



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:44 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 Full wwPDB EM Validation 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

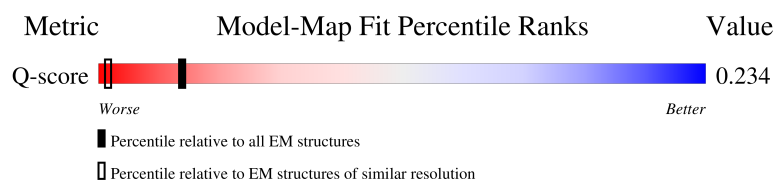
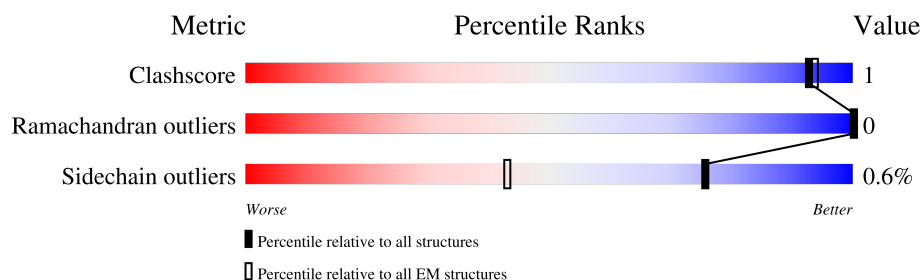
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 ≥ 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	66% 94%
1	B	1587	69% 93%
1	C	1587	66% 94%
1	D	1587	69% 94%

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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

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
1	A	1541	Total	C	N	O	S	0	0
			12805	8291	2104	2370	40		
1	B	1534	Total	C	N	O	S	0	0
			12756	8265	2094	2358	39		
1	C	1541	Total	C	N	O	S	0	0
			12805	8291	2104	2370	40		
1	D	1534	Total	C	N	O	S	0	0
			12756	8265	2094	2358	39		

- Molecule 2 is a protein called Portal protein.

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

- 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).



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

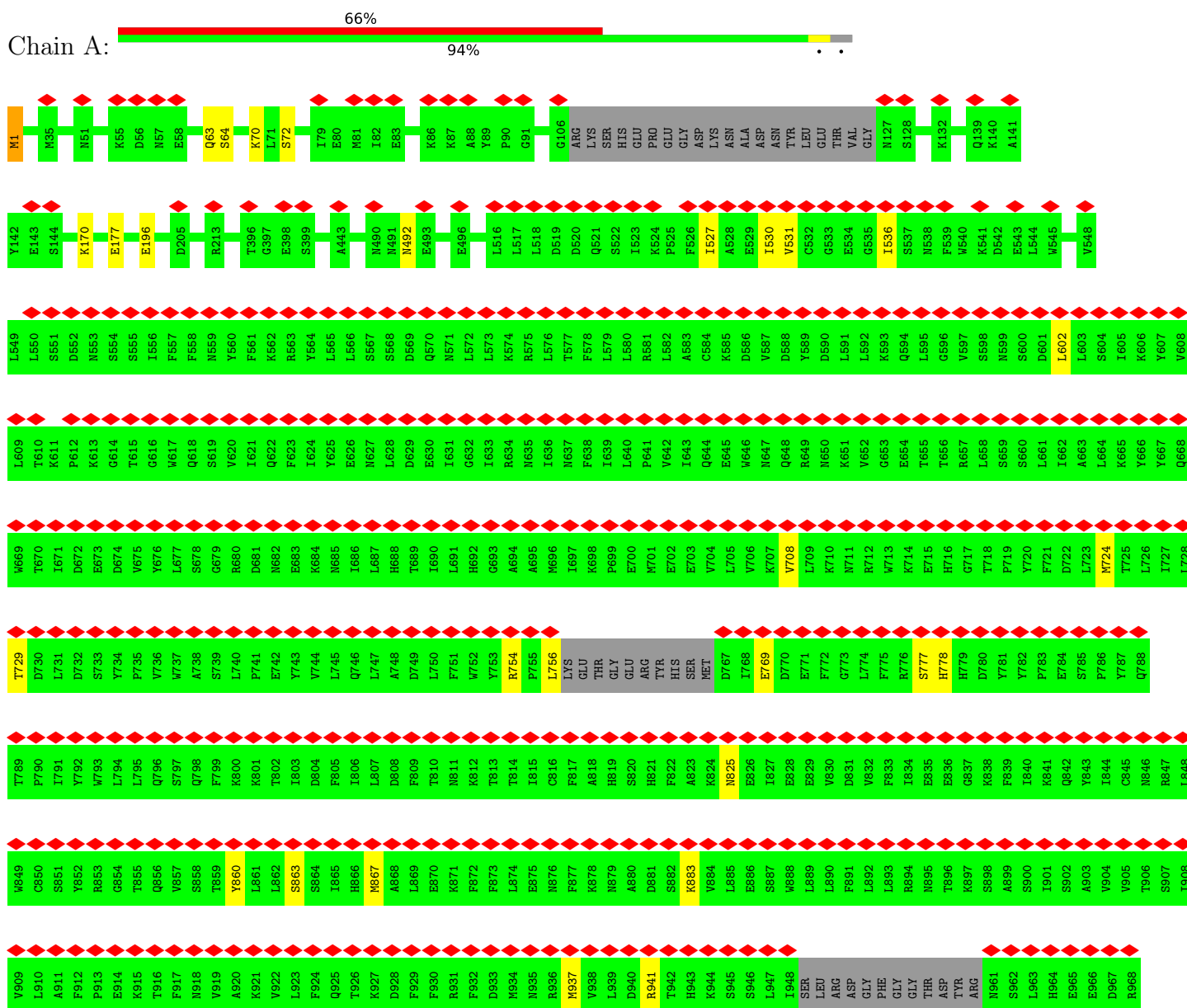
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total Mg 1 1	0
4	B	1	Total Mg 1 1	0
4	C	1	Total Mg 1 1	0
4	D	1	Total Mg 1 1	0

3 Residue-property plots

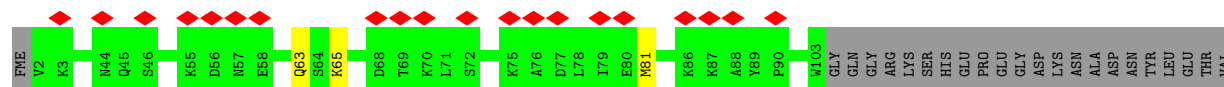
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ATP-binding protein Avs4

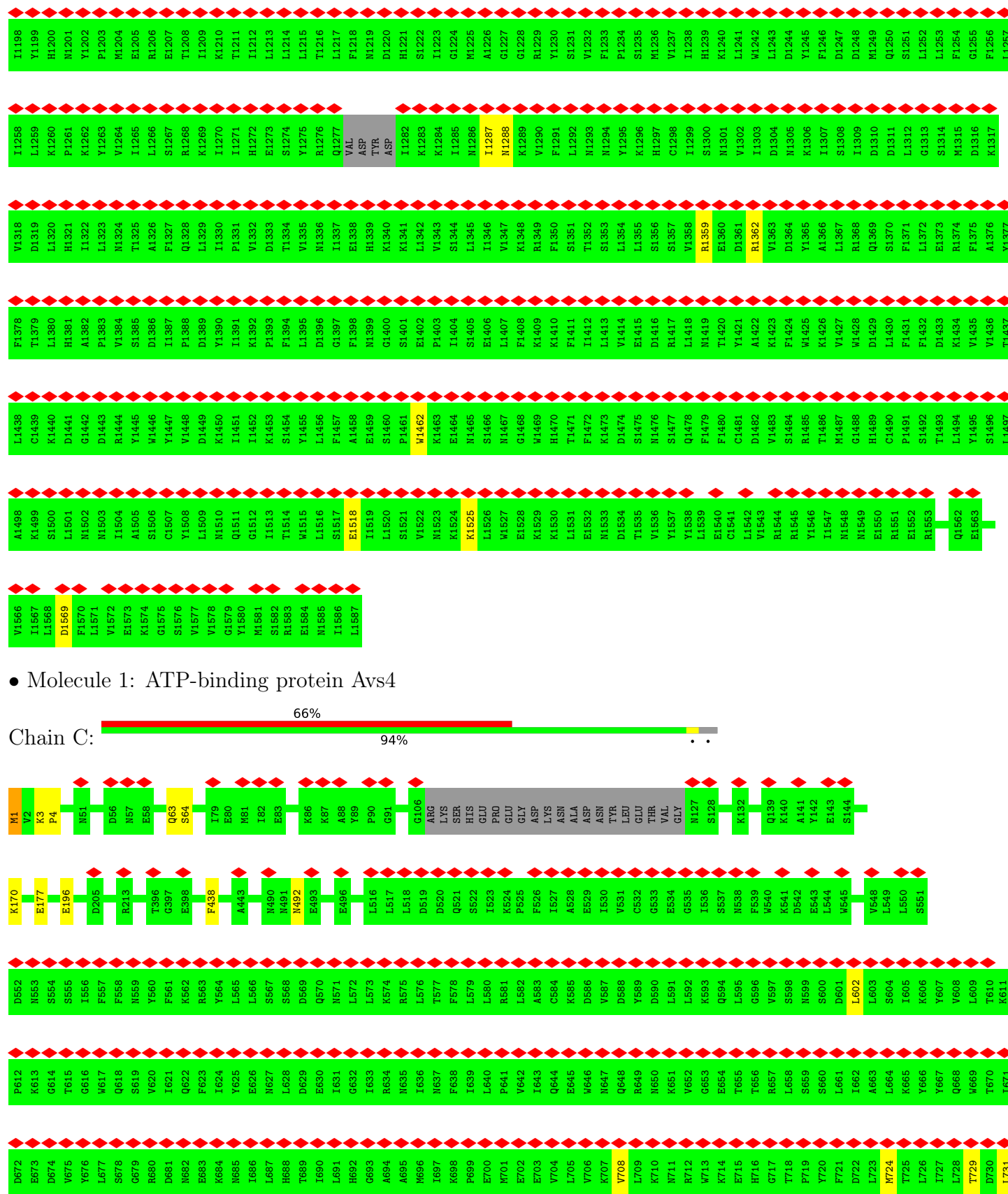


V1578	G1579	Y1580	M1581	S1582	N1585	I1586	L1587
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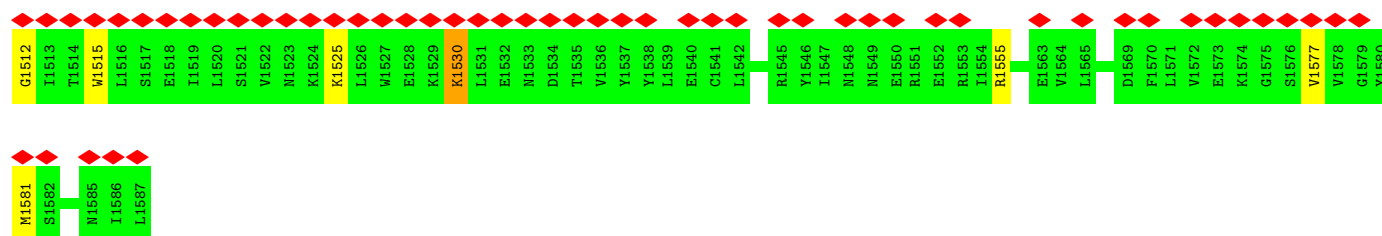
Chain B:



G1138	N1078	Q1018	ASP	S898	K838	H778	T718	L658	S598	N538	K311	GLY
N1139	S1079	L1019	TYR	A899	F839	H779	P719	S659	N599	F539	K321	ASN
I1140	E1080	P1020	ARG	S900	I840	D780	Y720	S660	N599	W540	K322	ASN
P1141	H1081	D1021		I901	K841	Y781	F721	L661	D601	K541		
A1142	M1082	E1022		S902	S962	Y782	D722	I662	L602	D542	N331	
D1143	K1083	A1023		A903	Y843	P783	L723	A663	L603	E543	Y332	
Y1084	Y1084	Q1024		V904	L844	E784	M724	L664	S604	L544	L333	
C1145	V1085	E1025		V905	C845	S785	T725	K665	I605	W545	I133	
S1146	T1086	T1026		T906	N846	P786	L726	Y666	K606	V546	D335	
V1147	L1087	E1027		S907	R847	Y787	I727	Y667	Y607	A547	L336	
K1088	L1088	A1028		I908	L848	Q788	L728	Q668	V608	V548	N337	
L1149	L1089	D1029		V909	W849	T789	T729	W669	L609	L549	Y338	
W1090	W1090	K1030		L910	C850	P790	D730	I670	T610	L550	A339	
A1091	A1091	T1031		A911	S851	I791	L731	I671	K611	S551	F340	
S1092	S1092	W1032		F912	Y852	Y792	D732	D672	P612	D552	I341	
Y1093	Y1093	R1033		P913	R853	Y793	S733	E673	K613	N553	D342	
K1094	K1094	L1034		E914	G854	L794	Y734	D674	G614	S554	I343	
R1095	R1095	C1035		K915	T855	L795	P735	V675	T615	S555	Y344	
E1096	E1096	L1036		T916	Q856	Q796	V736	Y676	G616	I556	K345	
K1097	K1097	A1037		F917	W857	S797	W737	L677	W617	F557	I346	
D1098	D1098	R1038		N918	S858	Q798	A738	S678	Q618	F558	T347	
E1099	E1099	M1039		V919	T859	F799	S739	G679	S619	N559	E357	
R1100	R1100	D1040		Y980	Y860	K800	L740	R680	V620	Y560		
Y1101	Y1101	L981		K921	L861	K801	P741	D681	I621	F561	E363	
K1102	K1102	E982		V922	L862	T802	E742	N682	Q622	K562		
N1103	N1103	K1043		L923	S863	I803	Y743	E683	F623	R563	D366	
Y1104	Y1104	M1044		F924	S864	D804	V744	K684	I624	Y564	T396	
G1105	G1105	K1045		Q925	T865	F805	L745	N685	Y625	L565	G397	
M1106	M1106	I1046		T926	H866	I806	Q746	I686	E626	S567	E398	
Y1107	Y1107	T1047		K927	K867	L807	L747	L687	N627	S568		
E1108	E1108	T1048		D928	A868	D808	A748	H688	L628	D569	M492	
D1109	D1109	K1049		F929	L869	F809	D749	T689	D629	D569		
N1110	N1110	E1050		F930	E870	T810	L750	I690	E630	Q570	E500	
P1111	P1111	K1051		R931	K871	N811	F751	L691	I631	N571		
Q1112	Q1112	D1052		R992	F872	F812	W752	H692	G632	L572	R515	
I1113	I1113	E1053		D933	F873	T813	Y753	G693	I633	L573	L516	
A1114	A1114	G1054		N934	L874	T814	R754	A694	R634	K574	L517	
P1115	P1115	I1055		N935	E875	L815	P755	A695	N635	R575	L518	
Q1116	Q1116	E1056		R936	N876	C816	L756	M696	I636	L576	D519	
E1117	E1117	I1057		N937	F877	F817	LYS	I697	N637	T577	D520	
T1118	T1118	S1058		V938	K878	A818	GLU	K698	F638	F578	Q521	
K1119	K1119	F1059		L939	N879	H819	THR	P699	I639	L579	Q522	
E1120	E1120	M1060		D940	A880	S820	GLY	E700	L639	L580	S523	
I1121	I1121	P1061		R941	D881	H821	GLU	M701	L640	R581	I523	
I1122	I1122	E1062		T942	S882	F822	TVR	E702	P641	L582	K524	
K1123	K1123	I1063		H943	K883	A823	HIS	E703	V642	L582	P525	
L1124	L1124	D1064		R1004	V884	K824	MET	E704	I643	A583	F526	
N1125	N1125	P1065		S945	L885	N825	D767	V704	Q644	C584	I527	
L1126	L1126	K1066		S946	E886	E826	I768	L705	E545	K585	A528	
E1127	E1127	L1067		L947	S887	I827	E769	V706	W646	D586	E529	
E1128	E1128	K1068		I948	W888	E828	E770	K707	N647	V587	I530	
G1129	G1129	Q1069		I948	L889	E829	D770	V708	N647	D588	V531	
S1130	S1130	Y1070		LEU	L890	E829	E771	L709	Q648	Y589	C532	
E1131	E1131	S1071		ARG	K890	V830	F772	K710	R649	D590	G533	
D1132	D1132	E1072		ASP	F891	D831	G773	N711	N650	E534	E534	
F1133	F1133	E1073		GLY	L893	F833	L774	R713	V652	L591	G535	
R1134	R1134	A1074		PHE	R894	L834	F775	K714	E654	L536		
L1135	L1135	I1075		THR	N895	E835	S777	E715	T655	G596		
L1136	L1136	K1076		THR	T896	E836		H716	T656	V597	S537	
N1137	N1137	K1077			K897	E837		G717	R657			

