



Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 04:49 PM EST

PDB ID : 8DGF
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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

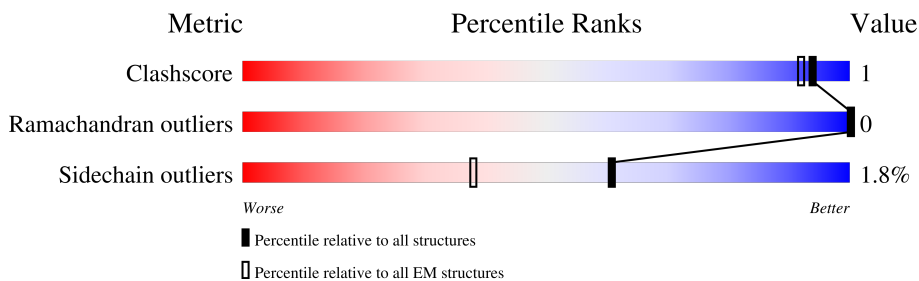
1 Overall quality at a glance i

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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% (Poor fit) 93% (0 outliers) 99% (1 outlier) 100% (2 outliers) 100% (3+ outliers)
1	B	1587	69% (Poor fit) 92% (0 outliers) 99% (1 outlier) 100% (2 outliers) 100% (3+ outliers)
1	C	1587	66% (Poor fit) 94% (0 outliers) 99% (1 outlier) 100% (2 outliers) 100% (3+ outliers)
1	D	1587	69% (Poor fit) 93% (0 outliers) 99% (1 outlier) 100% (2 outliers) 100% (3+ outliers)
2	E	535	82% (Poor fit) 76% (0 outliers) 82% (1 outlier) 87% (2 outliers) 95% (3+ outliers)
2	F	535	82% (Poor fit) 73% (0 outliers) 82% (1 outlier) 87% (2 outliers) 95% (3+ outliers)
2	G	535	82% (Poor fit) 79% (0 outliers) 82% (1 outlier) 87% (2 outliers) 95% (3+ outliers)
2	H	535	82% (Poor fit) 74% (0 outliers) 82% (1 outlier) 87% (2 outliers) 95% (3+ outliers)

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 (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

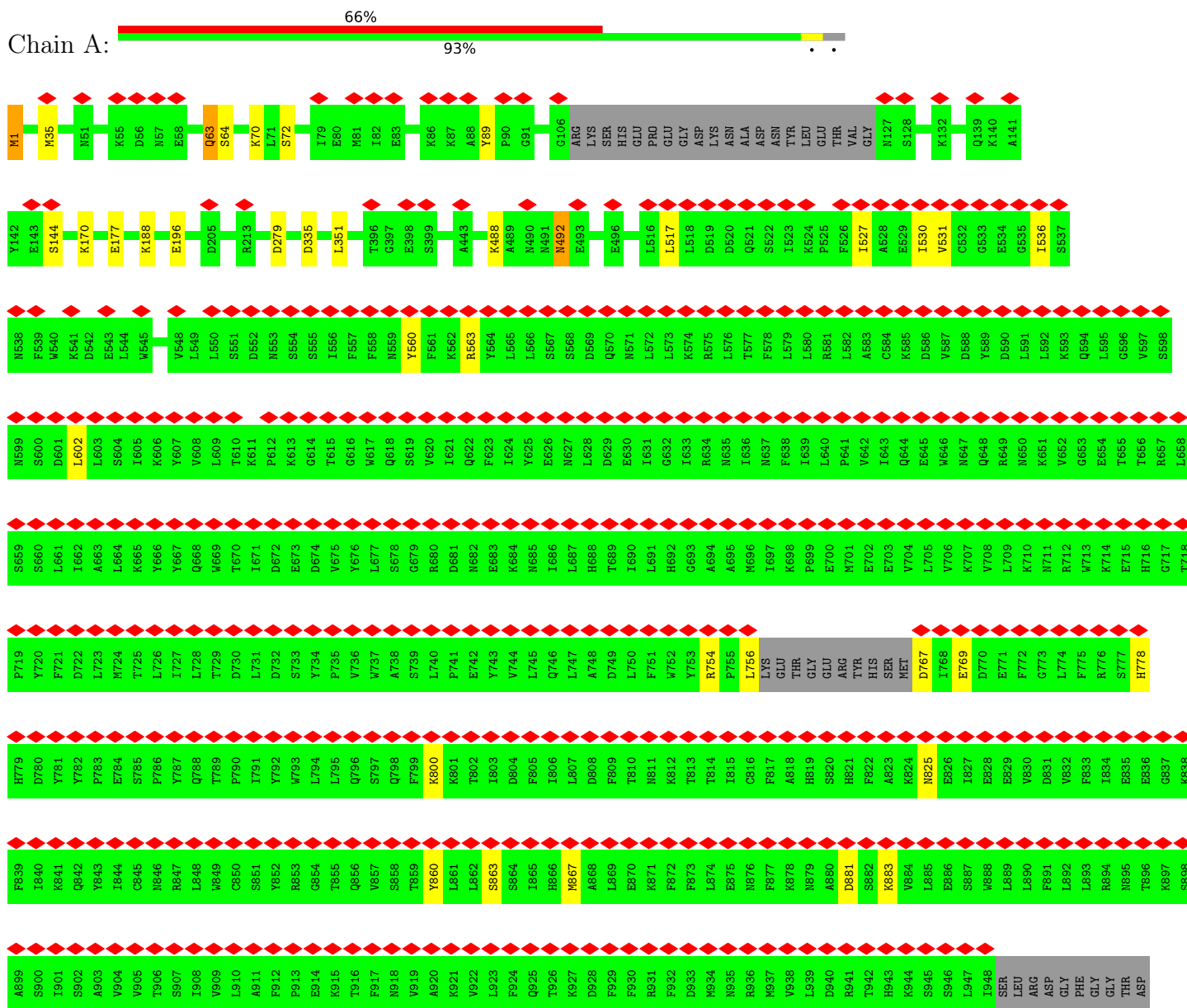
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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.

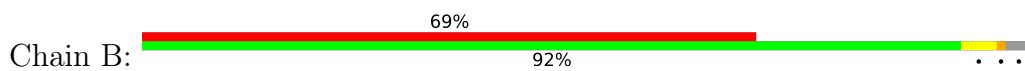
- Molecule 1: ATP-binding protein Avs4



TYR	ARG	L1019	L1020	L1021	E1022	A1023	Q1024	E1025	T1026	E1027	A1028	D1029	K1030	A971	C972	D973	D974	V975	H976	R977	R978	T979	Y980	L981	E982	N983	L984	A985	L986	H987	Y988	Y989	Y990	F991	A992	S993	E994	N995	V996	T997	E998	R999	D1000	A1001	I1002	E1003	R1004	Q1005	Q1006	V1007	L1008	M1009	D1010	I1011	F1012	D1013	K1014	Y1015	Y1016	M1017	Q1018
S1079	E1080	H1081	M1082	K1083	V1084	V1085	T1086	L1087	K1088	L1089	M1090	A1091	S1092	Y1093	K1094	Q1095	E1096	K1097	D1098	E1099	R1100	Y1101	K1102	M1103	Y1104	G1105	M1106	I1107	D1109	M1110	Q1111	Q1112	I1113	A1114	L1115	Q1116	E1117	T1118	K1119	E1120	I1121	I1122	K1123	K1124	L1125	M1126	E1127	E1128	G1129	G1130	E1131	D1132	F1133	R1134	L1135	L1136	M1137	G1138			
M1139	I1140	P1141	A1142	L1143	V1144	C1145	S1146	V1147	L1148	L1149	L1150	D1151	Y1152	F1153	M1154	Q1155	L1156	M1157	M1158	E1159	E1160	R1161	E1162	Y1163	C1164	G1165	D1166	I1167	L1168	L1169	A1170	Y1171	S1172	K1173	L1174	P1175	L1176	K1177	E1178	G1179	Y1180	M1181	I1182	Q1183	V1184	Q1185	D1186	G1187	T1188	T1189	G1190	A1191	I1192	S1193	L1194	A1195	L1196	V1197	I1198		
Y1199	H1200	M1201	Y1202	P1203	M1204	E1205	R1206	E1207	T1208	I1209	K1210	I1211	I1212	L1213	L1214	L1215	T1216	L1217	F1218	M1219	D1220	H1221	S1222	I1223	G1224	M1225	A1226	G1227	G1228	R1229	Y1230	S1231	S1232	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	I1258		
L1259	K1260	P1261	K1262	V1263	V1264	I1265	L1266	S1267	R1268	L1269	I1270	I1271	H1272	E1273	S1274	R1275	Y1276	Q1277	VAL	ASP	TVR	ASP	I1282	K1283	K1284	I1285	M1286	I1287	M1288	K1289	V1290	F1291	M1292	N1293	M1294	Y1295	K1296	H1297	C1298	I1299	S1300	M1301	V1302	I1303	D1304	M1305	K1306	I1307	S1308	I1309	D1310	D1311	G1313	S1314	M1315	L1316	K1317	V1318			
D1319	L1320	H1321	I1322	L1323	M1324	T1325	A1326	F1327	Q1328	L1329	I1330	P1331	V1332	D1333	T1334	V1335	M1336	I1337	E1338	H1339	K1340	K1341	L1342	V1343	S1344	L1345	I1346	V1347	K1348	R1349	F1350	S1351	L1352	S1353	L1354	L1355	E1356	S1357	V1358	R1359	E1360	D1361	R1362	V1363	L1364	Y1365	Y1366	A1366	L1367	R1368	Q1369	S1370	F1371	L1372	E1373	R1374	M1375	L1376	Y1377	F1378	
T1379	L1380	H1381	A1382	P1383	V1384	S1385	D1386	I1387	P1388	D1389	Y1390	I1391	K1392	P1393	F1394	L1395	D1396	G1397	F1398	M1399	G1400	S1401	E1402	P1403	I1404	S1405	E1406	L1407	F1408	K1409	K1410	F1411	I1412	L1413	V1414	E1415	D1416	R1417	L1418	M1419	T1420	Y1421	A1422	K1423	F1424	W1425	K1426	V1427	Y1428	D1429	L1430	F1431	S1432	D1433	K1434	V1435	A1436	T1437	L1438		
C1439	K1440	D1441	G1442	D1443	R1444	Y1445	V1446	Y1447	V1448	D1449	K1450	I1451	I1452	K1453	S1454	Y1455	L1456	F1457	A1458	E1459	S1460	P1461	V1462	K1463	E1464	N1465	S1466	N1467	G1468	W1469	H1470	T1471	K1472	K1473	D1474	S1475	N1476	S1477	Q1478	F1479	F1480	C1481	D1482	V1483	S1484	R1485	T1486	M1487	H1488	H1489	C1490	P1491	S1492	T1493	L1494	Y1495	A1496	L1497	A1498		
K1499	S1500	L1501	M1502	M1503	I1504	A1505	S1506	C1507	Y1508	L1509	M1510	Q1511	I1512	I1513	T1514	W1515	L1516	S1517	E1518	I1519	L1520	S1521	V1522	M1523	K1524	K1525	L1526	W1527	E1528	K1529	K1530	L1531	E1532	M1533	D1534	T1535	V1536	Y1537	Y1538	L1539	E1540	C1541	L1542	R1543	Y1544	I1545	M1546	M1547	E1548	M1549	E1550	R1551	E1552	R1553	I1554	R1555	E1556	V1557	L1558		

D1569	F1570	L1571	V1572	E1573	K1574	G1575	S1576	V1577	G1578	L1579	Y1580	M1581	S1582	M1585	I1586	L1587
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

• Molecule 1: ATP-binding protein Avs4

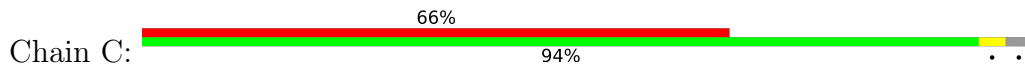


FME	V2	K3	M4	Q45	S46	K55	D56	N57	E58	Q63	S64	K65	D68	T69	K70	L71	S72	K75	A76	D77	L78	I79	E80	M81	K86	K87	A88	Y89	P90	W103	GLY	GLN	GLY	ARG	LYS	SER	HIS	GLU	PRO	GLU	GLY	ASP	LYS	ASN	ALA	ASP	ASN	ASN	TVR	LEU	GLU	THR	VAL
-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

