



wwPDB EM Validation Summary Report ⓘ

Apr 7, 2025 – 05:21 pm BST

PDB ID : 9GMA / pdb_00009gma
EMDB ID : EMD-51446
Title : MukBEF in a DNA capture state (dimer)
Authors : Burmann, F.; Lowe, J.
Deposited on : 2024-08-28
Resolution : 9.10 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.dev117
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) : 2.42

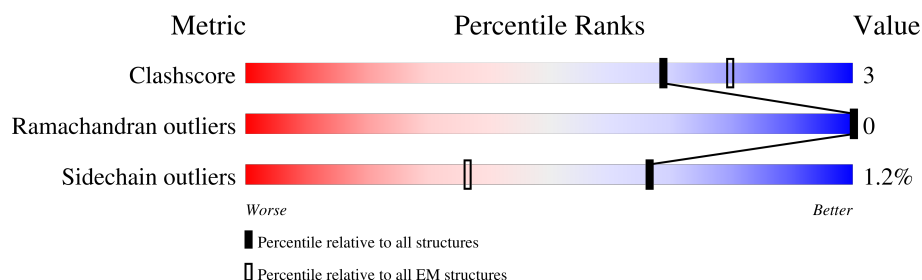
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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	A	1482	
1	B	1482	
1	O	1482	
1	P	1482	
2	C	440	
2	D	440	
3	E	240	
3	F	240	

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Mol	Chain	Length	Quality of chain
3	Q	240	
3	R	240	
4	G	78	
4	I	78	
4	M	78	
4	S	78	
5	K	2124	
6	L	2124	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	4HH	G	36	-	-	X	-
4	4HH	S	36	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 130919 atoms, of which 64362 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 Chromosome partition protein MukB.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1467	Total	C	H	N	O	S	0	0
			23547	7298	11707	2188	2314	40		
1	B	1467	Total	C	H	N	O	S	0	0
			23546	7298	11706	2188	2314	40		
1	O	1467	Total	C	H	N	O	S	0	0
			23547	7298	11707	2188	2314	40		
1	P	1467	Total	C	H	N	O	S	0	0
			23546	7298	11706	2188	2314	40		

- Molecule 2 is a protein called Chromosome partition protein MukF.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	C	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		
2	D	440	Total	C	H	N	O	S	0	0
			6982	2218	3451	614	686	13		

- Molecule 3 is a protein called Chromosome partition protein MukE.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	F	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		
3	Q	212	Total	C	H	N	O	S	0	0
			3441	1090	1719	301	322	9		
3	R	198	Total	C	H	N	O	S	0	0
			3246	1029	1627	284	298	8		

- Molecule 4 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms							AltConf	Trace
4	G	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	I	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	S	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		
4	M	72	Total	C	H	N	O	P	S	0	0
			1147	360	564	87	133	1	2		

- Molecule 5 is a DNA chain called pFB526.

Mol	Chain	Residues	Atoms							AltConf	Trace
5	K	73	Total	C	H	N	O	P		0	0
			2311	708	815	285	430	73			

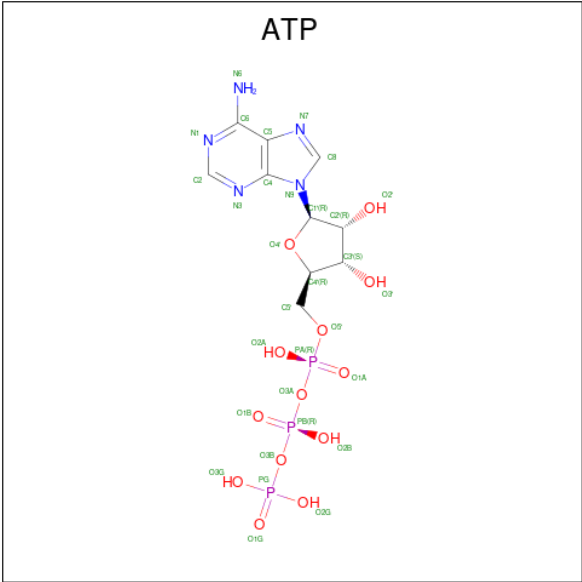
- Molecule 6 is a DNA chain called pFB526.

Mol	Chain	Residues	Atoms							AltConf	Trace
6	L	73	Total	C	H	N	O	P		0	0
			2320	711	823	267	446	73			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	
7	O	1	Total	Mg	0
			1	1	
7	P	1	Total	Mg	0
			1	1	

- Molecule 8 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

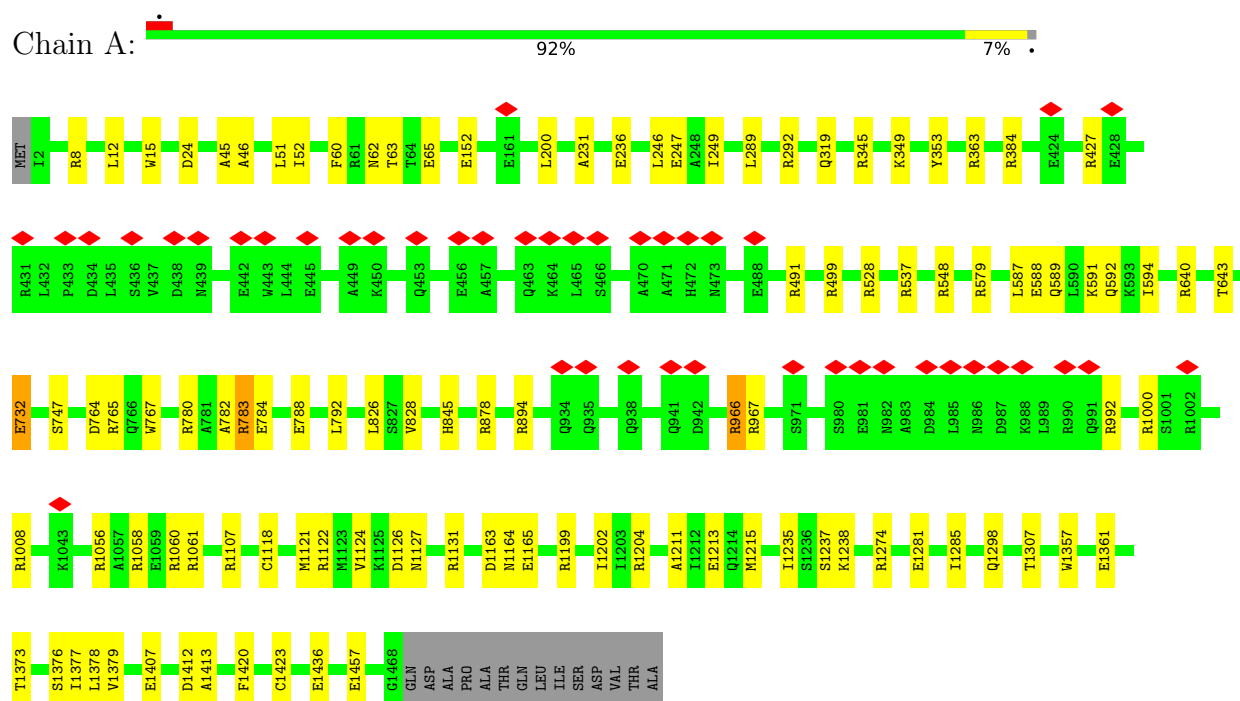


Mol	Chain	Residues	Atoms						AltConf
8	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	B	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	O	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
8	P	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

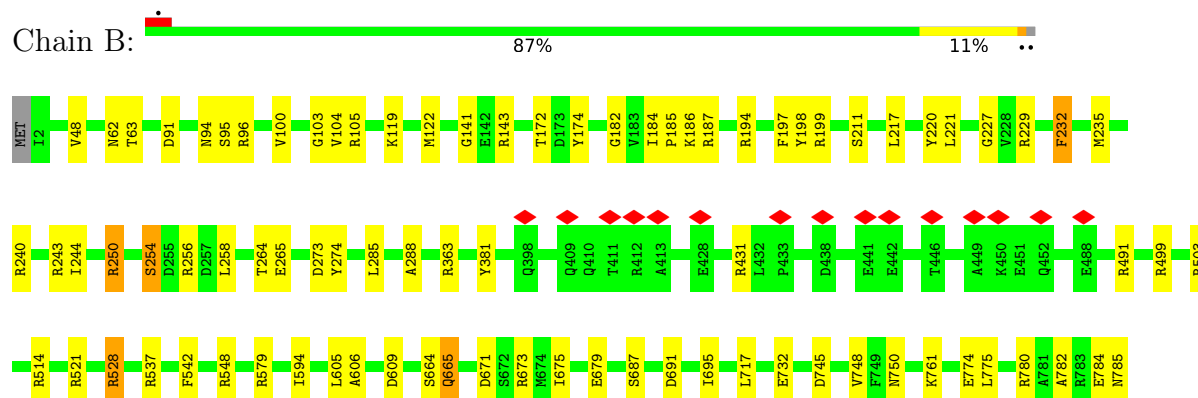
3 Residue-property plots

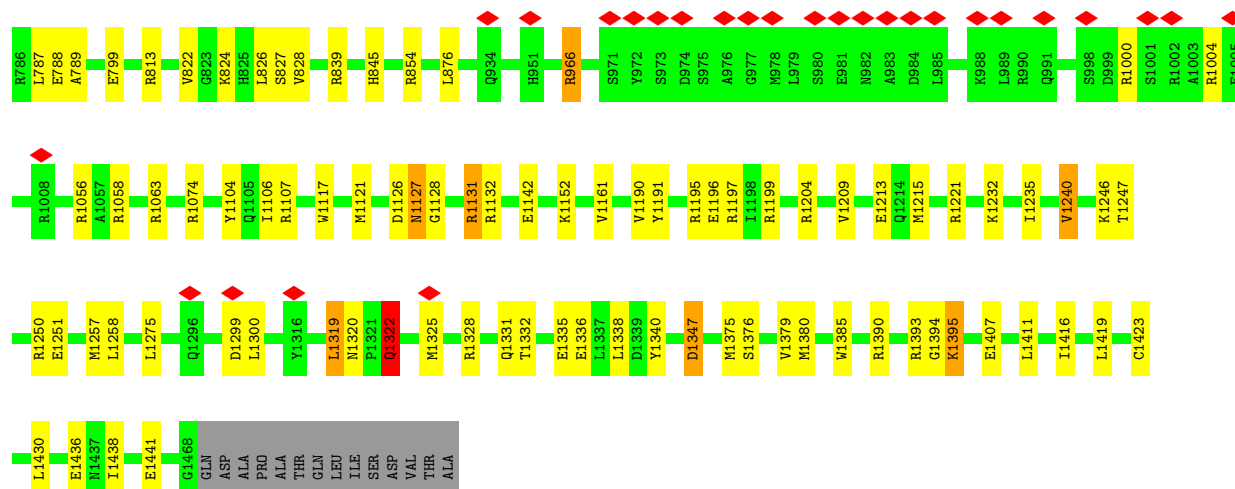
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Chromosome partition protein MukB

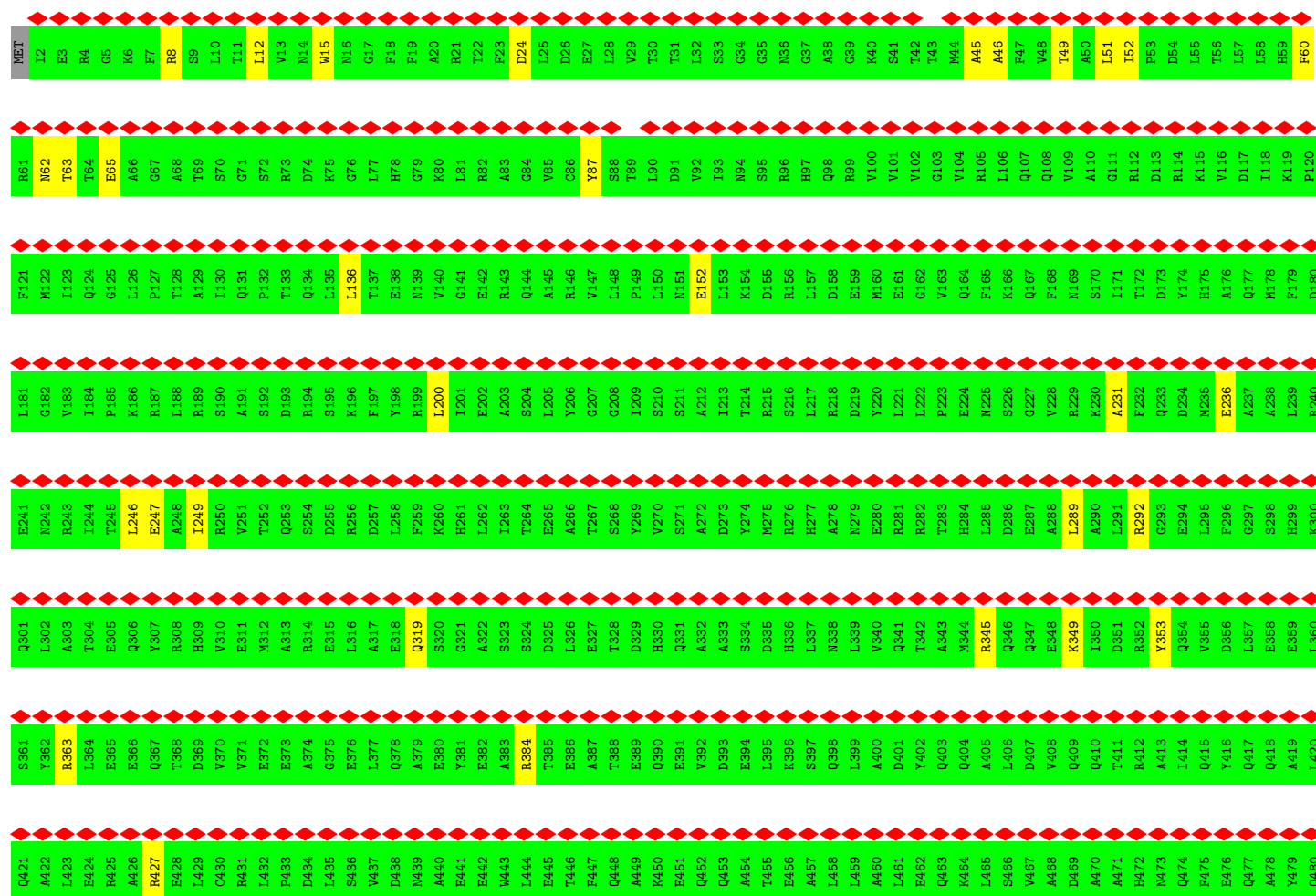
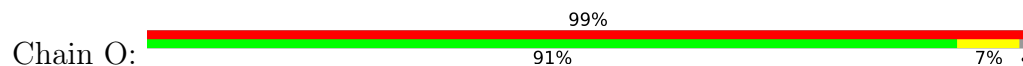


