



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 11:55 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:

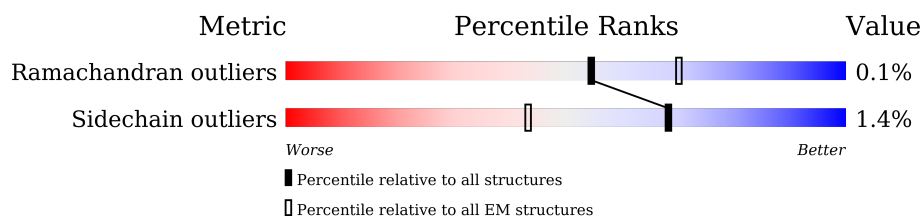
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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 $\leq 5\%$. 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	<div> <div>15%</div> <div>90%</div> <div>8%</div> </div>
1	O	234	<div> <div>37%</div> <div>97%</div> <div>•</div> </div>
2	B	261	<div> <div>28%</div> <div>79%</div> <div>19%</div> </div>
2	P	261	<div> <div>52%</div> <div>94%</div> <div>•</div> </div>
3	C	248	<div> <div>28%</div> <div>83%</div> <div>15%</div> </div>
3	Q	248	<div> <div>50%</div> <div>94%</div> <div>6%</div> </div>
4	D	241	<div> <div>28%</div> <div>94%</div> <div>6%</div> </div>
4	R	241	<div> <div>40%</div> <div>96%</div> <div>•</div> </div>
5	E	263	<div> <div>14%</div> <div>89%</div> <div>9%</div> </div>

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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

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		

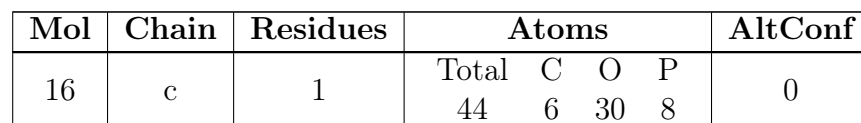
- Molecule 15 is a protein called Proteasome activator complex subunit 4.

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

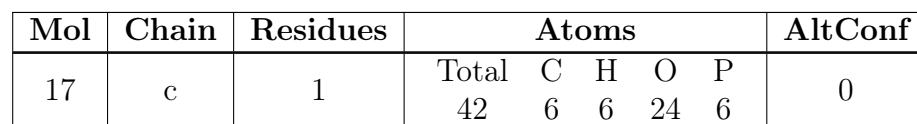
There are 37 discrepancies between the modelled and reference sequences:

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-tetraphosphonooxy-cyclohexyl] phosphono hydrogen phosphate (three-letter code: K0W) (formula: C₆H₂₀O₃₀P₈) (labeled as "Ligand of Interest" by depositor).



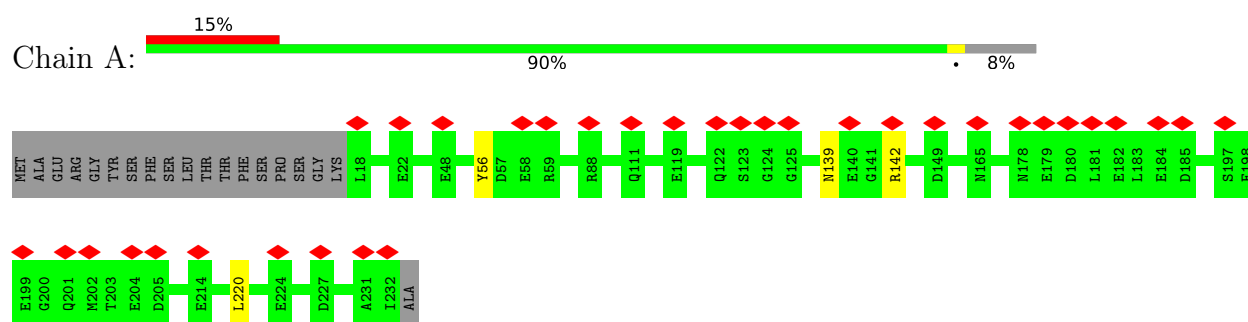
- Molecule 17 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



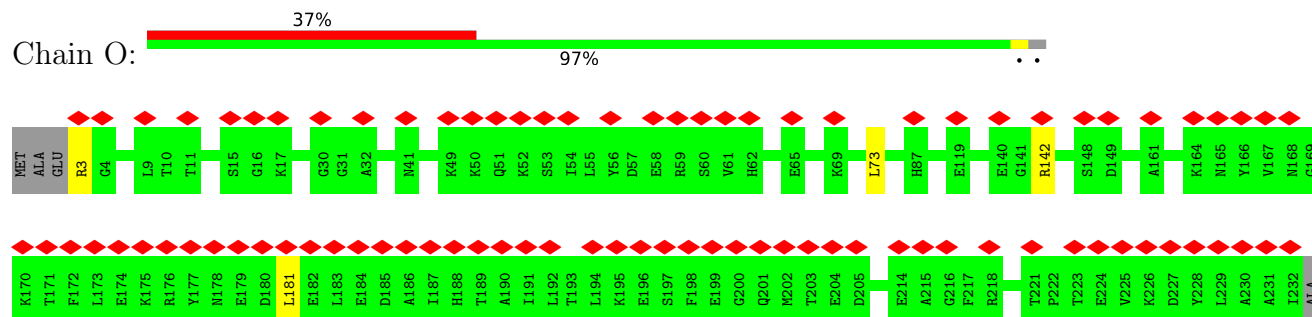
3 Residue-property plots [i](#)

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.

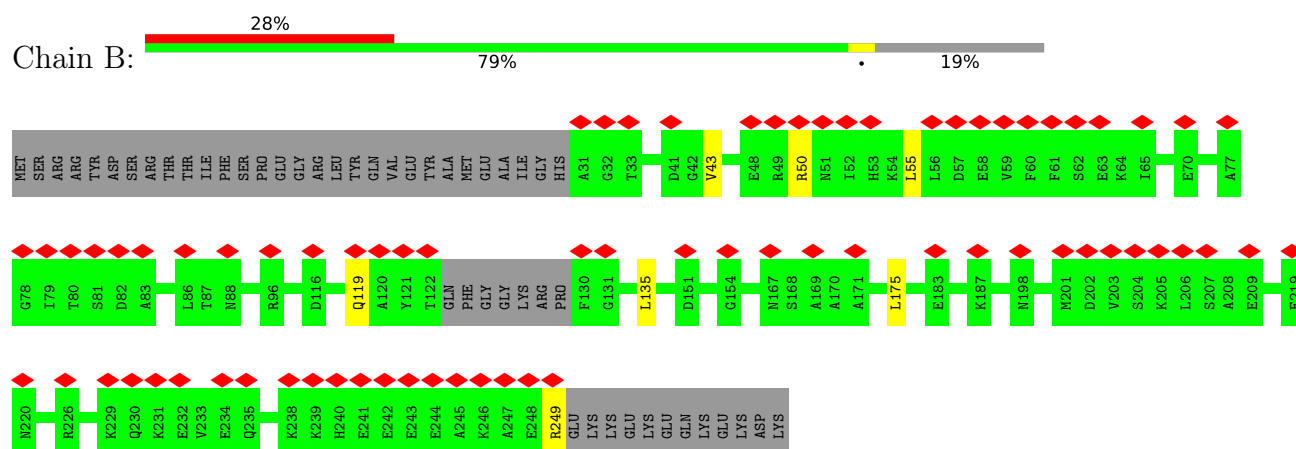
- Molecule 1: Proteasome subunit alpha type-2



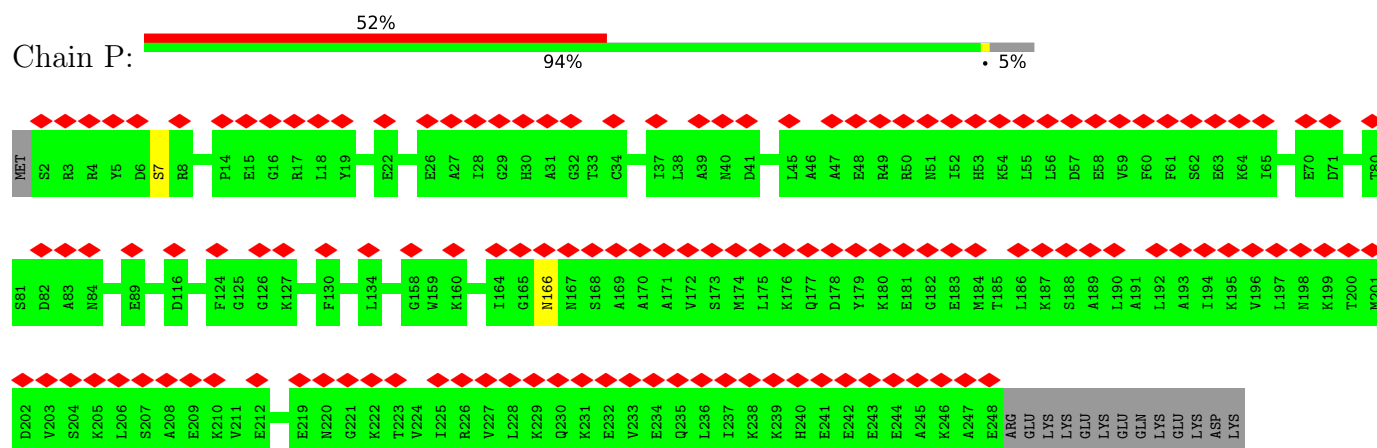
- Molecule 1: Proteasome subunit alpha type-2



