wwPDB EM Validation Summary Report

Mar 20, 2024 – 03:16 AM JST

PDB ID	:	6KWY
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:

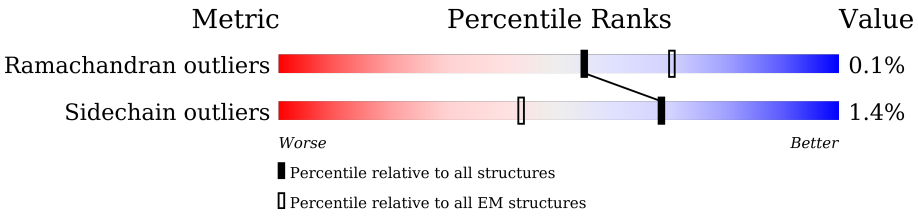
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

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

The reported resolution of this entry is 2.72 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)
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 <=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	15% 90% · 8%
1	O	234	37% 97% · ·
2	B	261	28% 79% · 19%
2	P	261	52% 94% · 5%
3	C	248	28% 83% · 15%
3	Q	248	50% 94% 6%
4	D	241	28% 94% 6%
4	R	241	40% 96% · ·
5	E	263	14% 89% · 9%

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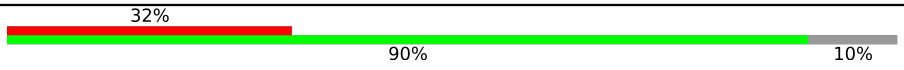
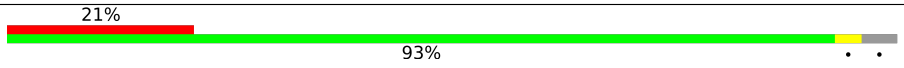
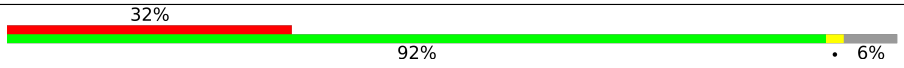
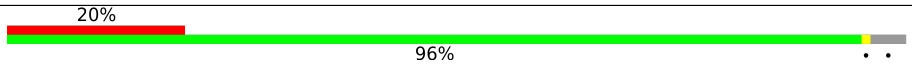
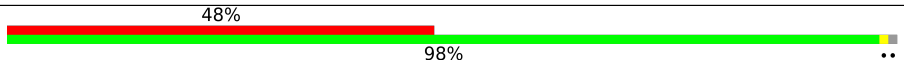
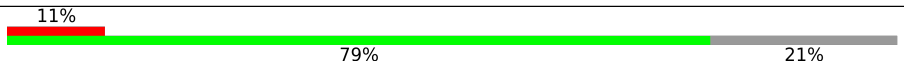
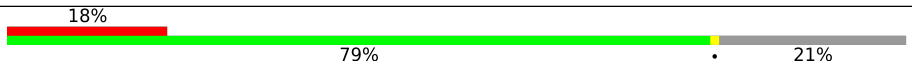
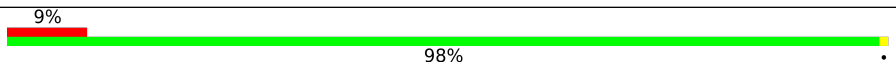
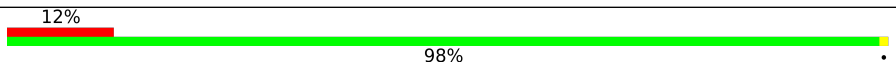
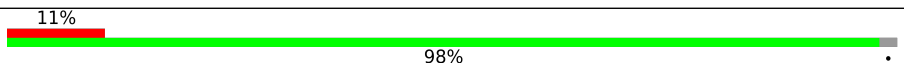
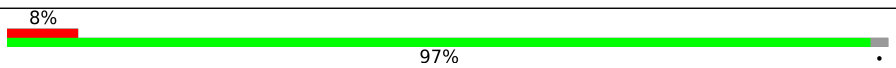
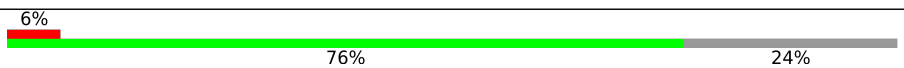
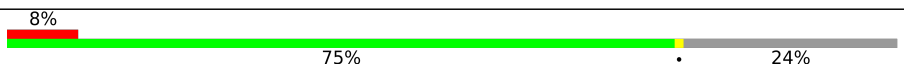
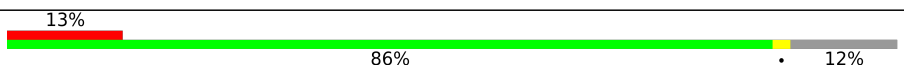
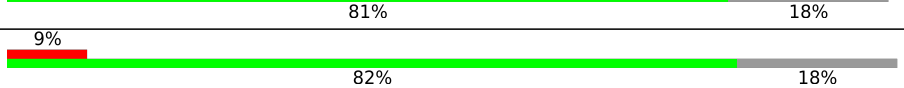
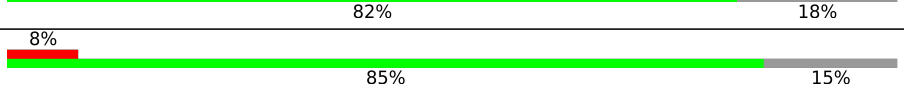
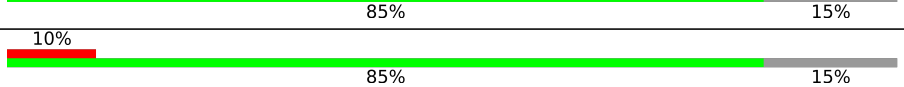
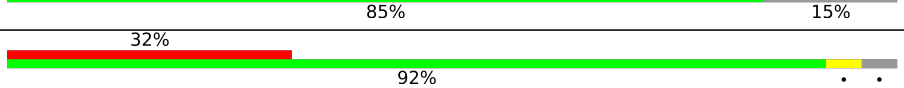
Mol	Chain	Length	Quality of chain
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	277	
8	V	277	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	263	
11	Y	263	
12	L	241	
12	Z	241	
13	M	264	
13	a	264	
14	N	239	
14	b	239	
15	c	1878	

2 Entry composition (i)

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 1574	C 1008	N 267	O 289	S 10	1	0

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

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

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

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

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

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

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

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

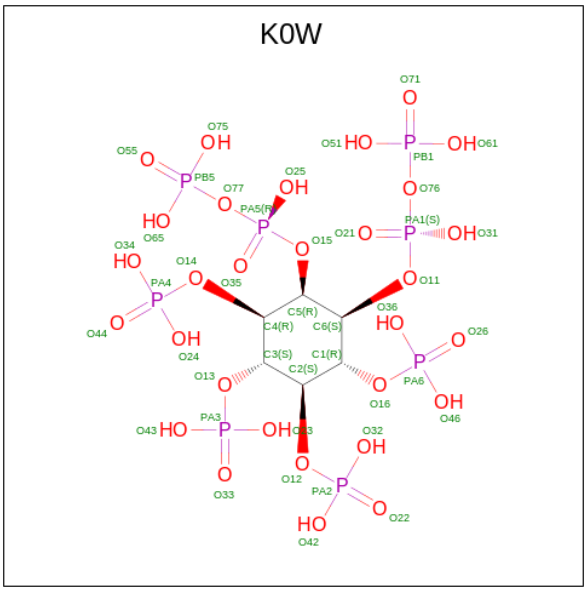
- Molecule 15 is a protein called Proteasome activator complex subunit 4.

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

There are 37 discrepancies between the modelled and reference sequences:

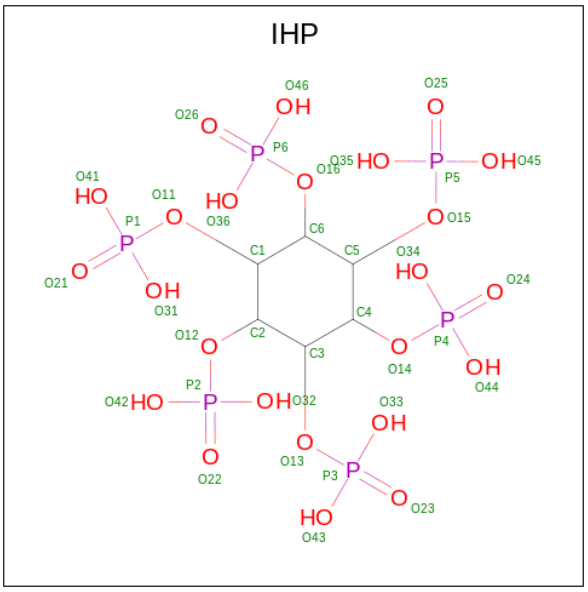
Chain	Residue	Modelled	Actual	Comment	Reference
c	-34	MET	-	initiating methionine	UNP Q14997
c	-33	GLY	-	expression tag	UNP Q14997
c	-32	THR	-	expression tag	UNP Q14997
c	-31	THR	-	expression tag	UNP Q14997
c	-30	ARG	-	expression tag	UNP Q14997
c	-29	SER	-	expression tag	UNP Q14997
c	-28	THR	-	expression 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-tetraphosphonooxy-cyclohexyl] phosphono hydrogen phosphate (three-letter code: K0W) (formula: $C_6H_{20}O_{30}P_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	c	1	44	6	30	8	0

- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).

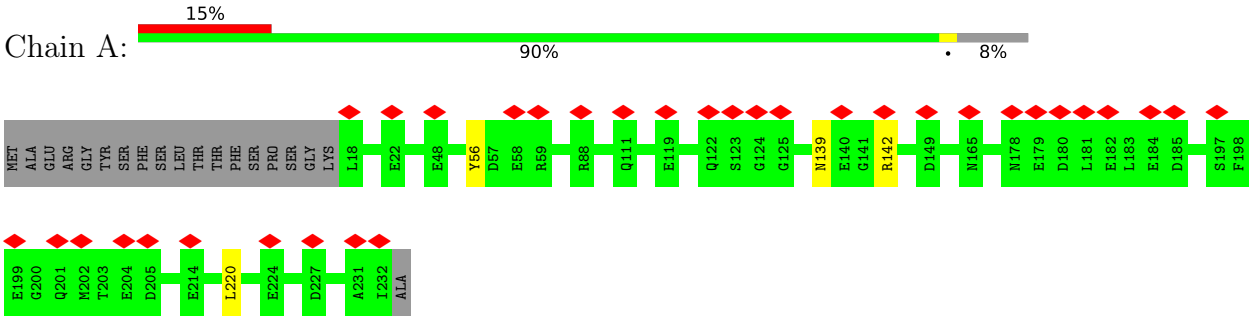


Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	O	P	
17	c	1	42	6	6	24	6	0

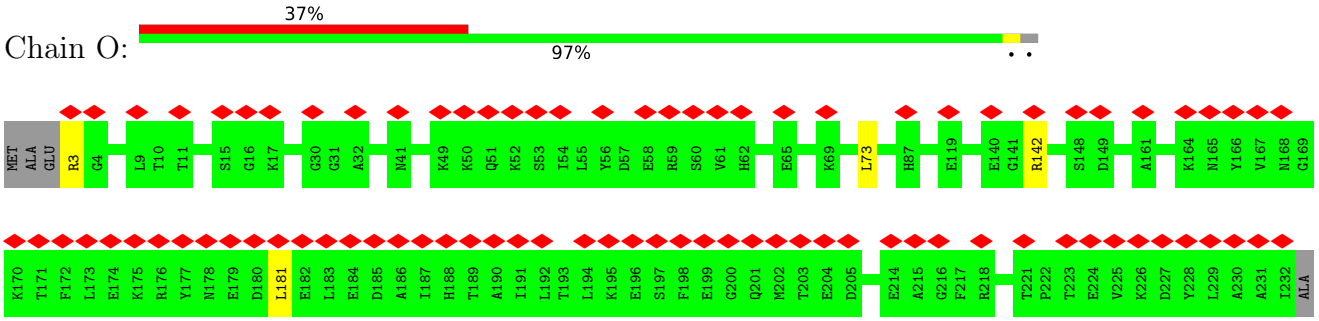
3 Residue-property plots (i)

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.

