



wwPDB EM Validation Summary Report ⓘ

Mar 10, 2026 – 01:06 AM UTC

PDB ID : 6KWY / pdb_00006kwy
EMDB ID : EMD-0781
Title : human PA200-20S complex
Authors : Ouyang, S.; Hongxin, G.
Deposited on : 2019-09-09
Resolution : 2.72 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

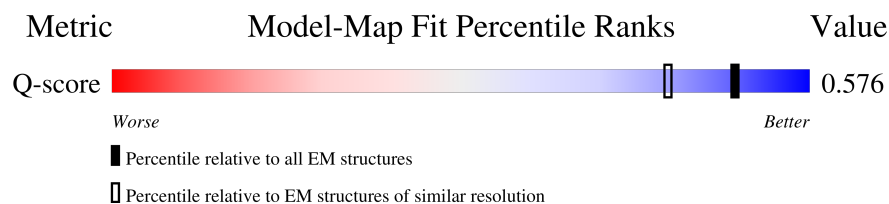
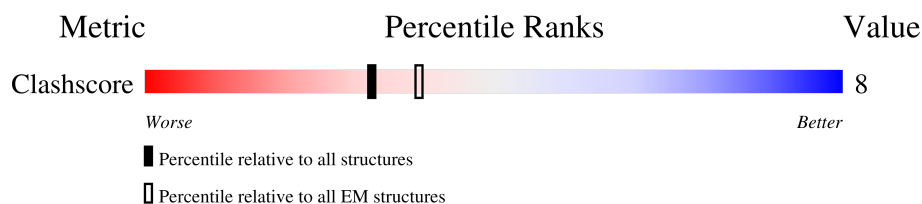
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

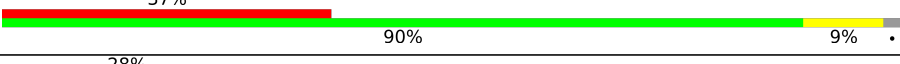
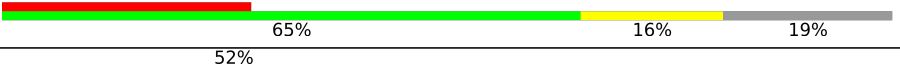
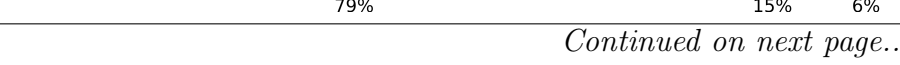
The reported resolution of this entry is 2.72 Å.

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	-
Q-score	-	25397	10355 (2.22 - 3.22)

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	234	
1	O	234	
2	B	261	
2	P	261	
3	C	248	
3	Q	248	

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Mol	Chain	Length	Quality of chain
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	263	
11	Y	263	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	239	
14	b	239	
15	c	1878	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	IHP	c	1902	-	-	X	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 62505 atoms, of which 6 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 Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	215	Total	C	N	O	S	0	0
			1671	1069	285	311	6		
1	O	230	Total	C	N	O	S	0	0
			1779	1136	301	336	6		

- Molecule 2 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	212	Total	C	N	O	S	0	0
			1645	1040	277	319	9		
2	P	247	Total	C	N	O	S	2	0
			1919	1211	326	371	11		

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	212	Total	C	N	O	S	0	0
			1641	1032	290	314	5		
3	Q	234	Total	C	N	O	S	0	0
			1817	1141	318	353	5		

- Molecule 4 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	227	Total	C	N	O	S	0	0
			1741	1099	286	345	11		
4	R	233	Total	C	N	O	S	0	0
			1768	1112	294	351	11		

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	240	Total	C	N	O	S	0	0
			1881	1180	339	350	12		
5	S	238	Total	C	N	O	S	3	0
			1871	1173	338	349	11		

- Molecule 6 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	245	Total	C	N	O	S	0	0
			1909	1210	326	361	12		
6	T	240	Total	C	N	O	S	1	0
			1867	1186	320	349	12		

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	237	Total	C	N	O	S	1	0
			1860	1183	309	355	13		
7	U	244	Total	C	N	O	S	0	0
			1885	1196	316	360	13		

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	220	Total	C	N	O	S	2	0
			1672	1053	286	320	13		
8	V	220	Total	C	N	O	S	2	0
			1655	1042	278	322	13		

- Molecule 9 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	204	Total	C	N	O	S	6	0
			1633	1039	274	301	19		
9	W	204	Total	C	N	O	S	2	0
			1604	1021	269	295	19		

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	196	Total	C	N	O	S	0	0
			1561	1001	264	287	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	196	Total	C	N	O	S	1	0
			1574	1008	267	289	10		

- Molecule 11 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	201	Total	C	N	O	S	0	0
			1543	974	267	293	9		
11	Y	199	Total	C	N	O	S	3	0
			1564	988	275	291	10		

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	213	Total	C	N	O	S	2	0
			1656	1048	283	314	11		
12	Z	213	Total	C	N	O	S	1	0
			1644	1043	281	309	11		

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		
13	a	216	Total	C	N	O	S	1	0
			1688	1065	291	320	12		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	1	0
			1515	951	258	293	13		
14	b	203	Total	C	N	O	S	1	0
			1526	958	259	296	13		

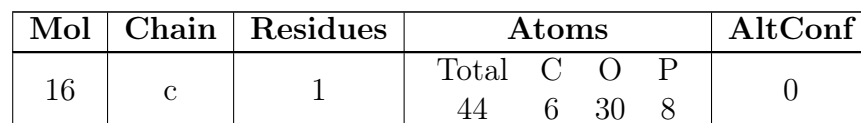
- Molecule 15 is a protein called Proteasome activator complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	1811	Total	C	N	O	S	0	0
			14643	9411	2500	2651	81		

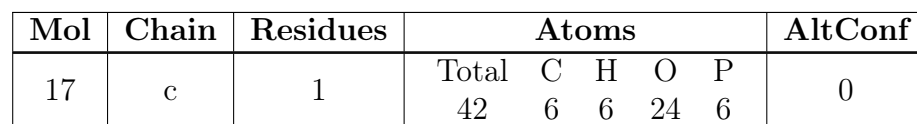
There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	-34	MET	-	initiating methionine	UNP Q14997
c	-33	GLY	-	expression tag	UNP Q14997
c	-32	THR	-	expression tag	UNP Q14997
c	-31	THR	-	expression tag	UNP Q14997
c	-30	ARG	-	expression tag	UNP Q14997
c	-29	SER	-	expression tag	UNP Q14997
c	-28	THR	-	expression tag	UNP Q14997
c	-27	MET	-	expression tag	UNP Q14997
c	-26	SER	-	expression tag	UNP Q14997
c	-25	TYR	-	expression tag	UNP Q14997
c	-24	TYR	-	expression tag	UNP Q14997
c	-23	HIS	-	expression tag	UNP Q14997
c	-22	HIS	-	expression tag	UNP Q14997
c	-21	HIS	-	expression tag	UNP Q14997
c	-20	HIS	-	expression tag	UNP Q14997
c	-19	HIS	-	expression tag	UNP Q14997
c	-18	HIS	-	expression tag	UNP Q14997
c	-17	ASP	-	expression tag	UNP Q14997
c	-16	TYR	-	expression tag	UNP Q14997
c	-15	ASP	-	expression tag	UNP Q14997
c	-14	ILE	-	expression tag	UNP Q14997
c	-13	PRO	-	expression tag	UNP Q14997
c	-12	THR	-	expression tag	UNP Q14997
c	-11	THR	-	expression tag	UNP Q14997
c	-10	GLU	-	expression tag	UNP Q14997
c	-9	ASN	-	expression tag	UNP Q14997
c	-8	LEU	-	expression tag	UNP Q14997
c	-7	TYR	-	expression tag	UNP Q14997
c	-6	PHE	-	expression tag	UNP Q14997
c	-5	GLN	-	expression tag	UNP Q14997
c	-4	GLY	-	expression tag	UNP Q14997
c	-3	ALA	-	expression tag	UNP Q14997
c	-2	MET	-	expression tag	UNP Q14997
c	-1	ASP	-	expression tag	UNP Q14997
c	0	PRO	-	expression tag	UNP Q14997
c	821	ILE	LEU	conflict	UNP Q14997
c	822	LEU	ILE	conflict	UNP Q14997

- Molecule 16 is [(1 {S},2 {R},3 {R},4 {S},5 {S},6 {R})-2-[oxidanyl(phosphonooxy)phosphoryl]oxy-3,4,5,6-tetrachosphonooxy-cyclohexyl] phosphono hydrogen phosphate (CCD ID: K0W) (formula: C₆H₂₀O₃₀P₈) (labeled as "Ligand of Interest" by depositor).



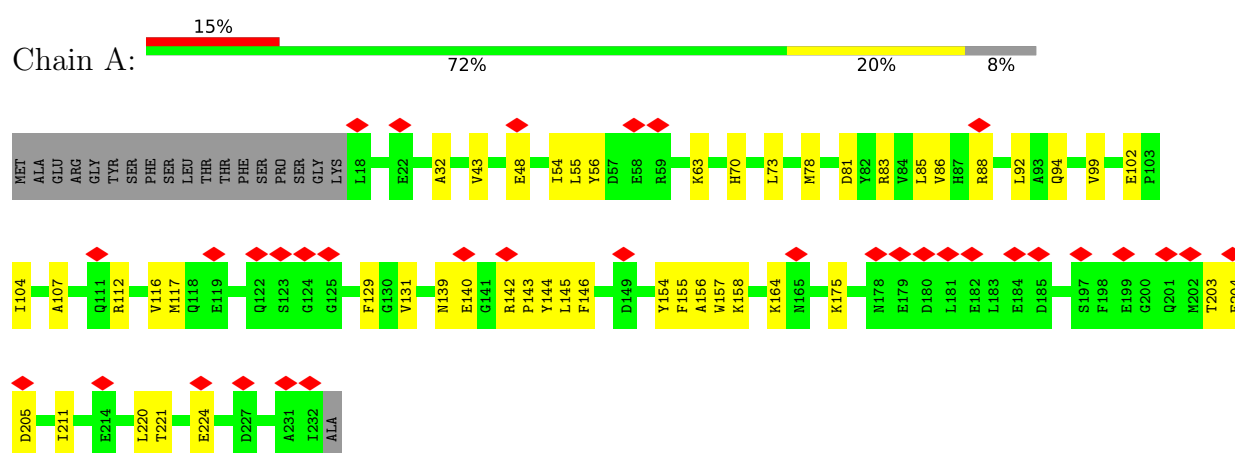
- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $\text{C}_6\text{H}_{18}\text{O}_{24}\text{P}_6$) (labeled as "Ligand of Interest" by depositor).



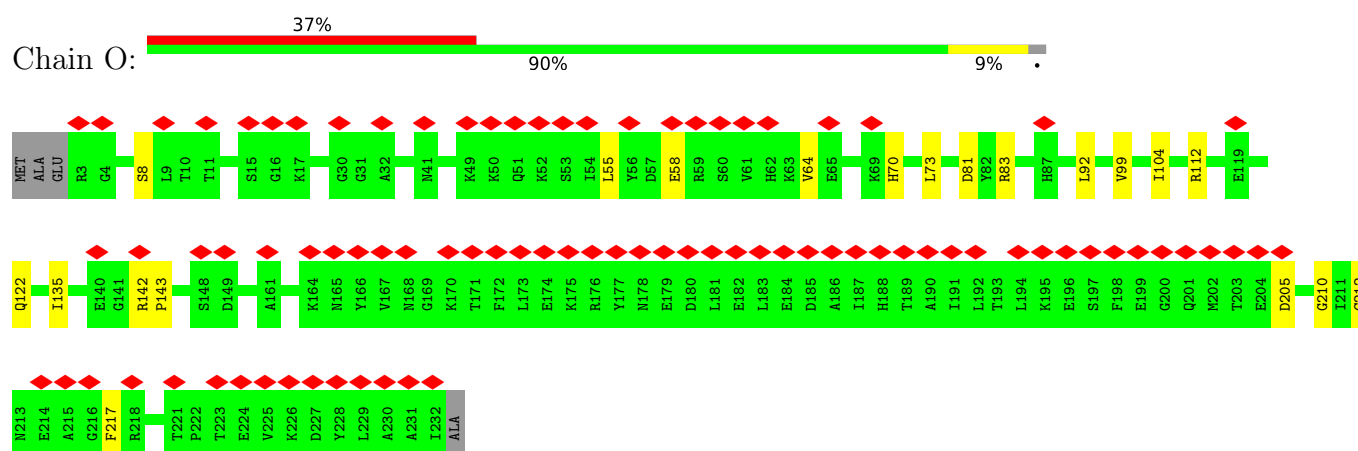
3 Residue-property plots

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

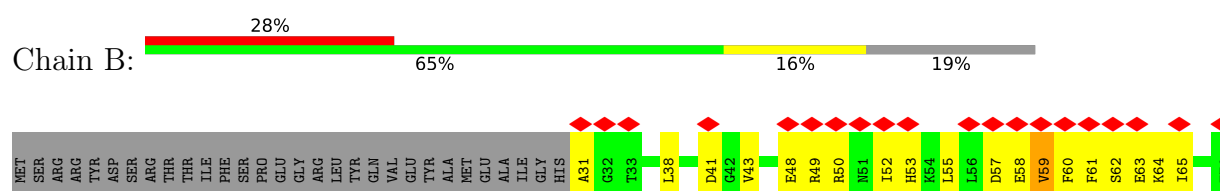
- Molecule 1: Proteasome subunit alpha type-2