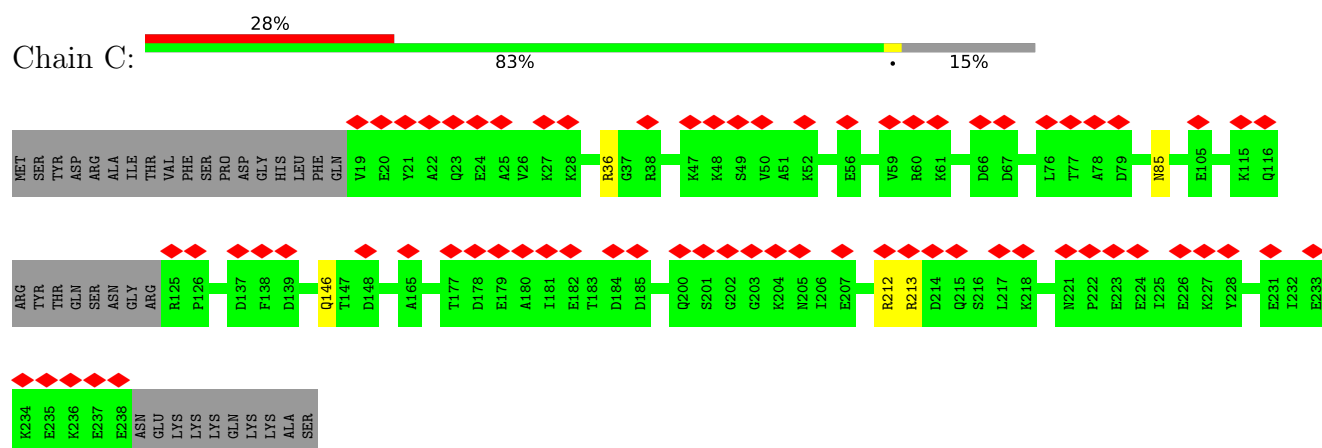
- Molecule 2: Proteasome subunit alpha type-4



- Molecule 2: Proteasome subunit alpha type-4



- Molecule 3: Proteasome subunit alpha type-7

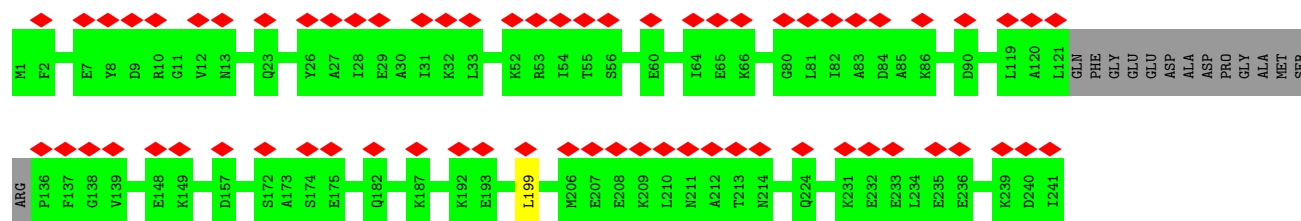


- Molecule 3: Proteasome subunit alpha type-7

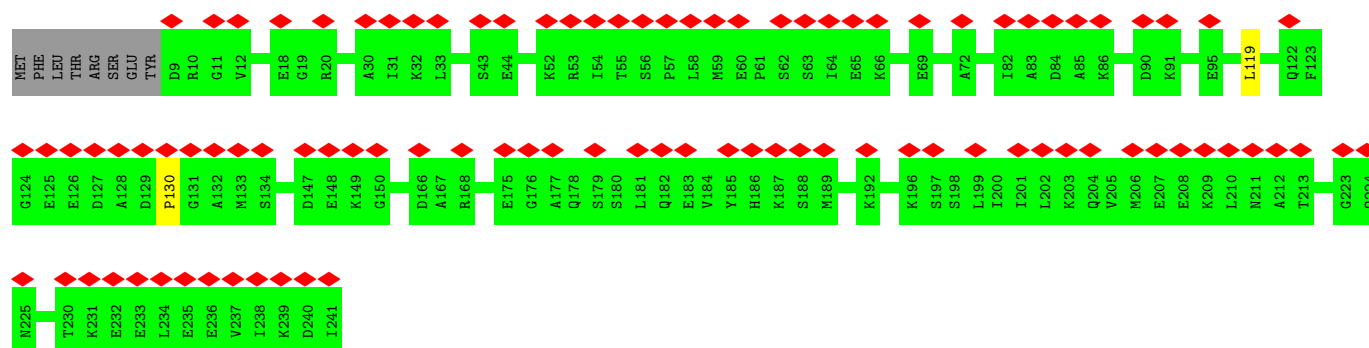
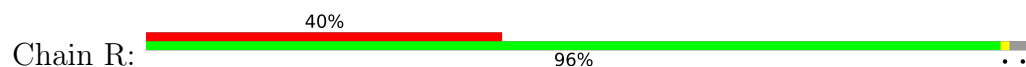


- Molecule 4: Proteasome subunit alpha type-5

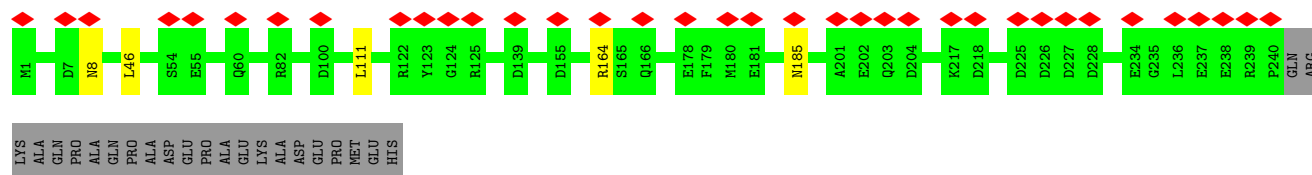
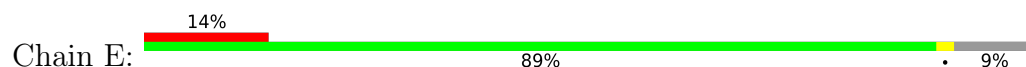




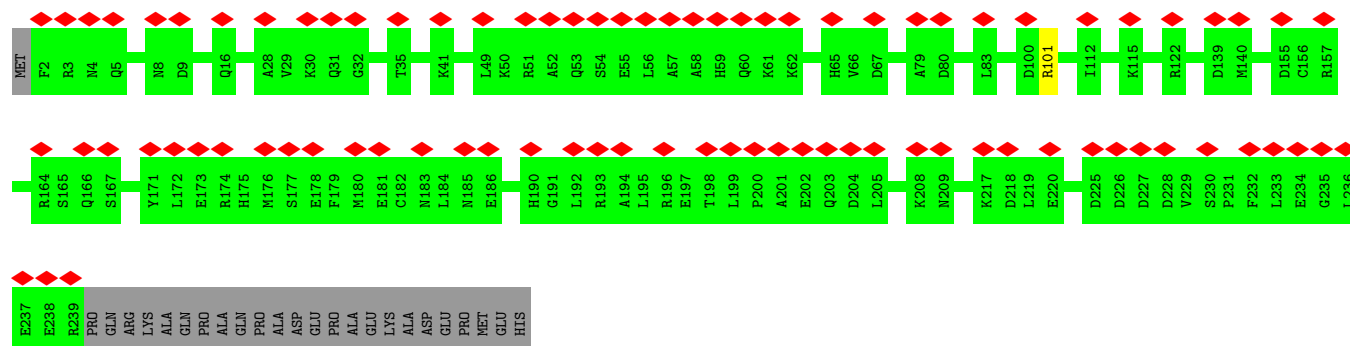
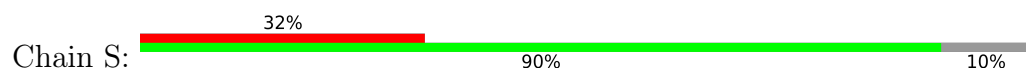
• Molecule 4: Proteasome subunit alpha type-5



• Molecule 5: Proteasome subunit alpha type-1

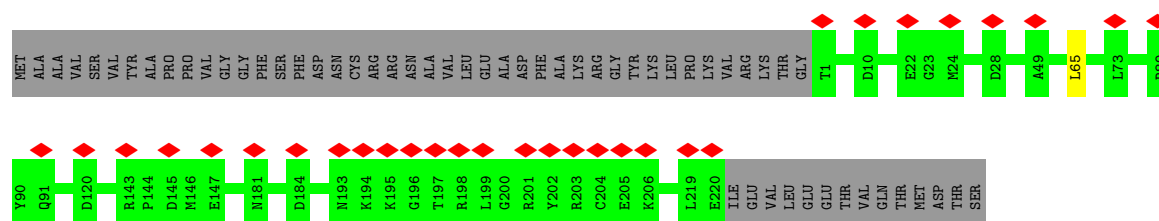
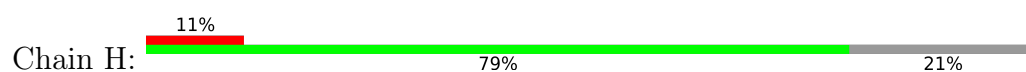