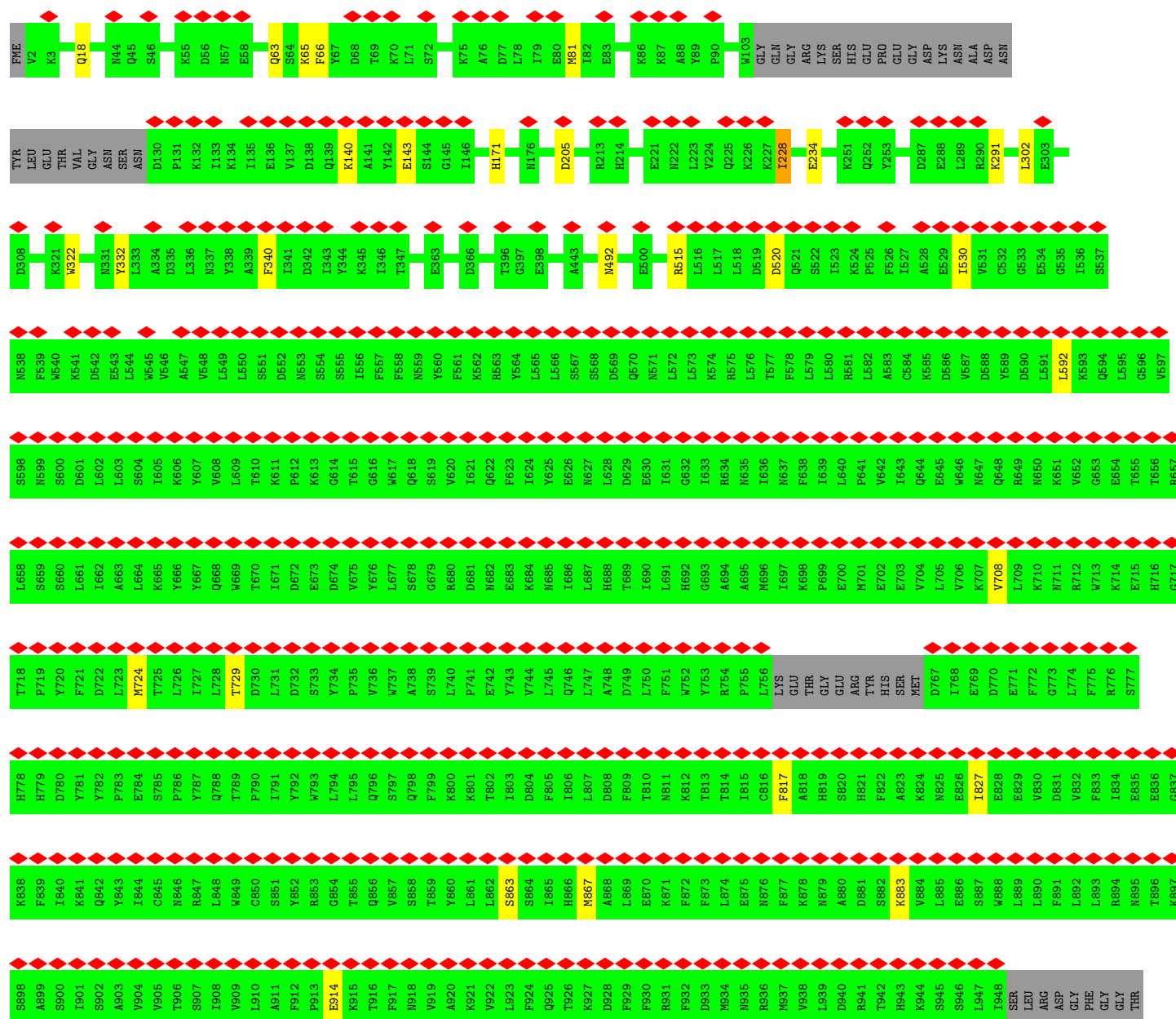


I1452	K1392	V1352	H1272	I1212	Y1152	S1092	V1032	C972	F912	Y852	Y792	D732
K1453	P1393	D1333	E1273	I1213	F1153	Y1093	R1033	D973	P913	R853	W93	S733
S1454	F1394	T1334	S1274	L1214	M1154	K1094	L1034	D974	E914	G854	L794	Y734
Y1455	L1395	V1335	Y1275	L1215	Q1155	R1095	C1035	V975	K915	T855	L795	P735
L1456	D1396	I1336	A1276	L1216	L1156	E1096	L1036	H976	T916	Q856	Q796	V736
F1457	G1397	I1337	Q1277	L1217	M1157	K1097	A1037	R977	F917	W857	W797	W737
A1458	F1398	E1338	VAL	F1218	M1158	D1098	A1038	N978	N918	S858	Q798	A738
E1459	M1399	H1339	ASP	M1219	E1159	E1099	M1039	T979	V919	T859	F799	S739
S1460	G1400	K1340	TYR	D1220	R1100	R1100	D1040	Y980	A920	Y860	K800	L740
S1461	S1401	K1341	ASP	H1221	E1161	Y1101	R1041	L981	K921	L861	K801	P741
E1462	E1402	L1342	I1282	S1222	E1162	K1102	R1042	E982	V922	L862	T802	E742
K1463	P1403	V1343	K1283	I1223	Y1163	M1103	K1043	N983	L923	S863	I803	Y743
E1464	I1404	S1344	K1284	G1224	C1164	Y1104	F924	L984	F924	S864	D804	V744
S1465	S1405	L1345	I1285	M1225	K1165	K1105	Q925	A985	Q925	I865	F805	L745
S1466	E1406	I1346	T1286	A1226	D1166	M1106	I1046	L986	T926	H866	I806	Q746
N1467	L1407	V1347	T1287	G1227	I1167	Y1107	T1047	H987	K927	M867	L807	L747
G1468	F1408	K1348	M1288	G1228	V1168	E1108	T1048	Y988	D928	A868	D808	A748
W1469	K1409	R1349	K1289	R1229	L1169	D1109	K1049	Q989	F929	L869	F809	D749
H1470	K1410	F1350	V1290	Y1230	A1170	M1110	E1050	I990	F930	E870	T810	L750
T1471	F1411	S1351	L1291	S1231	Y1171	P1111	K1051	F991	R931	K871	N811	F751
F1472	L1412	T1352	M1293	V1232	K1172	I1112	D1052	A992	F932	F872	K812	W752
K1473	L1413	S1353	M1294	F1233	S1173	I1113	E1053	S993	D933	F873	T813	Y753
D1474	V1414	L1354	Y1295	P1234	L1174	A1114	G1054	E994	M934	L874	T814	R754
S1475	E1415	L1355	K1296	S1235	P1175	L1115	I1055	N995	N935	E875	I815	P755
N1476	D1416	S1356	H1297	M1236	L1176	K1116	E1056	V996	R936	N876	C816	L756
S1477	R1417	K1357	C1298	V1237	K1177	E1117	I1057	T997	M937	F877	F817	LYS
Q1478	L1418	V1358	I1299	I1238	E1178	T1118	S1058	E998	V938	K878	A818	GLU
F1479	M1419	R1359	S1300	H1239	G1179	K1119	F1059	K999	L939	N879	H819	THR
F1480	L1420	E1360	M1301	K1240	M1180	E1120	M1060	D1000	D940	A880	S820	GLY
C1481	Y1421	D1361	V1302	L1241	Y1181	I1121	P1061	A1001	R941	S881	H821	GLU
D1482	A1422	R1362	I1303	W1242	Y1182	I1122	E1062	I1002	T942	S882	F822	ARG
V1483	K1423	V1363	D1304	L1243	Q1183	K1123	I1063	E1003	H943	K883	A823	TYR
S1484	F1424	D1364	M1305	D1244	Y1184	K1124	D1064	A1004	K944	V884	K824	SER
R1485	W1425	Y1365	K1306	L1245	Q1185	L1125	P1065	Q1005	S945	L885	N825	MET
T1486	K1426	A1366	T1307	F1246	D1186	M1126	K1066	Q1006	S946	E886	E826	I768
M1487	V1427	L1367	S1308	D1247	G1187	E1127	L1067	Q1007	L947	S887	I827	E769
G1488	W1428	R1368	I1309	D1248	T1188	E1128	K1068	L1008	I948	W888	E828	D770
H1489	D1429	Q1369	D1310	M1249	T1189	G1129	Q1069	W1009	SER	L889	E829	F772
C1490	L1430	S1370	D1311	Q1250	S1190	G1130	Y1070	D1010	LEU	L890	V830	G773
P1491	F1431	F1371	L1312	S1251	A1191	E1131	S1071	I1011	ASP	F891	D831	L774
S1492	F1432	L1372	G1313	L1252	I1192	D1132	E1072	F1012	ASP	L892	V832	F775
T1493	D1433	E1373	S1314	L1253	S1193	F1133	E1073	D1013	GLY	L893	F833	F776
L1494	K1434	R1374	M1315	F1254	A1194	R1134	A1074	K1014	GLY	R894	I834	R776
Y1495	V1435	F1375	D1316	G1255	L1195	L1135	I1075	Y1015	THR	N895	E835	S777
S1496	V1436	A1376	D1317	F1256	P1196	L1136	K1076	Y1016	ASP	T896	E836	H778
L1497	T1437	V1377	K1318	F1257	V1197	M1137	K1077	M1017	THR	K897	G837	H779
A1498	L1438	F1378	D1319	I1258	I1198	G1138	M1078	Q1018	ARG	S898	K838	D780
K1499	C1439	T1379	L1320	K1259	Y1199	M1139	S1079	L1019	N961	A899	F839	Y781
S1500	L1440	H1380	H1321	K1260	H1200	I1140	E1080	P1020	S962	S900	I840	Y782
N1502	D1441	L1381	I1322	P1261	M1201	P1141	H1081	D1021	L963	I901	K841	P783
M1503	G1442	A1382	L1323	K1262	Y1202	A1142	M1082	E1022	H964	S902	Q842	E784
I1504	D1443	P1383	M1324	Y1263	P1203	D1143	K1083	A1023	E965	A903	Y843	P786
A1505	R1444	V1384	T1325	V1264	M1204	V1144	Y1084	Q1024	E966	V904	I844	Y787
S1506	W1446	S1385	A1326	I1265	E1205	K1145	V1085	Q1025	D967	V905	C845	Q788
C1507	D1447	D1386	F1327	L1266	R1206	S1146	T1086	E1025	R968	T906	N846	W789
Y1508	F1447	T1387	Q1328	L1267	E1207	V1147	T1087	T1026	I969	T907	R847	P790
L1509	V1448	P1388	L1329	R1268	T1208	L1148	K1088	E1027	K970	S908	L848	I791
D1449	D1449	D1389	I1330	K1269	T1209	L1149	L1089	A1028	A971	V909	W849	
N1510	K1450	Y1390	P1331	I1270	K1210	L1150	W1090	K1030		L910	C850	
Q1511	I1451	T1391		I1271	T1211	D1151	A1091	T1031		A911	S851	



• Molecule 1: ATP-binding protein Avs4

Chain D:

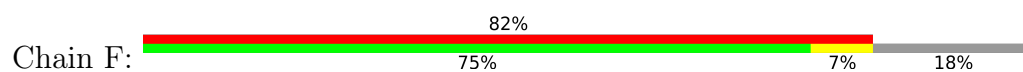


- Molecule 2: Portal protein

MET	ALA	SER	SER	GLN
K6	R7	E8	G9	F10
A11	E12	N13	G14	A15
K16	A17	V18	Y19	D20
A21	L22	K23	N24	D25
R26	N27	S28	Y29	E30
T31	R32	A33	E34	N35
C36	A37	X38	Y39	T40
I41	P42	S43	L44	F45
P46	K47	D48	S49	D50
N51	A52	S53	T54	D55
Y56	T57	T58	P59	V60