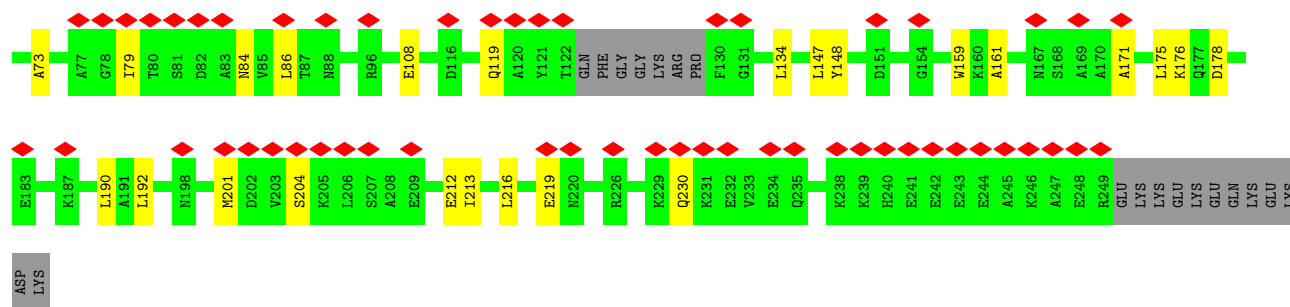


- Molecule 1: Proteasome subunit alpha type-2

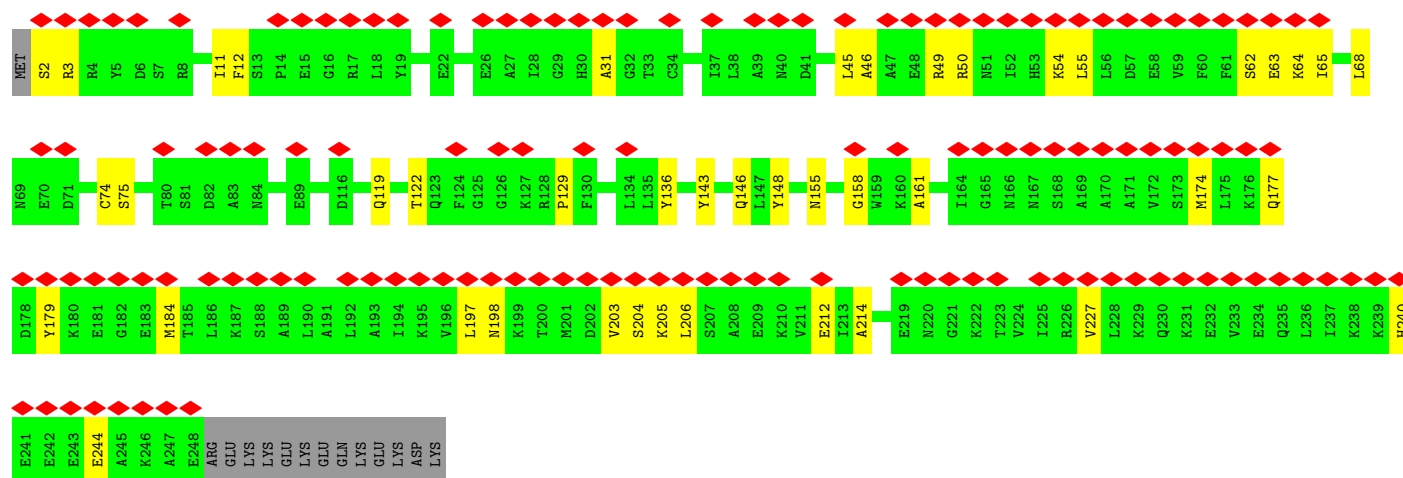
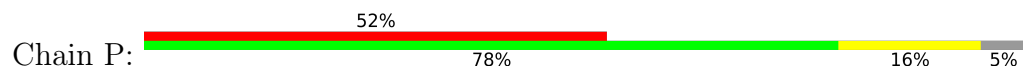


- Molecule 2: Proteasome subunit alpha type-4

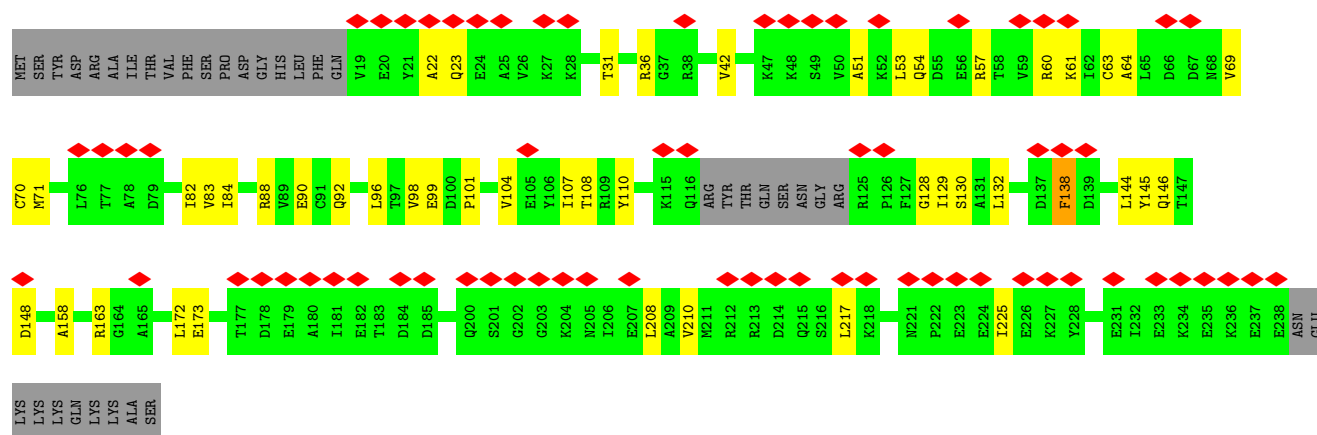




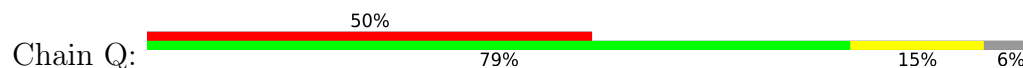
- Molecule 2: Proteasome subunit alpha type-4

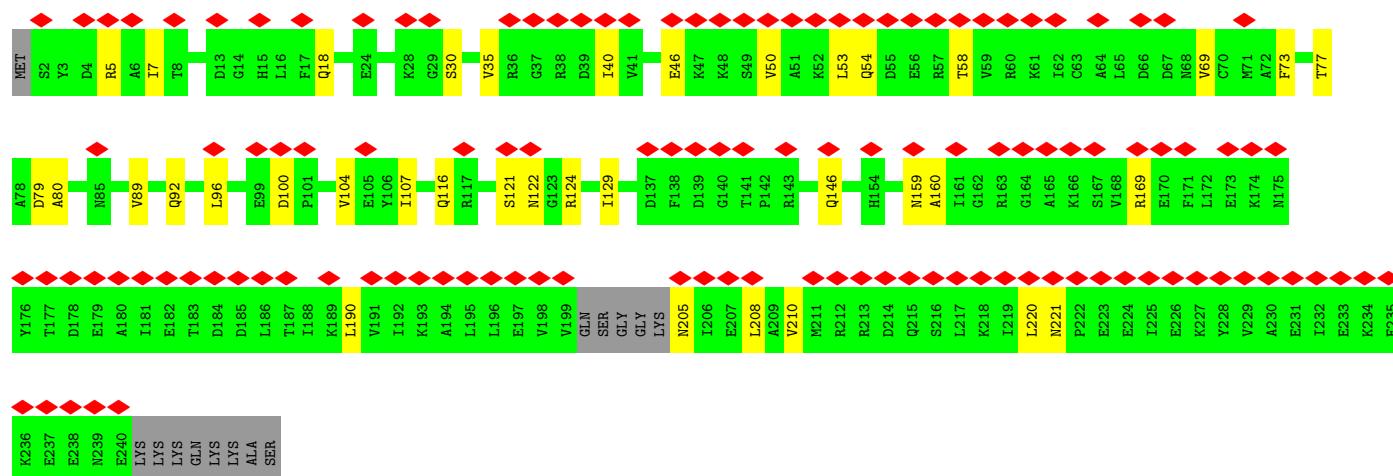


- Molecule 3: Proteasome subunit alpha type-7

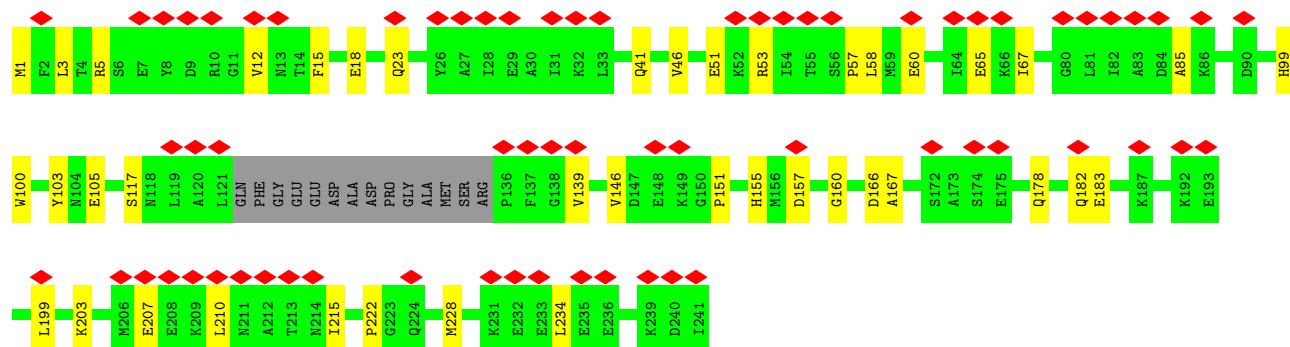
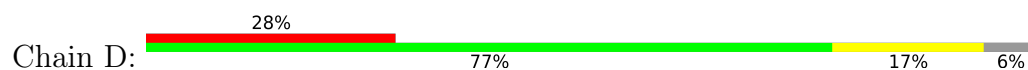


- Molecule 3: Proteasome subunit alpha type-7

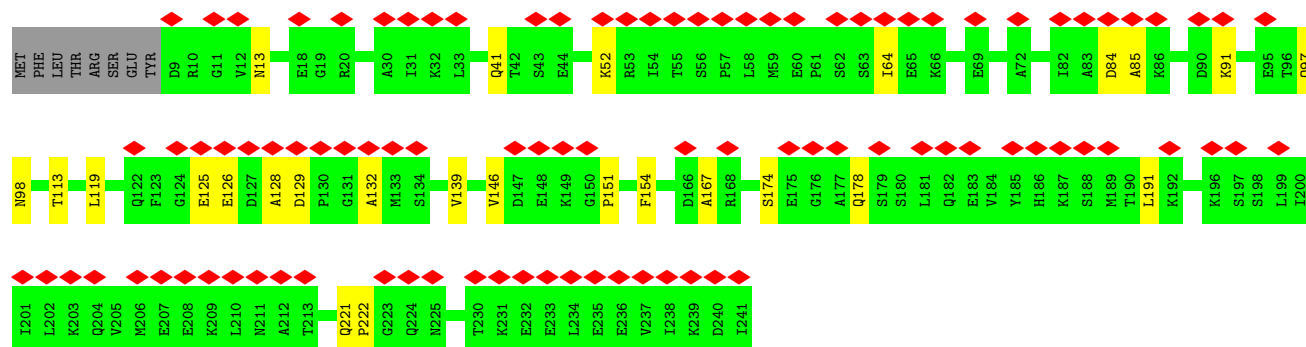
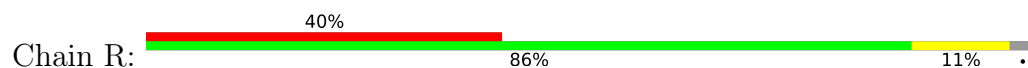




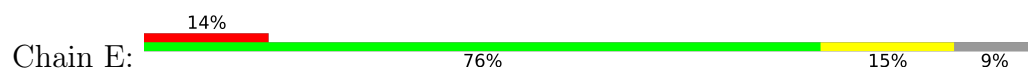
• Molecule 4: Proteasome subunit alpha type-5

