



## wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 06:40 PM UTC

PDB ID : 8DGF / pdb\_00008dgf  
EMDB ID : EMD-27422  
Title : Avs4 bound to phage PhiV-1 portal  
Authors : Wilkinson, M.E.; Gao, L.; Strecker, J.; Makarova, K.S.; Macrae, R.K.; Koonin, E.V.; Zhang, F.  
Deposited on : 2022-06-23  
Resolution : 2.90 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

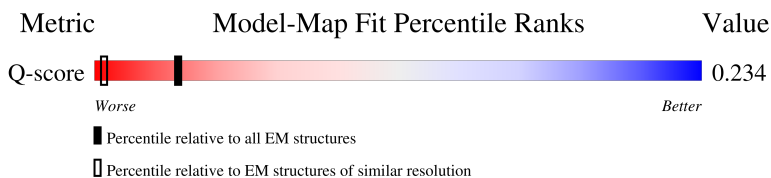
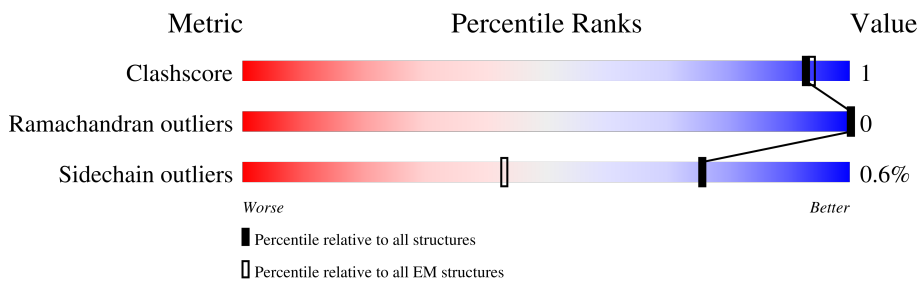
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 i

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	13054 ( 2.40 - 3.40 )

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  $\geq 3$ , 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	1587	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">66%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 66%, orange 66%, yellow 94%, green 94%, grey 94%);"></div> <div style="text-align: center;">94%</div> </div>
1	B	1587	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">69%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 69%, orange 69%, yellow 93%, green 93%, grey 93%);"></div> <div style="text-align: center;">93%</div> </div>
1	C	1587	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">66%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 66%, orange 66%, yellow 94%, green 94%, grey 94%);"></div> <div style="text-align: center;">94%</div> </div>
1	D	1587	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">69%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 69%, orange 69%, yellow 94%, green 94%, grey 94%);"></div> <div style="text-align: center;">94%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	535	82% 76% 5% 18%
2	F	535	82% 75% 7% 18%
2	G	535	82% 79% • 18%
2	H	535	82% 75% 7% • 18%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 64958 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 ATP-binding protein Avs4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1541	12805	8291	2104	2370	40	0	0
1	B	1534	12756	8265	2094	2358	39	0	0
1	C	1541	12805	8291	2104	2370	40	0	0
1	D	1534	12756	8265	2094	2358	39	0	0

- Molecule 2 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	438	3427	2165	565	678	19	0	0
2	F	438	3427	2165	565	678	19	0	0
2	G	438	3427	2165	565	678	19	0	0
2	H	438	3427	2165	565	678	19	0	0

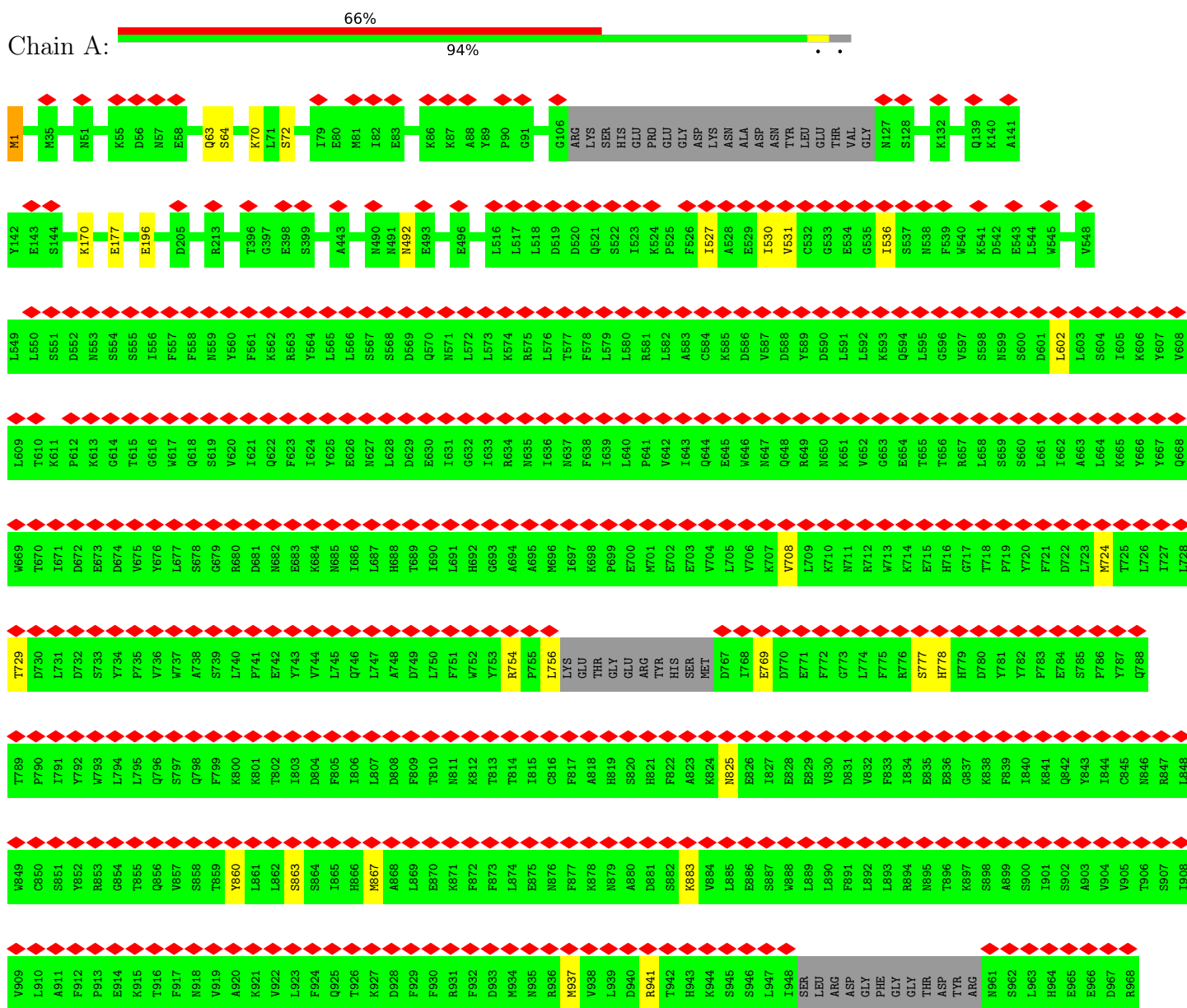
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



### 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: ATP-binding protein Avs4





G1138	N1078	Q1018	ASP	S898	K838	H778	T718	L658	S598	N538	K311	D130	GLY
N1139	S1079	L1019	TYR	A899	F839	H779	P719	S659	N699	F539	K321	ASW	ASN
I1140	E1080	P1020	ARG	S900	I840	D780	Y720	S660	S600	W540	W322	SER	ASN
P1141	H1081	D1021		I901	K841	Y781	F721	L661	D601	K541	N331	P131	D130
A1142	M1082	E1022		S902	Q842	Y782	D722	I662	L602	E542	Y332	K132	P131
D1143	K1083	A1023		A903	Y843	F783	L723	A663	S604	E543	L333	I133	K132
V1144	Y1084	Q1024		V904	I844	E784	W724	L664	I605	W545	A334	K134	I133
C1145	V1085	E1025		V905	C945	S785	T725	K665	I606	V546	D335	I135	K134
S1146	T1086	E1026		T906	M846	P786	L726	Y666	K606	A547	L336	E136	I135
V1147	L1087	E1027		S907	R847	Y787	I727	Y667	Y607	V548	N337	V137	E136
L1148	K1088	A1028		I908	L848	Q788	L728	Q667	V608	V549	Y338	V137	E136
L1149	L1089	D1029		V909	W849	Q789	T729	W669	L609	L549	A339	D138	Q139
L1150	W1090	K1030		L910	C850	P790	D730	I670	T610	S551	F340	Q139	Q139
D1151	A1091	T1031		A911	S851	I791	L731	T671	K611	D552	I341	K140	K140
Y1152	S1092	M1032		F912	Y852	Y792	D732	D672	P612	N553	D342	A141	A141
F1153	Y1093	R1033		P913	R853	W793	S733	E673	K613	S554	I343	Y142	Y142
M1154	K1094	L1034		V914	C854	L794	Y734	D674	G614	S555	Y344	Y143	Y143
Q1155	R1095	C1035		K915	T855	L795	P735	V675	T615	I556	K345	S144	S144
L1156	E1096	L1036		T916	Q856	Q796	V736	Y676	G616	F557	I346	G145	G145
N1157	K1097	A1037		F917	W857	S797	W737	L677	W617	F558	T347	I146	I146
D1158	D1098	M1038		N918	S858	Q798	A738	S678	Q618	N559	E357	H171	H171
E1159	E1099	M1039		T919	T859	F799	S739	G679	S619	Y560	E363	N176	N176
R1160	R1100	D1040		A920	W860	K600	L740	R680	V620	F561	E363	N176	N176
R1161	Y1101	R1041		K921	L861	K601	P741	D681	I621	K562	D366	D205	D205
E1162	K1102	R1042		V922	S863	T862	E742	N682	Q622	R563	D366	D205	D205
K1163	N1103	K1043		L923	S864	D804	V744	K684	I624	Y564	T396	R213	R213
C1164	Y1104	M1044		F924	S864	D804	V744	K684	I624	Y564	T396	R213	R213
K1165	G1105	K1045		Q925	I865	F905	L745	N685	Y625	L565	G397	H214	H214
L1166	M1106	I1046		T926	H866	I806	Q746	I866	E626	L566	E398	H214	H214
I1167	Y1107	T1047		K927	K867	L807	L747	L687	N627	S567	M492	L219	L219
E1168	E1108	T1048		D928	A868	D808	A748	H688	L628	S568	M492	L219	L219
L1169	D1109	K1049		F929	L869	F909	D749	T889	D629	D569	E500	H220	H220
A1170	N1110	E1050		F930	E870	T810	L750	I690	E630	Q570	E500	H220	H220
Y1171	P1111	E1051		R931	K871	N811	F751	I691	E630	N571	E500	H220	H220
Q1172	Q1112	D1052		F932	F872	K612	W752	H692	G632	L572	R515	L223	L223
K1173	I1113	E1053		D933	F873	T613	Y753	G693	I633	L573	L516	L223	L223
L1174	A1114	G1054		A934	L874	T614	R754	A694	R634	K574	L516	L223	L223
P1175	L1115	I1055		N935	E875	I615	P755	A695	N635	R575	L518	K226	K226
L1176	Q1116	E1056		R936	W876	C816	L756	M696	I636	L576	D520	K227	K227
K1177	E1117	I1057		N937	F877	F817	L756	I697	N637	T577	D520	K227	K227
E1178	T1118	S1058		V938	K878	A818	GLU	K698	N637	F578	Q521	K244	K244
G1179	K1119	F1059		L939	N879	H819	THR	P699	I639	L579	S522	E248	E248
Y1180	E1120	M1060		D940	A880	S820	GLY	E700	L640	L580	S522	E248	E248
N1181	I1121	P1061		R941	D881	H821	ARG	N701	P641	I523	K524	Q252	Q252
Y1182	I1122	E1062		T942	S882	F822	TYR	N702	L582	R581	F525	Y253	Y253
Q1183	K1123	I1063		H943	K883	A823	HIS	E703	I643	A583	F526	D287	D287
V1184	K1124	D1064		K944	W884	K824	MET	V704	Q644	C584	I527	E288	E288
Q1185	L1125	P1065		S945	L885	N825	D767	L705	E645	K855	A528	E288	E288
D1186	M1126	Q1006		S946	E886	E826	I768	V706	E645	D586	E529	L289	L289
G1187	E1127	V1007		S947	E887	I827	E769	K707	W646	V587	I530	R290	R290
T1188	E1128	L1067		I948	W888	E828	D770	V708	N647	D588	V531	K291	K291
T1189	G1129	K1068		W889	L889	E829	D770	L709	Q648	D588	V531	K291	K291
S1190	E1130	Q1069	SER	L890	L890	E829	E771	L709	R649	D590	C532	L302	L302
A1191	S1071	I1070	LEU	L890	W830	E829	F772	K710	R650	D590	C532	L302	L302
D1192	E1072	S1071	ARG	F891	D831	E829	G773	N711	K651	D590	C532	L302	L302
S1193	E1073	E1073	GLY	L892	W832	E829	L774	R712	V652	D590	C532	L302	L302
A1194	F1133	E1073	PHE	L893	F833	E829	F775	R713	G653	D590	C532	L302	L302
L1195	E1074	K1014	GLY	L894	L834	E829	R776	K714	V655	D590	C532	L302	L302
P1196	L1135	I1075	GLY	L895	W835	E829	S777	K715	T655	D590	C532	L302	L302
V1197	N1137	K1076	THR	N1017	T896	E836	G837	H716	T656	D590	C532	L302	L302
		K1077			K897			G717	R657	V597	S537		