• Molecule 5: Proteasome subunit alpha type-1

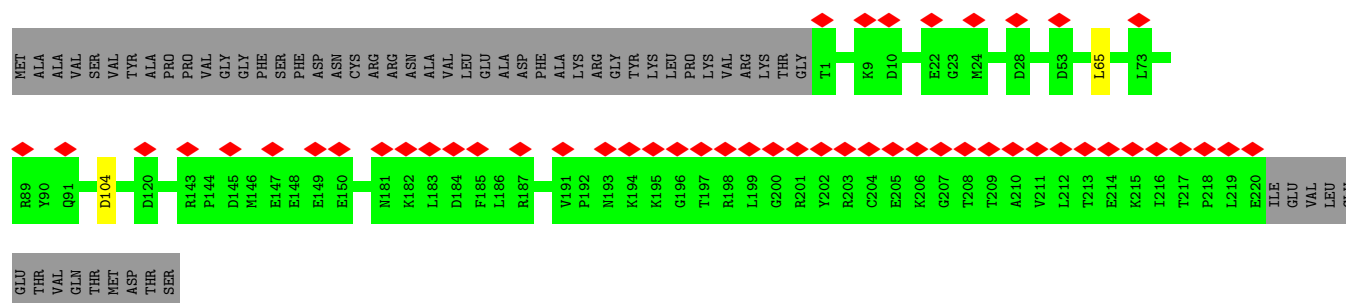
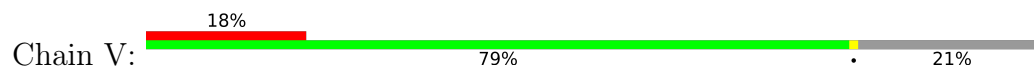


• Molecule 6: Proteasome subunit alpha type-3

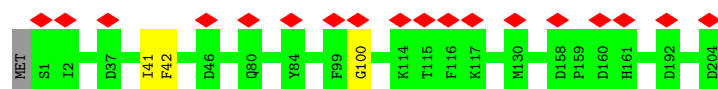




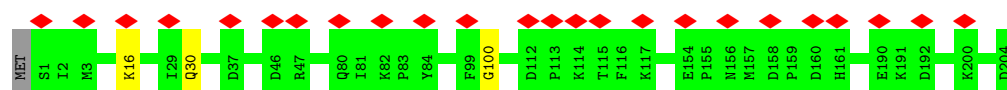
• Molecule 8: Proteasome subunit beta type-7



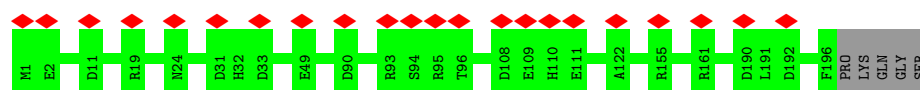
• Molecule 9: Proteasome subunit beta type-3



• Molecule 9: Proteasome subunit beta type-3

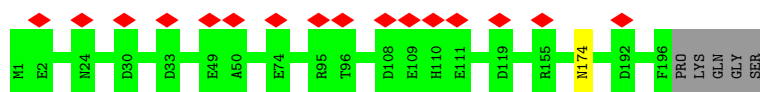


• Molecule 10: Proteasome subunit beta type-2

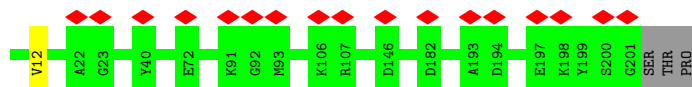
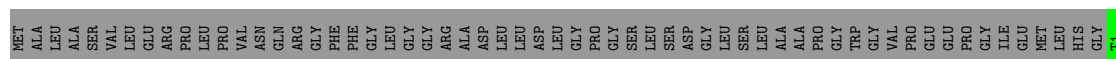
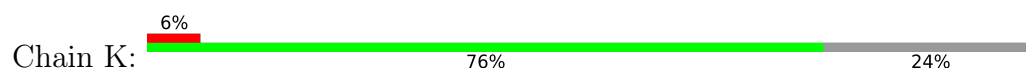


• Molecule 10: Proteasome subunit beta type-2

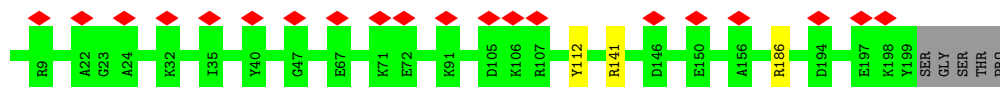
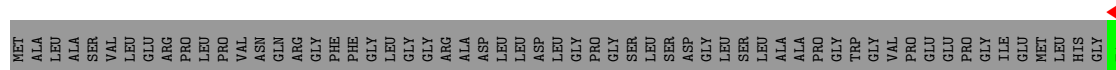
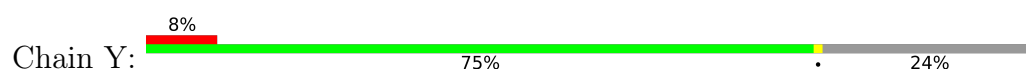




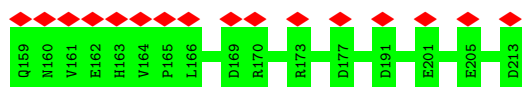
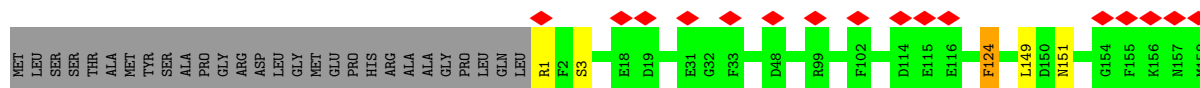
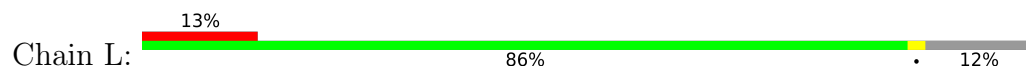
- Molecule 11: Proteasome subunit beta type-5



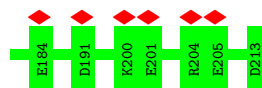
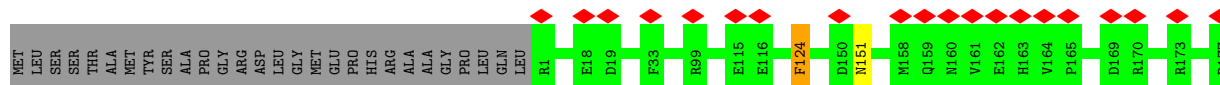
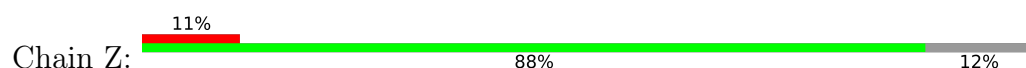
- Molecule 11: Proteasome subunit beta type-5



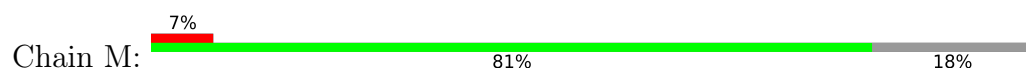
- Molecule 12: Proteasome subunit beta type-1

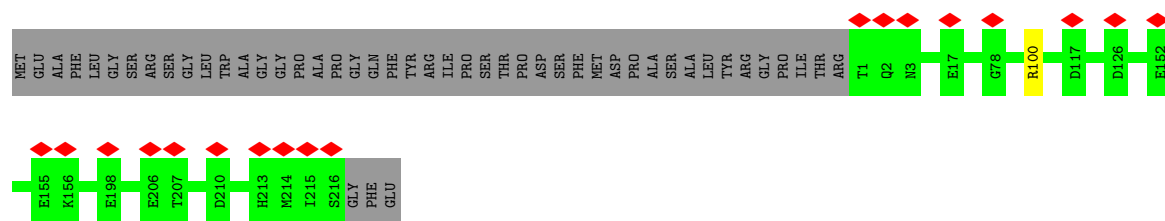


- Molecule 12: Proteasome subunit beta type-1

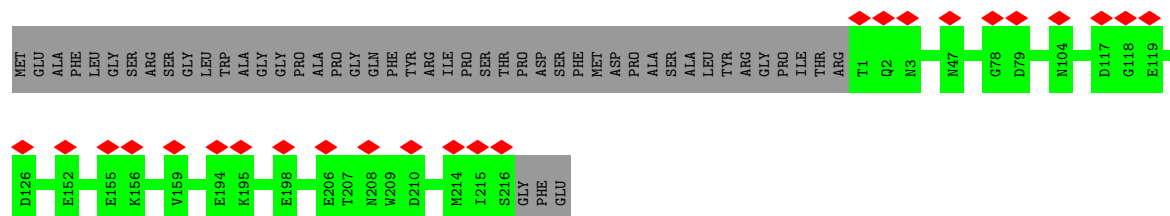
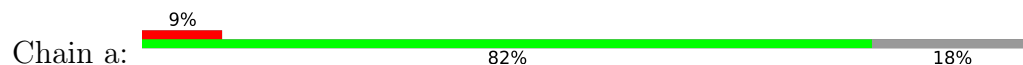


- Molecule 13: Proteasome subunit beta type-4

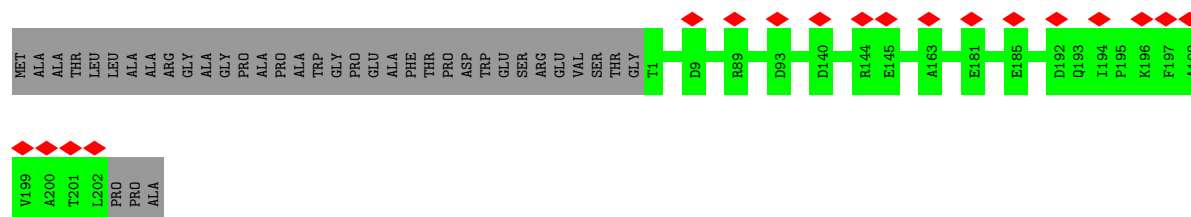
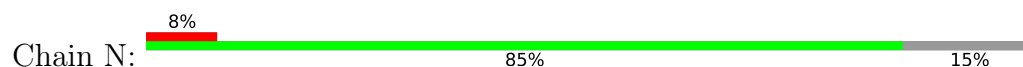