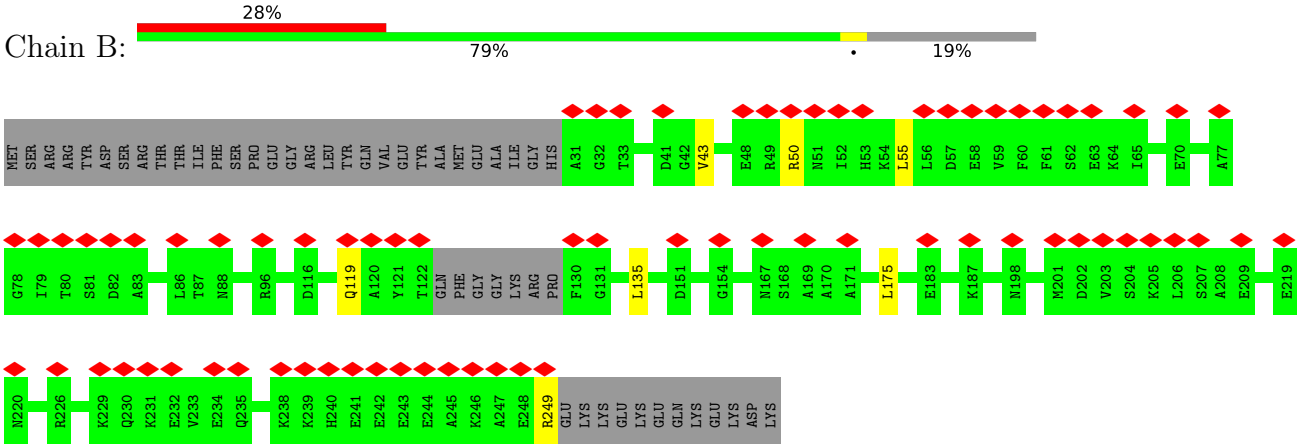
• Molecule 1: Proteasome subunit alpha type-2



• Molecule 1: Proteasome subunit alpha type-2

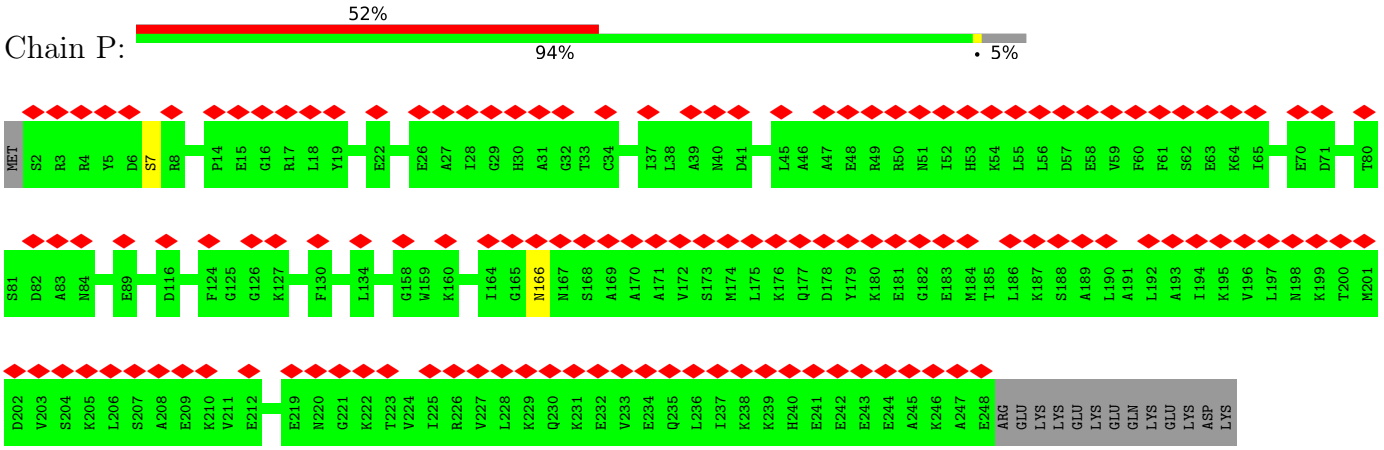


• Molecule 2: Proteasome subunit alpha type-4



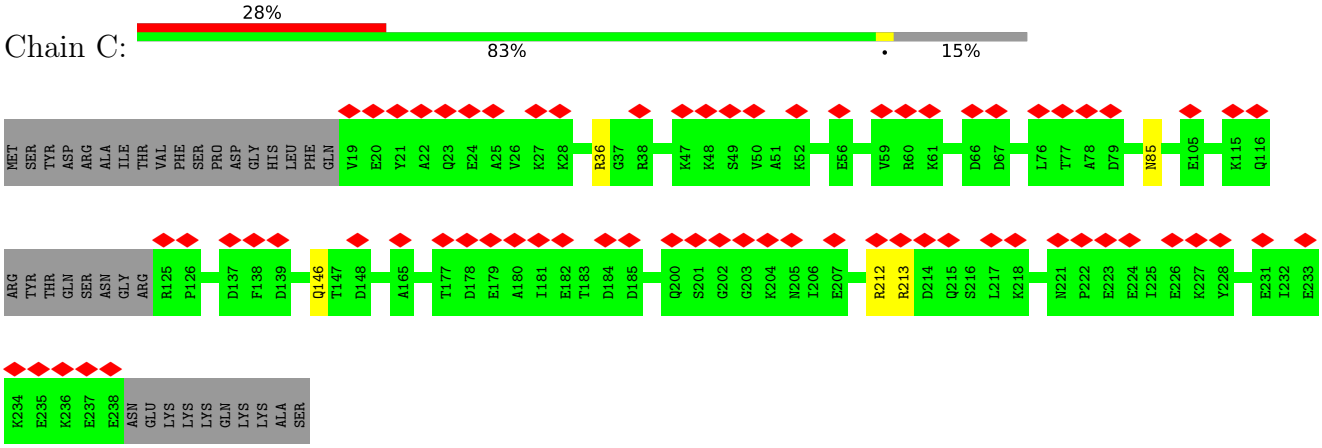
• Molecule 2: Proteasome subunit alpha type-4

Chain P:



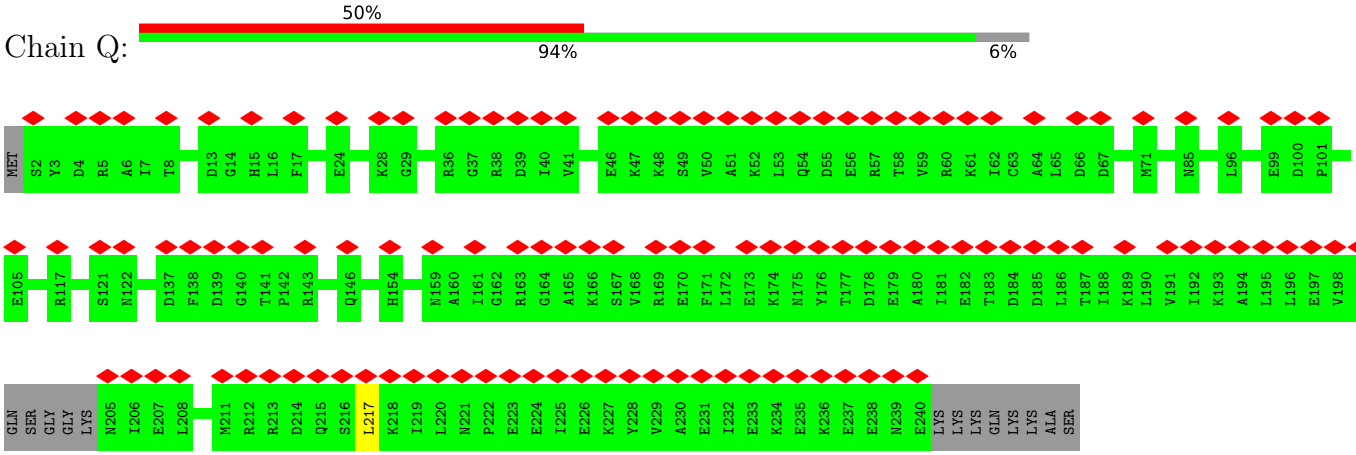
• Molecule 3: Proteasome subunit alpha type-7

Chain C:



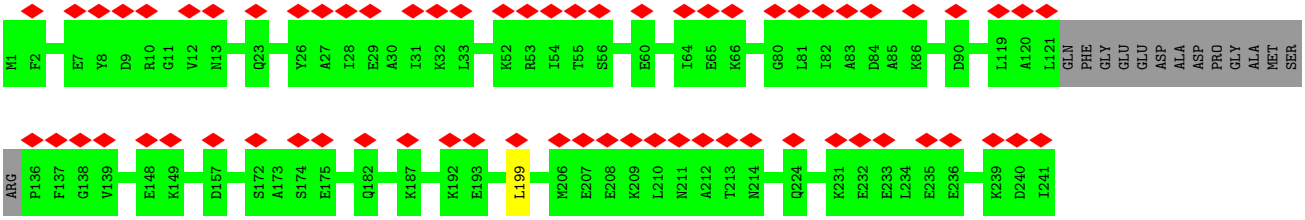
• Molecule 3: Proteasome subunit alpha type-7

Chain Q:



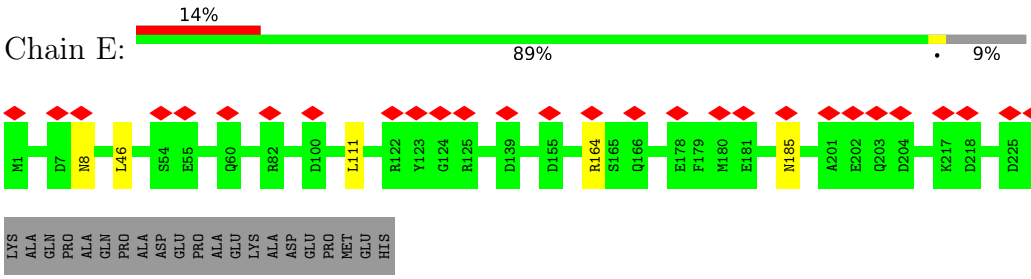
• Molecule 4: Proteasome subunit alpha type-5

Chain D:

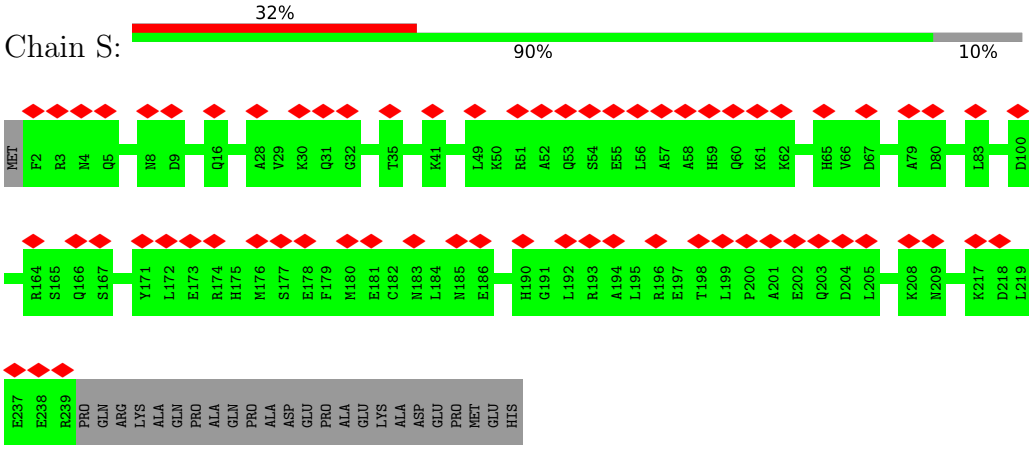


• Molecule 4: Proteasome subunit alpha type-5

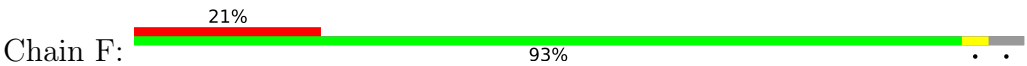
• Molecule 5: Proteasome subunit alpha type-1

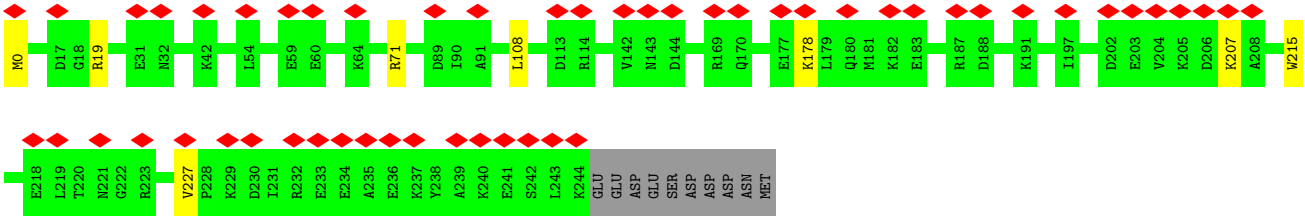


• Molecule 5: Proteasome subunit alpha type-1

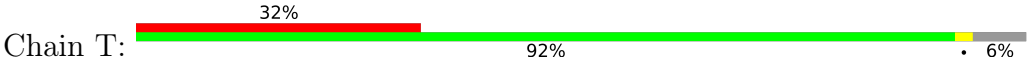


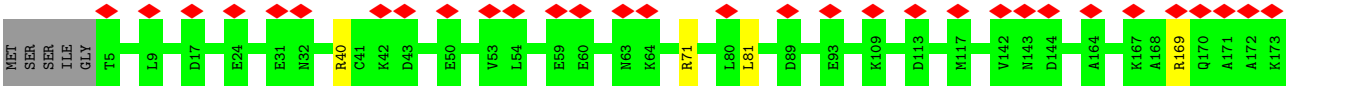
• Molecule 6: Proteasome subunit alpha type-3