• Molecule 1: Chromosome partition protein MukB





• Molecule 1: Chromosome partition protein MukB



L481	V482	K483	N484	I485	V486	G487	E488	T489	S490	R491	S492	E493	A494	W495	Q496	S497	A498	R499	E500	L501	L502	R503	D504	W505	P506	S507	Q508	R509	H510	L511	A512	D513	R514	V515	Q516	P517	L518	R519	M520	R521	L522	S523	E524	L525	E526	Q527	R528	L529	N530	N531	Q532	Q533	A535	E536	R537	L538	L539	S540		
E541	F542	C543	K544	R545	Q546	G547	R548	Q549	Y550	Q551	A552	E553	D554	L555	E556	A557	L558	Q559	N560	E561	L562	E563	A564	R565	Q566	E567	A568	L569	S570	L571	S572	V573	L574	E575	G576	G577	E578	R579	R580	M581	L582	M583	R584	Q585	E586	L587	E588	Q589	L590	K591	Q592	K593	I594	Q595	S596	L597	T598	A599	R600	
A601	P602	V603	W604	L605	A606	A607	Q608	D609	T610	L611	N612	R613	L614	C615	E616	L617	S618	G619	E620	T621	L622	A623	S624	R625	N626	D627	V628	T629	E630	Y631	M632	Q633	Q634	L635	L636	E637	R638	E639	R640	E641	A642	T643	V644	E645	Q646	D647	E648	V649	A650	A651	G711	Q652	K653	R654	E655	L656	E657	K658	Q659	I660
E661	R662	L663	S664	Q665	P666	S667	G668	A669	E670	D671	S672	R673	M674	I675	A676	L677	A678	E679	R680	F681	G682	G683	V684	L685	L686	S687	E688	I689	Y690	D691	D692	L693	T694	I695	D696	D697	A698	P699	Y700	F701	S702	A703	L704	W705	G706	F707	A708	R709	H710	G711	I712	V713	V714	F715	D716	L717	L718	L719	V720	
R721	P722	H723	L724	E725	T726	L727	E728	D729	C730	F731	E732	D733	L734	Y735	L736	I737	E738	G739	D740	F741	L742	S743	F744	S745	D746	S747	V748	F749	N750	A751	E752	E753	Q754	T755	L756	A757	V758	L759	V760	K761	S762	S763	D764	R765	Q766	L767	R768	Y769	S770	R771	V772	F773	E774	L775	P776	L777	F778	G779	R780	
A781	A782	R783	E784	N785	R786	L787	E788	A789	L790	N791	L792	E793	R794	D795	A796	L797	A798	E799	R800	Y801	A802	T803	L804	S805	F806	D807	V808	Q809	K810	I811	Q812	R813	A814	H815	Q816	A817	F818	S819	Q820	F821	V822	G823	K824	H825	L826	S827	V828	A829	F830	D831	T832	D833	P834	E835	A836	E837	I838	R839	E840	
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E901	M902	D903	E904	A905	Q906	E907	A908	A909	R910	F911	L912	Q913	Q914	H915	G916	S917	A918	L919	T920	K921	L922	E923	P924	M925	V926	A927	V928	L929	Q930	S931	D932	P933	Q934	Q935	H936	E937	Q938	L939	Q940	Q941	D942	Y943	E944	T945	A946	K947	H948	S949	Q950	H951	Q952	A953	K954	Q955	Q956	A957	F958	A959	L960	
V961	E962	I963	V964	Q965	R966	R967	V968	H969	F970	S971	Y972	S973	D974	S975	A976	G977	M978	L979	S980	E981	N982	A983	D984	L985	N986	D987	K988	L989	R990	Q991	R992	L993	E994	H995	A996	E997	S998	D999	R1000	S1001	R1002	A1003	R1004	E1005	Q1006	L1007	R1008	Q1009	Q1010	Q1011	A1012	Q1013	Y1014	S1015	Q1016	F1017	L1018	Q1019	V1020	
L1021	A1022	S1023	L1024	K1025	S1026	S1027	Y1028	E1029	T1030	K1031	Q1032	D1033	M1034	L1035	K1036	E1037	L1038	L1039	Q1040	E1041	M1042	K1043	D1044	I1045	G1046	V1047	Q1048	A1049	D1050	A1051	N1052	A1053	E1054	M1055	R1056	A1057	L1058	E1059	R1060	L1061	D1062	R1063	L1064	H1065	E1066	A1067	L1068	S1069	V1070	N1071	L1072	S1073	R1074	V1075	N1076	Q1077	L1078	E1079	K1080	
Q1081	I1082	A1083	F1084	C1085	E1086	A1087	E1088	M1089	E1090	N1091	V1092	Q1093	K1094	K1095	L1096	R1097	K1098	L1099	E1100	R1101	D1102	Y1103	Y1104	Q1105	I1106	R1107	E1108	Q1109	V1110	V1111	S1112	A1113	K1114	A1115	G1116	W1117	C1118	A1119	V1120	M1121	R1122	M1123	V1124	K1125	D1126	N1127	G1128	V1129	E1130	R1131	R1132	L1133	H1134	R1135	R1136	E1137	L1138	A1139	Y1140	
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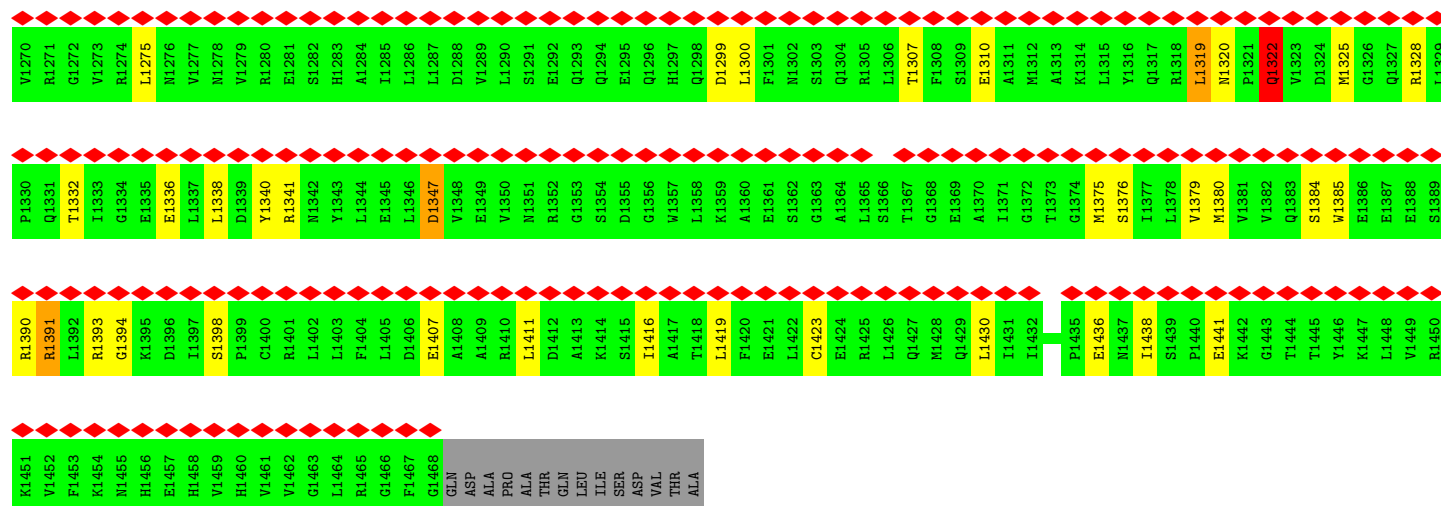
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V1381	V1382	G1383	S1384	V1385	E1386	E1387	E1388	S1389	R1390	R1391	L1392	R1393	G1394	K1395	D1396	I1397	S1398	P1399	C1400	R1401	L1402	L1403	F1404	L1405	D1406	E1407	A1408	A1409	R1410	L1411	D1412	A1413	K1414	S1415	I1416	A1417	T1418	L1419	F1420	E1421	L1422	C1423	E1424	R1425	L1426	Q1427	M1428	Q1429	L1430	I1431	I1432	A1433	A1434	P1435	E1436	N1437	I1438	S1439	P1440
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● Molecule 1: Chromosome partition protein MukB

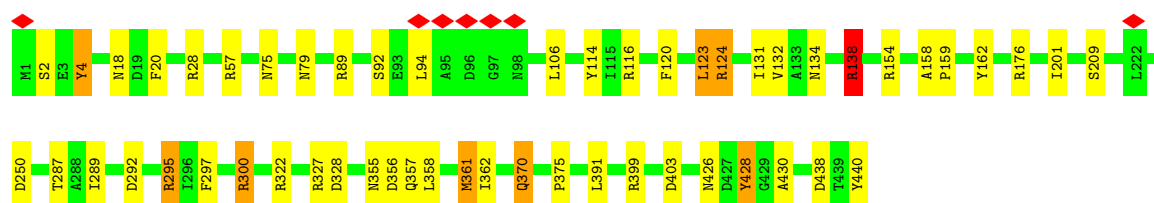
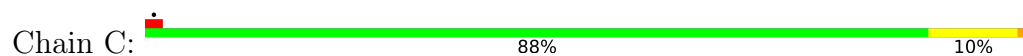


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E365	E366	Q367	T368	D369	V370	V371	E372	E373	A374	G375	E376	L377	Q378	A379	E380	Y381	E382	A383	R384	T385	E386	A387	T388	E389	Q390	E391	V392	D393	E394	L395	K396	S397	Q398	L399	A400	D401	Y402	Q403	Q404	L405	L406	D407	V408	Q409	Q410	Q411	R412	A413	T414	Q415	Y416	Q417	Q418	A419	Q420	Q421	A422	L423	E424	
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V183	I184	P185	K186	R187	L188	R189	S190	A191	S192	D193	R194	S195	K196	F197	Y198	R199	L200	L201	E202	A203	S204	L205	Y206	G207	G208	I209	S210	S211	A212	T213	T214	R215	S216	L217	R218	D219	Y220	L221	L222	P223	E224	N225	S226	G227	V228	R229	K230	A231	F232	Q233	D234	M235	E236	A237	A238	L239	R240	E241	N242	
M122	I123	Q124	G125	L126	P127	T128	A129	S130	Q131	P132	T133	Q134	L135	L136	T137	E138	N139	V140	G141	E142	R143	Q144	A145	G207	V147	L148	P149	L150	N151	E152	T153	L154	K154	D155	R156	L157	D158	E159	M160	E161	G162	V163	Q164	F165	K166	Q167	F168	N169	A170	S170	T171	T172	D173	Y174	Q177	M178	F179	D180	L181	G182
N62	T63	T64	E65	A66	G67	A68	T69	S70	G71	S72	R73	D74	K75	G76	L77	H78	G79	K80	L81	R82	A83	G84	V85	C86	S87	S88	T89	L90	D91	V92	I93	N94	S95	R96	H97	Q98	R99	V100	V101	V102	G103	V104	R105	L106	Q107	Q108	V109	A110	G111	R112	D113	R114	K115	V116	D117	I118	K119	P120	F121	
MET	I2	E3	R4	G5	K6	F7	R8	S9	L10	T11	V13	N14	W15	N16	G17	F18	F19	A20	R21	T22	F23	D24	L25	D26	E27	L28	V29	T30	T31	L32	S33	G34	G35	N36	G37	A38	G39	K40	S41	T42	T43	M44	A45	A46	F47	V48	T49	A50	L51	D54	L55	T56	L57	L58	H59	F60	R61			