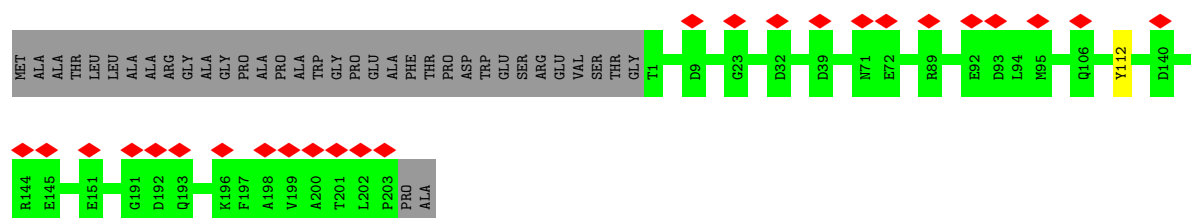
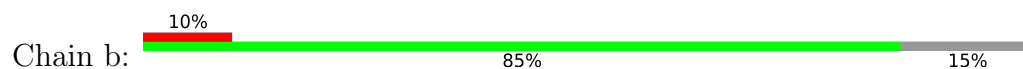
• Molecule 13: Proteasome subunit beta type-4



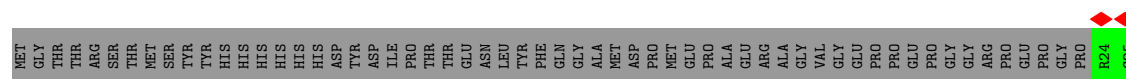
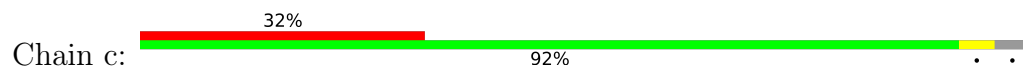
• Molecule 14: Proteasome subunit beta type-6

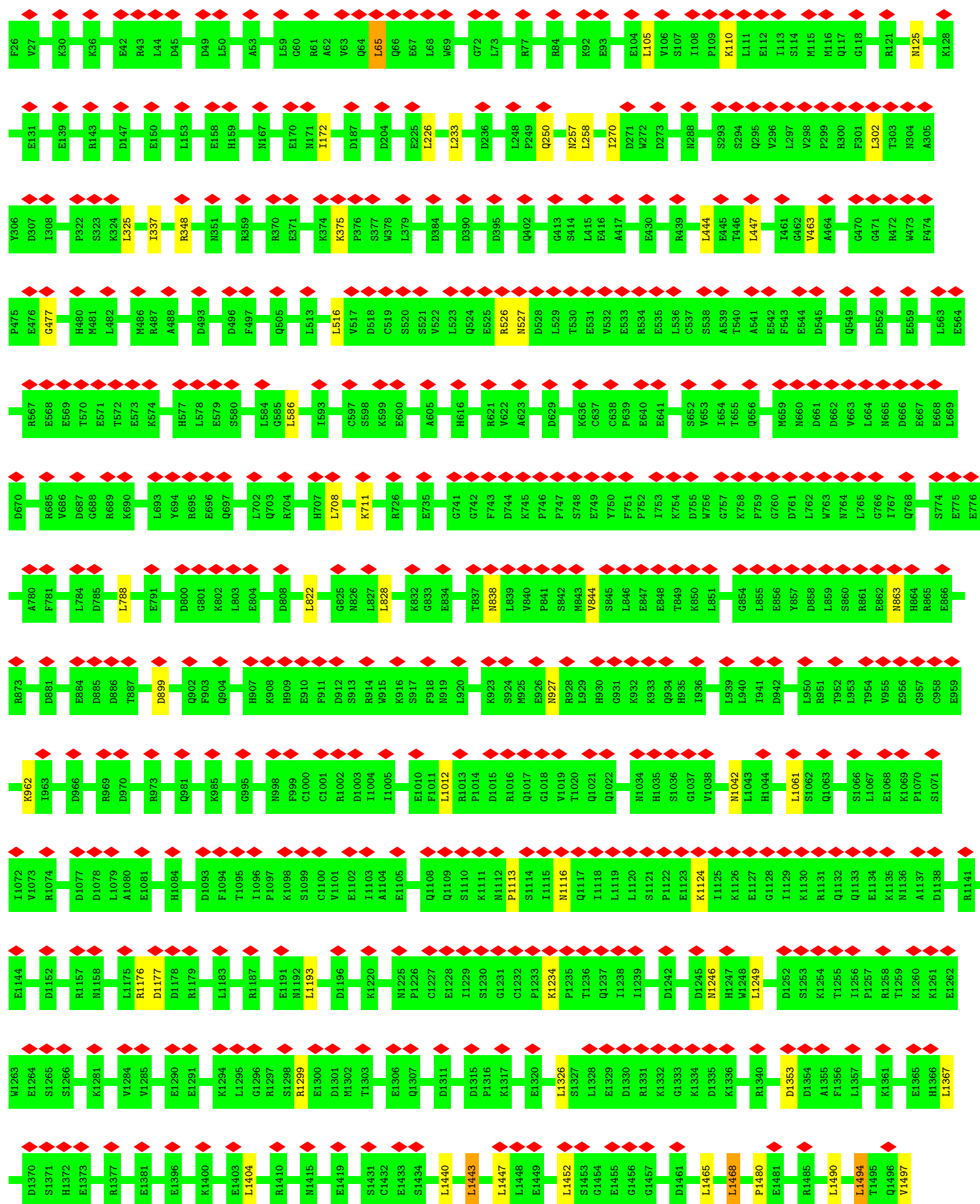


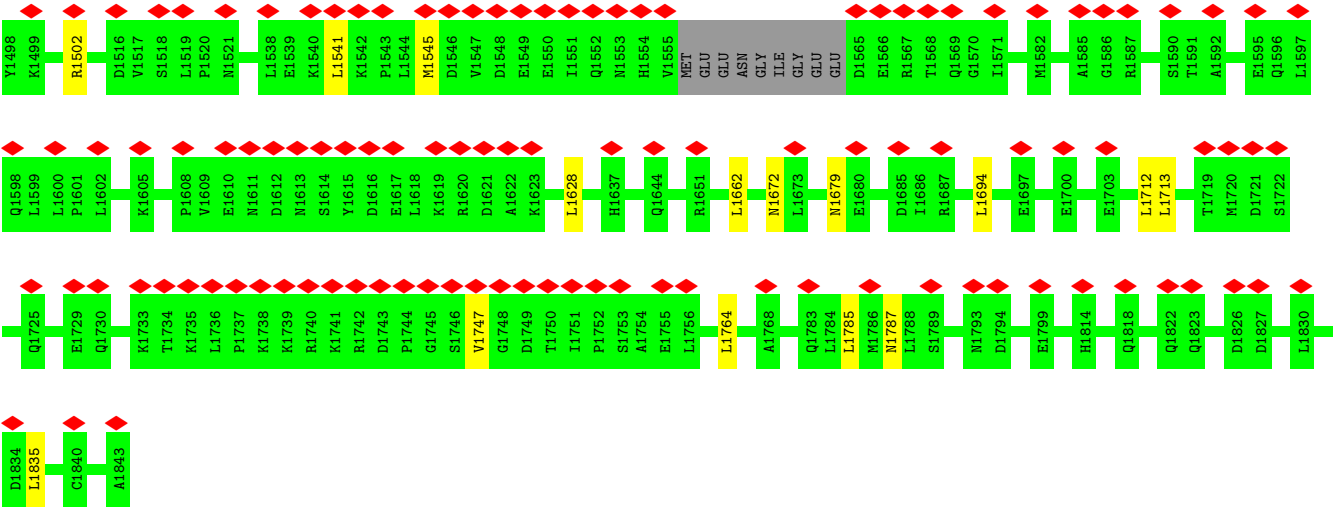
• Molecule 14: Proteasome subunit beta type-6



• Molecule 15: Proteasome activator complex subunit 4







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 (\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 (\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	0.55	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(°)	Ideal(°)
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

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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 ⓘ

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 ⓘ

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 monosaccharides 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
16	K0W	c	1901	-	40,44,44	1.27	4 (10%)	66,74,74	1.25	8 (12%)
17	IHP	c	1902	-	36,36,36	0.72	0	54,60,60	0.94	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	K0W	c	1901	-	-	8/42/66/66	0/1/1/1
17	IHP	c	1902	-	-	2/30/54/54	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(°)	Ideal(°)
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.