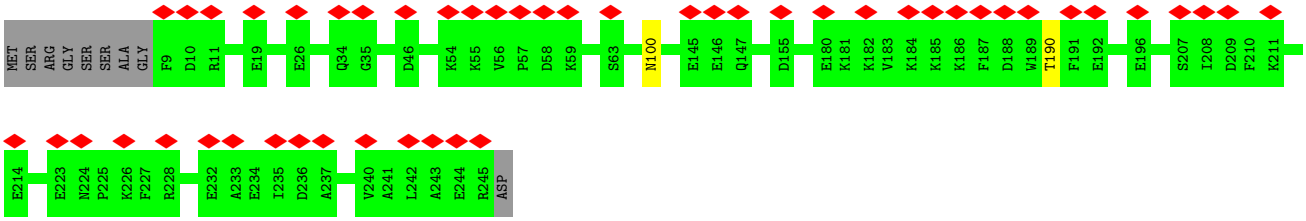


• Molecule 6: Proteasome subunit alpha type-3

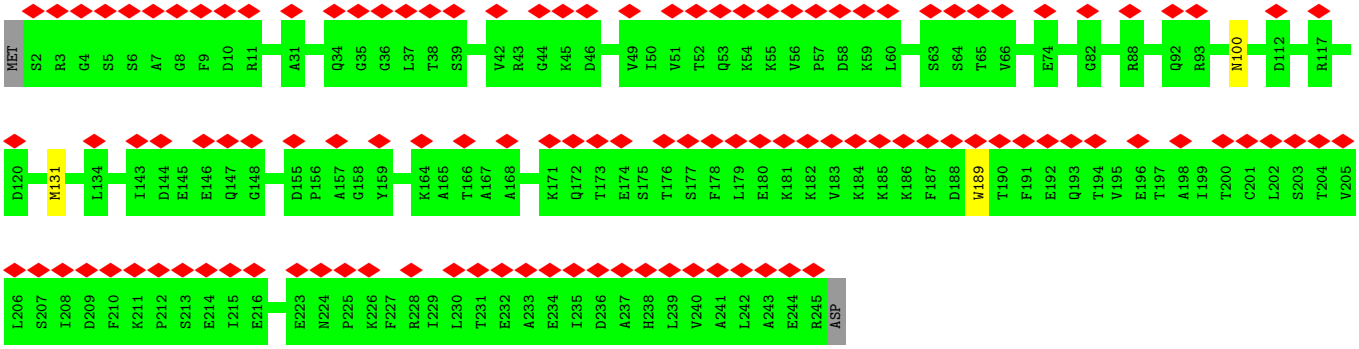




• Molecule 7: Proteasome subunit alpha type-6

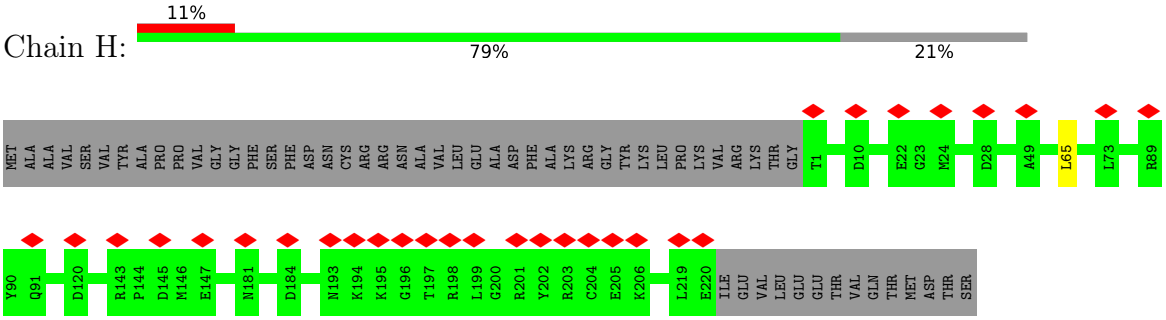


• Molecule 7: Proteasome subunit alpha type-6



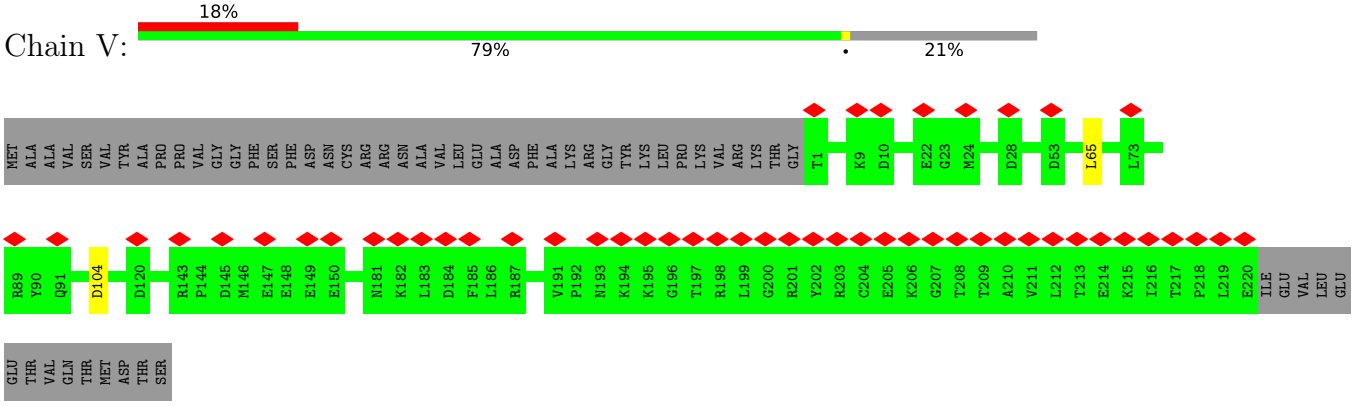
• Molecule 8: Proteasome subunit beta type-7

Chain H:



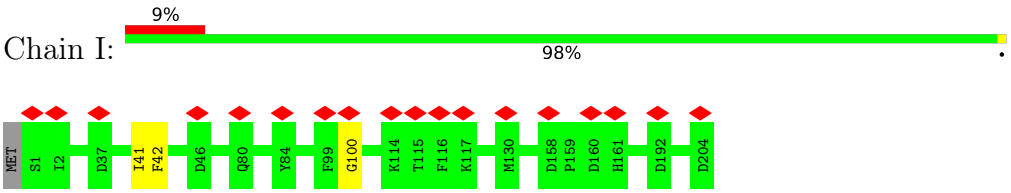
• Molecule 8: Proteasome subunit beta type-7

Chain V:



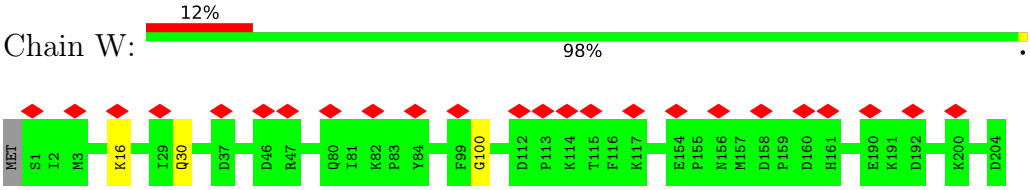
• Molecule 9: Proteasome subunit beta type-3

Chain I:



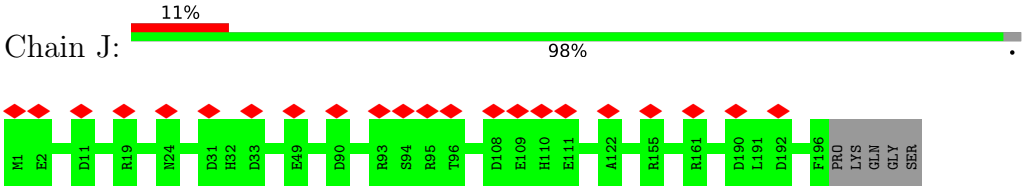
• Molecule 9: Proteasome subunit beta type-3

Chain W:



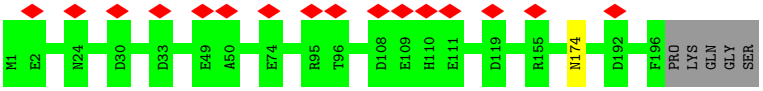
• Molecule 10: Proteasome subunit beta type-2

Chain J:

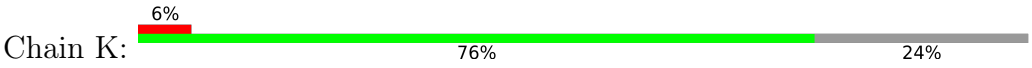


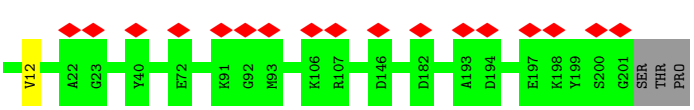
• Molecule 10: Proteasome subunit beta type-2

Chain X:

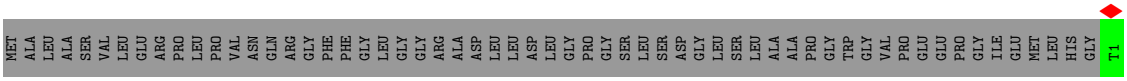


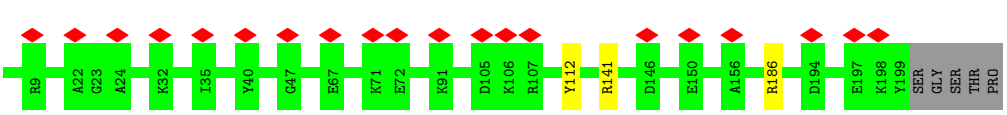
• Molecule 11: Proteasome subunit beta type-5



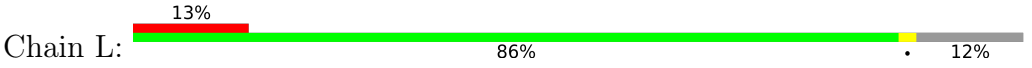


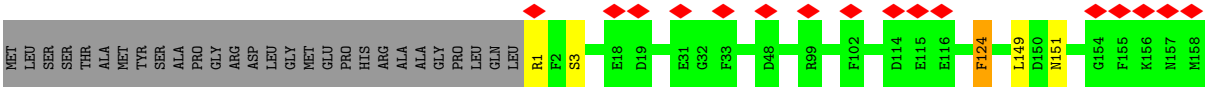
• Molecule 11: Proteasome subunit beta type-5

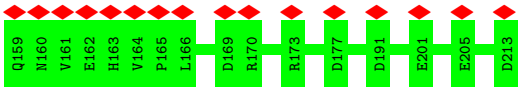




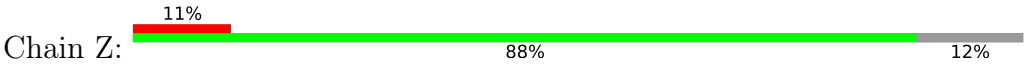
• Molecule 12: Proteasome subunit beta type-1

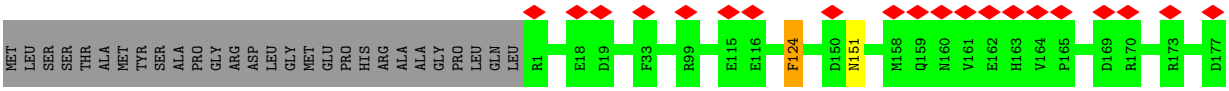


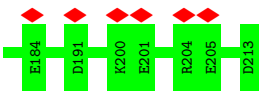




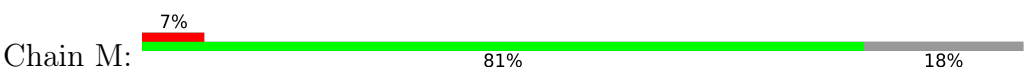
• Molecule 12: Proteasome subunit beta type-1