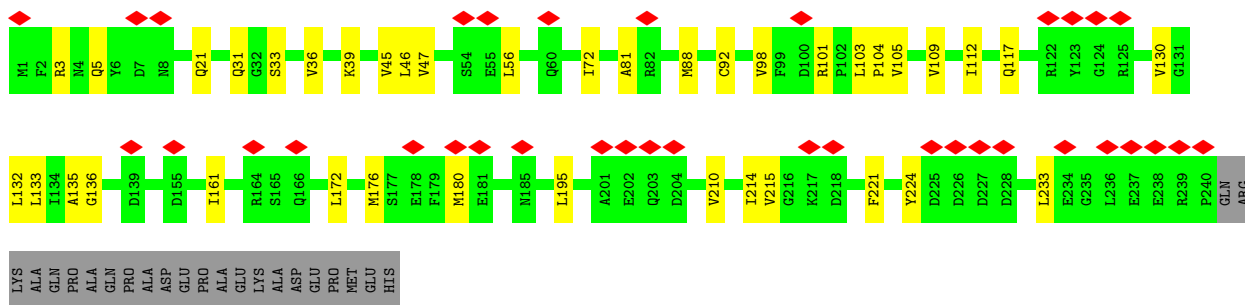


• Molecule 4: Proteasome subunit alpha type-5

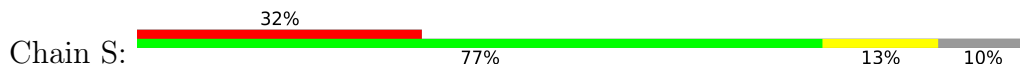


• Molecule 5: Proteasome subunit alpha type-1

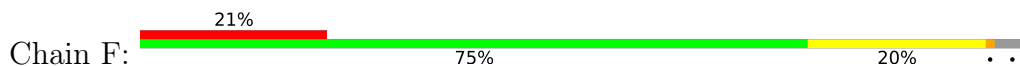




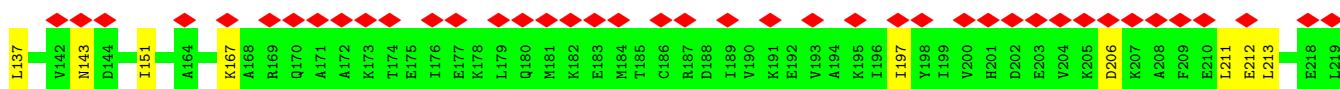
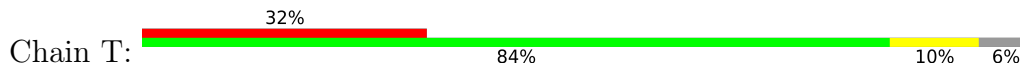
• Molecule 5: Proteasome subunit alpha type-1

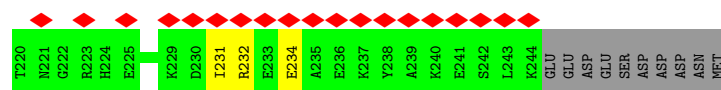


• Molecule 6: Proteasome subunit alpha type-3

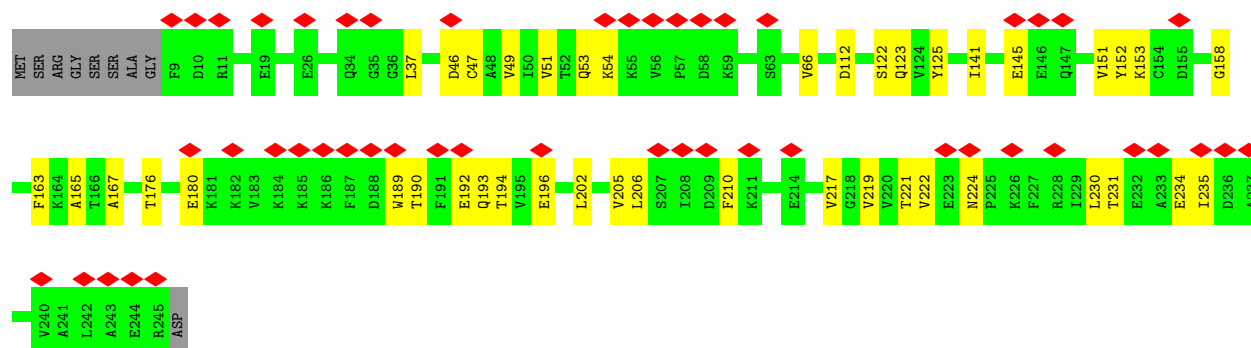
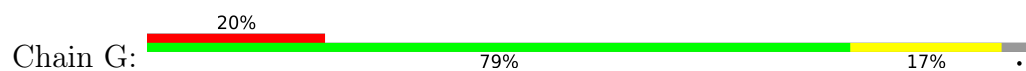


• Molecule 6: Proteasome subunit alpha type-3

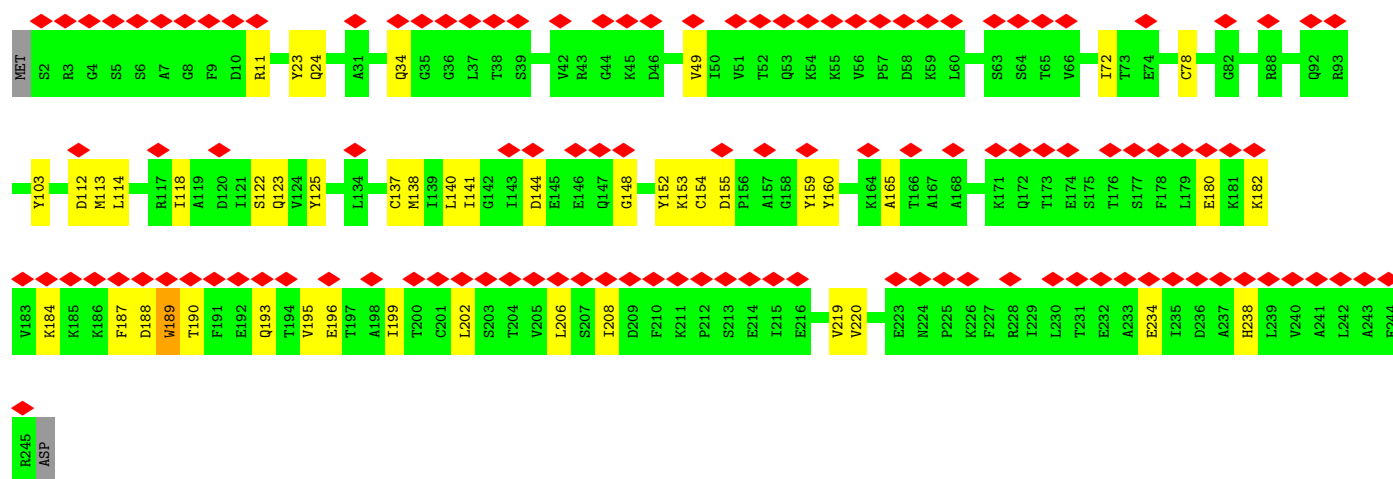
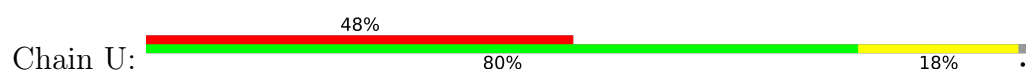




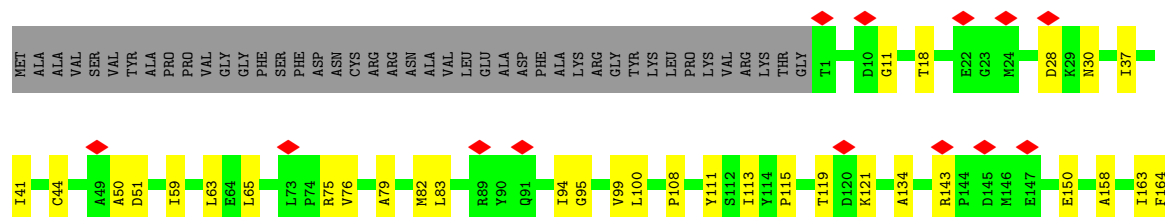
• Molecule 7: Proteasome subunit alpha type-6

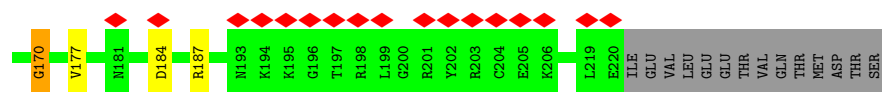


• Molecule 7: Proteasome subunit alpha type-6

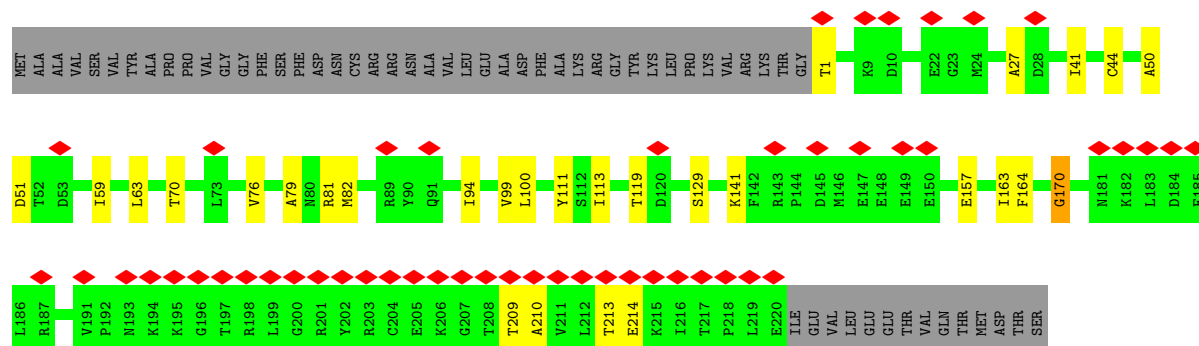


• Molecule 8: Proteasome subunit beta type-7

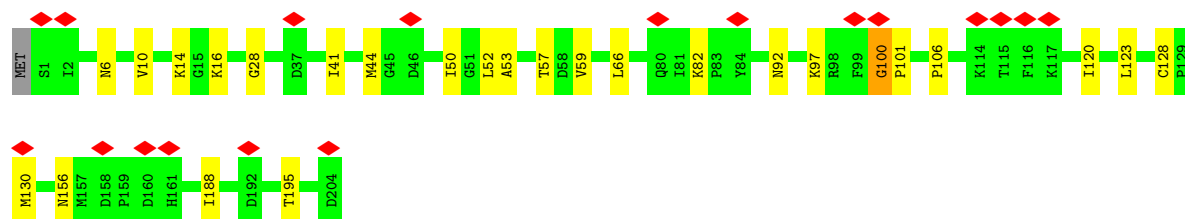
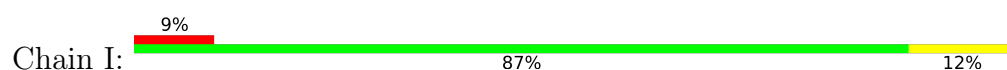




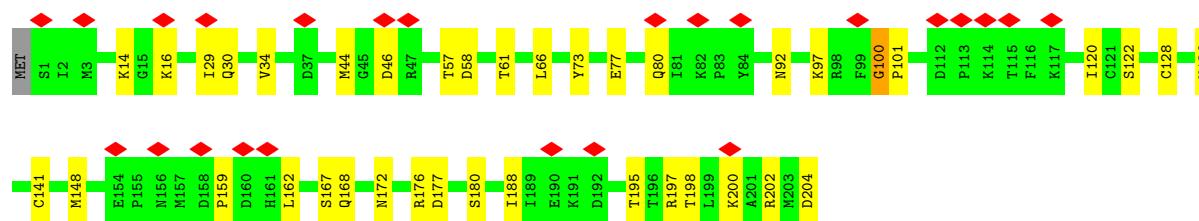
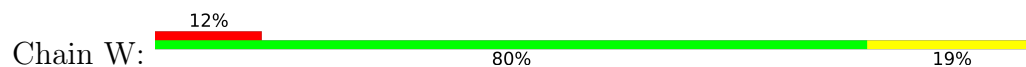
- Molecule 8: Proteasome subunit beta type-7



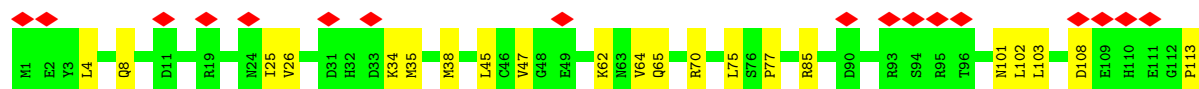
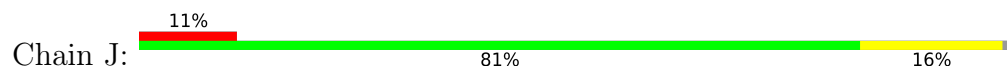
- Molecule 9: Proteasome subunit beta type-3