L1136	L1137	G1138	N1139	I1140	P1141	A1142	D1143	V1144	C1145	S1146	V1147	L1148	L1149	L1150	D1151	F1152	F1153	N1154	Q1155	L1156	N1157	N1158	E1159	E1160	R1161	E1162	Y1163	C1164	K1165	D1166	I1167	V1168	L1169	A1170	Y1171	C1172	K1173	L1174	P1175	L1176	K1177	E1178	G1179	Y1180	N1181	Y1182	Q1183	V1184	O1185	D1186	G1187	T1188	T1189	S1190	I1191	A1192	S1193	L1194	L1195				
K1076	K1077	N1078	S1079	E1080	H1081	K1082	K1083	Y1084	V1085	T1086	L1087	K1088	L1089	W1090	A1091	S1092	Y1093	K1094	R1095	E1096	K1097	D1098	E1099	R1100	R1101	K1102	N1103	Y1104	G1105	M1106	Y1107	E1108	D1109	N1110	P1111	Q1112	I1113	A1114	L1115	Q1116	E1117	T1118	K1119	E1120	I1121	I1122	K1123	K1124	L1125	N1126	E1127	K1066	L1067	K1068	Q1069	I1070	G1130	E1131	D1132	E1073	R1133	R1134	L1135
Y1016	N1017	Q1018	L1019	P1020	D1021	E1022	A1023	Q1024	E1025	T1026	E1027	A1028	D1029	K1030	T1031	M1032	R1033	L1034	C1035	L1036	A1037	R1038	M1039	D1040	R1041	R1042	K1043	M1044	K1045	I1046	T1047	T1048	K1049	E1050	K1051	D1052	E1053	G1054	I1055	E1056	I1057	S1058	F1059	M1060	P1061	E1062	I1063	D1064	P1065	K1066	L1067	K1068	Q1069	Y1070	G1130	E1131	D1132	E1073	A1074	I1075			
K1076	K1077	N1078	S1079	E1080	H1081	K1082	K1083	Y1084	V1085	T1086	L1087	K1088	L1089	W1090	A1091	S1092	Y1093	K1094	R1095	E1096	K1097	D1098	E1099	R1100	R1101	K1102	N1103	Y1104	G1105	M1106	Y1107	E1108	D1109	N1110	P1111	Q1112	I1113	A1114	L1115	Q1116	E1117	T1118	K1119	E1120	I1121	I1122	K1123	K1124	L1125	N1126	E1127	K1066	L1067	K1068	Q1069	Y1070	G1130	E1131	D1132	E1073	A1074	I1075	
T896	K897	S898	A899	S900	I901	S902	A903	V904	V905	T906	S907	I908	W909	L910	A911	F912	P913	E914	K915	T916	F917	N918	V919	A920	K921	V922	L923	F924	Q925	T926	K927	D928	R929	F930	R931	F932	E994	N995	V996	T997	N998	D1000	A1001	I1002	E1003	R1004	Q1005	Q1006	S946	L947	I948	SER	LEU	ARG	ASP	GLY	PHE	GLY	I1015				
E836	G837	K838	F839	I840	K841	Q842	Y843	I844	C845	M846	R847	L848	W849	C850	S851	Y852	K853	G854	T855	Q856	W857	S858	T859	Y860	L861	L862	S863	S864	T865	H866	K867	A868	L869	E870	K871	F872	L874	E875	H876	F877	A878	K878	N879	A880	D881	S882	K883	V884	L885	E886	S887	W888	L889	L890	V891	D892	L893	R894	N895				
R776	S777	H778	H779	D780	Y781	Y782	P783	E784	S785	P786	Y787	Q788	T789	P790	I791	Y792	W793	L794	L795	Q796	S797	Q798	F799	K800	L801	T802	L803	D804	F805	L806	L807	D808	F809	T810	N811	K812	T813	L814	L815	C816	F817	A818	H819	S820	S821	F822	A823	K824	N825	E826	L827	E828	E829	V830	D831	L832	F833	L834	E835				
H716	G717	T718	P719	Y720	D721	L722	L723	W724	T725	L726	I727	W728	L729	D730	L731	D732	S733	Y734	P735	W736	W737	A738	S739	L740	E741	E742	Y743	V744	L745	Q746	L747	A748	D749	L750	F751	W752	Y753	R754	P755	L756	LYS	THR	GLY	GLU	ARG	TYR	HIS	SER	MET	D767	I768	E769	D770	E771	F772	G773	L774	F775	K714	E715			
T856	R657	L658	S659	S660	L661	I662	A663	L664	K665	Y666	Y667	Q668	W669	T670	I671	D672	E673	D674	V675	W676	L677	S678	G679	R680	I681	N682	E683	K684	Y685	E686	L687	H688	T689	I690	L691	H692	G693	A694	A695	M696	I697	K698	P699	E700	M701	E702	E703	V704	L705	V706	K707	V708	L709	K710	K651	W652	R712	K714	E715				
I536	S537	N538	F539	W540	K541	D542	E543	L544	W545	V546	A547	V548	L549	L550	S551	D552	N553	S554	S555	I556	F557	F558	N559	Y560	F561	K562	Y564	L565	L566	S567	S568	D569	Q570	N571	L572	L573	K574	R575	L576	T577	F578	L579	L580	R581	L582	L583	C584	K585	D586	V587	D588	Y589	D590	L591	L592	K593	Q594	L595					
G596	V597	S598	N599	W600	D601	L602	L603	S604	I605	K606	Y607	W608	L609	T610	K611	P612	K613	G614	T615	G616	Q618	S619	W620	I621	Q622	F623	I624	Y625	E626	N627	L628	D629	E630	I631	G632	I633	R634	N635	I636	N637	F638	I639	L640	P641	V642	I643	Q644	E645	W646	N647	Q648	D649	M650	K651	W652	R712	E715						
D308	K311	K321	W322	M331	Y332	L333	A334	D335	V336	M337	Y338	A339	F340	I341	D342	I343	S344	K345	I346	T347	E357	E363	D366	T396	G397	E398	M492	E500	R515	L516	L517	L518	D519	D520	Q521	S522	I523	P525	F526	A528	E529	I530	C532	G533	E534	G535																	
GLY	ASN	SER	ASN	D130	P131	K132	I133	K134	I135	E136	V137	D138	Q139	K140	A141	Y142	E143	S144	G145	I146	H171	N176	D205	R213	H214	L219	H220	E221	N222	L223	V224	Q225	K226	K227	I228	E234	K244	E248	Q252	Y253	D287	E288	L289	R290	K291	L302	E303																

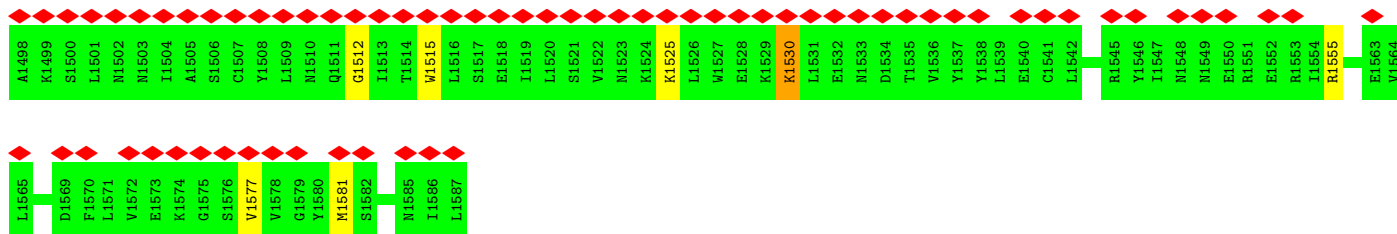
P1196	V1197	I1198	Y1199	H1200	N1201	Y1202	P1203	M1204	R1206	E1207	T1208	I1209	K1210	T1211	I1212	L1213	L1214	L1215	L1216	L1217	F1218	N1219	D1220	H1221	S1222	I1223	G1224	M1225	A1226	G1227	G1228	G1229	V1230	S1231	F1232	F1233	P1234	S1235	M1236	I1238	H1239	K1240	L1241	W1242	L1243	D1244	Y1245	F1246	D1247	D1248	N1249	Q1250	S1251	L1252	L1253	F1254	G1255		
F1256	L1257	I1258	L1259	K1260	P1261	K1262	Y1263	M1264	I1265	L1266	S1267	K1268	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	L1302	I1303	D1304	D1364	K1306	Y1307	S1308	I1309	D1310	L1311	L1312	L1313	S1314	M1315
D1316	K1317	V1318	D1319	L1320	H1321	I1322	L1323	M1324	T1325	A1326	F1327	Q1328	L1329	I1330	P1331	D1332	T1334	V1335	M1336	I1337	E1338	H1339	K1340	K1341	L1342	V1343	L1344	L1345	I1346	V1347	K1348	R1349	F1350	S1351	L1352	S1353	L1354	L1355	L1356	S1357	V1358	R1359	E1360	R1362	V1363	D1364	K1365	Y1366	A1366	L1367	I1368	Q1369	S1370	F1371	L1372	E1373	L1374	F1375	
A1376	Y1377	F1378	T1379	L1380	H1381	A1382	P1383	V1384	S1385	D1386	I1387	P1388	D1389	Y1390	I1391	K1392	P1393	F1394	L1395	D1396	M1396	G1397	F1398	N1399	G1400	K1401	E1402	P1403	I1404	S1405	E1406	L1407	F1408	K1409	K1410	F1411	I1412	L1413	V1414	E1415	D1416	R1417	L1418	N1419	T1420	A1422	K1423	F1424	Y1425	K1426	V1427	W1428	I1429	L1430	F1431	F1432	L1433	K1434	V1435
T1436	L1437	L1438	C1439	D1441	G1442	D1443	L1444	Y1445	W1446	Y1447	V1448	D1449	K1450	I1451	I1452	K1453	S1454	Y1455	L1456	F1457	A1458	E1459	S1460	P1461	W1462	K1463	E1464	N1465	S1466	N1467	G1468	W1469	H1470	L1471	F1472	K1473	D1474	S1475	N1476	N1477	Q1478	F1479	F1480	C1481	D1482	V1483	S1484	R1485	T1486	M1487	G1488	H1489	C1490	P1491	S1492	T1493	L1494	L1495	
S1496	L1497	A1498	K1499	S1500	N1501	M1502	N1503	I1504	A1505	S1506	C1507	Y1508	L1509	M1510	Q1511	I1512	I1513	T1514	W1515	L1516	S1517	E1518	I1519	L1520	S1521	V1522	N1523	K1524	K1525	L1526	V1527	E1528	L1529	M1530	L1531	E1532	N1533	D1534	T1535	V1536	Y1537	Y1538	E1540	C1541	V1543	R1544	R1545	Y1546	T1547	M1548	N1549	E1550	R1551	E1552	R1553	Q1562			
E1563	V1566	I1567	L1568	D1569	F1570	L1571	V1572	E1573	K1574	G1575	S1576	V1577	V1578	V1579	M1580	M1581	S1582	R1583	E1584	M1585	I1586	L1587																																					

• Molecule 1: ATP-binding protein Avs4

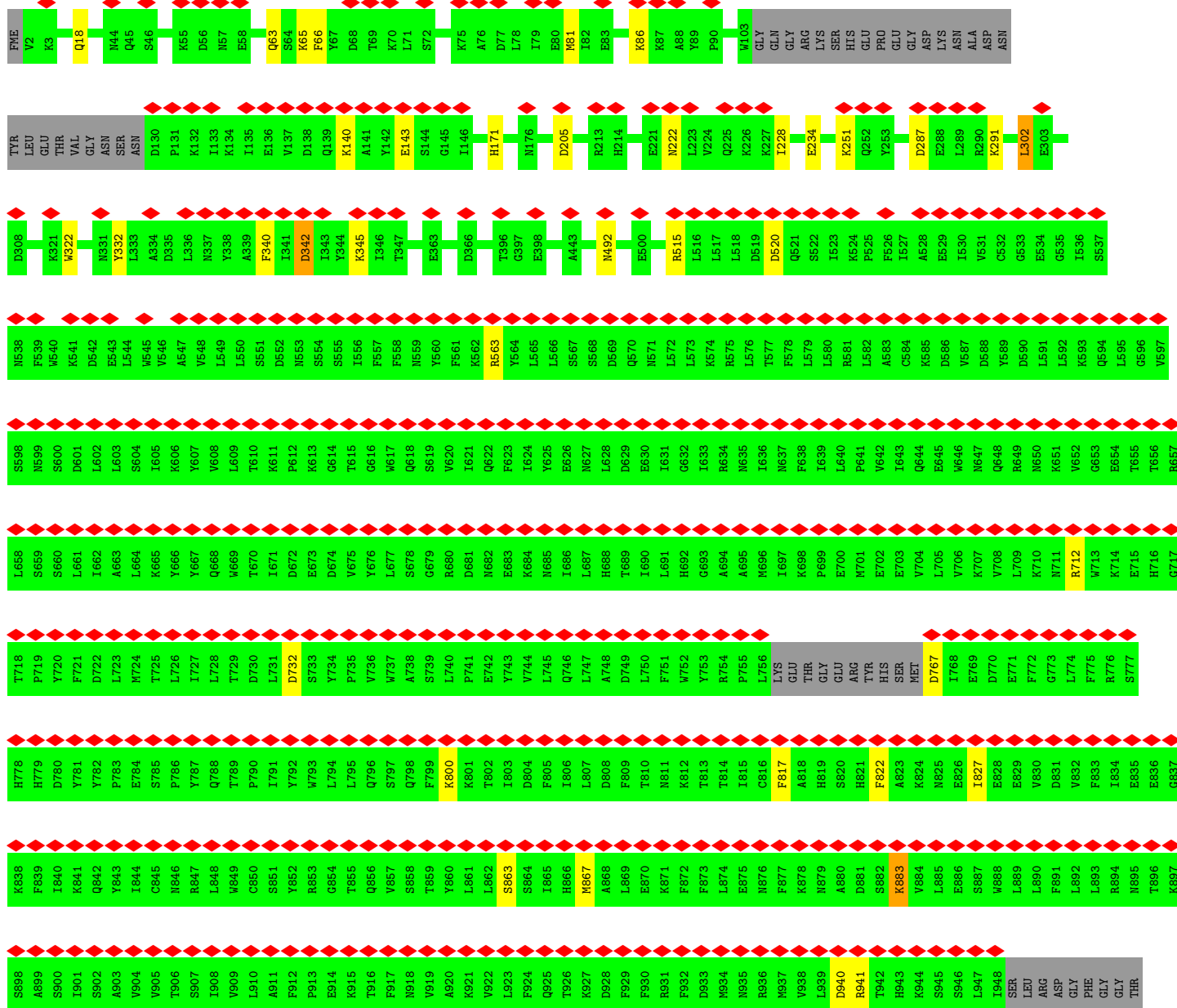
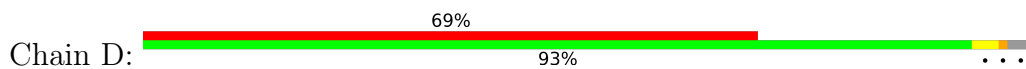


M1	V2	K3	P4	M35	N51	D56	N57	E58	Q63	S64	I79	E80	M81	I82	E83	K86	K87	A88	Y89	P90	G91	G106	ARG	N490	LYS	SER	HIS	GLU	PRO	GLY	GLY	ASP	LYS	ASN	ALA	ASP	ASN	TYR	LEU	GLU	THR	VAL	GLY	N127	S128	K132	Q139	K140	A141	Y142	E143										
S144	K170	E177	K188	D542	E196	D205	D211	R212	R213	D279	K611	D335	L351	T396	G397	E398	E398	F438	A443	K488	A489	N490	N491	N492	E493	E496	L516	L517	L518	D519	D520	Q521	S522	I523	K524	P525	F526	I527	A528	E529	I530	V531	D532	V531	E533	Q533	E534	G535	I536												
S537	N538	F539	W540	K541	E543	L544	W545	V548	L549	L550	S551	D552	N553	S554	S555	I556	F557	F558	N559	Y560	F561	K562	R563	Y564	L565	L566	N567	S568	S568	D569	Q570	N571	L572	L573	K574	R575	L576	T577	F578	L579	L580	R581	L582	A583	C584	K585	D586	V587	D588	Y589	D590	L591	L592	K593	Q594	L595	G596	V597			
S598	N599	S600	D601	L602	L603	S604	L644	I605	K606	V607	V608	L609	T610	K611	P612	K613	S614	G614	T615	G616	W617	F618	N619	Y620	I621	R622	F623	I624	N625	E626	N627	L628	D629	E630	I631	G632	I633	R634	M635	L636	N637	F638	I639	L640	P641	V642	I643	Q644	E645	W646	N647	D648	R649	N650	K651	R652	G653	E654	T655	G656	R657
L658	S659	S660	L661	I662	A663	L664	K665	V666	Q668	W669	I670	E671	D672	E673	D674	V675	Y676	L677	S678	G679	R680	D681	N682	E683	K684	N685	I686	L687	H688	T689	I690	H691	H692	G693	A694	A695	M696	I697	K698	P699	E700	M701	E702	E703	V704	L705	W706	K707	V708	L709	K710	N711	R712	W713	K714	E715	H716	G717			