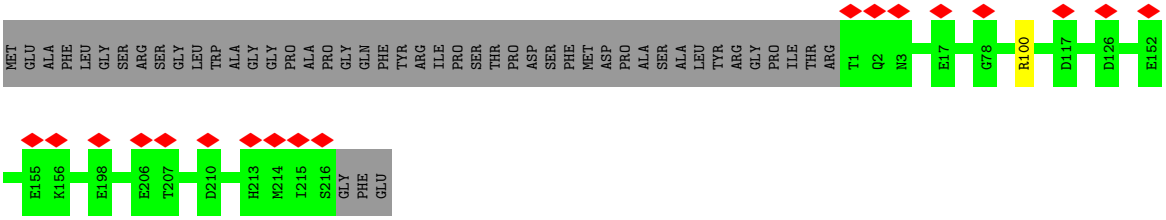






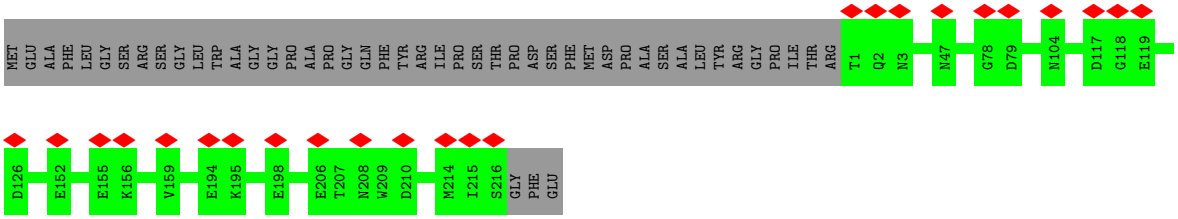
• Molecule 13: Proteasome subunit beta type-4





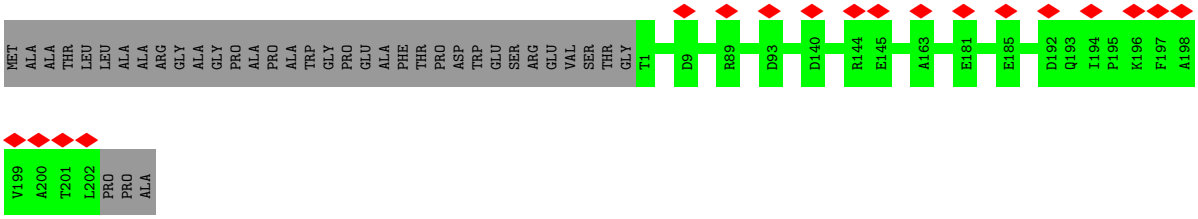
• Molecule 13: Proteasome subunit beta type-4

Chain a:



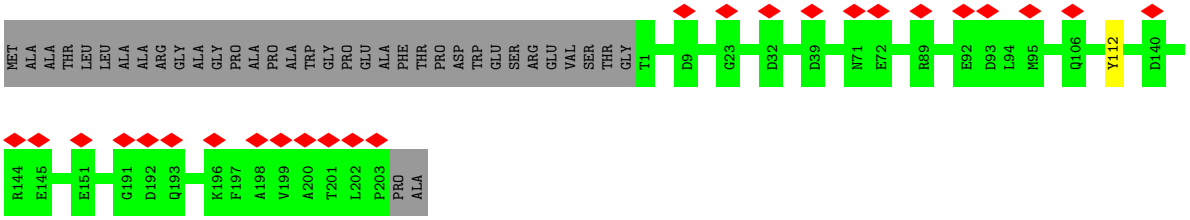
• Molecule 14: Proteasome subunit beta type-6

Chain N:



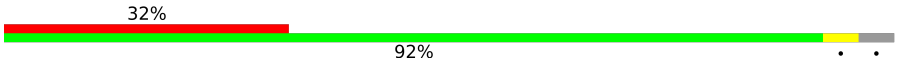
• Molecule 14: Proteasome subunit beta type-6

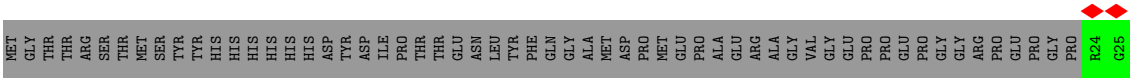
Chain b:

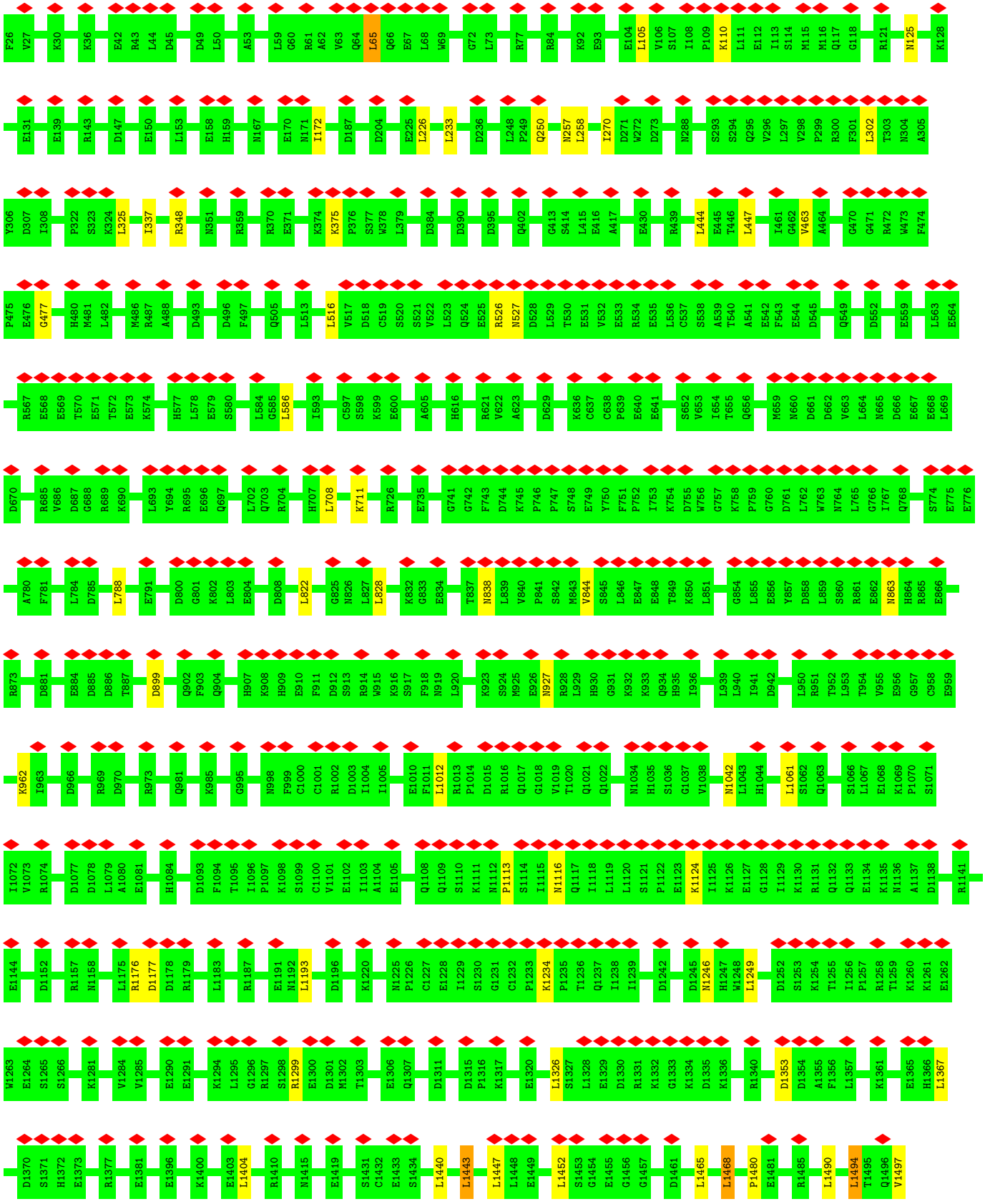


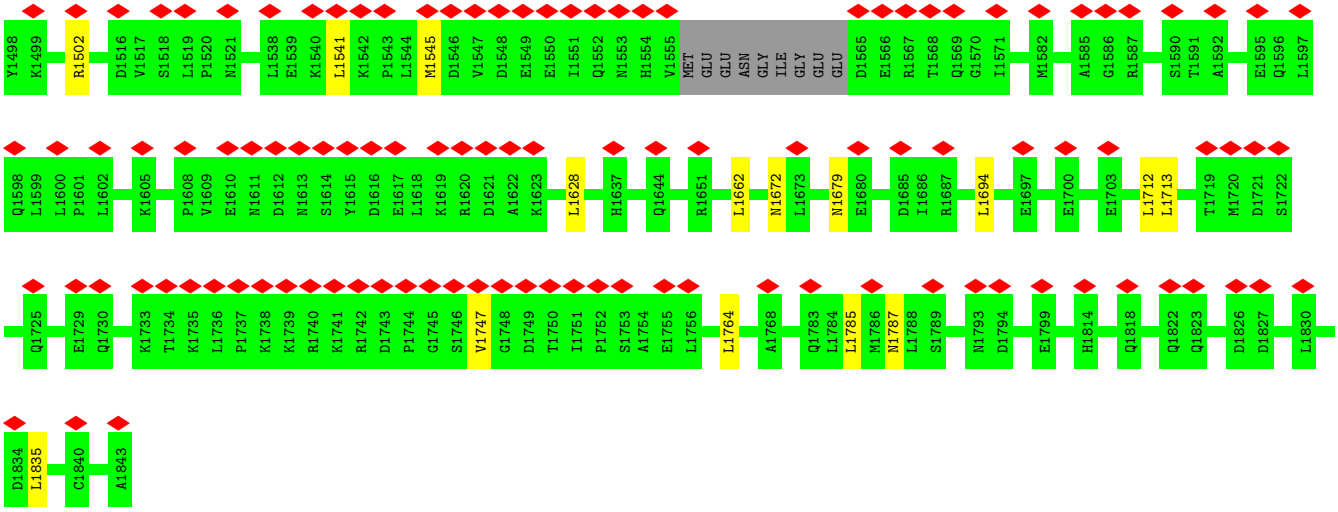
• Molecule 15: Proteasome activator complex subunit 4

Chain c:






P26 V27 K30 K36 E42 R43 L44 D45 D49 L50 A53 L59 G60 R61 A62 V63 Q64 L65 Q66 E67 L68 W69 G72 L73 R77 R84 K92 E93 E104 L105 V106 S107 I108 P109 K110 L111 E112 I113 S114 M115 M116 Q117 G118 R121 N125 K128
E131 E139 R143 D147 E150 L153 E158 H159 N167 E170 N171 I172 D187 D204 E225 L226 L233 D236 L248 P249 Q250 N257 L258 I270 D271 W272 D273 N288 S293 S294 Q295 V296 L297 V298 P299 R300 F301 L302 T303 N304 A305
Y306 D307 I308 P322 S323 K324 L325 I337 R348 N351 R359 R370 E371 K374 K375 P376 S377 W378 L379 D384 D390 D395 Q402 G413 S414 L415 E416 A417 E430 R439 L444 E445 T446 L447 I461 G462 V463 A464 G470 G471 R472 W473 F474
P475 E476 G477 H480 M481 L482 M486 R487 A488 D493 D496 F497 Q505 L513 L516 V517 D518 C519 S520 S521 V522 L523 Q524 E525 R526 N527 D528 L529 T530 E531 V532 E533 R534 E535 L536 C537 S538 A539 T540 A541 E542 F543 E544 D545 Q549 D552 E559 L563 E564
R567 E568 E569 T570 E571 T572 E573 K574 H577 L578 E579 S580 L584 G585 L586 I593 C597 S598 K599 E600 A605 H616 R621 V622 A623 D629 K636 C637 C638 P639 E640 E641 S652 V653 I654 T655 Q656 M659 N660 D661 D662 V663 L664 N665 D666 E667 E668 L669
D670 R685 V686 D687 G688 R689 K690 L693 Y694 R695 E696 Q697 L702 Q703 R704 H707 L708 K711 R726 E735 G741 G742 F743 D744 K745 P746 P747 S748 E749 Y750 F751 P752 I753 K754 D755 W756 G757 K758 P759 G760 D761 L762 W763 N764 L765 G766 I767 Q768 S774 E775 E776
A780 F781 L784 D785 L788 E791 D800 G801 K802 L803 E804 D808 L822 G825 N826 L827 L828 K832 G833 E834 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
R873 D881 E884 D885 D886 T887 D899 Q902 F903 Q904 H907 K908 H909 E910 F911 D912 S913 R914 W915 K916 S917 F918 N919 L920 K923 S924 M925 E926 N927 R928 L929 H930 G931 K932 K933 Q934 H935 I936 L939 L940 I941 D942 L950 R951 T952 L953 T954 V955 E956 G957 C958 E959
K962 I963 D966 R969 D970 R973 Q981 K985 G995 N998 F999 C1000 C1001 R1002 D1003 I1004 I1005 E1010 F1011 L1012 R1013 P1014 D1015 R1016 Q1017 G1018 V1019 T1020 Q1021 Q1022 N1034 H1035 S1036 G1037 V1038 N1042 L1043 H1044 L1061 S1062 Q1063 S1066 L1067 E1068 K1069 P1070 S1071
I1072 V1073 R1074 D1077 D1078 L1079 A1080 E1081 H1084 D1093 F1094 T1095 I1096 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
E1144 D1152 R1157 N1158 L1175 R1176 D1177 D1178 R1179 L1183 R1187 E1191 N1192 L1193 D1196 K1220 N1225 P1226 C1227 E1228 I1229 S1230 G1231 C1232 P1233 K1234 P1235 T1236 Q1237 I1238 I1239 D1242 D1245 N1246 H1247 W1248 L1249 D1252 S1253 K1254 T1255 I1256 P1257 R1258 T1259 K1260 K1261 E1262
W1263 E1264 S1265 S1266 K1281 V1284 V1285 E1290 E1291 K1294 L1295 G1296 R1297 S1298 R1299 E1300 D1301 M1302 T1303 E1306 Q1307 D1311 D1315 P1316 K1317 E1320 L1326 S1327 L1328 E1329 D1330 R1331 K1332 G1333 K1334 D1335 K1336 R1340 D1353 D1354 A1355 F1356 L1357 K1361 E1365 H1366 L1367
D1370 S1371 H1372 E1373 R1377 E1381 E1396 K1400 E1403 L1404 R1410 N1415 E1419 S1431 C1432 E1433 S1434 L1440 L1443 L1447 L1448 E1449 L1452 S1453 G1454 E1455 G1456 G1457 D1461 L1465 L1468 P1480 E1481 R1485 L1490 L1494 T1495 Q1496 V1497