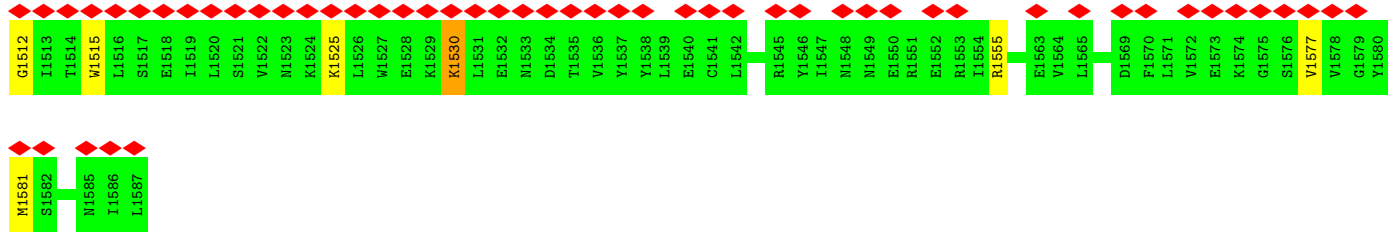
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I1258	L1259	K1260	P1261	K1262	Y1263	V1264	I1265	L1266	S1267	R1268	K1269	I1270	I1271	H1272	E1273	S1274	Y1275	R1276	Q1277	VAL	ASP	TYR	ASP	I1282	K1283	K1284	I1285	N1286	I1287	N1288	K1289	V1290	F1291	L1292	N1293	N1294	Y1295	K1296	H1297	C1298	I1299	S1300	N1301	K1302	V1303	D1304	D1305	Y1306	I1307	S1308	I1309	D1310	D1311	L1312	G1313	S1314	M1315	D1316	K1317																																																																																																										
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F1378	T1379	L1380	H1381	A1382	P1383	V1384	S1385	D1386	I1387	P1388	D1389	Y1390	I1391	K1392	P1393	F1394	L1395	L1396	G1397	F1398	N1399	G1400	S1401	E1402	P1403	I1404	S1405	E1406	L1407	F1408	K1409	K1410	F1411	I1412	L1413	V1414	E1415	D1416	R1417	L1418	N1419	T1420	Y1421	A1422	K1423	F1424	W1425	K1426	W1427	W1428	D1429	L1430	F1431	F1432	D1433	K1434	V1435	V1436	T1437																																																																																																										
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• Molecule 1: ATP-binding protein Avs4

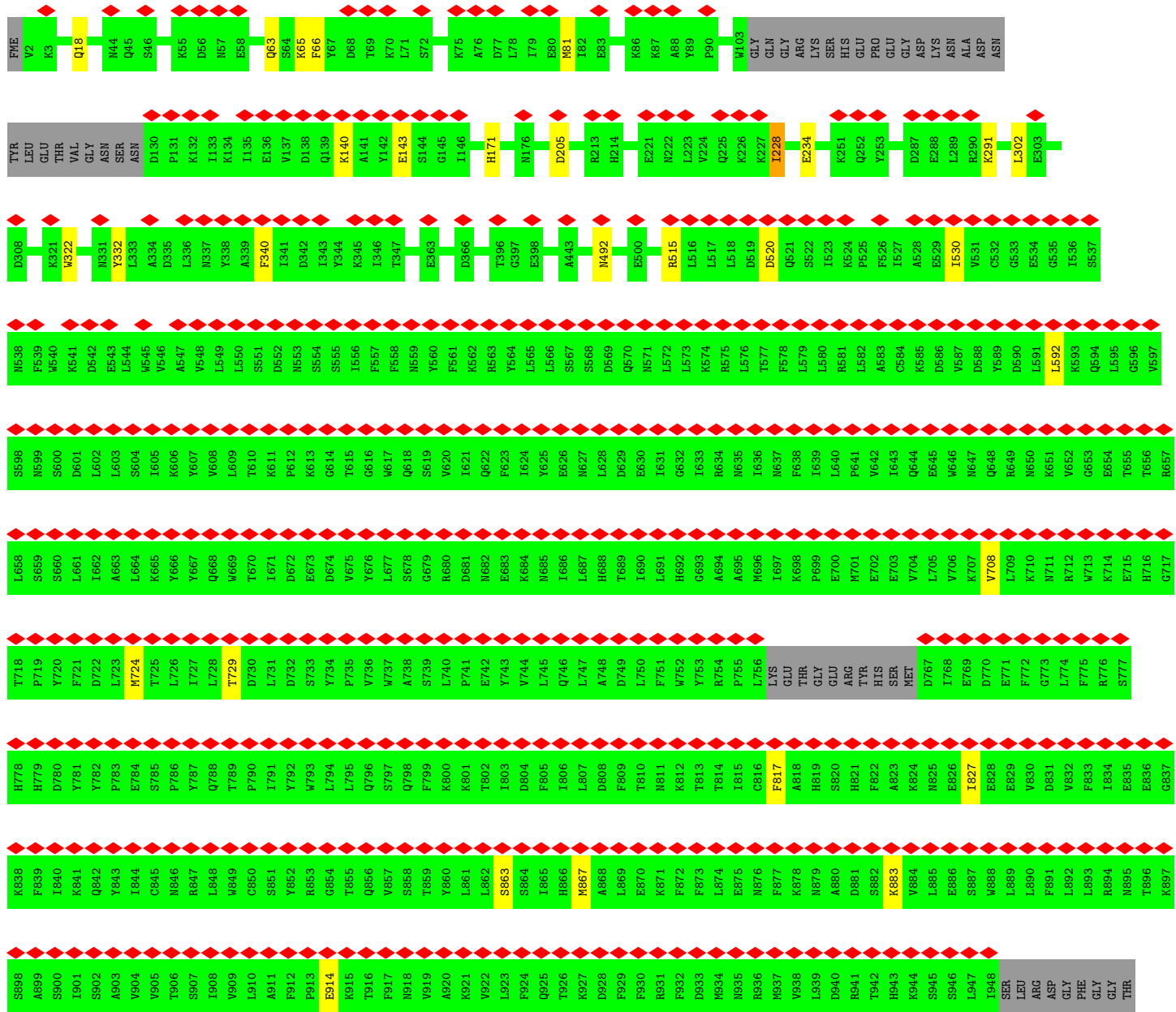


M1	V2	K3	P4	N51	D56	N57	E58	Q63	S64	I79	E80	M81	I82	E83	K86	K87	A88	Y89	P90	G91	G106	ARG	LYS	SER	HIS	GLU	PRD	GLU	GLY	ASP	ASN	ALA	ASN	TYR	LEU	GLU	THR	VAL	GLY	N127	S128	K132	Q139	W540	K140	A141	Y142	L544	E143	S144								
K170	E177	E196	D205	R213	T396	G397	E398	F438	A443	N490	N491	E493	E496	L516	L517	L518	D519	D520	Q521	S522	I523	K524	P525	F526	I527	A528	E529	I530	V531	C532	G533	E534	G535	E536	S537	N538	F539	W540	K541	D542	E543	L544	W545	V548	L549	L550	S551											
D552	N553	S554	S555	I556	F557	F558	N559	F561	K562	R563	Y564	L565	L566	S567	D568	Q570	N571	L572	L573	K574	R575	L576	T577	F578	L579	L580	R581	L582	A583	C584	K585	D586	V587	D588	Y589	L591	L592	K593	Q594	L595	G596	V597	S598	N599	S600	D601	L602	L603	S604	I605	K606	Y607	V608	L609	T610	K611		
P612	K613	G614	T615	G616	W617	Q618	S619	V620	I621	Q622	F623	K624	Y625	E626	N627	L628	D629	E630	I631	G632	I633	R634	N635	I636	N637	F638	I639	L640	P641	V642	I643	Q644	E645	W646	N647	Q648	N650	K651	V652	G653	Q654	T655	V656	R657	L658	S659	S660	D661	I662	A663	L664	K665	Y666	Y667	Q668	L669	T670	I671
D672	E673	D674	V675	Y676	L677	S678	G679	R680	D681	N682	E683	K684	N685	I686	L687	H688	T689	I690	L691	H692	G693	A694	A695	M696	I697	K698	P699	E700	M701	E702	E703	V704	L705	V706	K707	V708	K710	N711	R712	G713	K714	E715	H716	G717	T718	P719	Y720	F721	I662	A663	L664	K665	Y666	Y667	Q668	L669	T670	I671

I1452	K1392	V1332	H1272	I1212	Y1152	S1092	V1032	C972	F912	Y852	Y792	D732
K1453	P1393	D1333	E1273	L1213	F1153	Y1093	R1033	D973	P913	R853	W793	S733
S1454	F1394	T1334	S1274	L1214	M1154	K1094	L1034	D974	E914	G854	L794	Y734
Y1455	L1395	V1335	Y1275	L1215	Q1155	R1095	C1035	V975	K915	T855	L795	P735
L1456	D1396	M1336	L1276	L1216	L1156	E1096	A1036	H976	T916	Q856	Q796	W736
F1457	G1397	I1337	Q1277	L1217	M1157	K1097	A1037	R977	F917	V857	S797	V737
A1458	F1398	E1338	VAL	F1218	M1158	D1098	M1038	N978	N918	S858	Q798	A738
E1459	M1399	H1339	ASP	M1219	E1159	E1099	M1039	T979	V919	T859	F799	S739
S1460	G1400	K1340	TYR	D1220	E1160	R1100	D1040	Y980	Y910	Y860	K800	L740
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E1402	E1402	L1342	K1283	S1222	E1162	K1102	R1042	E982	V922	L862	T802	E742
P1403	P1403	V1343	K1284	I1223	Y1163	M1103	K1043	N983	L923	S863	I803	Y743
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L1407	L1407	V1347	M1288	G1227	I1167	Y1107	T1047	H987	K927	M867	L807	L747
F1408	F1408	K1348	K1289	G1228	V1168	E1108	T1048	Y988	D928	A868	D808	A748
K1409	K1409	R1349	F1290	R1229	L1169	D1109	K1049	Q989	F929	L869	F809	D749
K1410	K1410	F1350	F1291	Y1230	A1170	M1110	E1050	I990	F930	E870	T810	L750
F1411	F1411	S1351	L1292	S1231	Y1171	P1111	K1051	F991	R931	K871	N811	F751
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K1413	K1413	S1353	M1294	F1233	K1173	I1113	E1053	S993	D933	F873	T813	Y753
D1414	D1414	L1354	Y1295	P1234	L1174	A1114	G1054	E994	M934	L874	T814	R754
E1415	E1415	L1355	K1296	S1235	P1175	L1115	I1055	N995	N935	E875	I815	P755
D1416	D1416	S1356	H1297	M1236	L1176	Q1116	E1056	V996	R936	N876	C816	P756
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L1418	L1418	V1358	I1299	I1238	E1178	T1118	S1058	E998	V938	K878	LYS	
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T1420	T1420	E1360	M1301	K1240	M1180	E1120	M1060	D1000	D940	A880	GLY	
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A1422	A1422	R1362	I1303	W1242	Y1182	I1122	E1062	I1002	T942	S882	ARG	
K1423	K1423	V1363	D1304	L1243	Q1183	K1123	I1063	E1003	H943	K883	HIS	
F1424	F1424	D1364	M1305	D1244	Y1184	K1124	D1064	A1004	K944	V884	SER	
W1425	W1425	Y1365	K1306	Y1245	Q1185	L1125	P1065	Q1005	S945	L885	K824	
K1426	K1426	A1366	I1307	F1246	D1186	M1126	K1066	Q1006	S946	E886	N825	
V1427	V1427	L1367	S1308	D1247	G1187	E1127	L1067	V1007	L947	S887	E826	
W1428	W1428	R1368	I1309	D1248	T1188	E1128	K1068	L1008	I948	W888	E828	
D1429	D1429	Q1369	D1310	M1249	T1189	G1129	Q1069	W1009	SER	L889	E829	
L1430	L1430	S1370	D1311	Q1250	S1190	G1130	Y1070	D1010	LEU	L890	V830	
F1431	F1431	F1371	L1312	S1251	A1191	E1131	S1071	I1011	ARG	F991	D831	
D1432	D1432	L1372	G1313	L1252	I1192	F1132	E1072	F1012	ASP	S891	F831	
K1433	K1433	E1373	S1314	L1253	S1193	F1133	E1073	D1013	GLY	L892	V832	
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C1439	C1439	T1379	L1320	L1259	Y1199	M1139	S1079	L1019	ARG	S998	K838	
K1440	K1440	L1380	H1321	K1260	H1200	I1140	E1080	P1020	N961	S900	F839	
G1442	G1442	A1382	I1322	P1261	M1201	I1141	H1081	I0201	S962	I900	L840	
D1443	D1443	P1383	L1323	K1262	Y1202	A1142	M1082	E1022	L963	S902	Q842	
R1444	R1444	V1384	M1324	Y1263	P1203	D1143	K1083	A1023	H964	A903	Y843	
V1445	V1445	S1385	I1325	V1264	M1204	Y1144	Y1084	Q1024	E965	V904	L844	
W1446	W1446	D1386	A1326	I1265	E1205	C1145	V1085	I0205	R968	V905	C845	
C1507	C1507	F1327	F1327	L1266	R1206	S1146	T1086	T1026	I969	T906	N846	
V1448	V1448	Q1328	Q1328	S1267	E1207	W1147	L1087	E1027	K970	S907	R847	
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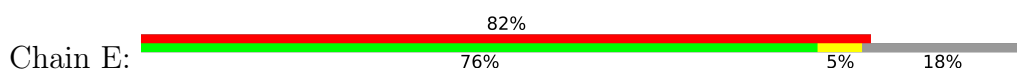