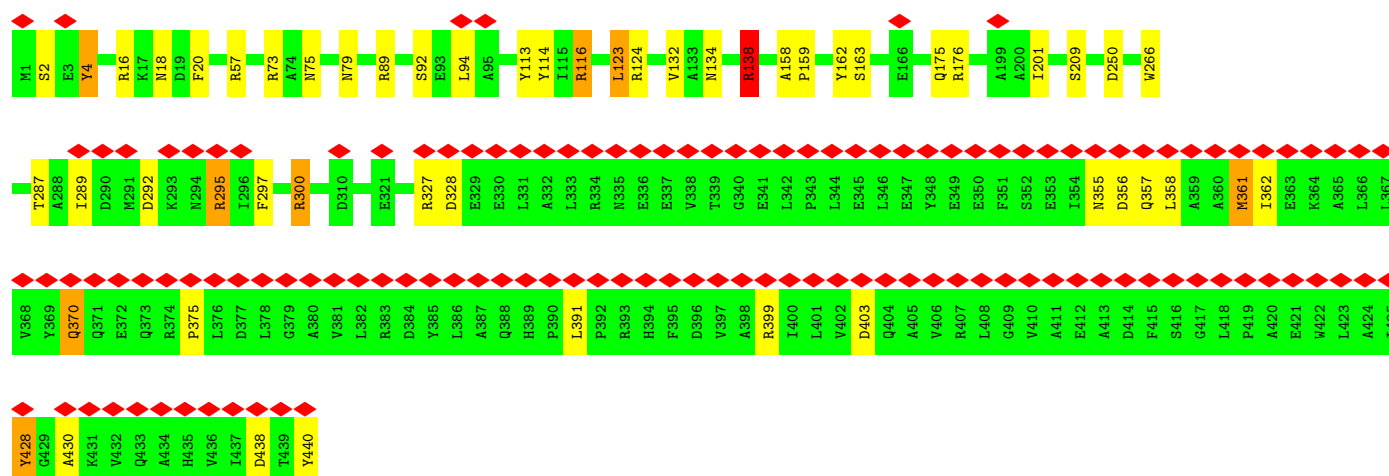
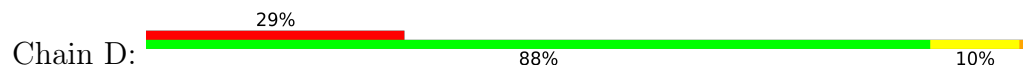
D1210	A1145	C1085	K1025	Q965	A905	H845	N785	E725	Q665	L605	R545	I485
A1211	L1146	E1086	S1026	R966	Q906	T846	R786	T726	P666	A606	Q546	V486
I1212	R1147	A1087	S1027	R967	E907	E847	E787	T728	S667	A607	G547	G487
E1213	S1148	E1088	Y1028	V968	A908	L848	E788	E728	G668	Q608	R548	E488
Q1214	M1149	M1089	E1029	H969	A909	E849	A789	D729	A669	D609	Q549	T489
M1215	S1150	E1090	T1030	F970	R910	R850	L790	C730	E870	T610	Y550	S490
E1216	D1151	N1091	K1031	S971	F911	E851	N791	F731	D671	L611	Q551	R491
I1217	K1152	V1092	Q1032	Y972	L912	V852	L792	E732	S672	N612	A552	S492
A1218	L1153	Q1093	D1033	S973	Q913	S853	E793	D733	R673	Q613	E553	E493
L1219	L1154	K1094	M1034	D974	Q914	R854	R794	L734	M674	L614	D554	A494
A1220	G1155	K1095	L1035	S975	H915	F855	D795	Y735	I675	C615	L555	W495
R1221	A1156	L1096	K1036	A976	G916	E856	A796	L736	A676	E616	E556	Q496
L1222	L1157	R1097	E1037	G977	S917	D857	L797	I737	A678	Q617	A557	S497
T1223	R1158	K1098	L1038	M978	A918	Q858	A798	E738	E678	S618	L558	A498
E1224	L1159	L1099	L1039	L979	L919	T859	E799	G739	E679	G619	Q559	R499
E1225	A1160	E1100	Q1040	S980	T920	Q860	R800	D740	R680	E620	Q560	E500
L1226	V1161	R1101	E1041	E981	K921	Q861	Y801	F741	F681	T621	E561	L501
T1227	E1165	D1102	M1042	N982	L922	Q862	A802	Q742	Q682	L622	L562	L502
A1228	H1166	Y1103	K1043	D984	E923	R863	T803	S743	G683	E563	E564	R503
R1229	L1167	Y1104	D1044	A984	P924	Q864	L804	F744	V684	S624	A564	D504
E1230	R1168	Q1105	I1045	L985	M925	Q865	S805	D745	L685	S625	R565	W505
Q1231	D1169	I1106	G1046	N986	V926	Y866	F806	D746	L686	N626	Q566	P506
L1232	R1172	R1107	V1047	D987	A927	A867	E747	S747	S687	D627	E567	Q508
A1234	E1175	E1108	Q1048	K988	V928	Q868	V808	V748	E688	V628	A568	Q509
I1235	D1176	Q1109	A1049	L989	L929	A869	Q809	F749	I689	T629	L569	R509
S1236	P1177	V1110	D1050	R990	Q930	K870	K810	N750	Y690	E630	S570	H510
T1237	R1178	S1112	M1052	Q991	D932	E871	I811	A751	D691	Y631	L571	L511
K1238	R1179	A1113	A1053	L993	P933	L873	R813	E752	I693	Q633	V573	D513
S1239	E1180	K1114	E1054	E994	Q934	T874	A814	Q754	T694	Q634	N574	R514
V1240	P1180	H1115	M1055	H995	Q935	T875	H815	T755	I695	L635	E575	V515
A1241	E1181	G1116	R1056	A996	H936	L876	Q816	N756	D696	L636	G576	Q516
I1242	R1182	W1117	A1057	E997	E937	N877	A817	A757	D697	E637	G577	P517
K1243	K1183	C1118	R1058	S998	Q938	R878	F818	V758	A698	R638	E578	L518
L1244	V1184	A1119	E1059	D999	L939	L879	S819	L759	P699	E639	R519	R519
Q1245	Q1185	V1120	R1060	R1000	Q940	I880	Q820	V760	Y700	R640	M520	M520
R1246	F1186	M1121	R1061	S1001	Q941	P881	F821	K761	F701	E641	M581	R521
T1247	F1187	R1122	D1062	R1002	D942	Q882	V822	S762	S702	A642	E582	L522
I1248	A1189	M1123	R1063	A1003	E943	V883	G823	D763	A703	T643	M583	S523
Q1249	E1190	V1124	L1064	R1004	E944	T884	K824	S764	L704	V644	R584	E524
R1250	Y1191	K1125	H1065	E1005	T945	L885	H825	R765	Y705	E645	Q585	L525
E1251	Q1192	D1126	E1066	Q1006	A946	L886	L826	Q766	G706	R646	E586	E526
Q1252	H1193	M1127	A1067	L1007	K947	L887	S827	V767	P707	D647	Q527	Q527
L1253	L1194	G1128	L1068	R1008	H948	D888	V828	R768	A708	E648	E588	R528
R1254	R1195	V1129	S1069	Q1009	S949	E889	A829	Y769	R709	V649	Q589	L529
E1196	R1197	E1130	V1070	Q1010	Q950	T890	F830	S770	A650	L590	L590	N530
T1255	R1198	R1131	M1071	Q1011	H951	L891	G711	R771	K591	A651	Q591	N531
R1256	R1199	R1132	R1072	A1012	Q952	I892	T832	V772	I712	Q652	Q592	Q532
M1257	E1200	L1133	S1073	Q1013	A953	D893	D833	F773	K593	K653	Q593	Q533
L1258	I1202	H1134	R1074	Y1014	K954	R894	P834	E774	V714	R654	I594	N534
N1259	I1203	R1135	V1075	S1015	Q955	V895	E835	L775	P715	E655	Q595	A535
Q1261	R1204	R1136	M1076	Q1016	Q956	E896	A836	P776	D716	L656	S596	E536
L1262	D1205	E1137	Q1077	F1017	A957	E897	E837	L777	L717	E657	R537	R537
Q1263	D1207	L1138	L1078	N1018	F958	V898	I838	F778	S718	K658	T598	L538
A1264	P1208	A1139	E1079	Q1019	A959	R899	R839	G779	L719	Q659	A599	L539
V1265	V1209	Y1140	K1080	V1020	L960	E900	E840	R780	I660	R600	S540	S540
L1266	E1142	M1141	Q1081	L1021	V961	E901	A781	A781	E661	P602	F542	F542
F1267	S1266	E1143	I1082	A1022	E962	N902	R842	A782	R722	R662	P602	F542
Q1268	G1144	G1143	F1084	S1023	I963	D903	Q843	R783	H723	L663	C543	K544



• Molecule 2: Chromosome partition protein MukF

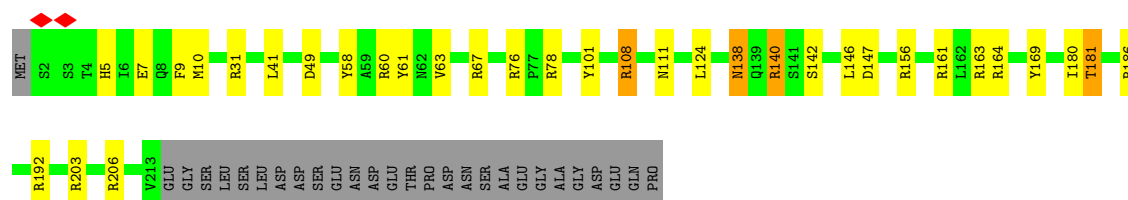


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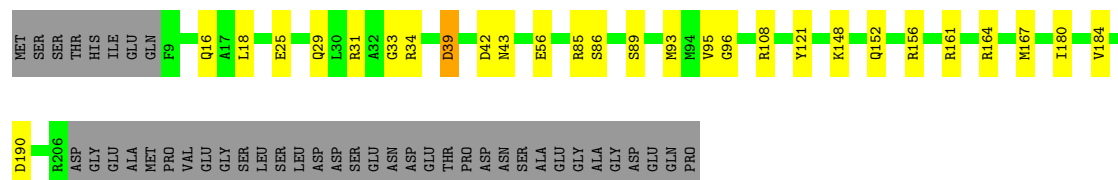


• Molecule 3: Chromosome partition protein MukE

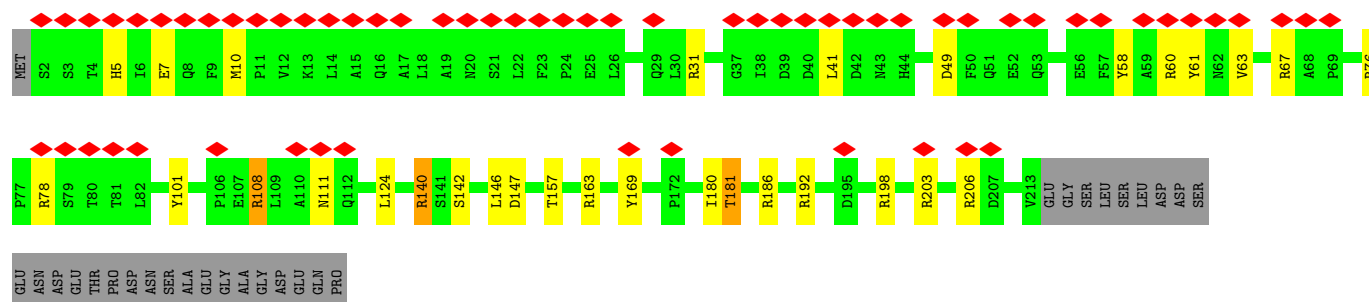
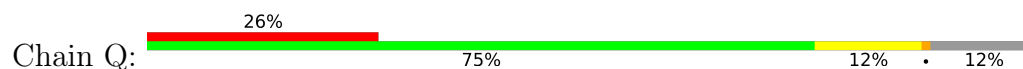




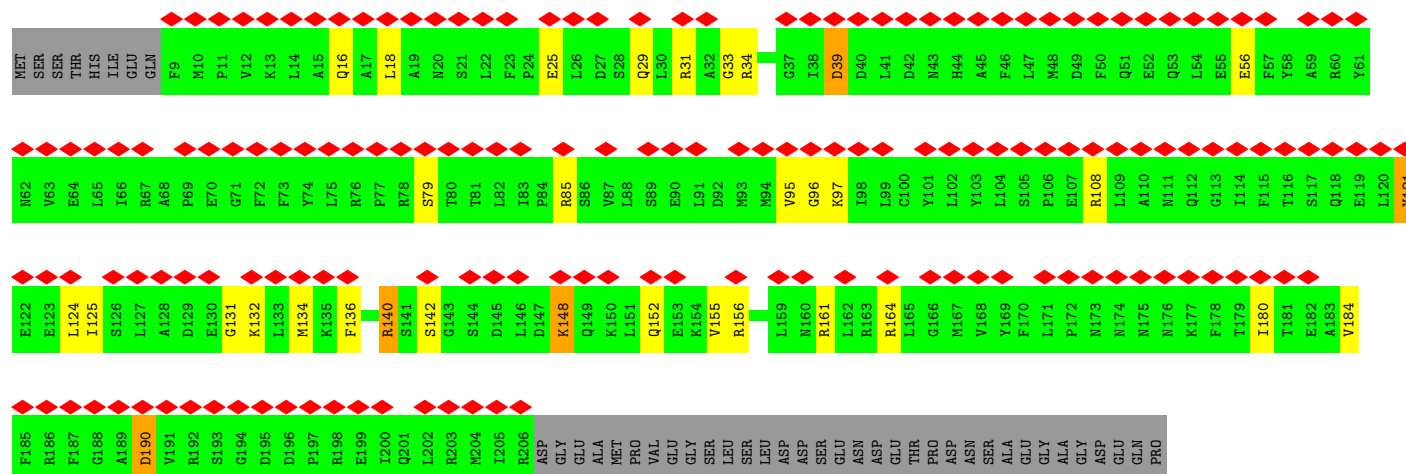
• Molecule 3: Chromosome partition protein MukE