Y1498 K1499 R1502 D1516 V1517 S1518 L1519 P1520 N1521 L1538 E1539 K1540 L1541 K1542 P1543 L1544 M1545 D1546 V1547 D1548 E1549 E1550 I1551 Q1552 N1553 H1554 V1555 MET GLU GLU ASN GLY ILE GLY GLU GLU D1565 E1566 R1567 T1568 Q1569 G1570 I1571 M1582 A1585 G1586 R1587 S1590 T1591 A1592 E1595 Q1596 L1597
Q1598 L1599 L1600 P1601 L1602 K1605 P1608 V1609 E1610 N1611 D1612 N1613 S1614 Y1615 D1616 E1617 L1618 K1619 R1620 D1621 A1622 K1623 L1628 H1637 Q1644 R1651 L1662 N1672 L1673 N1679 E1680 D1685 I1686 R1687 L1694 E1697 E1700 E1703 L1712 L1713 T1719 M1720 D1721 S1722
Q1725 E1729 Q1730 K1733 T1734 K1735 L1736 P1737 K1738 K1739 R1740 K1741 R1742 D1743 P1744 G1745 S1746 V1747 G1748 D1749 T1750 I1751 P1752 S1753 A1754 E1755 L1756 L1764 A1768 Q1783 L1784 L1785 M1786 N1787 L1788 S1789 N1793 D1794 E1799 H1814 Q1818 Q1822 Q1823 D1826 D1827 L1830
D1834 L1835 C1840 A1843

4 Experimental information (i)

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 ($e^-/Å^2$)	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 (Å)	374.4, 374.4, 374.4	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: IHP, K0W

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	0.55	0/1706	0.67	0/2314
1	O	0.46	0/1818	0.60	2/2467 (0.1%)
2	B	0.49	0/1666	0.69	0/2248
2	P	0.44	0/1955	0.61	0/2642
3	C	0.46	0/1660	0.69	0/2240
3	Q	0.40	0/1842	0.58	0/2496
4	D	0.49	0/1767	0.67	0/2386
4	R	0.42	0/1795	0.58	1/2424 (0.0%)
5	E	0.52	0/1917	0.69	0/2592
5	S	0.43	0/1915	0.60	0/2589
6	F	0.50	0/1944	0.70	0/2617
6	T	0.47	0/1905	0.65	2/2567 (0.1%)
7	G	0.53	0/1897	0.68	0/2566
7	U	0.43	0/1919	0.61	1/2596 (0.0%)
8	H	0.49	0/1705	0.67	1/2307 (0.0%)
8	V	0.47	0/1688	0.65	1/2288 (0.0%)
9	I	0.51	0/1668	0.70	4/2247 (0.2%)
9	W	0.49	0/1636	0.69	3/2205 (0.1%)
10	J	0.49	0/1593	0.61	0/2156
10	X	0.49	0/1609	0.61	0/2176
11	K	0.53	0/1574	0.66	0/2128
11	Y	0.53	0/1604	0.68	0/2165
12	L	0.50	0/1692	0.71	3/2281 (0.1%)
12	Z	0.51	0/1677	0.69	2/2260 (0.1%)
13	M	0.52	0/1720	0.63	0/2328
13	a	0.54	0/1724	0.66	0/2334
14	N	0.49	0/1544	0.61	0/2090
14	b	0.50	0/1556	0.64	0/2107
15	c	0.47	0/14985	0.79	39/20326 (0.2%)
All	All	0.48	0/63681	0.69	59/86142 (0.1%)

There are no bond length outliers.

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	c	1353	ASP	CB-CG-OD1	10.30	127.57	118.30
15	c	516	LEU	CA-CB-CG	8.78	135.49	115.30
15	c	1177	ASP	CB-CG-OD1	8.73	126.15	118.30
15	c	1468	LEU	CA-CB-CG	8.20	134.15	115.30
15	c	302	LEU	CA-CB-CG	8.04	133.79	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	213/234 (91%)	203 (95%)	10 (5%)	0	100	100
1	O	228/234 (97%)	219 (96%)	9 (4%)	0	100	100
2	B	208/261 (80%)	198 (95%)	10 (5%)	0	100	100
2	P	247/261 (95%)	238 (96%)	9 (4%)	0	100	100
3	C	208/248 (84%)	189 (91%)	19 (9%)	0	100	100
3	Q	230/248 (93%)	220 (96%)	9 (4%)	1 (0%)	34	58
4	D	223/241 (92%)	207 (93%)	16 (7%)	0	100	100
4	R	231/241 (96%)	219 (95%)	11 (5%)	1 (0%)	34	58
5	E	238/263 (90%)	223 (94%)	15 (6%)	0	100	100
5	S	239/263 (91%)	232 (97%)	7 (3%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
6	F	243/255 (95%)	229 (94%)	13 (5%)	1 (0%)	34 58
6	T	239/255 (94%)	232 (97%)	7 (3%)	0	100 100
7	G	236/246 (96%)	227 (96%)	9 (4%)	0	100 100
7	U	242/246 (98%)	237 (98%)	5 (2%)	0	100 100
8	H	220/277 (79%)	213 (97%)	7 (3%)	0	100 100
8	V	220/277 (79%)	209 (95%)	11 (5%)	0	100 100
9	I	208/205 (102%)	199 (96%)	9 (4%)	0	100 100
9	W	204/205 (100%)	194 (95%)	9 (4%)	1 (0%)	29 53
10	J	194/201 (96%)	185 (95%)	9 (5%)	0	100 100
10	X	195/201 (97%)	186 (95%)	9 (5%)	0	100 100
11	K	199/263 (76%)	192 (96%)	7 (4%)	0	100 100
11	Y	200/263 (76%)	192 (96%)	8 (4%)	0	100 100
12	L	213/241 (88%)	208 (98%)	5 (2%)	0	100 100
12	Z	212/241 (88%)	206 (97%)	6 (3%)	0	100 100
13	M	214/264 (81%)	202 (94%)	12 (6%)	0	100 100
13	a	215/264 (81%)	203 (94%)	12 (6%)	0	100 100
14	N	201/239 (84%)	197 (98%)	4 (2%)	0	100 100
14	b	202/239 (84%)	195 (96%)	7 (4%)	0	100 100
15	c	1807/1878 (96%)	1634 (90%)	167 (9%)	6 (0%)	41 65
All	All	7929/8754 (91%)	7488 (94%)	431 (5%)	10 (0%)	54 77

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	R	130	PRO
9	W	30	GLN
15	c	325	LEU
15	c	477	GLY
15	c	962	LYS

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	173/191 (91%)	169 (98%)	4 (2%)	50	77
1	O	184/191 (96%)	182 (99%)	2 (1%)	73	89
2	B	175/221 (79%)	168 (96%)	7 (4%)	31	58
2	P	201/221 (91%)	198 (98%)	3 (2%)	65	85
3	C	173/211 (82%)	168 (97%)	5 (3%)	42	70
3	Q	190/211 (90%)	190 (100%)	0	100	100
4	D	192/203 (95%)	191 (100%)	1 (0%)	88	95
4	R	192/203 (95%)	192 (100%)	0	100	100
5	E	202/224 (90%)	197 (98%)	5 (2%)	47	75
5	S	202/224 (90%)	201 (100%)	1 (0%)	88	95
6	F	201/212 (95%)	194 (96%)	7 (4%)	36	63
6	T	194/212 (92%)	191 (98%)	3 (2%)	65	85
7	G	204/210 (97%)	202 (99%)	2 (1%)	76	90
7	U	204/210 (97%)	202 (99%)	2 (1%)	76	90
8	H	183/228 (80%)	183 (100%)	0	100	100
8	V	180/228 (79%)	178 (99%)	2 (1%)	73	89
9	I	178/174 (102%)	178 (100%)	0	100	100
9	W	174/174 (100%)	174 (100%)	0	100	100
10	J	165/171 (96%)	165 (100%)	0	100	100
10	X	168/171 (98%)	167 (99%)	1 (1%)	86	94
11	K	153/202 (76%)	152 (99%)	1 (1%)	84	93
11	Y	157/202 (78%)	152 (97%)	5 (3%)	39	67
12	L	179/199 (90%)	174 (97%)	5 (3%)	43	71
12	Z	176/199 (88%)	174 (99%)	2 (1%)	73	89
13	M	179/215 (83%)	178 (99%)	1 (1%)	86	94
13	a	179/215 (83%)	179 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	b	159/181 (88%)	158 (99%)	1 (1%)	86	94
15	c	1650/1705 (97%)	1610 (98%)	40 (2%)	49	76
All	All	6724/7389 (91%)	6624 (98%)	100 (2%)	68	85

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	Z	124	PHE
15	c	527	ASN
15	c	1835	LEU
14	b	112	TYR
15	c	250	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
15	c	250	GLN
15	c	907	HIS
15	c	310	HIS
15	c	789	GLN
15	c	1132	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	54,60,60	0.94	0
16	K0W	c	1901	-	40,44,44	1.27	4 (10%)	66,74,74	1.25	8 (12%)

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	-	-	8/42/66/66	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	c	1901	K0W	PA3-O13	3.45	1.65	1.59
16	c	1901	K0W	PA6-O16	2.92	1.64	1.59
16	c	1901	K0W	PA4-O14	2.77	1.64	1.59
16	c	1901	K0W	PA2-O12	2.74	1.64	1.59

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	c	1901	K0W	O77-PA5-O15	3.39	109.33	102.48
16	c	1901	K0W	C5-C6-C1	3.37	117.78	110.41
16	c	1901	K0W	C5-C4-C3	2.78	116.50	110.41
16	c	1901	K0W	PA1-O76-PB1	-2.68	123.61	132.83
16	c	1901	K0W	C4-C3-C2	2.61	116.12	110.41

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

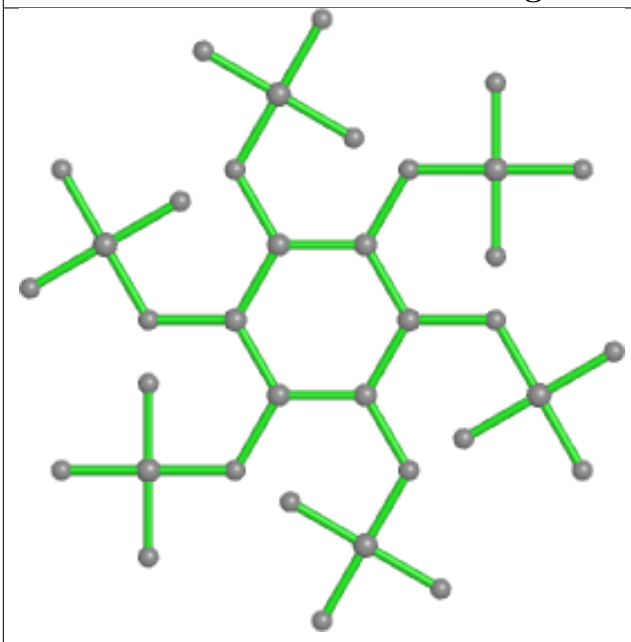
Mol	Chain	Res	Type	Atoms
16	c	1901	K0W	C4-C3-O13-PA3
16	c	1901	K0W	C2-O12-PA2-O22
17	c	1902	IHP	C3-O13-P3-O43
16	c	1901	K0W	C6-O11-PA1-O76
16	c	1901	K0W	C3-O13-PA3-O23

There are no ring outliers.