• Molecule 1: ATP-binding protein Avs4



ASP	TYR	ARG	R961	S962	L963	R964	E965	E966	D967	R968	R969	R970	A971	C972	D973	D974	V975	H976	R977	R978	T979	Y980	L981	E982	R983	L984	A985	L986	H987	Y988	Q989	Y990	F991	R992	S993	E994	N995	Y996	T997	E998	R999	D1000	A1001	I1002	E1003	Q1004	Q1005	Q1006	V1007	L1008	W1009	D1010	I1011	F1012	D1013	K1014	Y1015	I1016	M1017
Q1018	L1019	P1020	D1021	E1022	A1023	Q1024	E1025	T1026	E1027	A1028	D1029	K1030	T1031	W1032	R1033	L1034	C1035	L1036	A1037	R1038	M1039	D1040	R1041	R1042	K1043	M1044	L1045	K1046	T1047	T1048	K1049	M1100	K1050	D1052	E1053	G1054	I1055	E1056	I1057	S1058	F1059	N1060	P1061	E1062	I1063	D1064	P1065	K1066	V1007	L1008	W1009	D1010	I1011	F1012	D1013	K1014	Y1015	I1016	M1017
M1078	S1079	E1080	H1081	M1082	K1083	V1084	V1085	T1086	L1087	K1088	L1089	W1090	A1091	S1092	Y1093	K1094	R1095	E1096	K1097	D1098	E1099	R1100	Y1101	M1102	M1103	Y1104	G1105	M1106	Y1107	E1108	D1109	M1110	P1111	Q1112	I1113	L1114	L1115	Q1116	E1117	T1118	K1119	E1120	I1121	I1122	K1123	K1124	L1125	M1126	E1127	E1128	G1129	E1130	E1131	D1132	F1133	R1134	L1135	L1136	M1137
G1138	M1139	I1140	P1141	D1142	D1143	V1144	C1145	S1146	V1147	L1148	L1149	L1150	D1151	Y1152	F1153	L1154	Q1155	L1156	M1157	E1158	E1159	E1160	R1161	E1162	Y1163	C1164	K1165	D1166	I1167	V1168	L1169	A1170	Y1171	S1172	K1173	L1174	P1175	L1176	K1177	E1178	G1179	Y1180	M1181	Y1182	K1183	V1184	Q1185	D1186	G1187	T1188	T1189	S1190	A1191	I1192	F1193	A1194	L1195	F1196	V1197
I1198	Y1199	H1200	N1201	Y1202	P1203	M1204	E1205	R1206	E1207	T1208	I1209	K1210	D1211	Y1212	F1213	L1214	L1215	T1216	L1217	F1218	M1219	D1220	H1221	S1222	I1223	G1224	M1225	A1226	G1227	G1228	R1229	Y1230	I1231	V1232	F1233	P1234	S1235	M1236	V1237	I1238	H1239	K1240	L1241	W1242	L1243	D1244	Y1245	F1246	D1247	T1248	M1249	Q1250	S1251	I1252	L1253	F1254	G1255	F1256	L1257
L1268	L1269	P1261	Y1262	V1263	V1264	I1265	L1266	S1267	R1268	K1269	I1270	I1271	H1272	E1273	S1274	Y1275	R1276	Q1277	VAL	ASP	TYR	ASP	I1282	K1283	K1284	I1285	M1286	I1287	N1288	K1289	V1290	F1291	L1292	M1293	N1294	Y1295	K1296	H1297	C1298	I1299	S1300	N1301	V1302	I1303	D1304	N1305	K1306	I1307	S1308	I1309	D1310	D1311	L1312	G1313	S1314	M1315	K1317		
V1318	D1319	L1320	H1321	L1322	L1323	N1324	T1325	A1326	F1327	Q1328	L1329	P1331	V1332	D1333	L1334	V1335	M1336	I1337	E1338	H1339	G1340	K1341	L1342	V1343	S1344	L1345	I1346	V1347	K1348	L1349	F1350	S1351	T1352	S1353	L1354	L1355	S1356	R1357	V1358	R1359	E1360	D1361	R1362	V1363	D1364	Y1365	A1366	V1367	R1368	Q1369	S1370	F1371	L1372	D1373	S1374	M1375	A1376	Y1377	
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L1438	C1439	K1440	D1441	G1442	D1443	R1444	Y1445	W1446	V1447	V1448	D1449	K1450	I1451	I1452	K1453	S1454	Y1455	L1456	F1457	A1458	E1459	S1460	W1461	K1463	E1464	M1465	S1466	M1467	G1468	V1469	H1470	L1471	F1472	K1473	D1474	S1475	N1476	S1477	Q1478	F1479	F1480	C1481	D1482	V1483	S1484	L1485	T1486	M1487	G1488	H1489	C1490	S1491	S1492	T1493	L1494	S1495	S1496	L1497	
A1498	K1499	S1500	L1501	M1502	M1503	I1504	A1505	S1506	C1507	Y1508	L1509	M1510	Q1511	G1512	I1513	T1514	W1515	L1516	S1517	E1518	I1519	L1520	S1521	V1522	K1524	K1525	L1526	W1527	E1528	K1529	K1530	L1531	E1532	M1533	D1534	Y1535	V1536	Y1537	Y1538	L1539	E1540	C1541	L1542	V1543	R1544	L1545	Y1546	I1547	M1548	M1549	E1550	R1551	E1552	R1553	Q1562	E1563			
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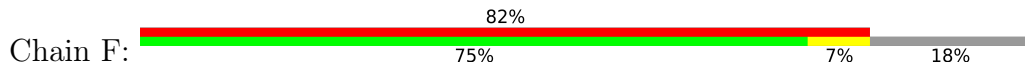
• Molecule 2: Portal protein



WET	ALA	SER	GLN	R6	R7	E8	O9	F10	A11	E12	M13	G14	A15	K16	A17	V18	Y19	D20	A21	L22	K23	N24	D25	R26	S28	Y29	E30	T31	R32	A33	E34	N35	C36	A37	K38	Y39	T40	I41	P42	S43	L44	F45	P46	R47	D48	S49	D50	N51	A52	S53	T54	D55	V56	T57	L58	P59	H60
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Q61	M121	V181	D241	N501	ALA	A421	ILE
A62	Y122	T182	A242	P302	VAL	V422	LEU
V63	I123	L183	S243	A303	GLN	E423	LYS
G64	E124	D184	Y244	G304	THR	P424	PRO
A65	S125	K185	P245	I305	GLY	T425	GLU
R66	M126	T186	V246	T306	GLU	T426	GLU
G67	S127	A187	D247	Q307	VAL	S427	GLN
L68	Y128	Y188	A248	V308	THR	T428	GLN
N69	R129	A189	C249	R309	ALA	G429	MET
N70	V130	A190	P250	R310	ALA	M430	ALA
L71	T131	L191	Y251	L311	E372	E431	GLU
A72	L132	P192	I252	T312	I374	A432	ALA
S73	F133	E193	P253	K313	R375	L433	ALA
K74	E134	D194	V254	A314	V376	G434	GLY
L75	T135	V195	R255	Q315	V377	R435	THR
M76	L136	R196	M256	T316	A378	G436	ALA
L77	K137	A197	V257	G317	S379	Q437	LEU
A78	Q138	A198	R258	D318	E380	D438	ASN
L79	L139	M199	I259	F319	L381	A439	ALA
F80	V140	D200	D260	V320	E382	L439	ALA
P81	V141	S201	G261	S321	D383	D440	ALA
M82	A142	G202	E262	G322	T384	K441	SER
Q83	G143	Q203	S263	R323	L385	E442	ALA
T84	M144	E204	Y264	P324	G386	R444	ALA
M85	A145	H205	H265	E325	G387	C445	ALA
M86	L146	K206	R266	D326	V388	T446	GLY
K87	L147	G207	S267	I327	Y389	A447	LEU
L88	Y148	D208	Y268	S328	S390	A448	ALA
T89	I149	E209	C269	F329	I391	W449	THR
I90	P150	M210	E270	L330	L392	A450	ALA
S91	E151	I211	E271	Q331	S393	A451	SER
E92	P152	D212	Y272	L332	Q394	L452	PRO
F93	E153	V213	L273	E333	E395	A453	GLU
E94	G154	Y214	G274	K334	L396	P454	MET
A95	A155	T215	D275	A335	Q397	M455	GLU
K96	Y156	H216	L276	A336	L398	ALA	ALA
Q97	M157	I217	R277	D337	P399	ASN	ALA
L98	P158	Y218	S278	F338	M400	PRO	ALA
V99	M159	L219	L279	S339	V401	ASP	GLN
A100	K160	D220	E280	V340	R402	ASP	PRO
Q101	L161	E221	M281	I341	V403	ASP	ILE
P102	P162	E222	L282	K342	L404	ASP	ILE
A103	R163	S223	Q283	A343	L405	THR	ALA
E104	L164	G224	E284	V344	K406	ILE	ALA
L105	S165	E225	E285	V345	Q407	LYS	ILE
A106	S166	Y226	I286	E346	L408	LEU	LEU
K107	Y167	L227	V287	E347	Q409	ILE	ILE
V108	V168	K228	K288	I348	A410	ALA	ALA
E109	V169	Y229	M289	E349	T411	ASN	ALA
E110	Q170	E230	E290	G350	M412	ALA	ALA
G111	R171	E231	M291	R351	Q413	GLY	ILE
L112	D172	I232	I292	L352	T414	ILE	ILE
S113	A173	D233	S293	S353	P415	THR	ASP
M114	F174	G234	A294	Y354	E416	SER	THR
V115	G175	V235	K295	A355	L417	ALA	SER
E116	T176	E236	V296	F356	P418	GLY	GLY
R117	V177	V237	I297	M357	R419	ASP	ASP
L118	L178	D238	G298	L358	E420	THR	THR
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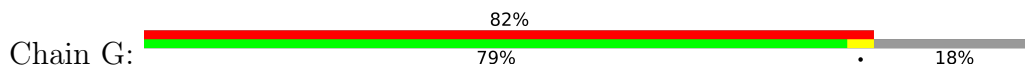
• Molecule 2: Portal protein



MET	Q61	Y121	V181	L22	Q61	M121	V181	D241
ALA	A62	Y122	T182	L22	A62	Y122	T182	A242
SER	V63	I123	L183	L22	V63	I123	L183	S243
GLM	G64	E124	D184	L22	G64	E124	D184	Y244
K6	R66	S125	K185	L22	R66	S125	K185	P245
R7	G67	M126	T186	L22	G67	M126	T186	V246
E8	S127	S127	A187	L22	S127	S127	A187	D247
G9	Y128	Y128	Y188	L22	Y128	Y128	Y188	A248
F10	R129	R129	A189	L22	R129	R129	A189	C249
A11	V130	V130	A190	L22	V130	V130	A190	P250
E12	T131	T131	L191	L22	T131	T131	L191	Y251
N13	L132	L132	P192	L22	L132	L132	P192	I252
G14	F133	F133	E193	L22	F133	F133	E193	P253
A15	S73	S73	D194	L22	S73	S73	D194	V254
K16	K74	K74	L75	L22	K74	K74	L75	R255
A17	L75	L75	M76	L22	L75	L75	M76	M256
V18	M76	M76	L77	L22	M76	M76	L77	V257
Y19	L77	L77	A78	L22	L77	L77	A78	R258
D20	A78	A78	L79	L22	A78	A78	L79	I259
A21	L79	L79	F80	L22	L79	L79	F80	D260
L22	F80	F80	P81	L22	F80	F80	P81	G261
K23	M82	M82	Q83	L22	M82	M82	Q83	E262
N24	Q83	Q83	T84	L22	Q83	Q83	T84	S263
D25	T84	T84	M85	L22	T84	T84	M85	Y264
R26	M85	M85	M86	L22	M85	M85	M86	G265
N27	M86	M86	K87	L22	M86	M86	K87	R266
S28	K87	K87	L88	L22	K87	K87	L88	S267
Y29	L88	L88	T89	L22	L88	L88	T89	Y268
E30	T89	T89	I90	L22	T89	T89	I90	C269
T31	I90	I90	S91	L22	I90	I90	S91	E270
R32	S91	S91	E92	L22	S91	S91	E92	E271
A33	E92	E92	F93	L22	E92	E92	F93	Y272
E34	F93	F93	E94	L22	F93	F93	E94	L273
N35	E94	E94	A95	L22	E94	E94	A95	G274
C36	A95	A95	K96	L22	A95	A95	K96	D275
A37	K96	K96	Q97	L22	K96	K96	Q97	L276
K38	Q97	Q97	L98	L22	Q97	Q97	L98	R277
Y39	L98	L98	V99	L22	L98	L98	V99	S278
T40	V99	V99	A100	L22	V99	V99	A100	L279
I41	A100	A100	Q101	L22	A100	A100	Q101	E280
P42	Q101	Q101	P102	L22	Q101	Q101	P102	M281
S43	P102	P102	A103	L22	P102	P102	A103	E221
L44	A103	A103	E104	L22	A103	A103	E104	S223
F45	E104	E104	L105	L22	E104	E104	L105	G224
P46	L105	L105	A106	L22	L105	L105	A106	S225
K47	A106	A106	K107	L22	A106	A106	K107	E226
D48	K107	K107	V108	L22	K107	K107	V108	L227
S49	V108	V108	E109	L22	V108	V108	E109	K228
D50	E109	E109	N51	L22	E109	E109	N51	Y229
A52	N51	N51	A52	L22	N51	N51	A52	E230
S53	A52	A52	T54	L22	A52	A52	T54	E231
D55	T54	T54	M114	L22	T54	T54	M114	I232
Y56	M114	M114	V115	L22	M114	M114	V115	D233
T57	V115	V115	E116	L22	V115	V115	E116	G234
S58	E116	E116	R117	L22	E116	E116	R117	V235
M60	R117	R117	L118	L22	R117	R117	L118	E236
	L118	L118	L119	L22	L118	L118	L119	V237
	L119	L119	M120	L22	L119	L119	M120	D238
	M120	M120		L22	M120	M120		G239
				L22				T240