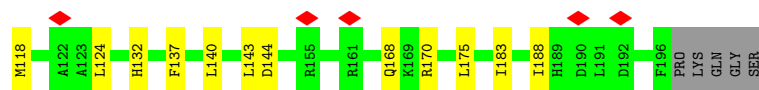


- Molecule 9: Proteasome subunit beta type-3

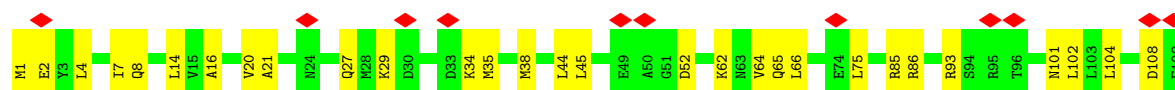
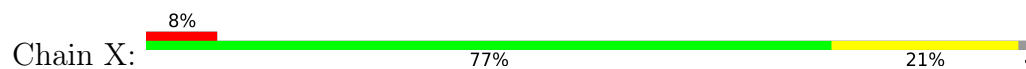


- Molecule 10: Proteasome subunit beta type-2

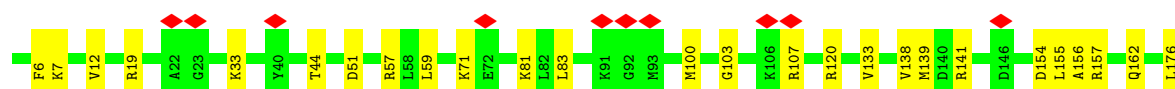
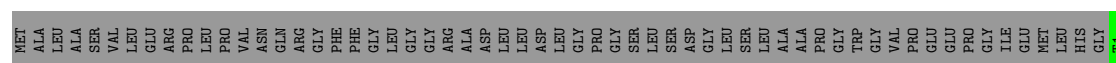




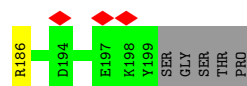
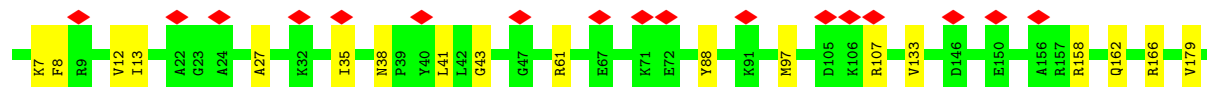
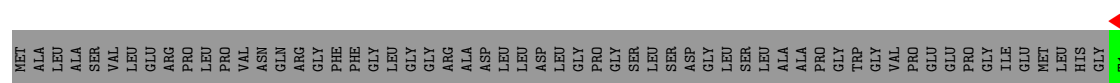
- Molecule 10: Proteasome subunit beta type-2



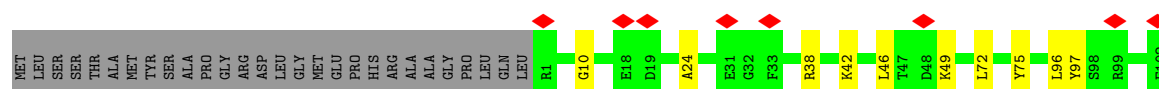
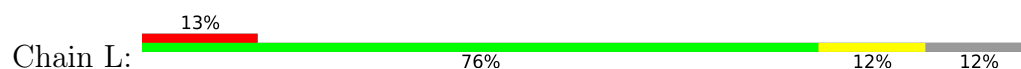
- Molecule 11: Proteasome subunit beta type-5

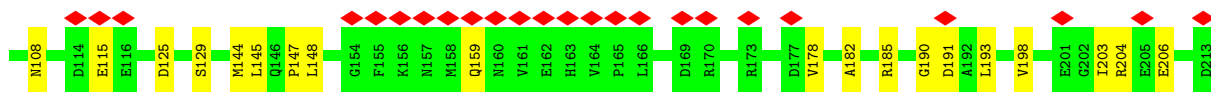


- Molecule 11: Proteasome subunit beta type-5

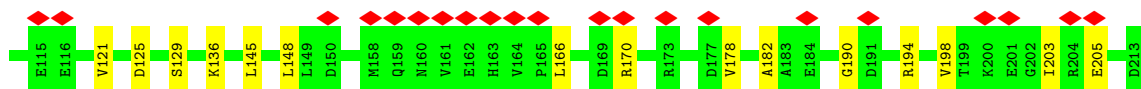
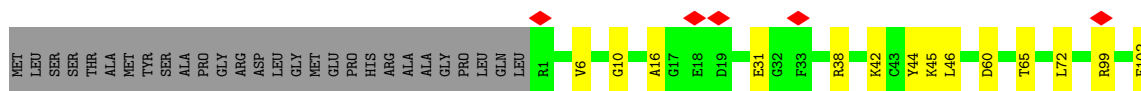
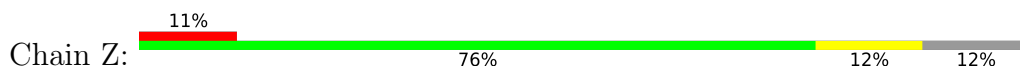


- Molecule 12: Proteasome subunit beta type-1

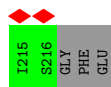
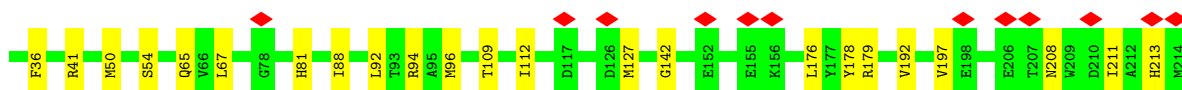
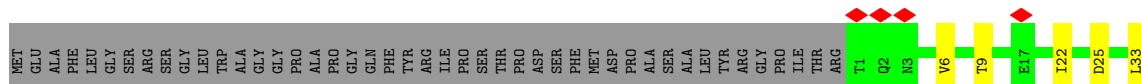




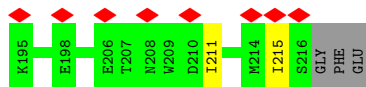
- Molecule 12: Proteasome subunit beta type-1



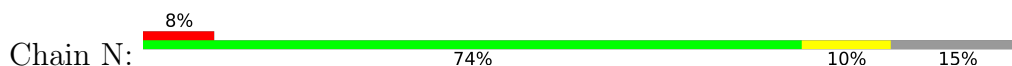
- Molecule 13: Proteasome subunit beta type-4

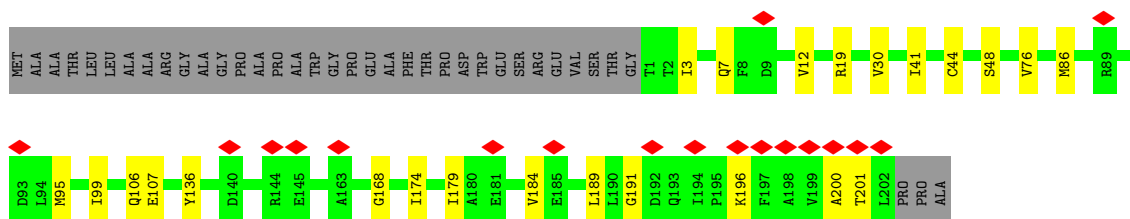


- Molecule 13: Proteasome subunit beta type-4

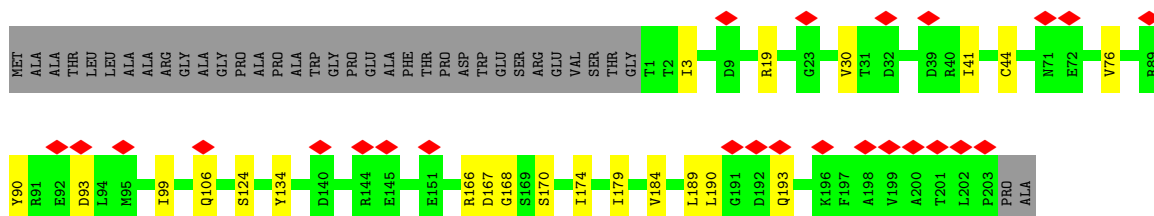
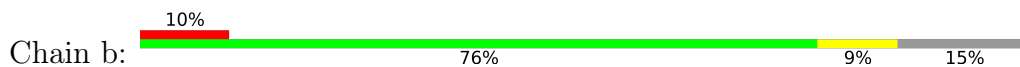


- Molecule 14: Proteasome subunit beta type-6

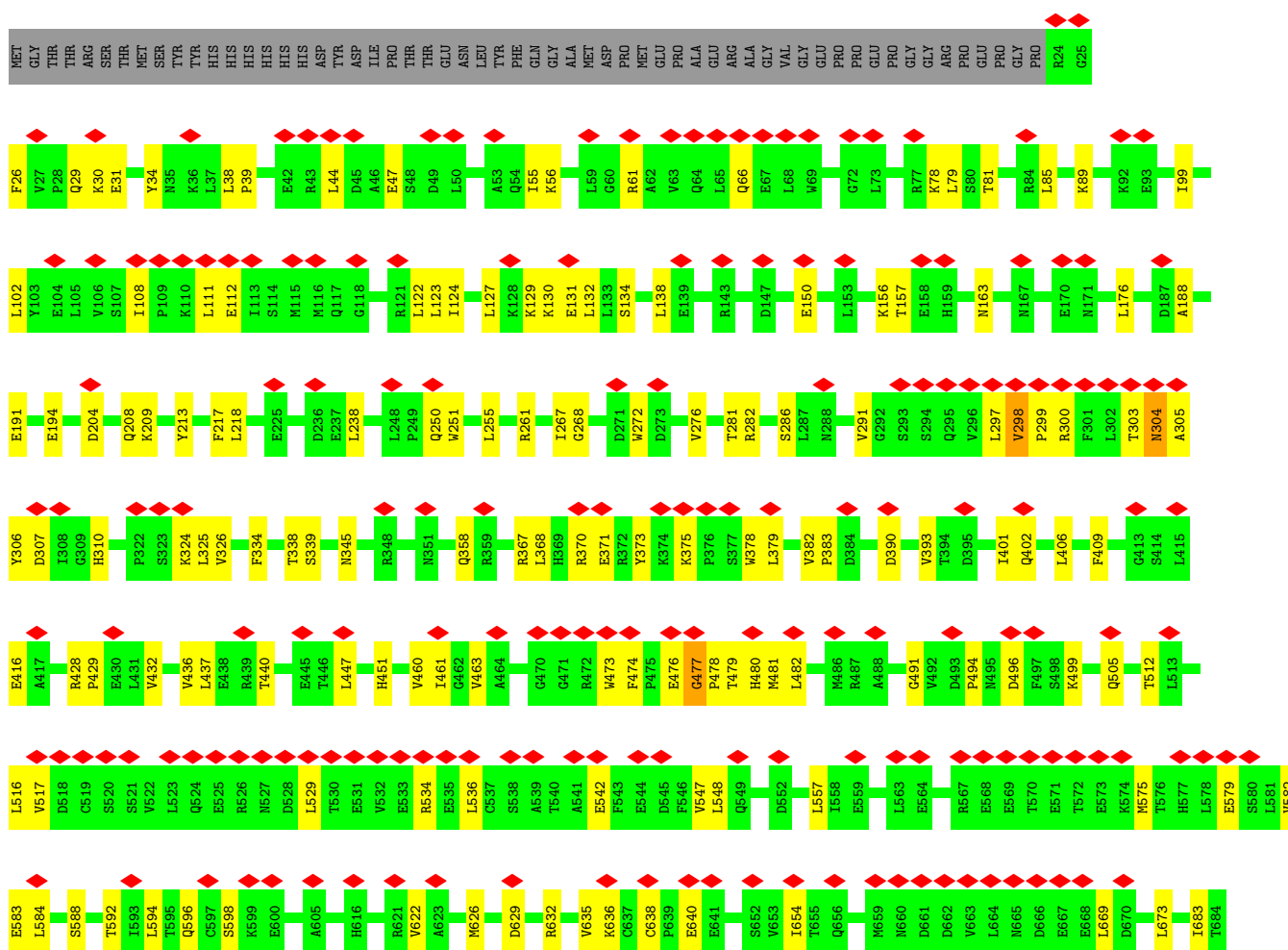




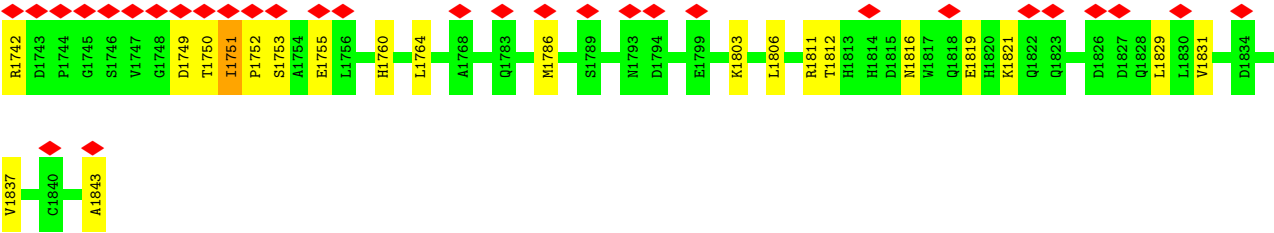
• Molecule 14: Proteasome subunit beta type-6