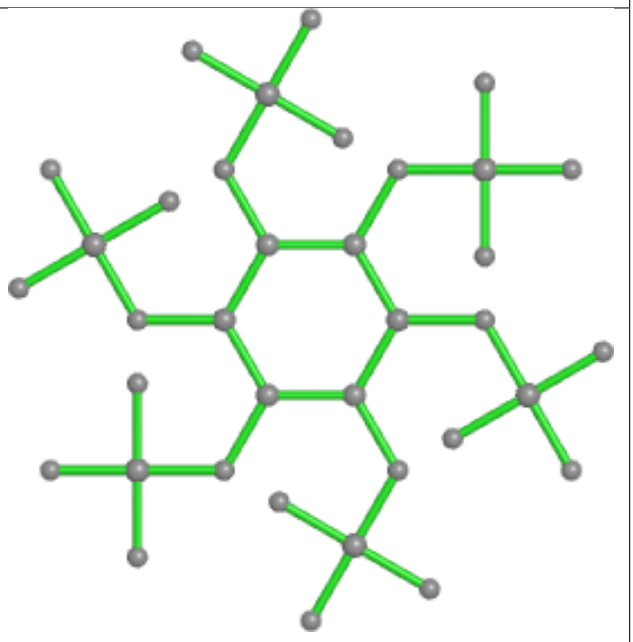
No monomer is involved in short contacts.

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 then 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.

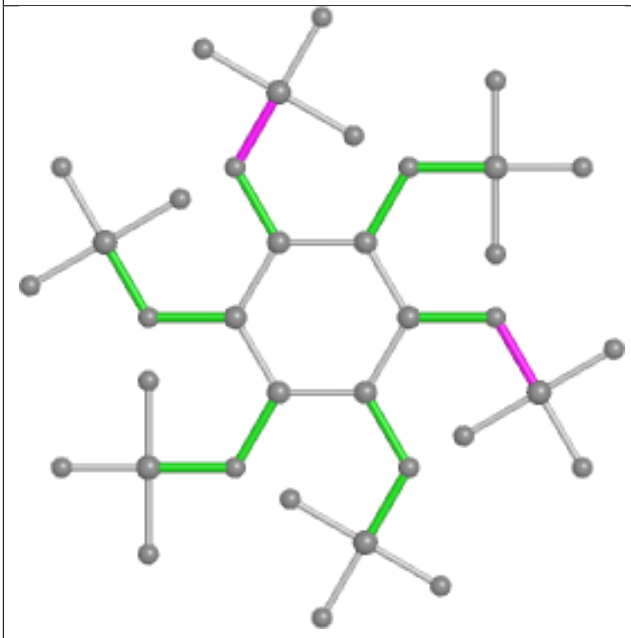
Ligand IHP c 1902



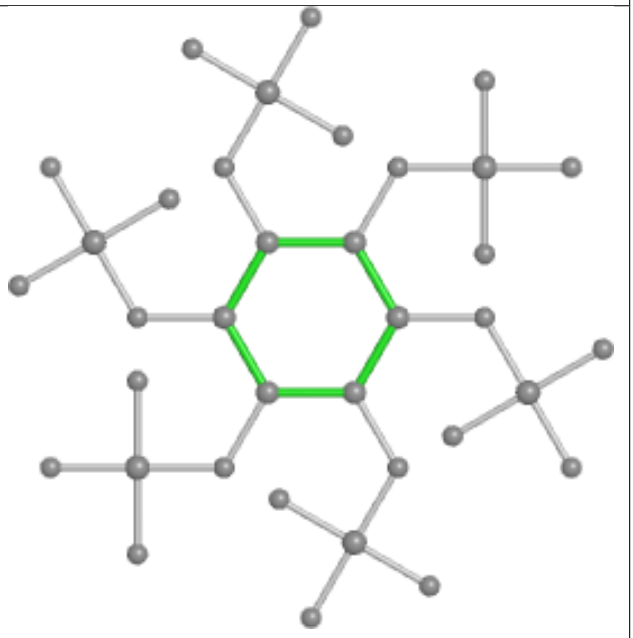
Bond lengths



Bond angles

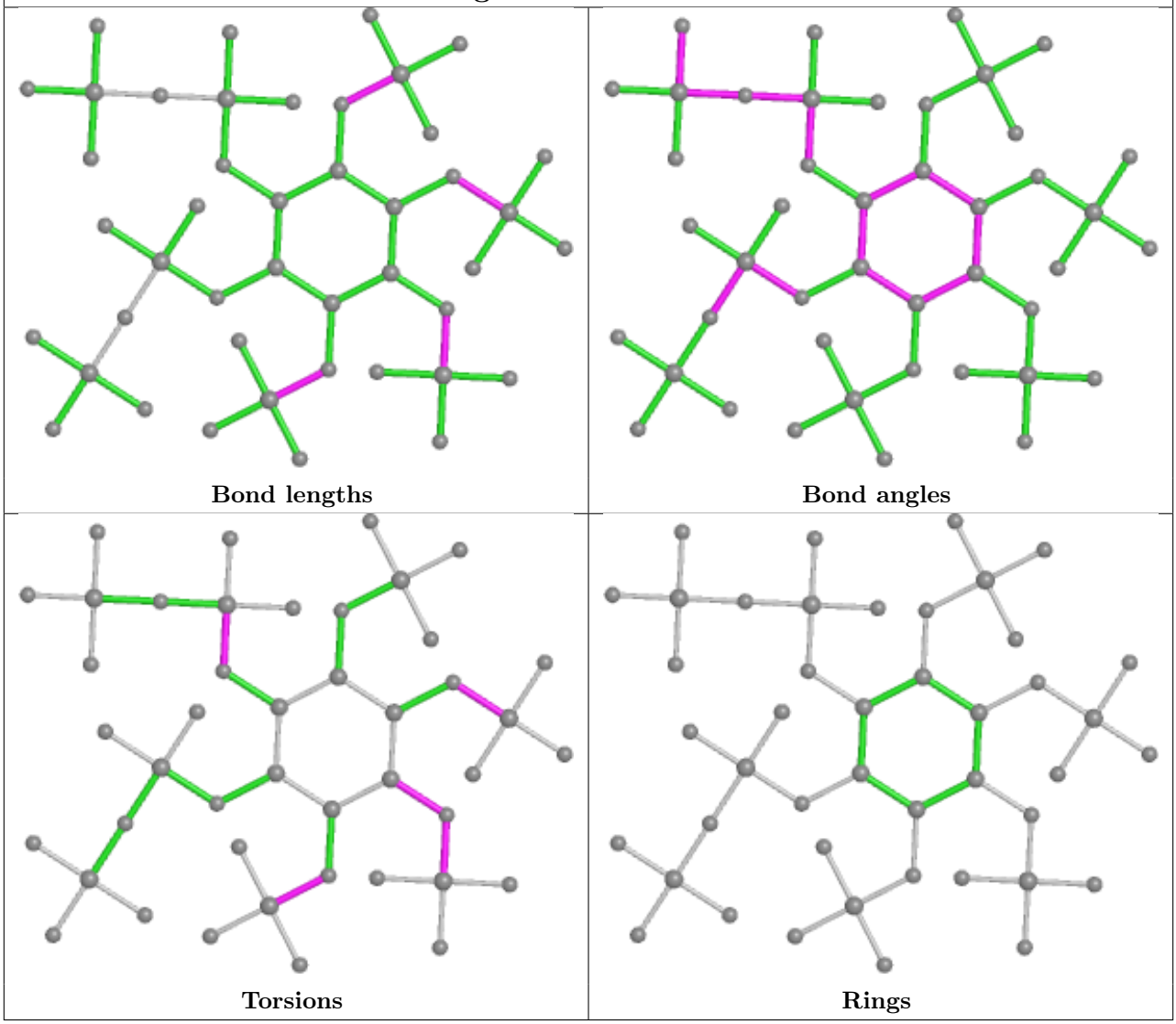


Torsions



Rings

Ligand K0W c 1901



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.

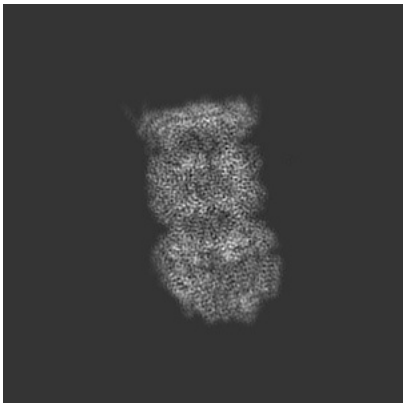
6 Map visualisation

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.

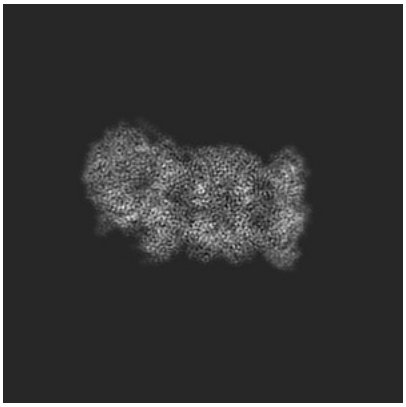
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

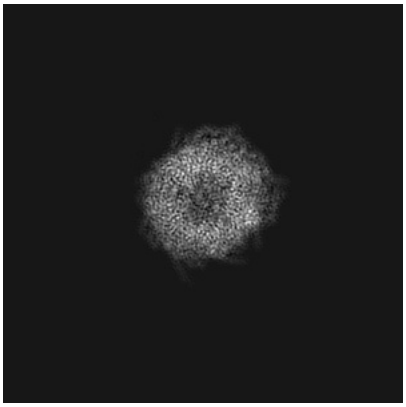
6.1.1 Primary map



X



Y



Z

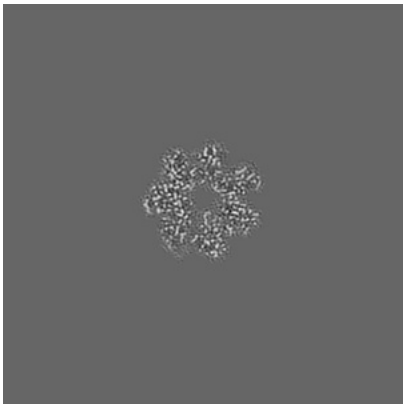
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 180

Y Index: 180



Z Index: 180

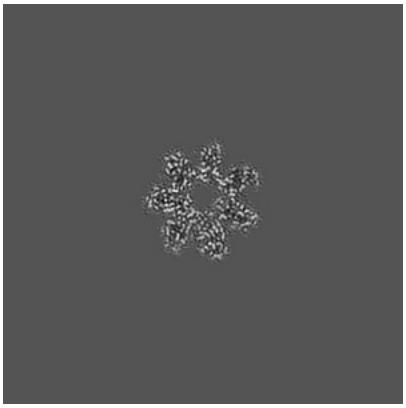
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 207

Y Index: 208

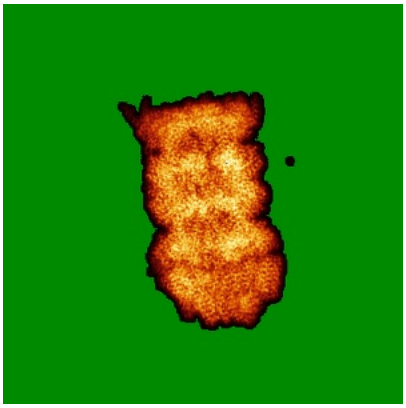


Z Index: 177

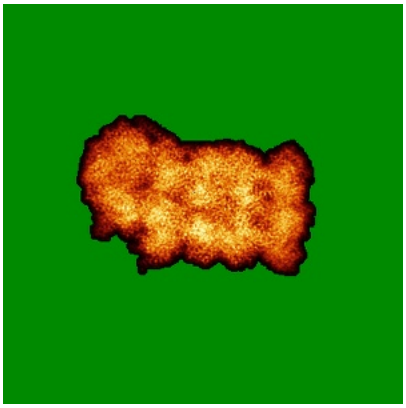
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