• Molecule 3: Chromosome partition protein MukE

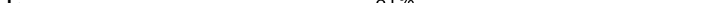


• Molecule 3: Chromosome partition protein MukE



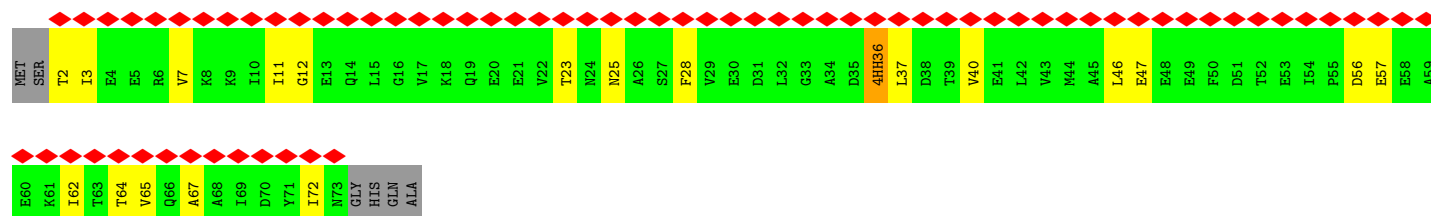
• Molecule 4: Acyl carrier protein


MET	SER	T2	T3	I11	G12	T23	N24	N25	F28	4HH36	L37	V40	L46	E47	D56	E57	I62	Te3	T64	V65	Q66	A67	I72	N73	GLY	HIS	GLN	ALA
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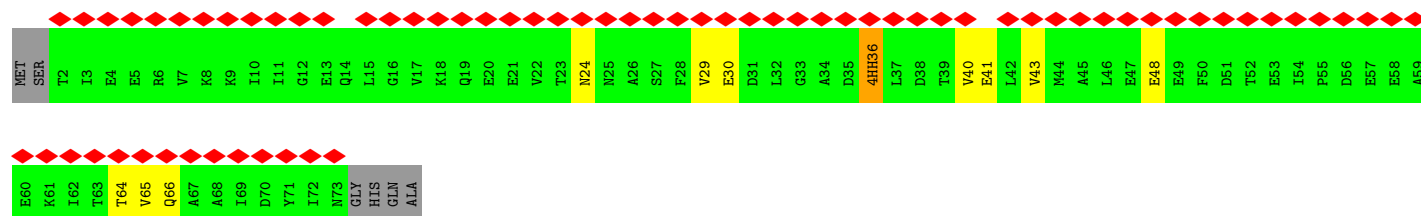
- Chain I:  81% 10% 8%



- Chain S:  92% 67% 24% 8%



- Chain M:  90% 78% 13% 8%



- Chain K: 97%





[illegible]

- Molecule 6: pFB526

Chain L:

[illegible]



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3754	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.346	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	720.7206, 720.7206, 720.7206	wwPDB
Map dimensions	166, 166, 166	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	4.34169, 4.34169, 4.34169	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4HH, MG, ATP

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	0.47	1/11999 (0.0%)	0.79	21/16166 (0.1%)
1	B	0.96	59/11999 (0.5%)	1.05	57/16166 (0.4%)
1	O	0.47	1/11999 (0.0%)	0.79	22/16166 (0.1%)
1	P	1.01	72/11999 (0.6%)	1.08	60/16166 (0.4%)
2	C	0.68	1/3592 (0.0%)	0.99	13/4862 (0.3%)
2	D	0.68	1/3592 (0.0%)	1.01	13/4862 (0.3%)
3	E	1.32	16/1753 (0.9%)	1.37	17/2361 (0.7%)
3	F	1.41	19/1648 (1.2%)	1.24	5/2218 (0.2%)
3	Q	1.32	16/1753 (0.9%)	1.36	17/2361 (0.7%)
3	R	1.42	25/1648 (1.5%)	1.26	10/2218 (0.5%)
4	G	0.25	0/558	0.42	0/754
4	I	0.25	0/558	0.41	0/754
4	M	0.25	0/558	0.41	0/754
4	S	0.25	0/558	0.42	0/754
5	K	1.61	1/1680 (0.1%)	2.66	199/2589 (7.7%)
6	L	1.59	3/1676 (0.2%)	2.55	174/2586 (6.7%)
All	All	0.89	215/67570 (0.3%)	1.13	608/91737 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	O	0	3
1	P	0	3
2	C	0	6
2	D	0	6
3	E	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	Q	0	2
5	K	0	19
6	L	0	17
All	All	0	65

The worst 5 of 215 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	295	ARG	C-N	-13.11	1.03	1.34
2	D	295	ARG	C-N	-13.07	1.03	1.34
1	A	589	GLN	C-N	7.64	1.51	1.34
1	O	589	GLN	C-N	7.60	1.51	1.34
3	R	85	ARG	CZ-NH2	-7.48	1.23	1.33

The worst 5 of 608 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	187	ARG	NE-CZ-NH2	11.30	125.95	120.30
6	L	29	DA	N1-C6-N6	-11.16	111.90	118.60
2	C	295	ARG	C-N-CA	10.48	147.90	121.70
2	D	295	ARG	C-N-CA	10.43	147.77	121.70
5	K	46	DA	N1-C6-N6	-10.34	112.39	118.60

There are no chirality outliers.

5 of 65 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1058	ARG	Sidechain
1	A	966	ARG	Sidechain
1	A	967	ARG	Sidechain
1	B	528	ARG	Sidechain
1	B	966	ARG	Sidechain

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	11840	11707	11705	58	0
1	B	11840	11706	11705	82	0
1	O	11840	11707	11705	61	0
1	P	11840	11706	11705	90	0
2	C	3531	3451	3450	69	0
2	D	3531	3451	3450	69	0
3	E	1722	1719	1718	12	0
3	F	1619	1627	1626	13	0
3	Q	1722	1719	1718	13	0
3	R	1619	1627	1626	12	0
4	G	583	564	563	24	0
4	I	583	564	563	8	0
4	M	583	564	563	9	0
4	S	583	564	563	26	0
5	K	1496	815	816	13	0
6	L	1497	823	822	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	A	31	12	12	0	0
8	B	31	12	12	0	0
8	O	31	12	12	0	0
8	P	31	12	12	0	0
All	All	66557	64362	64346	455	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 3.

The worst 5 of 455 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:C:158:ALA:HB1	2:D:123:LEU:HG	1.19	1.18
2:C:162:TYR:HB3	2:D:124:ARG:HG3	1.23	1.15
2:C:158:ALA:CB	2:D:123:LEU:HG	1.82	1.10
2:C:131:ILE:HD11	2:D:163:SER:OG	1.56	1.06
4:S:36:4HH:CL3	4:S:40:VAL:HG21	1.87	1.05

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100	100
1	B	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
1	O	1465/1482 (99%)	1423 (97%)	42 (3%)	0	100	100
1	P	1465/1482 (99%)	1413 (96%)	52 (4%)	0	100	100
2	C	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
2	D	438/440 (100%)	426 (97%)	12 (3%)	0	100	100
3	E	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
3	F	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
3	Q	210/240 (88%)	206 (98%)	4 (2%)	0	100	100
3	R	196/240 (82%)	191 (97%)	5 (3%)	0	100	100
4	G	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
4	I	69/78 (88%)	67 (97%)	2 (3%)	0	100	100
4	M	69/78 (88%)	66 (96%)	3 (4%)	0	100	100
4	S	69/78 (88%)	68 (99%)	1 (1%)	0	100	100
All	All	7824/8080 (97%)	7587 (97%)	237 (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	1269/1281 (99%)	1260 (99%)	9 (1%)	81	87
1	B	1269/1281 (99%)	1257 (99%)	12 (1%)	75	83
1	O	1269/1281 (99%)	1260 (99%)	9 (1%)	81	87
1	P	1269/1281 (99%)	1257 (99%)	12 (1%)	75	83
2	C	376/376 (100%)	364 (97%)	12 (3%)	34	53
2	D	376/376 (100%)	364 (97%)	12 (3%)	34	53
3	E	189/212 (89%)	185 (98%)	4 (2%)	48	66
3	F	177/212 (84%)	174 (98%)	3 (2%)	56	72
3	Q	189/212 (89%)	186 (98%)	3 (2%)	58	73
3	R	177/212 (84%)	174 (98%)	3 (2%)	56	72
4	G	62/66 (94%)	62 (100%)	0	100	100
4	I	62/66 (94%)	62 (100%)	0	100	100
4	M	62/66 (94%)	62 (100%)	0	100	100
4	S	62/66 (94%)	62 (100%)	0	100	100
All	All	6808/6988 (97%)	6729 (99%)	79 (1%)	66	78

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	1060	ARG
1	P	1322	GLN
1	O	1165	GLU
1	P	673	ARG
3	Q	181	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	111	ASN
3	Q	111	ASN
2	C	198	GLN
2	D	75	ASN
2	D	134	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	4HH	S	36	4	21,26,27	0.45	0	27,35,37	3.13	4 (14%)
4	4HH	I	36	4	21,26,27	0.46	0	27,35,37	1.72	3 (11%)
4	4HH	G	36	4	21,26,27	0.45	0	27,35,37	3.13	4 (14%)
4	4HH	M	36	4	21,26,27	0.47	0	27,35,37	1.73	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	4HH	S	36	4	-	5/32/35/37	-
4	4HH	I	36	4	-	6/32/35/37	-
4	4HH	G	36	4	-	5/32/35/37	-
4	4HH	M	36	4	-	6/32/35/37	-

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	36	4HH	O1P-P-OG	11.65	161.86	107.75
4	S	36	4HH	O1P-P-OG	11.64	161.82	107.75
4	S	36	4HH	OG-P-O2P	-8.87	74.39	109.07
4	G	36	4HH	OG-P-O2P	-8.86	74.46	109.07
4	G	36	4HH	P-OG-CB	6.13	157.62	121.68

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	36	4HH	N-CA-CB-OG
4	I	36	4HH	CB-OG-P-O1P
4	M	36	4HH	N-CA-CB-OG
4	M	36	4HH	CB-OG-P-O1P
4	G	36	4HH	CJ-O3P-P-OG

There are no ring outliers.

4 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	36	4HH	16	0
4	I	36	4HH	1	0
4	G	36	4HH	15	0
4	M	36	4HH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
8	ATP	O	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)
8	ATP	A	1502	7	26,33,33	0.61	0	31,52,52	1.13	3 (9%)
8	ATP	B	1502	7	26,33,33	0.63	0	31,52,52	1.12	3 (9%)
8	ATP	P	1502	7	26,33,33	0.63	0	31,52,52	1.12	3 (9%)

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
8	ATP	O	1502	7	-	1/18/38/38	0/3/3/3
8	ATP	A	1502	7	-	1/18/38/38	0/3/3/3
8	ATP	B	1502	7	-	2/18/38/38	0/3/3/3
8	ATP	P	1502	7	-	2/18/38/38	0/3/3/3

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(°)
8	P	1502	ATP	C5-C6-N6	2.39	123.99	120.35
8	B	1502	ATP	C5-C6-N6	2.37	123.96	120.35
8	A	1502	ATP	C5-C6-N6	2.35	123.92	120.35
8	A	1502	ATP	O2'-C2'-C3'	-2.32	104.30	111.82
8	O	1502	ATP	O2'-C2'-C3'	-2.31	104.36	111.82

There are no chirality outliers.

