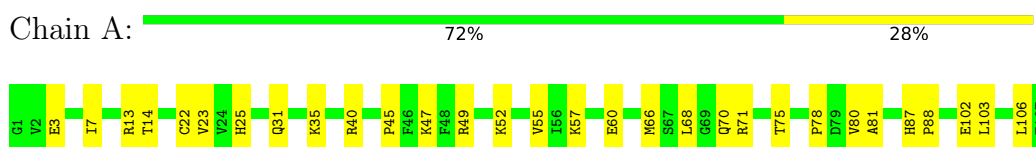
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Mol	Chain	Residues	Atoms		AltConf
7	E	1	Total 1	Ca 1	0
7	G	1	Total 1	Ca 1	0
7	J	1	Total 1	Ca 1	0

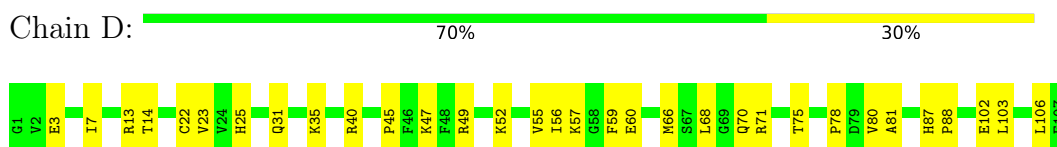
3 Residue-property plots [i](#)

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.

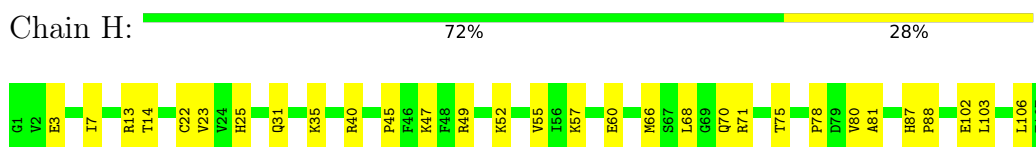
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



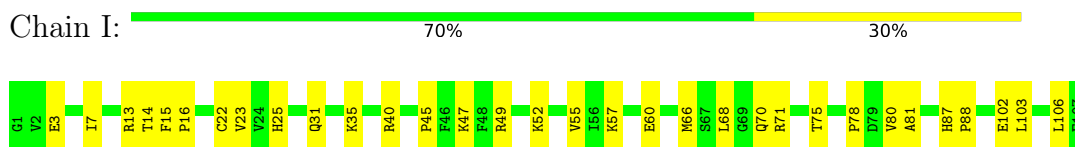
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



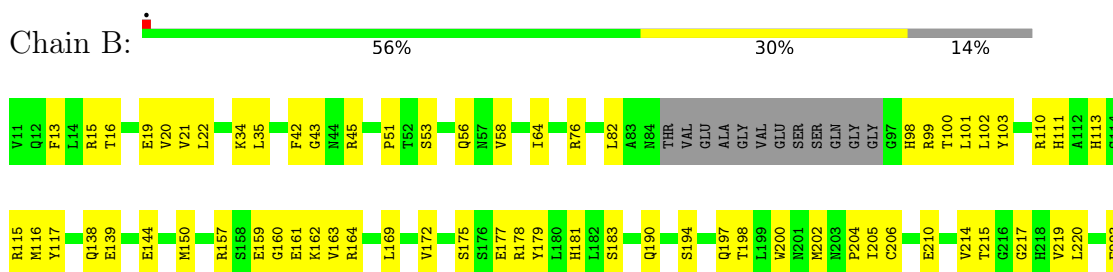
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B



- Molecule 2: Ryanodine receptor 1



A1578	M1579	F1580	R1584	R1594	L1595	Q1598	M1599	L1600	M1601	P1609	F1612	V1615	E1616	T1617	R1618	L1619	A1620	G1621	E1622	R1623	L1624	G1625	V1626	A1627	M1637	A1638	L1639	H1640	I1641	P1642	E1643	M1644	N1645	R1646	C1647	M1648	Q1559	E1560	V1561	L1563	I1562	E1565	Q1568	R1661	F1662	H1665	Y1670	R1671	A1672	V1673			
N1482	V1483	H1484	S1485	C1489	M1494	V1495	W1496	G1497	G1498	V1501	S1502	G1504	GLN	GLY	R1508	L1514	D1522	A1523	M1527	K1547	L1548	F1549	P1550	A1551	V1552	F1553	V1554	L1555	L1546	C1647	M1648	Q1559	E1560	G1451	W1452	V1453	T1454	P1455	M1462	K1570	L1466	V1474	T1475	M1573	P1574	G1477	L1575	V1673					
MET	MET	THR	GLN	PRO	ALA	THR	PRO	ALA	THR	PRO	ALA	GLY	GLY	GLY	PRO	ALA	N1420	R1421	D1422	D1423	P1424	E1425	I1426	T1430	T1431	T1432	Y1433	Y1434	Y1435	V1439	Q1443	C1447	V1448	V1449	V1450	G1451	W1452	V1453	T1454	P1455	M1462	K1570	L1466	V1474	T1475	M1476	G1477	D1478					
SER	ALA	GLY	GLY	TRP	GLY	GLU	ALA	ALA	ALA	GLY	GLY	LYS	GLY	GLY	PRO	GLY	THR	PRO	GLN	PRO	GLY	VAL	GLY	VAL	ALA	GLN	PRO	ARG	ALA	GLY	ASN	GLY	LYS	ASP	ALA	ALA	ALA	ALA	GLY	PRO	ASP	PRO	THR	GLY	PHE	LEU	PHE	LYS	ALA	LYS	LYS	ALA	ALA
M1260	D1261	P1268	C1269	L1270	R1271	L1272	A1273	H1274	L1287	F1288	L1289	R1290	L1291	S1292	L1293	P1294	F1297	H1298	Q1299	R1302	C1303	T1304	GLY	GLY	ALA	THR	PRO	LEU	ALA	GLY	GLN	PRO	PRO	ALA	ALA	ASP	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA				
R1158	T1159	I1160	I1161	F1162	T1163	L1164	V1168	S1171	S1175	E1176	A1178	F1179	R1180	F1181	I1182	F1188	L1189	V1191	C1192	P1196	V1199	G1200	D1207	S1210	Q1220	F1223	A1227	M1230	V1234	W1237	Q1244	F1245	E1246	P1247	P1248	P1249	H1252	E1256	V1257														
GLN	VAL	GLU	N1065	Q1066	S1067	R1068	W1069	D1070	R1071	V1072	R1073	F1075	R1076	A1077	E1078	Y1081	T1082	V1083	G1086	R1087	F1092	V1095	M1100	R1101	W1104	A1105	L1115	G1116	Y1122	V1123	F1124	N1125	R1128	G1129	Q1130	R1131	W1132	H1133	P1138	D1147	M1152	I1153	D1154	L1155	T1156	E1157							
L867	I870	R871	E872	K873	L874	A875	E876	R877	I878	H879	R886	I887	W891	T892	Y893	Q894	R897	K901	R902	L903	H904	P905	C906	L907	H911	S912	L913	E917	L922	L929	K930	T931	L932	R935	I936	C937	R938	V939	G940	E947	L950	K951	Y959	P969	L970								
D971	L972	A976	L977	T978	P979	A980	Q981	L984	V985	H993	R1000	W1005	S1006	Y1007	S1008	I1013	R1016	R1017	M1018	C906	L907	H911	S912	L913	E917	L922	L929	K930	T931	L932	R935	I936	C937	R938	V939	G940	E947	L950	K951	Y959	P969	L970											
T642	R645	P646	N647	W650	E654	T657	G660	K661	Y662	F664	E665	V666	M667	V668	D669	A677	T680	H681	L682	R683	A687	L688	W702	D717	L721	W722	A727	R728	P733	L738	A739	P740	E741	V744	S745	G746	C747	L748	T635	M636	L637	P753	S754										
I755	S756	F757	I759	W760	G761	C762	E769	D774	P779	V780	Y781	S782	F783	S784	V787	K788	V789	R790	F791	L792	G795	G798	F799	F800	A801	F802	Y808	H812	L821	R822	L823	E824	R825	I826	R835	H838	L839	V840	G841	P842	T849	V852	T858										
C393	Q394	Q395	E396	M403	F421	K424	L551	P431	R553	L443	I449	T560	L561	E562	V563	V574	R469	S470	L471	R472	R473	R474	Q475	E480	E481	Q482	M483	L486	V487	I491	D492	R615	G618	I621	L633	G634	T635	M636	L637	P753	S754												
L539	F540	S541	D545	W546	V547	V548	K550	R551	D552	L554	E555	T560	L561	E562	V563	V574	R469	S470	L471	R472	R473	R474	Q475	E480	E481	Q482	M483	L486	V487	I491	D492	R615	G618	I621	L633	G634	T635	M636	L637	P753	S754												
K320	L323	ASP	THR	ALA	PRO	LYS	ARG	ASP	VAL	GLY	MET	GLY	PRO	PRO	E338	I339	K340	Y341	C346	F347	V348	Q349	G354	L355	W356	L357	T358	Y359	A360	A361	P362	D363	P364	K365	A366	L369	G370	V371	L372	K373	K374	K375	A376	I377	L378	G382	A387	L388	F389	L390	T391	F316	R392
H224	G225	H226	E229	C230	L231	T232	I233	S234	R242	V245	Y246	Y247	E248	V252	H255	A256	R257	S258	R261	L262	S265	W269	S270	G271	S272	H273	L274	W275	R276	G277	L280	H284	V285	T286	L292	L293	L299	C305	H308	T312	S313	F314	C315	F316									



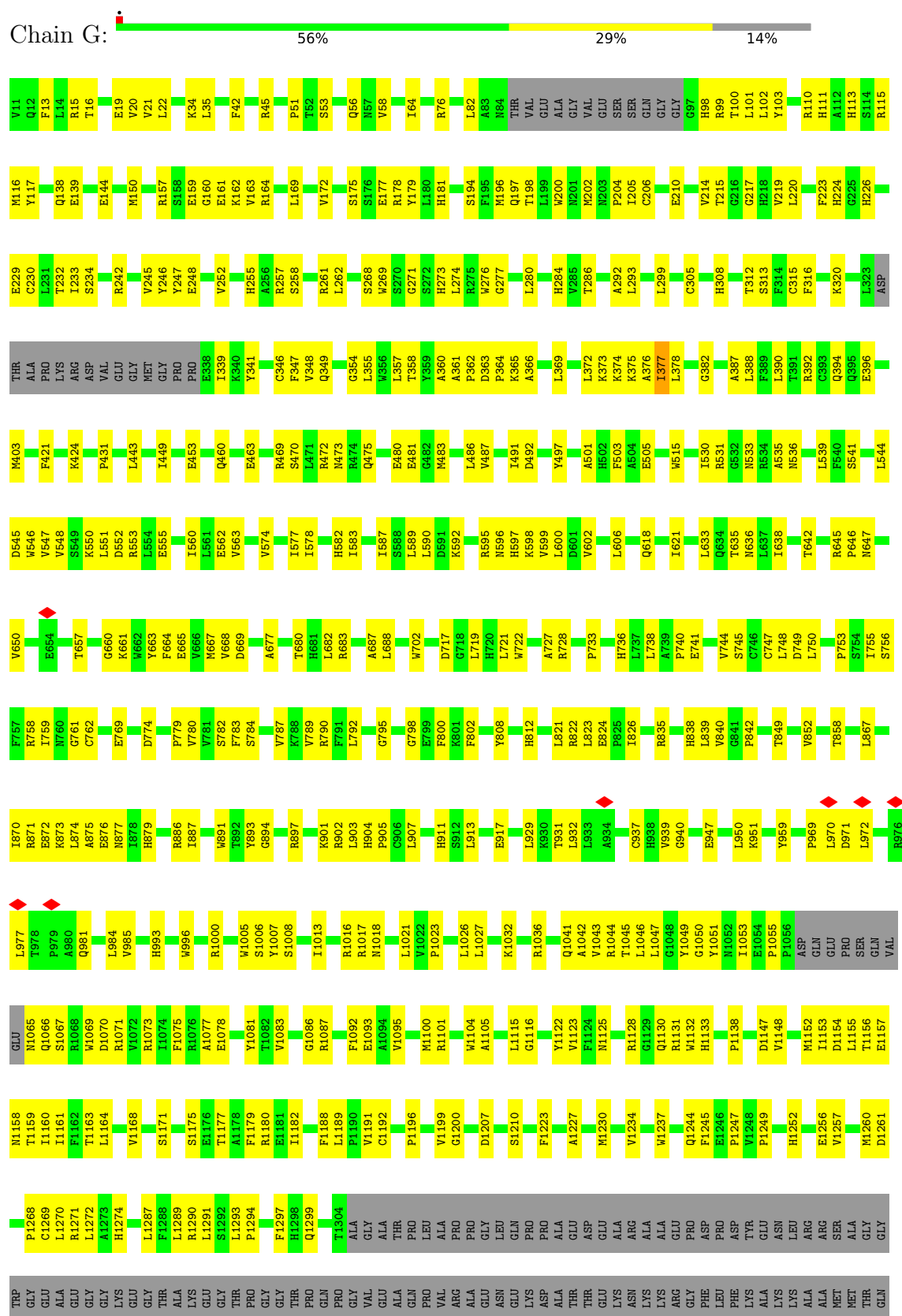
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LEU	GLU	R4161	M4044	N3806	D3717	L3603	L3509	I3413	M3335	M3239	L3143	D3060	L2964
ARG	ALA	N4162	V4045	G3807	H3605	H3604	T3510	R3414	R3337	C3240	F3144	V3065	R2965
ARG	ASP	F4163	M4046	G3808	Y3720	E3607	A3512	Y3415	V3340	I3243	H3145	L3068	D2967
THR	GLU	L4164	M4047	V3812	L3721	E3607	T3513	V3416	F3341	P3244	H3146	H3069	D2968
ALA	ASP	F4165	V4048	V3812	Y3722	E3607	L3514	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLU	L4166	V4049	V3812	Y3722	E3607	L3514	Y3416	F3341	P3244	H3146	H3069	D2968
GLY	GLY	A4167	V4055	M3816	A3724	T3612	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLY	L4171	V4055	M3816	Y3725	T3612	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLU	L4171	V4055	M3816	Y3725	T3612	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
THR	ALA	L4181	K4069	L3833	I3728	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	ALA	E4182	F4061	L3835	K3731	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
LEU	ALA	L4183	F4062	L3835	K3731	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLU	M4184	D4063	L3838	S3732	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLY	L4184	M4064	L3838	S3732	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLY	L4184	M4064	L3838	S3732	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
LEU	ALA	R4189	F4065	L3842	L3735	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
LEU	GLU	L4190	L4066	L3843	E3740	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
THR	GLU	E4191	K4067	L3844	ASN	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLY	R4192	L4068	N3845	GLY	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
VAL	ALA	L4197	I4071	A3846	GLU	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLY	I4197	V4072	L3849	ALA	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ARG	ALA	B4202	V4081	Q3850	GLU	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLY	A4203	V4081	Q3851	GLU	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
GLY	GLY	Q4204	V4081	Q3852	GLU	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	ALA	L4087	L4087	L3856	E3747	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	ALA	M4207	L4088	L3856	S3752	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
GLY	GLY	S4089	P4208	F3753	F3753	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	THR	K4090	K4090	F3754	E3754	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
GLY	VAL	V4210	M4097	L3865	E3755	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	ALA	K4211	M4097	L3866	K3756	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	ALA	K4211	M4097	L3866	K3756	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
GLY	ALA	K4214	F4103	L3868	E3757	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	GLY	V4222	I4108	G3871	M3758	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	THR	V4222	I4108	E3872	Q3766	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
LEU	ALA	G4225	L4112	L3873	Q3767	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ARG	ARG	G4225	L4112	L3873	S3768	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
LEU	LEU	K4230	A4117	L3885	R3769	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
THR	ALA	K4230	A4117	L3885	R3769	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
GLY	ALA	F4234	E4121	L3887	H3771	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
SER	ALA	V4235	M4122	L3888	R3772	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	ALA	T4241	M4122	L3888	R3772	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	ARG	L4242	I4123	Q3889	G3773	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
GLY	ALA	F4243	P4135	L3891	A3775	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
GLY	ALA	M4244	I4139	C3892	M3778	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
LEU	GLY	M4245	I4139	E3893	Q3779	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
VAL	LEU	Q4246	N4142	G3894	L3780	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
GLU	GLY	T4247	L4146	H3895	Q3782	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
TYR	TYR	A4248	L4147	Q3900	M3782	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
ALA	ALA	L4251	L4147	M4023	G3788	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
LYS	SER	L4251	V4025	R3904	E3789	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
LEU	LEU	E4252	M4026	L3905	T3790	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
VAL	ARG	E4253	S4151	Q3906	T3790	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
THR	ARG	PRO	H4152	L4027	M3793	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
VAL	VAL	GLY	H4153	L4028	M3793	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968
THR	VAL	GLY	V4154	M4039	L3802	L3603	L3515	Y3416	F3341	P3244	H3146	H3069	D2968