• Molecule 15: Proteasome activator complex subunit 4



L1665	Q1666	T1667	M1668	V1669	F1670	Y1671	T1672	L1673	F1674	L1677	M1678	N1679	E1680	D1685	I1686	R1687	V1690	L1693	E1697	Q1698	L1699	E1700	V1701	R1702	E1703	M1704	A1705	A1706	L1712	L1713	Q1714	T1719	M1720	D1721	S1722	P1723	M1724	Q1725	E1729	Q1730	L1731	C1732	T1733	K1734	A1735	A1650	L1736	P1737	K1738	K1739	R1740	K1741		
A1585	Q1586	R1587	S1590	T1591	A1592	E1595	Q1596	L1597	Q1598	L1599	L1600	P1601	L1602	F1603	P1604	K1605	P1608	V1609	E1610	N1611	D1612	D1613	S1614	Y1615	D1616	E1617	L1618	K1619	R1620	D1621	A1622	K1623	L1624	L1628	Q1631	H1637	Q1638	Q1644	Q1648	T1649	A1650	R1651	W1655	T1660	V1661	L1662	T1663	Y1664						
V1501	R1502	I1505	L1509	T1510	Y1511	L1512	F1513	D1516	V1517	S1518	L1519	P1520	M1521	L1538	E1539	K1540	L1541	L1443	F1444	E1445	L1446	L1447	L1448	E1449	A1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L1486	L1490	Q1496	K1499	N1500							
E1403	C1406	L1409	R1410	N1415	E1419	C1427	S1431	C1432	E1433	S1434	R1435	K1439	L1440	L1443	F1444	E1445	L1446	L1447	L1448	E1449	A1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L1486	L1490	Q1496	K1499	N1500											
I1323	L1326	S1327	L1328	D1329	R1331	K1332	G1333	D1335	K1336	R1340	R1341	K1346	F1349	R1350	F1352	D1353	D1354	A1355	F1356	L1357	L1360	K1361	P1362	H1363	L1364	E1365	H1366	D1370	S1371	H1372	E1373	R1377	A1380	E1381	T1382	I1383	L1386	W1393	E1396	K1397	V1398	E1399	K1400	L1401	W1402									
E1403	C1406	L1409	R1410	N1415	E1419	C1427	S1431	C1432	E1433	S1434	R1435	K1439	L1440	L1443	F1444	E1445	L1446	L1447	L1448	E1449	A1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L1486	L1490	Q1496	K1499	N1500											
V1501	R1502	I1505	L1509	T1510	Y1511	L1512	F1513	D1516	V1517	S1518	L1519	P1520	M1521	L1538	E1539	K1540	L1541	L1443	F1444	E1445	L1446	L1447	L1448	E1449	A1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L1486	L1490	Q1496	K1499	N1500							
A1585	Q1586	R1587	S1590	T1591	A1592	E1595	Q1596	L1597	Q1598	L1599	L1600	P1601	L1602	F1603	P1604	K1605	P1608	V1609	E1610	N1611	D1612	D1613	S1614	Y1615	D1616	E1617	L1618	K1619	R1620	D1621	A1622	K1623	L1624	L1628	Q1631	H1637	Q1638	Q1644	Q1648	T1649	A1650	R1651	W1655	T1660	V1661	L1662	T1663	Y1664						
L762	W763	N764	L765	G766	Q767	W769	S774	E775	E776	F779	A780	F781	L784	D785	L788	Q789	E791	D800	G801	L724	L803	E804	D808	H818	N819	L822	G825	N826	L827	L828	K832	G833	E834	P835	V836	T837	N838	L839	V840	P841	S842	M843	V844	S845	L846	E847	E848							
T849	K850	L851	G854	L855	E856	Y857	D858	L859	S860	R861	E862	N863	H864	R865	E866	V867	I868	R873	L876	L880	D881	E884	D885	D886	T887	L890	F891	L892	I893	I894	D899	Q902	F903	Q904	H907	K908	H909	E910	F911	D912	S913	R914	W915	K916	S917	F918	N919	L920	V921	K922				
K923	S924	M925	N926	R928	L929	H930	G931	K932	K933	Q934	H935	I936	L939	L940	I941	D942	R943	E949	L950	R951	T952	L953	T954	V955	E956	G957	C958	E959	Y960	K961	K962	I963	D966	M967	L968	R969	D970	L971	L972	R973	L974	S980	Q981	V982	R983	N984	K985	F990	G995	N998	F999			
C1000	C1001	R1002	D1003	I1004	I1005	L1009	E1010	R1013	P1014	D1015	R1016	Q1017	G1018	V1019	T1020	Q1021	Q1022	M1034	H1035	S1036	G1037	V1038	A1041	H1044	V1050	Q1051	T1052	V1053	P1054	A1055	I1056	V1057	L1061	S1062	Q1063	A1064	M1065	L1067	E1068	K1069	P1070	S1071	I1072	V1073	R1074	D1077	D1078	L1079	A1080	E1081				
K1082	I1083	H1084	R1085	Q1086	G1091	L1092	D1093	F1094	T1095	P1097	K1098	S1099	C1100	V1101	E1102	I1103	A1104	E1105	Q1108	Q1109	S1110	K1111	N1112	P1113	S1114	I1115	N1116	Q1117	I1118	L1119	L1120	S1121	P1122	E1123	K1124	I1125	K1126	E1127	G1128	I1129	K1130	R1131	Q1132	Q1133	E1134	K1135	N1136	A1137	D1138	R1141	Y1143	E1144	N1145	L1146
V1147	D1152	G1153	V1154	R1157	N1158	K1162	I1168	G1169	L1170	L1175	R1176	D1177	D1178	R1179	V1180	L1181	P1182	L1183	I1186	R1187	E1191	N1192	L1193	N1194	H1195	D1196	K1213	K1216	K1220	E1224	N1225	P1226	C1227	E1228	I1229	S1230	D1231	C1232	P1233	K1234	P1235	T1236	Q1237	I1238	I1239	D1242								
D1245	N1246	H1247	D1252	S1253	K1254	T1255	I1256	P1257	L1258	T1259	K1260	K1261	E1262	W1263	E1264	S1265	S1266	V1269	E1270	K1271	H1273	W1274	K1281	V1284	V1285	Y1286	E1290	E1291	K1294	L1295	G1296	R1297	S1298	R1299	E1300	D1301	M1302	T1303	E1306	Q1307	I1308	D1311	D1315	P1316	K1317	E1320	Q1321	L1322						
I1323	L1326	S1327	L1328	D1329	R1331	K1332	G1333	D1335	K1336	R1340	R1341	K1346	F1349	R1350	F1352	D1353	D1354	A1355	F1356	L1357	L1360	K1361	P1362	H1363	L1364	E1365	H1366	D1370	S1371	H1372	E1373	R1377	A1380	E1381	T1382	I1383	L1386	W1393	E1396	K1397	V1398	E1399	K1400	L1401	W1402									
E1403	C1406	L1409	R1410	N1415	E1419	C1427	S1431	C1432	E1433	S1434	R1435	K1439	L1440	L1443	F1444	E1445	L1446	L1447	L1448	E1449	A1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L1486	L1490	Q1496	K1499	N1500											
V1501	R1502	I1505	L1509	T1510	Y1511	L1512	F1513	D1516	V1517	S1518	L1519	P1520	M1521	L1538	E1539	K1540	L1541	L1443	F1444	E1445	L1446	L1447	L1448	E1449	A1450	P1451	L1452	S1453	G1454	E1455	G1456	G1457	D1461	A1462	L1468	Q1475	E1476	V1477	R1478	E1481	L1482	R1485	L1486	L1490	Q1496	K1499	N1500							
A1585	Q1586	R1587	S1590	T1591	A1592	E1595	Q1596	L1597	Q1598	L1599	L1600	P1601	L1602	F1603	P1604	K1605	P1608	V1609	E1610	N1611	D1612	D1613	S1614	Y1615	D1616	E1617	L1618	K1619	R1620	D1621	A1622	K1623	L1624	L1628	Q1631	H1637	Q1638	Q1644	Q1648	T1649	A1650	R1651	W1655	T1660	V1661	L1662	T1663	Y1664						



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	87000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.179	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KOW, IHP

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	0.48	0/1706	0.71	4/2314 (0.2%)
1	O	0.38	0/1818	0.59	0/2467
2	B	0.44	0/1666	0.71	3/2248 (0.1%)
2	P	0.38	0/1955	0.59	1/2642 (0.0%)
3	C	0.42	0/1660	0.81	3/2240 (0.1%)
3	Q	0.33	0/1842	0.65	2/2496 (0.1%)
4	D	0.45	0/1767	0.66	0/2386
4	R	0.38	0/1795	0.59	2/2424 (0.1%)
5	E	0.49	0/1917	0.69	0/2592
5	S	0.39	0/1915	0.61	2/2589 (0.1%)
6	F	0.45	0/1944	0.73	4/2617 (0.2%)
6	T	0.40	0/1905	0.64	0/2567
7	G	0.45	0/1897	0.72	1/2566 (0.0%)
7	U	0.37	0/1919	0.67	3/2596 (0.1%)
8	H	0.44	0/1705	0.66	2/2307 (0.1%)
8	V	0.41	0/1688	0.64	2/2288 (0.1%)
9	I	0.48	1/1668 (0.1%)	0.69	4/2247 (0.2%)
9	W	0.46	0/1636	0.74	7/2205 (0.3%)
10	J	0.44	0/1593	0.61	0/2156
10	X	0.44	0/1609	0.61	0/2176
11	K	0.46	0/1574	0.61	0/2128
11	Y	0.44	0/1604	0.64	0/2165
12	L	0.45	0/1692	0.66	2/2281 (0.1%)
12	Z	0.46	0/1677	0.67	2/2260 (0.1%)
13	M	0.47	0/1720	0.61	0/2328
13	a	0.48	0/1724	0.65	0/2334
14	N	0.45	0/1544	0.57	0/2090
14	b	0.45	0/1556	0.60	0/2107
15	c	0.46	0/14985	0.87	35/20326 (0.2%)
All	All	0.44	1/63681 (0.0%)	0.71	79/86142 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	41	ILE	C-N	5.86	1.43	1.33

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	c	303	THR	N-CA-C	12.09	124.46	111.28
7	U	189	TRP	N-CA-C	11.72	128.34	109.24
15	c	1270	GLU	N-CA-C	10.46	122.75	111.36
15	c	1112	ASN	CA-C-N	9.46	131.66	119.84
15	c	1112	ASN	C-N-CA	9.46	131.66	119.84

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	1671	0	1665	58	0
1	O	1779	0	1747	12	0
2	B	1645	0	1655	48	0
2	P	1919	0	1895	31	0
3	C	1641	0	1664	41	0
3	Q	1817	0	1786	34	0
4	D	1741	0	1738	37	0
4	R	1768	0	1756	27	0
5	E	1881	0	1862	27	0
5	S	1871	0	1855	22	0
6	F	1909	0	1900	66	0
6	T	1867	0	1847	15	0
7	G	1860	0	1866	41	0
7	U	1885	0	1881	35	0
8	H	1672	0	1703	23	0
8	V	1655	0	1661	20	0
9	I	1633	0	1660	15	0
9	W	1604	0	1626	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1561	0	1558	25	0
10	X	1574	0	1578	32	0
11	K	1543	0	1495	25	0
11	Y	1564	0	1539	15	0
12	L	1656	0	1655	19	0
12	Z	1644	0	1644	17	0
13	M	1687	0	1666	19	0
13	a	1688	0	1666	18	0
14	N	1515	0	1492	16	0
14	b	1526	0	1503	15	0
15	c	14643	0	14837	428	0
16	c	44	0	0	15	0
17	c	36	6	6	12	0
All	All	62499	6	62406	1055	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 8.