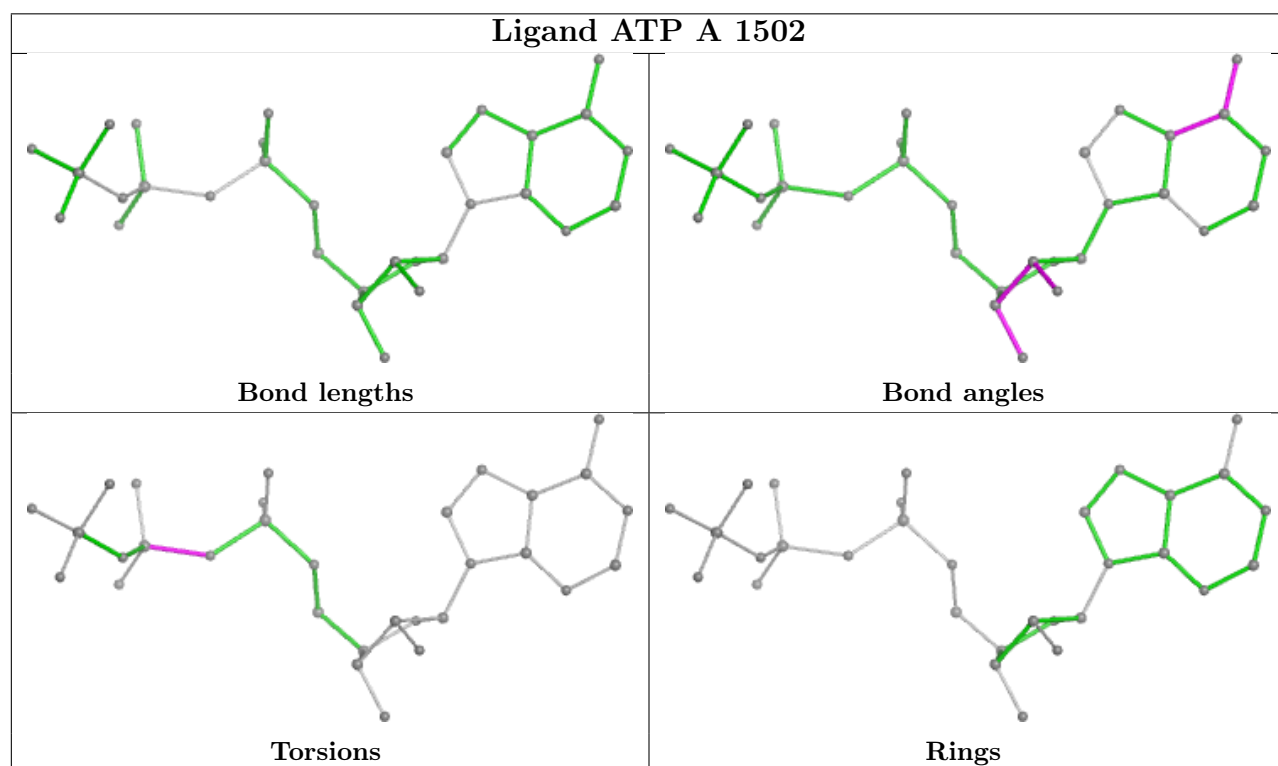
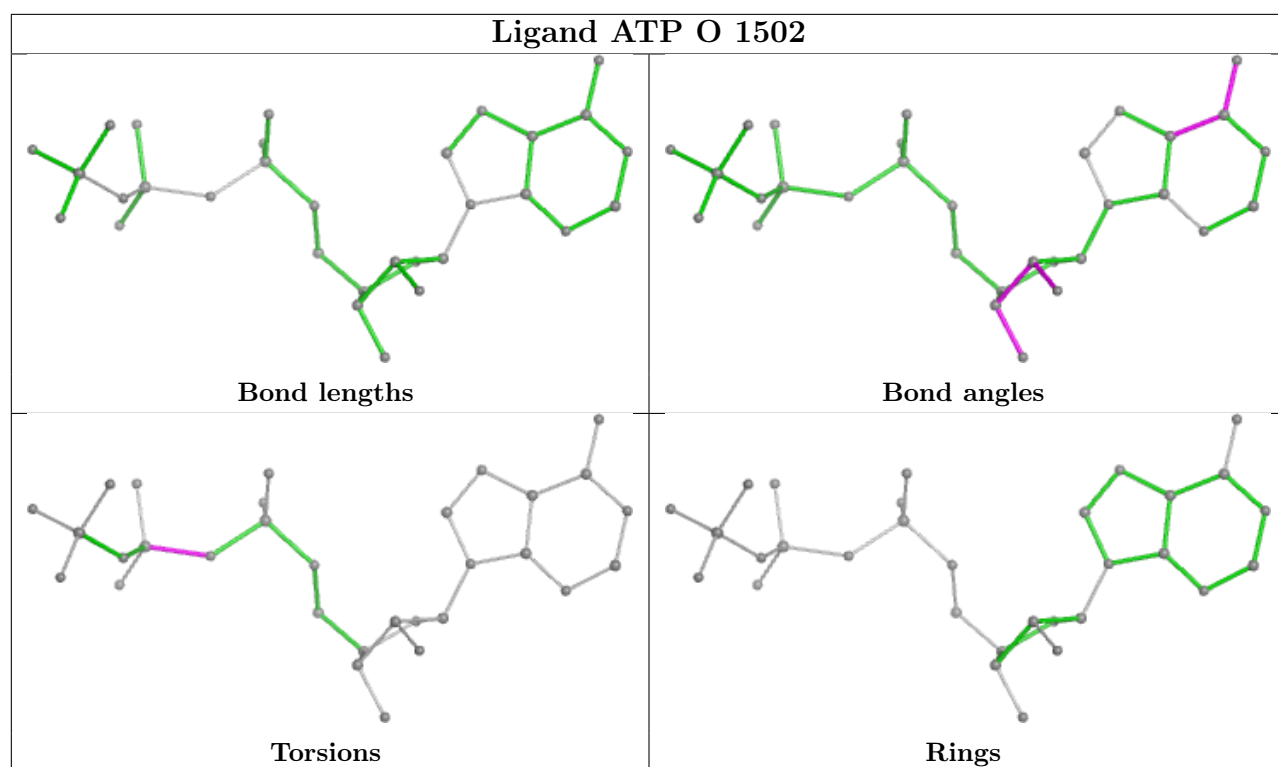
5 of 6 torsion outliers are listed below:

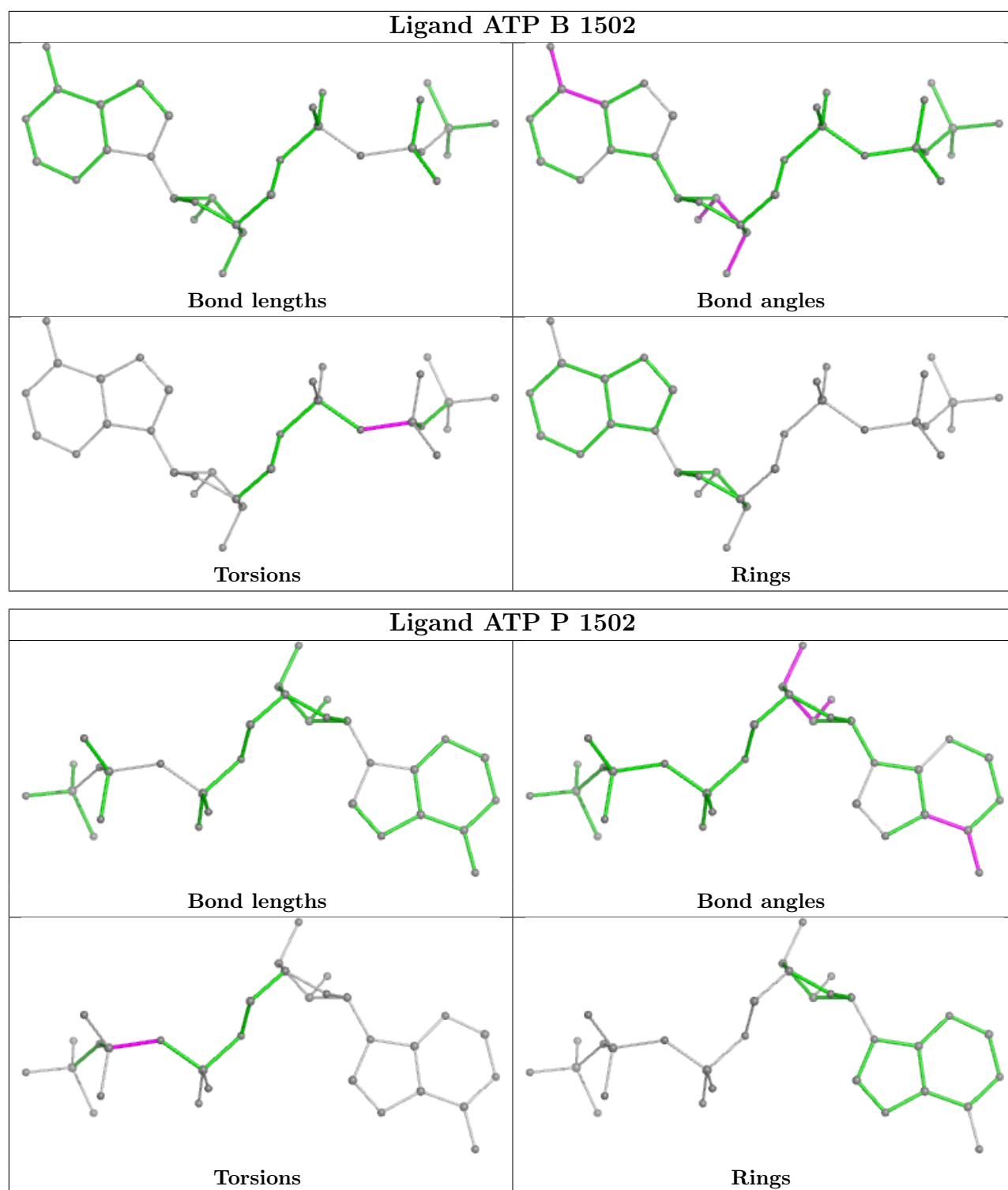
Mol	Chain	Res	Type	Atoms
8	A	1502	ATP	PA-O3A-PB-O2B
8	O	1502	ATP	PA-O3A-PB-O2B
8	B	1502	ATP	PA-O3A-PB-O1B
8	B	1502	ATP	PA-O3A-PB-O2B
8	P	1502	ATP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	295:ARG	C	296:ILE	N	1.04
1	C	295:ARG	C	296:ILE	N	1.03

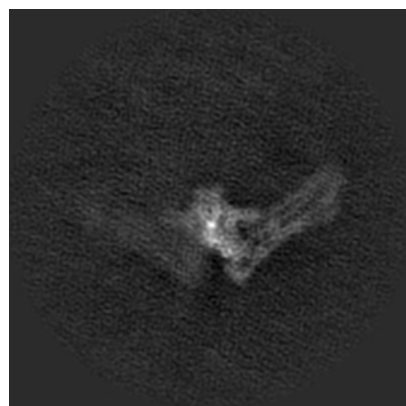
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-51446. These allow visual inspection of the internal detail of the map and identification of artifacts.

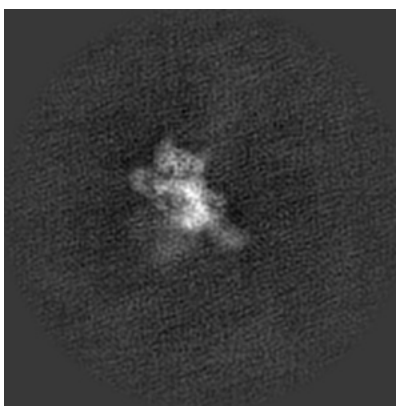
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

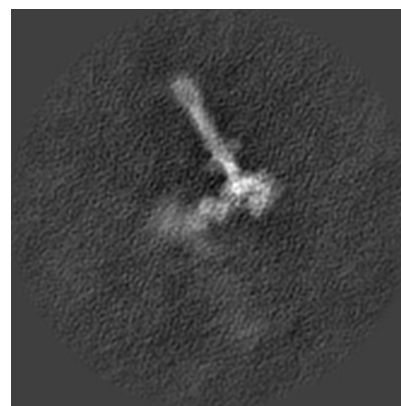
6.1.1 Primary map



X

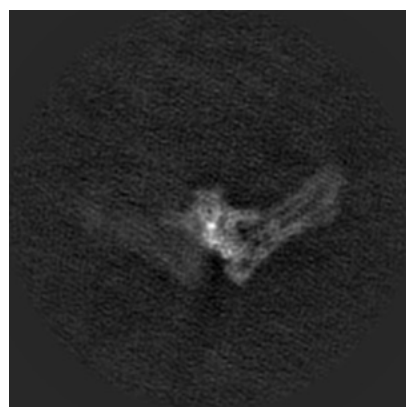


Y

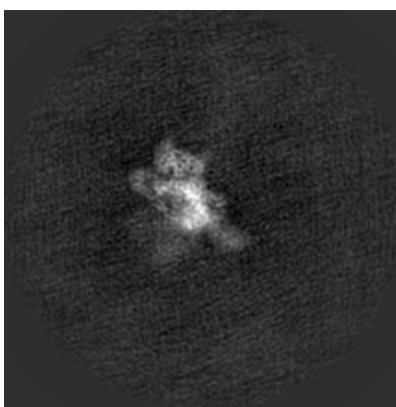


Z

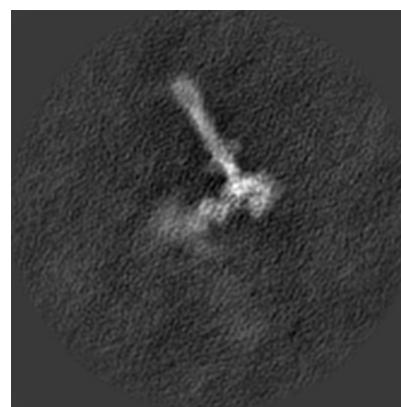
6.1.2 Raw map



X



Y

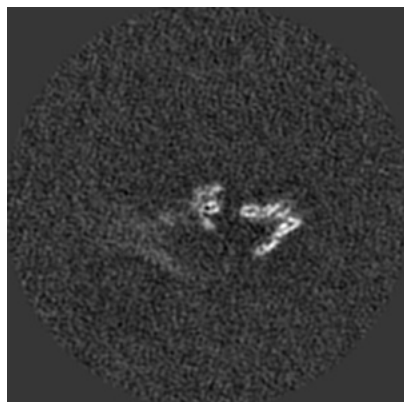


Z

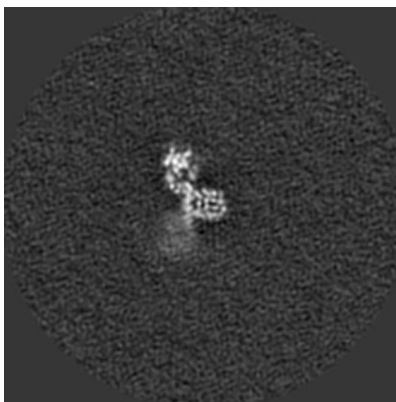
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