ILE	A421	ALA	N301	D241	V181	N121	Q61
LEU	V422	VAL	P302	A242	T182	Y122	A62
LYS	E423	GLN	A303	A243	L183	I123	V63
THR	P424	ARG	G304	Y244	D184	E124	G64
GLU	T425	THR	I305	P245	K185	S125	A65
GLU	T426	GLU	T306	V246	T186	N126	R66
GLN	S427	VAL	Q307	D247	Q187	S127	G67
GLN	T428	THR	V308	A248	Y188	Y128	L68
GLU	G429	ALA	R309	C249	A189	R129	N69
MET	M430	E372	R310	P250	A190	V130	N70
ALA	E431	E373	L311	Y251	L191	T131	L71
GLU	A432	I374	T312	I252	P192	L132	A72
ALA	L433	R375	K313	P253	E193	F133	S73
GLN	L434	Y376	A314	V254	D194	E134	K74
GLY	G434	V377	Q315	R255	V195	T135	L75
THR	R435	A378	T316	M256	R196	L136	M76
ALA	G436	S379	G317	V257	N197	K137	L77
LEU	Q437	E380	D318	R258	A198	Q138	A78
ASN	D438	L381	F319	I259	M199	L139	A79
ALA	L439	E382	V320	D260	D200	V140	F80
ALA	D440	D383	S321	G261	S201	V141	P81
SER	K441	T384	G322	E262	G202	A142	M82
GLY	L442	L385	R323	S263	Q203	G143	Q83
ALA	E443	G386	P324	Y264	E204	N144	T84
GLY	R444	G387	E325	G265	H205	A145	W85
ALA	C445	V388	D326	R266	K206	L146	M86
GLY	T446	Y389	I327	S267	G207	L147	K87
LEU	A447	S390	S328	Y268	D208	Y148	L88
ALA	A448	I391	F329	C269	E209	I149	T89
THR	W449	S393	L330	E270	M210	P150	I90
ALA	S450	SER	Q331	E271	I211	E151	S91
PRO	A451	Q394	L332	Y272	D212	P152	E92
GLU	L452	E395	E333	L273	V213	E153	F93
ASN	A453	L396	K334	G274	Y214	G154	E94
MET	P454	Q397	A335	D275	T215	A155	A95
ALA	M455	L398	A336	L276	H216	Y156	K96
ALA	GLN	P399	D337	R277	I217	N157	Q97
ALA	ASN	M400	F338	S278	Y218	P158	L98
GLN	PRO	V401	S339	L279	L219	M159	V99
ALA	ASP	R402	V340	E280	D220	K160	A100
GLY	ILE	V403	A341	N281	E221	L161	Q101
MET	ASN	L404	K342	L282	E222	Y162	P102
VAL	ILE	L405	A343	Q283	G224	R163	A103
PRO	ALA	K406	V344	E284	G224	L164	E104
ASN	THR	ILE	S345	A285	E225	S165	L105
	LYS	Q407	E346	I286	Y226	S166	A106
	LEU	LEU	Q409	V287	L227	Y167	K107
	ILE	ALA	Q347	K287	K228	V168	V108
	ALA	ASN	I348	M289	Y229	V169	E109
	ASN	ALA	T411	E349	M289	R171	G111
	ILE	GLY	M412	G350	E230	Q170	E110
	GLY	ILE	Q413	R351	M291	R171	G111
	ILE	ASP	I414	L352	I292	D172	L112
	THR	THR	P415	S353	S293	A173	S113
	SER	SER	E416	Y354	A294	F174	M114
	GLY	GLY	L417	A355	K295	G175	V115
			P418	F356	V296	T176	E116
			K419	M357	I297	V177	R117
			E420	L358	G298	L178	I118
				N359	L299	Q179	L119
				SER	V300	T180	M120

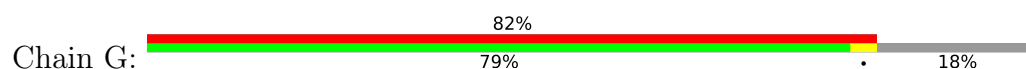
• Molecule 2: Portal protein



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	N27	S28	Y29	E30	T31	R32	A33	E34	N35	C36	A37	K38	Y39	T40	I41	P42	S43	L44	F45	P46	K47	D48	S49	D50	N51	A52	S53	T54	D55	Y56	T57	T58	P59	W60		
	Q61	A62	V63	G64	A65	R66	Q67	L68	N69	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	A106	K107	V108	E109	E110	G111	L112	M113	V114	L115	E116	R117	I118	L119	M120
	N121	Y122	I123	E124	S125	N126	S127	Y128	R129	V130	T131	L132	F133	E134	T135	L136	K137	Q138	L139	V140	V141	A142	G143	N144	A145	L146	L147	Y148	I149	P150	E151	P152	E153	G154	A155	Y156	N157	M158	M159	K160	L161	Y162	R163	L164	S165	S166	Y167	V168	V169	Q170	R171	D172	A173	F174	G175	T176	V177	L178	Q179	I180
	V181	T182	L183	D184	K185	T186	A187	L188	A189	A190	L191	P192	E193	D194	V195	R196	N197	A198	M199	D200	S201	G202	Q203	E204	H205	K206	G207	D208	E209	M210	I211	D212	V213	Y214	T215	H216	I217	Y218	L219	D220	E221	E222	S223	G224	E225	Y226	L227	K228	Y229	E230	E231	I232	D233	G234	V235	E236	V237	D238	G239	T240
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	E280	N281	L282	Q283	E284	A285	I286	V287	K288	M289	S290	M291	I292	S293	A294	K295	V296	I297	G298	L299	V300	

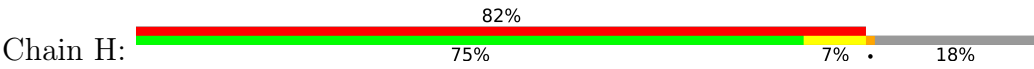
ILE	LEU	LYS	THR	PRO	GLU	GLU	GLN	GLN	GLU	MET	ALA	ALA	ALA	GLN	GLY	THR	ALA	LEU	GLU	ASN	ALA	ALA	GLY	GLY	ALA	GLY	LEU	ALA	THR	ALA	SER	PRO	GLU	ASN	MET	GLU	ALA	ALA	ALA	ALA	ALA	ASN	ASP	PRO	GLN	GLY	GLY	MET	VAL	PRO	ASN									
A421	V422	E423	P424	T425	I426	S427	T428	G429	M430	E431	A432	L433	G434	R435	G436	Q437	D438	L439	D440	K441	L442	E443	R444	C445	I446	A447	A448	W449	S450	A451	L452	A453	P454	M455	GLN	ASN	ASP	PRO	ASP	ILE	ASN	ILE	ILE	ALA	THR	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ILE	ILE	GLY	ILE	ASP	THR	SER	GLY
ALA	VAL	GLN	ARG	THR	GLY	GLU	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	M400	V401	R402	V403	L404	L405	K406	Q407	L408	Q409	A410	T411	N412	Q413	I414	P415	E416	L417	P418	K419	E420		
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	

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ILE	LEU	LYS	THR	PRO	GLU	GLU	GLN	GLN	GLU	MET	ALA	GLU	ALA	GLN	GLY	THR	ALA	GLU	GLU	ASN	ALA	ALA	ALA	SER	GLY	ALA	GLY	ALA	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY
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• Molecule 2: Portal protein



ILE	A421	VAL	N301	D241	V181	N121	Q61	MET
	LEU	V422		GLN	A242	T182	Y122	
LYS	E423	ARG	P302	S243	L183	I123	V63	SER
THR	P424	THR	A503	Y244	D184	E123	G64	GLN
GLU	T425	GLY	I305	P245	K185	S125	A65	K6
GLU	I426	GLU	T306	V246	T186	N126	R66	R7
LYS	S427	ARG	Q307	D247	A187	S127	G67	E8
GLN	T428	VAL	V308	A248	Y188	S127	L68	G9
GLN	G429	THR	R309	C249	A189	R129	N69	F10
GLU	M430	ALA	R310	P250	A190	V130	N70	GLU
ALA	E431	I374	L311	Y251	L191	T131	L71	A11
ALA	A432	R375	T312	T252	P192	L132	A72	E12
GLN	L433	Y376	K313	P253	E193	F133	S73	N13
GLY	G434	A314	A314	R254	D194	E134	K74	G14
THR	R435	V377	Q315	R255	V195	T135	L75	A15
ALA	G436	A378	T316	M256	R196	L136	M76	K16
LEU	Q437	S379	G317	V257	N197	K137	L77	A17
GLU	D438	E380	D318	R258	A198	Q138	A78	V18
ASN	L439	L381	F319	I259	M199	L139	L79	Y19
ALA	A440	D382	V320	D260	D200	V140	F80	D20
ALA	SER	T384	S321	G261	S201	V141	P81	A21
ALA	K441	L442	G322	E262	G202	A142	M82	L22
GLY	E443	L385	R323	S263	Q203	G143	Q83	K23
ALA	R444	G386	P324	Y264	E204	N144	T84	N24
GLY	C445	G387	E325	G265	H205	A145	W85	D25
ALA	I446	V388	D326	R266	K206	L146	M86	R26
ALA	A447	Y389	I327	S267	G207	L147	K87	N27
LEU	A448	S390	S328	Y268	D208	Y148	L88	S28
ALA	THR	I391	F329	C269	E209	E149	T89	Y29
THR	W449	L392	L330	E270	M210	P150	I90	E30
SER	S450	S393	Q331	E271	T211	E151	S91	T31
PRO	A451	Q394	L332	Y272	D212	P152	E92	R32
GLU	L452	E395	E333	L273	V213	E153	F93	A33
ASN	A453	L396	K334	G274	E214	G154	E94	E34
MET	P454	Q397	A335	D275	T215	A155	A95	N35
GLU	M455	L398	A336	L276	H216	Y156	K96	C36
ALA	GLN	P399	D337	R277	I217	N157	Q97	A37
ALA	ASN	P399	ASP	S278	Y218	P158	L98	K38
ALA	PRO	M400	F338	L279	L219	M159	V99	Y39
GLN	ASP	V401	S339	R402	D220	K160	A100	T40
GLY	ILE	R403	V340	E280	E221	L161	Q101	I41
ASN	ASN	V403	A341	N281	E222	Y162	P102	P42
MET	ILE	L404	K342	L282	E223	R163	A103	S43
VAL	ALA	L405	A343	Q283	G224	L164	E104	L44
PRO	THR	K406	V344	E284	E225	S165	L105	F45
ASN	LYS	Q407	S345	A285	Y226	S166	A106	P46
	LEU	L408	E346	I286	V226	V167	K107	K47
	ARG	Q409	Q347	V287	L227	V167	A107	D48
	ALA	A410	T348	K288	K228	V168	V108	S49
	ASN	T411	E349	M289	Y229	V169	E109	D50
	ALA	N412	G350	S290	E230	Q170	E110	N51
	ILE	Q413	R351	M291	E231	R171	G111	A52
	GLY	I414	L352	T292	I232	D172	L112	S53
ASP	THR	P415	S353	S293	D233	A173	S113	T54
SER	SER	E416	Y354	A294	G234	F174	M114	D55
THR	GLY	L417	A355	K295	V235	G175	V115	S56
GLY		P418	F356	V296	E236	T176	E116	Y56
		K419	M357	T297	V237	V177	R117	T57
		E420	L358	G298	D238	L178	L118	P58
			N359	L299	Q239	Q179	L119	P69
			SER	V300	T240	I180	M120	W60

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 ($\text{\AA}$)	372.3703, 372.3703, 372.3703	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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%)

All (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
2	H	324	PRO	CG-CD	-10.60	1.14	1.50
2	E	324	PRO	CA-C	6.51	1.63	1.52

All (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
2	H	324	PRO	N-CD-CG	-10.84	86.94	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	324	PRO	CA-CB-CG	-10.58	84.40	104.50
2	F	324	PRO	CA-N-CD	-8.73	99.78	112.00
2	H	324	PRO	CA-N-CD	-8.48	100.13	112.00
2	F	324	PRO	CA-CB-CG	-7.88	89.52	104.50
2	H	324	PRO	CA-CB-CG	-7.34	90.55	104.50
2	E	324	PRO	N-CA-CB	-7.14	96.70	103.41
2	F	398	LEU	CB-CG-CD2	-6.74	90.47	110.70
2	E	324	PRO	N-CD-CG	-6.66	93.22	103.20
2	G	454	PRO	N-CA-CB	-6.60	96.45	103.38
1	C	777	SER	CA-C-N	6.57	129.97	120.38
1	C	777	SER	C-N-CA	6.57	129.97	120.38
1	A	777	SER	CA-C-N	6.10	128.74	120.38
1	A	777	SER	C-N-CA	6.10	128.74	120.38
1	A	1530	LYS	CB-CG-CD	5.69	124.39	111.30
1	C	1530	LYS	CB-CG-CD	5.69	124.38	111.30
2	G	454	PRO	CA-N-CD	-5.62	104.13	112.00
2	G	398	LEU	CB-CG-CD2	-5.60	93.89	110.70
2	E	398	LEU	CB-CG-CD2	-5.36	94.63	110.70
2	H	151	GLU	CA-CB-CG	5.06	124.22	114.10