Y2192	Q2107	Q2036	LYS	Y1712	M1601	G1498	LEU	GLY	A1273	V1168	R1069	Q981	L874
H2193	E2108	L2039	GLU	D1713	P1609	V1501	PRO	LYS	H1274	V1168	W1069	Q981	A875
Q2194	D2109	A2040	ASP	L1714	L1714	S1502	ARG	GLU	L1287	S1171	D1070	Q981	E876
N2195	Y2110		ALA	L1715	P1829	P1503	LEU	GLY	L1287	S1171	R1071	Q981	N877
N2196	Q2111	Q2045	LYS	I1718	F1612	P1504	PRO	THR	L1288	S1175	V1072	Q981	H878
N2197	S2113		GLU	H1719	V1615	G1504	HIS	ALA	L1289	E1176	I1074	Q981	I879
P2114	P2114		GLU	R1727	E1616	GLN	ASP	LYS	R1290	T1177	F1075	Q981	R886
V2117			GLU	R1727	R1618	GLY	VAL	GLU	L1291	T1177	F1075	Q981	I887
S2121	Q2045		ALA	M1730	R1618	R1508	PRO	THR	S1292	F1179	A1077	Q981	W891
S2122	P1840		ALA	M1731	R1619	R1508	PRO	PRO	P1294	F1180	E1078	Q981	S892
S2123	P1841		GLU	L1731	A1620	L1514	ASP	GLY	F1297	E1181	Y1081	Q981	Y893
L2124	L1849		GLY	E1733	E1621	G1518	R1421	THR	H1296	T1182	T1082	Q981	G894
H2125	V1850		LYS	Y1734	E1622	L1519	D1422	PRO	Q1299	F1188	V1083	Q981	
R2126	M1851		GLU	I1735	R1623	L1522	D1423	GLN	Q1299	L1189	V1083	Q981	R897
Q2127	G1852		ASP	P1740	G1625	L1522	P1424	PRO	T1304	G1192	G1086	Q981	
Y2128	I1853		LEU	A1627	A1523	A1523	I1426	VAL	ALA	C1192	R1087	Q981	K901
E2133	F1854		LEU	R1743	M1527	M1527	I1426	GLU	ALA	P1196	F1092	Q981	R902
L2134	D1858		SER	P1749	K1547	K1547	T1430	ALA	ALA	P1196	F1092	Q981	L903
L2135	I1862		ARG	R1758	L1548	L1548	T1431	ALA	THR	P1199	E1093	Q981	H904
R2136	I1862		LEU	R1759	P1549	P1549	T1432	PRO	PRO	G1200	A1094	Q981	P905
L2138	M1865		SER	P1763	P1550	P1550	Y1433	VAL	ALA	G1200	V1095	Q981	C906
P2139	I1866		LEU	R1771	A1551	A1551	Y1435	ARG	PRO	D1207	M1100	Q981	L907
R2140	F1871		LYS	L1771	F1552	F1552	Y1435	ALA	PRO	S1210	R1101	Q981	H911
I2144	F1946		THR	R1772	V1554	V1554	V1439	ASN	GLY	Q1220	W1104	Q981	S912
V2149	G1874		VAL	P1773	P1556	P1556	Q1443	LYS	PRO	G1116	G1116	Q981	L913
T2152	GLU		ARG	H1776	Q1559	Q1559	C1447	ASP	PRO	F1223	Y1122	Q981	E917
L2156	GLU		LEU	H1776	E1652	E1652	V1448	ALA	ALA	A1227	A1227	Q981	L929
E2157	GLU		LYS	V1783	L1653	L1653	V1449	THR	GLU	M1125	M1125	Q981	R930
R2163	GLU		LYS	L1786	R1656	R1656	W1450	GLU	ALA	Q1041	A1041	Q981	T931
V2168	GLU		GLU	P1787	R1661	R1661	G1451	LYS	ALA	V1043	V1043	Q981	L932
Q2169	GLU		GLU	ALA	F1662	F1662	W1452	ASN	ARG	R1128	G1128	Q981	L933
M2170	GLU		GLU	ALA	F1662	F1662	V1453	LYS	ALA	Q1130	T1044	Q981	A934
Q2173	GLU		GLU	E1793	R1670	R1670	T1494	ALA	ALA	W1237	L1046	Q981	C937
E2174	GLU		LEU	E1793	Y1670	Y1670	P1455	ARG	PRO	Q1244	W1132	Q981	H938
S2255	GLU		PRO	R1797	A1672	A1672	M1476	GLY	PRO	F1245	H1133	Q981	V939
N2256	GLU		ALA	R1797	V1673	V1673	G1477	PHE	ASP	E1246	Y1049	Q981	G940
L2257	ASP		ASP	P1800	L1676	L1676	D1478	LYS	ASP	P1247	G1048	Q981	G940
M2178	GLU		GLU	L1804	R1680	R1680	M1462	LEU	ASP	Y1051	Y1051	Q981	E947
I2179	GLU		GLU	L1804	R1680	R1680	M1462	PHE	ASP	D1147	D1147	Q981	E947
Q2180	GLU		GLU	R1808	L1694	L1694	N1482	LYS	TYR	V1148	V1148	Q981	L950
S2181	GLU		LYS	D1809	L1694	L1694	H1483	ALA	GLU	M1152	M1152	Q981	K951
I2182	GLU		GLU	K1810	L1698	L1698	H1483	LYS	ASN	E1054	E1054	Q981	K951
G2264	ASP		ASP	K1810	L1698	L1698	S1485	LYS	LEU	P1055	P1055	Q981	Y959
G2264	GLU		GLU	M1814	L1703	L1703	N1482	ALA	ARG	ASP	ASP	Q981	Y959
L2265	GLU		GLU	L1815	P1704	P1704	M1482	ALA	ARG	GLN	GLN	Q981	P969
G2266	GLU		GLU	G1816	P1704	P1704	H1483	MET	SER	GLU	GLU	Q981	L970
T2185	GLU		GLU	G1816	P1704	P1704	H1483	THR	GLY	PRO	PRO	Q981	D971
M2186	GLU		GLU	R1708	Q1598	Q1598	S1485	GLN	GLY	D1261	D1261	Q981	L972
Q2189	GLU		GLU	R1708	Q1598	Q1598	S1485	PRO	TRP	P1268	P1268	Q981	R976
			H2035		L1600	L1600	G1497	ALA	GLY	C1269	C1269	Q981	L977
					L1600	L1600	G1497	THR	ALA	L1270	L1270	Q981	L977
					L1600	L1600	G1497	PRO	ALA	R1271	R1271	Q981	L977
					L1600	L1600	G1497	PRO	ALA	L1272	L1272	Q981	P979
					L1600	L1600	G1497	ALA	GLY			Q981	A980

L3429	V3446	L3249	L3075	L2977	H2902	K2825	K2750	E2669	M2546	L2457	S2374	P2272
N3430	S3447	M3250	D3076	E2978	H2902	A2826	L2751	L2672	M2550	R2458	G2375	L2273
V3438	A3251	D3252	T3079	A2979	L2905	R2827	D2752	H2673	L2550	L2460	L2376	A2277
F3442	R3351	I3253	V3080	V2981	V2906	E2828	S2753	F2754	C2555	G2468	L2380	A2278
W3445	E3352	L3266	G3084	R2985	D2909	G2929	F2755	R2676	L2659	L2470	E2381	S2279
H3449	L3353	A3261	V3088	K2996	T2910	L2911	A2759	K2677	L2678	L2471	E2382	L2286
K3452	H3355	R3262	R3093	L3003	A2913	T2912	F2679	F2679	T2563	S2471	A2383	A2287
E3455	I3359	E3265	E3097	P3004	K2914	R2915	G2681	G2681	L2577	L2472	L2384	L2288
Q3456	P3360	P3267	S3098	M3007	E2915	K2916	D2684	D2684	M2578	L2474	R2385	Q2291
M3467	R3364	H3268	E3101	C3014	R2920	L2920	S2685	S2685	M2582	P2477	P2395	P2395
T3471	R3368	I3270	E3102	L3015	Q2924	T2924	H2688	H2688	L2583	L2478	VAL	Q2293
K3475	K3371	P3275	F3104	L3018	K2928	T2928	Y2691	Y2691	T2585	D2482	ARG	K2297
SER	V3372	M3276	K3105	P3021	Q2931	Q2931	E2694	E2694	G2592	L2485	ARG	V2298
LYS	E3375	L3277	M3106	A3022	Y2935	Y2935	L2695	L2695	L2595	K2489	GLU	V2299
ALA	Q3378	C3278	V3107	K3023	R2939	R2939	R2697	R2697	Q2599	A2492	HIS	G2303
LYS	L3379	L3194	R3110	V3024	L2935	L2935	M2698	M2698	R2600	S2483	GLY	G2306
ALA	R3380	R3197	L3111	L3025	Y2936	Y2936	H2700	H2700	E2604	F2494	PHE	L2307
ALA	L3381	A3198	LEU	E3037	R2939	R2939	F2701	F2701	E2605	V2495	GLY	L2313
ASP	L3384	M3201	GLY	H3030	GLY	GLY	E2709	E2709	L2603	S2501	GLU	Y2318
ALA	A3385	P3202	LYS	A3031	LEU	LEU	L2710	L2710	E2604	M2502	PRO	Y2318
E3386	E3386	V3203	SER	S3032	LEU	LEU	P2711	P2711	D2497	G2508	PRO	L2321
A3387	A3387	V3203	ALA	K3033	ASP	ASP	Y2714	Y2714	H2498	V2509	GLU	G2322
GLY	P3303	M3214	ARG	E3037	MET	MET	E2724	E2724	D2605	G2511	GLU	V2323
GLY	C3304	Y3219	THR	E3037	L2946	L2946	K2795	K2795	L2608	L2512	N2324	N2324
SER	T3305	Y3219	GLN	S3041	S2950	S2950	THR	THR	C2611	L2518	P2335	P2335
GLN	L3312	K3222	LYS	L3042	K2953	K2953	ALA	ALA	L2619	L2522	R2330	R2330
ARG	N3313	S3223	GLY	F3043	R2954	R2954	S2797	S2797	Q2620	G2525	D2333	D2333
THR	S3314	S3224	VAL	G3044	F2955	F2955	ASP	ASP	H2621	F2526	F2334	F2334
LYS	L3315	R3225	GLY	K3045	A2956	A2956	GLY	GLY	L2622	L2527	L2335	L2335
LYS	L3316	E3226	N3128	L3049	F2957	F2957	LYS	LYS	R2624	R2531	R2336	R2336
LYS	I3323	R3227	Y3131	V3050	G2958	G2958	ALA	ALA	R2625	L2518	F2340	F2340
ARG	V3324	A3228	Y3131	R3051	F2959	F2959	THR	THR	L2626	L2522	L2429	L2429
GLY	L3329	I3229	L3137	V3054	Q2961	Q2961	VAL	VAL	V2627	L2522	L2430	L2430
ASP	L3327	L3230	P3138	F3057	Q2962	Q2962	ASP	ASP	A2637	G2525	D2431	D2431
ARG	I3329	G3231	V3139	F3057	L2963	L2963	GLY	GLY	M2639	R2435	R2435	R2435
TYR	V3334	S3235	T3142	D3060	R2965	R2965	N2734	N2734	P2640	A2437	A2437	A2437
M3336	M3336	M3239	L3143	V3065	V2966	V2966	P2737	P2737	K2642	A2445	A2445	A2445
K3336	K3336	C3240	Q3144	L3068	D2968	D2968	R2738	R2738	L2643	G2446	G2446	G2446
R3337	R3337	C3240	H3146	L3068	L2969	L2969	P2739	P2739	T2644	D2537	R2359	R2359
V3340	V3340	I3243	I3147	H3069	S2970	S2970	V2740	V2740	T2645	T2538	G2448	G2448
F3341	F3341	P3244	I3147	I3070	Q2971	Q2971	K2809	K2809	R2650	F2541	R2452	R2452
A3342	A3342	V3245	D3155	L3071	E2972	E2972	L2813	L2813	S2542	S2542	I2453	I2453
Q3343	Q3343	L3246	V3156	A3072	F2973	F2973	K2814	K2814	T2544	T2544	R2454	R2454
P3344	P3344	D3247	L3157	R3073	L2974	L2974	A2815	A2815	Y2655	Y2655	A2455	A2455
N3428	N3428	R3248	L3158	S3074	A2975	A2975	E2748	E2748	S2668	S2668	I2456	I2456