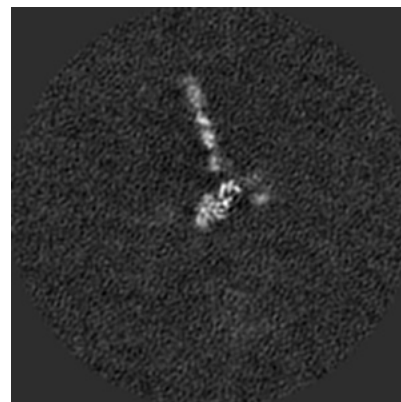
6.2.1 Primary map



X Index: 83

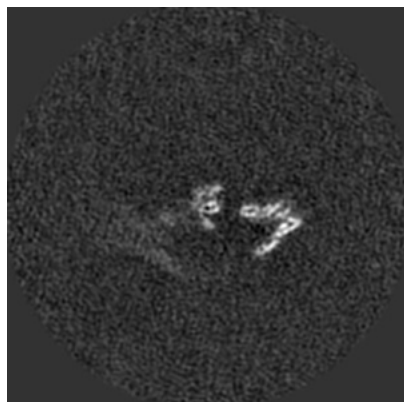


Y Index: 83

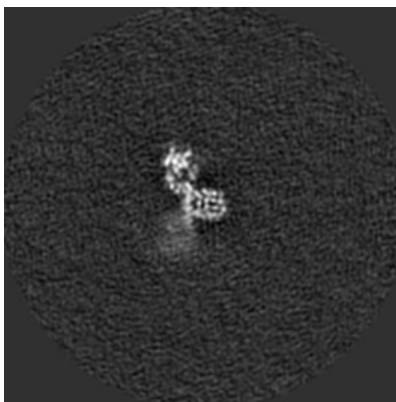


Z Index: 83

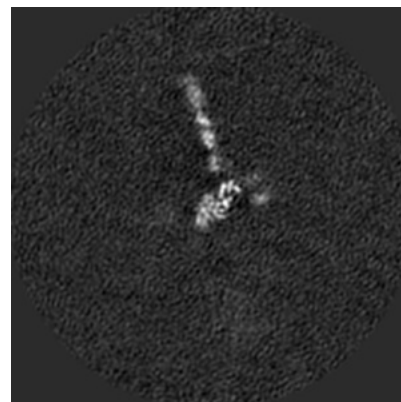
6.2.2 Raw map



X Index: 83



Y Index: 83

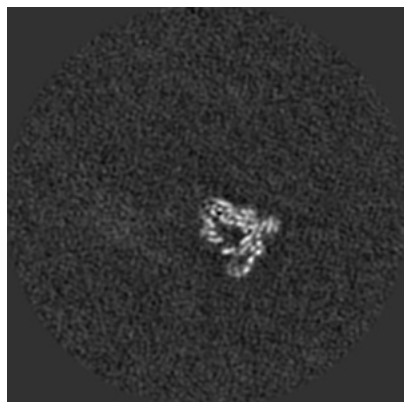


Z Index: 83

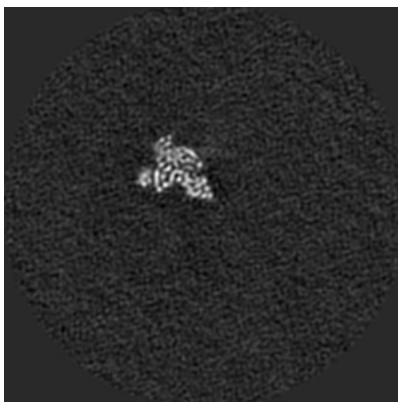
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

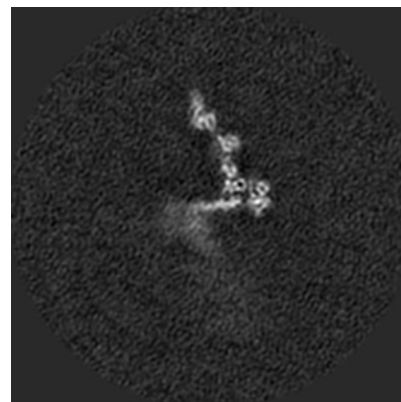
6.3.1 Primary map



X Index: 90

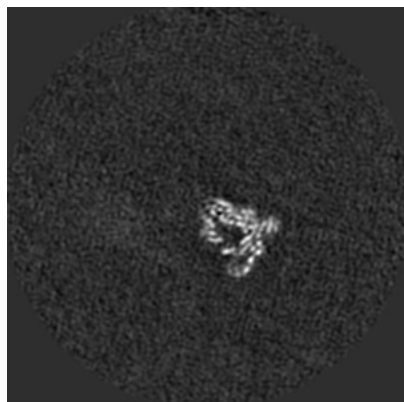


Y Index: 90

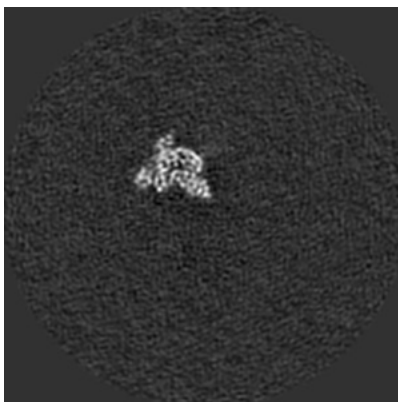


Z Index: 76

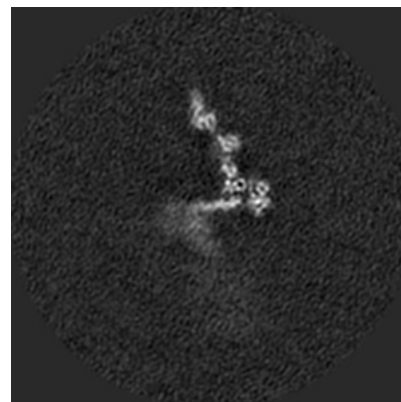
6.3.2 Raw map



X Index: 90



Y Index: 91

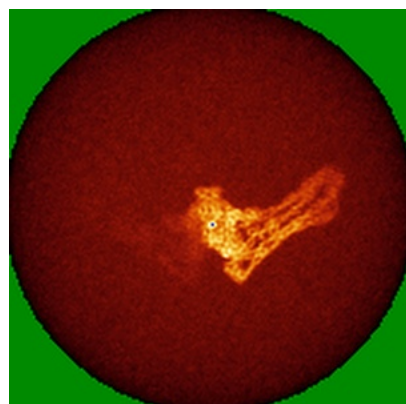


Z Index: 76

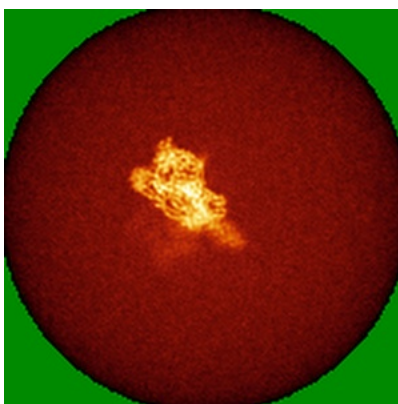
The images above show the largest variance slices of the map in three orthogonal directions.

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

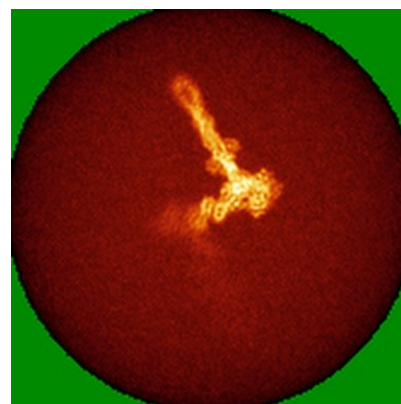
6.4.1 Primary map



X

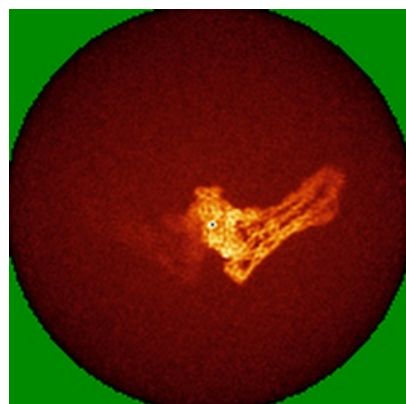


Y

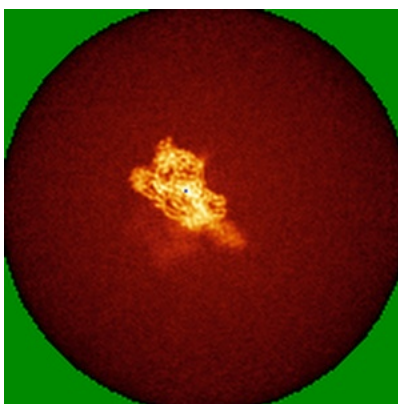


Z

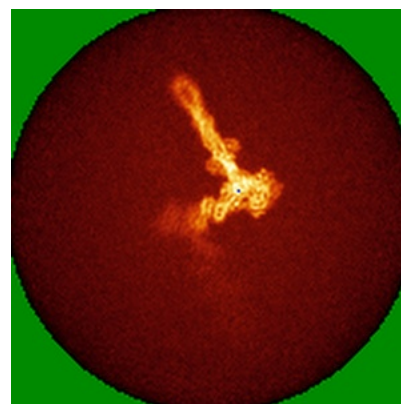
6.4.2 Raw map



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.

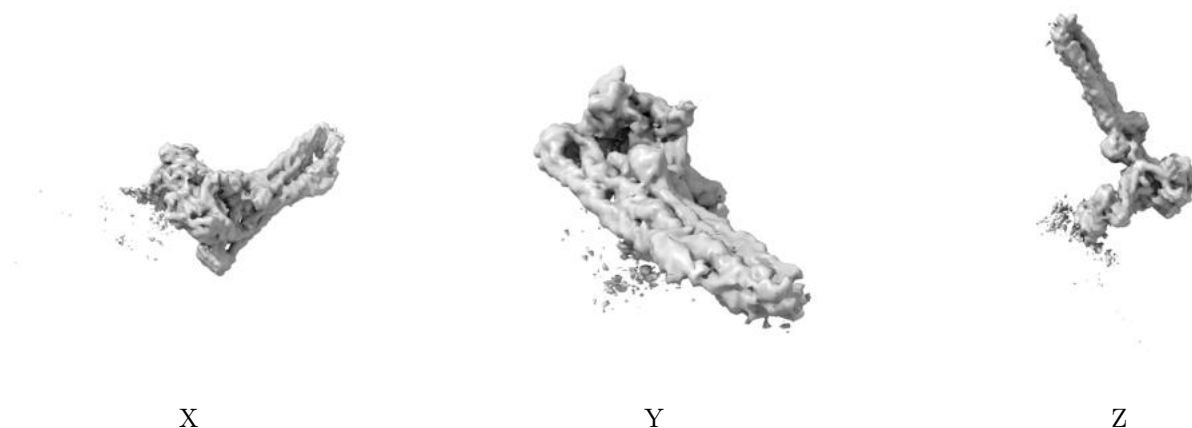
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

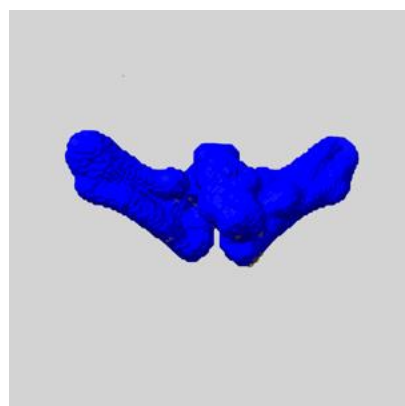
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

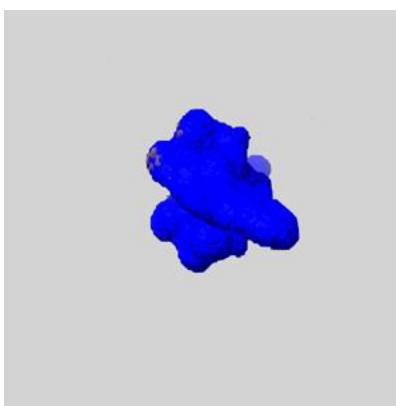
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