L1438	F1378	V1318	I1258	I1198	G1138	M1076	Q1018	ASP	S898	K838	H778	T718
C1439	T1379	D1319	L1259	Y1199	M1139	S1079	L1019	TYR	A899	F839	H779	P719
K1440	L1380	L1320	K1260	H1200	I1140	E1080	P1020	ARG	S900	I840	D780	Y720
D1441	H1381	H1321	P1261	N1201	P1141	H1081	D1021		I901	K841	F781	F721
G1442	A1382	I1322	K1262	N1202	A1142	M1082	E1022		S902	Q842	Y782	D722
D1443	P1383	L1323	Y1263	P1203	D1143	K1083	A1023		A903	P843	P783	L723
R1444	V1384	N1324	V1264	M1204	V1144	Y1084	Q1024		V904	I844	E784	M724
Y1445	S1385	T1325	I1265	E1205	C1145	V1085	E1025		V905	C845	S785	T725
M1446	D1386	A1326	L1266	R1206	S1146	L1086	T1026		T906	R846	P786	L726
V1447	F1387	F1327	S1267	E1207	V1147	L1087	E1027		S907	R847	Y787	I727
V1448	P1388	Q1328	R1268	T1208	L1148	K1088	A1028		I908	R848	Q788	L728
D1449	D1389	L1329	K1269	I1209	L1149	L1089	D1029		V909	W849	T789	T729
K1450	Y1390	I1330	I1270	K1210	L1150	M1090	K1030		L910	C850	P790	D730
I1451	I1391	V1331	I1271	T1211	D1151	A1091	T1031		A911	S851	I791	L731
K1452	K1392	V1332	H1272	I1212	Y1152	S1092	F1032		F912	Y852	Y792	D732
K1453	P1393	L1333	E1273	L1213	F1153	Y1093	R1033		P913	R853	W793	S733
S1454	F1394	T1334	S1274	L1214	M1154	K1094	L1034		E914	G854	L794	Y734
L1455	L1395	V1335	Y1275	L1215	Q1155	K1095	C1035		K915	S855	L795	P735
L1456	D1396	M1336	R1276	T1216	L1156	E1096	L1036		T916	Q856	Q796	V736
F1457	G1397	I1337	Q1277	L1217	M1157	K1097	A1037		F917	V857	S797	W737
A1458	F1398	E1338	VAL	F1218	M1158	D1098	A1038		N918	S858	Q798	A738
E1459	M1399	H1339	ASP	M1219	E1159	E1099	R1039		V919	W859	F799	S739
S1460	G1400	K1340	TYR	D1220	E1160	R1100	M1040		A920	Y860	K800	L740
P1461	S1401	K1341	ASP	H1221	R1161	Y1101	R1041		K921	L861	K801	P741
W1462	E1402	L1342	I1282	S1222	E1162	K1102	R1042		V922	L862	T802	E742
K1463	P1403	L1343	K1283	I1223	Y1163	M1103	K1043		L923	S863	Y803	Y743
E1464	I1404	S1344	K1284	G1224	C1164	Y1104	M1044		F924	S864	D804	V744
S1405	S1405	L1345	I1285	M1225	K1165	G1105	K1045		Q925	I865	F805	L745
E1406	E1406	L1346	M1286	A1226	K1166	M1106	I1046		T926	H866	I806	Q746
L1407	V1347	I1347	I1287	A1227	D1167	V1107	T1047		K927	V867	L807	L747
F1408	F1408	K1348	K1289	G1228	V1168	E1108	T1048		D928	A868	D808	A748
K1409	K1409	R1349	R1290	R1229	L1169	D1109	K1049		F929	L869	F809	D749
K1410	F1350	F1350	F1291	Y1230	A1170	M1110	E1050		F930	E870	T810	L750
F1411	S1351	T1351	L1292	I1231	Y1171	K1111	K1051		R931	K871	N811	F751
I1412	I1412	T1352	M1293	V1232	S1172	Q1112	D1052		F932	F872	K812	W752
L1413	M1294	S1353	M1294	F1233	K1173	I1113	E1053		D933	F873	T813	Y753
V1414	Y1295	L1354	Y1295	P1234	L1174	A1114	G1054		M934	L874	T814	R754
E1415	K1296	L1355	K1296	S1235	P1175	L1115	I1055		N935	E875	I815	P755
D1416	H1297	M1356	H1297	M1236	L1176	Q1116	E1056		R936	N876	C816	L756
R1417	C1298	V1357	C1298	V1237	K1177	E1117	I1057		M937	F877	F817	LYS
L1418	I1299	V1358	I1299	I1238	E1178	S1058	S1058		V938	K878	A818	GLU
M1419	S1300	R1359	S1300	H1239	G1179	K1119	F1059		L939	H819	A819	THR
F1420	M1301	E1360	M1301	K1240	Y1180	E1120	M1060		D940	A880	S820	GLU
Y1421	D1361	D1361	V1302	L1241	M1181	I1121	P1061		R941	D881	H821	ARG
A1422	R1362	R1362	I1303	W1242	Y1182	I1122	E1062		T942	S882	F822	THR
K1423	D1304	K1243	D1304	W1243	Q1183	K1123	I1063		H943	K883	A823	HIS
F1424	D1364	D1244	M1305	D1244	Y1184	K1124	D1064		K944	V884	K824	MET
W1425	Y1365	Y1245	K1306	Y1245	Q1185	L1125	P1065		S945	L885	N825	D767
K1426	A1366	F1246	K1307	F1246	D1186	M1126	K1066		S946	E886	E826	I768
W1428	L1367	D1247	S1308	D1247	G1187	E1127	L1067		L947	S887	I827	E769
D1429	R1368	D1248	I1309	D1248	T1188	E1128	K1068		I948	W888	E828	D770
L1430	Q1369	M1249	D1310	M1249	T1189	G1129	Q1069		SER	L889	E829	E771
P1431	S1370	Q1250	D1311	Q1250	S1190	G1130	Y1070		ARG	L890	E830	F772
F1432	L1372	L1252	L1312	L1252	A1191	I1131	S1071		ASP	F891	D831	G773
D1433	L1373	L1253	G1313	L1253	I1192	D1132	E1072		GLY	L892	V832	L774
K1434	L1374	F1254	S1314	L1253	S1193	F1133	E1073		PHE	L893	F833	F775
L1435	R1374	G1255	L1315	F1254	A1194	R1134	A1074		GLY	N894	I834	R776
Y1436	F1375	F1256	D1316	F1256	L1195	L1135	T1075		THR	E895	E835	S777
A1376	A1376	Y1377	K1317	F1256	P1196	L1136	K1076			T896	E836	
L1497					V1197	M1137	K1077			K897	G837	

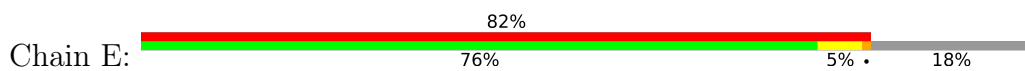


• Molecule 1: ATP-binding protein Avs4



ASP	TYR	ARG	R961	S962	L963	R964	E965	E966	D967	R968	I969	R970	A971	C972	D973	D974	V975	H976	L977	R978	T979	Y980	L981	E982	R983	L984	A985	L986	H987	Y988	Q989	I990	F991	R992	S993	E994	N995	Y996	T997	E998	R999	D1000	A1001	I1002	E1003	R1004	Q1005	Q1006	V1007	L1008	W1009	D1010	I1011	F1012	D1013	K1014	Y1015	L1016	M1017
L1018	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	K1045	L1046	T1047	T1048	K1049	E1050	K1051	D1052	E1053	G1054	I1055	E1056	I1057	S1058	F1059	N1060	P1061	E1062	I1063	D1064	P1065	K1066	V1007	L1008	W1009	D1010	I1011	F1012	D1013	K1014	Y1015	L1016	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	G1114	L1115	Q1116	E1117	T1118	K1119	E1120	I1121	I1122	K1123	R1124	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	M1154	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	I1182	K1183	V1184	Q1185	D1186	G1187	T1188	T1189	G1190	E1191	I1192	D1193	F1194	A1195	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	L1228	R1229	Y1230	I1231	V1232	F1233	P1234	S1235	M1236	V1237	I1238	H1239	K1240	L1241	W1242	L1243	D1244	Y1245	F1246	G1247	T1248	M1249	Q1250	A1251	I1252	L1253	F1254	G1255	F1256	L1257
L1268	L1269	K1270	P1261	K1262	Y1263	V1264	I1265	L1266	S1267	R1268	K1269	I1270	L1271	H1272	E1273	S1274	Y1275	R1276	Q1277	VAL	ASP	TYR	ASP	I1282	K1283	K1284	I1285	M1286	I1287	M1288	K1289	V1290	F1291	L1292	M1293	N1294	Y1295	K1296	H1297	C1298	I1299	S1300	N1301	V1302	I1303	D1304	M1305	K1306	I1307	S1308	I1309	D1310	D1311	L1312	G1313	S1314	M1315	K1316	K1317
V1318	D1319	L1320	H1321	L1322	L1323	M1324	T1325	A1326	F1327	Q1328	L1329	I1330	P1331	V1332	D1333	L1334	V1335	M1336	I1337	E1338	H1339	K1340	K1341	L1342	V1343	S1344	L1345	I1346	K1348	R1349	F1350	L1351	T1352	S1353	L1354	L1355	S1356	S1357	V1358	R1359	E1360	D1361	R1362	V1363	D1364	Y1365	A1366	V1367	R1368	Q1369	S1370	F1371	L1372	D1373	S1374	M1375	A1376	Y1377	
F1378	T1379	L1380	H1381	A1382	P1383	V1384	S1385	D1386	I1387	P1388	D1389	Y1390	I1391	K1392	P1393	F1394	L1395	D1396	G1397	F1398	M1399	G1400	S1401	E1402	P1403	I1404	S1405	E1406	F1408	K1409	K1410	F1411	I1412	L1413	V1414	E1415	D1416	R1417	L1418	M1419	T1420	Y1421	A1422	K1423	F1424	Y1425	K1426	V1427	W1428	D1429	L1430	F1431	F1432	D1433	K1434	Y1435	V1436	T1437	
L1438	C1439	K1440	D1441	G1442	R1444	Y1445	W1446	S1447	V1448	D1449	K1450	I1451	I1452	K1453	S1454	Y1455	L1456	F1457	A1458	E1459	S1460	W1461	W1462	K1463	E1464	M1465	S1466	M1467	G1468	V1469	H1470	T1471	F1472	K1473	D1474	S1475	N1476	S1477	Q1478	F1479	F1480	C1481	D1482	S1484	R1485	T1486	M1487	G1488	H1489	C1490	S1492	T1493	L1494	Y1495	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	W1527	E1528	K1529	K1530	E1532	M1533	D1534	Y1535	V1536	Y1537	Y1538	L1539	E1540	C1541	V1543	R1544	R1545	Y1546	I1547	M1548	M1549	E1550	R1551	E1552	R1553	Q1562	E1563						
V1566	I1567	L1568	D1569	F1570	L1571	V1572	E1573	K1574	G1575	S1576	V1577	V1578	G1579	M1580	M1581	S1582	R1583	E1584	M1585	I1586	L1587	I1519	L1520	S1521	V1522	K1524	K1525	W1527	E1528	K1529	K1530	E1532	M1533	D1534	Y1535	V1536	Y1537	Y1538	L1539	E1540	C1541	V1543	R1544	R1545	Y1546	I1547	M1548	M1549	E1550	R1551	E1552	R1553	Q1562	E1563					

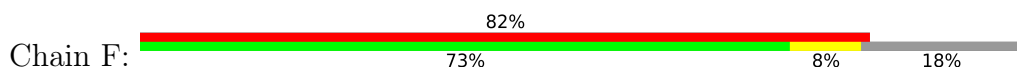
• Molecule 2: Portal protein



WET	ALA	SER	GLN	R6	R7	E8	O9	F10	A11	E12	M13	G14	A15	K16	A17	V18	Y19	D20	A21	L22	R23	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	S58	P59	H60
-----	-----	-----	-----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Q61	M121	V181	D241	N501	A421	ALA	ILE
A62	Y122	T182	A242	P302	V422	VAL	LEU
V63	I123	L183	S243	A303	E423	GLN	LYS
G64	E124	D184	Y244	G304	P424	THR	PRO
A65	S125	K185	P245	I305	T425	GLY	GLU
R66	S126	T186	V246	T306	T426	GLU	GLY
G67	S127	A187	D247	Q307	S427	VAL	GLN
L68	Y128	Y188	A248	V308	T428	THR	GLN
N69	R129	A189	C249	R309	G429	ALA	GLU
N70	V130	A190	P250	R310	M430	ALA	ALA
L71	T131	L191	Y251	L311	E431	E372	GLU
A72	L132	P192	I252	T312	A432	E373	ALA
S73	F133	E193	P253	K313	L433	I374	ALA
K74	E134	D194	V254	A314	G434	R375	GLN
L76	T135	V195	R255	Q315	R435	Y376	GLY
M76	L136	R196	M256	T316	G436	V377	THR
L77	K137	A197	V257	S379	Q437	A378	ALA
A78	Q138	A198	R258	D318	D438	E380	ASN
L79	L139	M199	I259	F319	L439	L381	ALA
F80	V140	D200	D260	V320	D440	E382	ALA
P81	V141	S201	G261	S321	K441	D383	SER
M82	A142	G202	E262	G322	L442	T384	ALA
Q83	G143	Q203	S263	R323	E443	L385	GLY
T84	M144	E204	Y264	P324	R444	G386	ALA
M85	A145	H205	G265	E325	C445	G387	GLY
M86	L146	K206	R266	D326	T446	V388	ALA
K87	L147	G207	S267	I327	A447	Y389	GLY
L88	Y148	D208	Y268	S328	A448	S390	LEU
T89	I149	E209	C269	F329	W449	I391	ALA
I90	P150	M210	E270	L330	S450	L392	ALA
S91	E151	I211	E271	Q331	A451	S393	SER
E92	P152	D212	Y272	L332	L452	Q394	PRO
F93	E153	V213	L273	E333	A453	E395	GLU
E94	G154	Y214	G274	K334	P454	L396	ASN
A95	A155	T215	D275	A335	M455	Q397	GLU
K96	Y156	H216	L276	A336	GLN	L398	ALA
Q97	M157	I217	R277	D337	ASN	P399	ALA
L98	P158	Y218	S278	F338	PRO	M400	ALA
V99	M159	L219	L279	S339	ASP	V401	GLN
A100	K160	D220	E280	V340	ASP	R402	ALA
Q101	L161	E221	M281	V403	ILE	V403	GLY
P102	P162	I222	L282	K342	ILE	L404	VAL
A103	R163	S223	Q283	A343	THR	L405	PRO
E104	L164	G224	E284	V344	ILE	K406	ALA
L105	S165	E225	A285	S345	LYS	Q407	ILE
A106	S166	Y226	I286	E346	LEU	L408	LEU
K107	Y167	L227	V287	Q347	ILE	Q409	ALA
V108	V168	K228	K288	I348	ALA	A410	ALA
E109	V169	Y229	M289	E349	ASN	T411	ASN
E110	Q170	E230	S290	G350	ALA	M412	ALA
G111	R171	E231	M291	R351	GLY	Q413	ILE
L112	D172	I232	I292	L352	ILE	T414	ILE
S113	A173	D233	S293	S353	THR	P415	ASP
M114	F174	G234	A294	Y354	SER	E416	THR
V115	G175	V235	K295	A355	GLY	L417	SER
E116	T176	E236	V296	F356	ALA	P418	GLY
R117	V177	V237	I297	M357	R419	K419	ASP
L118	L178	D238	G298	L358	SER	E420	THR
L119	Q179	G239	L299	M359	GLY		SER
M120	I180	T240	V300	SER			