• Molecule 2: Ryanodine receptor 1





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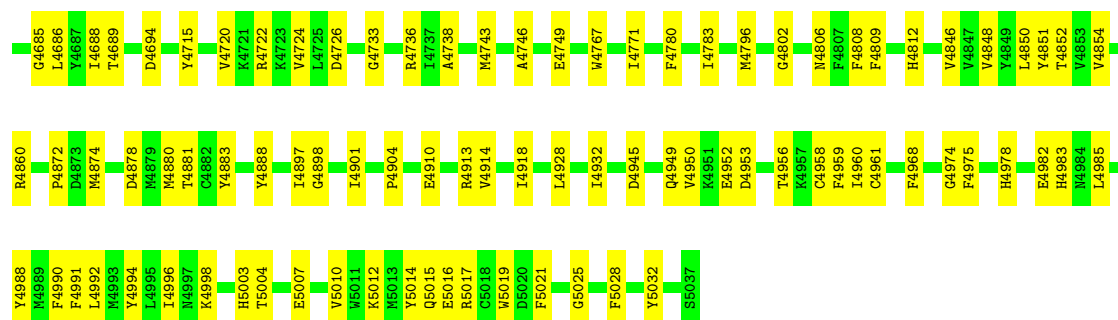
- Molecule 2: Ryanodine receptor 1

M403	L323	G225	V116	V11
F421	ASP	H226	Y117	Q12
K424	THR	E229	L118	L14
P431	ALA	C230	S119	R15
L443	PRO	L231	G136	T16
I449	LYS	T232	L137	E19
E453	ARG	I233	G138	V20
Q460	ASP	S234	E139	V21
E463	VAL	R242	E144	L22
R469	GLY	V245	M150	K34
S470	MET	Y246	M150	L35
L471	PRO	Y247	R157	F42
R472	PRO	E248	S158	R45
M473	E338	V252	E159	R45
E474	L339	H255	G160	P51
Q475	K340	A256	E161	T52
E480	Y341	R257	K162	S53
F481	G346	S258	R164	Q56
M483	C347	R261	L169	R57
L486	V348	L262	V172	V58
V487	Q349	S268	S175	I64
I491	G354	V269	S176	R76
D492	L357	S270	E177	
Y497	A360	G271	R178	L82
A501	C361	S272	Y179	A83
F503	P362	H273	L180	N84
E505	D363	L274	H181	THR
M515	P364	R275	S194	VAL
I520	K365	G277	Q197	GLU
E530	A366	L280	T198	GLY
G532	L369	H284	L199	VAL
F503	L372	V285	M200	GLU
E505	K373	T286	M202	SER
M515	C374	A292	M203	GLN
I530	K375	L293	P204	GLY
G532	A376	L299	I205	GLY
F503	I377	L299	C206	G97
E505	L378	C305	E210	H98
M515	A387	H308	V214	R99
I530	C389	T312	T215	T100
G532	R392	S313	G216	L101
F503	C393	F314	G217	T102
E505	L390	S315	H218	L103
M515	C395	F316	L220	R110
I530	E396	V220	F223	H111
G532			R224	A112
F503				H113
E505				S114
M515				R115

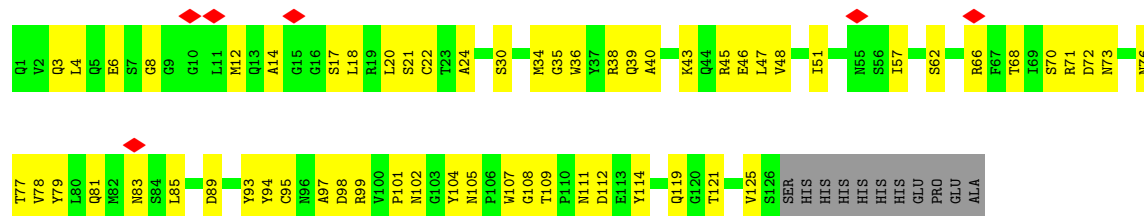


L3172	V3088	R9985	L2905	R2827	S2753	H2673	L2550	S2459	L2376	L2273	Y2192	E2108	L2039
Y3173	R3093	K2996	D2909	E2828	F2754	R2676	C2555	L2460	L2377	A2277	P2195	D2109	A2040
L3176	E3097	L3003	T2910	G2829	A2759	K2677	L2559	G2468	T2380	A2278	N2196	Y2111	Q2046
T3178	S3098	P3004	T2912	E2830	T2762	F2679	T2563	I2470	E2382	S2279	L2197	Q2112	L2046
V3183	E3101	N3007	A2913	GLU	K2765	W2680	T2563	S2471	A2383	L2286	W2198	S2113	LEU
L3186	D3102	C3014	K2915	THR	W2766	W2681	T2577	L2472	R2384	A2287	R2199	Q2114	GLY
L3187	I3103	E2915	K2916	GLU	A2767	D2684	M2578	L2473	R2385	A2288	A2200	L2116	GLY
L3190	E3104	L3015	E2920	LYS	A2768	S2685	M2582	L2474	P2395	Q2291	L2201	L2117	GLU
G3191	K3105	L3018	R2924	LYS	D2769	H2688	T2585	T2475	GLY	E2292	G2202	F2121	GLU
C3192	L3106	L3018	Q2924	THR	K2770	Y2691	T2585	L2479	VAL	Q2293	H2204	S2122	PRO
L3194	L3110	K3023	K2928	LYS	T2771	E2694	R2588	D2482	ARG	K2297	M2208	L2123	GLU
A3195	R3111	S3024	E2935	ILE	Q2772	L2695	R2588	L2485	ARG	W2299	M2211	L2124	GLU
R3196	L3125	L3025	Y2935	GLN	W2773	W2696	G2592	K2489	ARG	V2212	V2214	Q2126	THR
L3197	H3030	H3030	R2939	THR	W2774	R2697	L2595	K2489	GLU	A2303	W2213	Y2128	LEU
A3198	A3031	A3031	GLY	ALA	W2775	M2698	Q2599	A2492	HIS	G2304	V2214	E2133	SER
M3201	N3032	N3032	LEU	GLN	S2776	A2699	Q2600	S2493	PHE	G2305	G2216	L2134	SER
P3202	K3034	K3034	LYS	THR	Y2777	M2700	R2600	F2494	GLY	G2306	GLY	L2135	ARG
V3203	E3035	E3035	ASP	TYR	W2780	P2701	I2603	W2495	GLU	L2307	GLY	R2136	ARG
V3203	K3036	K3036	PRO	GLU	Y2781	C2702	E2604	P2496	PRO	L2313	THR	A2137	SER
N3214	E3037	E3037	ARG	GLU	W2782	I2706	D2605	D2497	PRO	Y2318	LYS	L2138	LEU
Y3219	S3041	S3041	L2946	GLY	E2783	A2709	M2608	H2498	GLU	T2321	I2223	R2140	GLU
K3222	L3042	L3042	E2950	LYS	E2783	L2710	K2499	A2500	N2414	W2322	T2230	I2144	VAL
S3223	G3043	G3043	K2953	GLY	K2786	P2711	C2611	S2501	L2418	W2323	T2230	V2149	ARG
P3224	E3044	E3044	R2954	THR	T2787	Y2714	L2619	M2502	G2419	N2324	R2234	V2149	LEU
R3225	L3049	L3049	F2955	ALA	W2788	V2715	Q2620	R2508	A2420	W2325	R2234	T2152	VAL
E3226	V3050	V3050	A2956	LYS	R2789	K2724	H2621	W2509	H2420	R2330	Y2238	L2156	LYS
R3227	R3051	R3051	F2957	THR	L2791	E2725	L2623	Y2510	A2421	D2333	Y2238	L2157	LYS
A3228	G2958	G2958	G2958	GLY	R2792	LYS	R2624	G2511	N2423	F2334	I2242	E2157	GLY
I3229	F2959	F2959	F2959	ALA	R2793	ALA	R2625	L2512	Y2426	R2336	Q2245	R2163	LYS
L3230	L2960	L2960	Q2961	THR	Y2794	THR	L2626	L2518	L2429	R2336	N2246	V2168	PRO
G3231	Q2962	Q2962	L2963	VAL	R2795	VAL	V2627	L2522	D2431	F2340	Q2247	Q2169	GLY
L3232	L2964	L2964	R2965	ALA	T2796	ASP	V2627	L2522	D2431	F2340	Q2247	M2170	GLY
S3235	R2965	R2965	Y2966	GLU	F2797	ALA	A2637	L2522	D2431	V2352	F2251	L2177	LEU
M3239	V2966	V2966	V2966	GLY	S2798	GLY	W2639	G2525	R2435	W2353	L2254	Q2173	PRO
C3240	D2967	D2967	D2967	THR	E2799	N2734	M2639	F2526	R2435	W2353	L2254	E2174	ALA
I3243	L2968	L2968	E2969	LYS	K2800	E2879	P2640	L2527	C2436	R2354	S2255	E2174	ALA
P3244	T2969	T2969	S2970	GLU	D2801	R2737	L2642	R2531	A2437	R2355	Y2256	E2175	GLY
V3245	Q2971	Q2971	E2972	THR	L2802	R2738	L2643	R2531	A2445	L2356	L2257	N2176	GLY
L3246	F2972	F2972	E2973	LYS	E2803	P2739	L2644	L2536	G2446	L2357	L2258	L2177	K2089
D3247	E2973	E2973	E2973	GLY	E2803	V2740	T2645	D2537	K2447	R2358	L2258	M2178	L2094
R3248	L2974	L2974	A2975	LYS	K2809	V2745	R2650	T2538	G2448	R2359	S2261	I2179	L2094
L3249	H2976	H2976	H2976	THR	L2810	L2746	Y2655	F2541	R2452	R2360	G2262	S2181	Q2095
M3250	L2977	L2977	E2978	GLU	L2813	L2747	S2542	T2542	I2453	G2264	L2263	I2182	E2096
A3251	E2978	E2978	E2978	LYS	A2815	P2748	T2543	T2543	R2454	A2367	L2265	Q2183	H2100
D3252	A2979	A2979	A2979	THR	E2749	E2749	S2668	T2544	I2455	L2368	G2266	M2184	W2101
I3253	V2980	V2980	V2980	GLY	K2750	E2749	E2669	E2545	I2456	L2368	M2267	I2185	R2104
L3256	V2981	V2981	V2981	GLY	L2751	K2750	E2669	M2546	R2458	S2374	Q2268	M2186	R2104
					E2820	L2751	E2669	M2546	R2458	S2374	Q2268	M2186	R2104
					W2821	D2752	L2672			P2272		K2189	Q2107
					E2824								
					K2825								
					A2826								

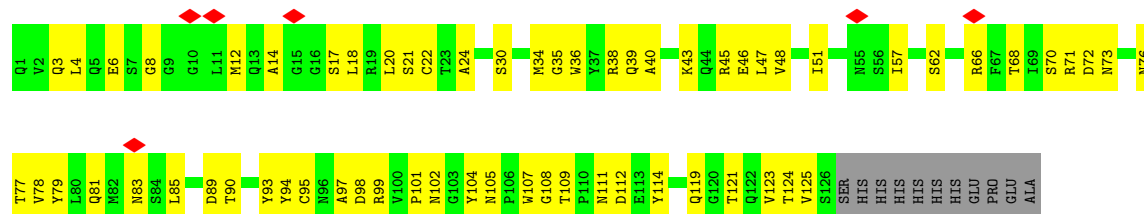




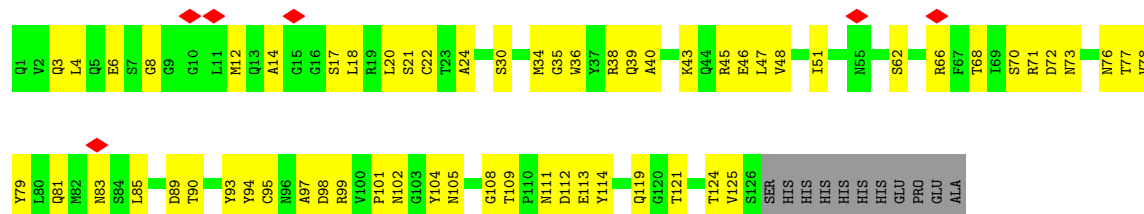
• Molecule 3: Nanobody 9657



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• Molecule 3: Nanobody 9657





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16530	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	3.003	Depositor
Minimum map value	-0.117	Depositor
Average map value	0.044	Depositor
Map value standard deviation	0.094	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, 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	0.11	0/834	0.38	0/1123
1	D	0.11	0/834	0.38	0/1123
1	H	0.11	0/834	0.38	0/1123
1	I	0.11	0/834	0.38	0/1123
2	B	0.13	0/34916	0.37	1/47328 (0.0%)
2	E	0.13	0/34916	0.37	1/47328 (0.0%)
2	G	0.13	0/34923	0.37	1/47336 (0.0%)
2	J	0.13	0/34916	0.37	1/47328 (0.0%)
3	C	0.19	0/987	0.55	0/1340
3	F	0.19	0/987	0.55	0/1340
3	K	0.19	0/987	0.55	0/1340
3	M	0.19	0/987	0.55	0/1340
All	All	0.14	0/146955	0.37	4/199172 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1503	PRO	N-CA-CB	6.06	110.23	103.44
2	E	1503	PRO	N-CA-CB	6.06	110.23	103.44
2	G	1503	PRO	N-CA-CB	6.06	110.23	103.44
2	J	1503	PRO	N-CA-CB	6.06	110.23	103.44