N301	P302	A303	G304	I305	T306	Q307	V308	R309	R310	L311	T312	K313	A314	Q315	T316	G317	D318	F319	V320	S321	G322	R323	P324	E325	D326	I327	S328	F329	L330	Q331	L332	E333	K334	A335	A336	D337	F338	S339	V340	A341	K342	A343	V344	S345	E346	Q347	I348	E349	G350	R351	L352	S353	Y354	A355	F356	M357	L358	N359	SER		
ALA	VAL	GLN	ARG	THR	GLY	GLU	ARG	VAL	THR	ALA	E372	E373	I374	R375	Y376	V377	A378	S379	E380	L381	E382	D383	T384	L385	G386	G387	V388	Y389	S390	I391	L392	S393	Q394	E395	L396	Q397	L398	P399	ASP	M400	V401	R402	V403	L404	L405	K406	Q407	L408	Q409	A410	T411	N412	Q413	I414	P415	E416	L417	P418	K419	E420	
A421	V422	E423	P424	T425	I426	S427	T428	G429	M430	E431	A432	L433	G434	R435	G436	Q437	D438	L439	D440	K441	L442	E443	R444	C445	I446	A447	A448	W449	S450	A451	L452	A453	P454	M455	GLN	ASN	ASP	PRO	ASP	ASP	ILE	R402	ASN	VAL	ILE	THR	ILE	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ILE	ILE	ASP	THR	THR	SER	GLY
ILE	LEU	LYS	THR	PRO	GLU	GLU	LYS	GLN	GLN	MET	ALA	ALA	ALA	GLY	THR	ALA	LEU	ASN	ALA	ALA	ALA	SER	GLY	GLY	ALA	ALA	GLY	ALA	ALA	THR	THR	ALA	PRO	PRO	ALA	ALA	ALA	ALA	GLN	GLN	ALA	ALA	GLY	GLY	MET	VAL	PRO	VAL	ASN												

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MET	ALA	SER	GLN	K6	R7	E8	G9	F10	A11	E12	M13	G14	A15	K16	A17	V18	Y19	D20	A21	L22	K23	N24	D25	R26	M27	S28	Y29	E30	T31	R32	A33	E34	M35	C36	A37	K38	Y39	T40	P42	P43	L44	F45	P46	K47	D48	S49	D50	M51	A52	S53	T54	D55	Y56	T57	T58	P59	W60				
Q61	A62	V63	L64	G65	R66	E67	L68	M69	A189	N70	L71	A72	S73	K74	L75	M76	L77	A78	L79	F80	P81	M82	Q83	T84	W85	M86	K87	L88	T89	I90	S91	E92	F93	E94	A95	K96	Q97	L98	V99	A100	Q101	P102	A103	E104	L105	S106	K107	D108	V109	E110	G111	L112	S113	M114	V115	E116	R117	L118	L119	M120	
M121	Y122	I123	E124	M125	N126	S127	Y128	R129	A189	V130	T131	L132	F133	E134	K135	L136	K137	Q138	L139	V140	S201	G202	Q203	E204	M205	L206	G207	D208	E209	M210	I211	D212	E213	G214	T215	H216	I217	Y218	L219	D220	E221	E222	S223	G224	E225	A285	I286	L287	K288	M289	S290	M291	I292	S293	A294	K295	V296	I297	G298	L299	V300
V181	T182	L183	D184	K185	T186	A187	Y188	A189	A190	L191	P192	E193	D194	V195	R196	N197	A198	M199	D200	S201	G202	Q203	E204	M205	L206	G207	D208	E209	M210	I211	D212	E213	G214	T215	H216	I217	Y218	L219	D220	E221	E222	S223	G224	E225	A285	I286	L287	K288	M289	S290	M291	I292	S293	A294	K295	V296	I297	G298	L299	V300	
D241	A242	S243	Y244	P245	V246	D247	A248	C249	P250	Y251	I252	P253	V254	R255	M256	V257	R258	I259	D260	G261	E262	S263	Y264	G265	R266	S267	Y268	C269	E270	E271	Y272	L273	G274	D275	L276	R277	S278	L279	N281	L282	Q283	E284	A285	I286	L287	K288	M289	S290	M291	I292	S293	A294	K295	V296	I297	G298	L299	V300			
N301	P302	A303	G304	I305	T306	Q307	V308	R309	R310	L311	T312	K313	A314	Q315	T316	G317	D318	F319	V320	S321	G322	R323	P324	E325	D326	I327	S328	F329	L330	Q331	L332	E333	K334	A335	A336	D337	F338	S339	V340	A341	K342	A343	V344	S345	E346	Q347	I348	E349	G350	R351	L352	S353	Y354	A355	F356	M357	L358	N359	SER		
ALA	VAL	GLN	ARG	THR	GLY	GLU	ARG	VAL	THR	ALA	E372	E373	I374	R375	Y376	V377	A378	S379	E380	L381	E382	D383	T384	L385	G386	G387	V388	Y389	S390	I391	L392	S393	Q394	E395	L396	Q397	L398	P399	ASP	M400	V401	R402	V403	L404	L405	K406	Q407	L408	Q409	A410	T411	N412	Q413	I414	P415	E416	L417	P418	K419	E420	
A421	V422	E423	P424	T425	I426	S427	T428	G429	M430	E431	A432	L433	G434	R435	G436	Q437	D438	L439	D440	K441	L442	E443	R444	C445	I446	A447	A448	W449	S450	A451	L452	A453	P454	M455	GLN	ASN	ASP	PRO	ASP	ASP	ILE	R402	ASN	VAL	ILE	THR	ILE	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ILE	ILE	ASP	THR	THR	SER	GLY
ILE	LEU	LYS	THR	PRO	GLU	GLU	LYS	GLN	GLN	MET	ALA	ALA	ALA	GLY	THR	ALA	LEU	ASN	ALA	ALA	ALA	SER	GLY	GLY	ALA	ALA	GLY	ALA	ALA	THR	THR	ALA	PRO	PRO	ALA	ALA	ALA	ALA	GLN	GLN	ALA	ALA	GLY	GLY	MET	VAL	PRO	VAL	ASN												

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## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	169977	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	31	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.138	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	372.3703, 372.3703, 372.3703	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.034362, 1.034362, 1.034362	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.34	0/13095	0.65	3/17695 (0.0%)
1	B	0.35	0/13056	0.65	0/17643
1	C	0.34	0/13095	0.65	3/17695 (0.0%)
1	D	0.34	0/13056	0.64	0/17643
2	E	0.73	4/3485 (0.1%)	0.93	6/4720 (0.1%)
2	F	0.44	1/3485 (0.0%)	0.76	4/4720 (0.1%)
2	G	0.52	1/3485 (0.0%)	0.81	5/4720 (0.1%)
2	H	0.45	1/3485 (0.0%)	0.78	4/4720 (0.1%)
All	All	0.40	7/66242 (0.0%)	0.69	25/89556 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	324	PRO	CG-CD	-31.12	0.45	1.50
2	G	454	PRO	CG-CD	-19.16	0.85	1.50
2	E	80	PHE	C-O	11.37	1.29	1.23
2	E	324	PRO	CB-CG	11.27	2.06	1.49
2	F	324	PRO	CG-CD	-11.14	1.12	1.50

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	324	PRO	CB-CG-CD	-33.13	0.07	106.10
2	G	454	PRO	N-CD-CG	-20.29	72.77	103.20
2	E	324	PRO	CA-N-CD	-15.57	90.20	112.00
2	G	454	PRO	CA-CB-CG	-11.59	82.49	104.50
2	F	324	PRO	N-CD-CG	-11.55	85.88	103.20

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	12805	0	12724	32	0
1	B	12756	0	12683	34	0
1	C	12805	0	12724	26	0
1	D	12756	0	12683	28	0
2	E	3427	0	3400	18	0
2	F	3427	0	3400	23	0
2	G	3427	0	3400	11	0
2	H	3427	0	3400	24	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	0	0
3	D	31	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	64958	0	64462	179	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 1.

The worst 5 of 179 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:F:117:ARG:HH12	2:F:121:ASN:HB2	1.39	0.87
2:H:117:ARG:HH12	2:H:121:ASN:HB2	1.46	0.79
1:C:937:MET:HG2	1:C:941:ARG:HH12	1.51	0.76
1:A:1359:ARG:O	1:A:1359:ARG:NH1	2.25	0.69
1:C:1359:ARG:O	1:C:1359:ARG:NH1	2.26	0.69

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	1531/1587 (96%)	1499 (98%)	32 (2%)	0	100	100
1	B	1524/1587 (96%)	1490 (98%)	34 (2%)	0	100	100
1	C	1531/1587 (96%)	1501 (98%)	30 (2%)	0	100	100
1	D	1524/1587 (96%)	1490 (98%)	34 (2%)	0	100	100
2	E	434/535 (81%)	422 (97%)	12 (3%)	0	100	100
2	F	434/535 (81%)	422 (97%)	12 (3%)	0	100	100
2	G	434/535 (81%)	419 (96%)	15 (4%)	0	100	100
2	H	434/535 (81%)	425 (98%)	9 (2%)	0	100	100
All	All	7846/8488 (92%)	7668 (98%)	178 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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	1422/1461 (97%)	1418 (100%)	4 (0%)	86	96
1	B	1418/1461 (97%)	1411 (100%)	7 (0%)	81	93
1	C	1422/1461 (97%)	1416 (100%)	6 (0%)	84	94
1	D	1418/1461 (97%)	1408 (99%)	10 (1%)	76	92
2	E	370/435 (85%)	367 (99%)	3 (1%)	73	90
2	F	370/435 (85%)	365 (99%)	5 (1%)	59	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	370/435 (85%)	369 (100%)	1 (0%)	86	96
2	H	370/435 (85%)	366 (99%)	4 (1%)	65	88
All	All	7160/7584 (94%)	7120 (99%)	40 (1%)	76	93

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	291	MET
2	G	320	VAL
2	E	320	VAL
2	F	86	MET
2	H	77	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	668	GLN
1	D	1137	ASN
2	F	413	GLN
1	B	650	ASN
1	B	644	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 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
1	FME	A	1	1	8,9,10	1.02	0	8,9,11	2.53	2 (25%)
1	FME	C	1	1	8,9,10	1.02	0	8,9,11	2.62	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	A	1	1	-	6/7/9/11	-
1	FME	C	1	1	-	6/7/9/11	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	FME	CA-N-CN	-5.49	114.38	122.82
1	A	1	FME	CA-N-CN	-5.30	114.67	122.82
1	C	1	FME	O1-CN-N	4.57	137.12	125.32
1	A	1	FME	O1-CN-N	4.42	136.74	125.32

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	O-C-CA-CB
1	C	1	FME	O1-CN-N-CA
1	C	1	FME	O-C-CA-CB
1	A	1	FME	CB-CG-SD-CE

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	2	0
1	C	1	FME	2	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
3	ATP	C	1601	4	32,33,33	0.93	2 (6%)	48,52,52	0.42	0
3	ATP	B	1601	4	32,33,33	1.13	2 (6%)	48,52,52	0.41	0
3	ATP	D	1601	4	32,33,33	1.13	2 (6%)	48,52,52	0.41	0
3	ATP	A	1601	4	32,33,33	0.94	2 (6%)	48,52,52	0.41	0

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
3	ATP	C	1601	4	-	1/22/38/38	0/3/3/3
3	ATP	B	1601	4	-	0/22/38/38	0/3/3/3
3	ATP	D	1601	4	-	0/22/38/38	0/3/3/3
3	ATP	A	1601	4	-	1/22/38/38	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1601	ATP	PA-O3A	-5.52	1.53	1.59
3	B	1601	ATP	PA-O3A	-5.51	1.53	1.59
3	A	1601	ATP	PA-O3A	-3.64	1.55	1.59
3	C	1601	ATP	PA-O3A	-3.58	1.55	1.59
3	A	1601	ATP	PB-O3B	-3.04	1.56	1.59

There are no bond angle outliers.

There are no chirality outliers.

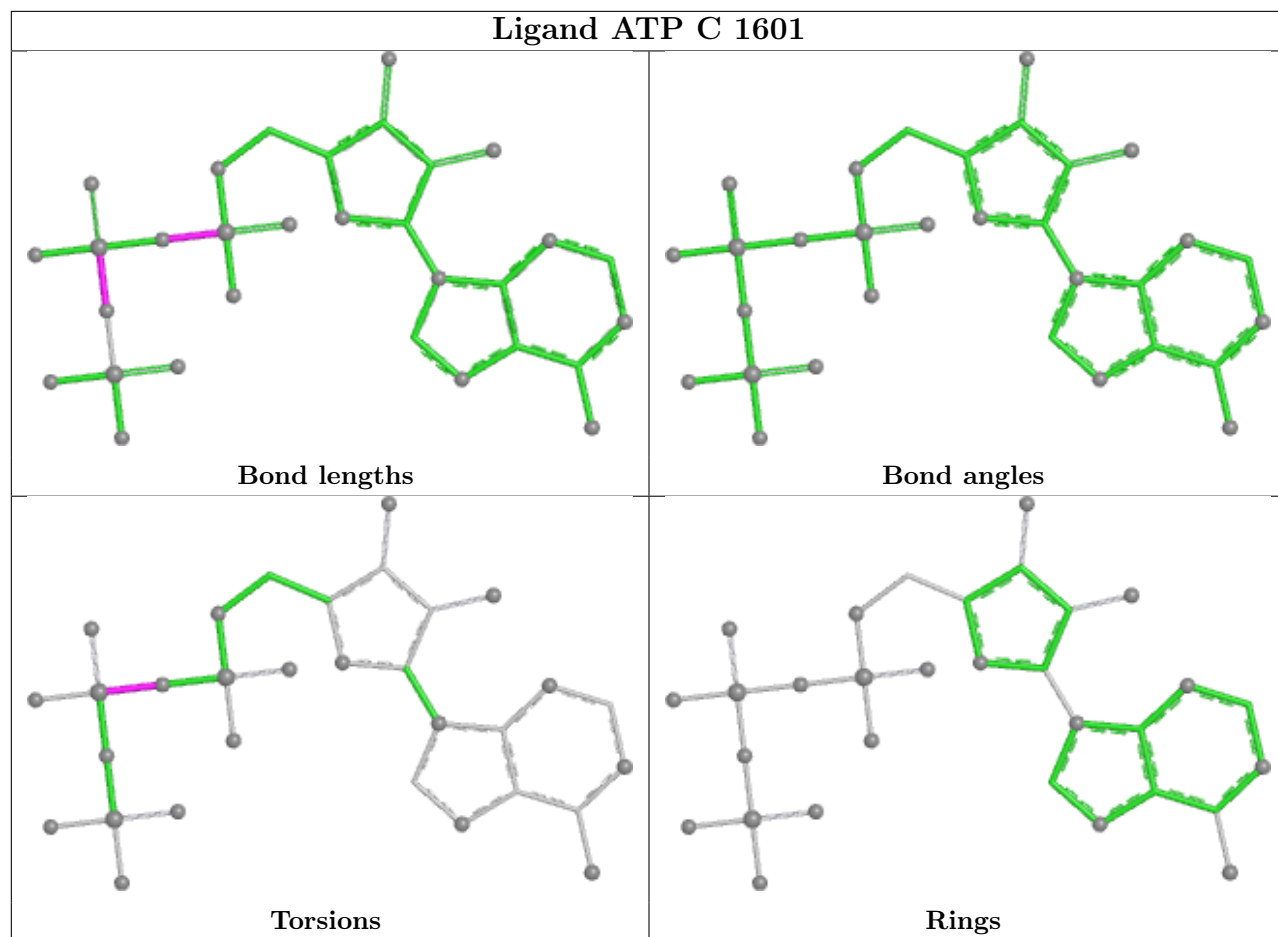
All (2) torsion outliers are listed below:

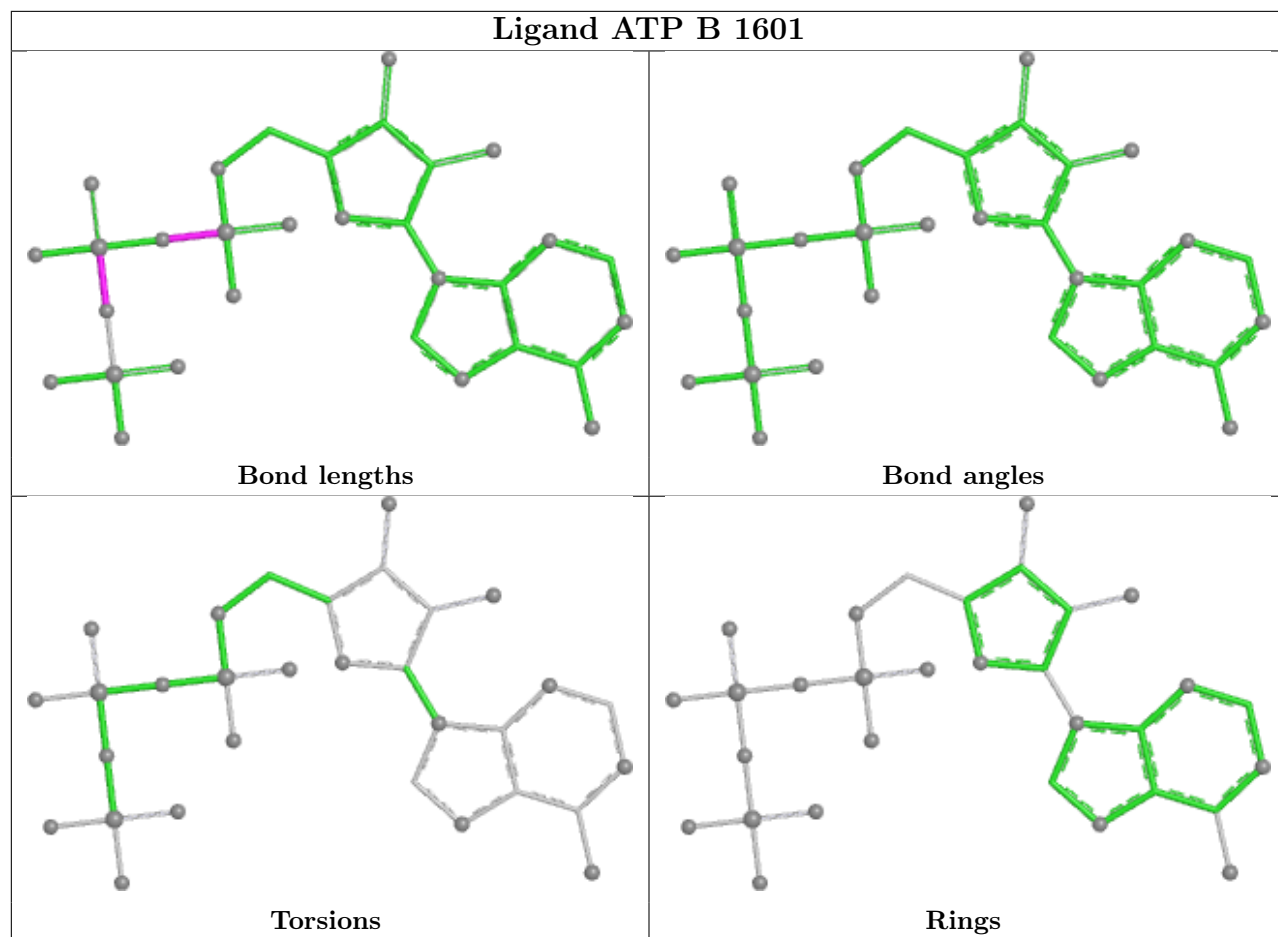
Mol	Chain	Res	Type	Atoms
3	A	1601	ATP	PA-O3A-PB-O2B
3	C	1601	ATP	PA-O3A-PB-O2B

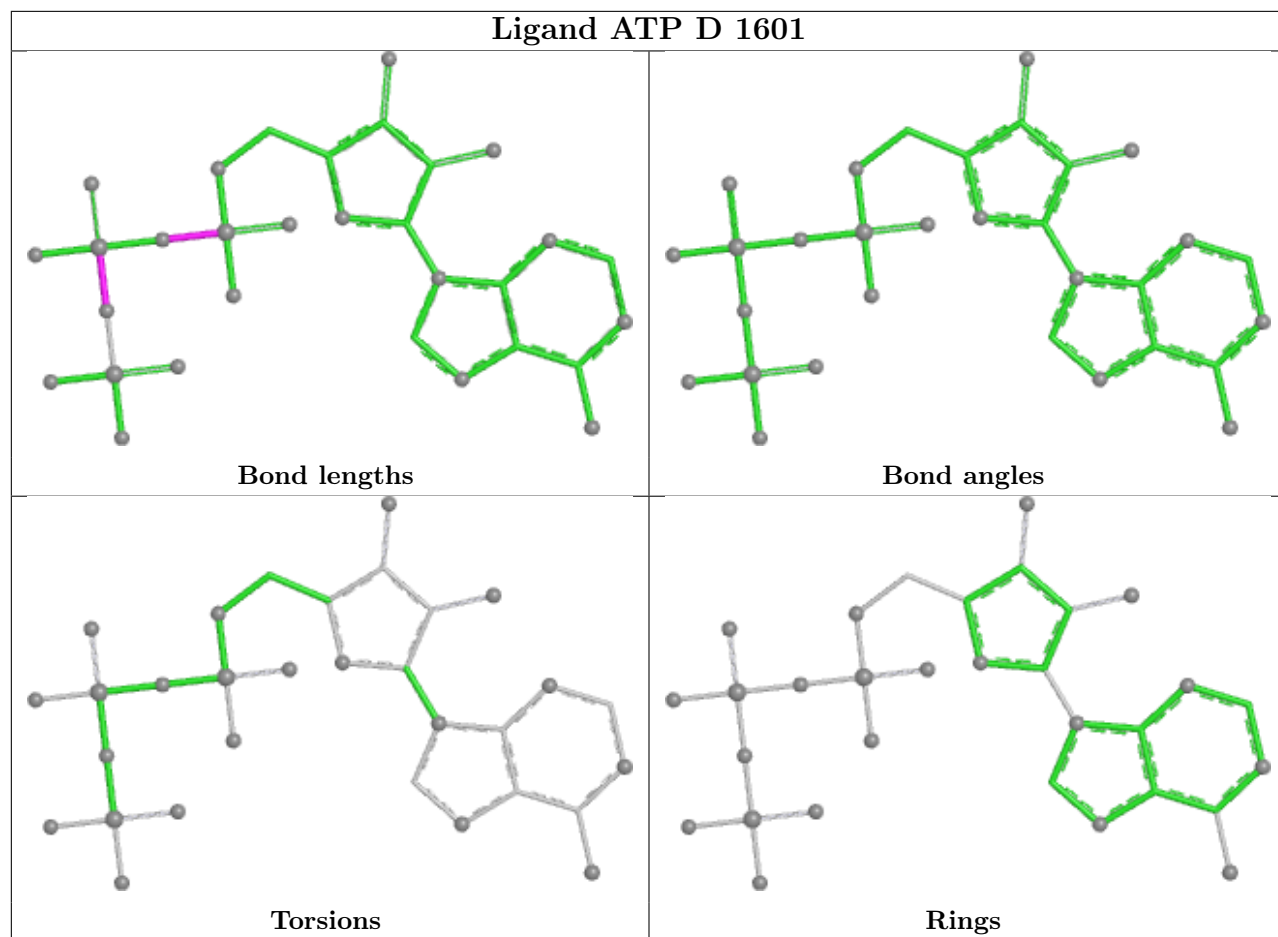
There are no ring outliers.

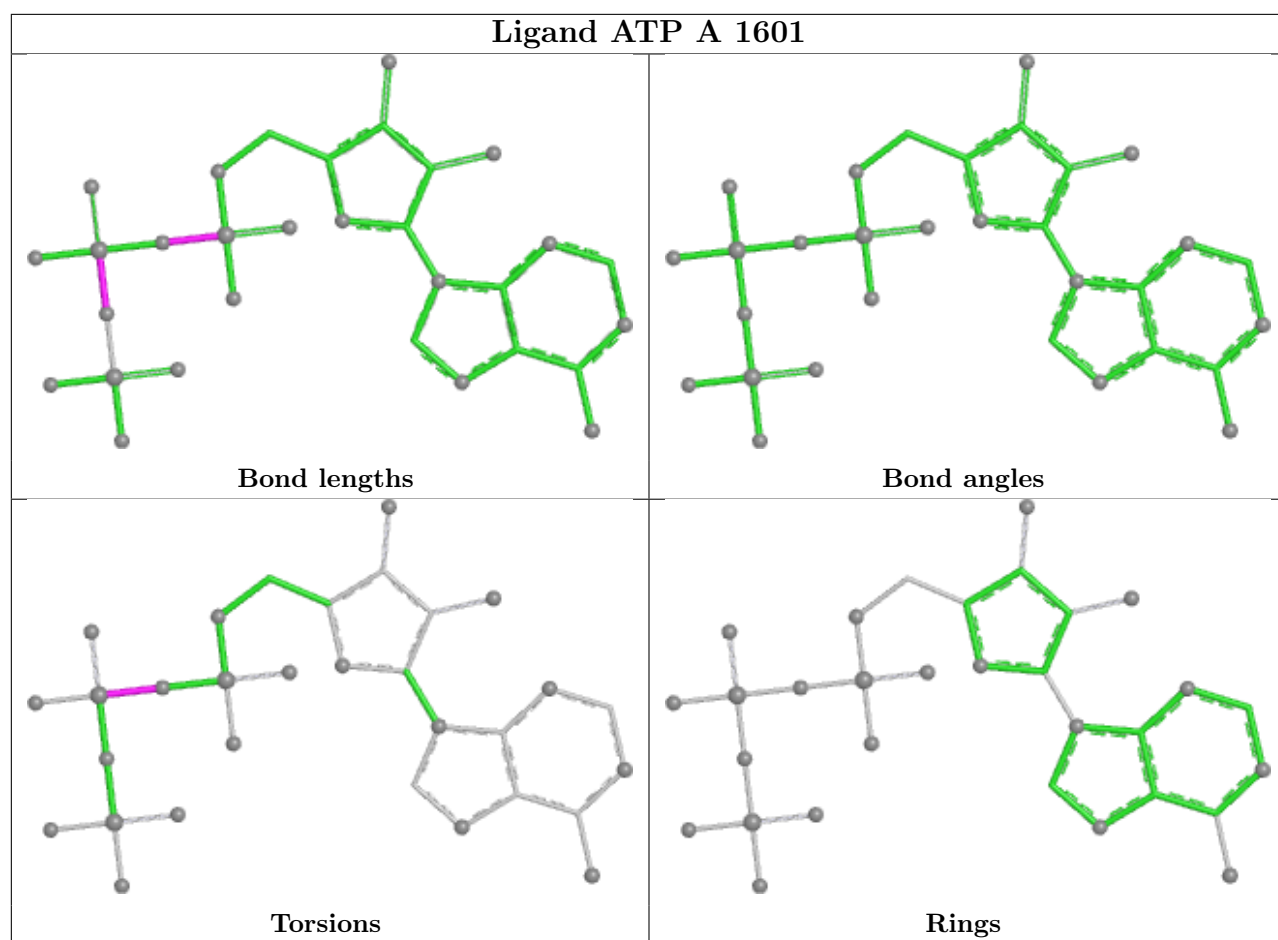
No monomer is involved in short contacts.

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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

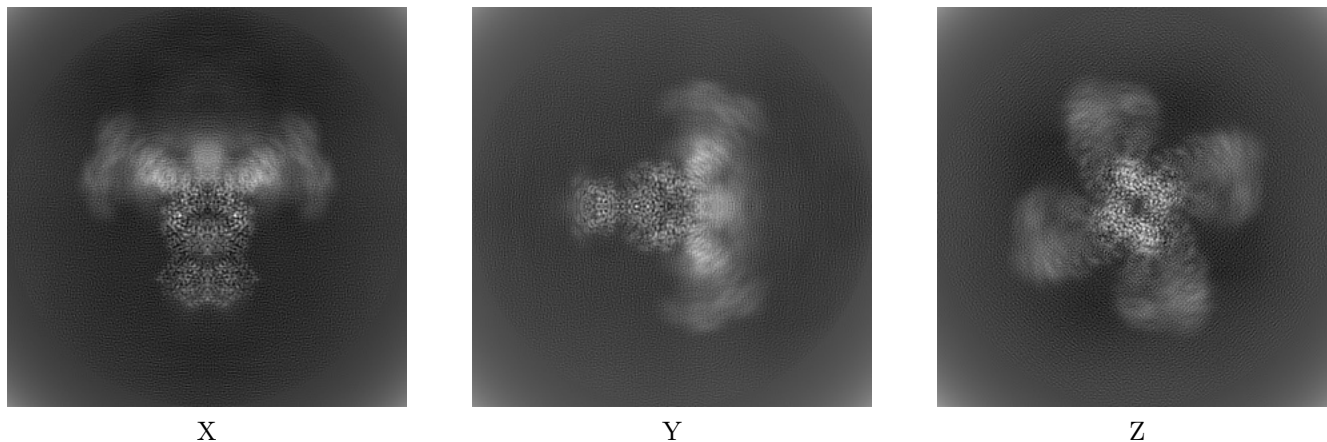
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27422. These allow visual inspection of the internal detail of the map and identification of artifacts.