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
2:E:84:THR:HA	2:E:120:MET:HE1	1.73	0.69
2:E:257:VAL:HG12	2:E:266:ARG:H	1.58	0.68
2:G:257:VAL:HG12	2:G:266:ARG:H	1.59	0.68
2:E:83:GLN:HG3	2:E:431:GLU:HG2	1.77	0.67
1:C:1026:THR:OG1	1:C:1027:GLU:OE2	2.13	0.66
2:H:83:GLN:HG3	2:H:431:GLU:HG2	1.78	0.66
2:G:84:THR:HA	2:G:120:MET:HE1	1.77	0.65
1:D:515:ARG:NH2	1:D:520:ASP:OD2	2.30	0.64
1:A:1226:ALA:HB2	2:E:384:THR:HG23	1.81	0.63
1:C:708:VAL:HG21	1:C:724:MET:HE3	1.81	0.62
1:A:708:VAL:HG21	1:A:724:MET:HE3	1.82	0.62
2:F:83:GLN:HG3	2:F:431:GLU:HG2	1.82	0.62
1:B:1106:MET:SD	1:B:1106:MET:N	2.73	0.61
1:B:1462:TRP:O	2:F:375:ARG:NH2	2.34	0.61
1:D:1462:TRP:O	2:H:375:ARG:NH2	2.34	0.61
1:C:1027:GLU:OE2	1:C:1027:GLU:N	2.33	0.61
2:F:149:ILE:HD11	2:F:400:MET:HG3	1.83	0.60
1:D:302:LEU:HD11	1:D:332:TYR:CD1	2.37	0.60
1:B:302:LEU:HD11	1:B:332:TYR:CD1	2.37	0.59
1:D:1106:MET:N	1:D:1106:MET:SD	2.74	0.59
1:D:708:VAL:HG21	1:D:724:MET:HE3	1.85	0.59
1:B:308:ASP:HA	1:B:311:LYS:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:VAL:HG21	1:B:724:MET:HE3	1.84	0.59
2:H:315:GLN:HG2	2:H:318:ASP:HB2	1.85	0.58
1:A:1525:LYS:H	1:A:1525:LYS:HD2	1.69	0.58
2:F:308:VAL:HG22	2:F:309:ARG:HH21	1.69	0.58
1:C:1525:LYS:HD2	1:C:1525:LYS:H	1.69	0.58
2:E:237:VAL:O	2:E:240:THR:OG1	2.21	0.57
2:H:114:MET:HE1	2:H:117:ARG:HE	1.69	0.57
2:H:257:VAL:HG12	2:H:266:ARG:H	1.69	0.57
2:G:237:VAL:O	2:G:240:THR:OG1	2.22	0.57
1:B:1359:ARG:HH11	1:B:1362:ARG:HD3	1.69	0.56
2:H:330:LEU:HG	2:H:334:LYS:HB2	1.87	0.56
2:F:118:ILE:HG21	2:F:413:GLN:HE21	1.72	0.55
2:H:330:LEU:HD12	2:H:333:GLU:HB3	1.88	0.55
2:H:152:PRO:HA	2:H:157:ASN:OD1	2.06	0.55
2:H:149:ILE:HD11	2:H:400:MET:HG3	1.88	0.55
1:A:196:GLU:OE1	1:A:196:GLU:N	2.40	0.54
1:A:1044:MET:HE3	1:A:1059:PHE:HB3	1.89	0.54
1:C:196:GLU:N	1:C:196:GLU:OE2	2.40	0.54
1:D:302:LEU:HD21	1:D:332:TYR:CE1	2.43	0.54
1:A:825:ASN:HD22	2:E:54:THR:C	2.17	0.53
2:F:118:ILE:HD13	2:F:413:GLN:NE2	2.23	0.53
2:H:309:ARG:HH12	2:H:313:LYS:HD3	1.74	0.53
1:A:1:FME:O1	1:D:171:HIS:ND1	2.43	0.52
1:B:1112:GLN:O	1:B:1116:GLN:HG3	2.09	0.52
1:D:1041:ARG:HE	2:H:316:THR:HG23	1.73	0.52
1:B:1525:LYS:H	1:B:1525:LYS:HE2	1.74	0.52
1:C:941:ARG:HB2	1:C:941:ARG:NH1	2.24	0.52
1:B:171:HIS:ND1	1:C:1:FME:O1	2.43	0.52
1:D:1112:GLN:O	1:D:1116:GLN:HG3	2.09	0.52
1:D:1525:LYS:HE2	1:D:1525:LYS:H	1.75	0.52
2:G:132:LEU:HD21	2:G:400:MET:HE1	1.92	0.51
1:A:937:MET:HE2	1:A:941:ARG:HE	1.74	0.51
1:C:1469:TRP:CD1	2:G:373:GLU:HG3	2.45	0.51
1:A:1469:TRP:CD1	2:E:373:GLU:HG3	2.45	0.51
2:E:132:LEU:HD21	2:E:400:MET:HE1	1.93	0.50
2:F:153:GLU:H	2:F:157:ASN:HD21	1.58	0.50
1:C:1044:MET:HE3	1:C:1059:PHE:HB3	1.92	0.50
1:A:937:MET:HE2	1:A:941:ARG:NE	2.26	0.50
1:D:63:GLN:HG2	1:D:81:MET:SD	2.52	0.50
1:B:515:ARG:NH2	1:B:520:ASP:OD2	2.44	0.50
1:D:228:ILE:HG21	1:D:340:PHE:CZ	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:LYS:O	1:B:248:GLU:HG2	2.12	0.50
1:B:63:GLN:HG2	1:B:81:MET:SD	2.52	0.49
1:B:228:ILE:HG21	1:B:340:PHE:CZ	2.48	0.49
1:B:302:LEU:HD21	1:B:332:TYR:CE1	2.48	0.49
1:B:1059:PHE:HB2	2:F:296:VAL:HG13	1.95	0.48
2:F:297:ILE:HG22	2:F:330:LEU:HD23	1.94	0.48
1:A:1530:LYS:HA	1:A:1530:LYS:HE2	1.95	0.48
1:A:1:FME:HE2	1:A:1:FME:HB3	1.71	0.48
1:B:1134:ARG:HH11	1:B:1134:ARG:HB3	1.78	0.48
2:F:86:MET:HE1	2:F:120:MET:HE3	1.94	0.48
2:F:152:PRO:HA	2:F:157:ASN:ND2	2.29	0.48
2:G:159:MET:HE3	2:G:159:MET:HB2	1.62	0.48
1:C:1530:LYS:HA	1:C:1530:LYS:HE2	1.95	0.47
2:F:80:PHE:CE2	2:F:397:GLN:HG2	2.49	0.47
2:F:118:ILE:HD13	2:F:413:GLN:HE22	1.80	0.47
2:F:80:PHE:HE2	2:F:397:GLN:HG2	1.78	0.47
1:A:530:ILE:HD12	1:A:536:ILE:HD13	1.96	0.47
2:H:302:PRO:HD3	2:H:326:ASP:HB2	1.97	0.47
1:B:291:LYS:HB3	1:B:322:TRP:CE3	2.50	0.46
1:D:1134:ARG:HB3	1:D:1134:ARG:HH11	1.79	0.46
2:F:151:GLU:HA	2:F:407:GLN:HE21	1.80	0.46
1:A:170:LYS:NZ	1:A:177:GLU:O	2.48	0.46
1:B:825:ASN:HD22	2:F:54:THR:C	2.23	0.46
2:H:86:MET:HE1	2:H:120:MET:HE3	1.98	0.46
1:B:990:ILE:HG23	1:B:991:PHE:HD2	1.80	0.46
1:B:132:LYS:H	1:B:132:LYS:HE2	1.81	0.46
1:D:291:LYS:HB3	1:D:322:TRP:CE3	2.50	0.46
2:F:426:ILE:HG22	2:F:428:THR:HG23	1.98	0.46
2:H:117:ARG:NH1	2:H:121:ASN:HB2	2.24	0.46
1:B:65:LYS:HA	1:B:65:LYS:HD3	1.81	0.45
1:B:1041:ARG:HE	2:F:316:THR:HG23	1.81	0.45
2:H:80:PHE:CE2	2:H:397:GLN:HG2	2.51	0.45
1:A:754:ARG:HH12	1:A:756:LEU:HD23	1.81	0.45
1:C:1469:TRP:HD1	2:G:373:GLU:HG3	1.81	0.45
1:A:863:SER:O	1:A:867:MET:HG3	2.17	0.45
1:D:65:LYS:HD3	1:D:65:LYS:HA	1.82	0.45
1:D:205:ASP:OD2	1:D:205:ASP:N	2.50	0.45
1:C:170:LYS:NZ	1:C:177:GLU:O	2.50	0.45
1:B:1134:ARG:HB3	1:B:1134:ARG:NH1	2.32	0.44
1:D:1134:ARG:HB3	1:D:1134:ARG:NH1	2.32	0.44
1:C:1:FME:HE2	1:C:1:FME:HB3	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1059:PHE:HB2	2:H:296:VAL:HG13	1.98	0.44
1:B:1287:ILE:HD12	1:B:1288:ASN:N	2.33	0.44
1:C:492:ASN:OD1	1:C:492:ASN:N	2.50	0.44
1:C:784:GLU:HG2	1:C:867:MET:HE1	1.98	0.44
1:B:205:ASP:OD2	1:B:205:ASP:N	2.49	0.44
2:H:157:ASN:HD22	2:H:157:ASN:HA	1.53	0.44
2:G:79:LEU:HB3	2:G:80:PHE:CD2	2.52	0.44
1:B:1120:GLU:O	1:B:1123:LYS:HE2	2.18	0.43
1:A:778:HIS:CE1	1:A:860:TYR:HD1	2.36	0.43
1:A:1112:GLN:CD	1:A:1112:GLN:H	2.26	0.43
2:H:84:THR:HA	2:H:120:MET:HE1	2.00	0.43
1:A:1469:TRP:HD1	2:E:373:GLU:HG3	1.82	0.43
1:D:1046:ILE:HD12	2:H:311:LEU:HB3	2.01	0.43
1:A:527:ILE:O	1:A:531:VAL:HG23	2.19	0.43
1:D:1359:ARG:NH1	1:D:1362:ARG:HD3	2.34	0.43
1:D:1524:LYS:HD2	1:D:1524:LYS:HA	1.78	0.43
2:F:307:GLN:OE1	2:F:309:ARG:HG2	2.18	0.43
1:B:914:GLU:H	1:B:914:GLU:CD	2.27	0.43
2:E:79:LEU:HB3	2:E:80:PHE:CD2	2.53	0.43
2:H:295:LYS:HE3	2:H:334:LYS:NZ	2.34	0.42
2:H:357:MET:HE1	2:H:385:LEU:HD11	2.01	0.42
1:C:883:LYS:HD3	1:C:883:LYS:N	2.34	0.42
2:H:77:LEU:HD12	2:H:77:LEU:HA	1.89	0.42
1:A:492:ASN:OD1	1:A:492:ASN:N	2.50	0.42
1:C:1099:GLU:O	1:C:1102:LYS:HG3	2.20	0.42
2:E:151:GLU:HA	2:E:152:PRO:HD3	1.90	0.42
2:G:84:THR:HA	2:G:120:MET:CE	2.46	0.42
2:H:151:GLU:HA	2:H:407:GLN:HE21	1.83	0.42
1:D:914:GLU:CD	1:D:914:GLU:H	2.27	0.42
2:G:257:VAL:HG11	2:G:266:ARG:HB2	2.01	0.42
1:B:883:LYS:HD2	1:B:883:LYS:H	1.85	0.42
1:C:1577:VAL:O	1:C:1581:MET:HG3	2.20	0.42
1:D:863:SER:O	1:D:867:MET:HG3	2.20	0.42
1:D:883:LYS:H	1:D:883:LYS:HD2	1.85	0.42
2:G:83:GLN:OE1	2:G:84:THR:N	2.53	0.42
1:A:1026:THR:OG1	1:A:1027:GLU:OE2	2.34	0.41
1:B:817:PHE:CE2	1:B:827:ILE:HD11	2.54	0.41
2:E:76:MET:HE3	2:E:129:ARG:HE	1.85	0.41
2:F:194:ASP:OD2	2:F:195:VAL:N	2.52	0.41
1:B:1113:ILE:H	1:B:1113:ILE:HG12	1.70	0.41
1:C:3:LYS:HG2	1:C:4:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1577:VAL:O	1:A:1581:MET:HG3	2.20	0.41
1:B:140:LYS:O	1:B:143:GLU:HG3	2.21	0.41
2:E:257:VAL:HG11	2:E:266:ARG:HB2	2.02	0.41
2:F:117:ARG:HH22	2:F:121:ASN:HD22	1.69	0.41
1:A:1512:GLY:HA2	1:A:1515:TRP:CE3	2.56	0.41
1:D:18:GLN:NE2	1:D:66:PHE:O	2.54	0.41
1:A:883:LYS:N	1:A:883:LYS:HD3	2.35	0.41
1:C:438:PHE:HE1	1:C:1555:ARG:HH12	1.68	0.41
1:A:990:ILE:HD11	2:E:311:LEU:HD13	2.03	0.41
1:A:1106:MET:HE2	1:A:1107:TYR:CZ	2.56	0.41
1:C:1512:GLY:HA2	1:C:1515:TRP:CE3	2.56	0.41
1:B:863:SER:O	1:B:867:MET:HG3	2.21	0.41
1:C:1119:LYS:HA	1:C:1122:ILE:HG22	2.03	0.41
2:E:380:GLU:HA	2:E:384:THR:OG1	2.21	0.41
1:C:1106:MET:HE2	1:C:1107:TYR:CZ	2.56	0.40
2:E:315:GLN:HG2	2:E:318:ASP:HB2	2.02	0.40
1:A:1099:GLU:O	1:A:1102:LYS:HG3	2.20	0.40
1:B:228:ILE:HD13	1:B:340:PHE:CZ	2.57	0.40
1:C:63:GLN:OE1	1:C:64:SER:N	2.54	0.40
1:D:1272:HIS:ND1	1:D:1272:HIS:C	2.79	0.40
1:A:70:LYS:NZ	1:A:72:SER:OG	2.54	0.40
1:A:769:GLU:HG2	1:A:778:HIS:CE1	2.57	0.40
1:D:140:LYS:O	1:D:143:GLU:HG3	2.20	0.40
1:D:817:PHE:CE2	1:D:827:ILE:HD11	2.56	0.40
2:E:381:LEU:O	2:E:385:LEU:HD23	2.22	0.40
2:F:357:MET:HE1	2:F:385:LEU:HD11	2.03	0.40
2:E:398:LEU:HA	2:E:398:LEU:HD23	1.93	0.40
1:A:63:GLN:OE1	1:A:64:SER:N	2.54	0.40
1:B:1569:ASP:N	1:B:1569:ASP:OD1	2.51	0.40

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	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 ⓘ

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
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

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	602	LEU
1	A	729	THR

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Mol	Chain	Res	Type
1	A	990	ILE
1	A	1081	HIS
1	B	228	ILE
1	B	492	ASN
1	B	530	ILE
1	B	592	LEU
1	B	729	THR
1	B	1003	GLU
1	B	1518	GLU
1	C	602	LEU
1	C	729	THR
1	C	731	LEU
1	C	914	GLU
1	C	941	ARG
1	C	1081	HIS
1	D	228	ILE
1	D	234	GLU
1	D	492	ASN
1	D	530	ILE
1	D	592	LEU
1	D	729	THR
1	D	1003	GLU
1	D	1155	GLN
1	D	1272	HIS
1	D	1518	GLU
2	E	214	TYR
2	E	291	MET
2	E	320	VAL
2	F	22	LEU
2	F	77	LEU
2	F	86	MET
2	F	112	LEU
2	F	114	MET
2	G	320	VAL
2	H	22	LEU
2	H	77	LEU
2	H	86	MET
2	H	199	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	165	ASN
1	A	220	HIS
1	A	337	ASN
1	A	350	ASN
1	A	355	ASN
1	A	384	ASN
1	A	423	GLN
1	A	644	GLN
1	A	668	GLN
1	A	821	HIS
1	A	825	ASN
1	A	925	GLN
1	A	987	HIS
1	A	1112	GLN
1	A	1137	ASN
1	A	1324	ASN
1	A	1328	GLN
1	A	1465	ASN
1	B	31	GLN
1	B	337	ASN
1	B	355	ASN
1	B	384	ASN
1	B	644	GLN
1	B	650	ASN
1	B	668	GLN
1	B	688	HIS
1	B	821	HIS
1	B	825	ASN
1	B	976	HIS
1	B	1081	HIS
1	B	1297	HIS
1	B	1324	ASN
1	B	1328	GLN
1	C	31	GLN
1	C	165	ASN
1	C	214	HIS
1	C	337	ASN
1	C	350	ASN
1	C	355	ASN
1	C	384	ASN
1	C	423	GLN
1	C	637	ASN

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Mol	Chain	Res	Type
1	C	644	GLN
1	C	650	ASN
1	C	668	GLN
1	C	779	HIS
1	C	925	GLN
1	C	943	HIS
1	C	1137	ASN
1	C	1324	ASN
1	C	1328	GLN
1	D	31	GLN
1	D	337	ASN
1	D	355	ASN
1	D	384	ASN
1	D	644	GLN
1	D	668	GLN
1	D	976	HIS
1	D	1137	ASN
1	D	1324	ASN
1	D	1328	GLN
2	E	281	ASN
2	F	157	ASN
2	F	281	ASN
2	F	413	GLN
2	G	281	ASN
2	G	359	ASN
2	H	281	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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.