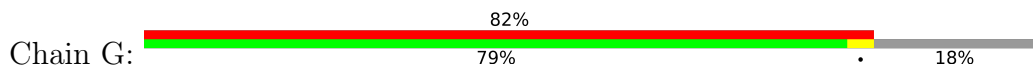
Molecule 2: Portal protein



MET	Q61	Y121	V181	D241	N501	A421	ILE
ALA	A62	Y122	T182	A242	P302	V422	LEU
SER	V63	I123	L183	S243	A303	E423	LYS
GLM	G64	E124	D184	Y244	G304	P424	THR
K6	R66	S125	K185	P245	I305	T425	GLU
R7	R66	S126	T186	V246	T306	T426	GLU
E8	G67	S127	A187	D247	Q307	S427	GLN
G9	L68	Y128	Y188	A248	V308	T428	GLN
F10	N69	R129	A189	C249	R309	G429	GLU
A11	N70	V130	A190	P250	R310	M430	ALA
E12	L71	T131	L191	Y251	L311	E431	GLU
N13	A72	L132	P192	I252	T312	A432	ALA
G14	S73	F133	E193	P253	K313	L433	ALA
A15	K74	E134	D194	V254	A314	G434	GLY
K16	L76	T135	V195	R255	Q315	R435	THR
A17	M76	L136	R196	M256	T316	G436	ALA
V18	L77	K137	A197	V257	S379	Q437	LEU
Y19	A78	Q138	R258	D318	D438	E380	ASN
D20	L79	L139	I259	F319	L439	L381	ALA
A21	F80	V140	D260	V320	D440	E382	ALA
L22	P81	V141	G261	S321	K441	D383	SER
K23	M82	A142	E262	G322	L442	T384	ALA
N24	Q83	G143	S263	R323	E443	L385	GLY
D25	T84	M144	Y264	P324	R444	G386	ALA
R26	M85	A145	G265	E325	C445	G387	GLY
N27	M86	L146	R266	D326	T446	V388	ALA
S28	K87	L147	S267	I327	A447	Y389	GLY
Y29	L88	Y148	Y268	S328	A448	S390	LEU
E30	T89	I149	C269	F329	W449	I391	ALA
T31	I90	P150	E270	L330	S450	L392	ALA
R32	S91	E151	E271	Q331	A451	S393	SER
A33	E92	P152	Y272	L332	L452	Q394	PRO
E34	F93	E153	L273	E333	A453	E395	GLU
N35	E94	G154	G274	K334	P454	L396	ASN
C36	A95	A155	D275	A335	M455	Q397	GLU
A37	K96	Y156	L276	A336	GLN	L398	ALA
K38	Q97	M157	R277	D337	ASN	P399	ALA
Y39	L98	P158	S278	F338	PRO	M400	ALA
T40	V99	M159	L279	S339	ASP	V401	GLN
I41	A100	K160	E280	V340	ASP	R402	ALA
P42	Q101	L161	M281	V403	ILE	V403	GLY
S43	P102	P162	L282	K342	ILE	L404	VAL
S44	A103	R163	Q283	A343	THR	L405	PRO
F45	E104	L164	E284	V344	ILE	K406	ALA
P46	L105	S165	A285	S345	LYS	Q407	ILE
K47	A106	S166	I286	E346	LEU	L408	LEU
D48	K107	Y167	V287	Q347	ILE	Q409	ALA
S49	V108	V168	K288	I348	ALA	A410	ALA
D50	E109	V169	M289	E349	ASN	T411	ASN
N51	Q170	E230	S290	G350	ALA	M412	ALA
A52	G111	E231	M291	R351	GLY	Q413	ILE
S53	L112	I232	I292	L352	ILE	T414	ILE
T54	S113	D233	S293	S353	THR	P415	ASP
D55	M114	F174	A294	Y354	SER	E416	THR
Y56	V115	G175	K295	A355	GLY	L417	SER
T57	E116	V235	V296	F356	ALA	P418	GLY
T58	R117	E236	I297	M357	R419	K419	ASP
P59	I118	D238	G298	L358	SER	E420	THR
M60	L119	G239	L299	M359	GLY		SER
	M120	I180	V300				

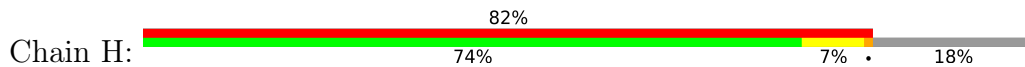
N301	P302	A303	G304	I305	T306	Q307	V308	R309	R310	L311	T312	K313	A314	Q315	T316	G317	D318	F319	V320	S321	G322	R323	P324	E325	D326	I327	S328	F329	L330	Q331	L332	E333	K334	A335	A336	D337	F338	S339	V340	A341	K342	A343	V344	S345	E346	Q347	I348	E349	G350	R351	S352	S353	Y354	A355	F356	M357	L358	N359	SER											
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	E349	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	ILE	ASN	ASN	ILE	ALA	THR	ILE	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ALA	ILE	ILE	LEU	ARG	ILE	ALA	ASN	ALA	ALA	ILE	ILE	GLY	ASP	THR	SER	GLY
ILE	LEU	LYS	THR	PRO	GLU	GLU	LYS	GLN	GLN	GLU	MET	ALA	ALA	ALA	GLY	THR	ALA	LEU	GLU	ASN	ALA	ALA	ALA	ALA	GLY	GLY	ALA	ALA	ALA	THR	THR	ALA	PRO	PRO	ALA	ALA	ALA	ALA	ALA	GLN	GLN	GLN	GLY	GLY	MET	VAL	PRO	PRO	ASN																					

• 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	M35	C36	A37	K38	Y39	T40	P42	P43	S43	L44	F45	P46	K47	D48	S49	D50	M51	A52	S53	T54	D55	Y56	T57	T58	P59	W60												
Q61	A62	V63	G64	A65	R66	G67	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	Y99	A100	Q101	P102	A103	E104	L105	S106	K107	D108	V108	E109	G110	L111	L112	S113	M114	V115	E116	R117	L118	L119	M120									
M121	Y122	I123	E124	M126	S127	Y128	R129	V130	L131	L132	F133	E134	T135	L136	K137	Q138	L139	V140	S201	V141	A142	G143	N144	A145	L146	L147	Y148	E209	M210	I211	D212	E153	G154	A155	Y156	P157	L158	M159	K160	L161	R163	L164	S165	A166	Y167	K228	Y229	E230	E231	I232	D233	A173	G234	V235	E236	V237	D238	G239	T240											
V181	T182	L183	D184	K185	T186	A187	Y188	A190	L191	P192	D193	E194	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	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	E280	N281	Q282	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	S352	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	E349	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	ILE	ASN	ASN	ILE	ALA	THR	ILE	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ALA	ILE	ILE	LEU	ARG	ILE	ALA	ASN	ALA	ALA	ILE	ILE	GLY	ASP	THR	SER	GLY
ILE	LEU	LYS	THR	PRO	GLU	GLU	LYS	GLN	GLN	GLU	MET	ALA	ALA	ALA	GLY	THR	ALA	LEU	GLU	ASN	ALA	ALA	ALA	GLY	GLY	ALA	ALA	ALA	THR	THR	ALA	PRO	PRO	ALA	ALA	ALA	ALA	ALA	ALA	GLN	GLN	GLN	GLY	GLY	MET	VAL	PRO	PRO	ASN																					

• Molecule 2: Portal protein



MET	ALA	SER	GLN	K6	R7	E8	G9	F10	A11	E12	N13	G14	A15	K16	A17	V18	Y19	D20	A21	L22	K23	N24	D25	K26	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	G67	L68	N69	N70	L71	A72	S73	K74	L75	M76	L77	A78	L79	F80	P81	M82	Q83	T84	M85	M86	K87	L88	T89	I90	S91	E92	F93	E94	A95	K96	Q97	P98	L99	M100	Q101	P102	A103	E104	L105	A106	K107	V108	E109	N110	G111	L112	S113	M114	V115	E116	R117	I118	L119	M120	
M121	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	M157	P158	M159	K160	L161	L162	R163	L164	S165	S166	Y167	V168	V169	Q170	R171	D172	A173	F174	G175	T176	V177	L178	Q179	I180	
V181	T182	L183	D184	L185	T186	A187	V188	A189	A190	L191	P192	E193	D194	V195	R196	M197	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	M281	L282	Q283	E284	A285	I286	V287	K288	M289	S290	M291	I292	S293	A294	K295	V296	I297	G298	L299	V300	
M301	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	T348	E349	G350	R351	L352	S353	Y354	A355	F356	M357	L358	N359	SER	
ALA	VAL	GLN	ARG	THR	GLY	GLU	ARG	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	I410	A411	ASN	ALA	M412	I413	I414	P415	E416	L417	P418	R419	E420
A421	V422	E423	P424	T425	I426	S427	T428	G429	M430	E431	A432	L433	G434	R435	G436	Q437	D438	L439	D440	R441	L442	E443	R444	C445	I446	A447	A448	W449	S450	A451	L452	A453	P454	M455	GLN	ASN	ASP	PRO	ASP	ILE	ASN	ASN	ALA	THR	ILE	LYS	LEU	ARG	ILE	ALA	ASN	ALA	ILE	GLY	ILE	ASP	THR	SER	GLY	
ILE	LEU	LYS	THR	PRO	GLU	GLY	LYS	GLN	GLU	MET	ALA	ALA	ALA	GLN	GLY	THR	ALA	LEU	ASN	ALA	ALA	SER	ALA	GLY	GLY	ALA	GLY	ALA	LEU	ALA	THR	ALA	PRO	GLU	ASN	ASN	MET	GLU	ALA	ALA	ALA	ALA	ALA	ALA	GLY	MET	VAL	PRO	ASN											

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	0.39	0/13095	0.66	6/17695 (0.0%)
1	B	0.40	0/13056	0.67	8/17643 (0.0%)
1	C	0.39	0/13095	0.66	6/17695 (0.0%)
1	D	0.40	0/13056	0.66	8/17643 (0.0%)
2	E	0.73	3/3485 (0.1%)	0.89	8/4720 (0.2%)
2	F	0.48	2/3485 (0.1%)	0.80	10/4720 (0.2%)
2	G	0.54	1/3485 (0.0%)	0.81	6/4720 (0.1%)
2	H	0.47	1/3485 (0.0%)	0.82	13/4720 (0.3%)
All	All	0.44	7/66242 (0.0%)	0.70	65/89556 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	324	PRO	CG-CD	-32.03	0.45	1.50
2	G	454	PRO	CG-CD	-19.71	0.85	1.50
2	F	324	PRO	CG-CD	-11.44	1.12	1.50
2	E	324	PRO	CB-CG	11.21	2.06	1.50
2	H	324	PRO	CG-CD	-10.89	1.14	1.50
2	F	257	VAL	CB-CG1	-5.43	1.41	1.52
2	E	324	PRO	CA-C	5.39	1.63	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	324	PRO	CB-CG-CD	-27.29	0.07	106.50
2	G	454	PRO	N-CD-CG	-20.29	72.77	103.20
2	E	324	PRO	CA-N-CD	-15.21	90.20	111.50
2	F	398	LEU	CB-CG-CD2	-12.07	90.47	111.00
2	F	324	PRO	N-CD-CG	-11.55	85.88	103.20
2	G	454	PRO	CA-CB-CG	-11.32	82.49	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	324	PRO	N-CD-CG	-10.84	86.94	103.20
2	E	324	PRO	CA-CB-CG	-10.32	84.40	104.00
2	G	398	LEU	CB-CG-CD2	-10.07	93.89	111.00
2	E	398	LEU	CB-CG-CD2	-9.63	94.63	111.00
1	B	342	ASP	CB-CG-OD1	8.81	126.23	118.30
1	D	342	ASP	CB-CG-OD1	8.80	126.22	118.30
2	H	383	ASP	CB-CG-OD2	8.77	126.19	118.30
2	H	398	LEU	CB-CG-CD2	-8.40	96.71	111.00
2	F	324	PRO	CA-N-CD	-8.37	99.78	111.50
2	H	324	PRO	CA-N-CD	-8.12	100.13	111.50
2	H	330	LEU	CB-CG-CD1	-8.02	97.37	111.00
2	H	330	LEU	CA-CB-CG	7.93	133.54	115.30
2	F	324	PRO	CA-CB-CG	-7.62	89.52	104.00
2	H	324	PRO	CA-CB-CG	-7.08	90.55	104.00
1	D	287	ASP	CB-CG-OD1	7.02	124.62	118.30
1	B	287	ASP	CB-CG-OD1	6.91	124.52	118.30
1	C	351	LEU	CA-CB-CG	6.86	131.08	115.30
2	H	199	MET	CG-SD-CE	6.84	111.14	100.20
1	D	302	LEU	CB-CG-CD1	-6.79	99.46	111.00
2	E	323	ARG	C-N-CD	6.68	142.43	128.40
1	A	351	LEU	CA-CB-CG	6.67	130.65	115.30
2	E	324	PRO	N-CD-CG	-6.66	93.22	103.20
2	F	398	LEU	CB-CG-CD1	6.63	122.28	111.00
1	C	1186	ASP	CB-CG-OD1	6.14	123.83	118.30
2	H	172	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	1064	ASP	CB-CG-OD1	6.10	123.79	118.30
2	F	172	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	1186	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	1186	ASP	CB-CG-OD1	6.05	123.75	118.30
1	C	1064	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	1186	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	1064	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	517	LEU	CA-CB-CG	5.97	129.04	115.30
1	A	517	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	302	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	1064	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	1098	ASP	CB-CG-OD1	5.92	123.62	118.30
1	C	1098	ASP	CB-CG-OD1	5.81	123.53	118.30
2	H	326	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	1569	ASP	CB-CG-OD2	5.72	123.45	118.30
2	E	320	VAL	CG1-CB-CG2	-5.63	101.89	110.90
1	D	1098	ASP	CB-CG-OD1	5.60	123.34	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1569	ASP	CB-CG-OD2	5.60	123.34	118.30
2	G	454	PRO	N-CA-CB	-5.59	96.45	102.60
1	B	1098	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	251	LYS	CD-CE-NZ	5.51	124.36	111.70
2	F	194	ASP	CB-CG-OD2	5.51	123.26	118.30
2	G	320	VAL	CG1-CB-CG2	-5.38	102.29	110.90
2	E	324	PRO	N-CA-CB	-5.36	96.70	102.60
2	H	330	LEU	CB-CG-CD2	5.34	120.07	111.00
1	A	881	ASP	CB-CG-OD1	5.29	123.06	118.30
2	G	454	PRO	CA-N-CD	-5.27	104.13	111.50
2	F	442	LEU	CA-CB-CG	5.24	127.36	115.30
2	F	404	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	B	878	LYS	CD-CE-NZ	5.20	123.66	111.70
1	C	881	ASP	CB-CG-OD1	5.19	122.97	118.30
2	H	114	MET	CG-SD-CE	5.16	108.45	100.20
2	H	132	LEU	CA-CB-CG	-5.09	103.60	115.30
2	F	199	MET	CG-SD-CE	5.01	108.21	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	25	0
1	B	12756	0	12683	32	0
1	C	12805	0	12724	22	0
1	D	12756	0	12683	26	0
2	E	3427	0	3400	16	0
2	F	3427	0	3400	22	0
2	G	3427	0	3400	9	0
2	H	3427	0	3400	21	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	156	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 (156) 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: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
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
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:B:308:ASP:HA	1:B:311:LYS:HG3	1.83	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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:F:153:GLU:H	2:F:157:ASN:HD21	1.58	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
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:B:1134:ARG:HH11	1:B:1134:ARG:HB3	1.78	0.48
2:F:152:PRO:HA	2:F:157:ASN:ND2	2.29	0.48
1:A:825:ASN:HD22	2:E:54:THR:C	2.17	0.47
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:286:ILE:HA	2:F:289:MET:HE3	1.96	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
2:G:84:THR:HA	2:G:120:MET:CE	2.46	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:D:1059:PHE:HB2	2:H:296:VAL:HG13	1.98	0.44
1:A:1081:HIS:HD1	1:A:1081:HIS:C	2.21	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:B:205:ASP:OD2	1:B:205:ASP:N	2.49	0.44
2:E:84:THR:HA	2:E:120:MET:CE	2.47	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:1469:TRP:HD1	2:E:373:GLU:HG3	1.82	0.43
2:G:83:GLN:O	2:G:120:MET:HE1	2.18	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:151:GLU:HA	2:H:407:GLN:HE21	1.83	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
1:D:1569:ASP:N	1:D:1569:ASP:OD1	2.53	0.42
2:G:83:GLN:OE1	2:G:84:THR:N	2.53	0.42
1:B:817:PHE:CE2	1:B:827:ILE:HD11	2.54	0.41
2:F:194:ASP:OD2	2:F:195:VAL:N	2.52	0.41
1:B:825:ASN:HD22	2:F:54:THR:C	2.23	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
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
1:C:1081:HIS:HD1	1:C:1081:HIS:C	2.24	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: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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:398:LEU:HA	2:E:398:LEU:HD23	1.93	0.40
2:H:84:THR:HA	2:H:120:MET:HE3	2.04	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 [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%)	1400 (98%)	22 (2%)	65	87
1	B	1418/1461 (97%)	1393 (98%)	25 (2%)	59	85
1	C	1422/1461 (97%)	1400 (98%)	22 (2%)	65	87
1	D	1418/1461 (97%)	1390 (98%)	28 (2%)	55	82
2	E	370/435 (85%)	363 (98%)	7 (2%)	57	84
2	F	370/435 (85%)	361 (98%)	9 (2%)	49	79
2	G	370/435 (85%)	366 (99%)	4 (1%)	73	92
2	H	370/435 (85%)	361 (98%)	9 (2%)	49	79
All	All	7160/7584 (94%)	7034 (98%)	126 (2%)	61	85