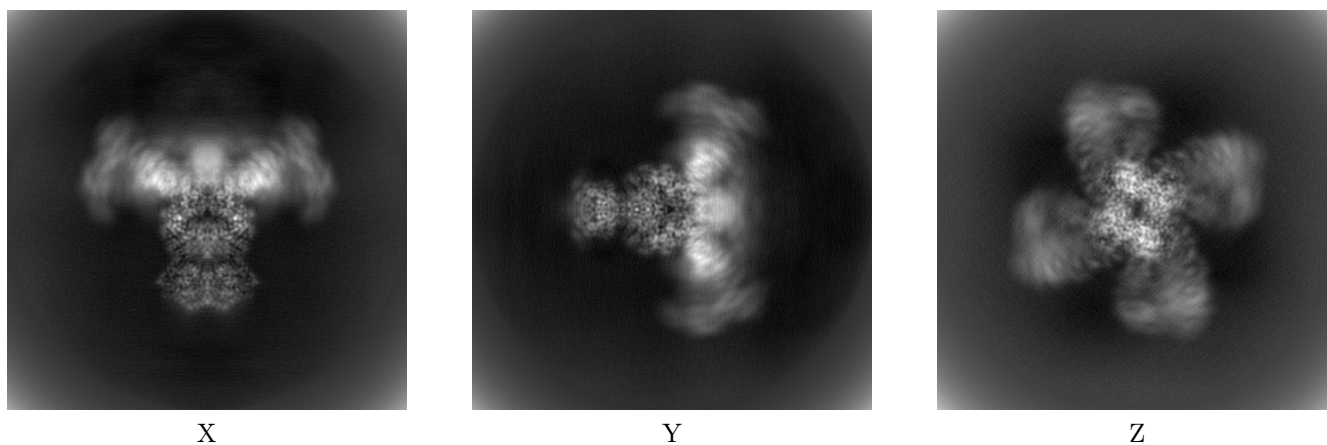
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

#### 6.1.1 Primary map



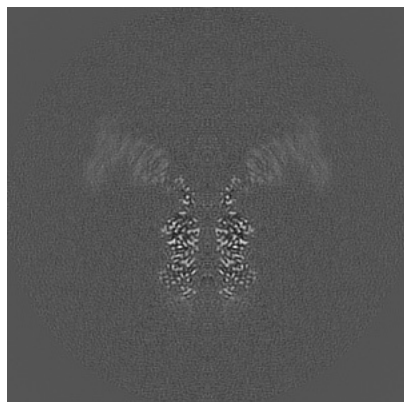
#### 6.1.2 Raw map



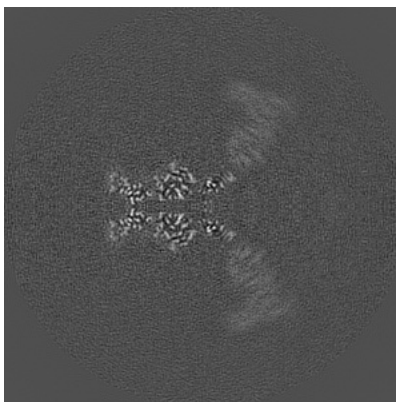
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

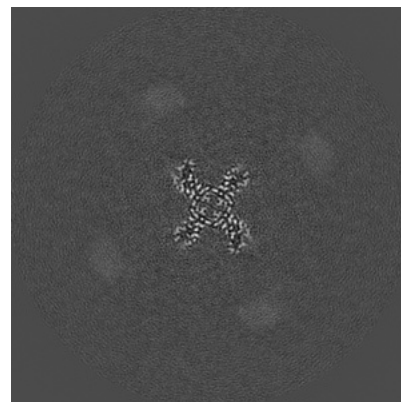
### 6.2.1 Primary map



X Index: 180

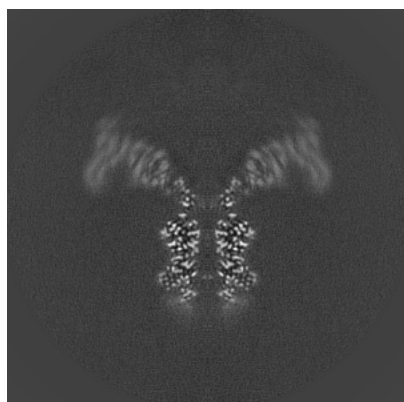


Y Index: 180

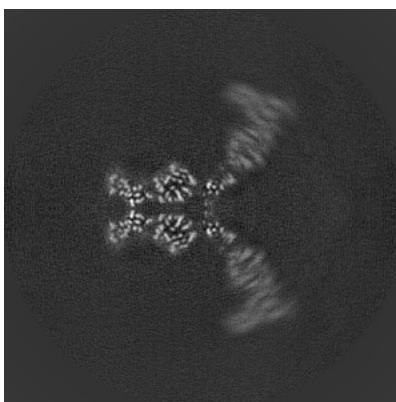


Z Index: 180

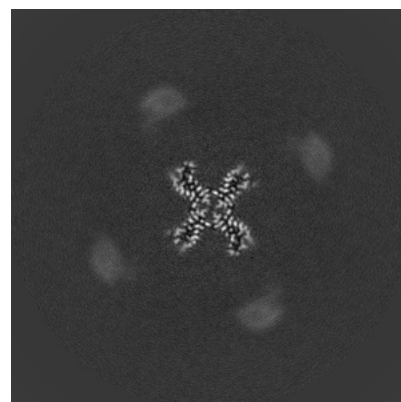
### 6.2.2 Raw map



X Index: 180



Y Index: 180

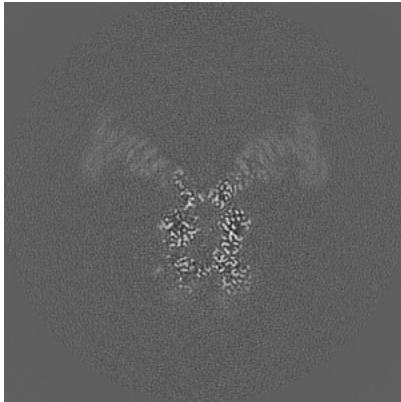


Z Index: 180

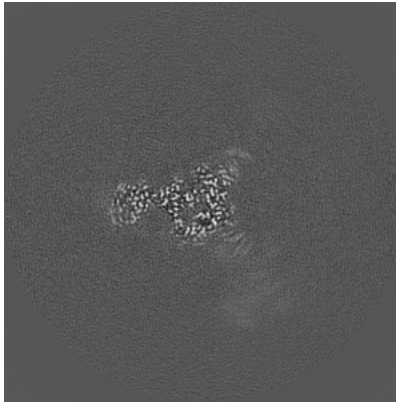
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

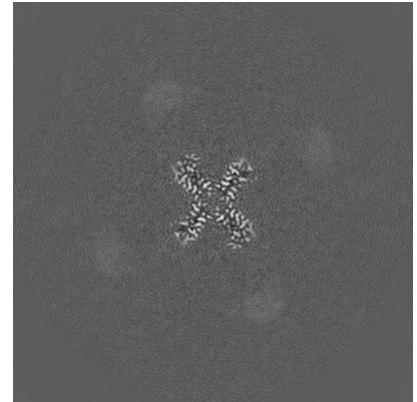
### 6.3.1 Primary map



X Index: 175

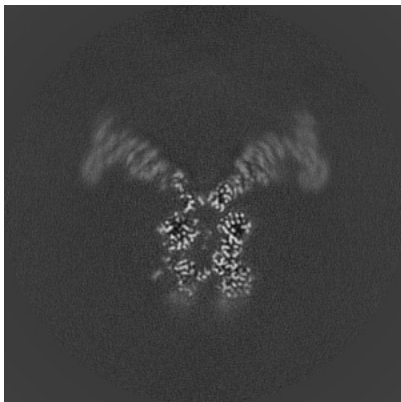


Y Index: 160

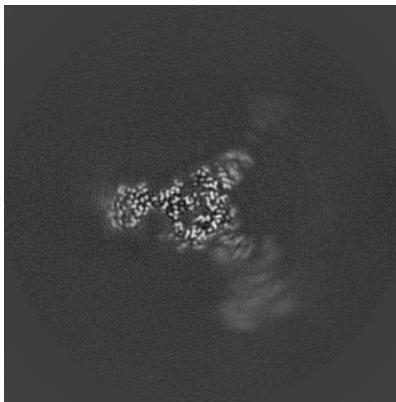


Z Index: 179

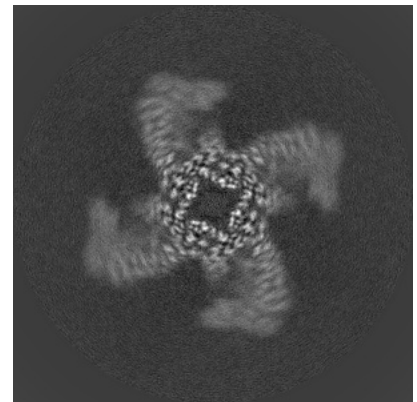
### 6.3.2 Raw map



X Index: 175



Y Index: 160

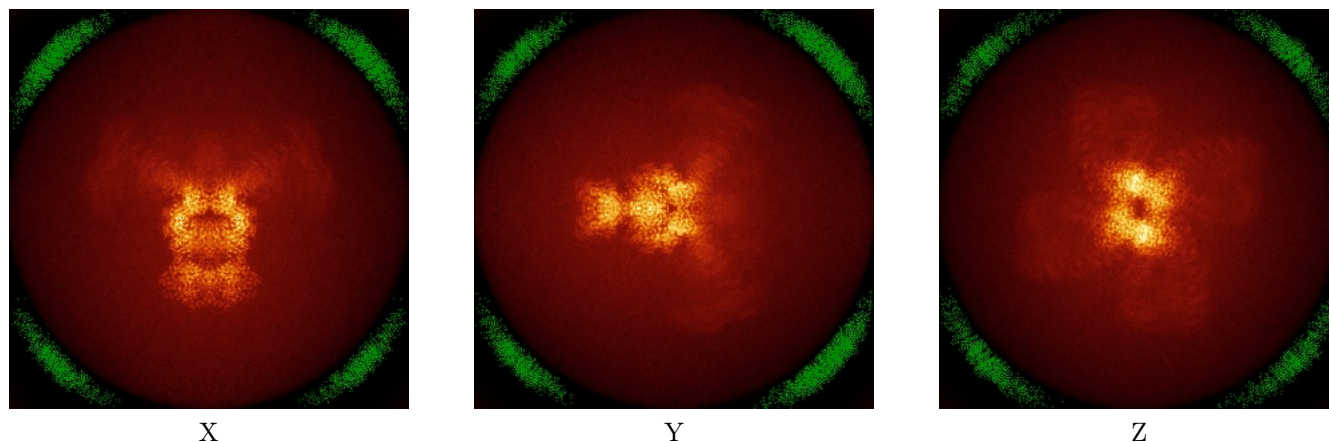


Z Index: 204

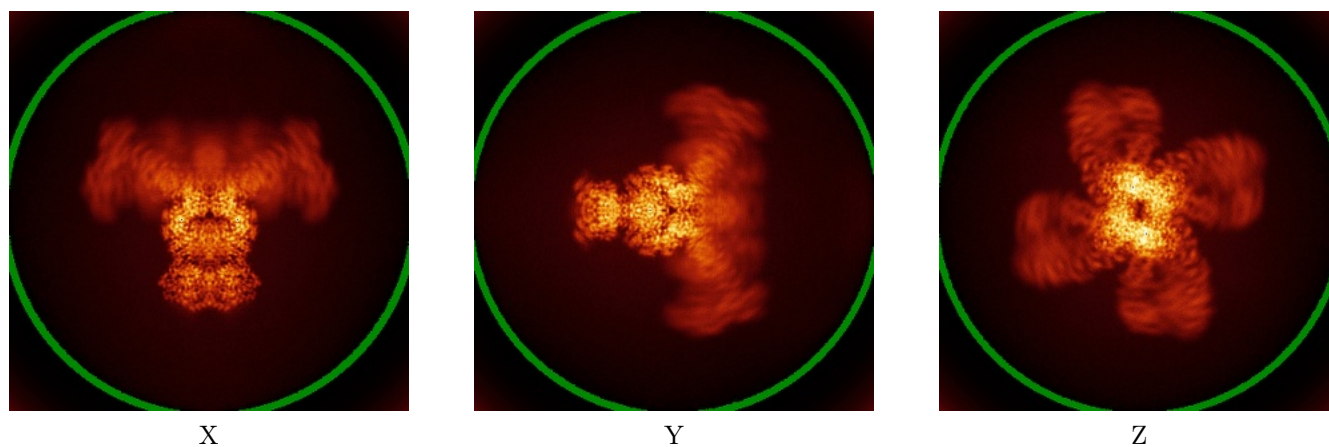
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



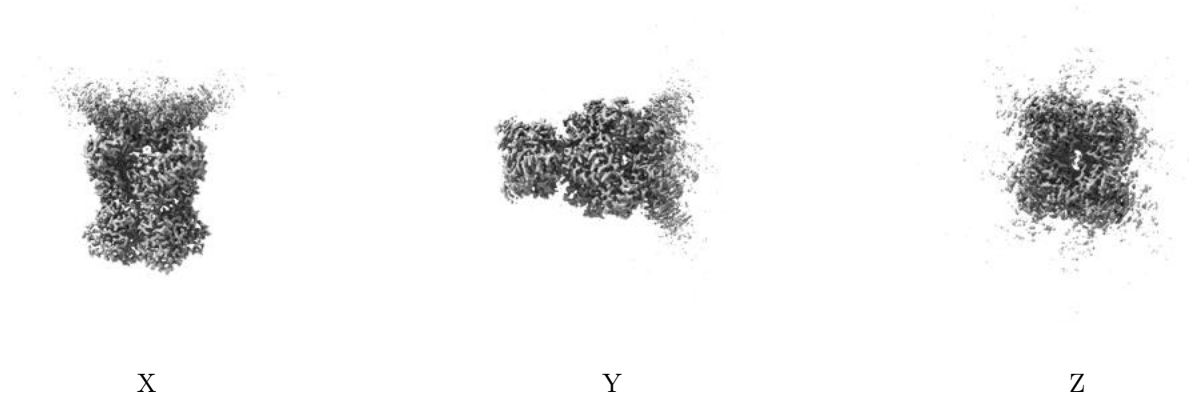
### 6.4.2 Raw map



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.