All (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
1	C	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
1	C	1	FME	N-CA-CB-CG
1	A	1	FME	CA-CB-CG-SD
1	C	1	FME	CA-CB-CG-SD
1	A	1	FME	C-CA-CB-CG
1	C	1	FME	C-CA-CB-CG

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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
3	C	1601	ATP	PB-O3B	-3.01	1.56	1.59
3	D	1601	ATP	PB-O3B	-2.43	1.56	1.59
3	B	1601	ATP	PB-O3B	-2.42	1.56	1.59

There are no bond angle outliers.

There are no chirality outliers.

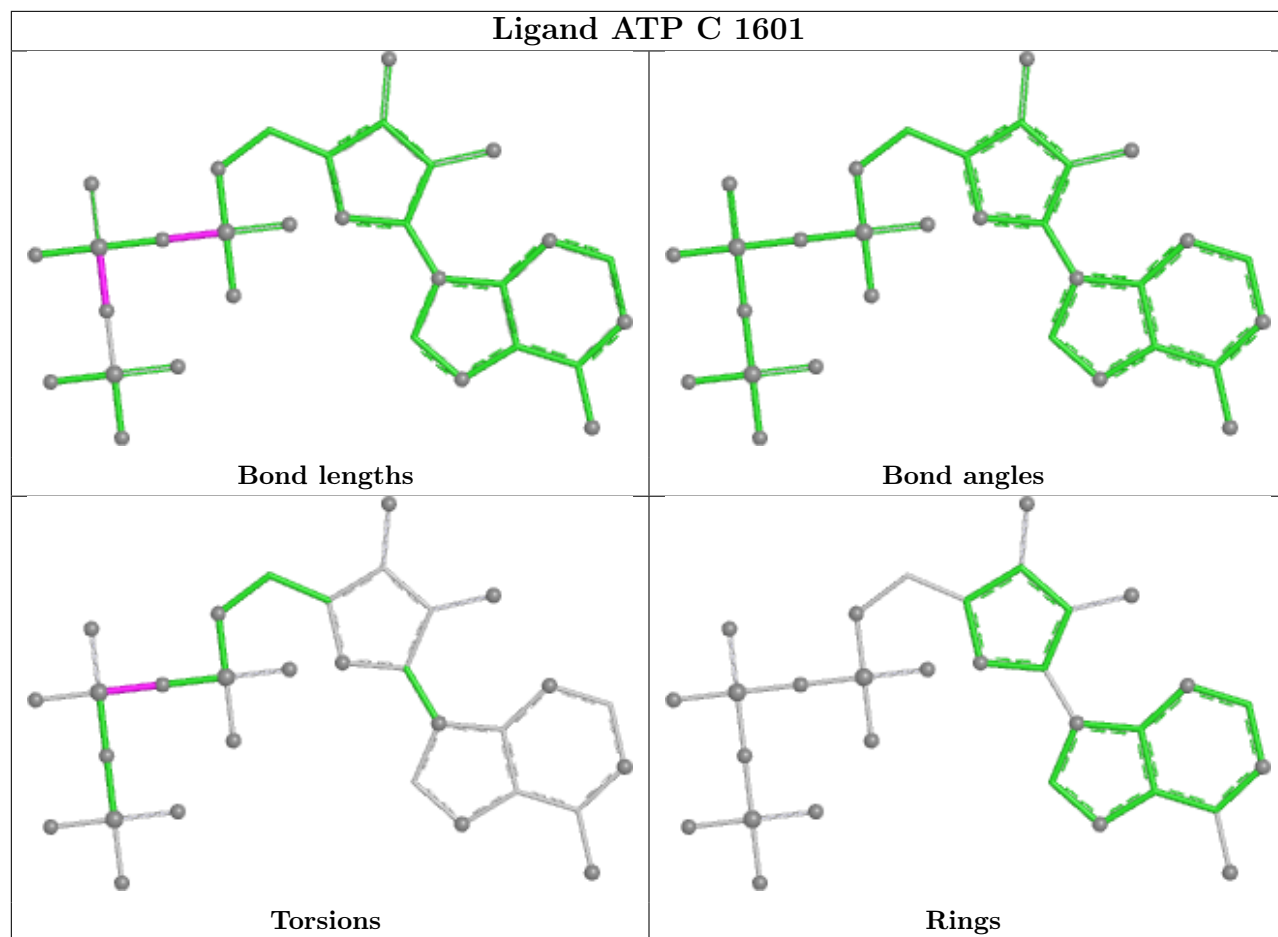
All (2) torsion outliers are listed below:

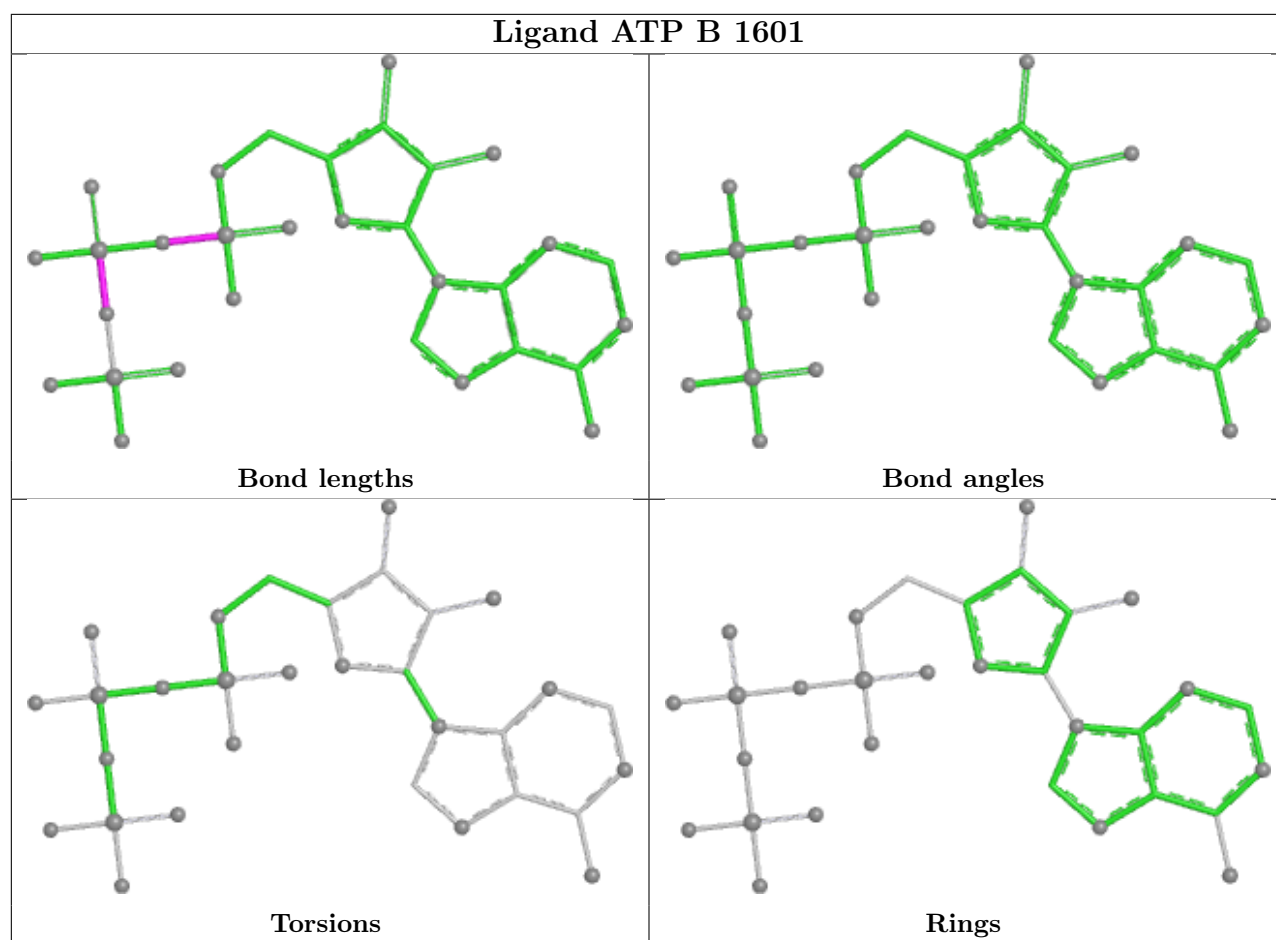
Mol	Chain	Res	Type	Atoms
3	A	1601	ATP	PA-O3A-PB-O2B
3	C	1601	ATP	PA-O3A-PB-O2B

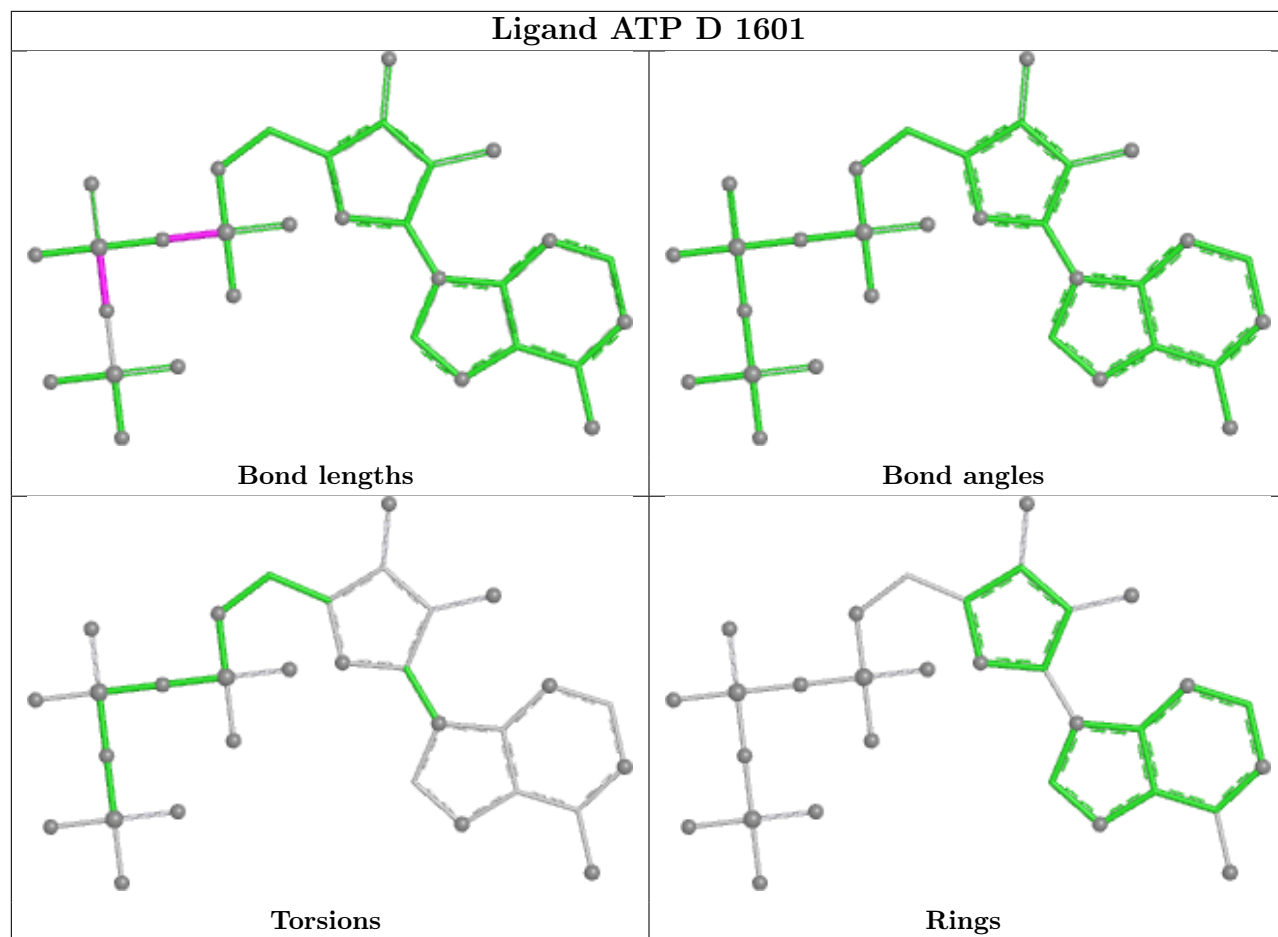
There are no ring outliers.