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	MET
1	A	63	GLN
1	A	89	TYR
1	A	144	SER
1	A	188	LYS
1	A	279	ASP
1	A	335	ASP
1	A	488	LYS
1	A	492	ASN
1	A	560	TYR
1	A	563	ARG
1	A	602	LEU
1	A	767	ASP
1	A	800	LYS
1	A	1041	ARG
1	A	1052	ASP
1	A	1081	HIS
1	A	1123	LYS
1	A	1359	ARG
1	A	1362	ARG
1	A	1428	TRP
1	A	1530	LYS
1	B	86	LYS
1	B	132	LYS
1	B	222	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	234	GLU
1	B	338	TYR
1	B	342	ASP
1	B	345	LYS
1	B	492	ASN
1	B	563	ARG
1	B	594	GLN
1	B	701	MET
1	B	712	ARG
1	B	767	ASP
1	B	800	LYS
1	B	883	LYS
1	B	940	ASP
1	B	1041	ARG
1	B	1095	ARG
1	B	1123	LYS
1	B	1289	LYS
1	B	1359	ARG
1	B	1360	GLU
1	B	1428	TRP
1	B	1518	GLU
1	B	1525	LYS
1	C	35	MET
1	C	63	GLN
1	C	89	TYR
1	C	144	SER
1	C	188	LYS
1	C	211	ASP
1	C	279	ASP
1	C	335	ASP
1	C	398	GLU
1	C	488	LYS
1	C	492	ASN
1	C	560	TYR
1	C	563	ARG
1	C	602	LEU
1	C	800	LYS
1	C	816	CYS
1	C	1041	ARG
1	C	1081	HIS
1	C	1123	LYS
1	C	1359	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	1428	TRP
1	C	1530	LYS
1	D	86	LYS
1	D	222	ASN
1	D	234	GLU
1	D	342	ASP
1	D	345	LYS
1	D	492	ASN
1	D	563	ARG
1	D	712	ARG
1	D	732	ASP
1	D	767	ASP
1	D	800	LYS
1	D	822	PHE
1	D	883	LYS
1	D	940	ASP
1	D	941	ARG
1	D	1041	ARG
1	D	1044	MET
1	D	1095	ARG
1	D	1106	MET
1	D	1123	LYS
1	D	1272	HIS
1	D	1289	LYS
1	D	1359	ARG
1	D	1360	GLU
1	D	1428	TRP
1	D	1518	GLU
1	D	1524	LYS
1	D	1525	LYS
2	E	86	MET
2	E	210	MET
2	E	214	TYR
2	E	320	VAL
2	E	323	ARG
2	E	326	ASP
2	E	437	GLN
2	F	22	LEU
2	F	86	MET
2	F	114	MET
2	F	117	ARG
2	F	210	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	323	ARG
2	F	326	ASP
2	F	354	TYR
2	F	455	MET
2	G	86	MET
2	G	109	GLU
2	G	320	VAL
2	G	323	ARG
2	H	22	LEU
2	H	86	MET
2	H	114	MET
2	H	117	ARG
2	H	194	ASP
2	H	199	MET
2	H	210	MET
2	H	323	ARG
2	H	354	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	825	ASN
1	B	825	ASN
2	F	157	ASN
2	F	413	GLN
2	H	205	HIS

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	1.04	0	7,9,11	2.72	2 (28%)
1	FME	C	1	1	8,9,10	1.05	0	7,9,11	2.81	2 (28%)

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	4.50	137.12	125.27
1	A	1	FME	O1-CN-N	4.36	136.74	125.27

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	1	0
1	C	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides 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	26,33,33	0.70	0	31,52,52	0.81	2 (6%)
3	ATP	B	1601	4	26,33,33	0.67	0	31,52,52	0.78	2 (6%)
3	ATP	A	1601	4	26,33,33	0.70	0	31,52,52	0.81	2 (6%)
3	ATP	D	1601	4	26,33,33	0.67	0	31,52,52	0.78	2 (6%)

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	-	1/18/38/38	0/3/3/3
3	ATP	B	1601	4	-	0/18/38/38	0/3/3/3
3	ATP	A	1601	4	-	1/18/38/38	0/3/3/3
3	ATP	D	1601	4	-	0/18/38/38	0/3/3/3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1601	ATP	PB-O3B-PG	2.24	140.50	132.83
3	A	1601	ATP	PB-O3B-PG	2.23	140.47	132.83
3	A	1601	ATP	C5-C6-N6	2.11	123.56	120.35
3	C	1601	ATP	C5-C6-N6	2.07	123.49	120.35
3	B	1601	ATP	PB-O3B-PG	2.06	139.91	132.83
3	D	1601	ATP	PB-O3B-PG	2.06	139.89	132.83
3	D	1601	ATP	C5-C6-N6	2.06	123.48	120.35
3	B	1601	ATP	C5-C6-N6	2.03	123.44	120.35

There are no chirality outliers.

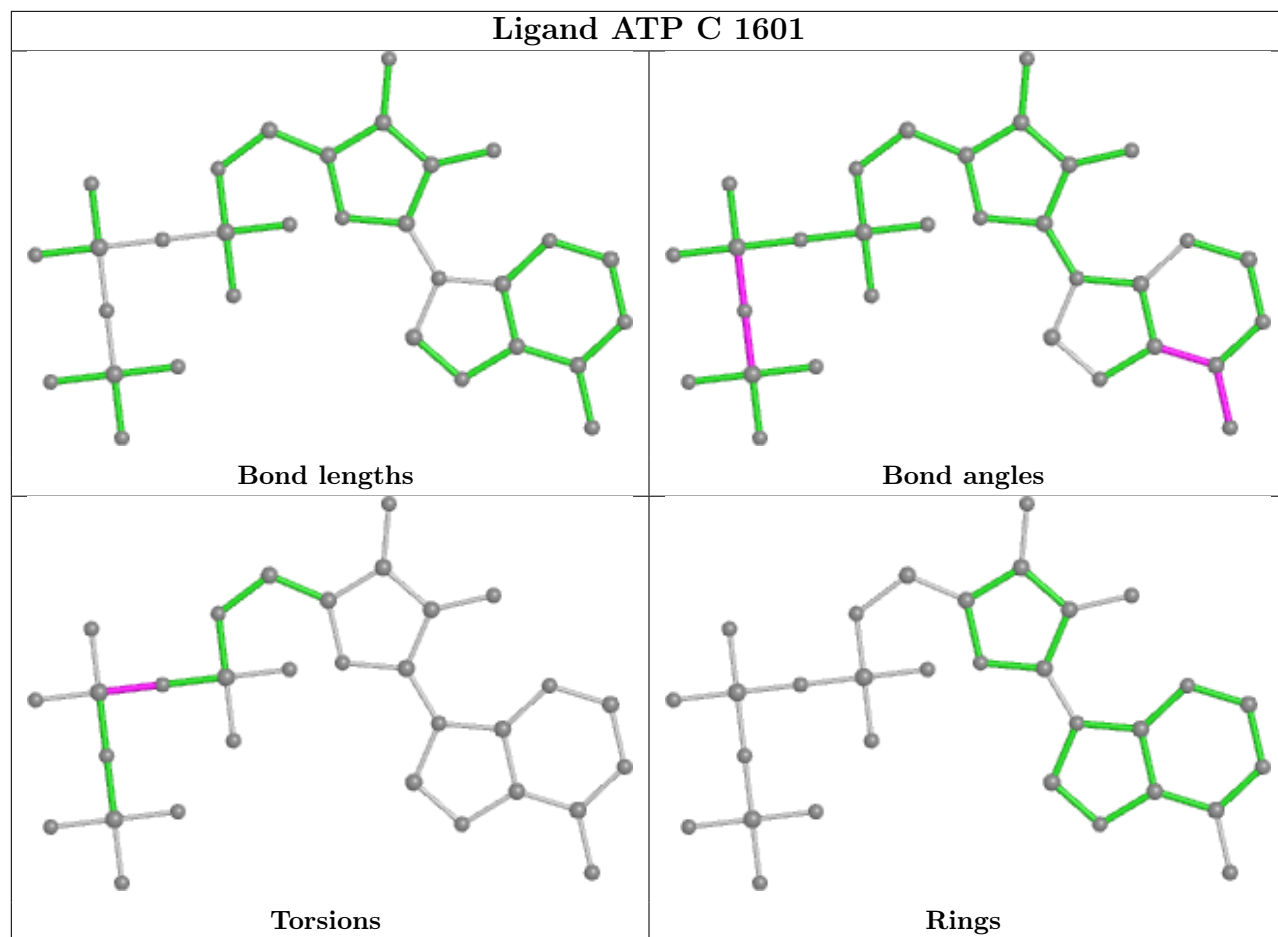
All (2) torsion outliers are listed below:

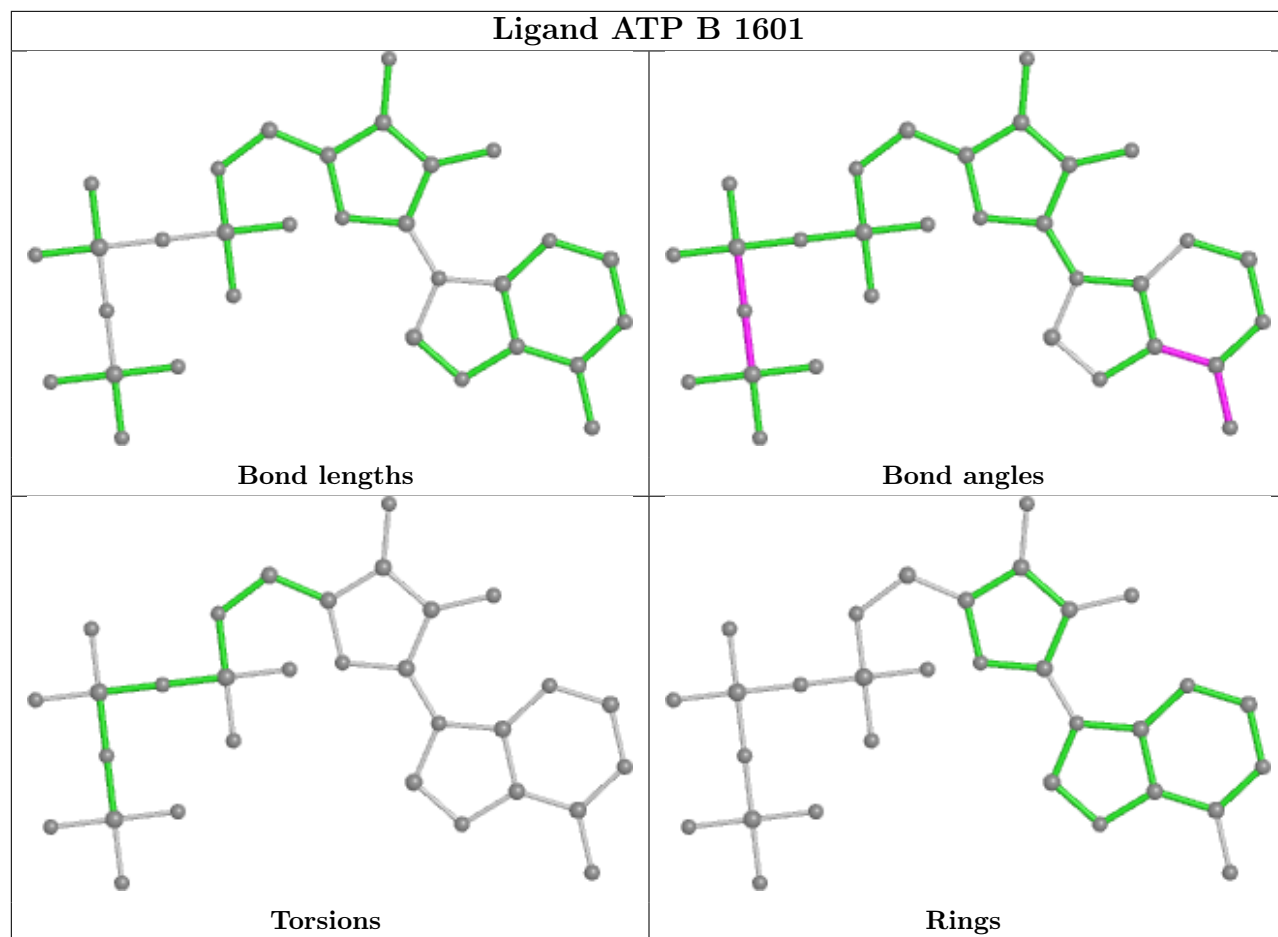
Mol	Chain	Res	Type	Atoms
3	A	1601	ATP	PA-O3A-PB-O2B
3	C	1601	ATP	PA-O3A-PB-O2B