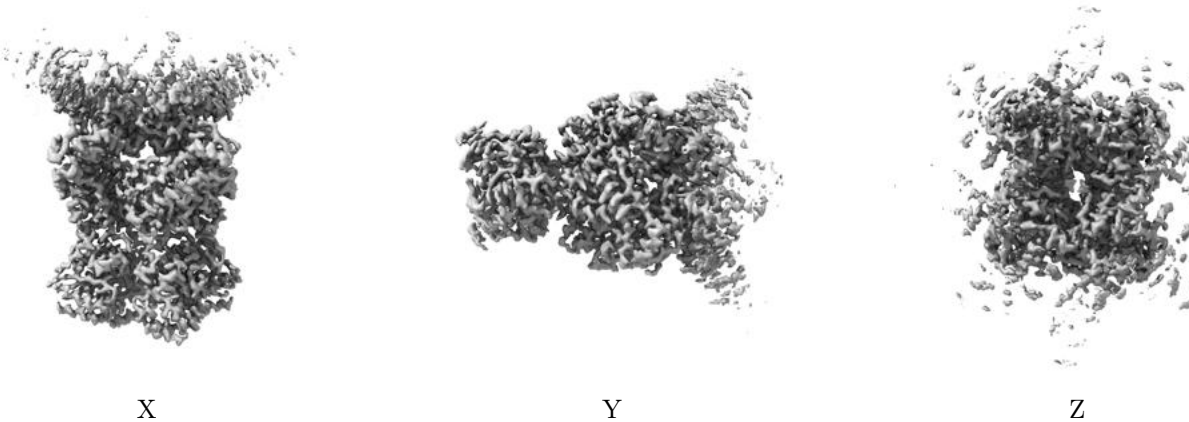
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

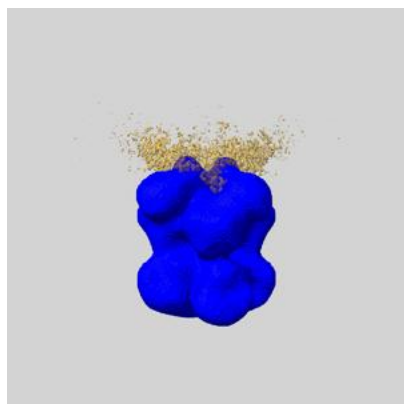
## 6.6 Mask visualisation [i](#)

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

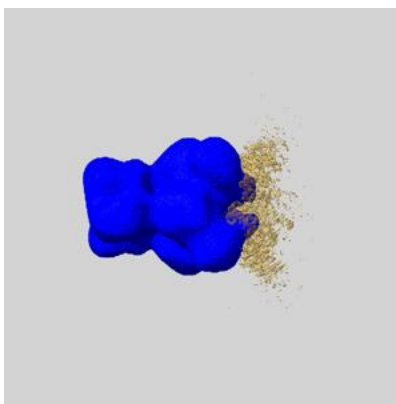
A mask typically either:

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

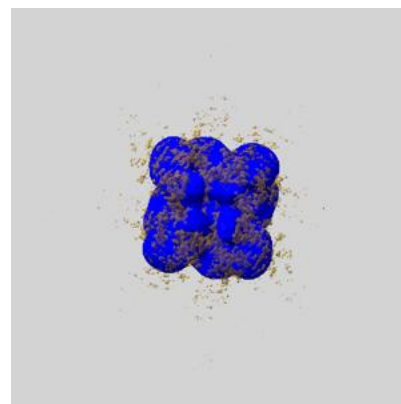
### 6.6.1 emd\_27422\_msk\_1.map [i](#)



X



Y

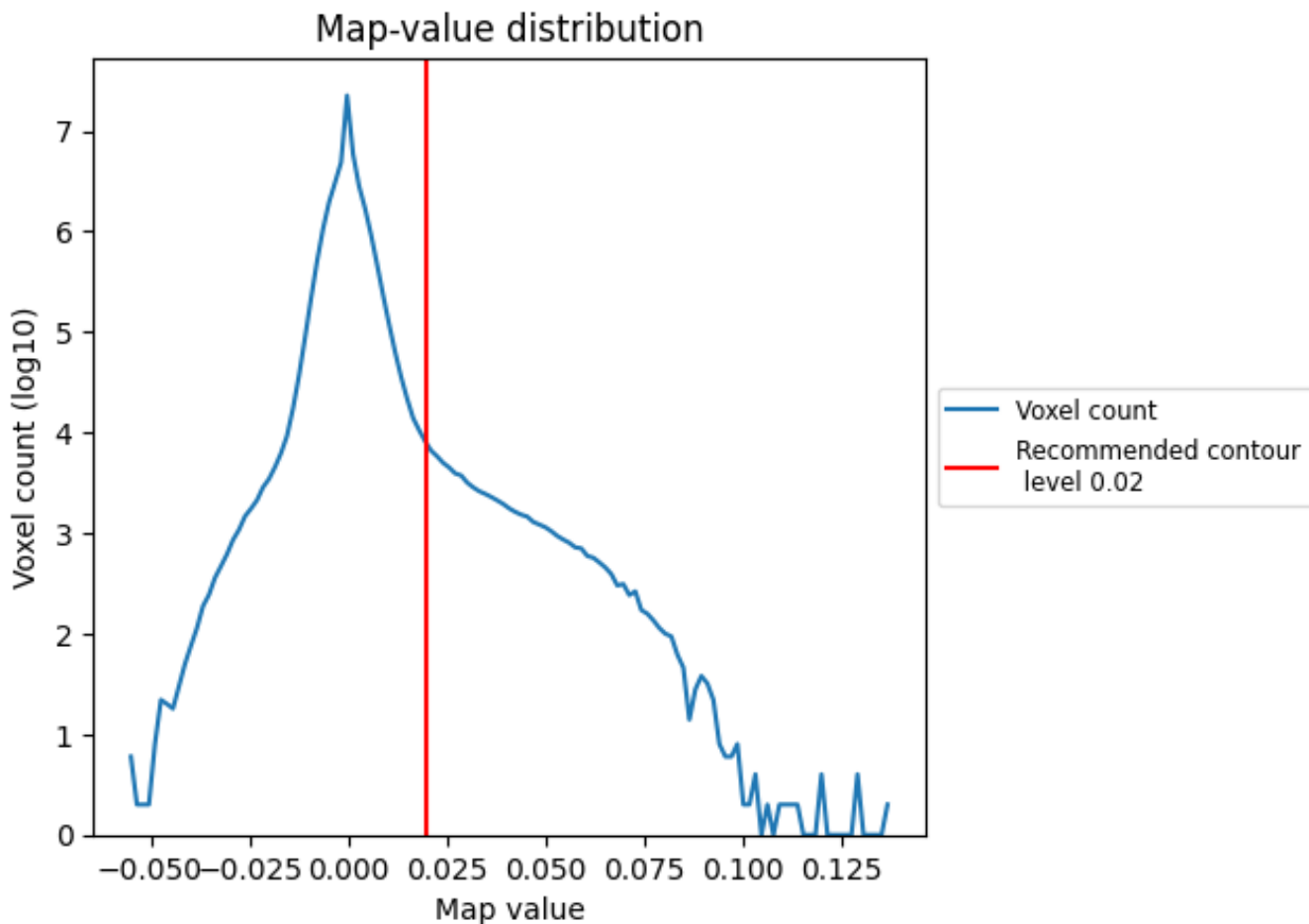


Z

## 7 Map analysis [i](#)

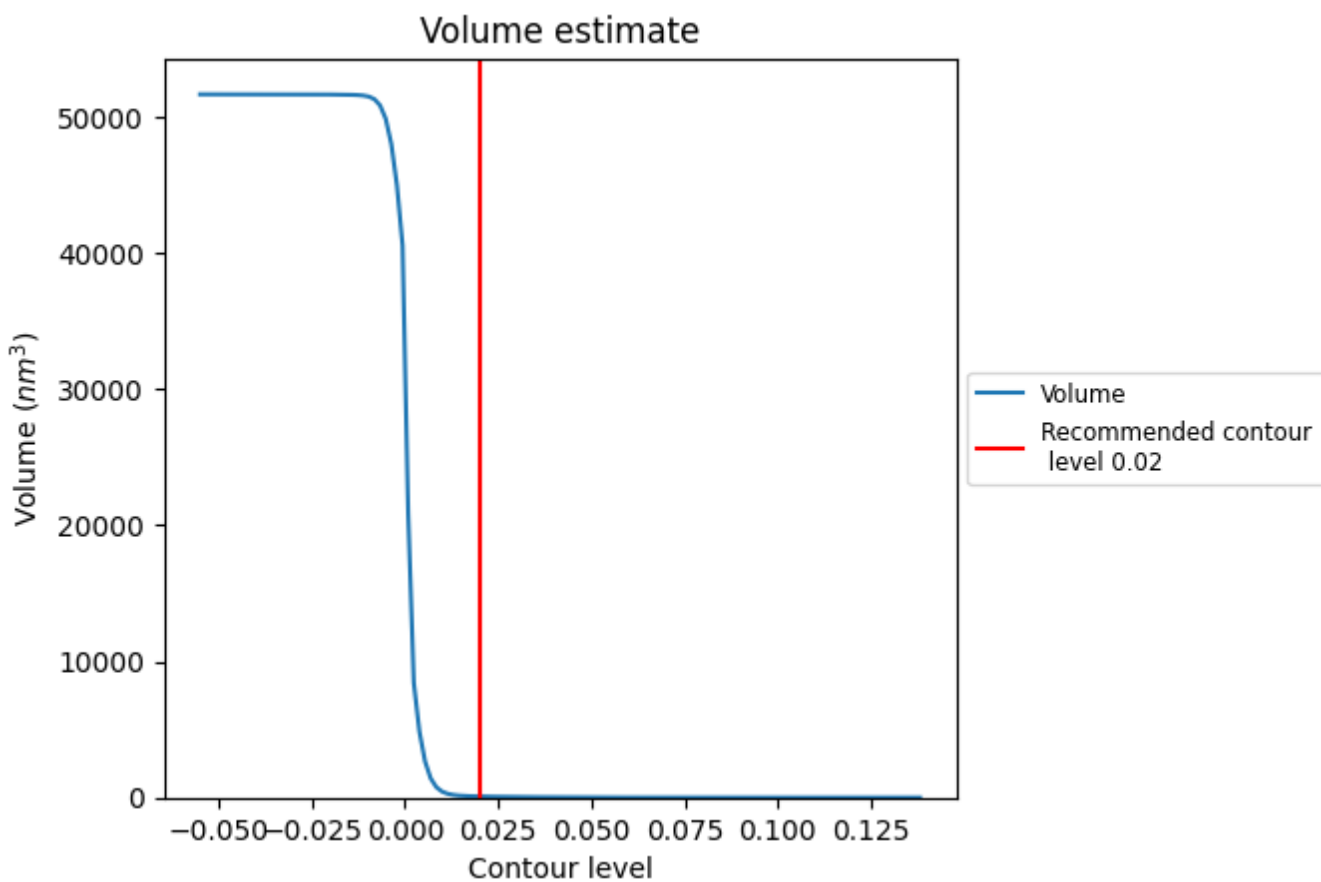
This section contains the results of statistical analysis of the map.