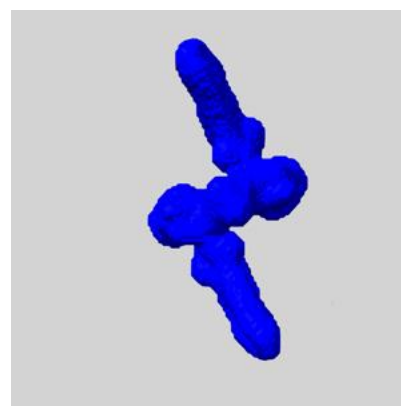
6.6.1 emd_51446_msk_1.map [i](#)



X



Y

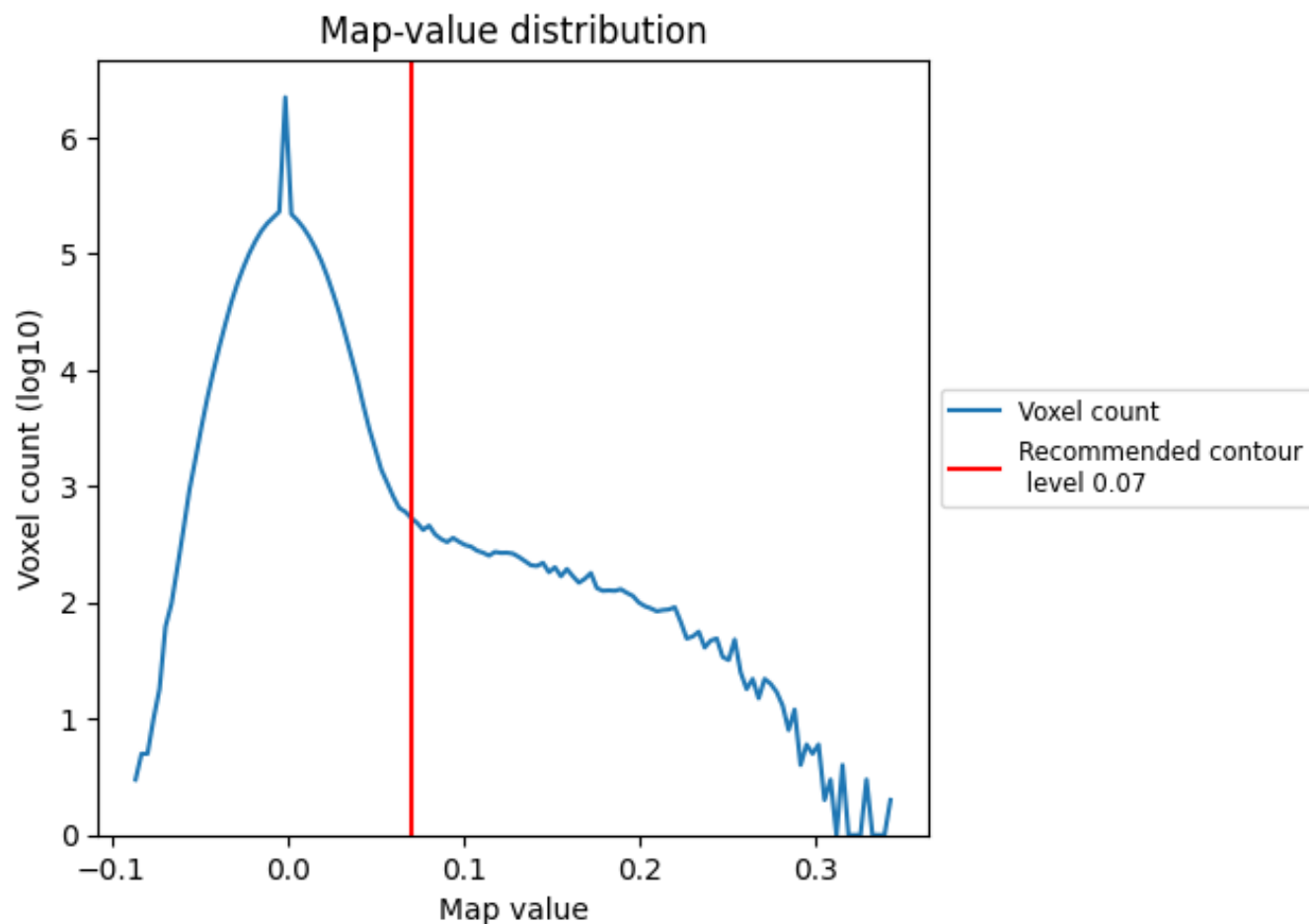


Z

7 Map analysis [i](#)

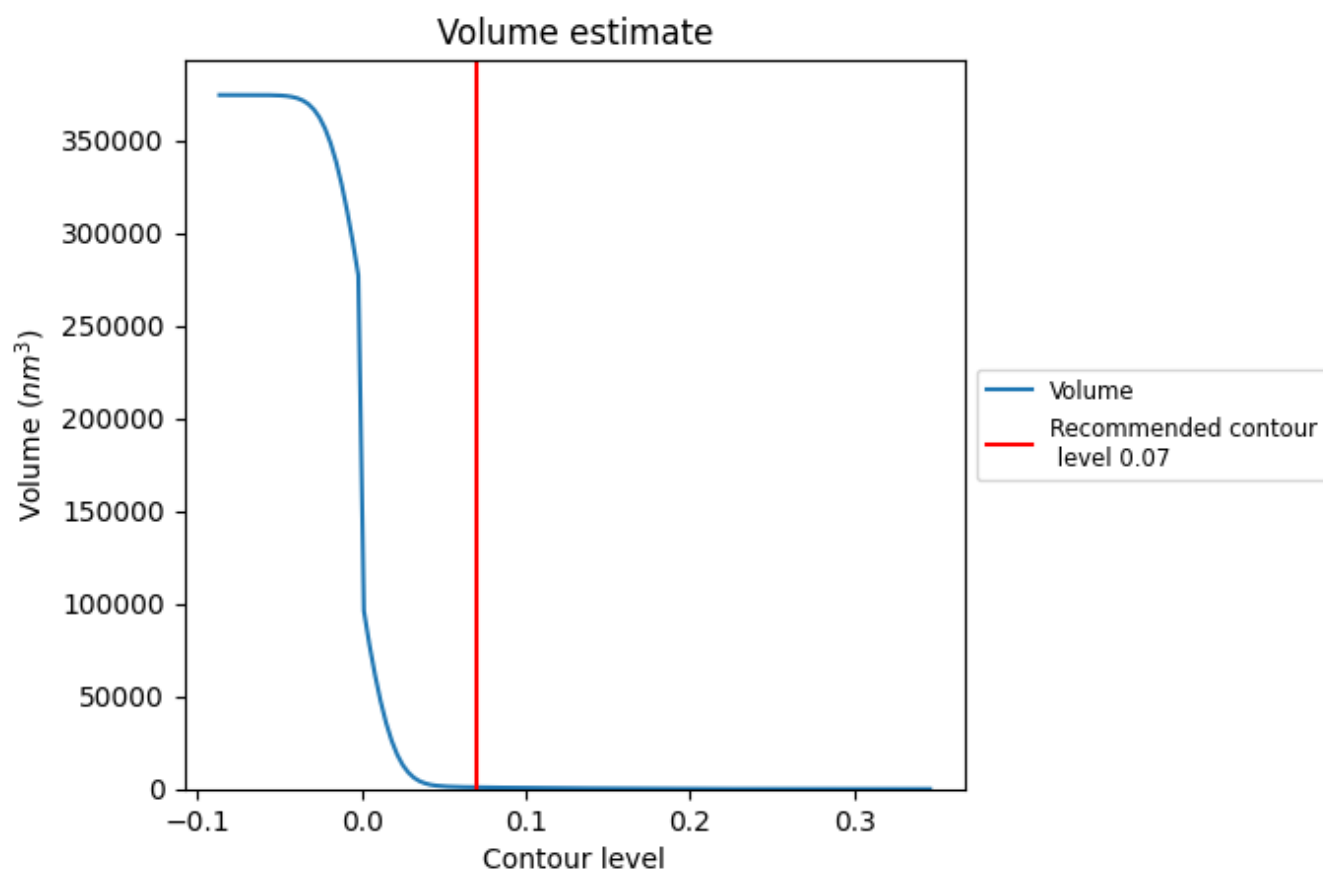
This section contains the results of statistical analysis of the map.

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.

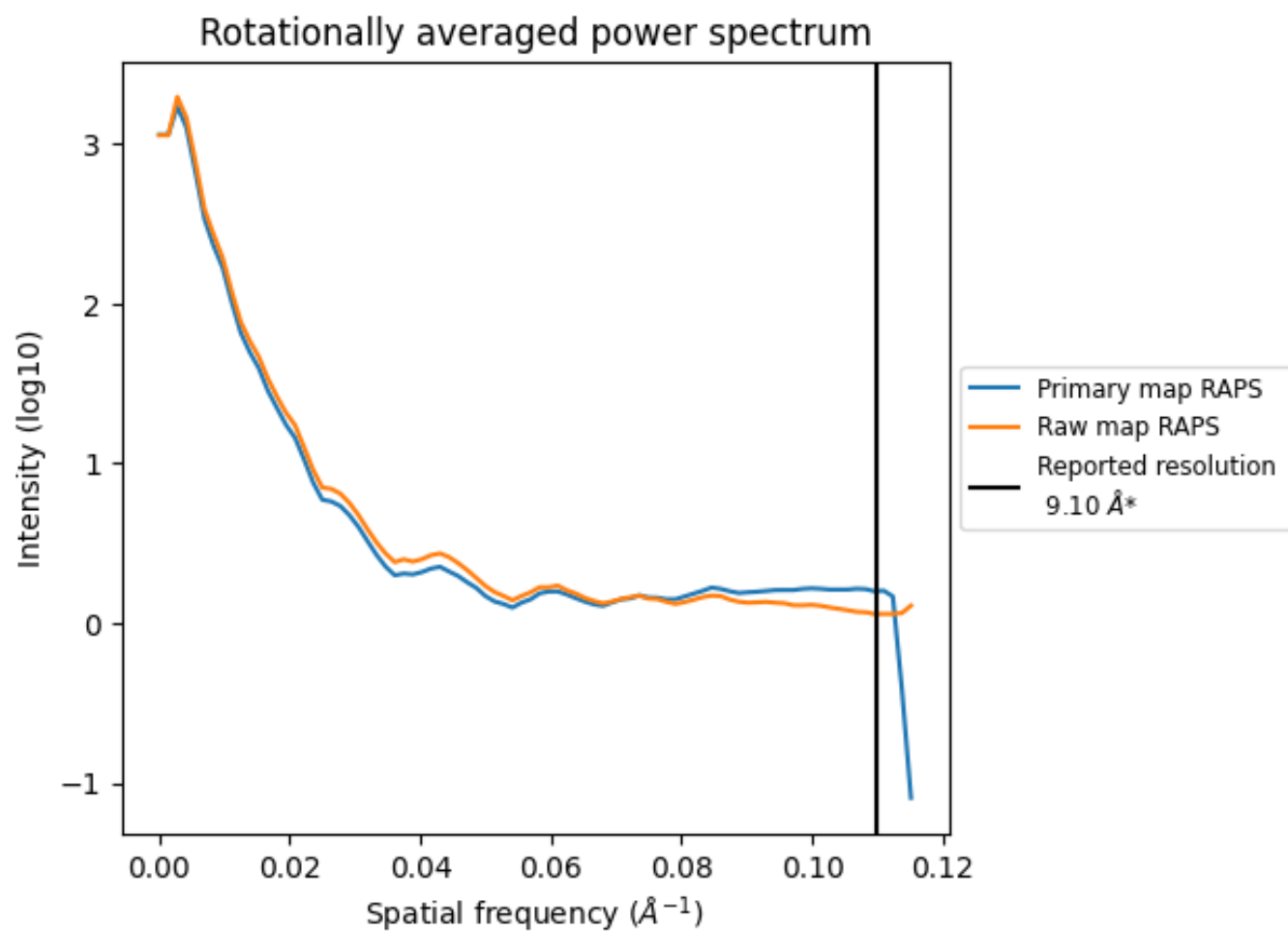
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 892 nm^3 ; this corresponds to an approximate mass of 806 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 [i](#)