The worst 5 of 1055 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)
15:c:972:LEU:HD11	15:c:1004:ILE:CD1	1.30	1.60
15:c:972:LEU:CD1	15:c:1004:ILE:HD11	1.34	1.52
15:c:300:ARG:NH1	15:c:1631:GLN:HG2	1.25	1.49
6:F:215:TRP:CZ2	6:F:227:VAL:HG13	1.48	1.47
6:F:215:TRP:NE1	6:F:227:VAL:HG22	1.36	1.36

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands 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	$\# Z > 2$
17	IHP	c	1902	-	36,36,36	0.72	0	60,60,60	0.96	0
16	K0W	c	1901	-	42,44,44	1.77	7 (16%)	68,74,74	1.15	6 (8%)

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
17	IHP	c	1902	-	-	2/30/54/54	0/1/1/1
16	K0W	c	1901	-	-	9/42/66/66	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	c	1901	K0W	PA5-O77	5.82	1.65	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	c	1901	K0W	PA1-O76	5.30	1.65	1.59
16	c	1901	K0W	PA3-O13	3.59	1.65	1.59
16	c	1901	K0W	PA6-O16	3.02	1.64	1.59
16	c	1901	K0W	PA4-O14	2.86	1.64	1.59

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	c	1901	K0W	C5-C6-C1	3.35	117.78	110.43
16	c	1901	K0W	C5-C4-C3	2.77	116.50	110.43
16	c	1901	K0W	C4-C3-C2	2.60	116.12	110.43
16	c	1901	K0W	C6-C1-C2	2.37	115.63	110.43
16	c	1901	K0W	PA6-O16-C1	-2.06	117.93	123.43

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	c	1901	K0W	C4-C3-O13-PA3
16	c	1901	K0W	C6-O11-PA1-O76
16	c	1901	K0W	C3-O13-PA3-O23
17	c	1902	IHP	C3-O13-P3-O43
16	c	1901	K0W	C2-C3-O13-PA3

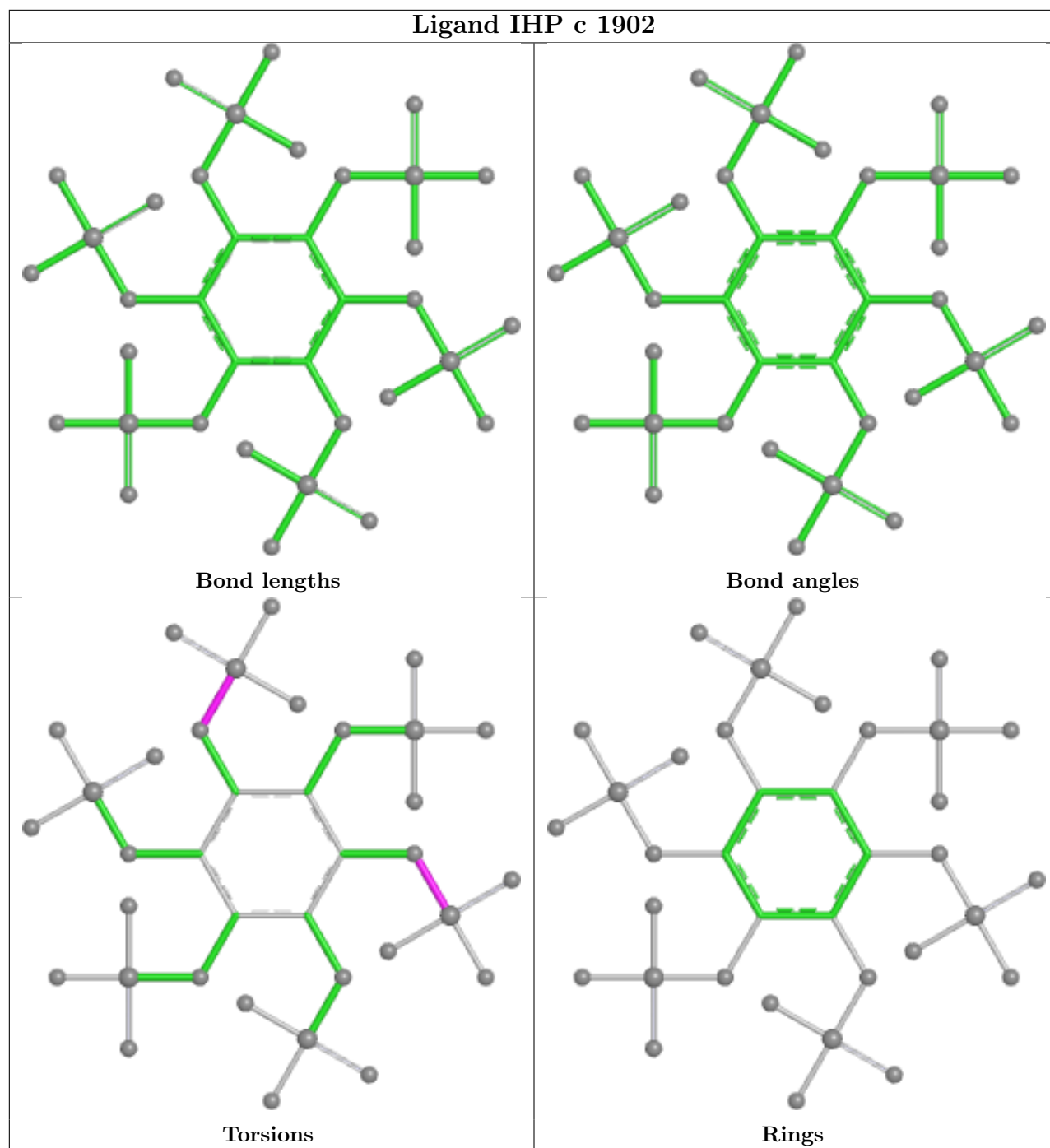
There are no ring outliers.

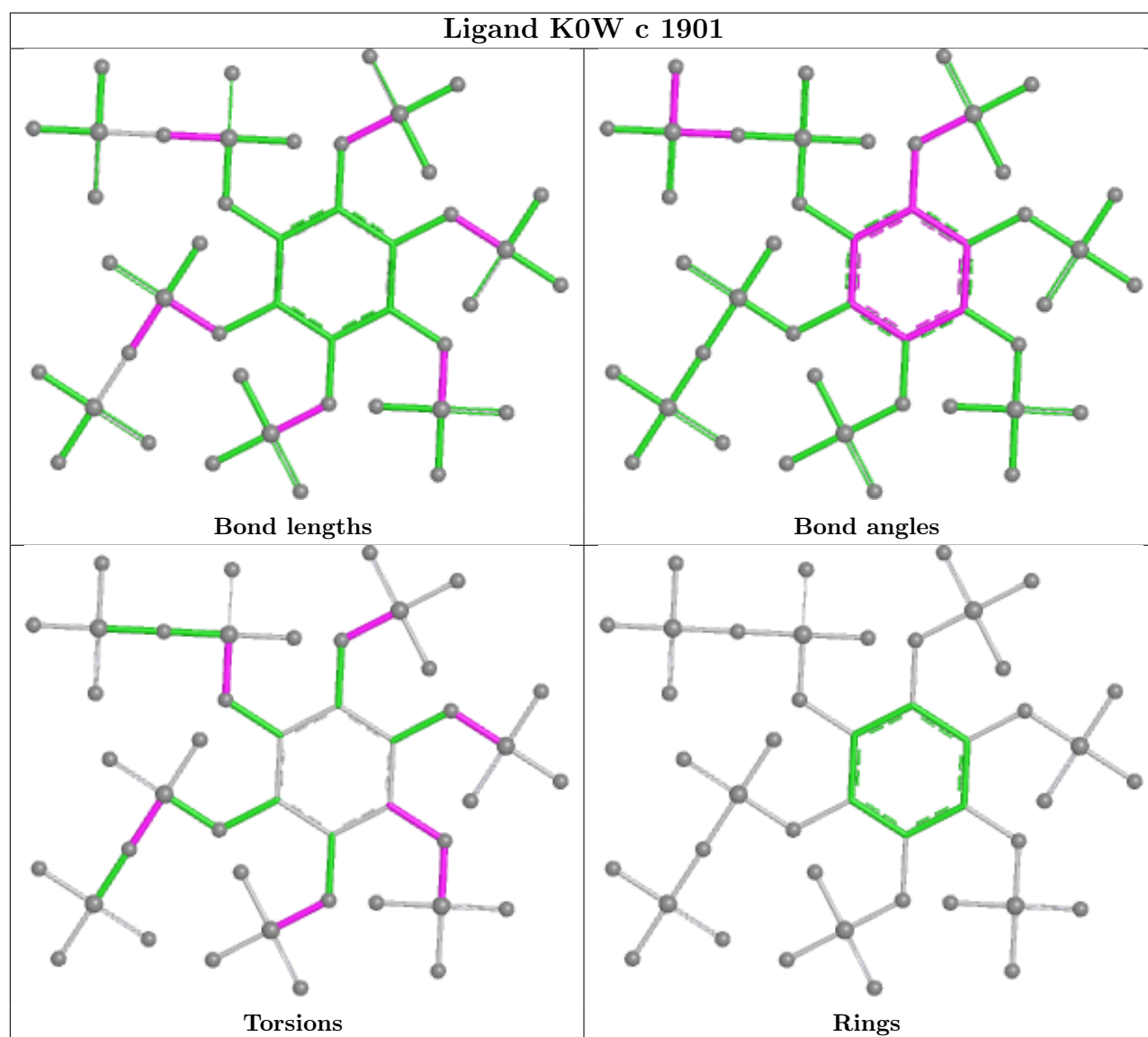
2 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	c	1902	IHP	12	0
16	c	1901	K0W	15	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

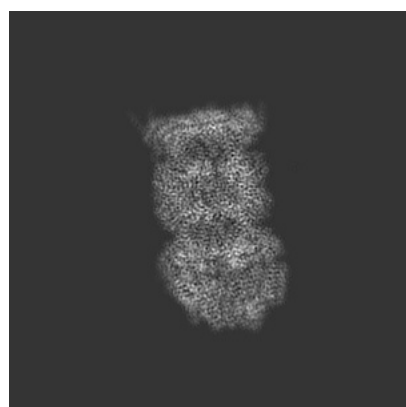
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0781. These allow visual inspection of the internal detail of the map and identification of artifacts.

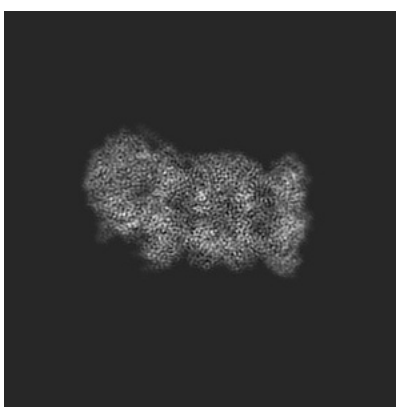
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

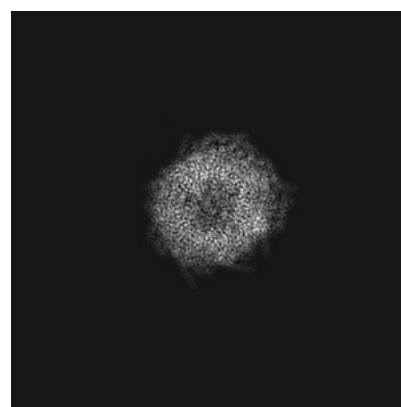
6.1.1 Primary map



X



Y



Z

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

6.2 Central slices [i](#)

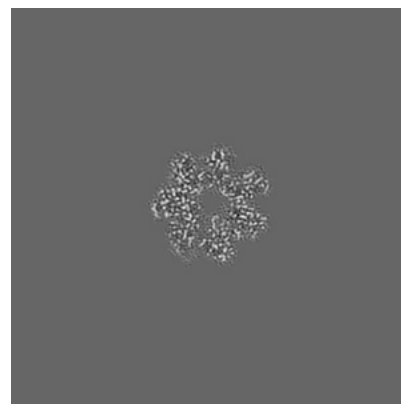
6.2.1 Primary map



X Index: 180



Y Index: 180

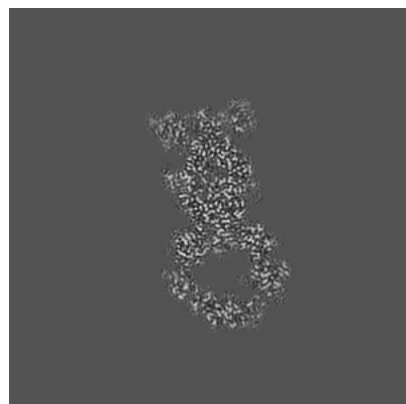


Z Index: 180

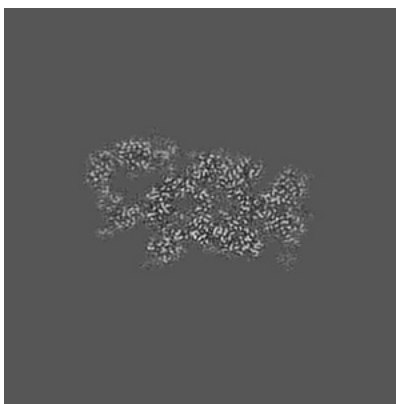
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

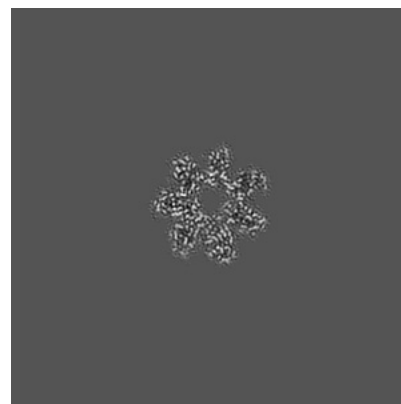
6.3.1 Primary map



X Index: 207



Y Index: 208

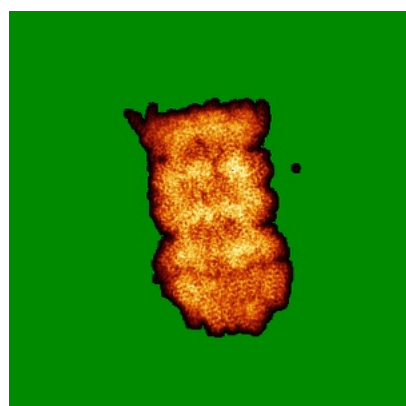


Z Index: 177

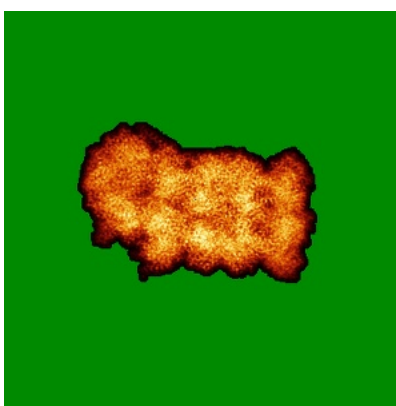
The images above show the largest variance slices of the map in three orthogonal directions.