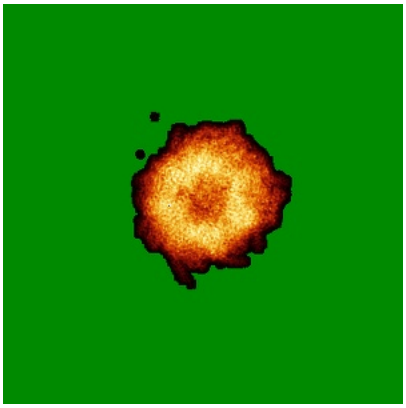
6.4.1 Primary map



X



Y

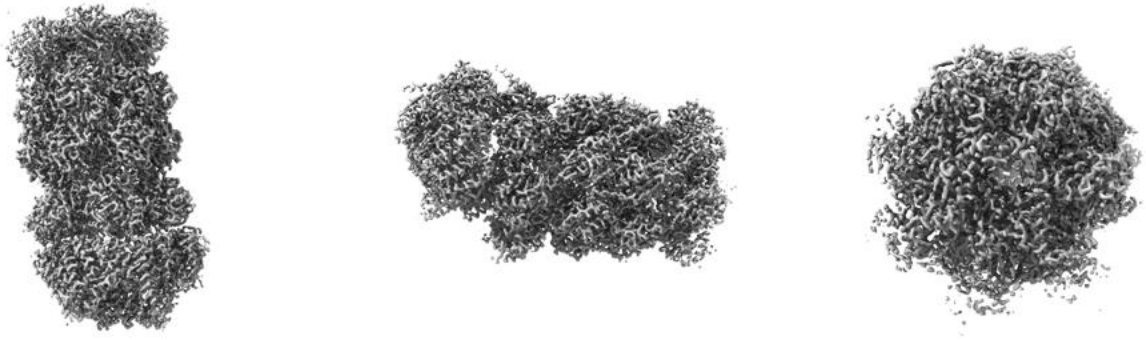


Z

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 (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

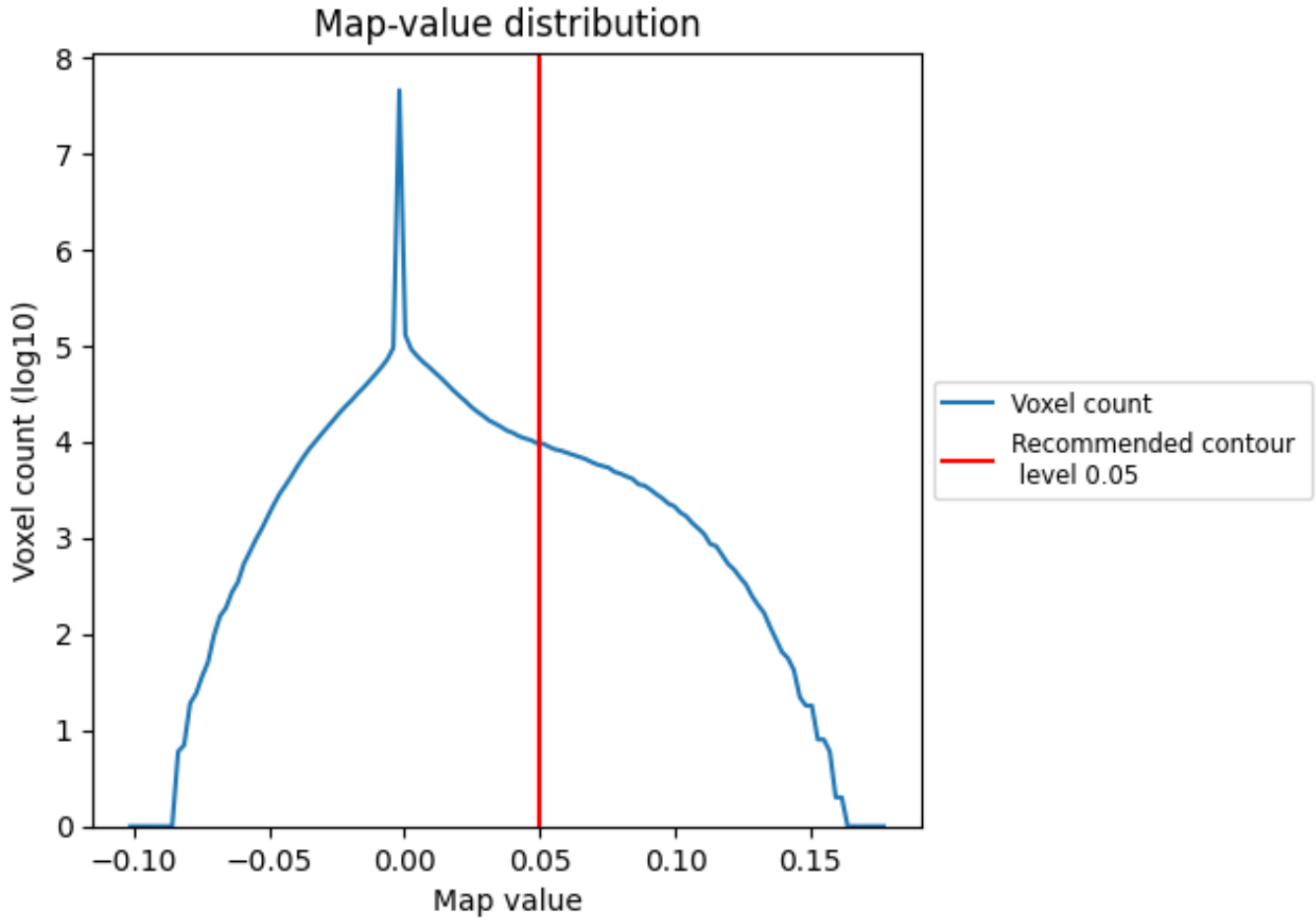
6.6 Mask visualisation (i)

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

7 Map analysis

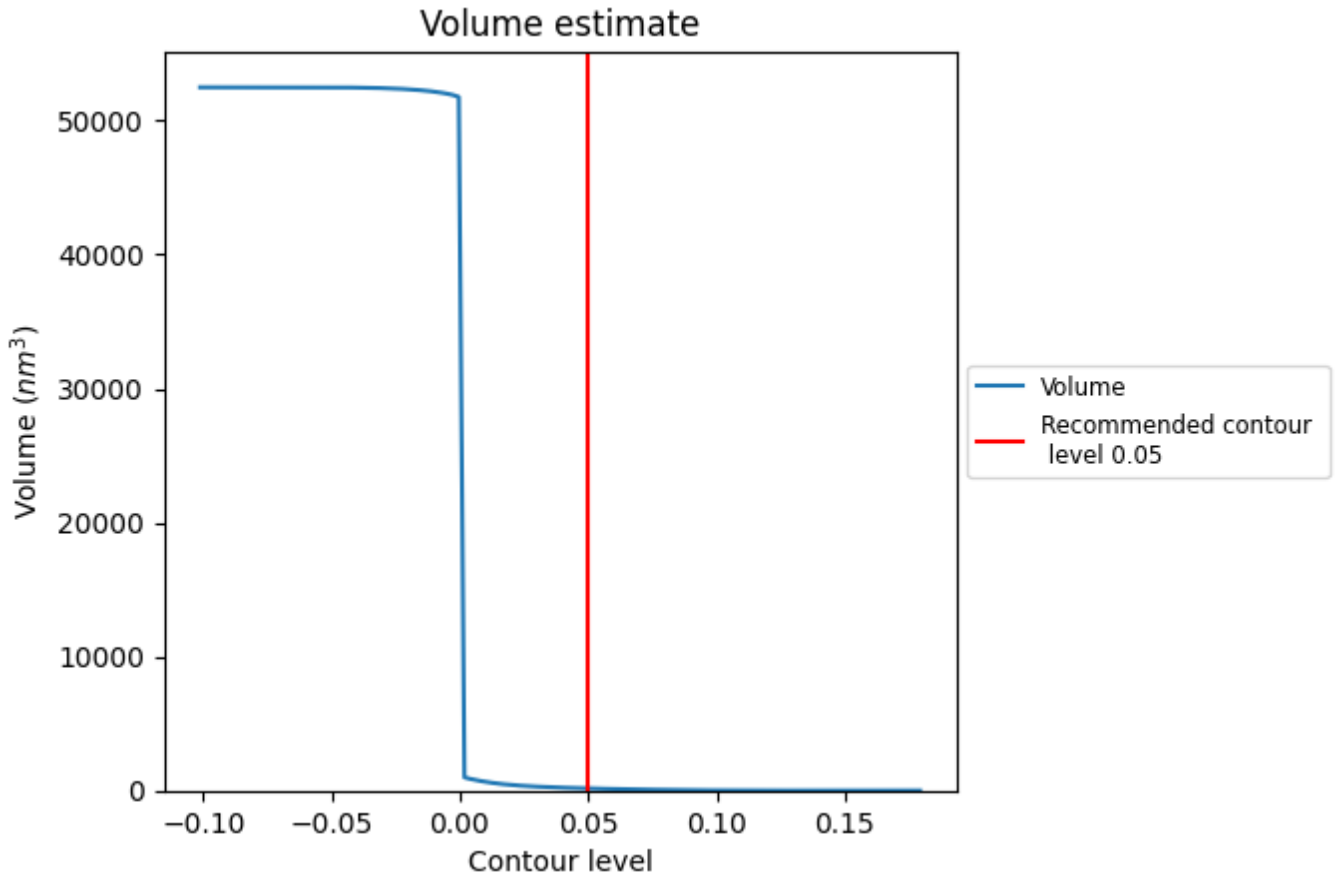
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

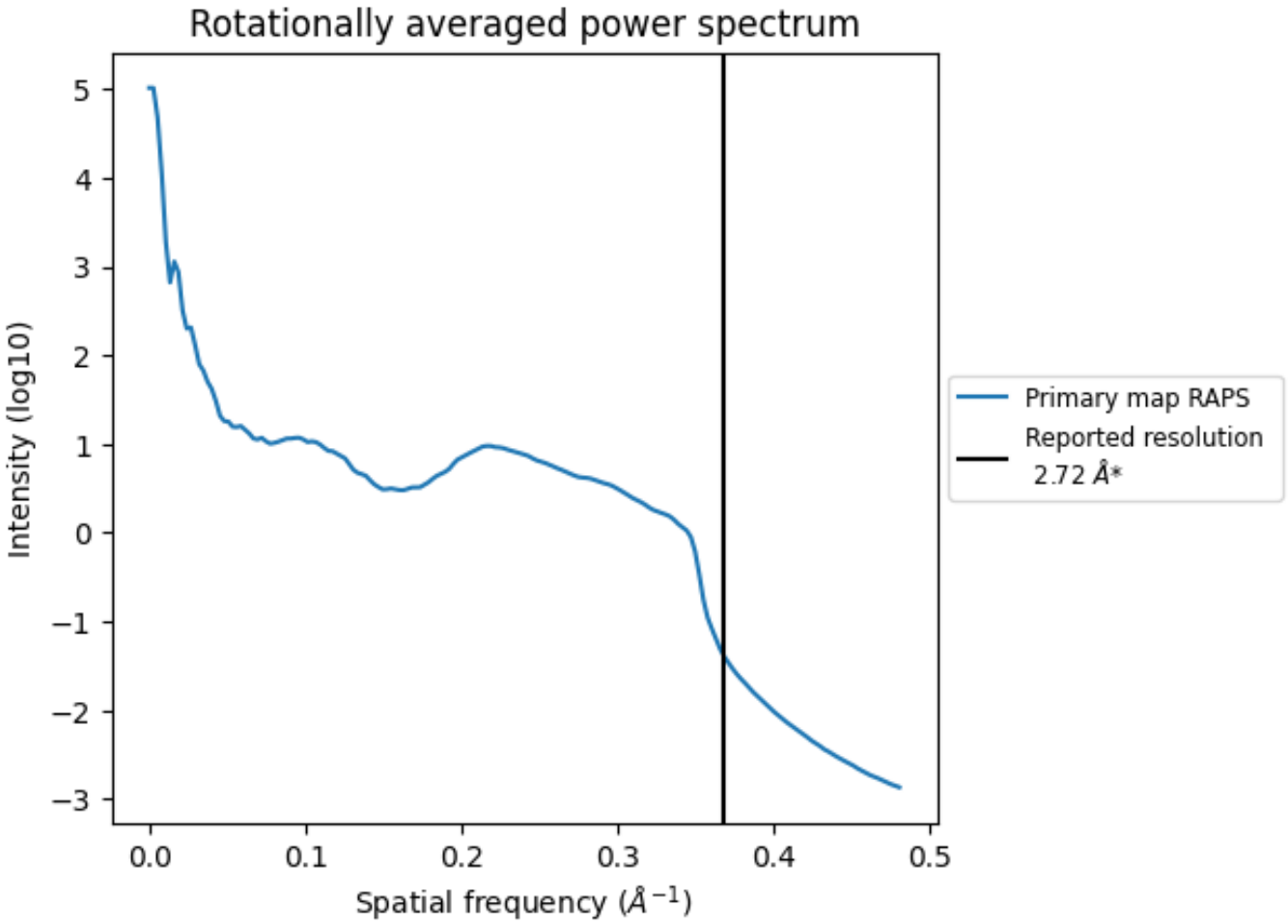
7.2 Volume estimate (i)