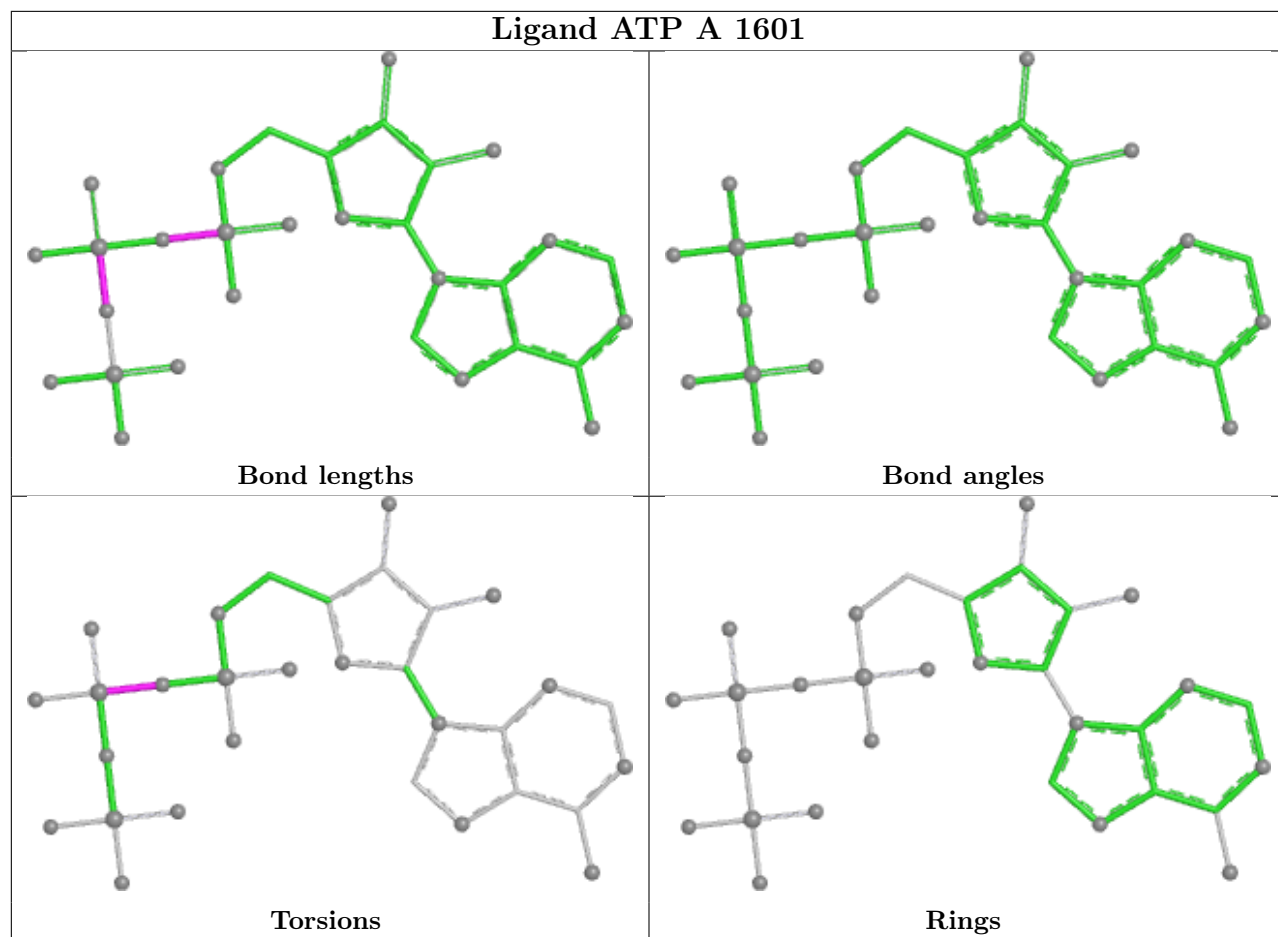
No monomer is involved in short contacts.

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.

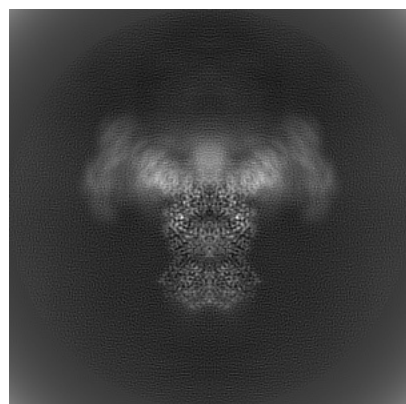
6 Map visualisation [i](#)

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.

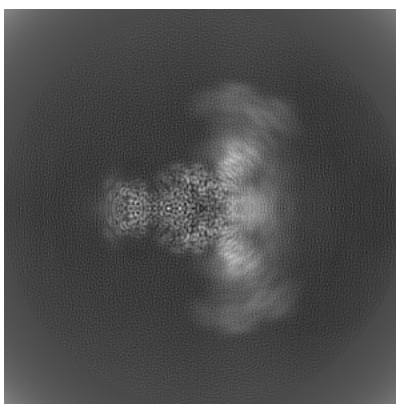
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

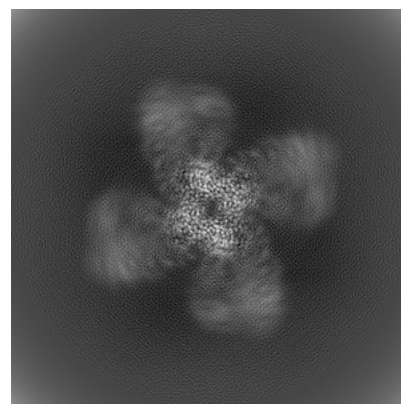
6.1.1 Primary map



X

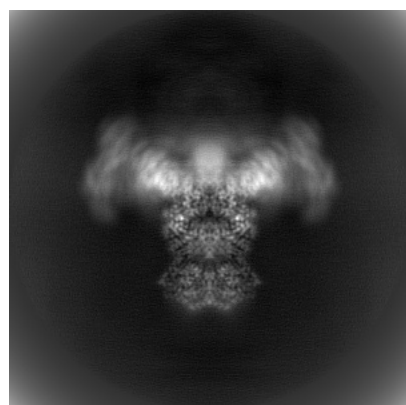


Y

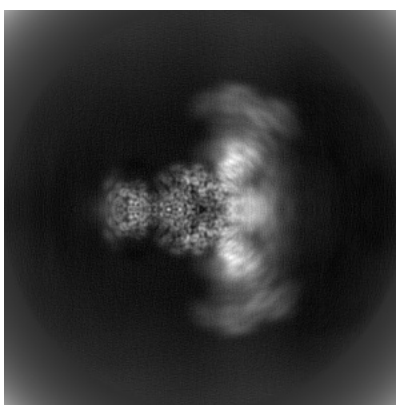


Z

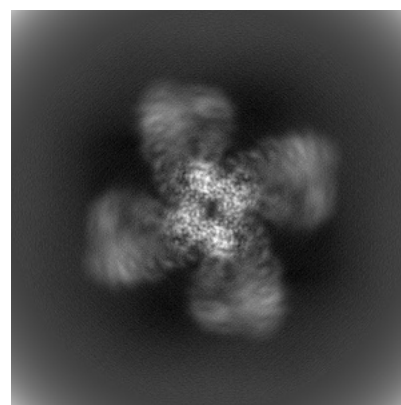
6.1.2 Raw map



X



Y

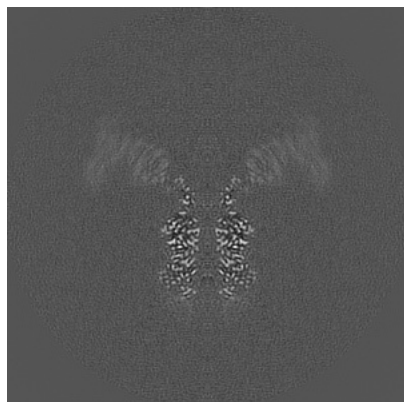


Z

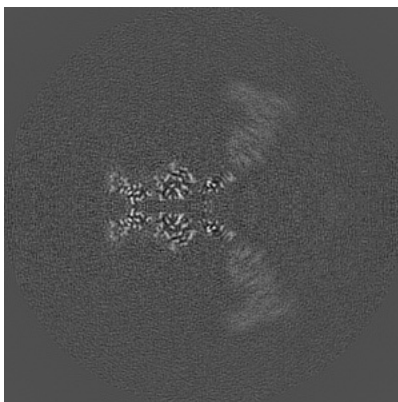
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

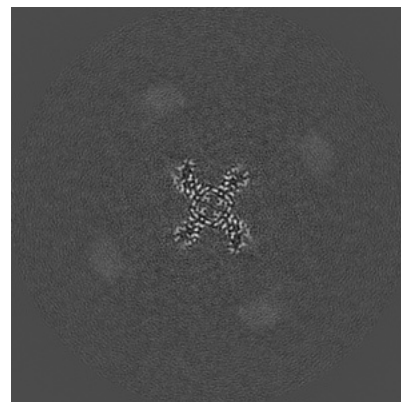
6.2.1 Primary map



X Index: 180

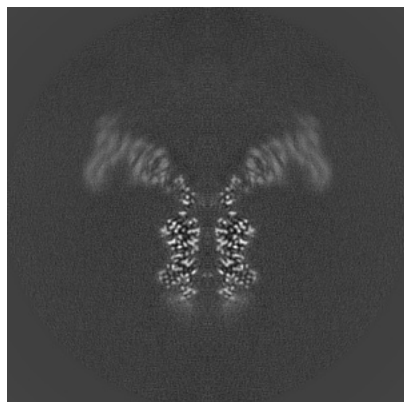


Y Index: 180

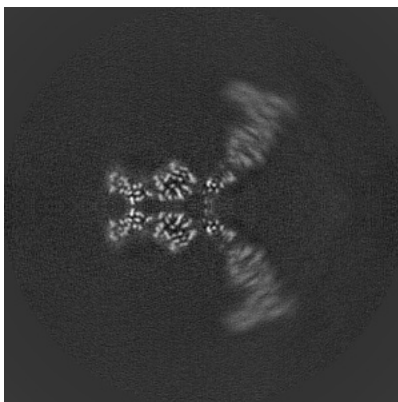


Z Index: 180

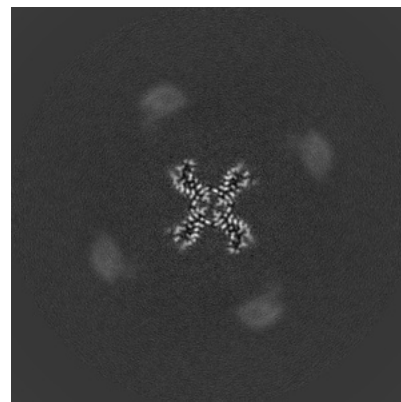
6.2.2 Raw map



X Index: 180



Y Index: 180

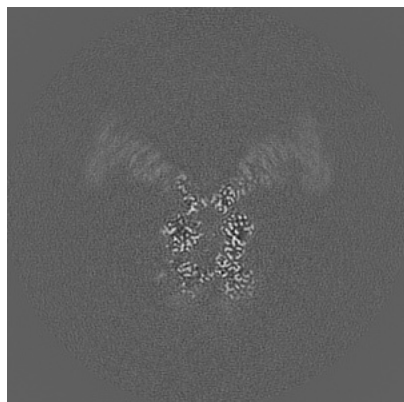


Z Index: 180

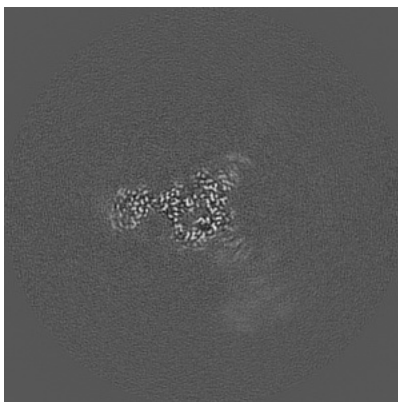
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

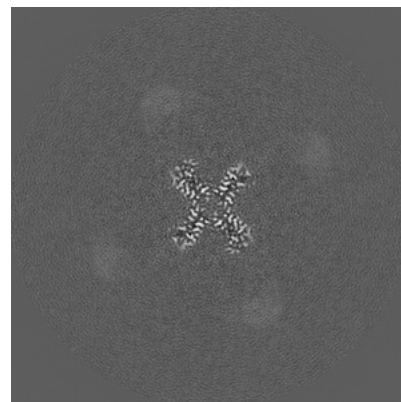
6.3.1 Primary map



X Index: 175

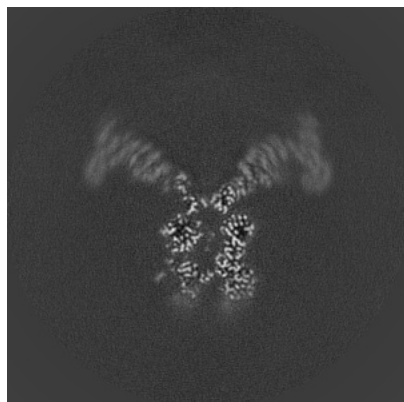


Y Index: 160

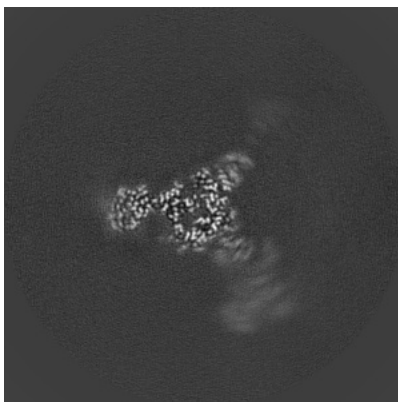


Z Index: 179

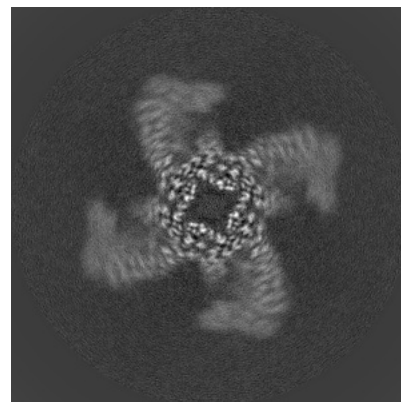
6.3.2 Raw map



X Index: 175



Y Index: 160

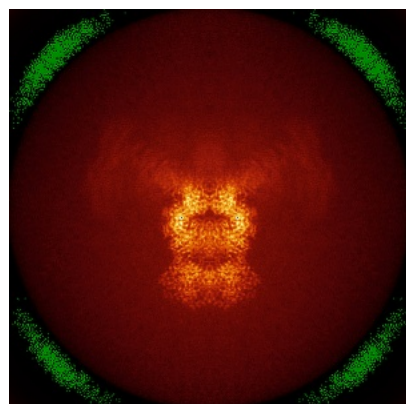


Z Index: 204

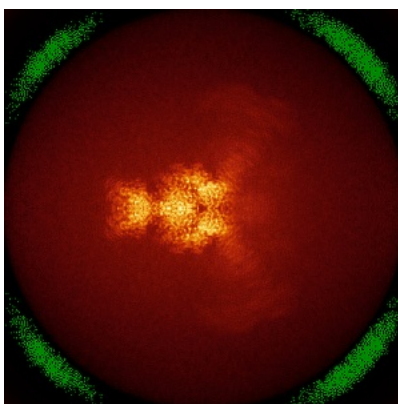
The images above show the largest variance slices of the map in three orthogonal directions.