### 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.

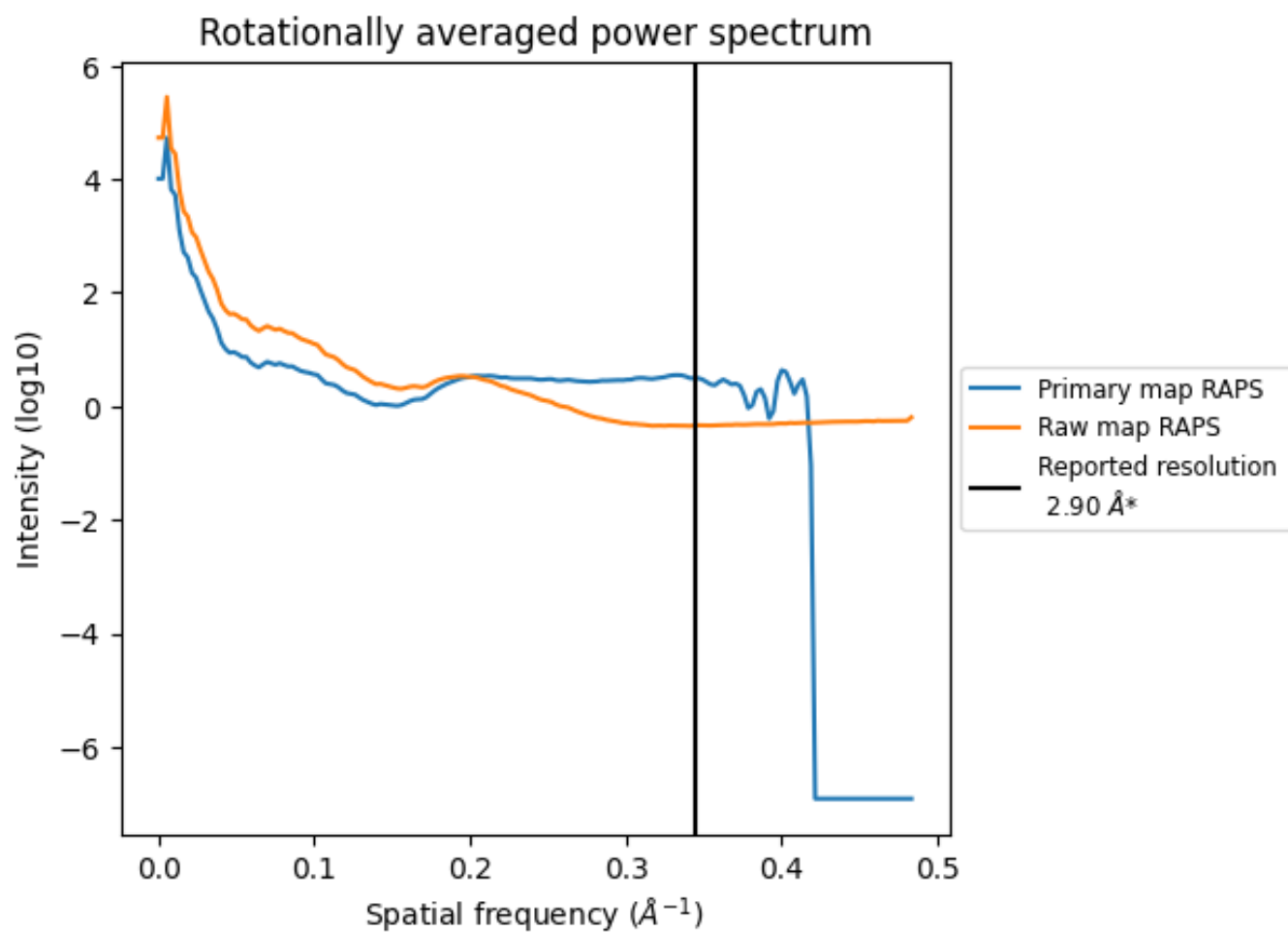
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $80 \text{ nm}^3$ ; this corresponds to an approximate mass of 73 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

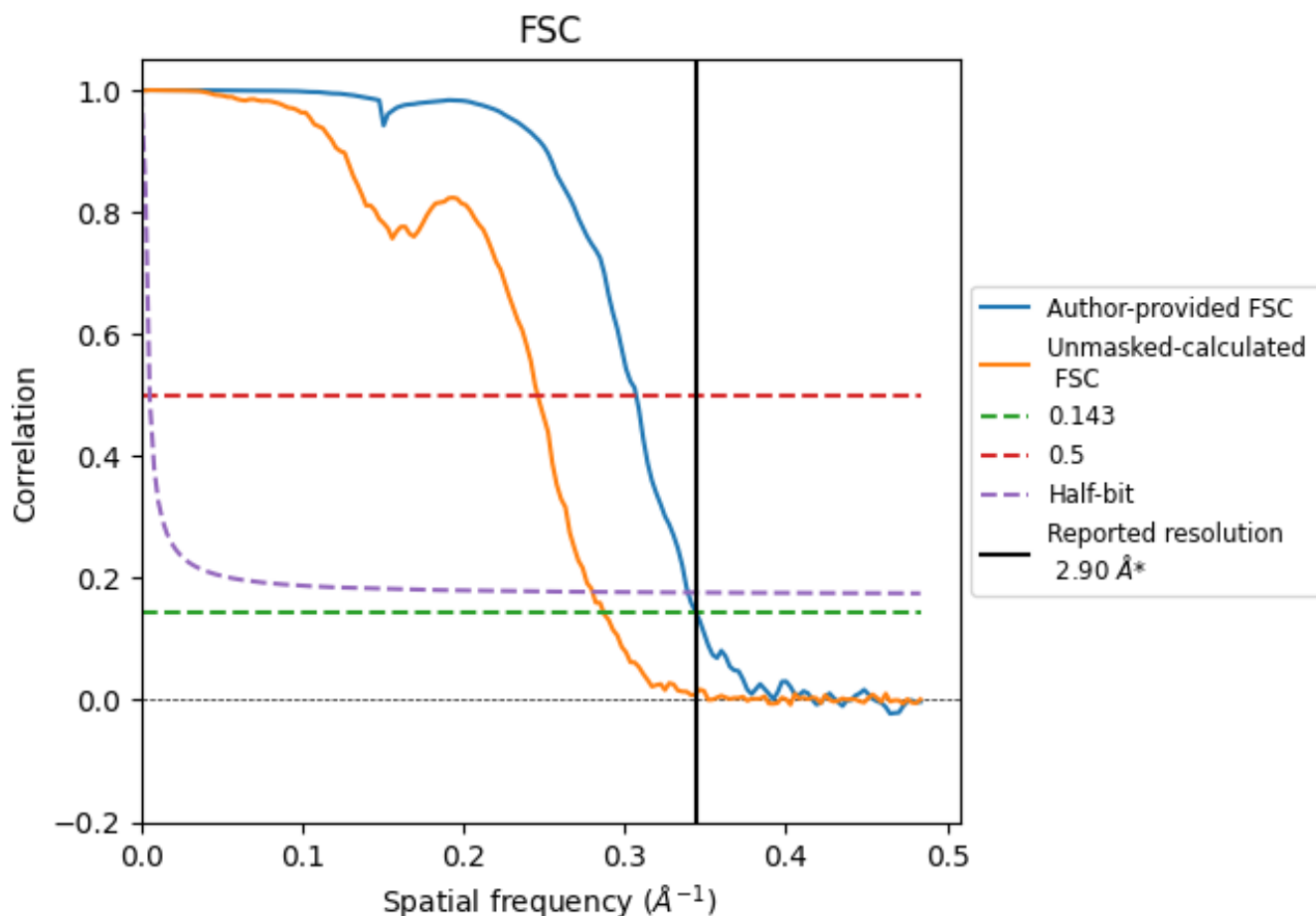


\*Reported resolution corresponds to spatial frequency of 0.345 Å<sup>-1</sup>

## 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  $0.345 \text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

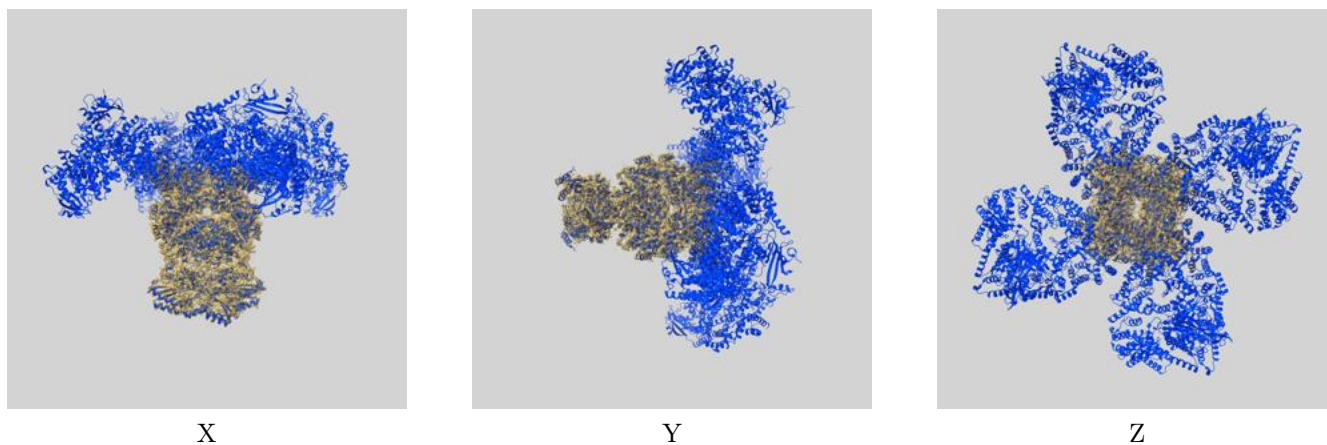
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.26	2.95
Unmasked-calculated*	3.48	4.07	3.57

\*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 3.48 differs from the reported value 2.9 by more than 10 %

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-27422 and PDB model 8DGF. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlay [i](#)



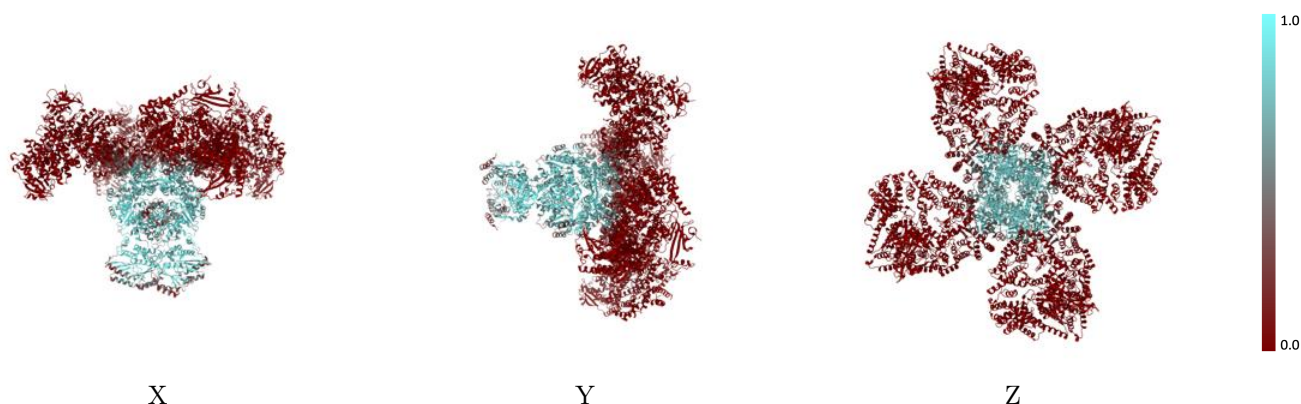
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



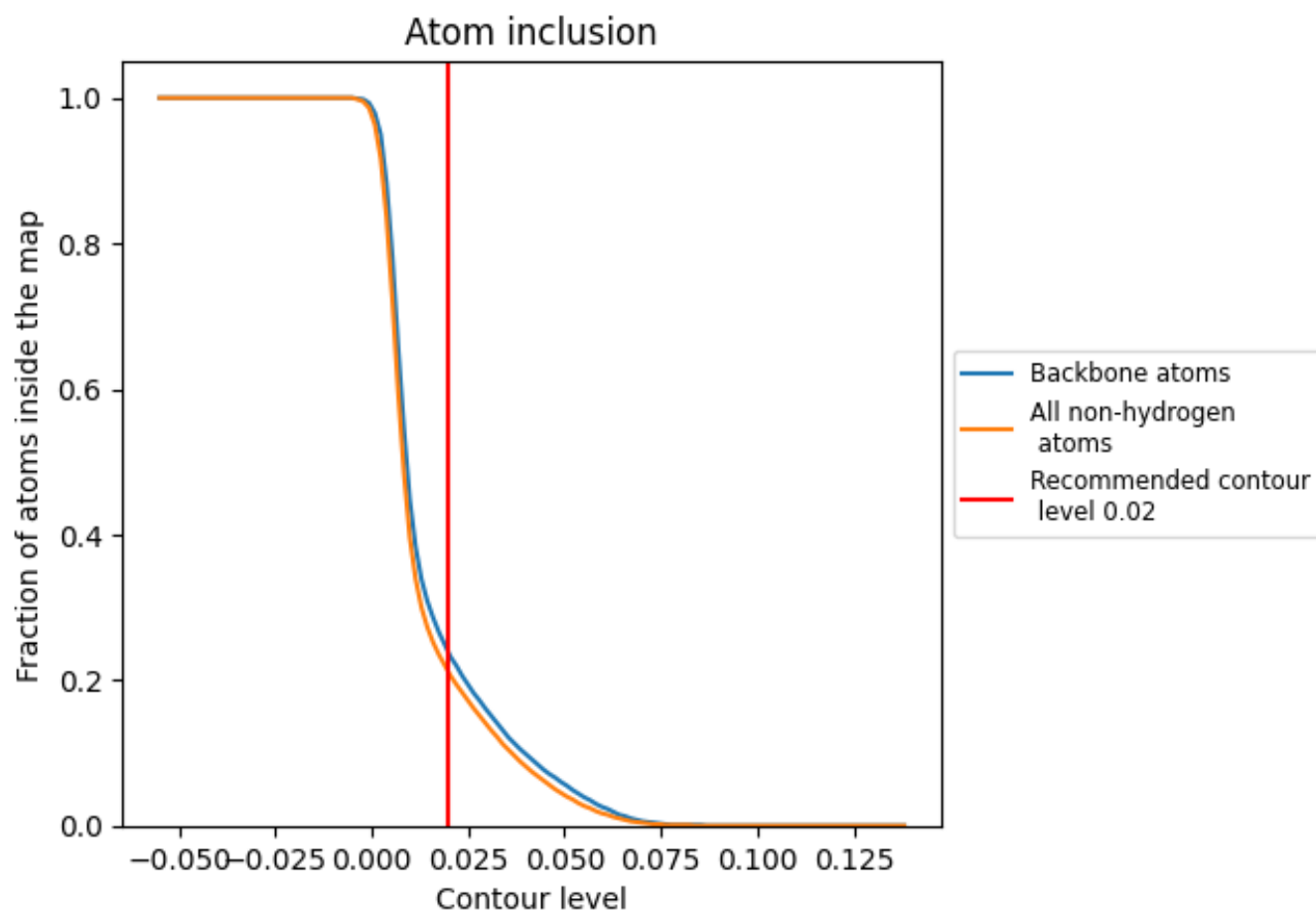
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 24% of all backbone atoms, 21% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2110	 0.2340
A	 0.2860	 0.2990
B	 0.2480	 0.2640
C	 0.2860	 0.3000
D	 0.2470	 0.2650
E	 0.0000	 0.0570
F	 0.0000	 0.0470
G	 0.0000	 0.0570
H	 0.0000	 0.0470