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	A	818	0	824	26	0
1	D	818	0	824	28	0
1	H	818	0	824	29	0
1	I	818	0	824	28	0
2	B	34143	0	33531	1090	0
2	E	34143	0	33531	1095	0
2	G	34150	0	33542	1090	0
2	J	34143	0	33531	1085	0
3	C	967	0	916	58	0
3	F	967	0	916	59	0
3	K	967	0	916	59	0
3	M	967	0	916	56	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	1	0
5	E	31	0	12	1	0
5	G	31	0	12	1	0
5	J	31	0	12	1	0
6	B	14	0	10	0	0
6	E	14	0	10	0	0
6	G	14	0	10	0	0
6	J	14	0	10	0	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	143907	0	141183	4640	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 4640 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)
2:B:2175:GLU:HA	2:B:2178:MET:HE2	1.45	0.98
2:E:2175:GLU:HA	2:E:2178:MET:HE2	1.45	0.96
2:G:2175:GLU:HA	2:G:2178:MET:HE2	1.45	0.96
2:J:2175:GLU:HA	2:J:2178:MET:HE2	1.45	0.96
2:E:3416:VAL:HG11	2:E:3516:LYS:HD3	1.51	0.93

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
1	D	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	H	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
1	I	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
2	B	4280/5027 (85%)	4144 (97%)	136 (3%)	0	100	100
2	E	4280/5027 (85%)	4142 (97%)	138 (3%)	0	100	100
2	G	4280/5027 (85%)	4142 (97%)	138 (3%)	0	100	100
2	J	4280/5027 (85%)	4140 (97%)	140 (3%)	0	100	100
3	C	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	F	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	K	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
3	M	124/137 (90%)	116 (94%)	8 (6%)	0	100	100
All	All	18036/21084 (86%)	17434 (97%)	602 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	88/88 (100%)	88 (100%)	0	100	100
1	D	88/88 (100%)	88 (100%)	0	100	100
1	H	88/88 (100%)	88 (100%)	0	100	100
1	I	88/88 (100%)	88 (100%)	0	100	100
2	B	3672/4270 (86%)	3672 (100%)	0	100	100
2	E	3672/4270 (86%)	3672 (100%)	0	100	100
2	G	3674/4270 (86%)	3673 (100%)	1 (0%)	100	100
2	J	3672/4270 (86%)	3672 (100%)	0	100	100
3	C	104/114 (91%)	104 (100%)	0	100	100
3	F	104/114 (91%)	104 (100%)	0	100	100
3	K	104/114 (91%)	104 (100%)	0	100	100
3	M	104/114 (91%)	104 (100%)	0	100	100
All	All	15458/17888 (86%)	15457 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	377	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 155 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	1035	ASN
3	F	73	ASN
2	J	2180	GLN
2	J	3909	ASN
3	M	3	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	E	5102	-	32,33,33	0.26	0	48,52,52	0.33	0
5	ATP	B	5102	-	32,33,33	0.26	0	48,52,52	0.33	0
6	CFF	G	5103	-	15,15,15	0.49	0	23,23,23	0.69	1 (4%)
6	CFF	J	5103	-	15,15,15	0.49	0	23,23,23	0.69	1 (4%)
5	ATP	G	5102	-	32,33,33	0.27	0	48,52,52	0.34	0
5	ATP	J	5102	-	32,33,33	0.27	0	48,52,52	0.33	0
6	CFF	B	5103	-	15,15,15	0.49	0	23,23,23	0.68	1 (4%)
6	CFF	E	5103	-	15,15,15	0.48	0	23,23,23	0.68	1 (4%)

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	E	5102	-	-	7/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	5102	-	-	7/22/38/38	0/3/3/3
6	CFF	G	5103	-	-	-	0/2/2/2
6	CFF	J	5103	-	-	-	0/2/2/2
5	ATP	G	5102	-	-	7/22/38/38	0/3/3/3
5	ATP	J	5102	-	-	7/22/38/38	0/3/3/3
6	CFF	B	5103	-	-	-	0/2/2/2
6	CFF	E	5103	-	-	-	0/2/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	5103	CFF	C12-N3-C2	2.23	121.22	117.33
6	J	5103	CFF	C12-N3-C2	2.23	121.22	117.33
6	B	5103	CFF	C12-N3-C2	2.21	121.18	117.33
6	E	5103	CFF	C12-N3-C2	2.20	121.16	117.33

There are no chirality outliers.

5 of 28 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	B	5102	ATP	C5'-O5'-PA-O3A
5	E	5102	ATP	C5'-O5'-PA-O1A
5	E	5102	ATP	C5'-O5'-PA-O2A

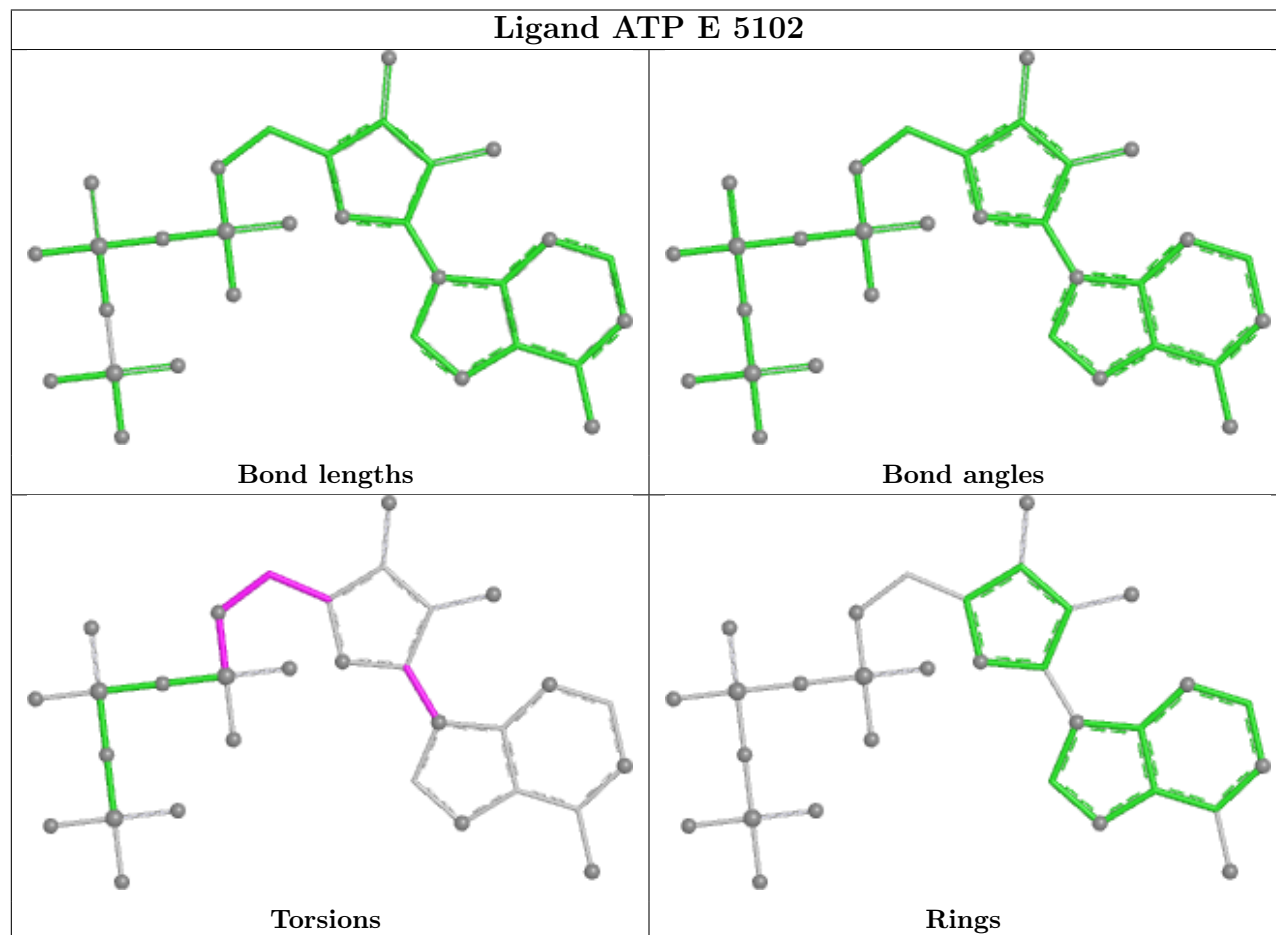
There are no ring outliers.

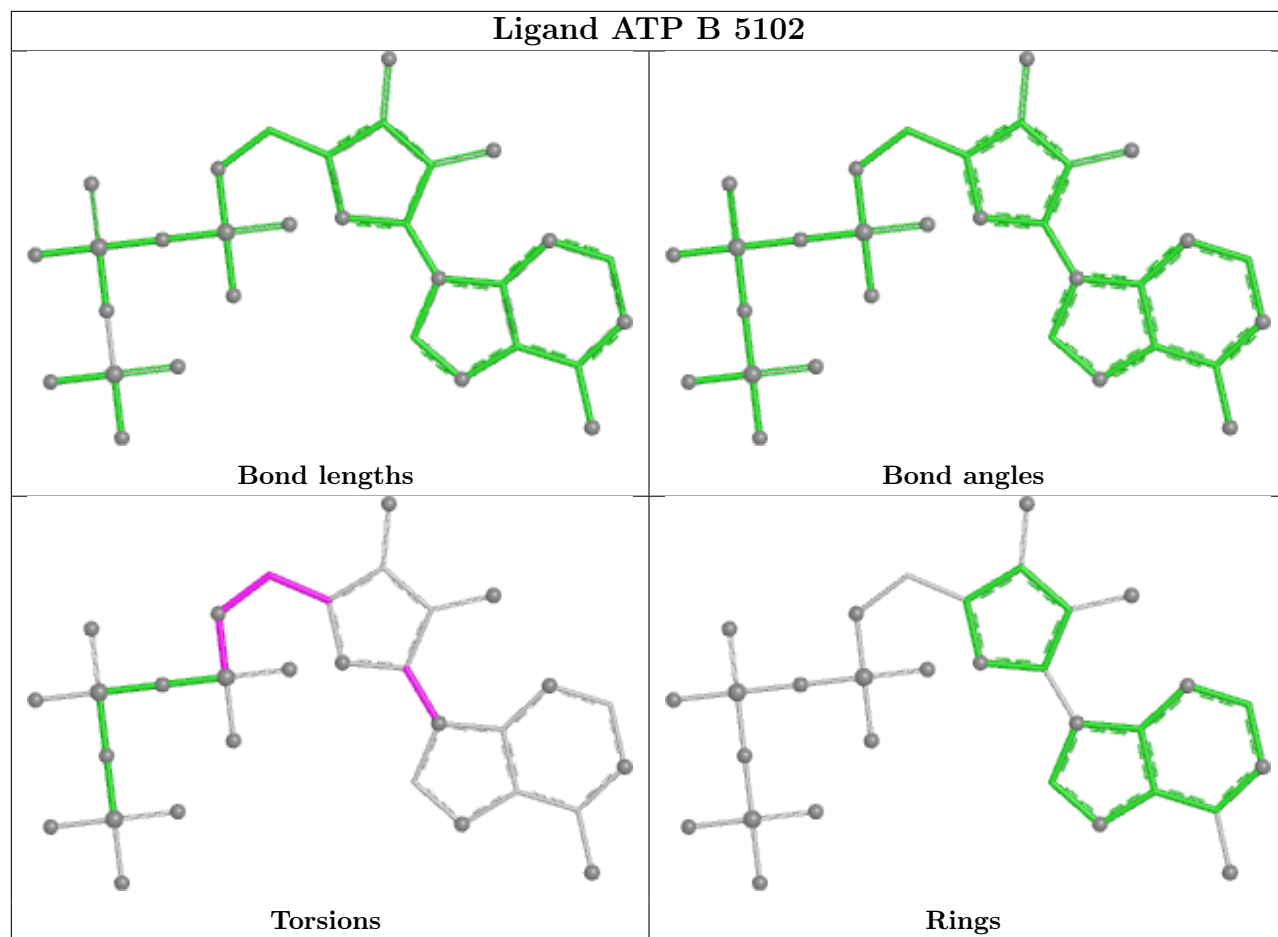
4 monomers are involved in 4 short contacts:

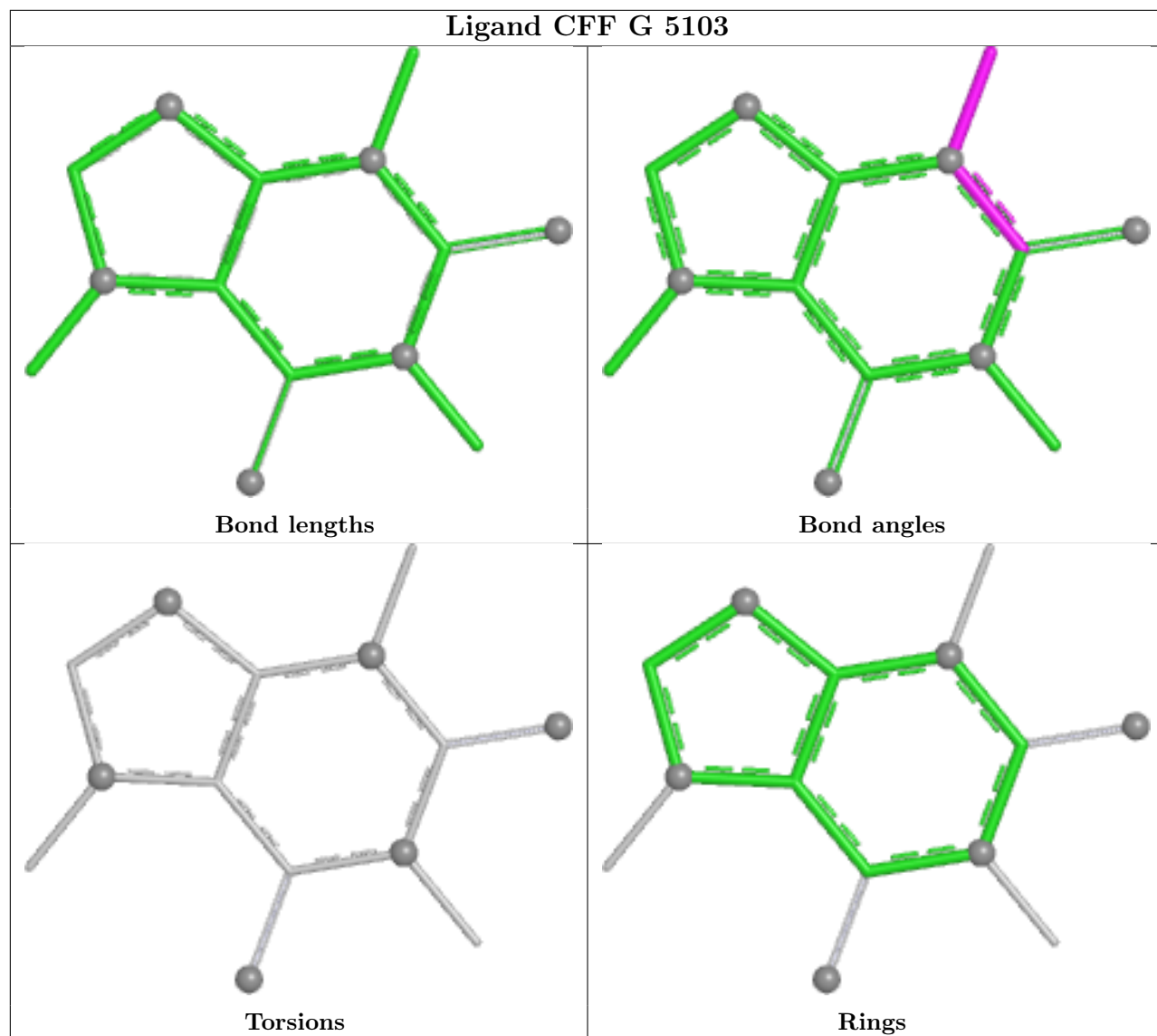
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	5102	ATP	1	0
5	B	5102	ATP	1	0
5	G	5102	ATP	1	0
5	J	5102	ATP	1	0

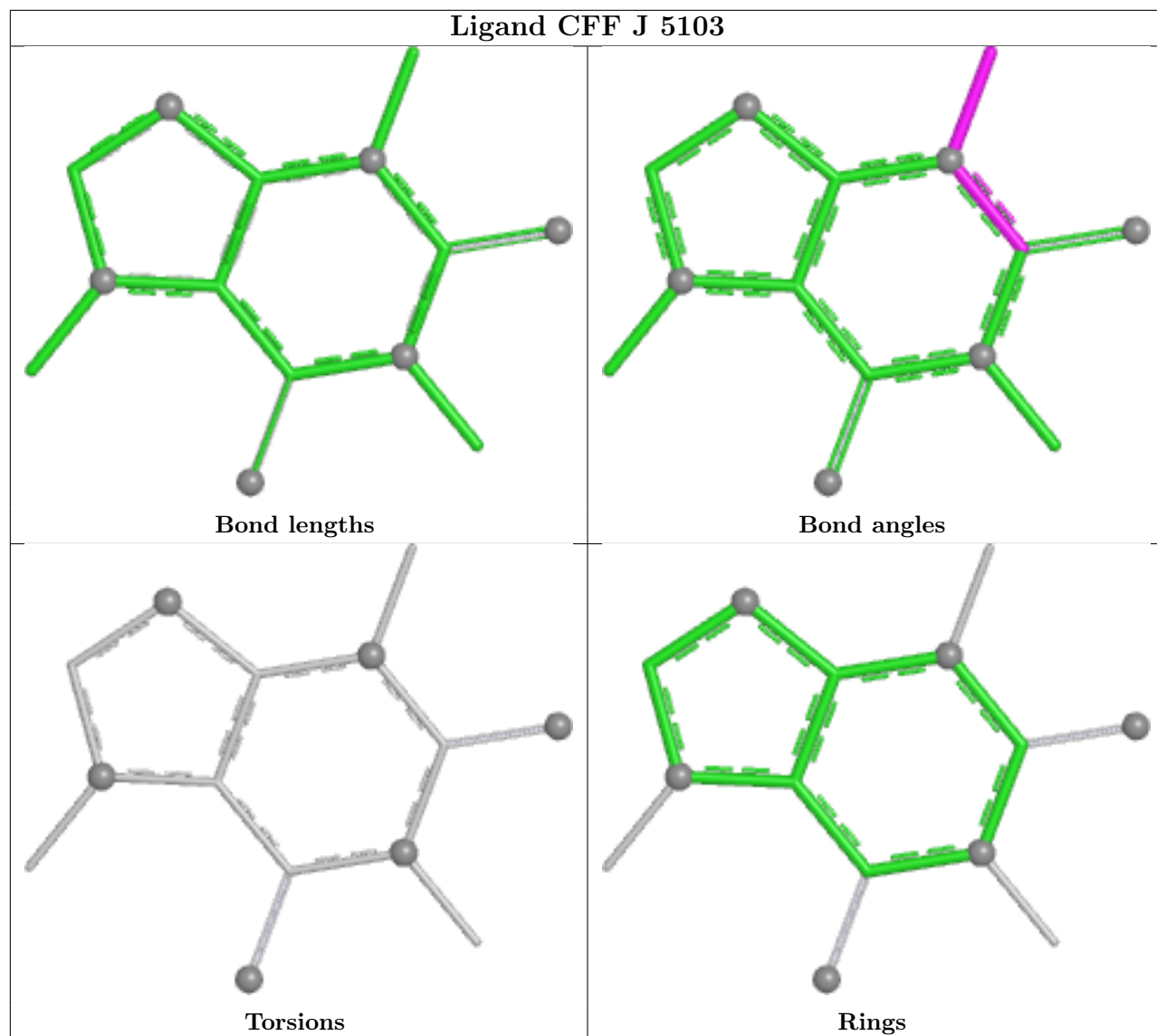
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

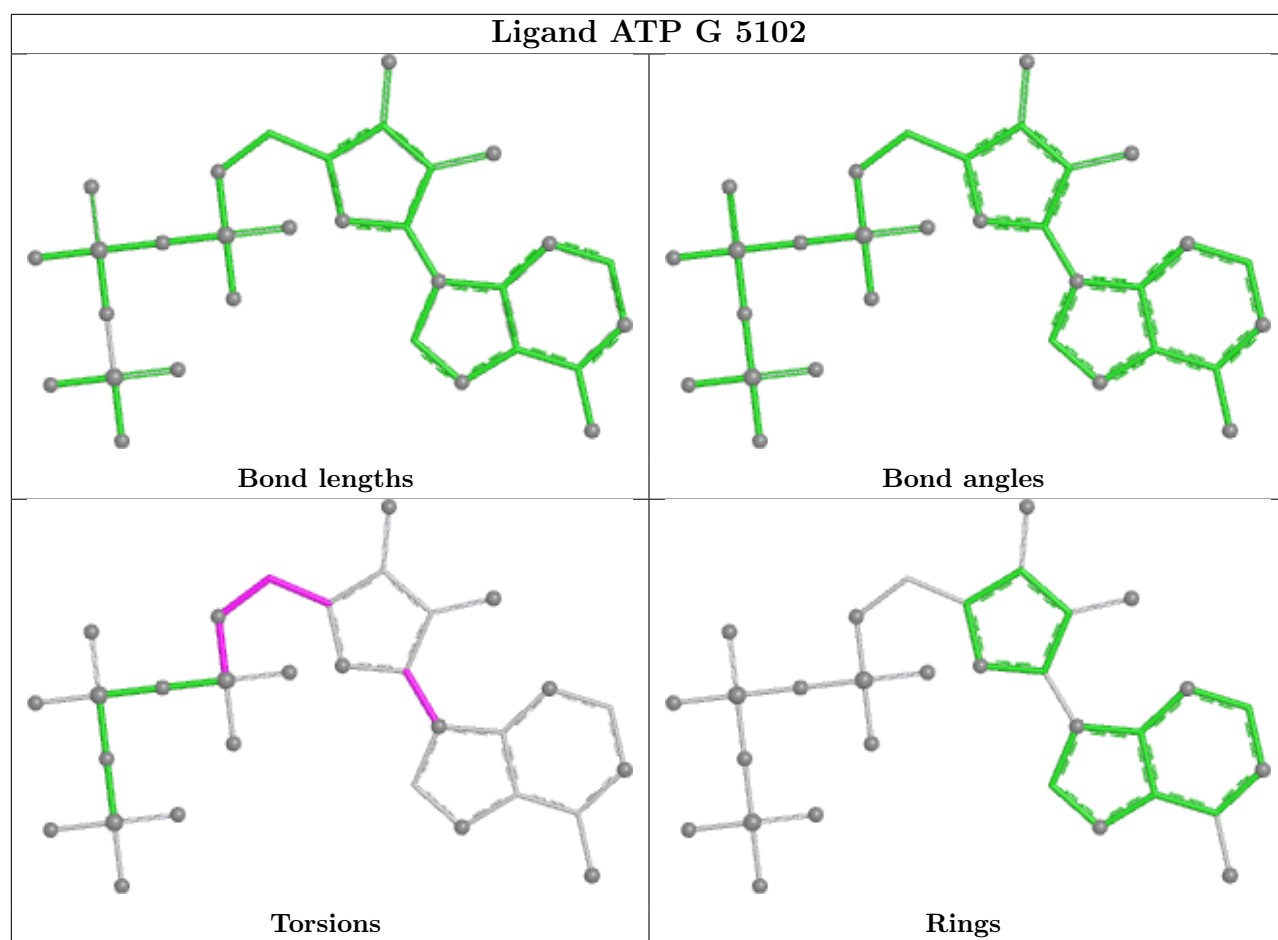
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