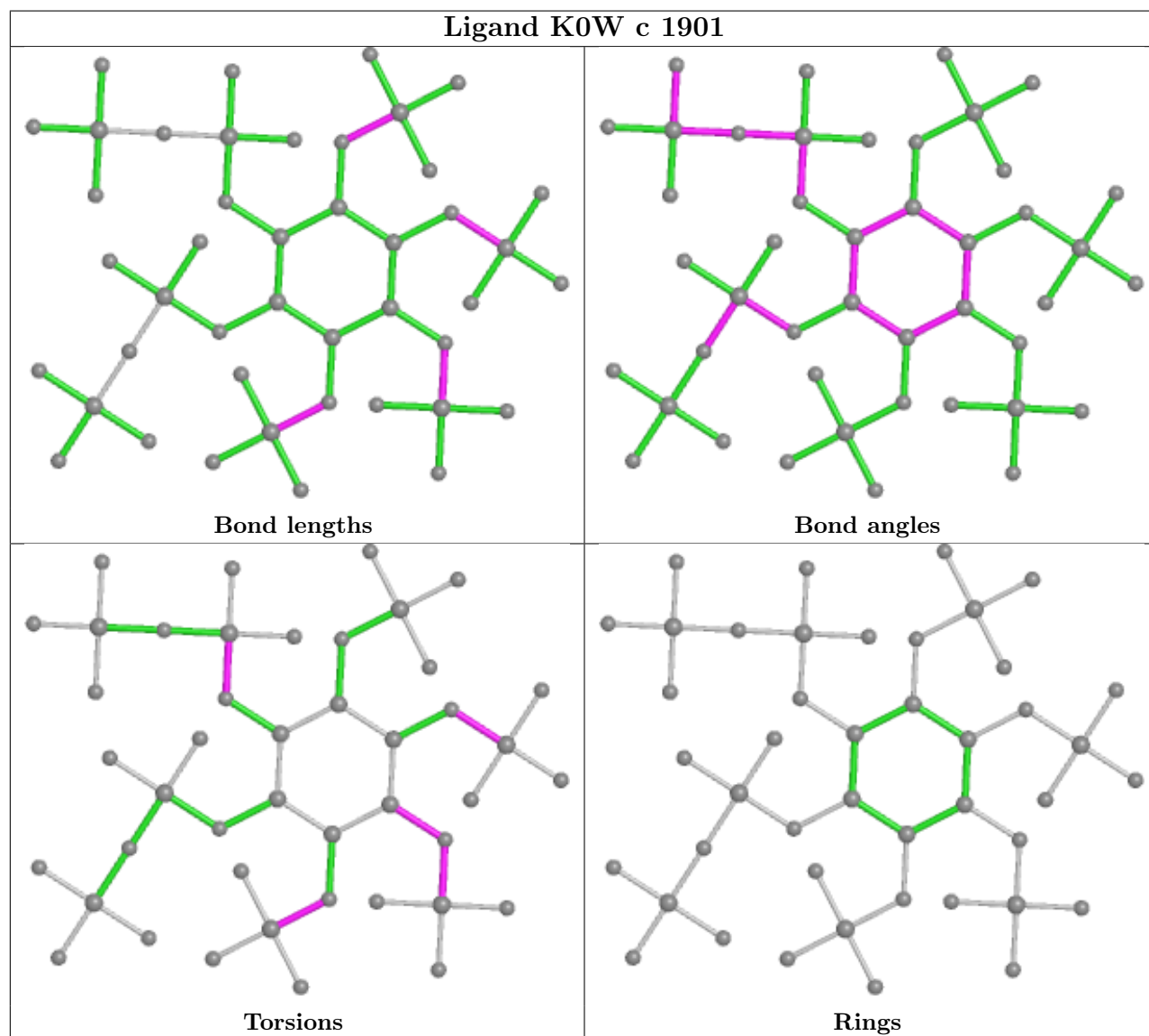
5 of 10 torsion outliers are listed below:

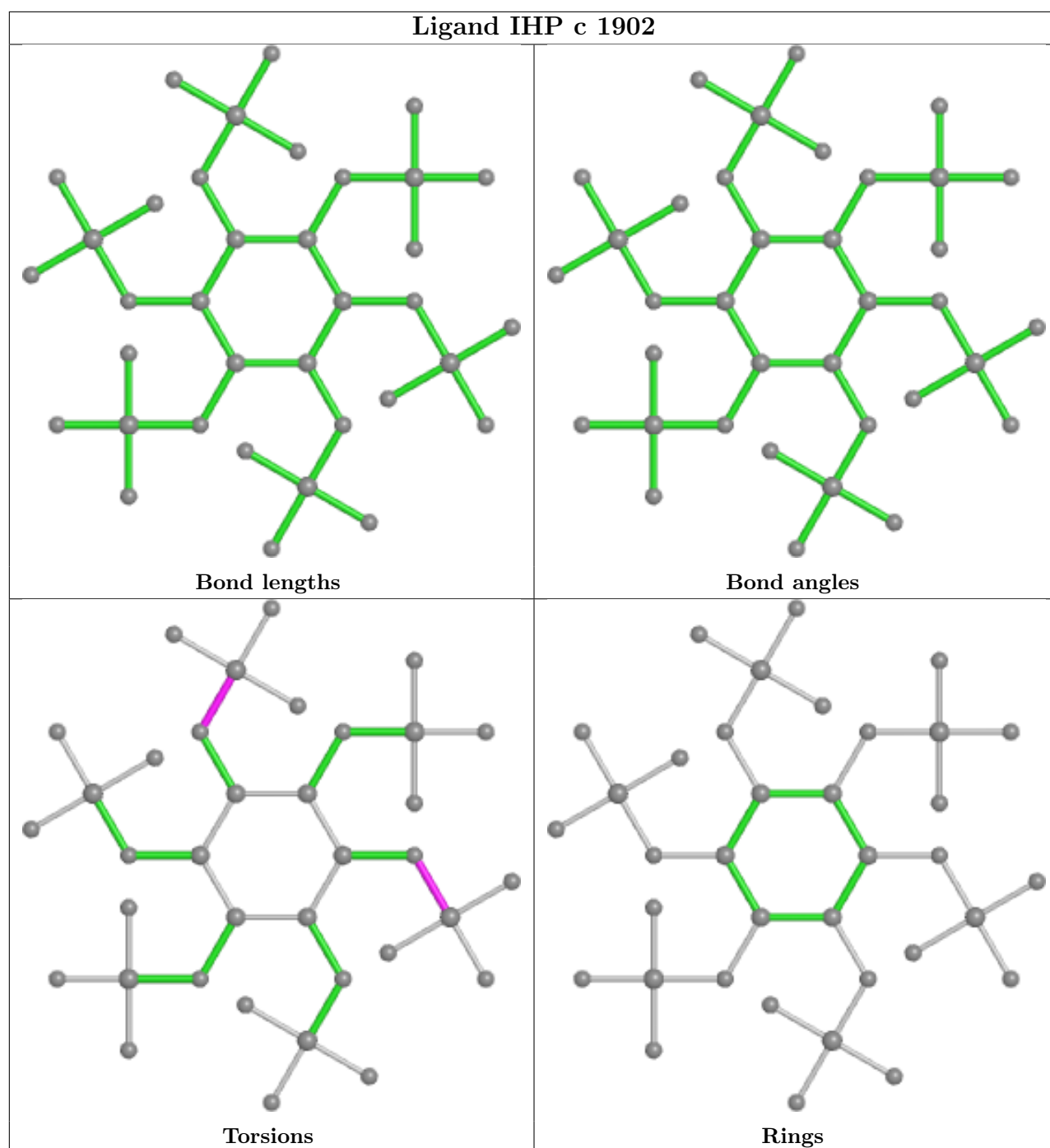
Mol	Chain	Res	Type	Atoms
16	c	1901	K0W	C4-C3-O13-PA3
16	c	1901	K0W	C2-O12-PA2-O22
17	c	1902	IHP	C3-O13-P3-O43
16	c	1901	K0W	C6-O11-PA1-O76
16	c	1901	K0W	C3-O13-PA3-O23

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 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.

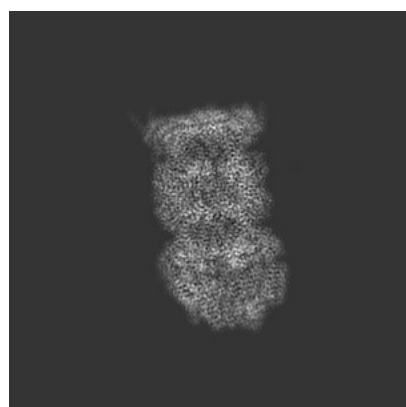
6 Map visualisation [i](#)

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.

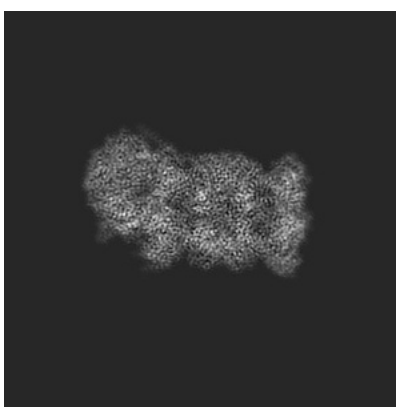
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

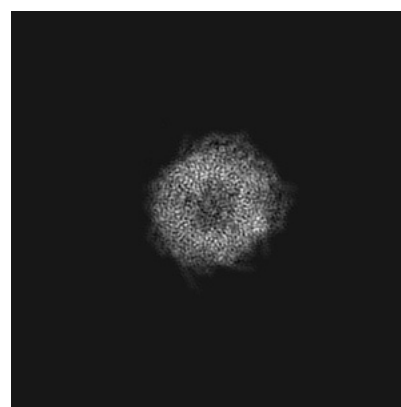
6.1.1 Primary map



X



Y



Z

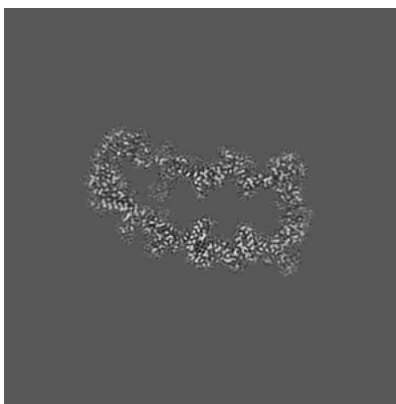
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