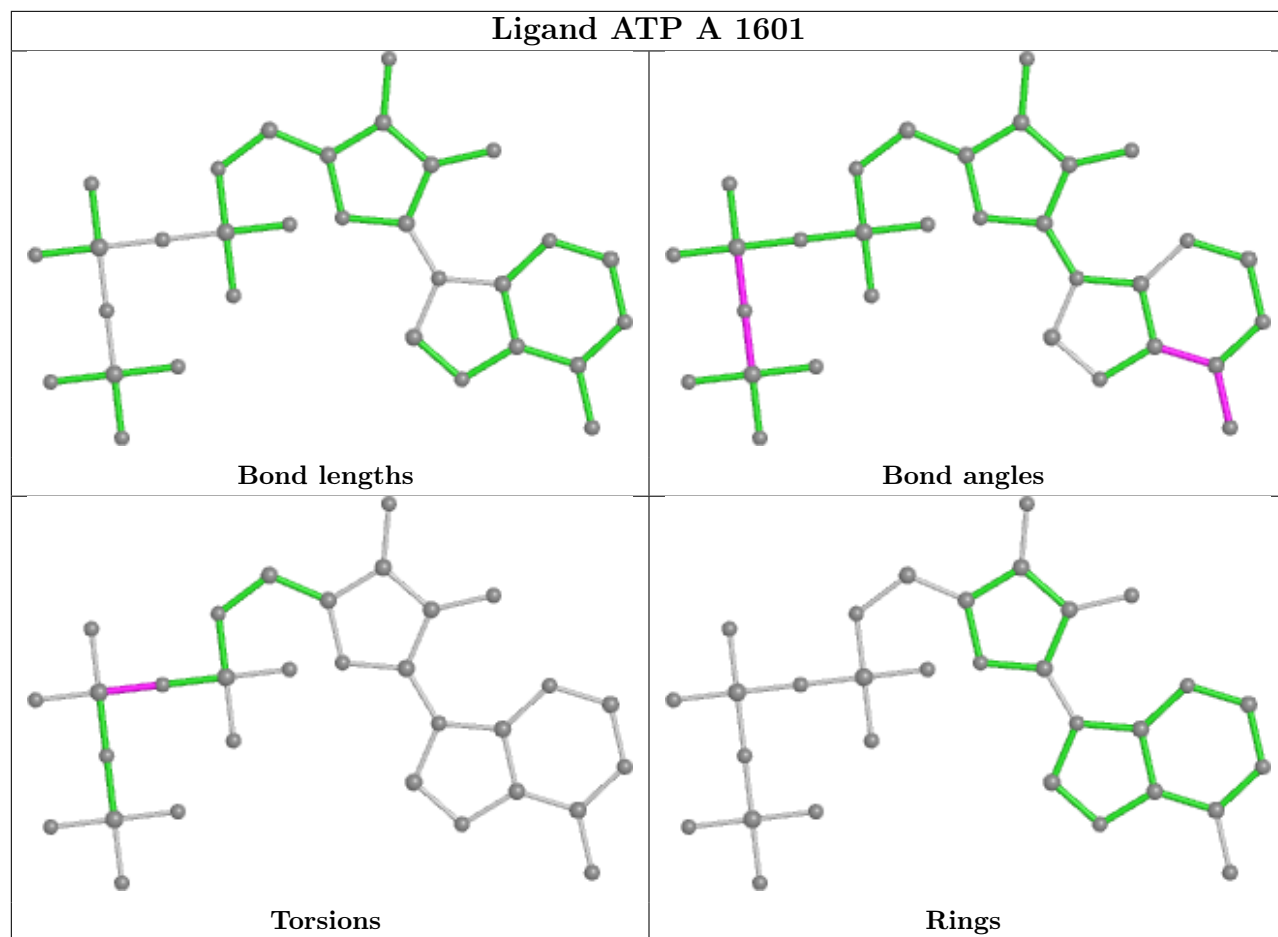
There are no ring outliers.

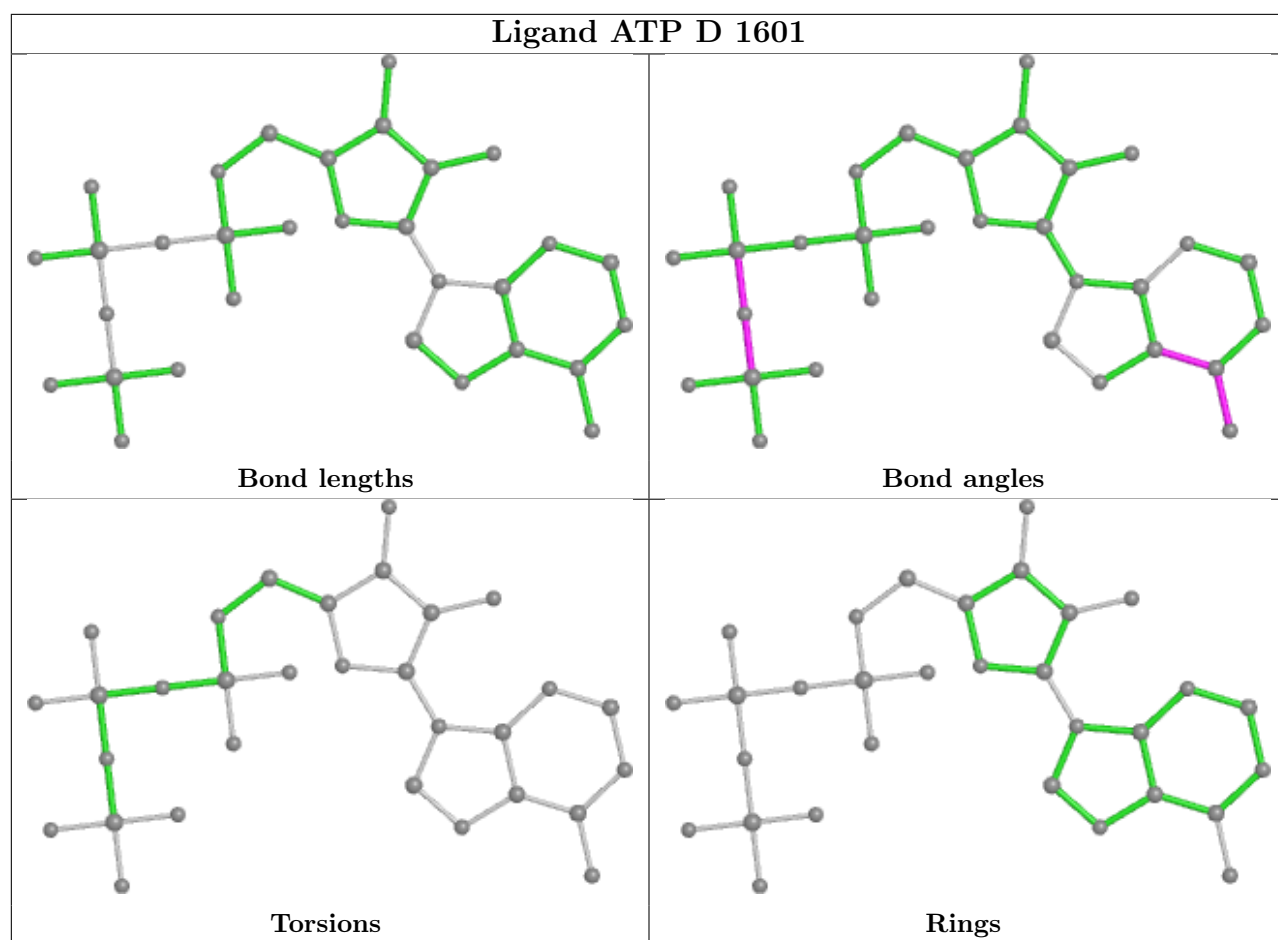
No monomer is involved in short contacts.

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.

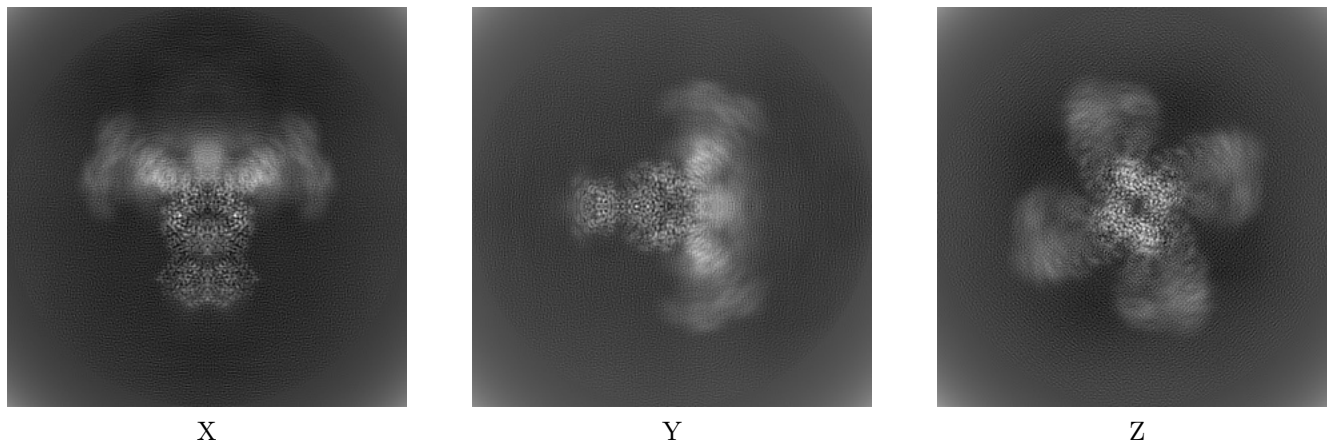
6 Map visualisation [i](#)

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.

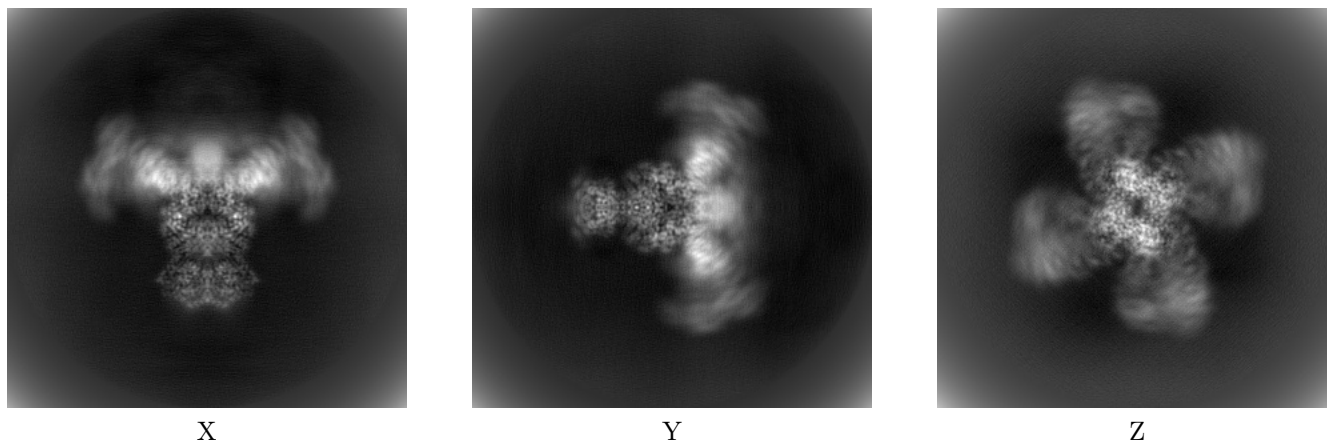
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



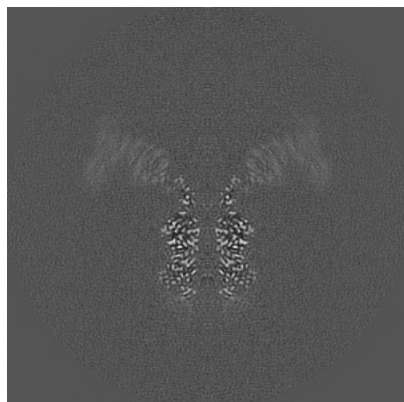
6.1.2 Raw map



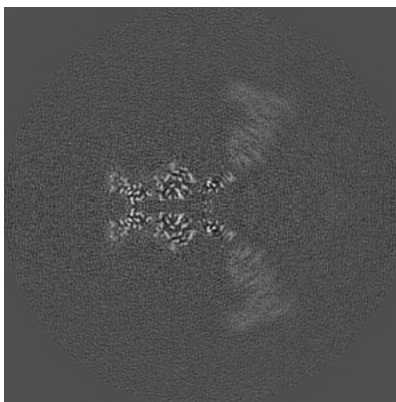
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

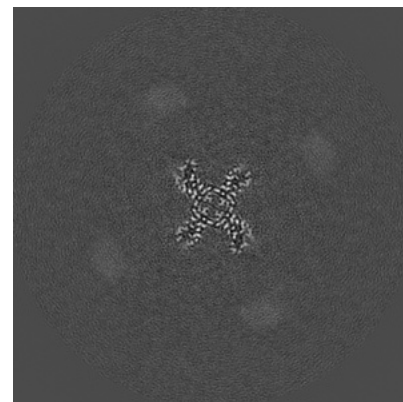
6.2.1 Primary map



X Index: 180

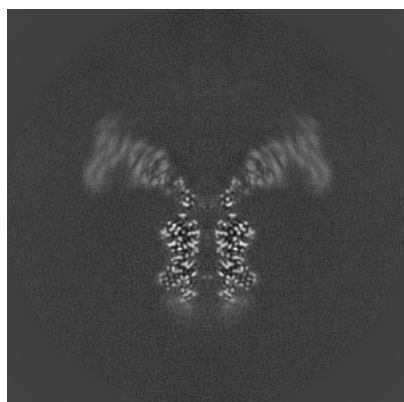


Y Index: 180

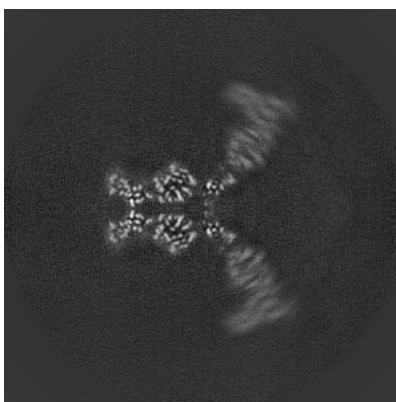


Z Index: 180

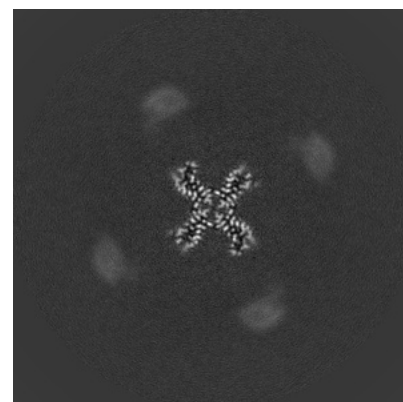
6.2.2 Raw map



X Index: 180



Y Index: 180

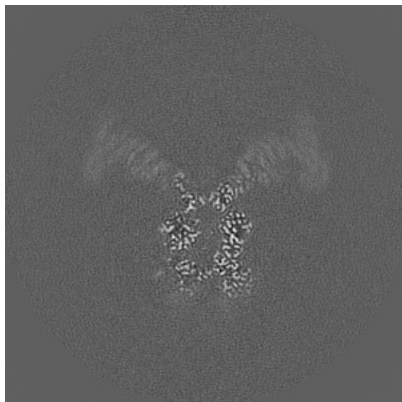


Z Index: 180

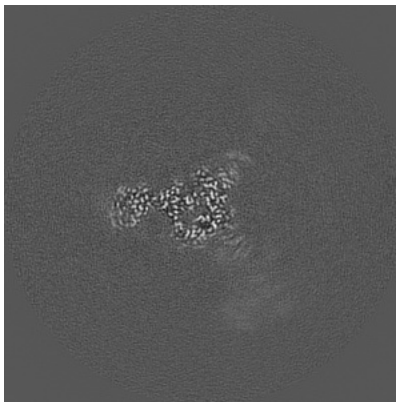
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