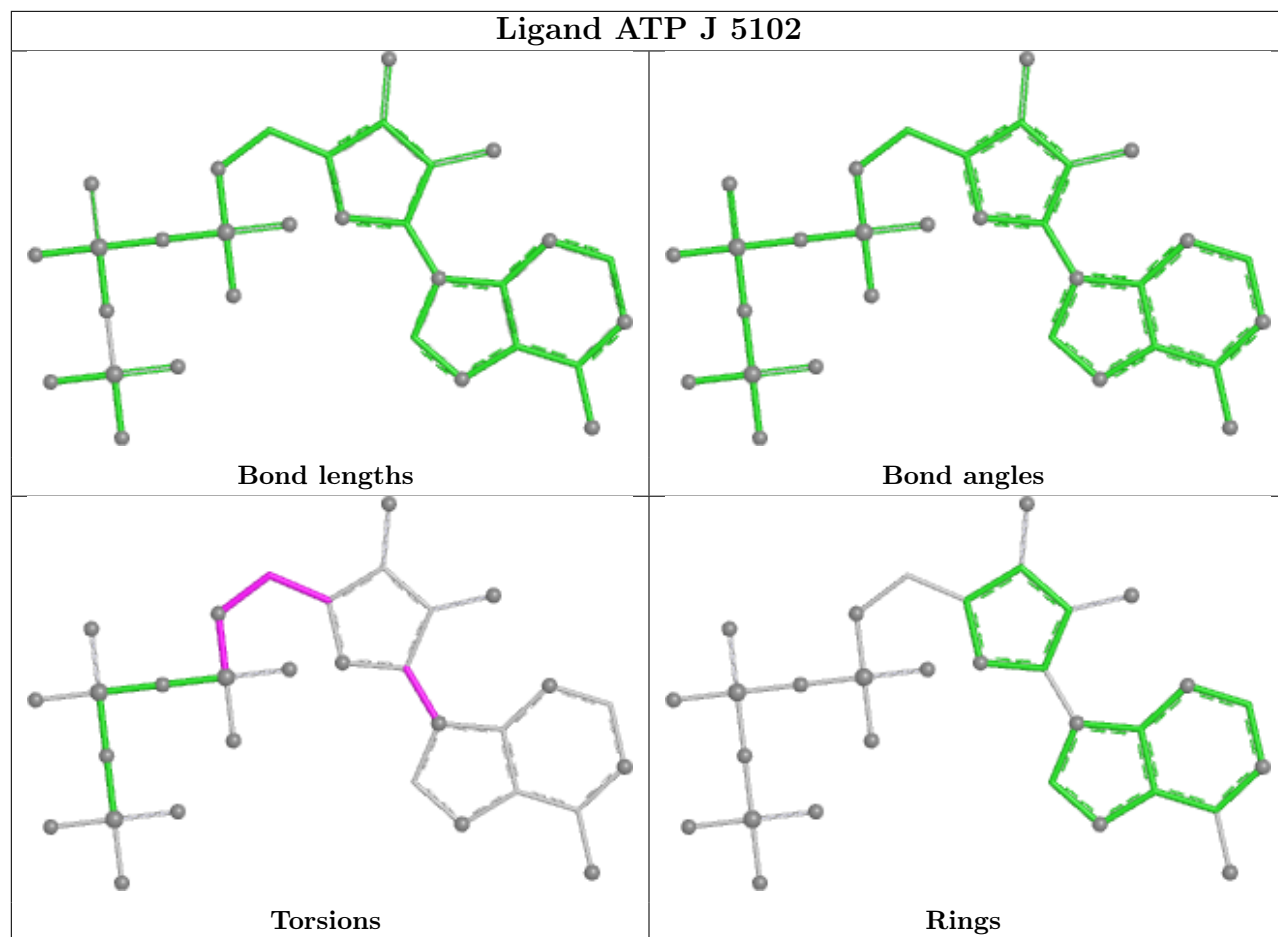


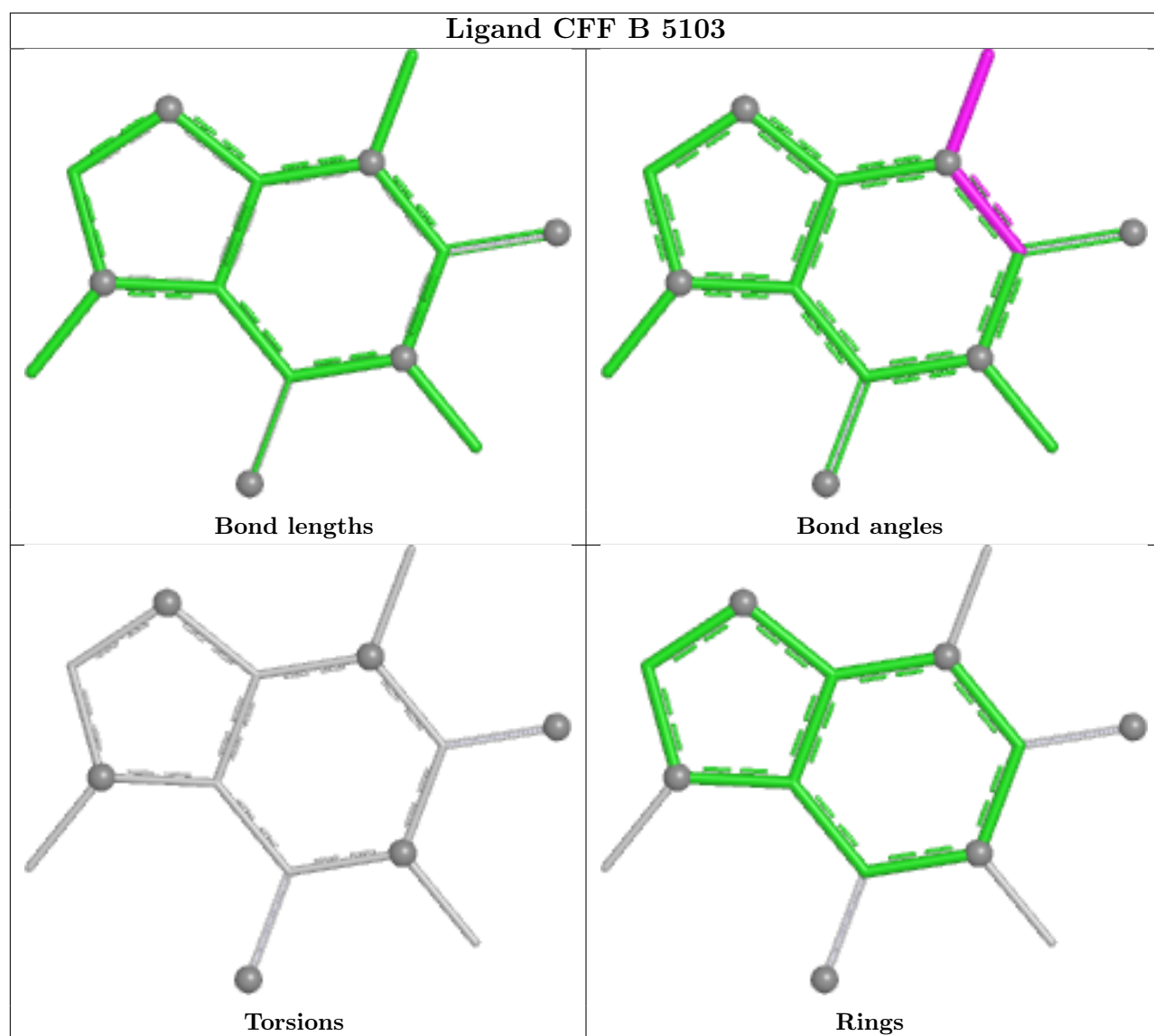


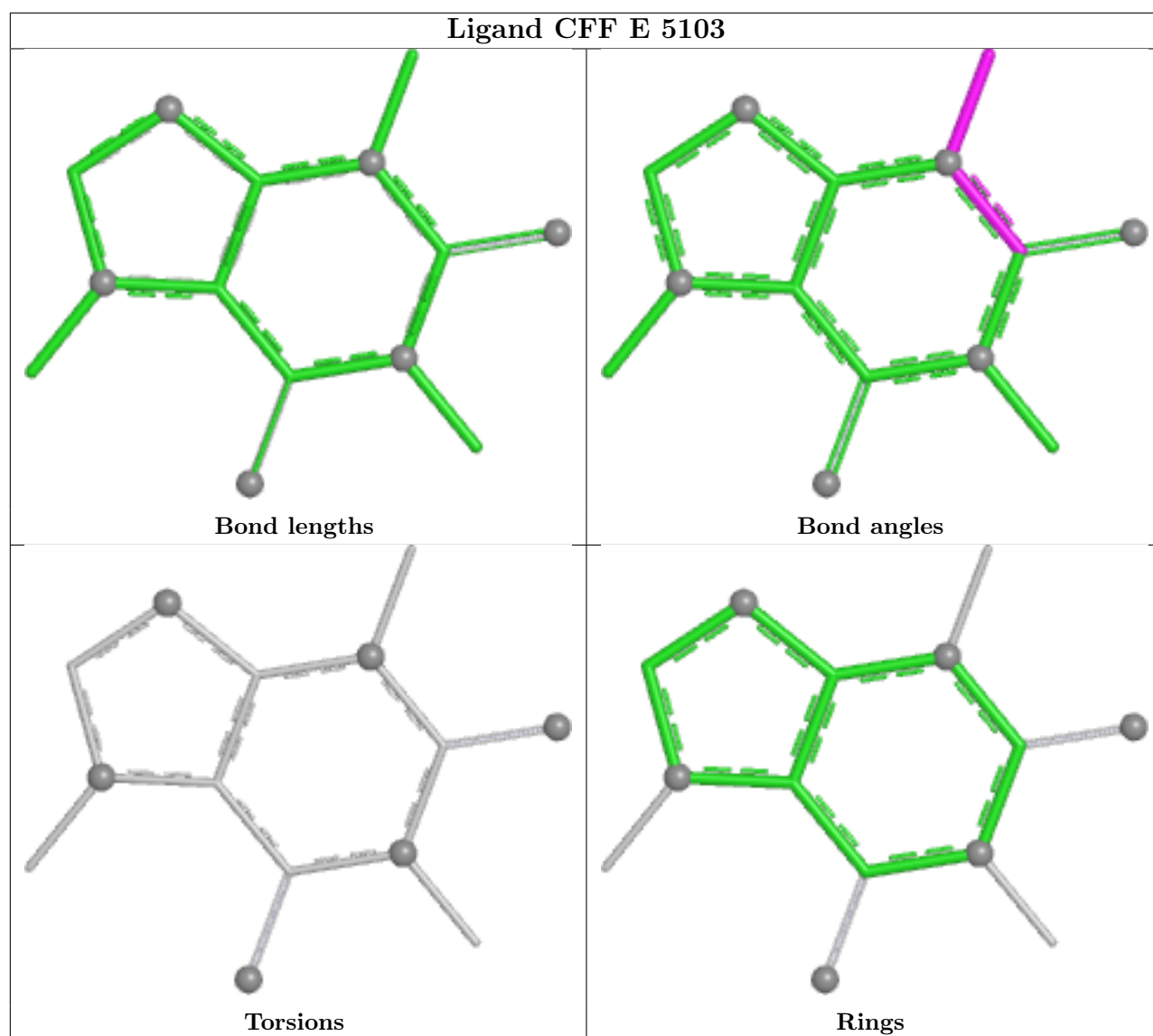












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

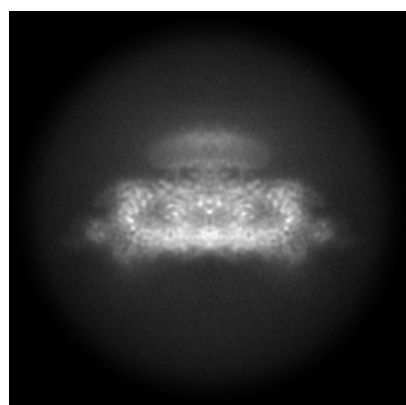
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19465. These allow visual inspection of the internal detail of the map and identification of artifacts.

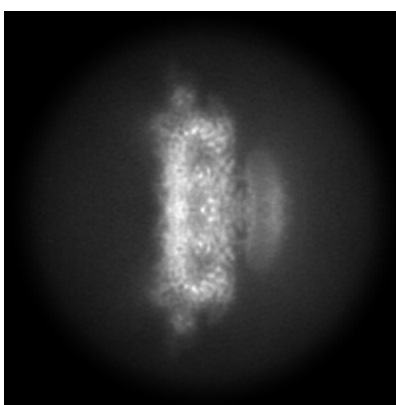
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

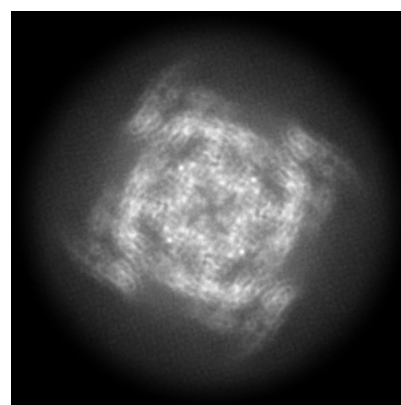
6.1.1 Primary map



X



Y

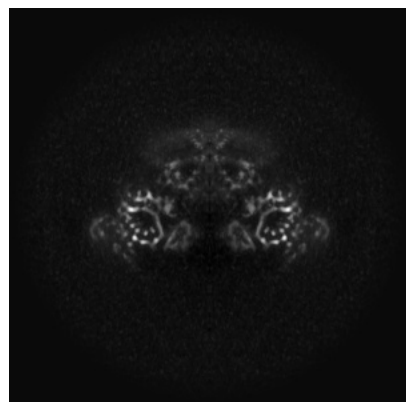


Z

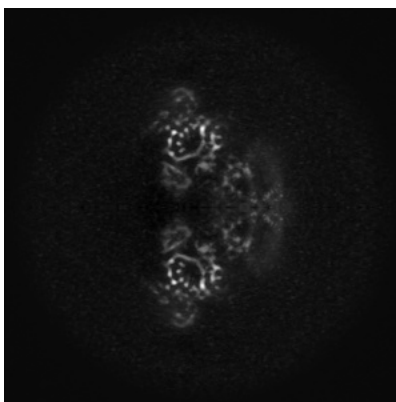
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

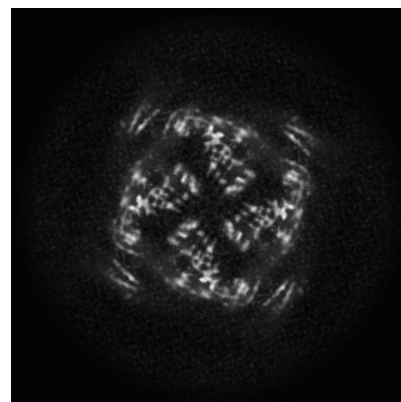
6.2.1 Primary map



X Index: 168



Y Index: 168

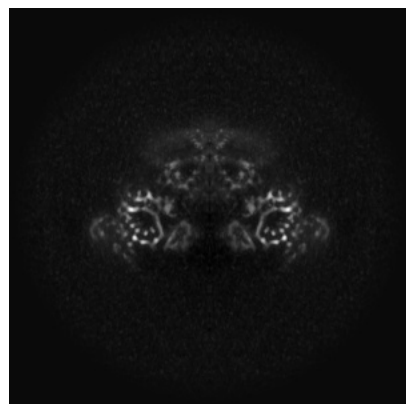


Z Index: 168

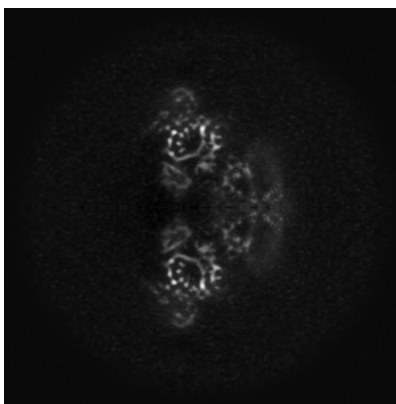
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

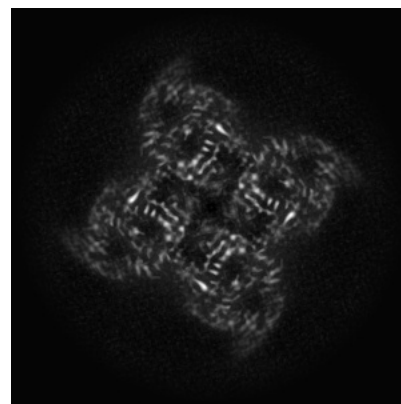
6.3.1 Primary map



X Index: 168



Y Index: 168

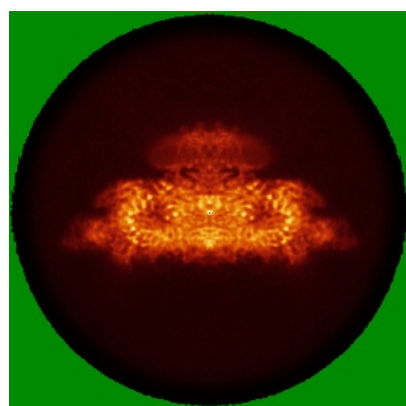


Z Index: 145

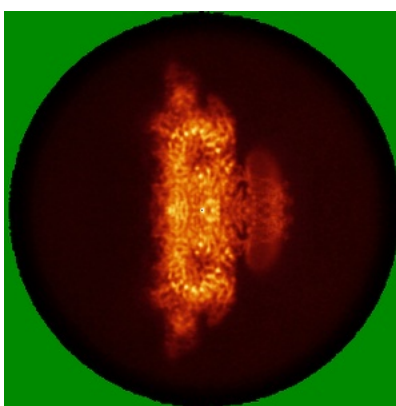
The images above show the largest variance slices of the map in three orthogonal directions.