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

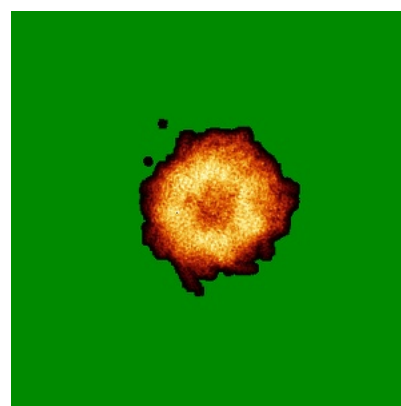
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

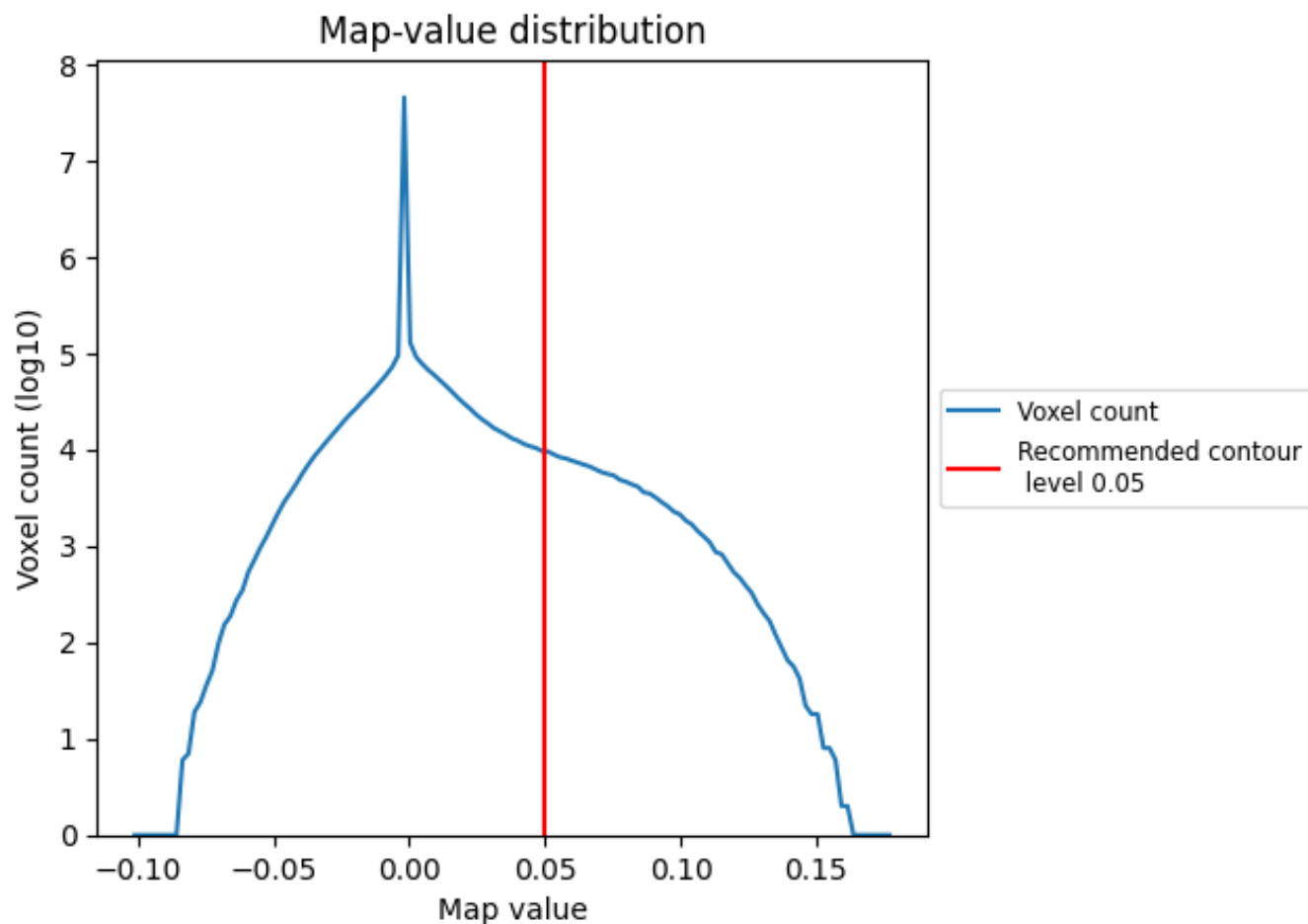
6.6 Mask visualisation

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

7 Map analysis [i](#)

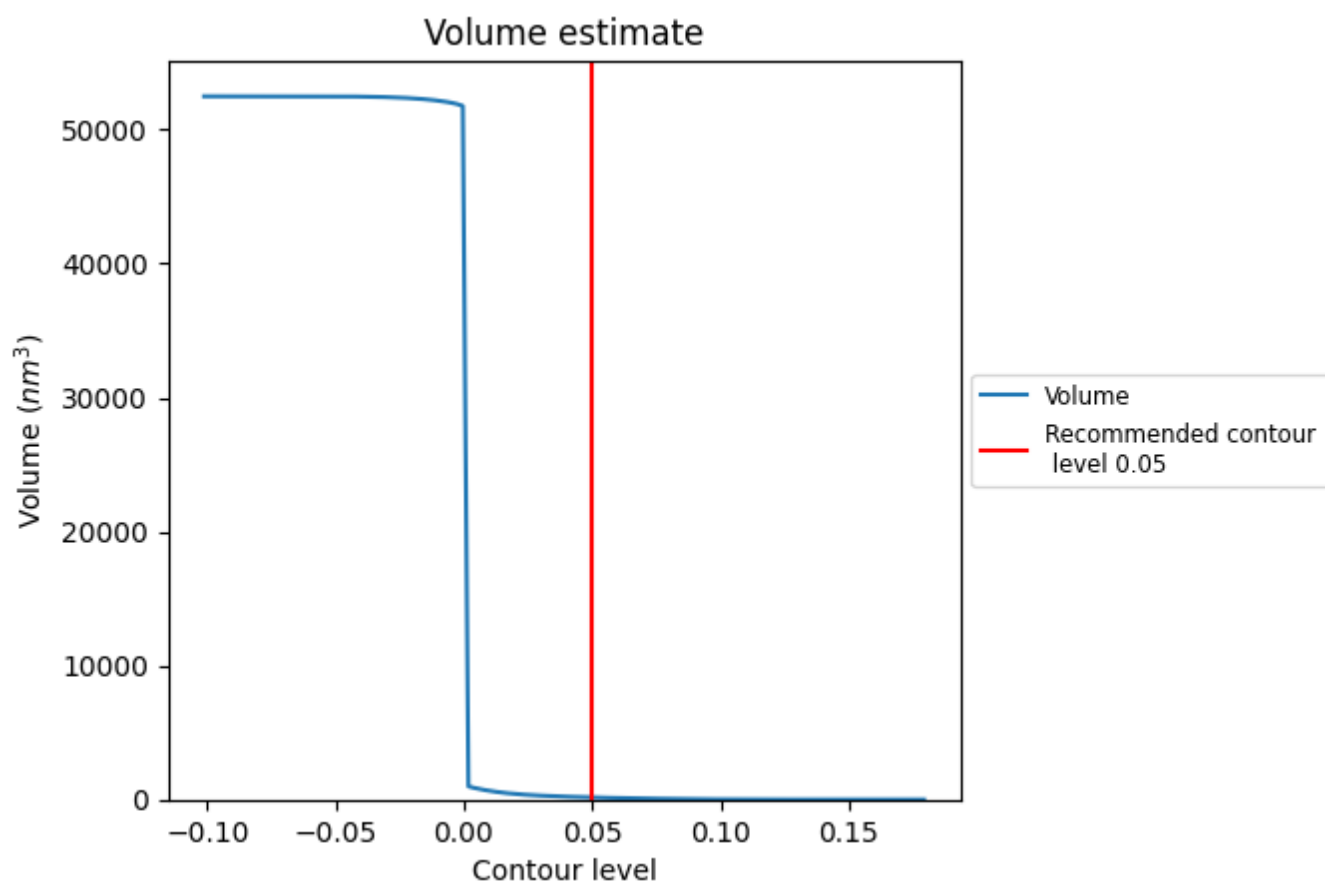
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

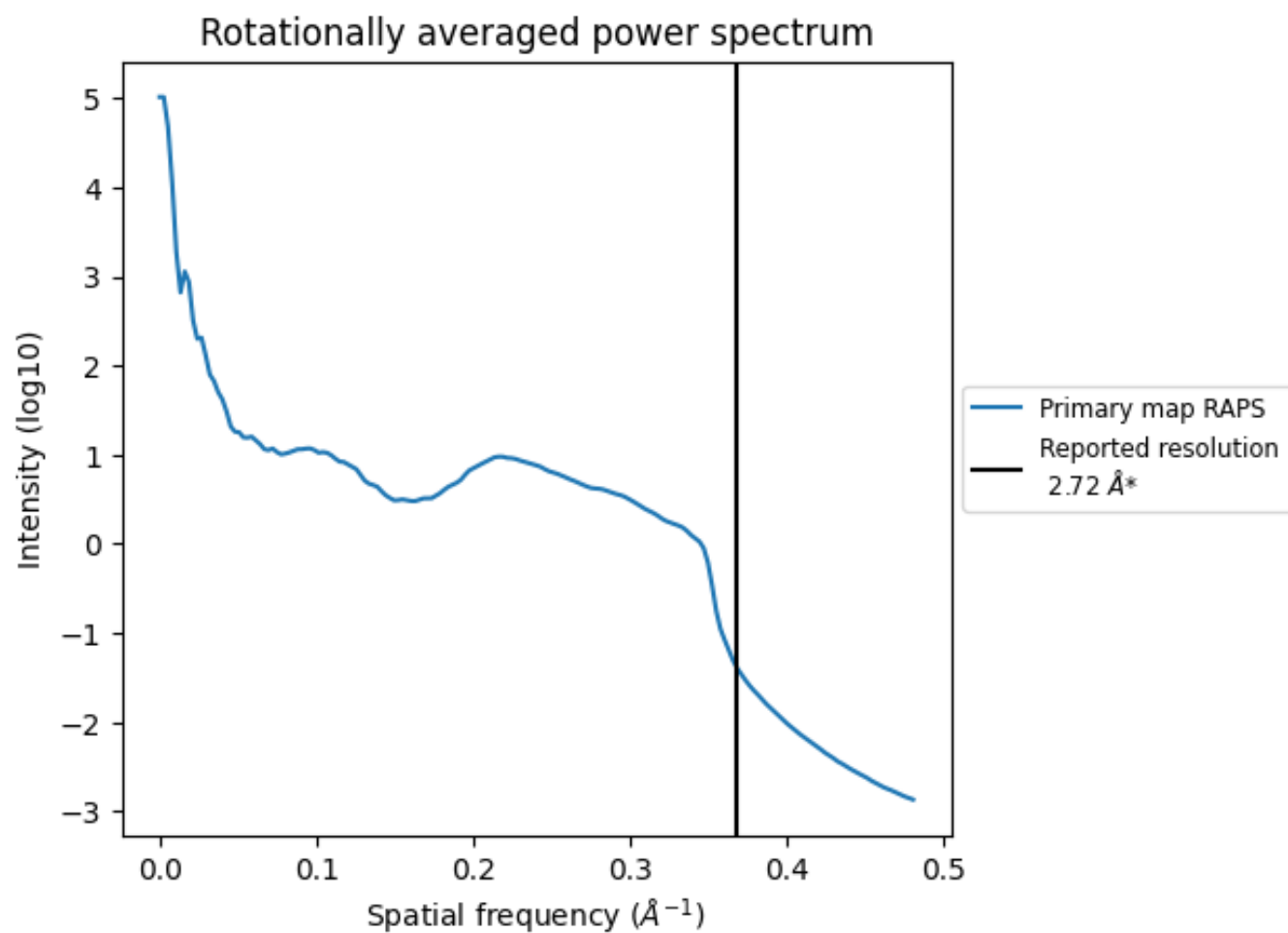
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm³; this corresponds to an approximate mass of 144 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 ⓘ