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

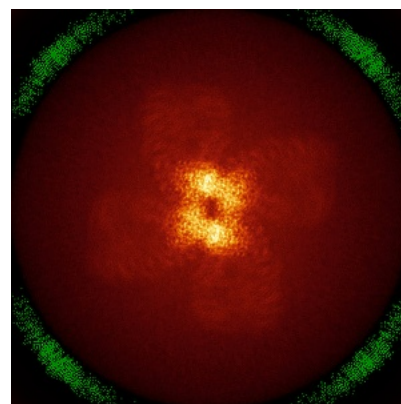
6.4.1 Primary map



X

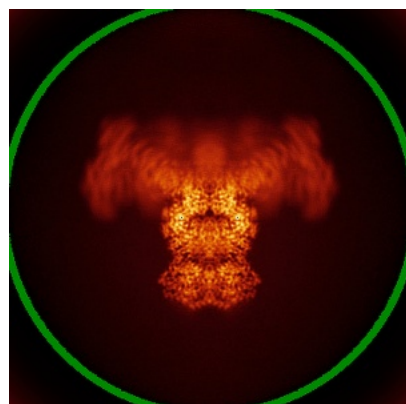


Y

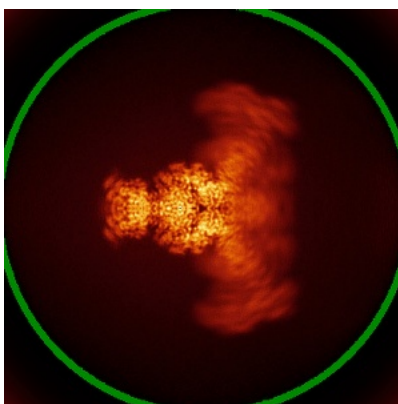


Z

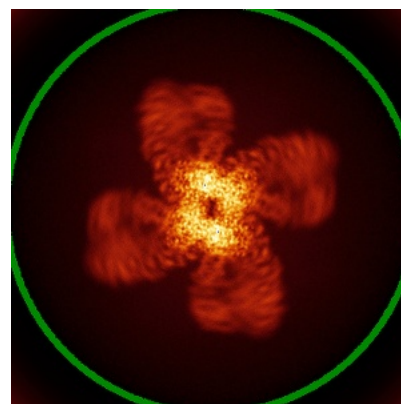
6.4.2 Raw map



X



Y

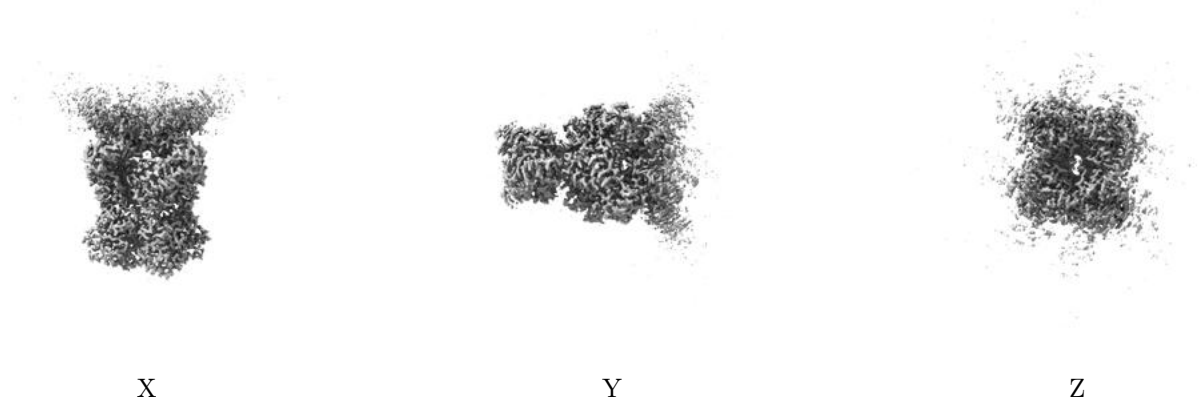


Z

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.

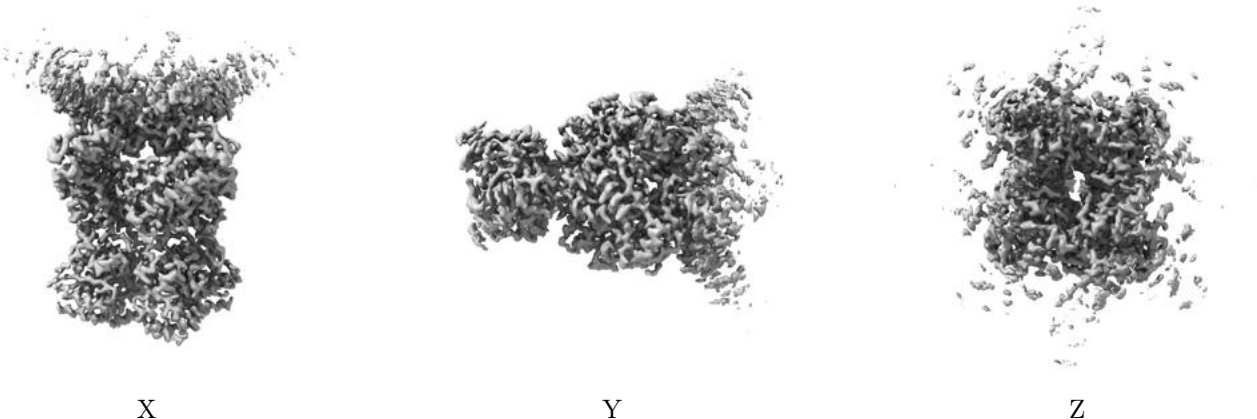
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

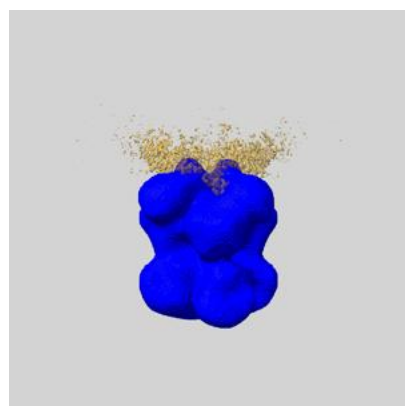
6.6 Mask visualisation [i](#)

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

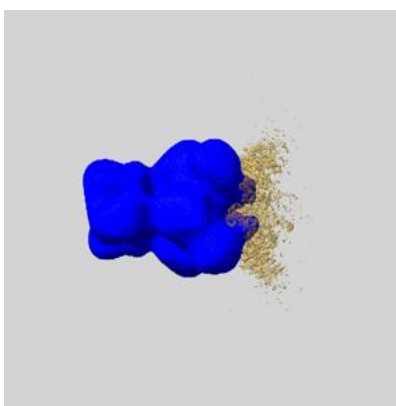
A mask typically either:

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

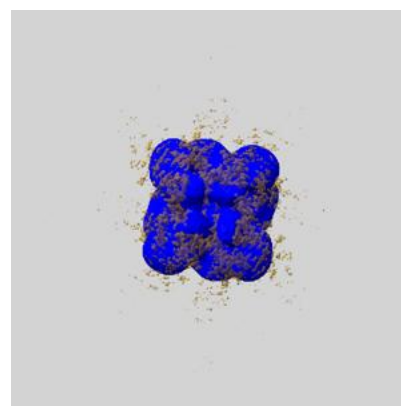
6.6.1 emd_27422_msk_1.map [i](#)



X



Y

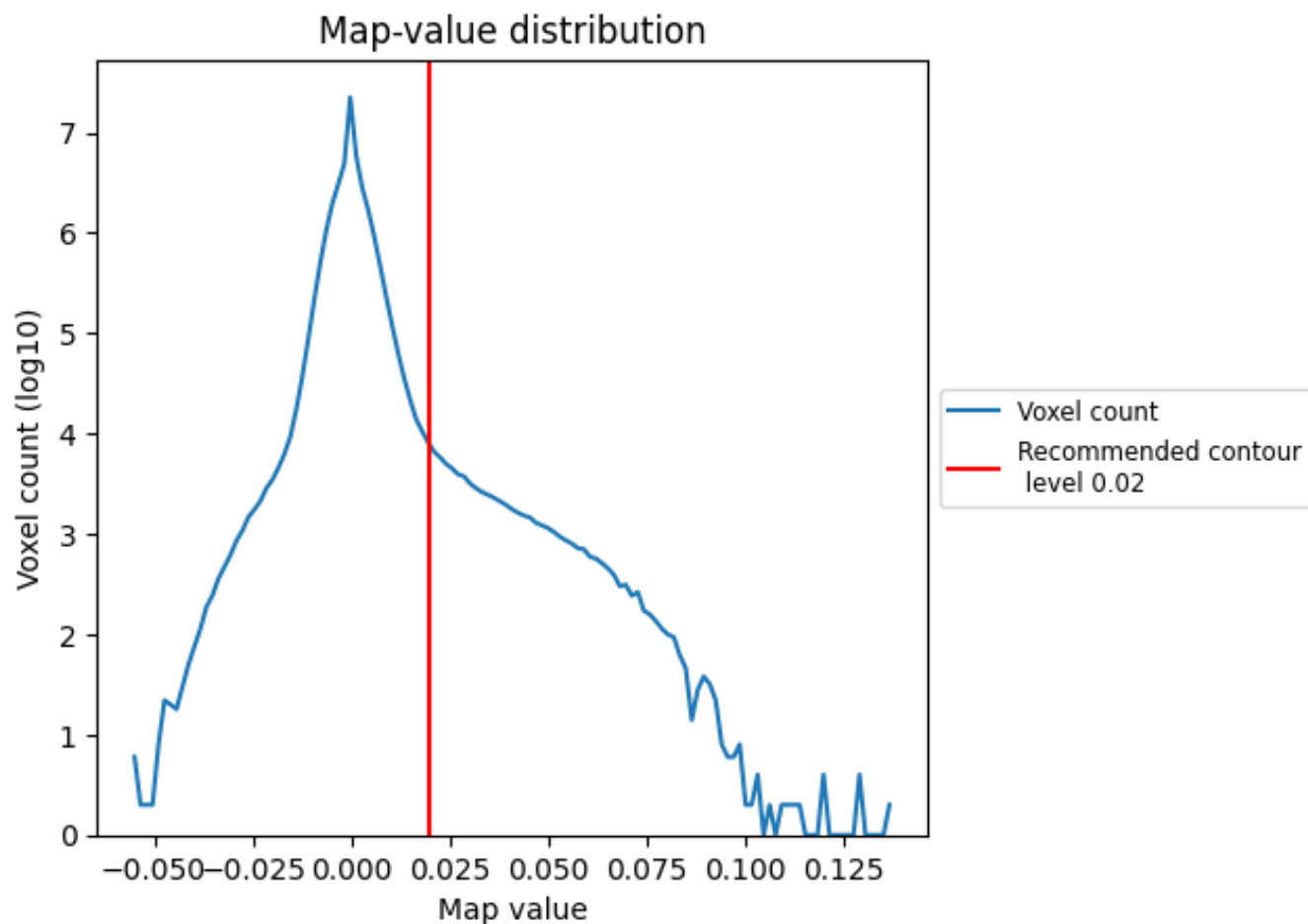


Z

7 Map analysis [i](#)

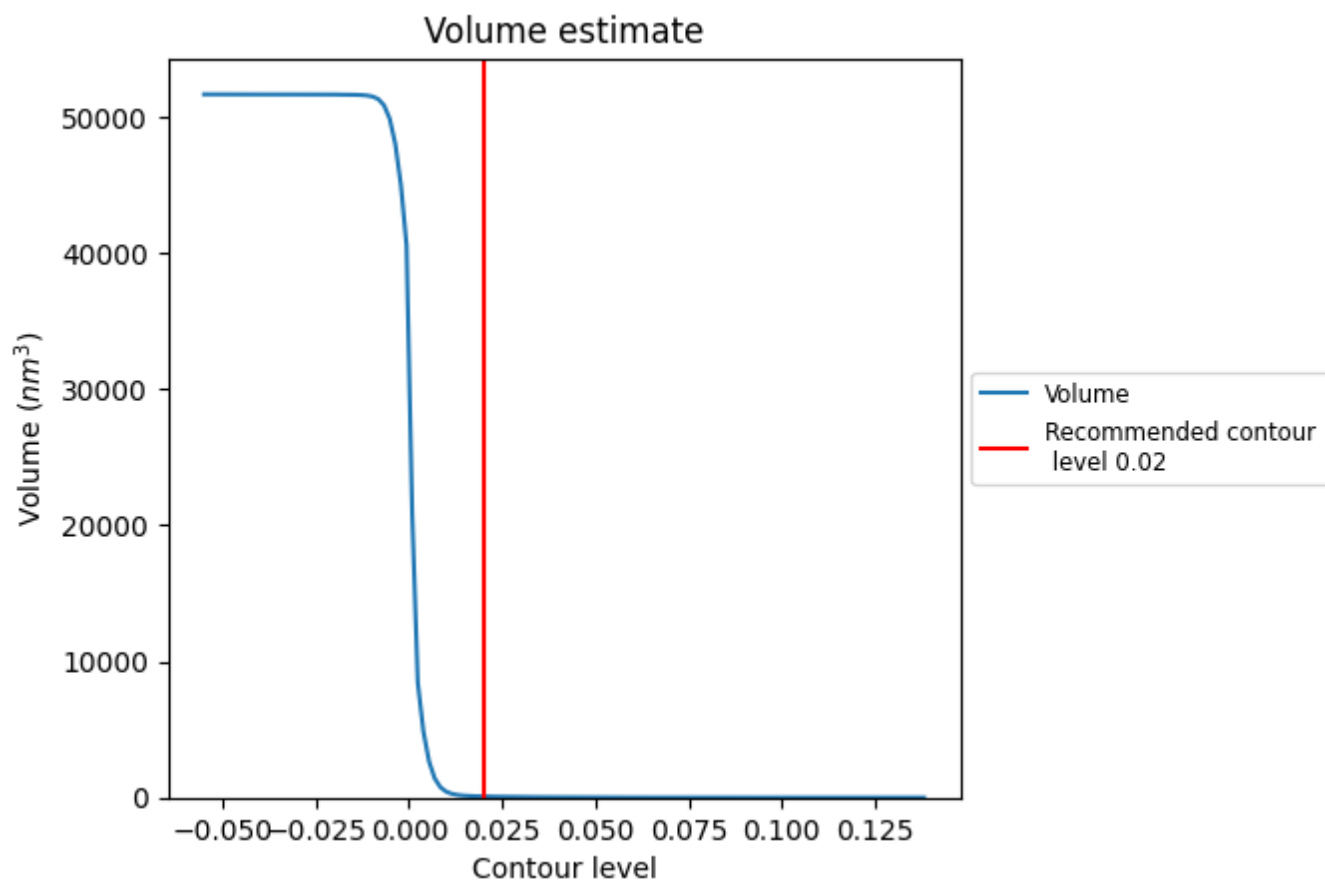
This section contains the results of statistical analysis of the map.

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.