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

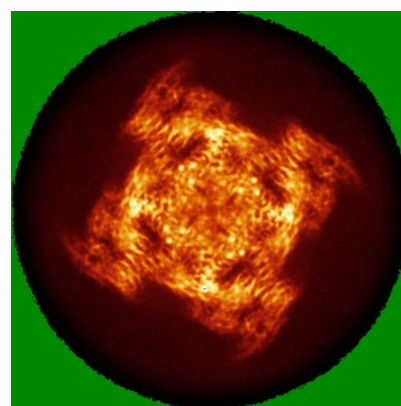
6.4.1 Primary map



X



Y

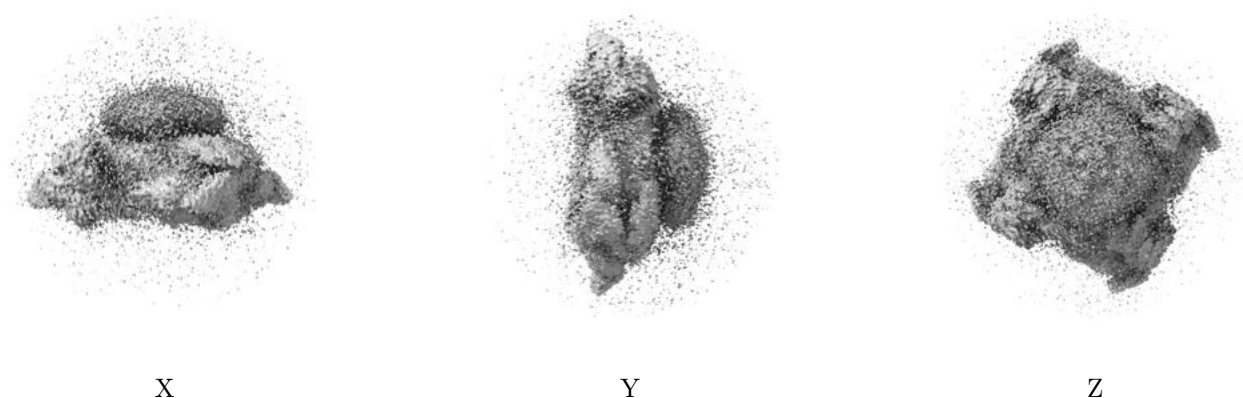


Z

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.

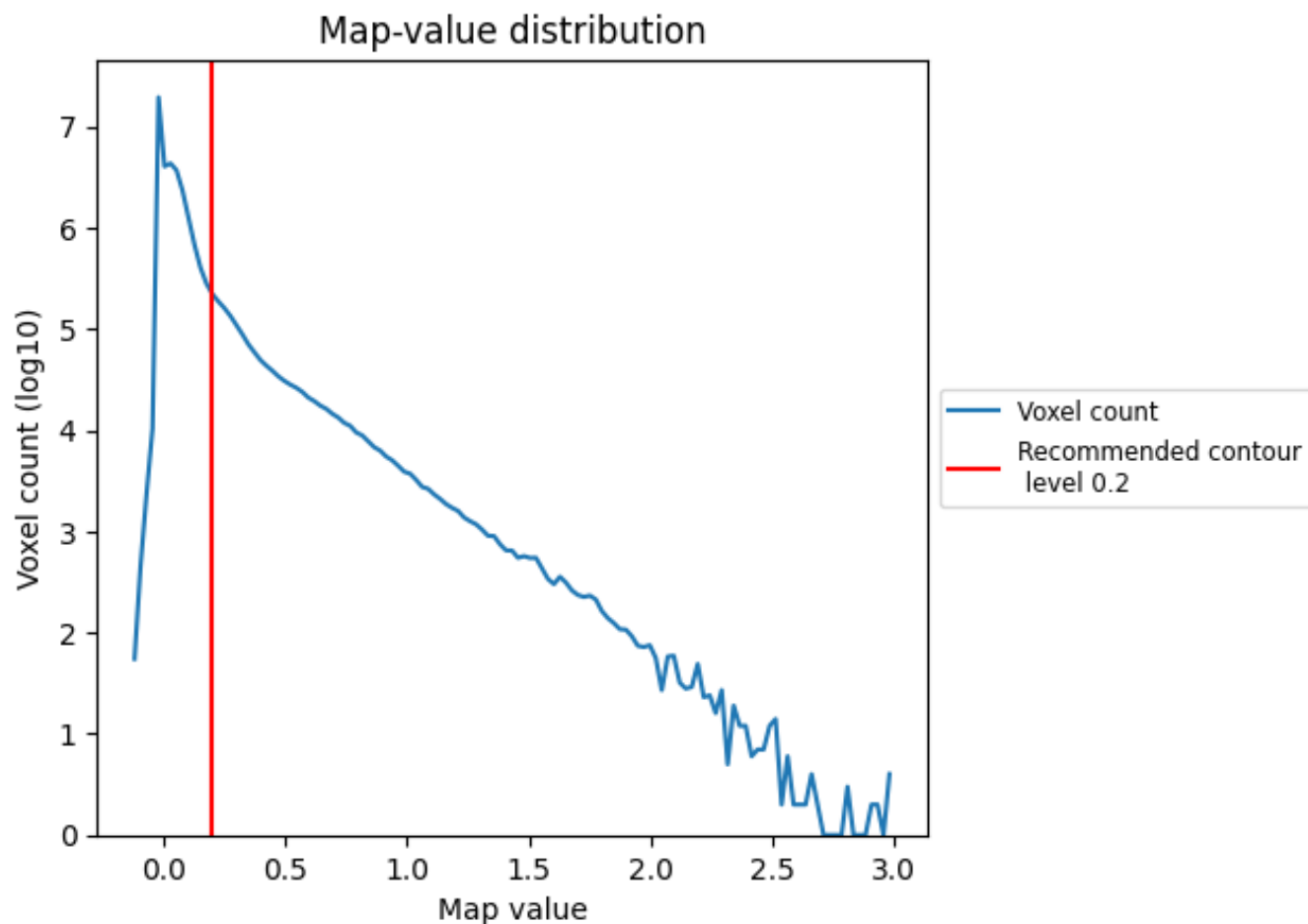
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

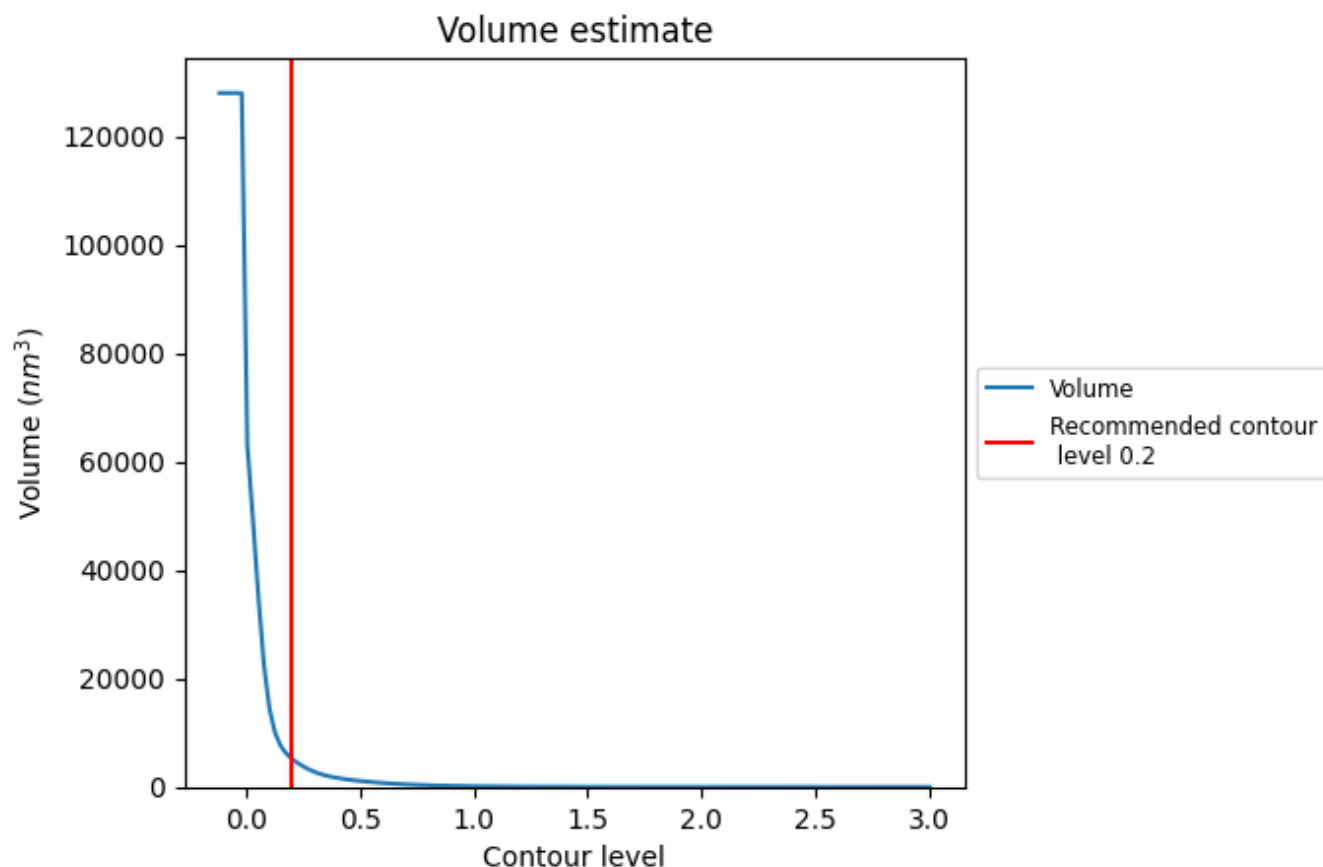
This section contains the results of statistical analysis of the map.

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.

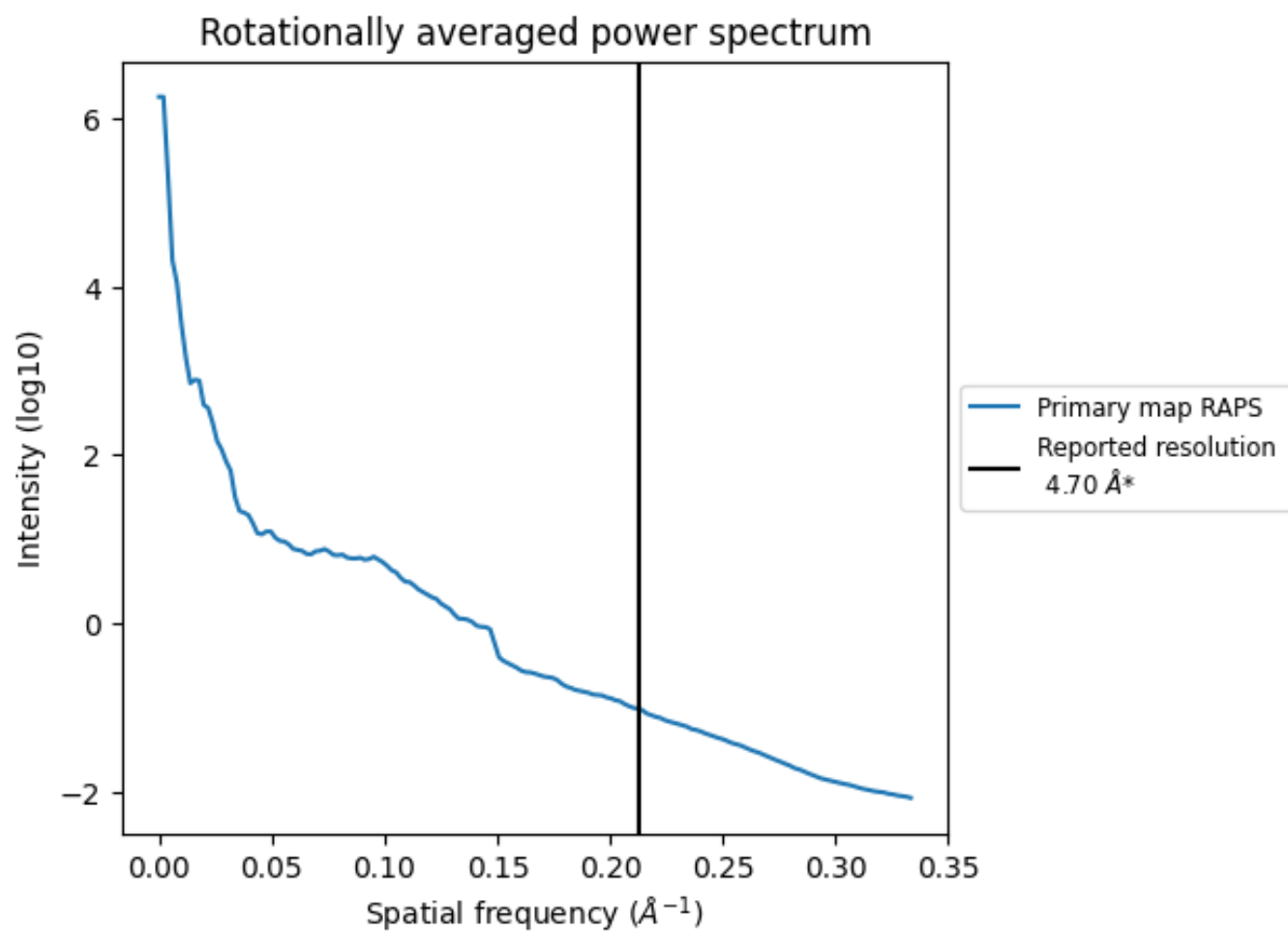
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5220 nm^3 ; this corresponds to an approximate mass of 4715 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 ⓘ