The volume at the recommended contour level is 159 nm^3; 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 (i)

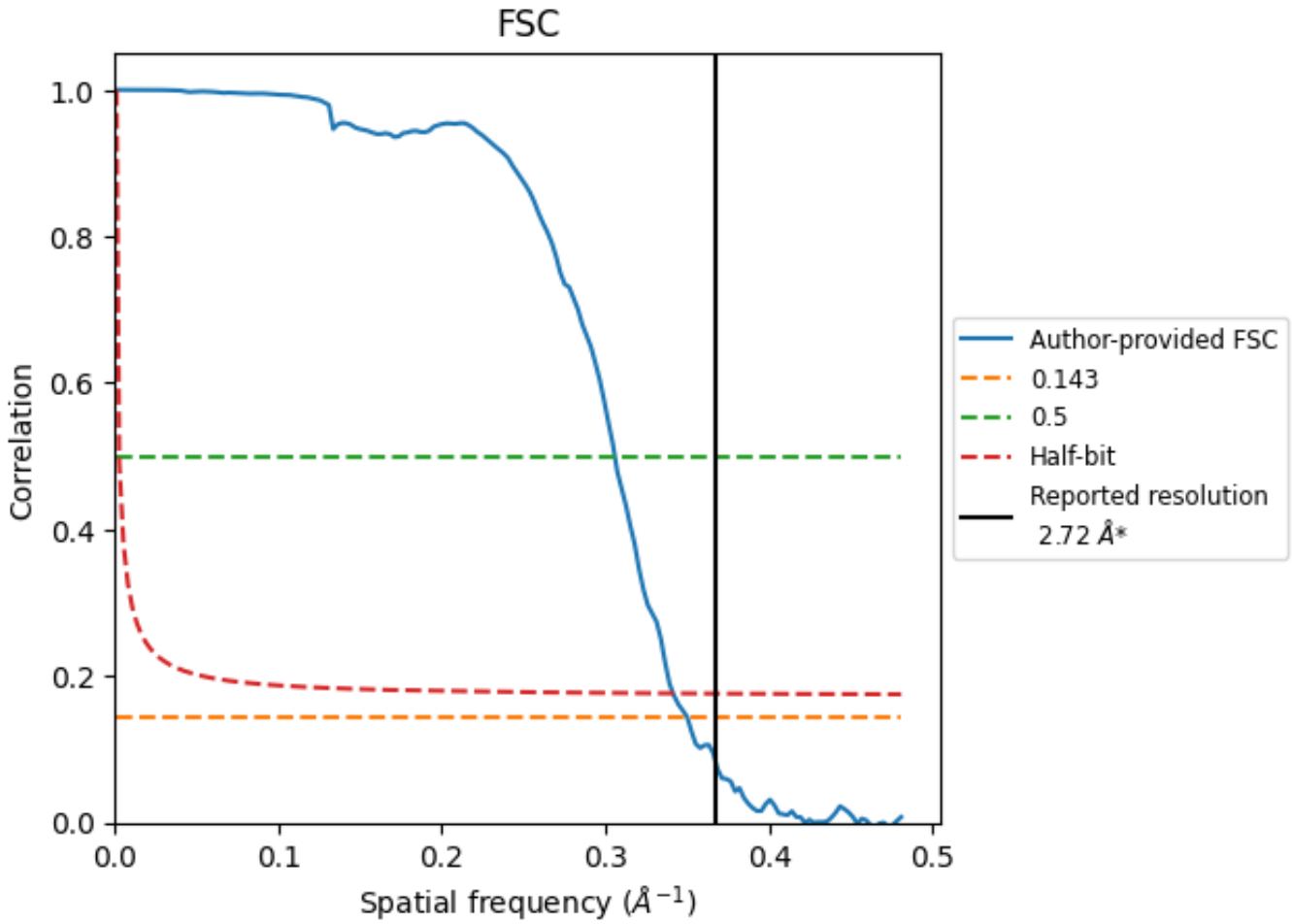


*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.368 Å^{-1}

8.2 Resolution estimates (i)

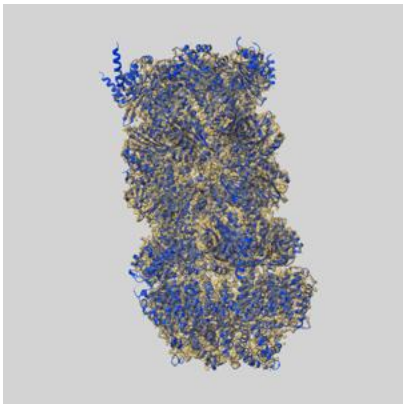
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.86	3.27	2.93
Unmasked-calculated*	-	-	-

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

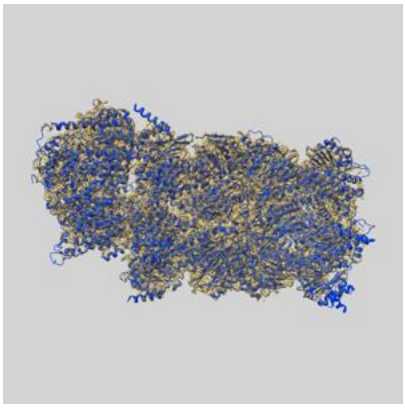
9 Map-model fit

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 9.

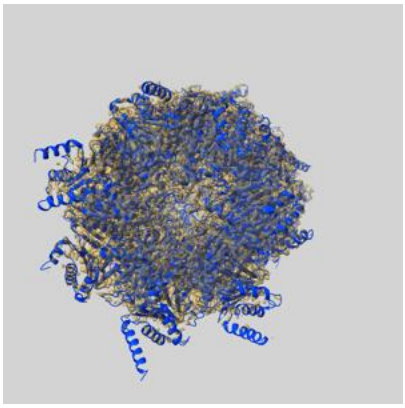
9.1 Map-model overlay



X



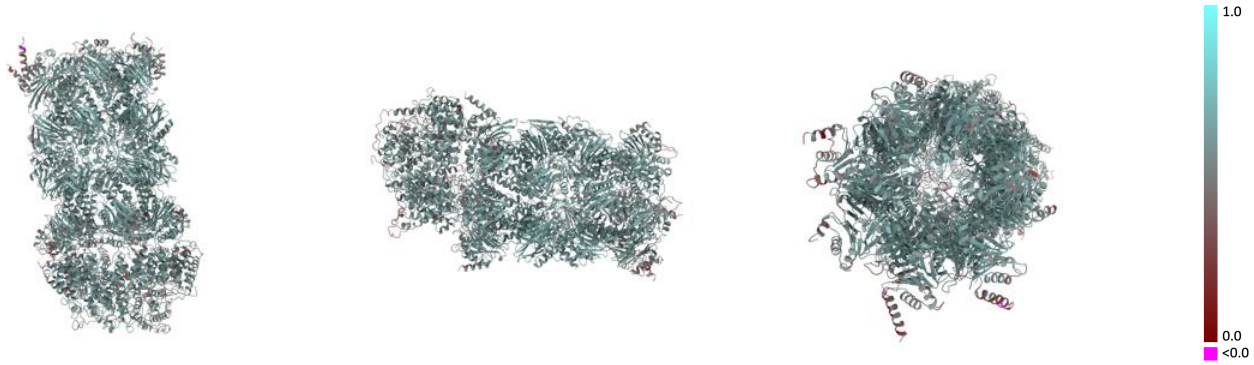
Y



Z

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.

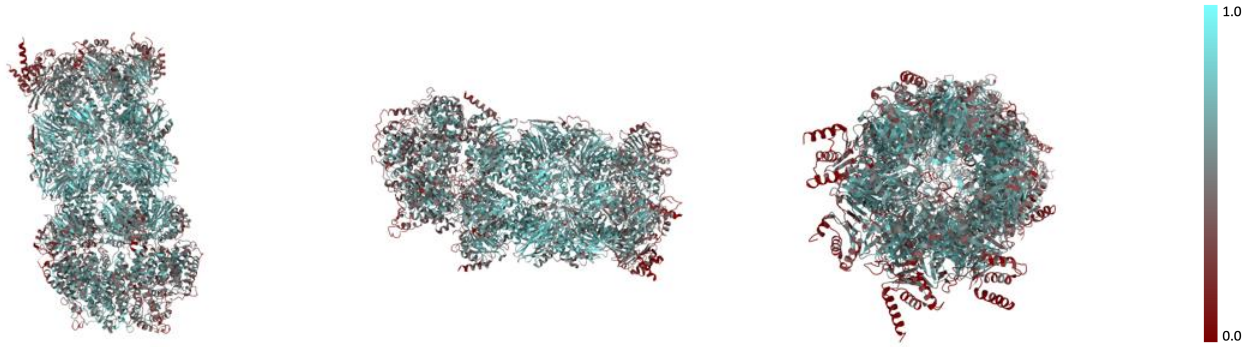
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

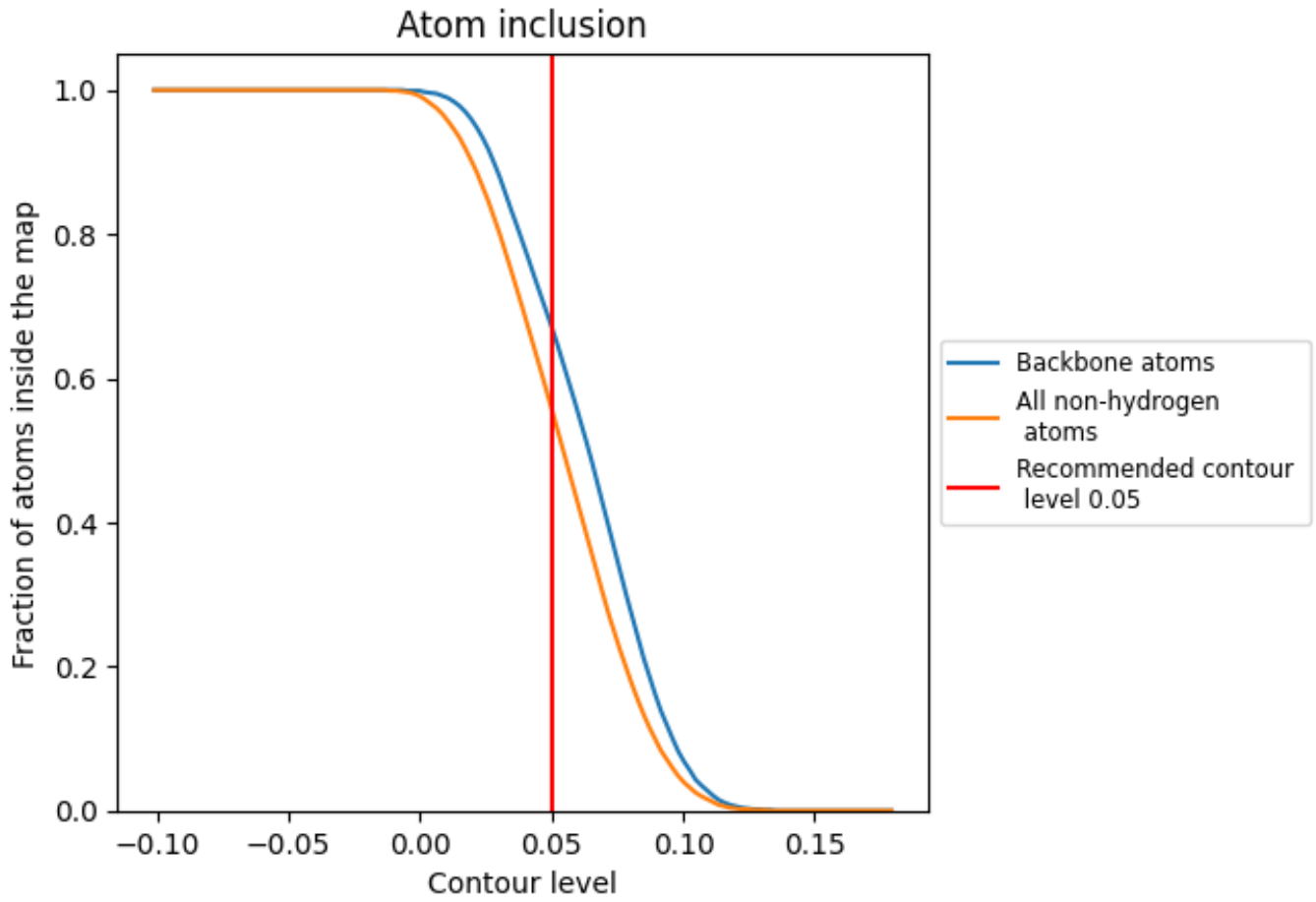
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.05).

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