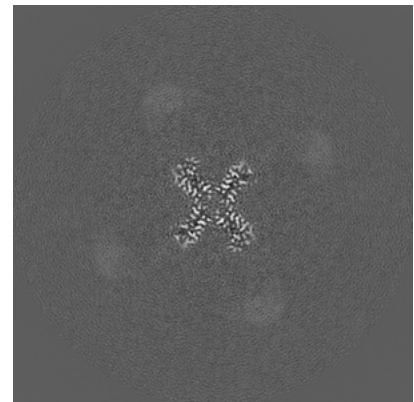
6.3.1 Primary map



X Index: 175

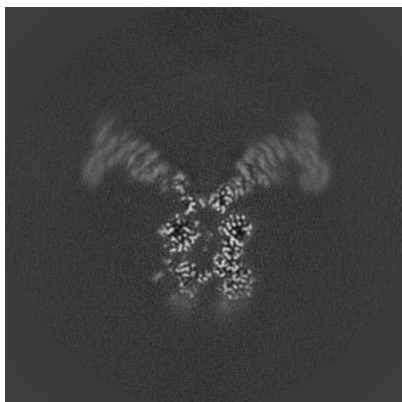


Y Index: 160

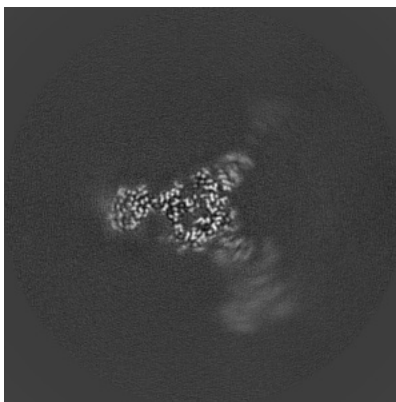


Z Index: 179

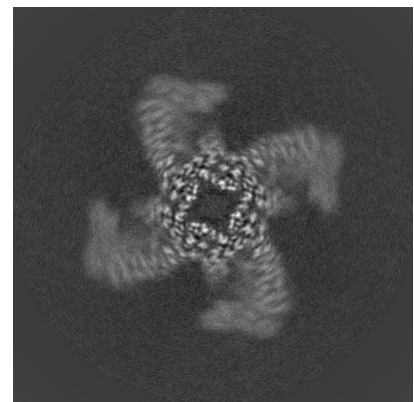
6.3.2 Raw map



X Index: 175



Y Index: 160

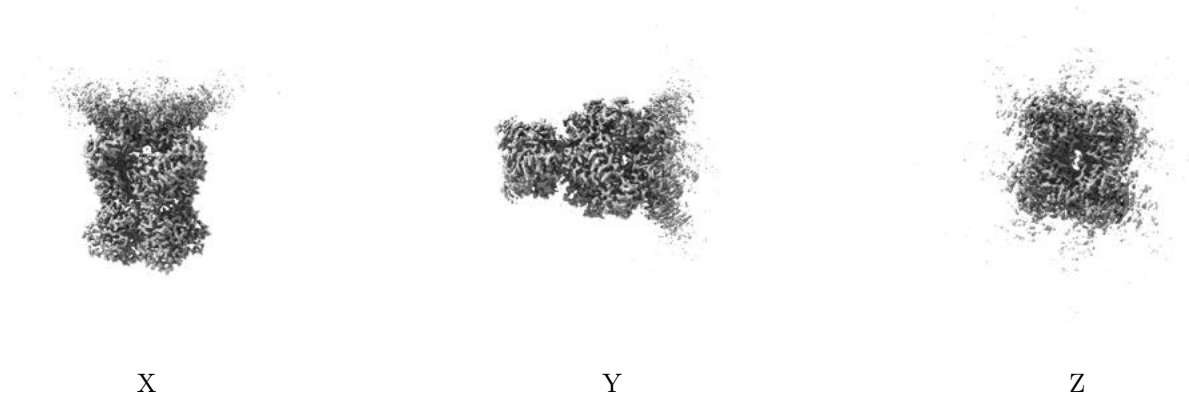


Z Index: 204

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

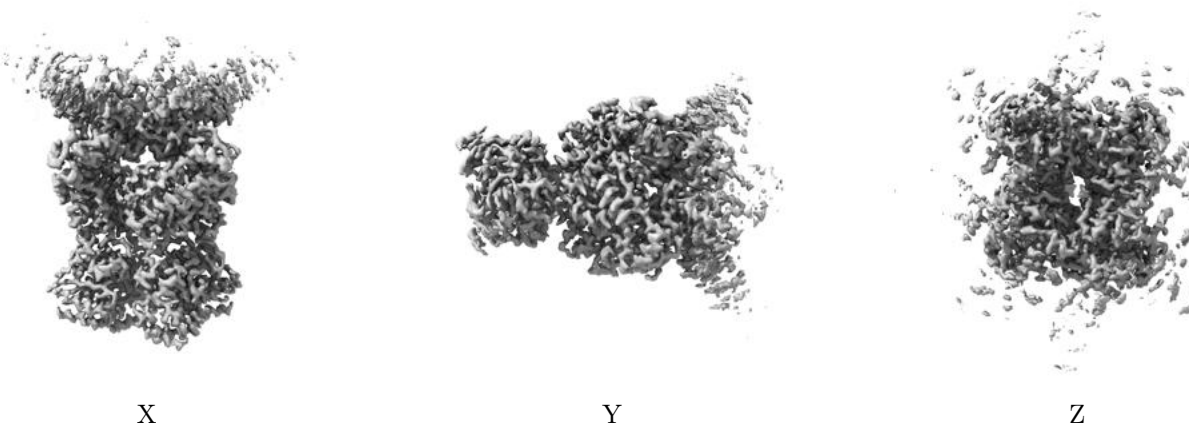
6.4 Orthogonal surface views [i](#)

6.4.1 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.

6.4.2 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.

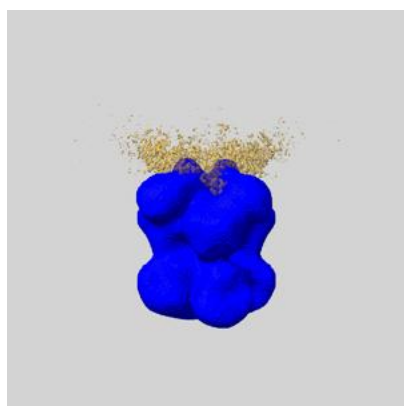
6.5 Mask visualisation [i](#)

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

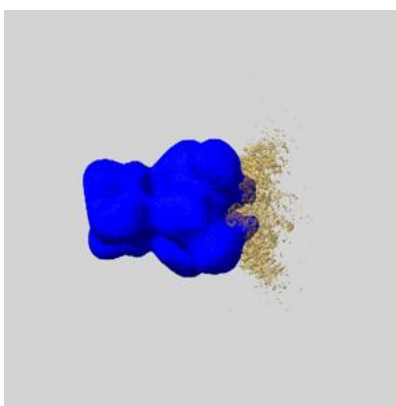
A mask typically either:

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

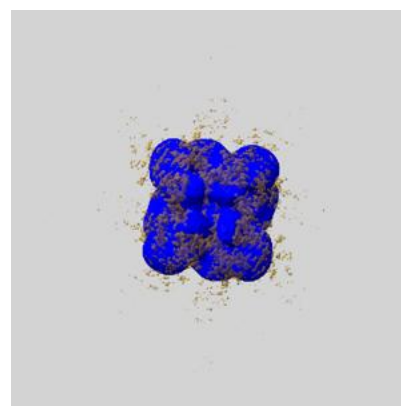
6.5.1 emd_27422_msk_1.map [i](#)



X



Y

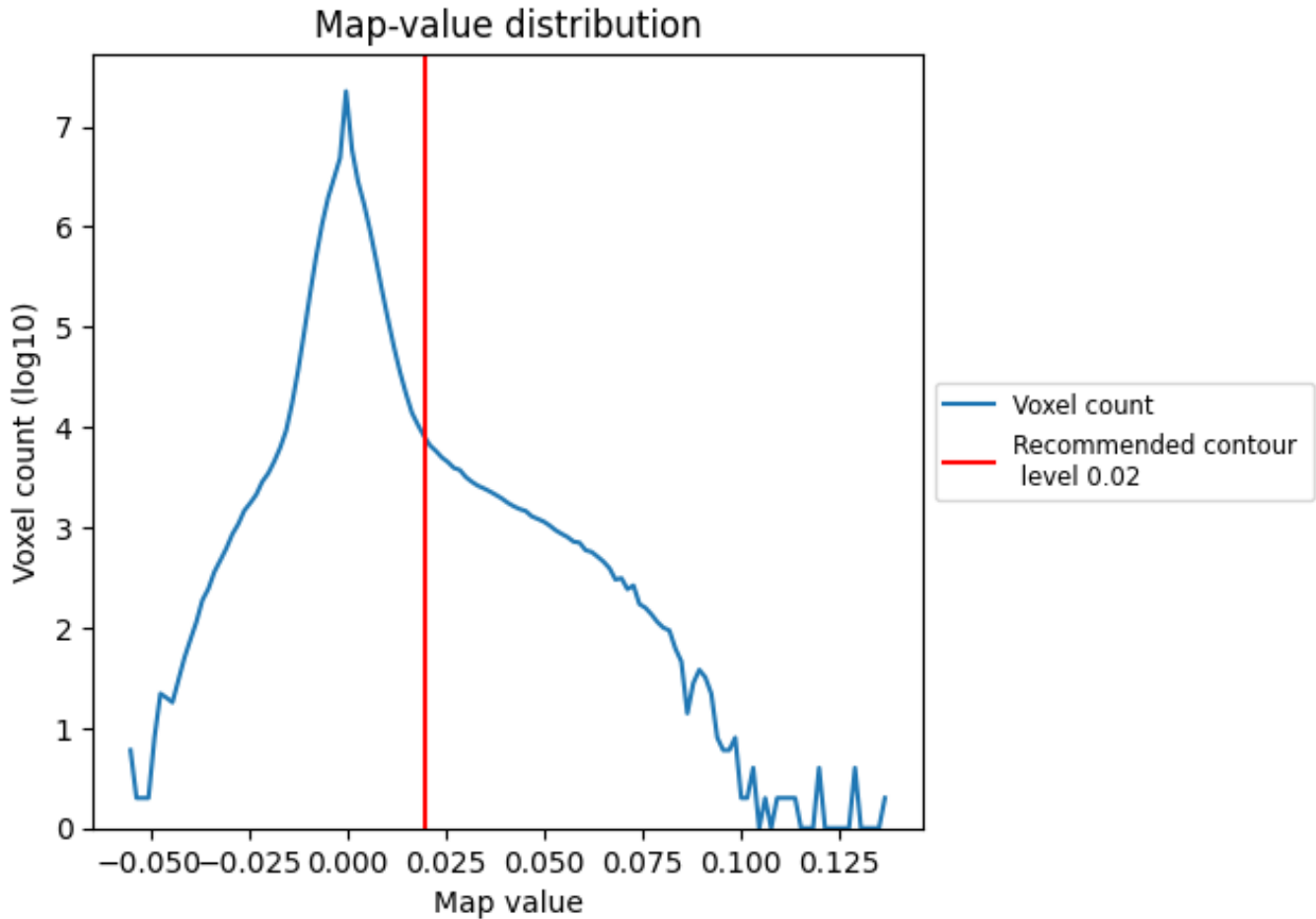


Z

7 Map analysis [i](#)

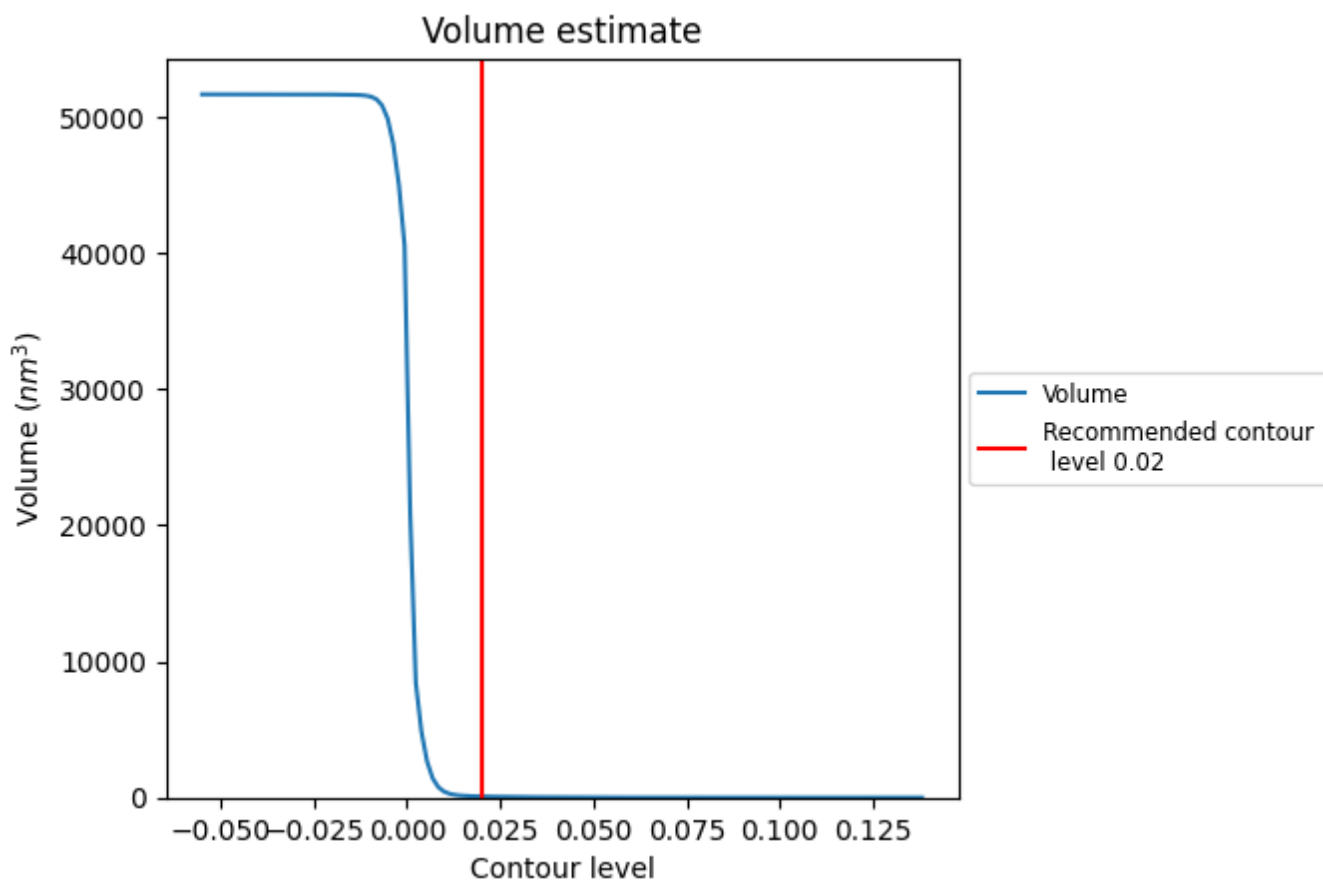
This section contains the results of statistical analysis of the map.

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.