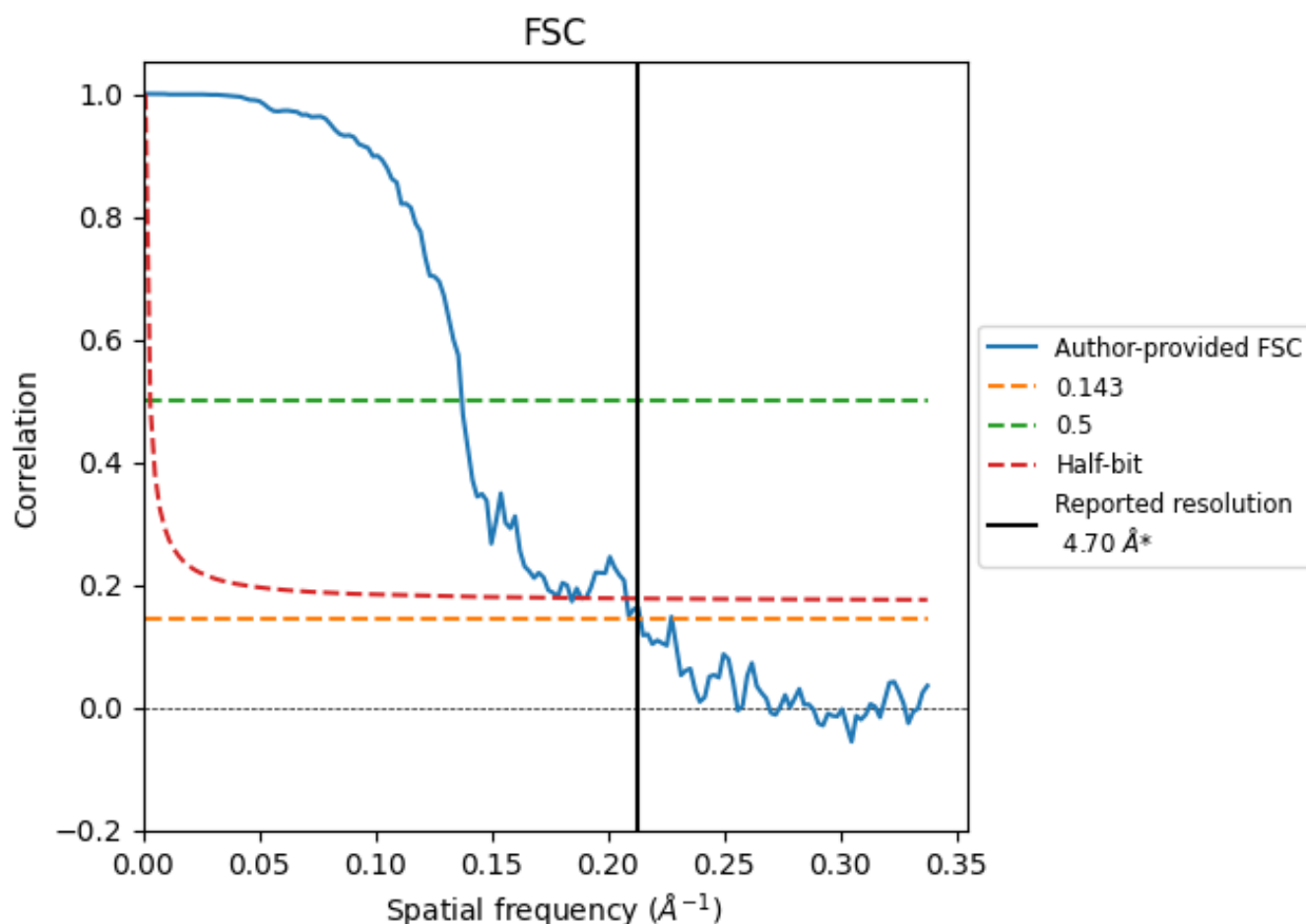


*Reported resolution corresponds to spatial frequency of 0.213 Å⁻¹

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 0.213 Å⁻¹

8.2 Resolution estimates [i](#)

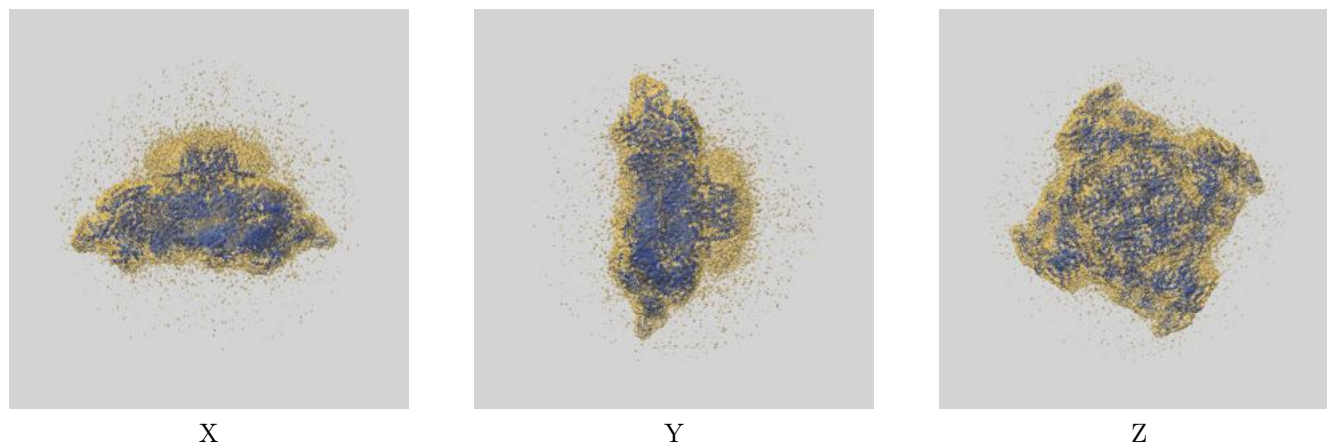
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	4.68	7.29	5.43
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

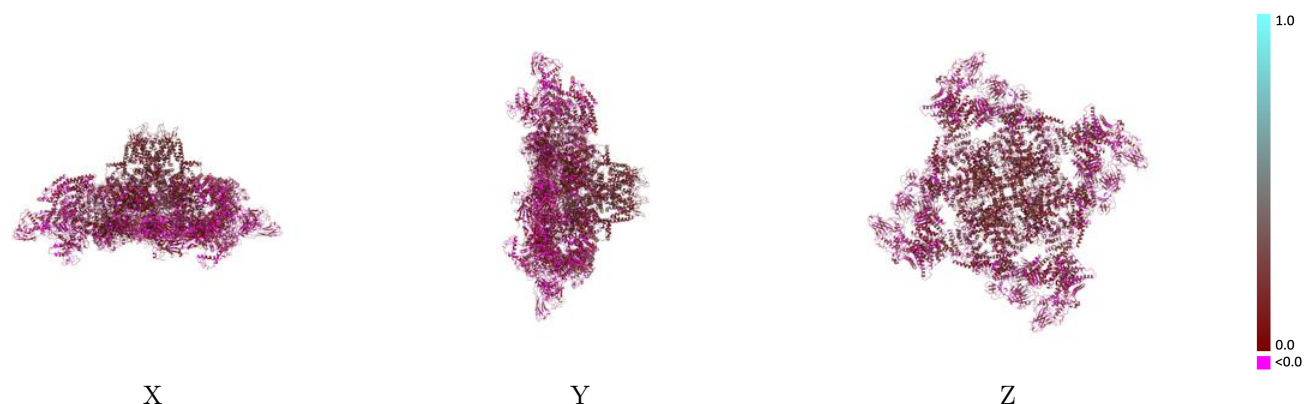
This section contains information regarding the fit between EMDB map EMD-19465 and PDB model 8RRU. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



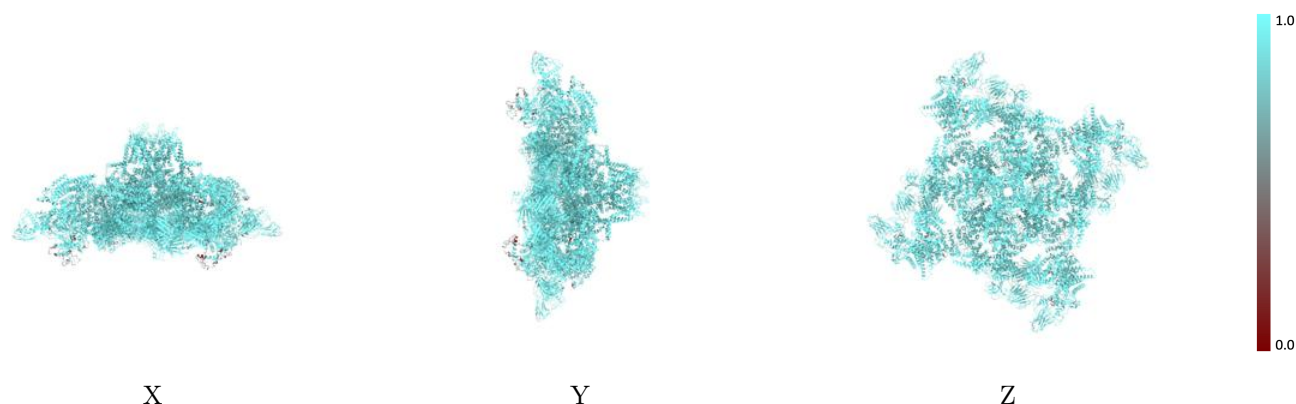
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



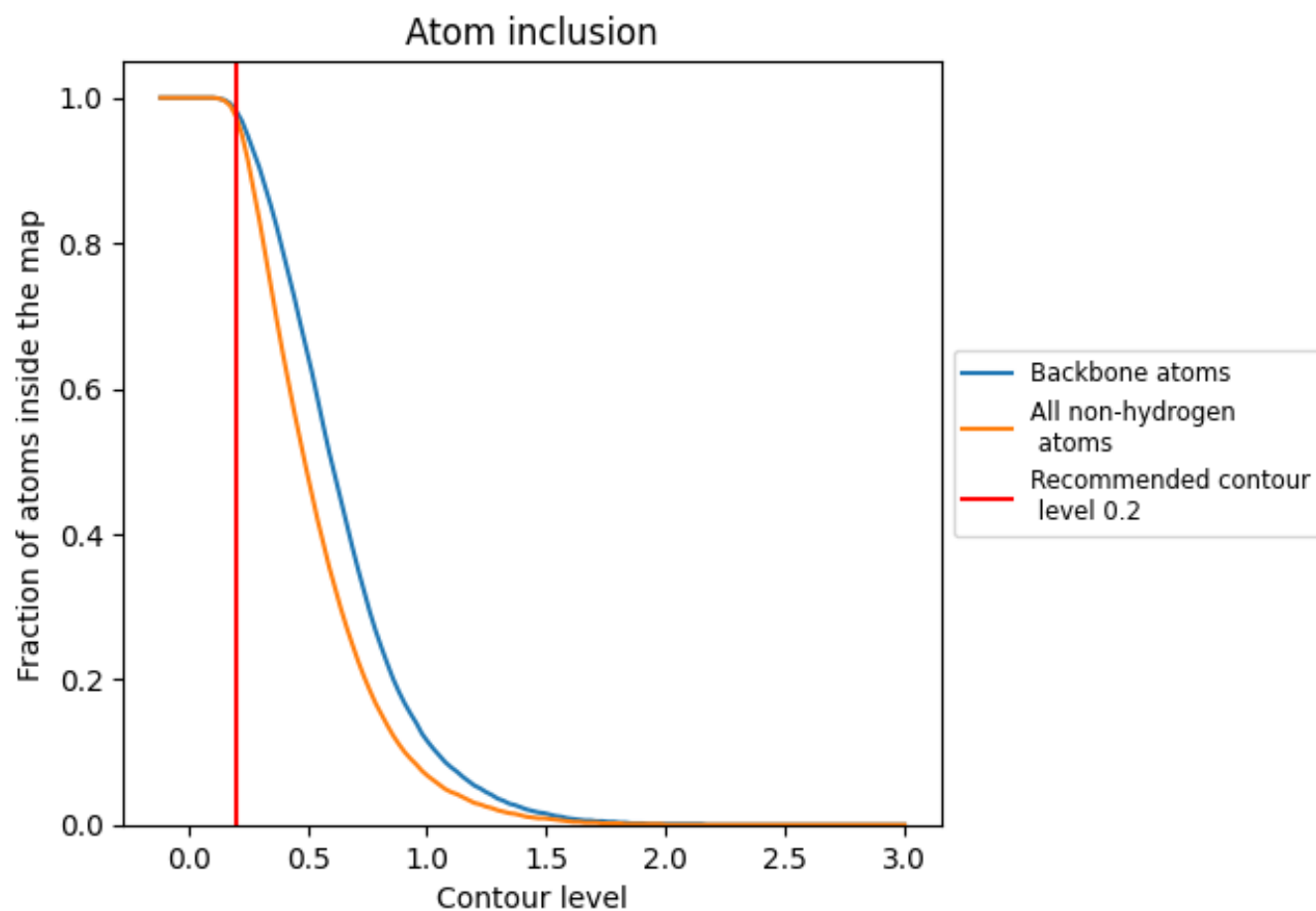
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 97% 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	0.9740	0.1100
A	0.9860	0.0460
B	0.9760	0.1140
C	0.9180	0.0580
D	0.9860	0.0440
E	0.9760	0.1130
F	0.9190	0.0590
G	0.9760	0.1140
H	0.9880	0.0460
I	0.9850	0.0440
J	0.9760	0.1140
K	0.9160	0.0570
M	0.9270	0.0610

1.0

0.0

<0.0