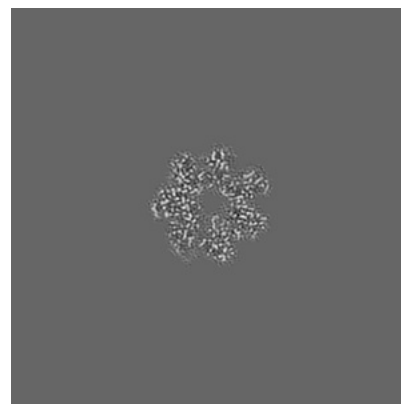
6.2.1 Primary map



X Index: 180



Y Index: 180

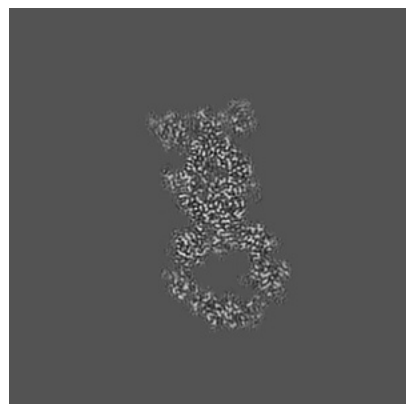


Z Index: 180

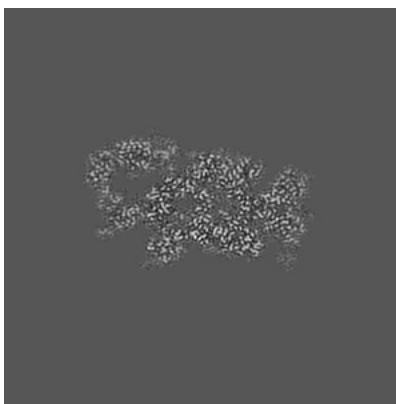
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

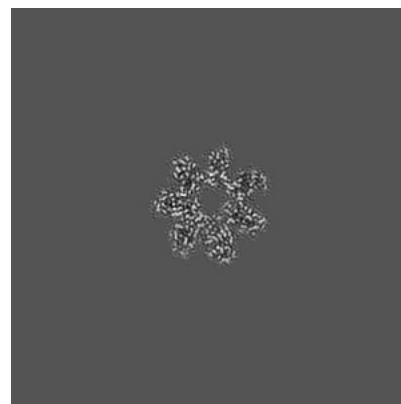
6.3.1 Primary map



X Index: 207



Y Index: 208

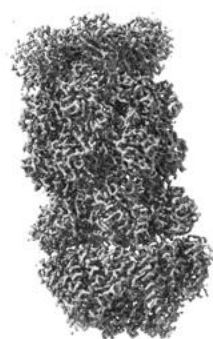


Z Index: 177

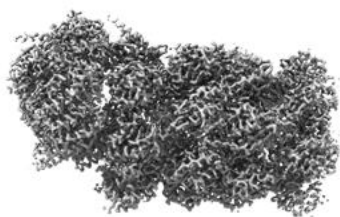
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 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.

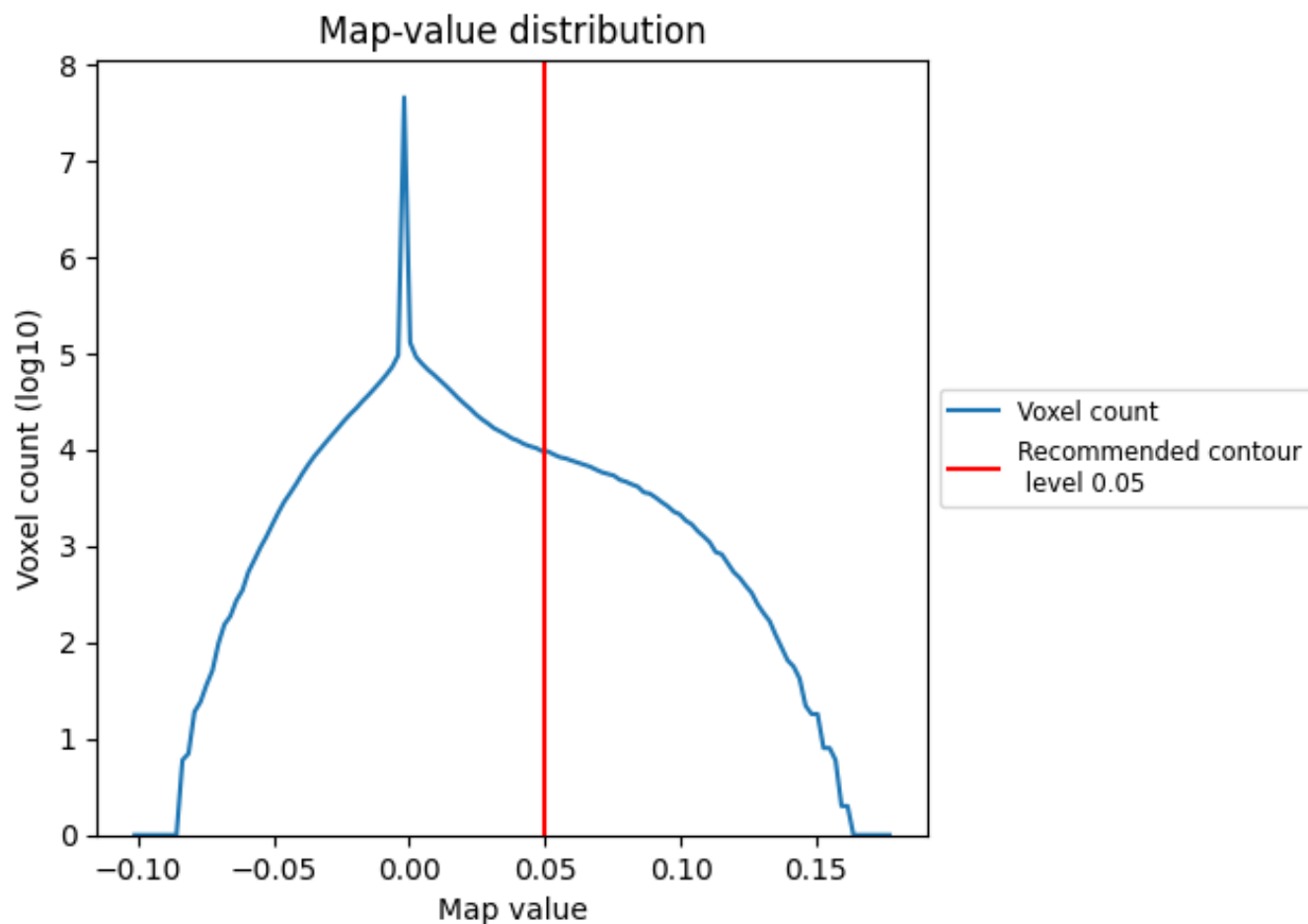
6.5 Mask visualisation

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

7 Map analysis [i](#)

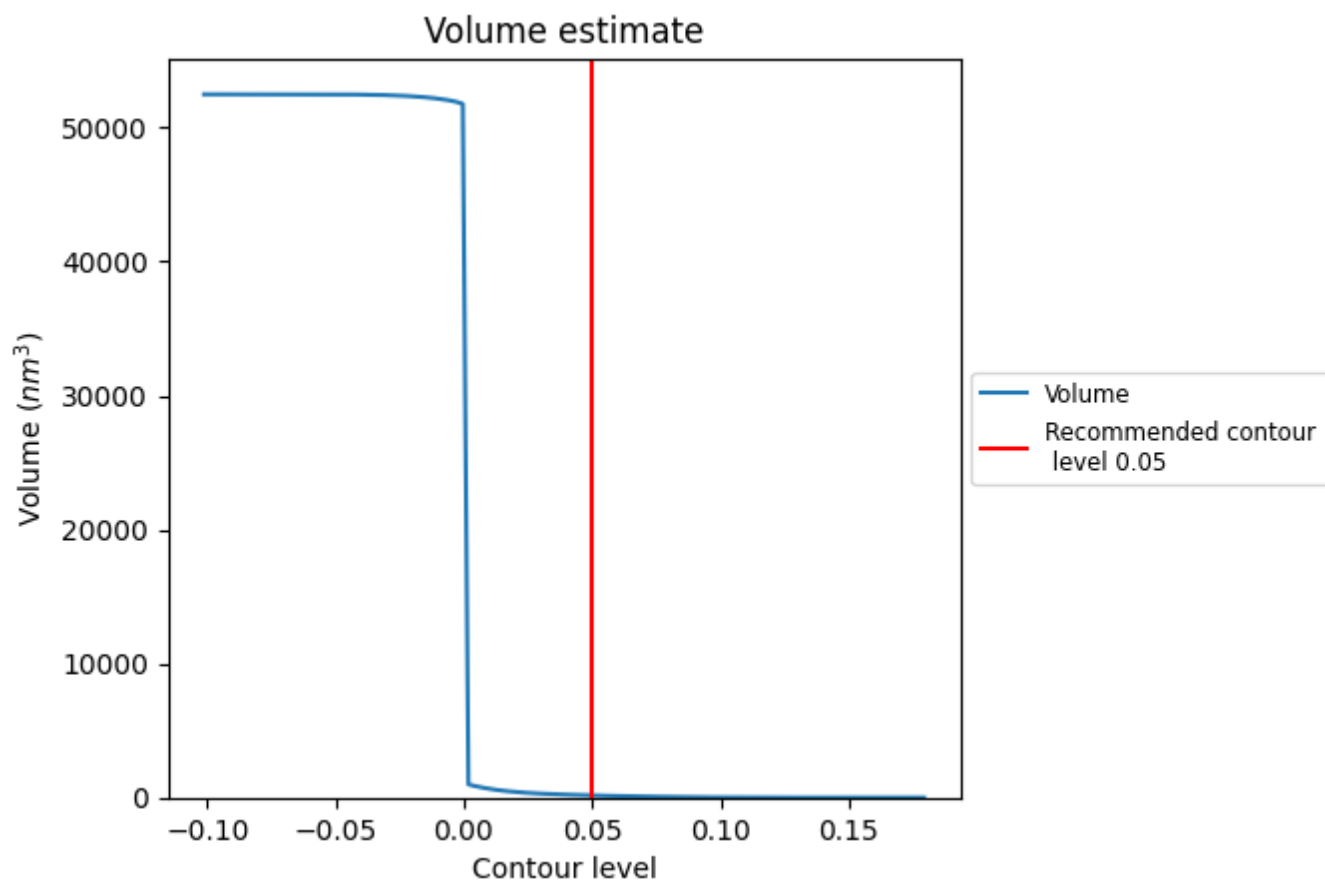
This section contains the results of statistical analysis of the map.