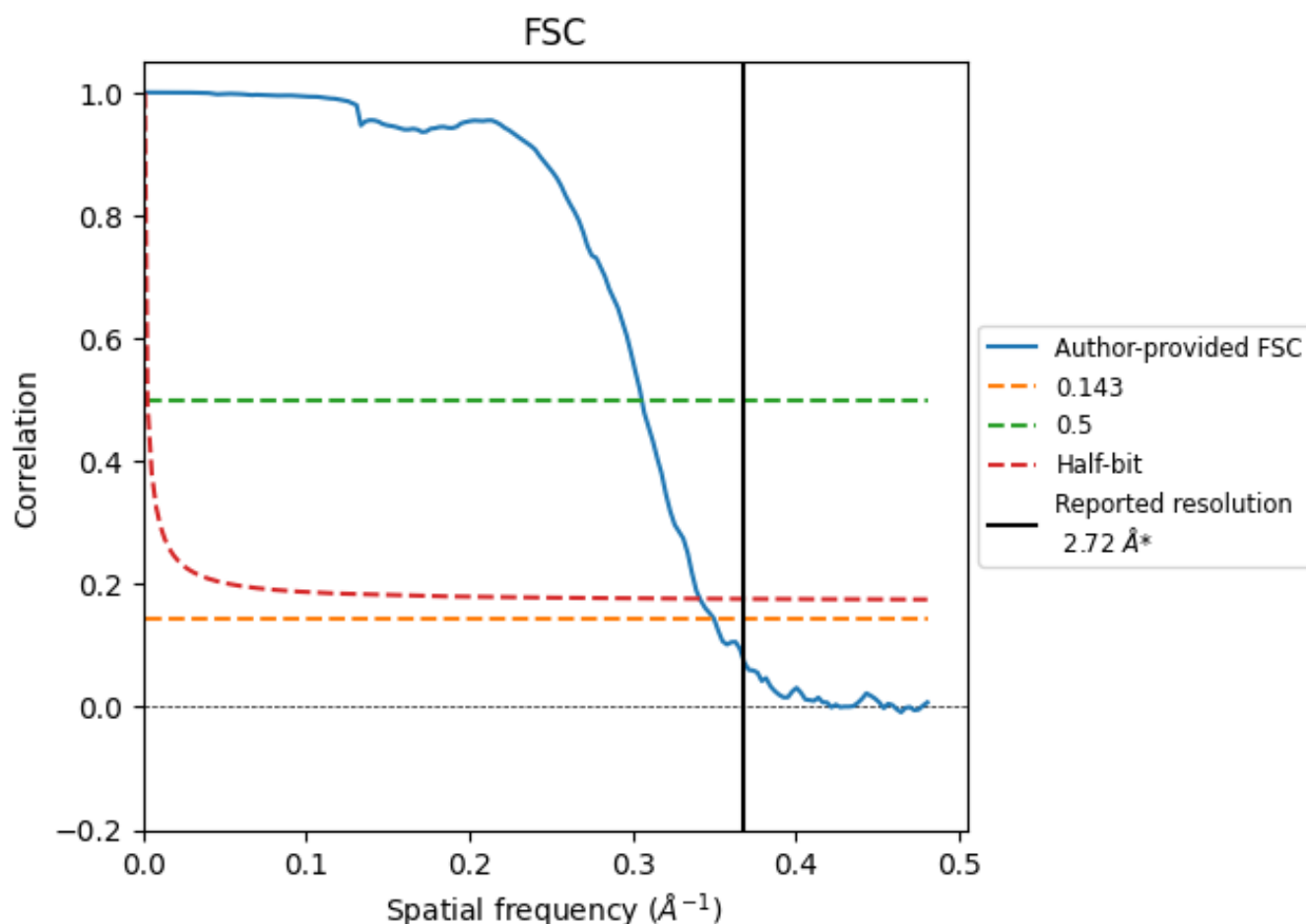


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

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 0.368 Å⁻¹

8.2 Resolution estimates [i](#)

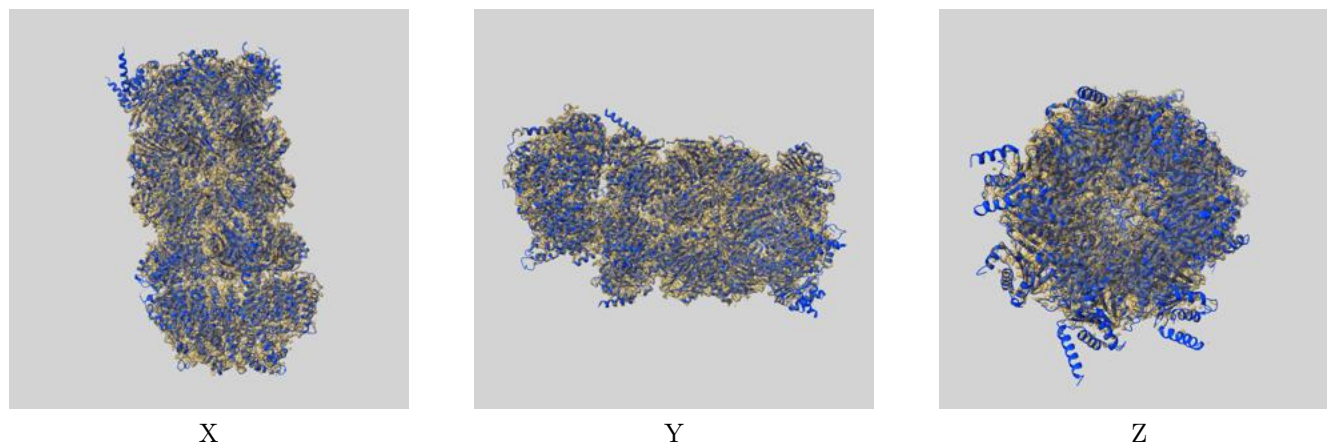
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.86	3.27	2.93
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

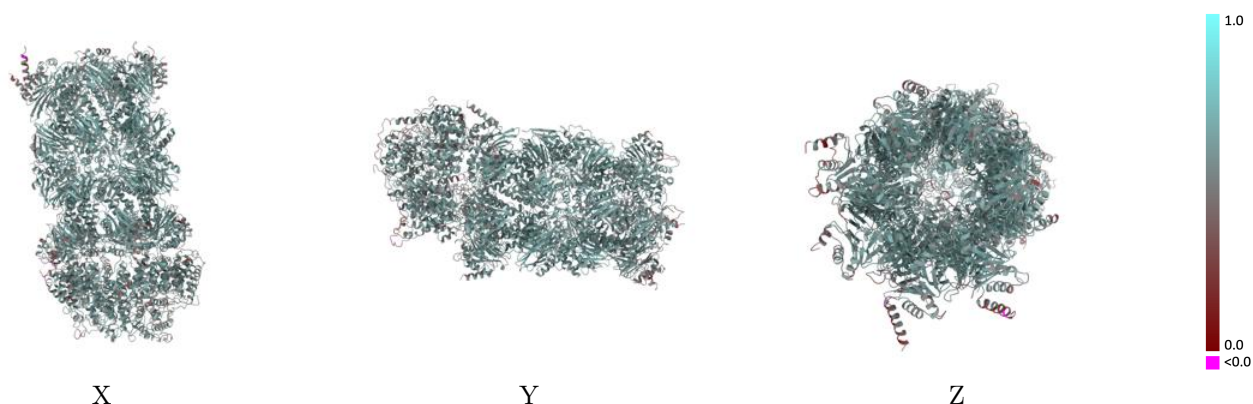
This section contains information regarding the fit between EMDB map EMD-0781 and PDB model 6KWY. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.05 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](#)

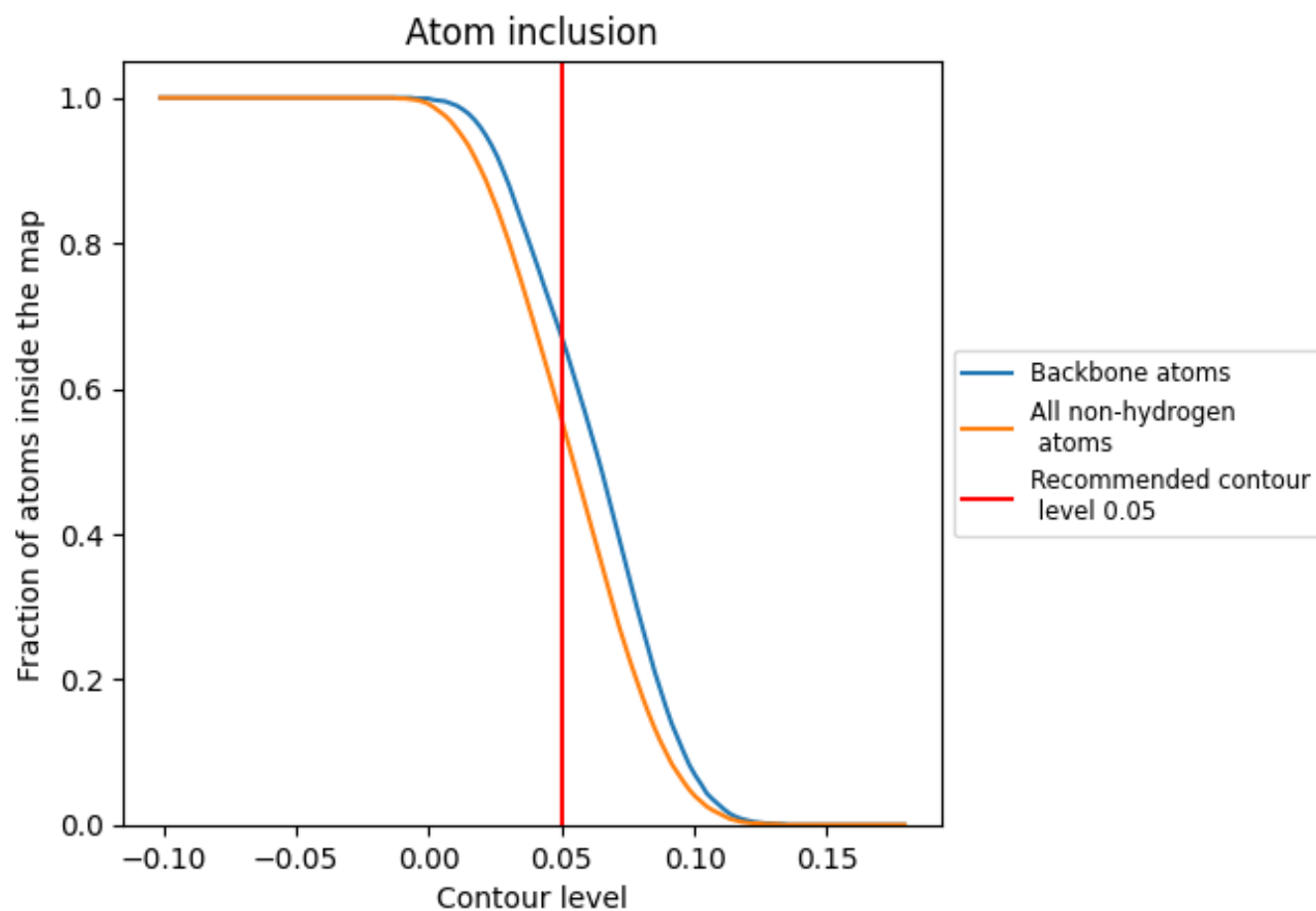


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 56% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5570	 0.5760
A	 0.6300	 0.5930
B	 0.5170	 0.5580
C	 0.5130	 0.5580
D	 0.5360	 0.5700
E	 0.6560	 0.5960
F	 0.5950	 0.5860
G	 0.5860	 0.5790
H	 0.6530	 0.6070
I	 0.6750	 0.6190
J	 0.6810	 0.6120
K	 0.6970	 0.6150
L	 0.6160	 0.5970
M	 0.6840	 0.6110
N	 0.7030	 0.6210
O	 0.4510	 0.5560
P	 0.3660	 0.5440
Q	 0.3640	 0.5450
R	 0.4600	 0.5740
S	 0.4930	 0.5700
T	 0.5090	 0.5630
U	 0.3960	 0.5460
V	 0.5760	 0.5770
W	 0.6500	 0.6110
X	 0.6730	 0.6090
Y	 0.6800	 0.6150
Z	 0.6350	 0.6100
a	 0.6790	 0.6120
b	 0.6680	 0.6120
c	 0.4890	 0.5400