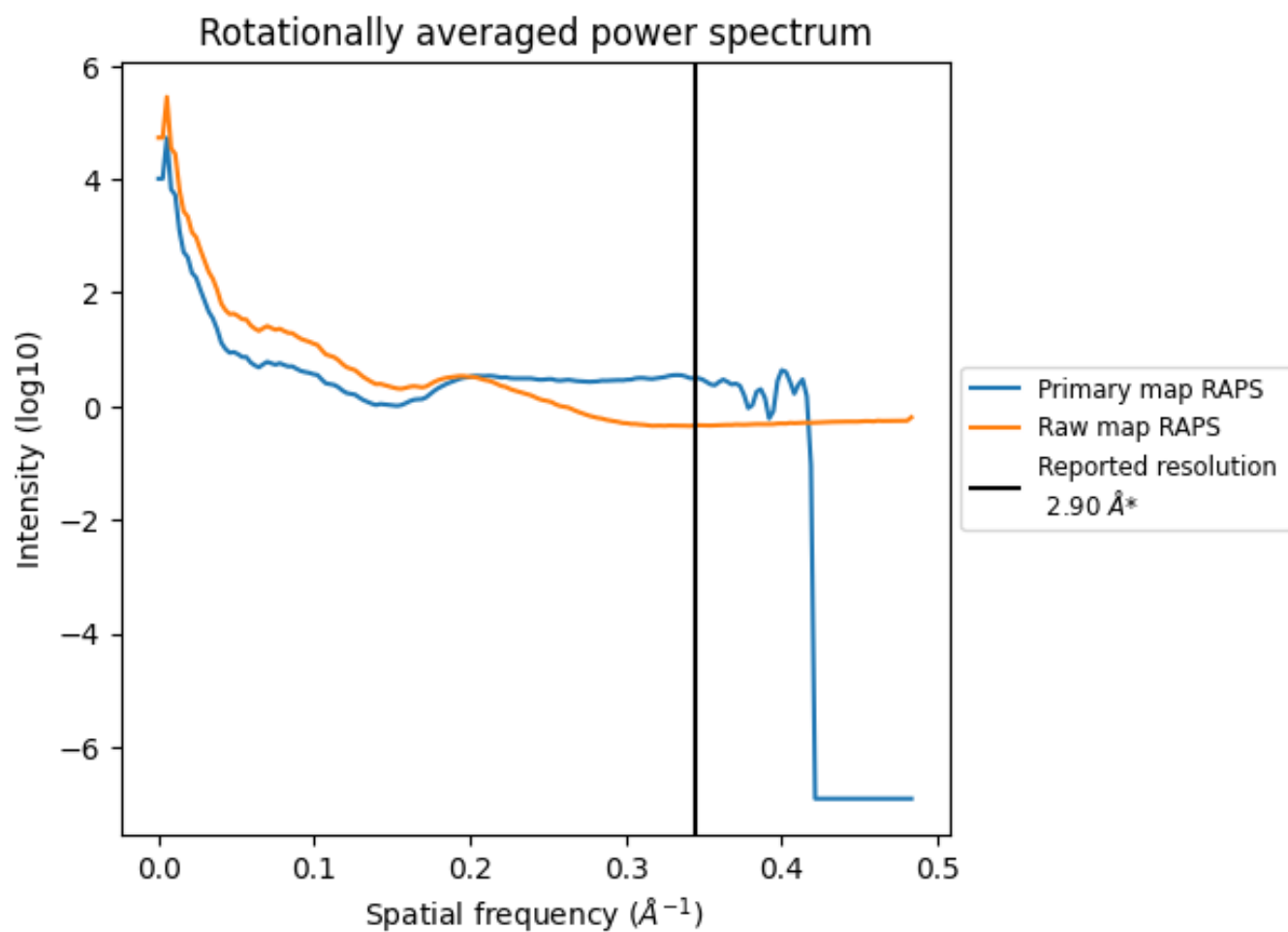
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm³; 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

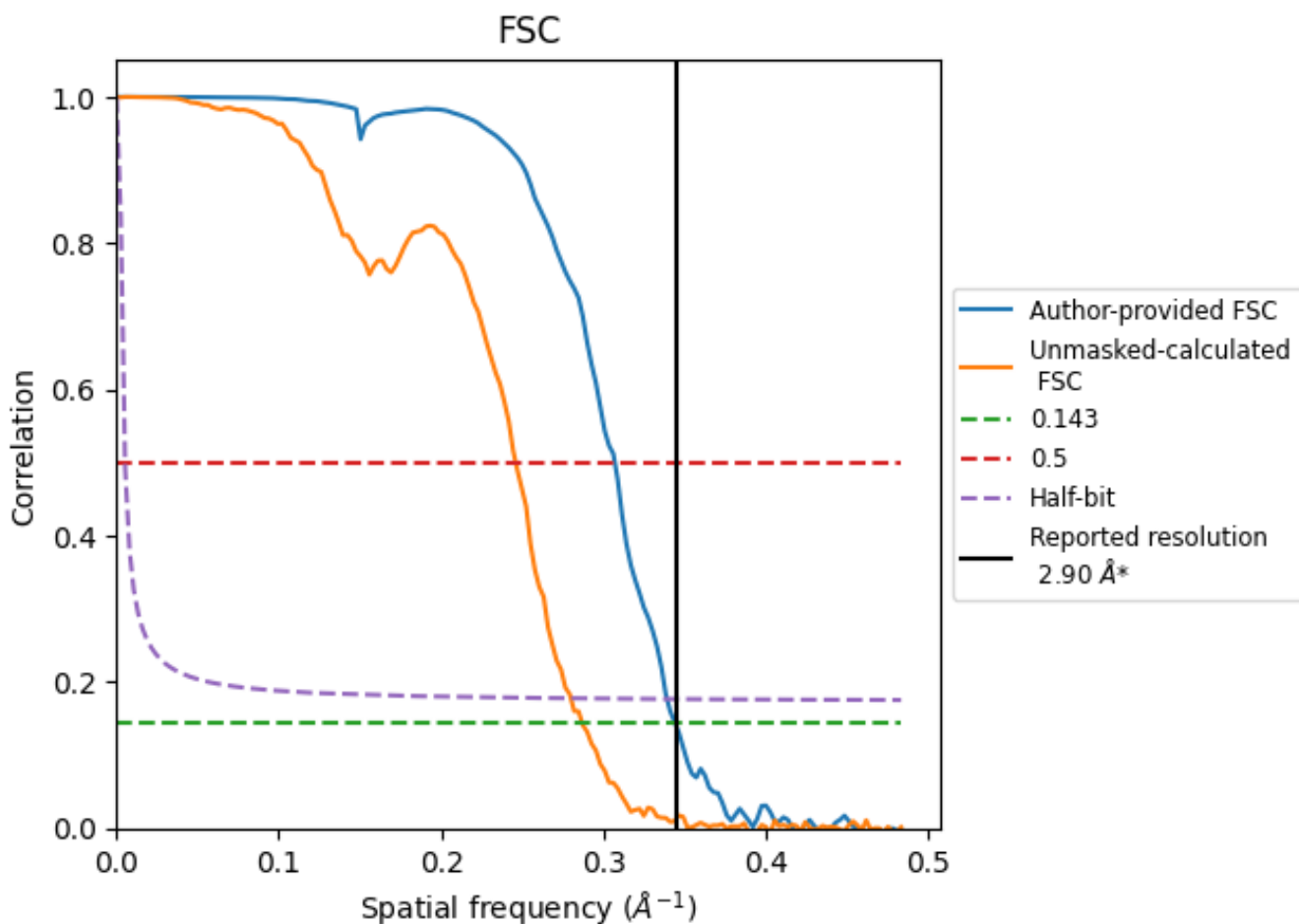


*Reported resolution corresponds to spatial frequency of 0.345 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

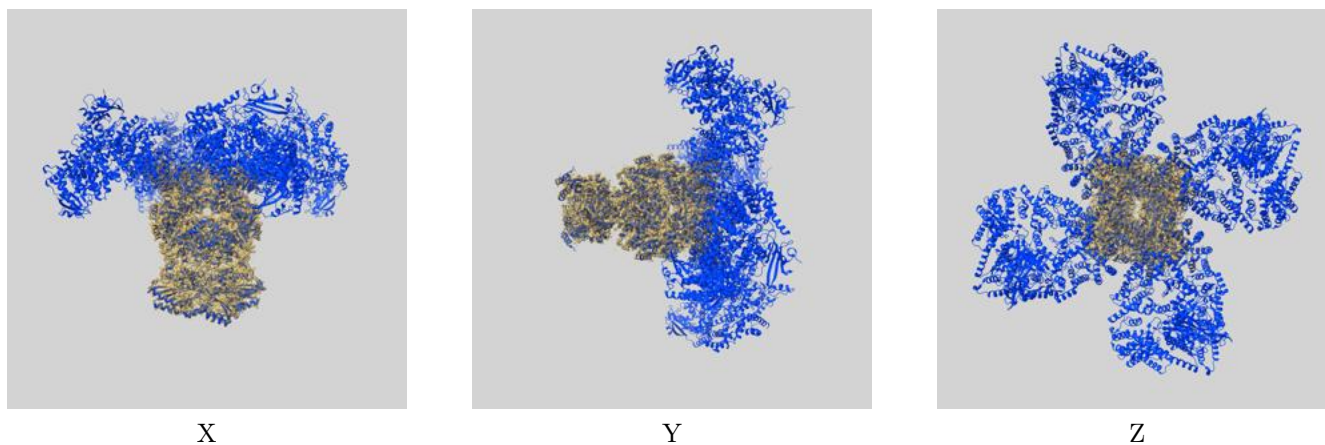
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.26	2.95
Unmasked-calculated*	3.48	4.07	3.57

*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 5.

9.1 Map-model overlay [i](#)



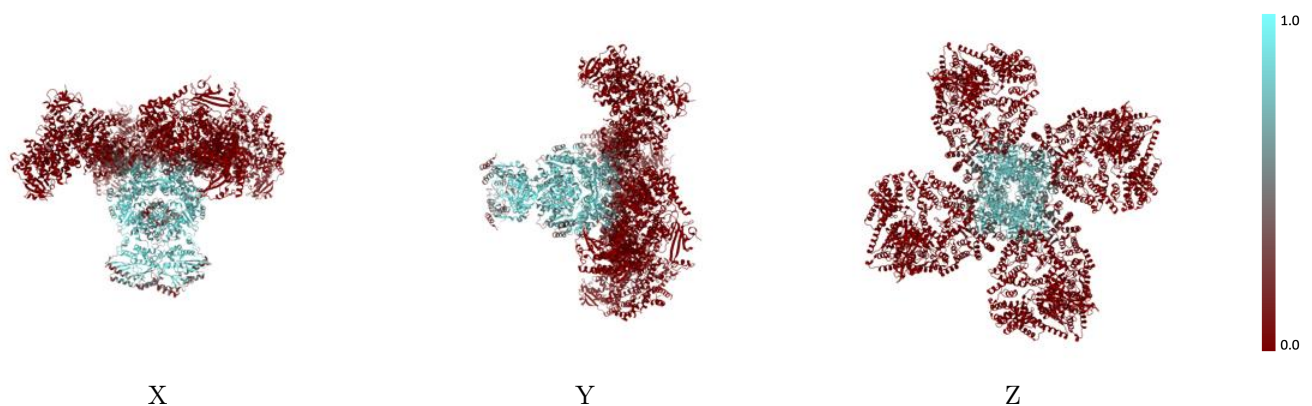
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



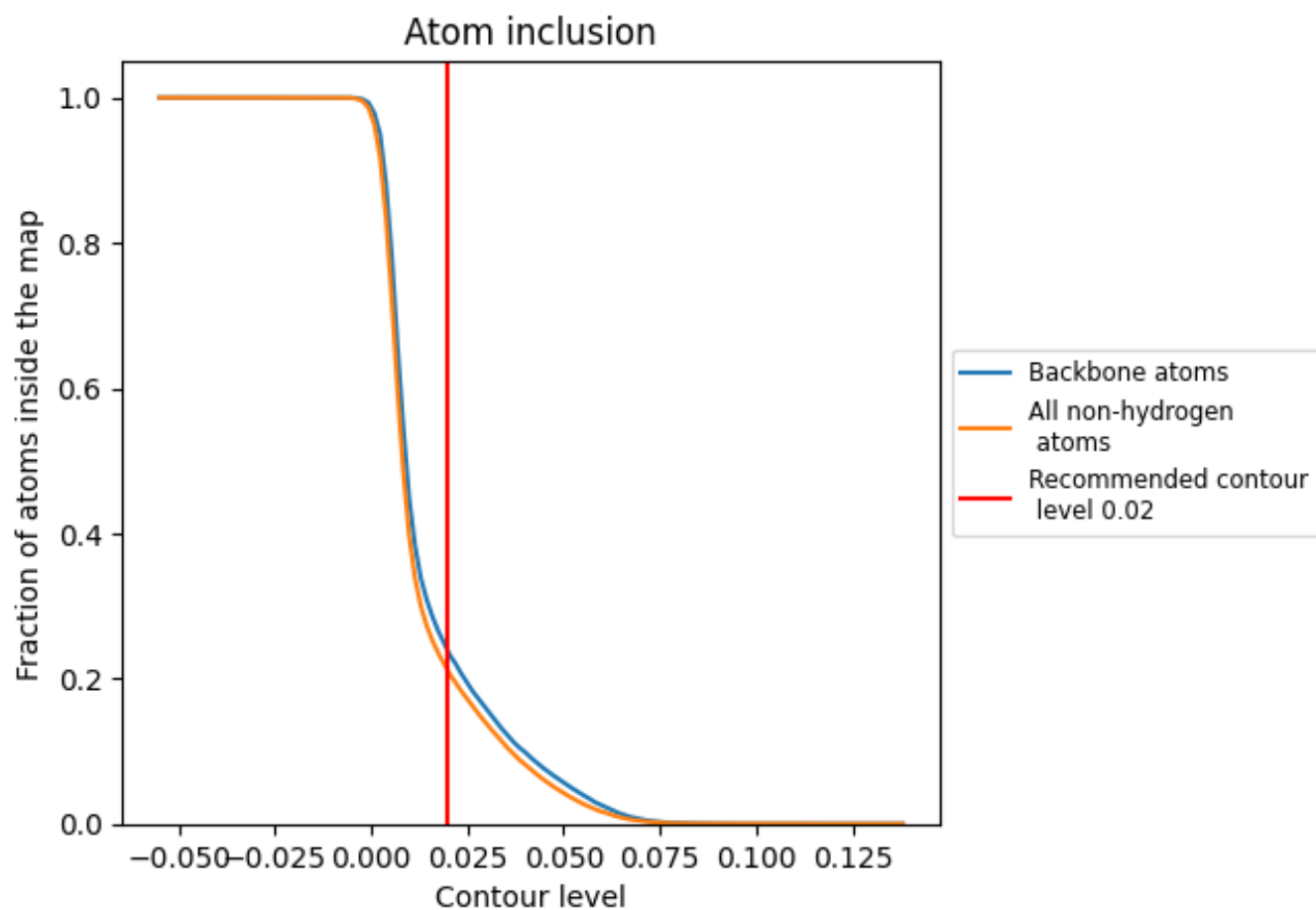
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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	 0.2108	 0.2340
A	 0.2863	 0.2990
B	 0.2481	 0.2640
C	 0.2865	 0.3000
D	 0.2473	 0.2650
E	 0.0000	 0.0570
F	 0.0000	 0.0470
G	 0.0000	 0.0570
H	 0.0000	 0.0470