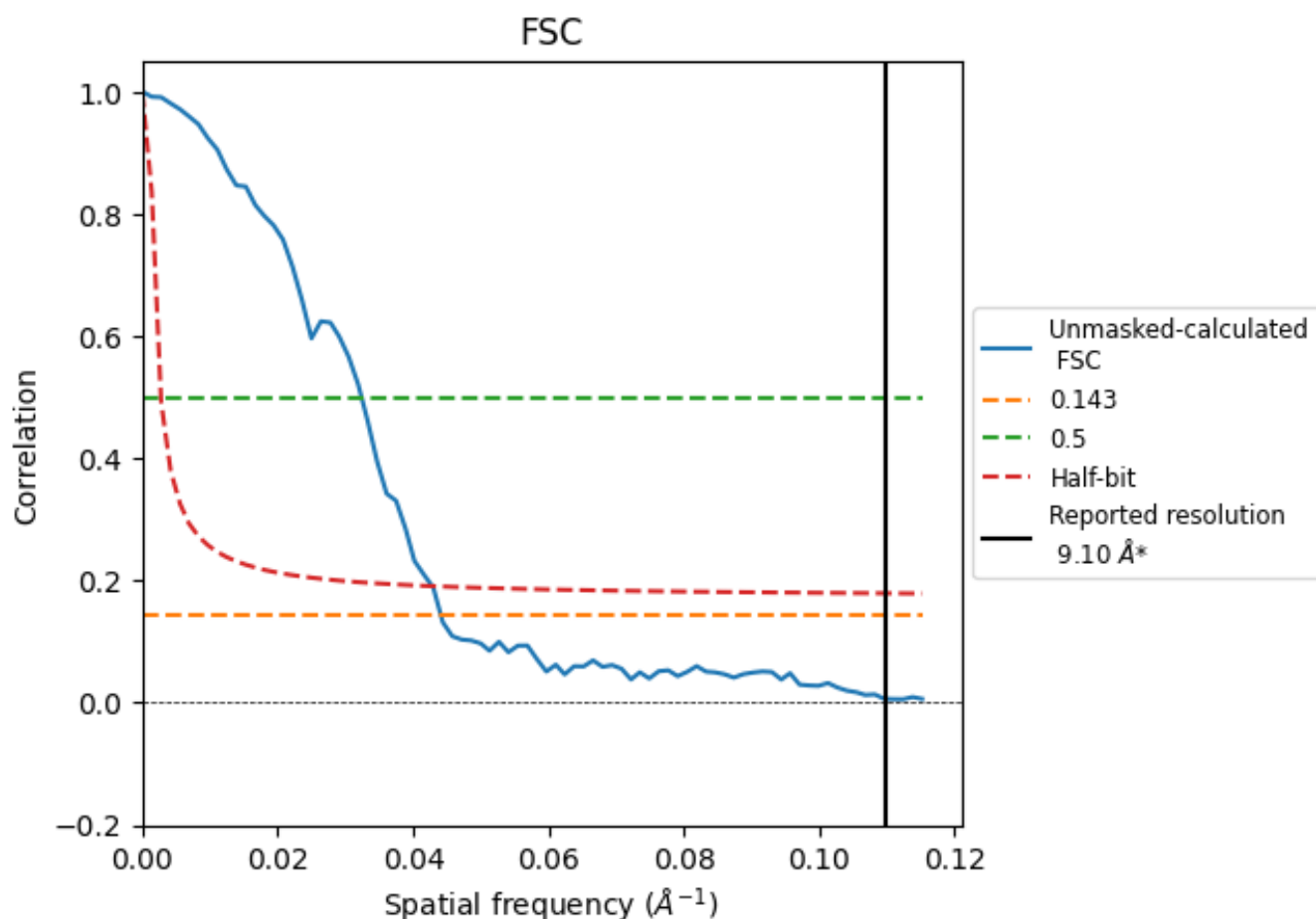


*Reported resolution corresponds to spatial frequency of 0.110 \AA^{-1}

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 0.110 Å⁻¹

8.2 Resolution estimates [i](#)

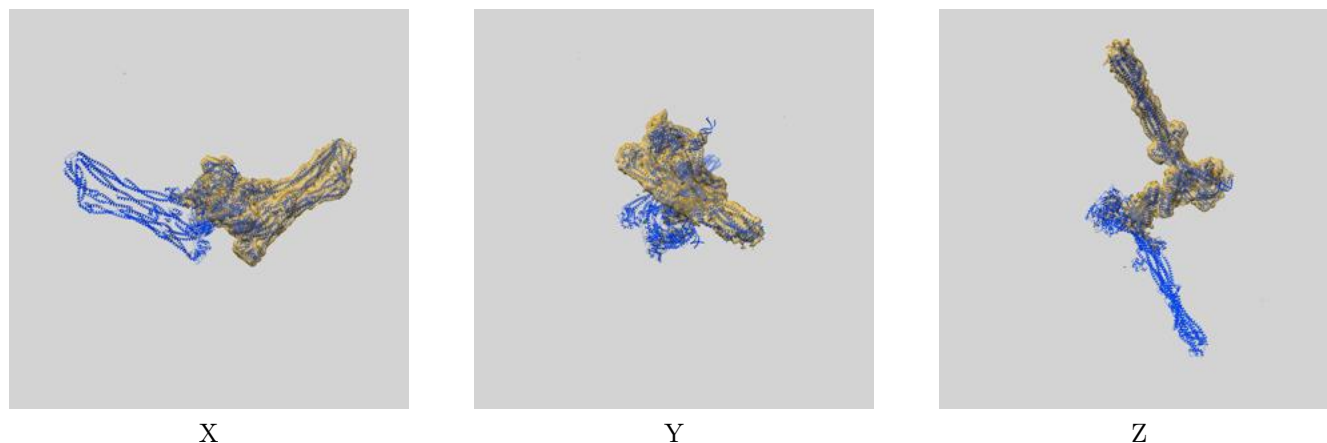
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	22.68	30.86	23.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 22.68 differs from the reported value 9.1 by more than 10 %

9 Map-model fit [i](#)

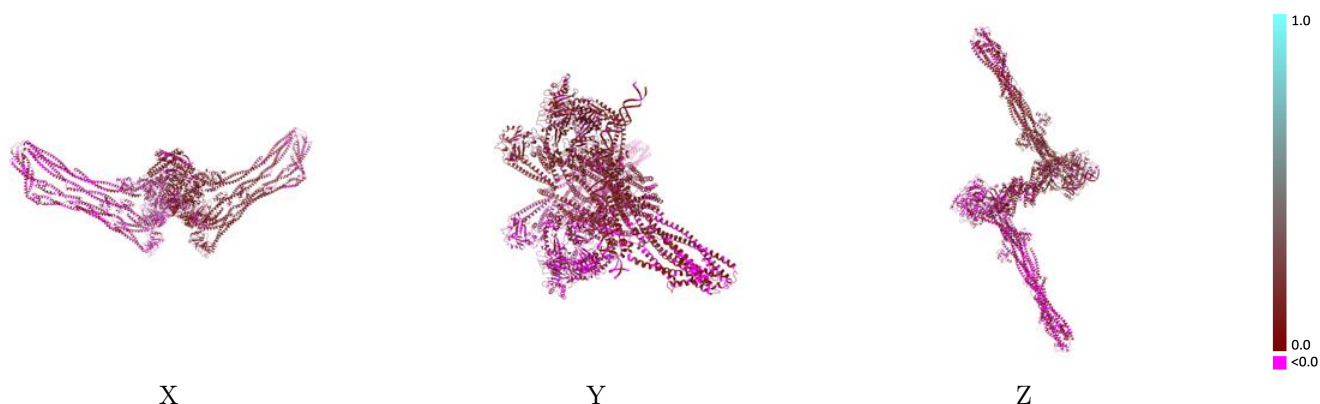
This section contains information regarding the fit between EMDB map EMD-51446 and PDB model 9GMA. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

9.1 Map-model overlay [i](#)



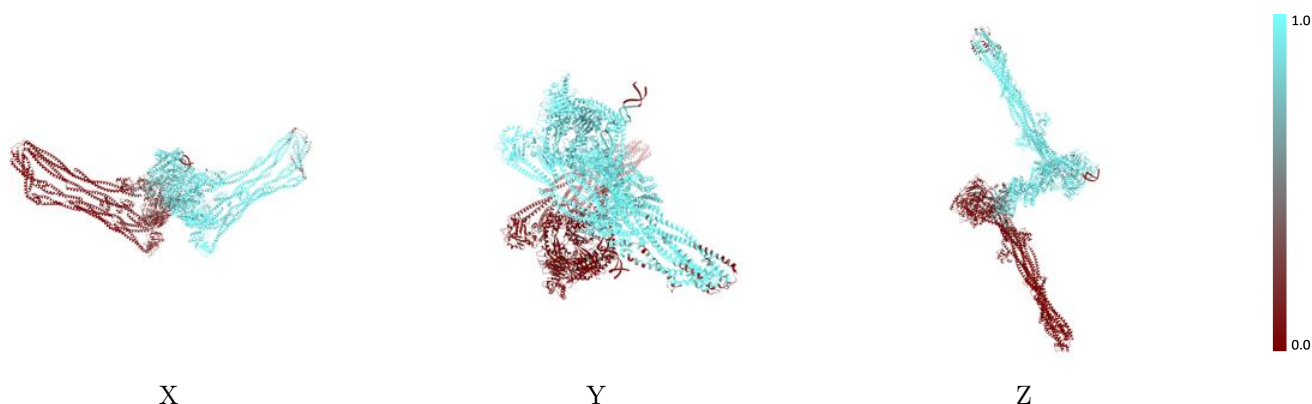
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



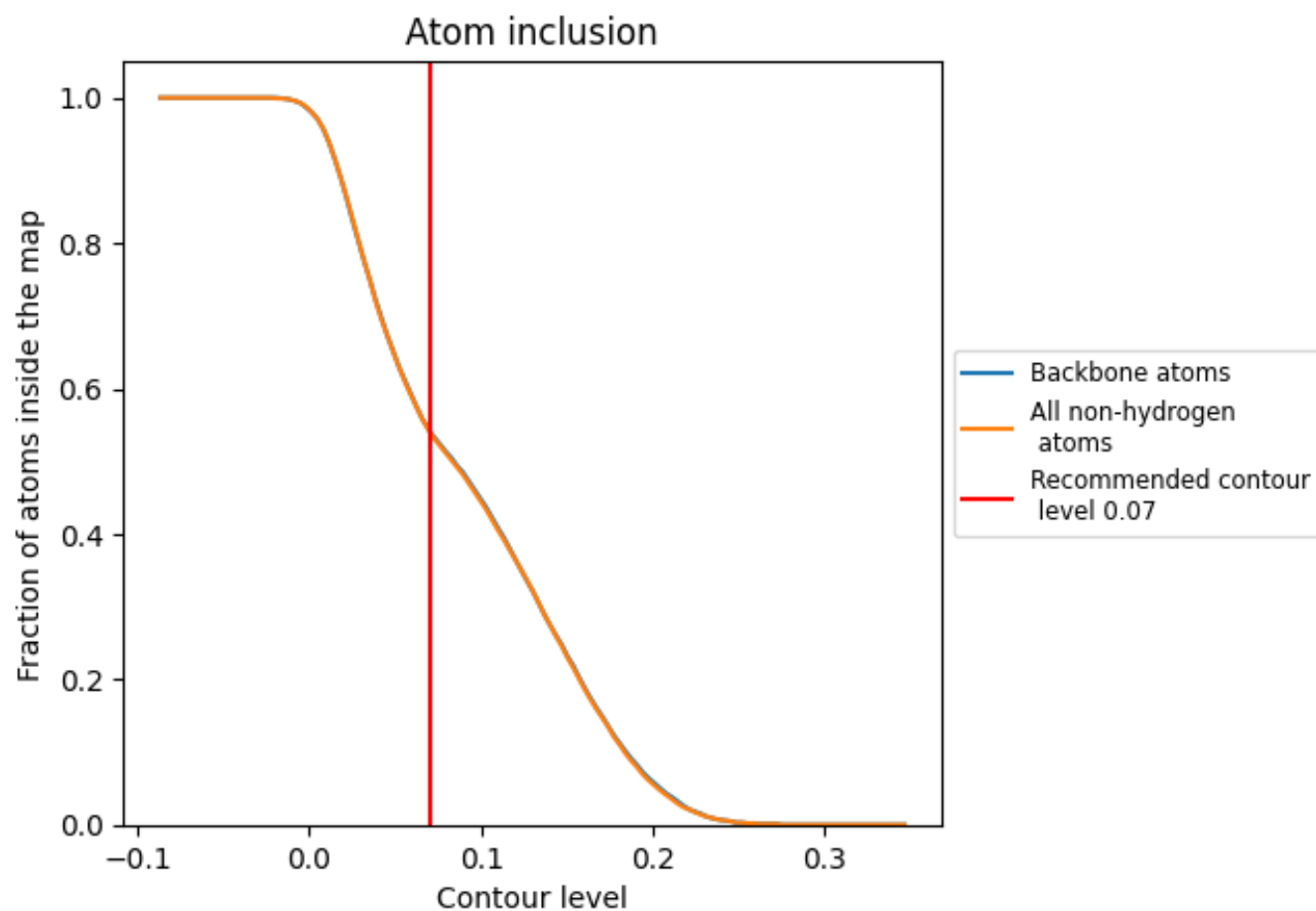
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 54% of all backbone atoms, 54% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5410	<div></div> 0.0750
A	<div></div> 0.9440	<div></div> 0.1220
B	<div></div> 0.9390	<div></div> 0.1190
C	<div></div> 0.9450	<div></div> 0.1200
D	<div></div> 0.6710	<div></div> 0.0760
E	<div></div> 0.9470	<div></div> 0.1300
F	<div></div> 0.9570	<div></div> 0.1330
G	<div></div> 0.9830	<div></div> 0.1350
I	<div></div> 0.9640	<div></div> 0.1490
K	<div></div> 0.6510	<div></div> 0.1010
L	<div></div> 0.6390	<div></div> 0.0990
M	<div></div> 0.0360	<div></div> 0.0260
O	<div></div> 0.0050	<div></div> 0.0160
P	<div></div> 0.0350	<div></div> 0.0200
Q	<div></div> 0.6600	<div></div> 0.0450
R	<div></div> 0.1760	<div></div> 0.0320
S	<div></div> 0.0000	<div></div> 0.0030

1.0

0.0

<0.0