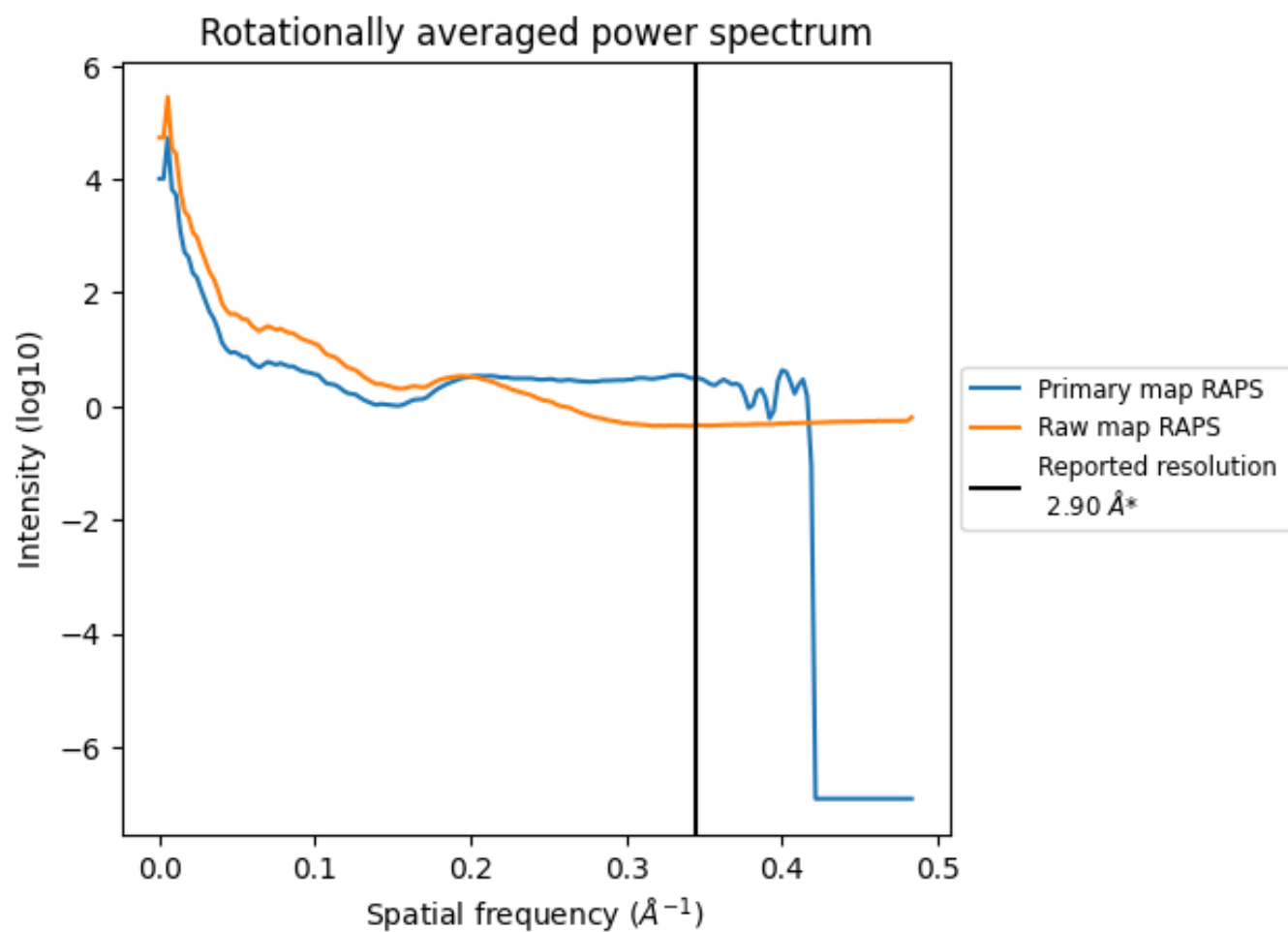
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 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 ⓘ

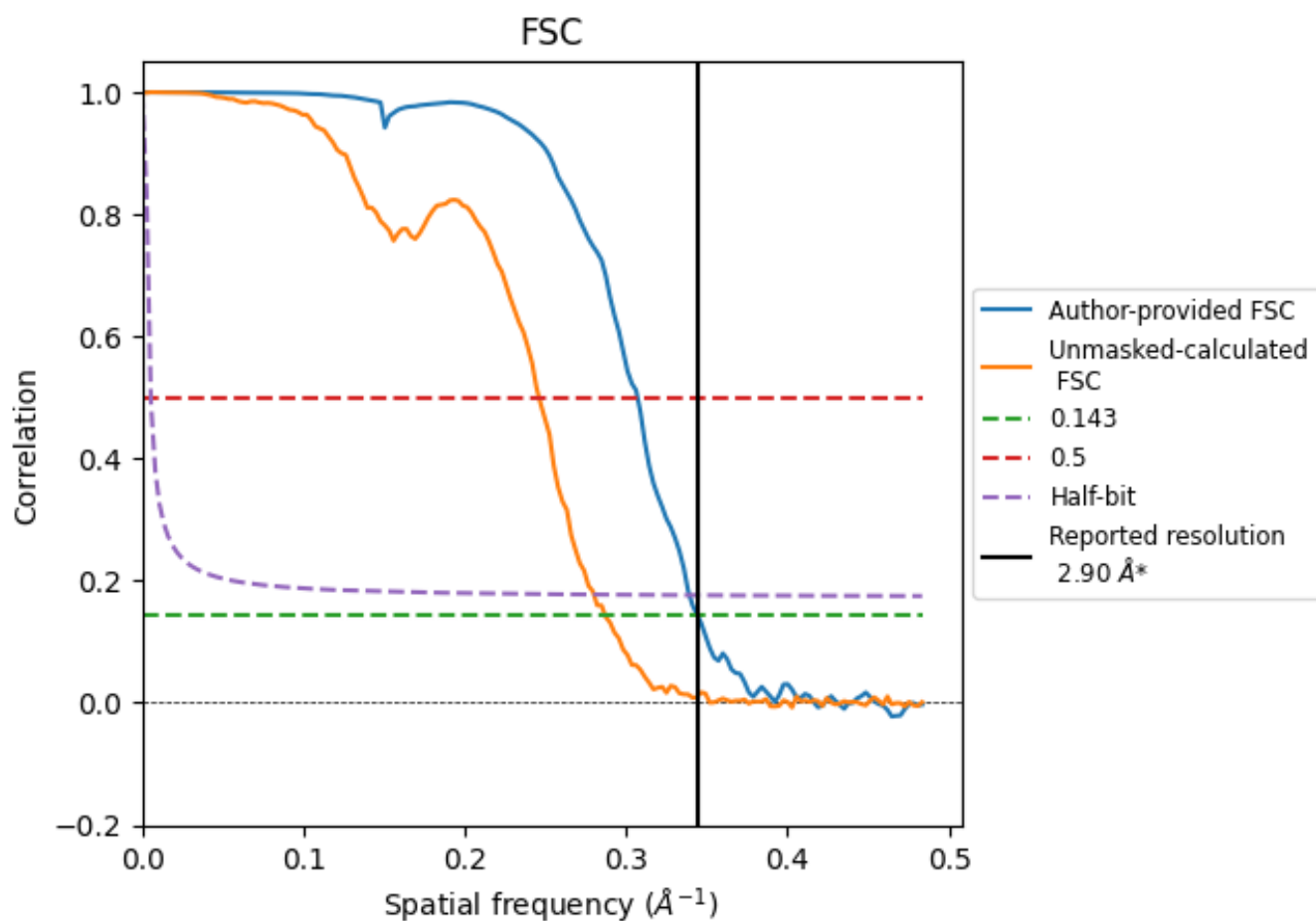


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

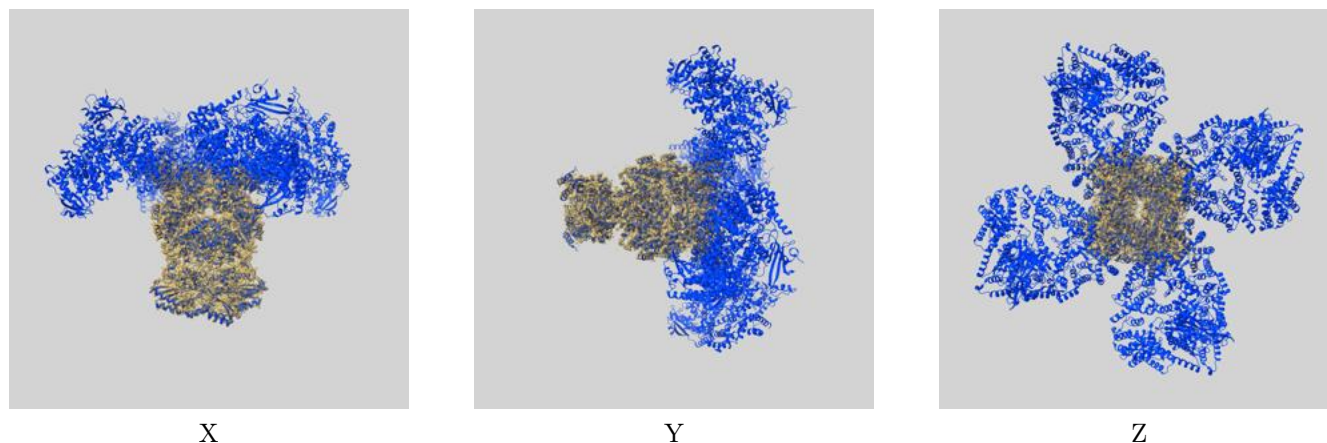
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.26	2.95
Unmasked-calculated*	3.48	4.07	3.57

*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](#)



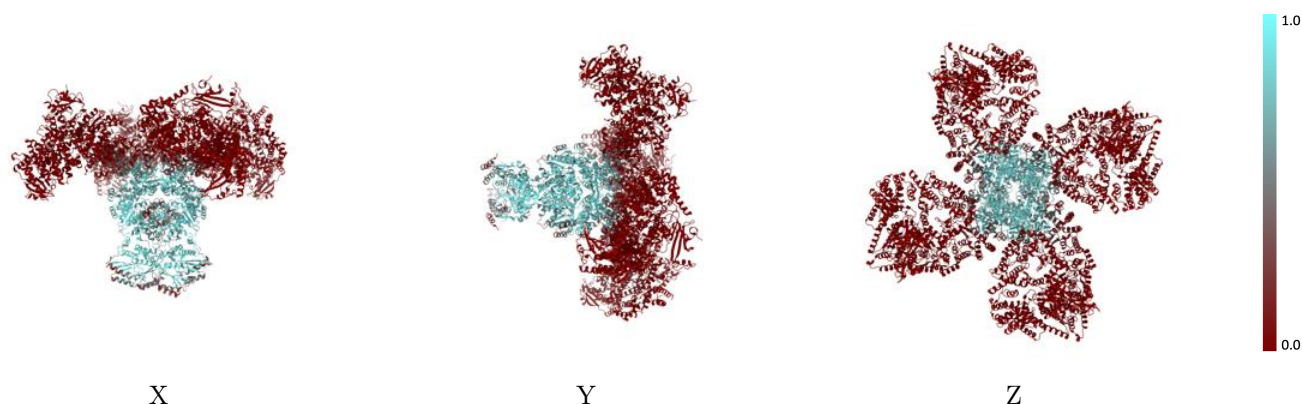
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



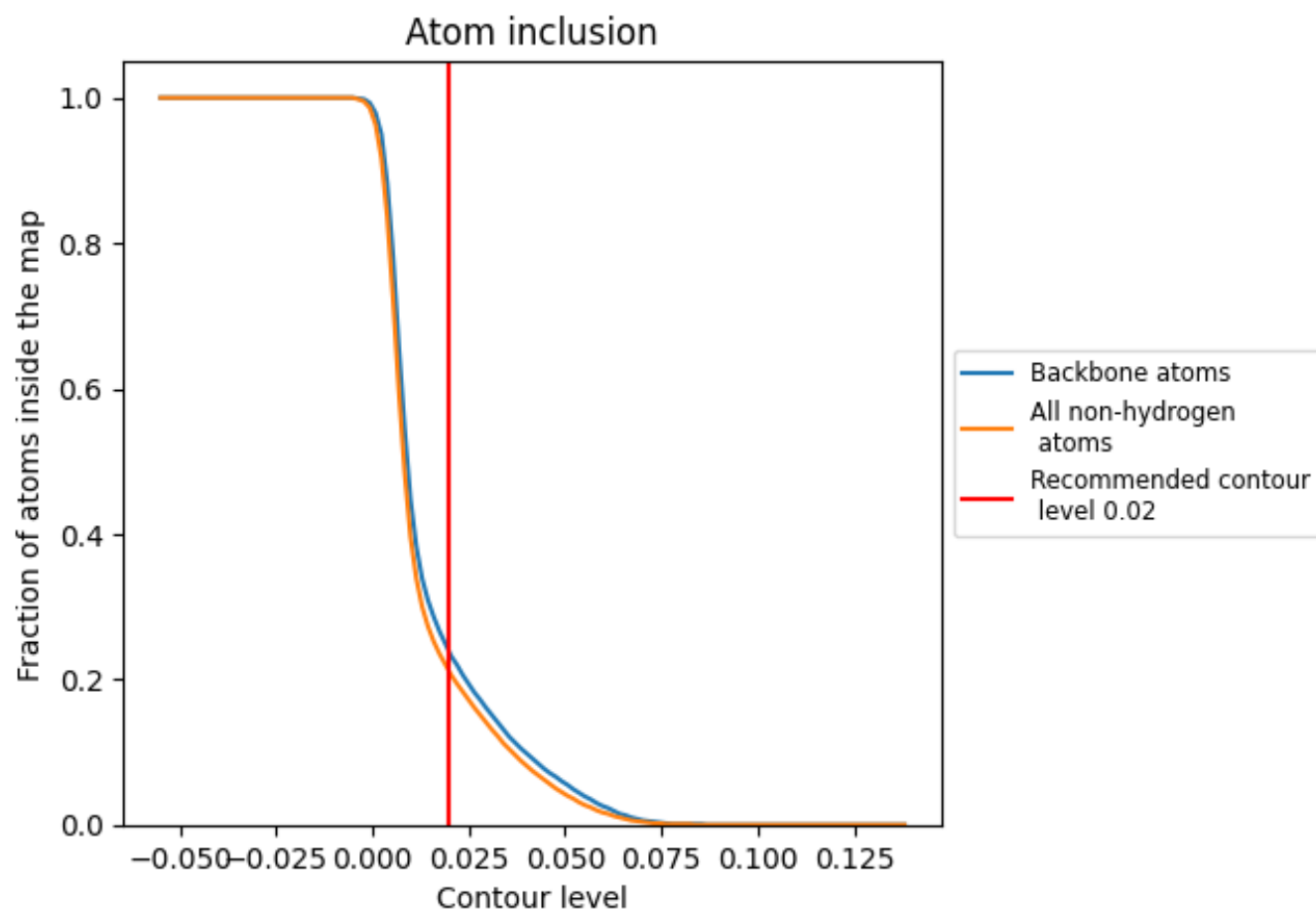
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

1.0

0.0

<0.0