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.

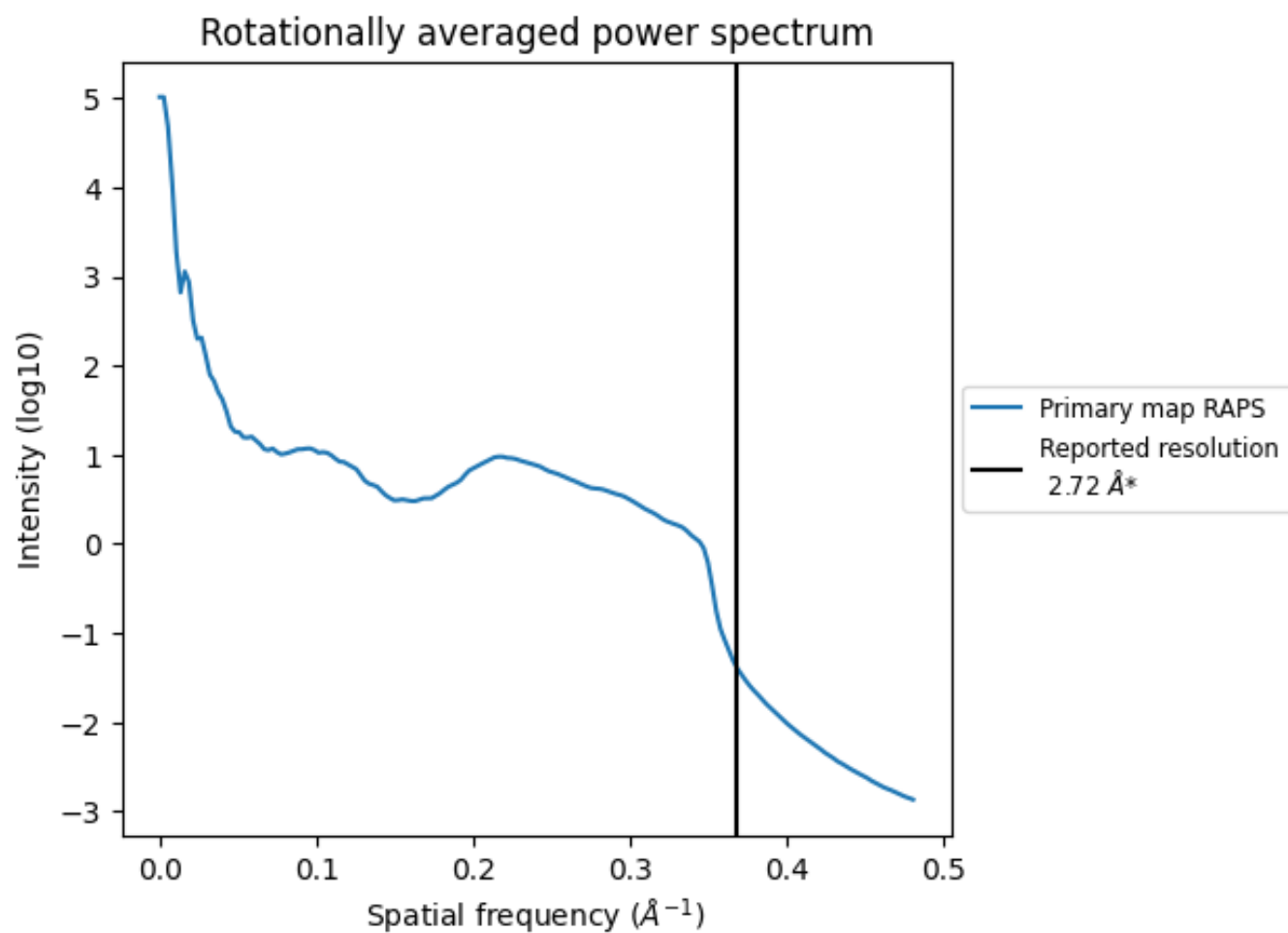
7.2 Volume estimate [i](#)



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 ⓘ

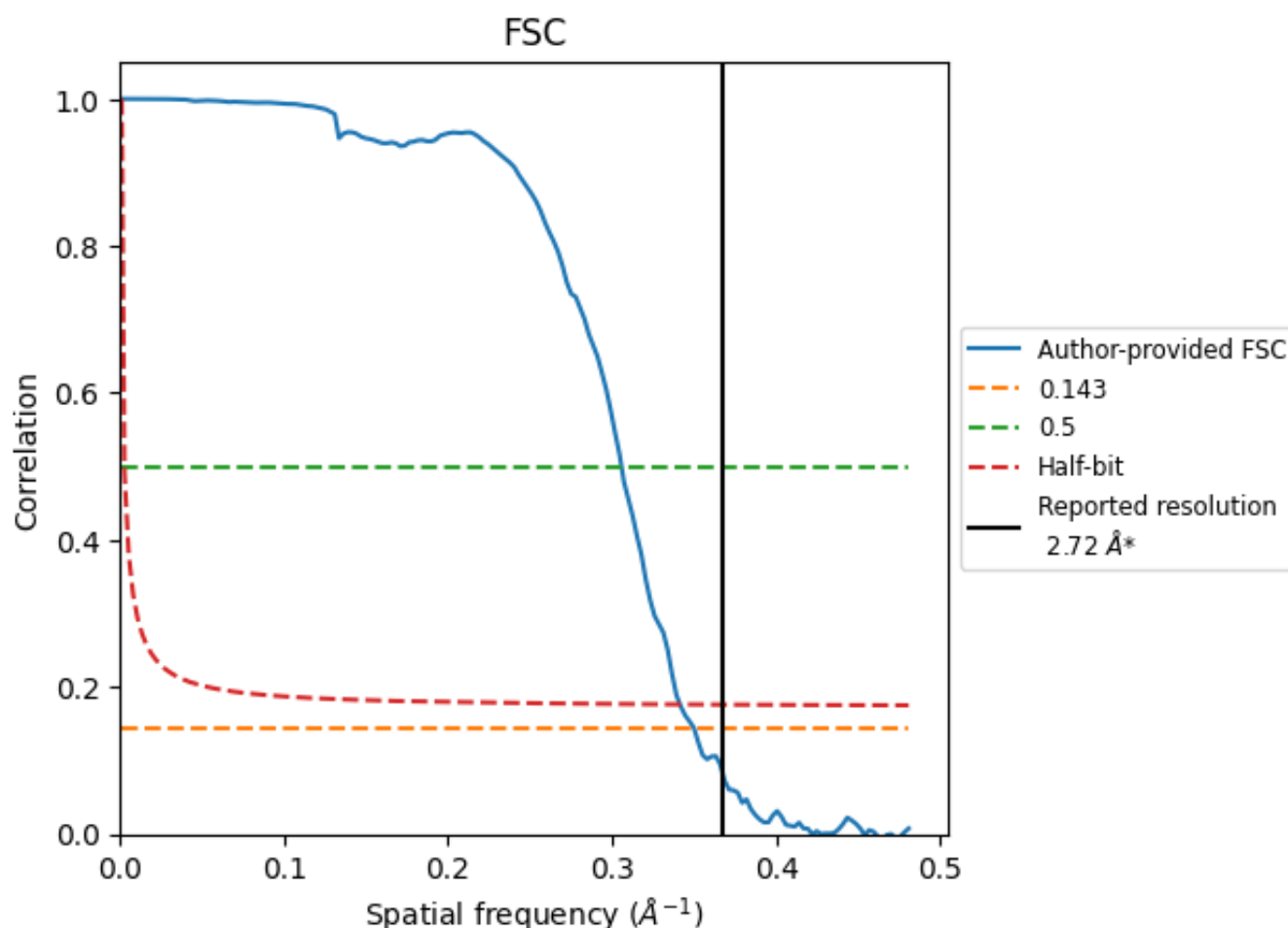


*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

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](#)

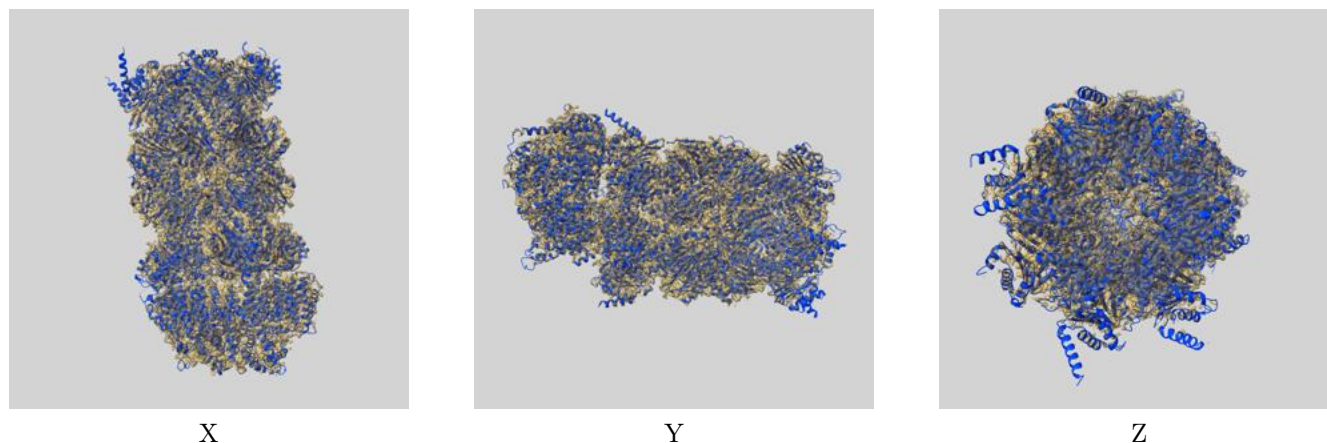
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.72	-	-
Author-provided FSC curve	2.86	3.27	2.93
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

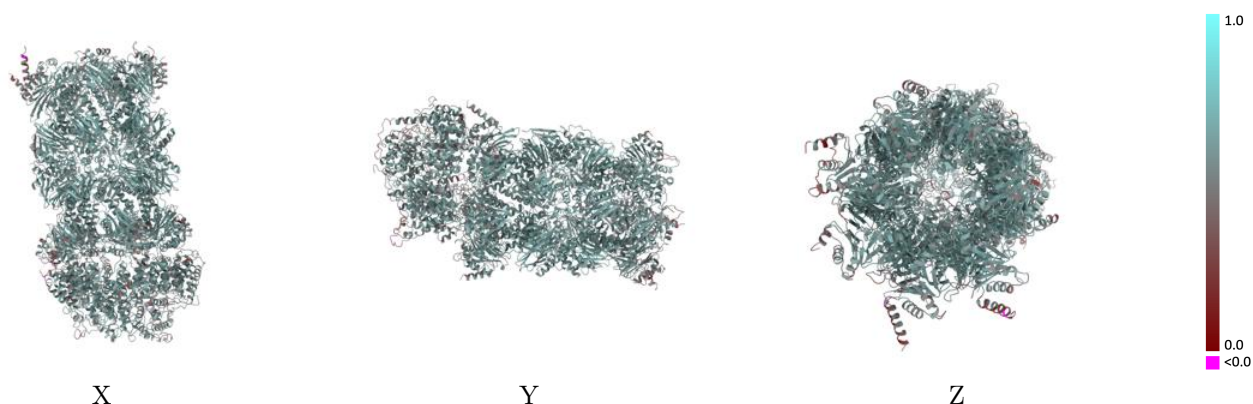
This section contains information regarding the fit between EMDB map EMD-0781 and PDB model 6KWY. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlay [i](#)



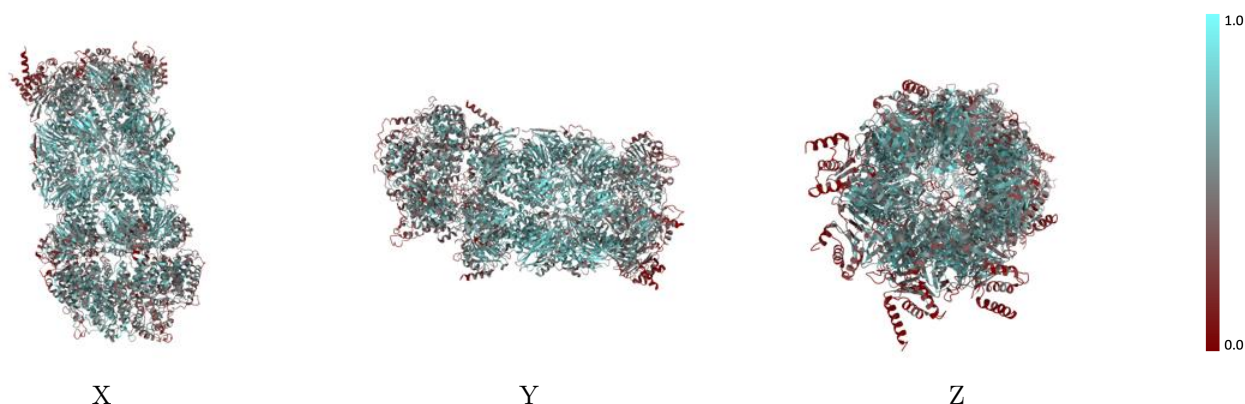
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



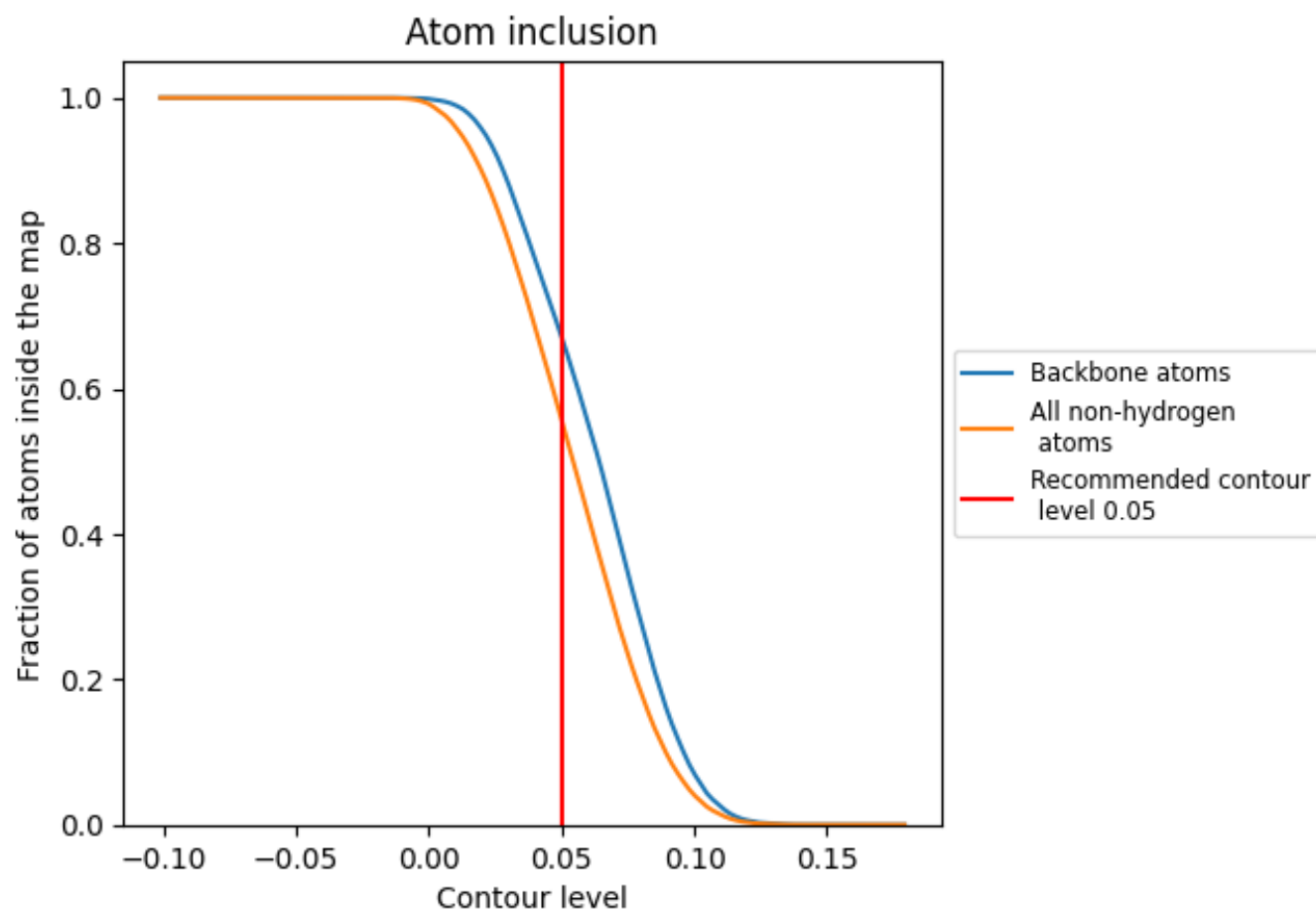
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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	 0.5571	 0.5760
A	 0.6302	 0.5930
B	 0.5167	 0.5580
C	 0.5128	 0.5580
D	 0.5365	 0.5700
E	 0.6563	 0.5960
F	 0.5948	 0.5860
G	 0.5863	 0.5790
H	 0.6528	 0.6070
I	 0.6754	 0.6190
J	 0.6809	 0.6120
K	 0.6974	 0.6150
L	 0.6159	 0.5970
M	 0.6837	 0.6110
N	 0.7030	 0.6210
O	 0.4509	 0.5560
P	 0.3664	 0.5440
Q	 0.3644	 0.5450
R	 0.4595	 0.5740
S	 0.4931	 0.5700
T	 0.5091	 0.5630
U	 0.3956	 0.5460
V	 0.5760	 0.5780
W	 0.6496	 0.6110
X	 0.6728	 0.6090
Y	 0.6796	 0.6150
Z	 0.6347	 0.6100
a	 0.6787	 0.6120
b	 0.6682	 0.6120
c	 0.4893	 0.5400

