Full wwPDB EM Validation Report (i)

Mar 20, 2024 – 04:33 PM JST

PDB ID	:	7DR6
EMDB ID	:	EMD-30824
Title	:	PA28alpha-beta in complex with immunoproteasome
Authors	:	Cong, Y.; Xu, C.
Deposited on	:	2020-12-26
Resolution	:	4.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

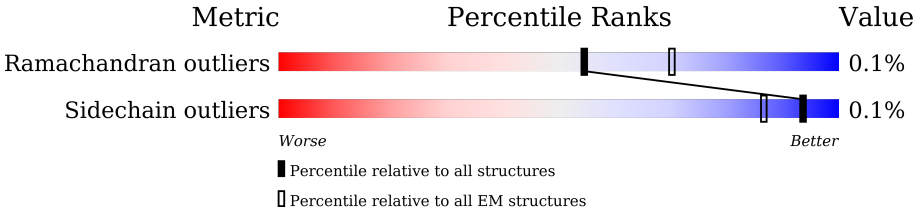
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.10 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	L	246	21% 96% .
1	e	246	34% 97% .
2	M	234	22% 97% .
2	f	234	26% 98% .
3	N	261	26% 94% 6%
3	g	261	30% 94% 6%
4	O	248	31% 94% 6%
4	a	248	30% 94% 6%
5	P	241	40% 97% .

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Mol	Chain	Length	Quality of chain
5	b	241	43% 97%
6	Q	263	32% 89% 11%
6	c	263	34% 89% 11%
7	R	255	24% 94% 6%
7	d	255	40% 94% 6%
8	A	239	50% 87% 13%
8	D	239	55% 85% 13%
8	F	239	64% 88% 12%
9	B	249	55% 85% 14%
9	C	249	54% 83% 17%
9	E	249	57% 83% 16%
9	G	249	55% 81% 18%
10	H	205	27% 100%
10	S	205	23% 99%
11	I	201	26% 99%
11	T	201	22% 98%
12	J	241	23% 88% 12%
12	U	241	24% 88% 12%
13	K	264	23% 81% 18%
13	V	264	24% 82% 18%
14	W	219	20% 91% 9%
14	Z	219	21% 91% 9%
15	1	273	20% 80% 20%
15	X	273	20% 79% 20%
16	2	276	18% 73% 27%

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Mol	Chain	Length	Quality of chain
16	Y	276	12% 73% 27%

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 59957 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	L	236	1850	1178	306	353	13	0	0
1	e	238	1856	1181	308	354	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	M	226	1763	1127	298	332	6	0	0
2	f	230	1793	1147	302	338	6	0	0

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	N	246	1936	1225	331	369	11	0	0
3	g	246	1936	1225	331	369	11	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	O	232	1824	1149	322	348	5	0	0
4	a	232	1824	1149	322	348	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	P	234	1790	1125	295	359	11	0	0
5	b	234	1790	1125	295	359	11	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	Q	235	1846	1156	330	349	11	0	0
6	c	235	1846	1156	330	349	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	R	240	1879	1191	321	356	11	0	0
7	d	240	1879	1191	321	356	11	0	0

- Molecule 8 is a protein called Proteasome activator complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	209	1684	1084	286	310	4	0	0
8	D	207	1678	1080	283	311	4	0	0
8	F	210	1695	1091	287	313	4	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PRO	HIS	variant	UNP Q9UL46
D	89	PRO	HIS	variant	UNP Q9UL46
F	89	PRO	HIS	variant	UNP Q9UL46

- Molecule 9 is a protein called Proteasome activator complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	213	1720	1102	292	320	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C	206	1663	1063	284	310	6	0	0
9	E	208	1685	1078	287	314	6	0	0
9	G	205	1654	1057	283	306	8	0	0

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H	204	1594	1015	265	295	19	0	0
10	S	204	1594	1015	265	295	19	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	I	198	1593	1023	270	292	8	0	0
11	T	197	1584	1017	268	291	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	J	213	1645	1042	282	311	10	0	0
12	U	213	1645	1042	282	311	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	K	216	1685	1065	289	319	12	0	0
13	V	216	1682	1063	289	318	12	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	W	199	1500	942	257	291	10	0	0
14	Z	199	1500	942	257	291	10	0	0

- Molecule 15 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	X	219	1611	1010	281	309	11	0	0
15	1	219	1611	1010	281	309	11	0	0

- Molecule 16 is a protein called Proteasome subunit beta type-8.

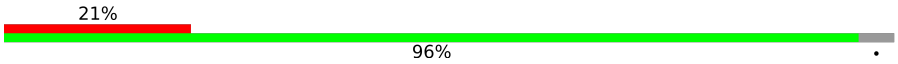
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	Y	201	1561	975	273	297	16	0	0
16	2	201	1561	975	273	297	16	0	0

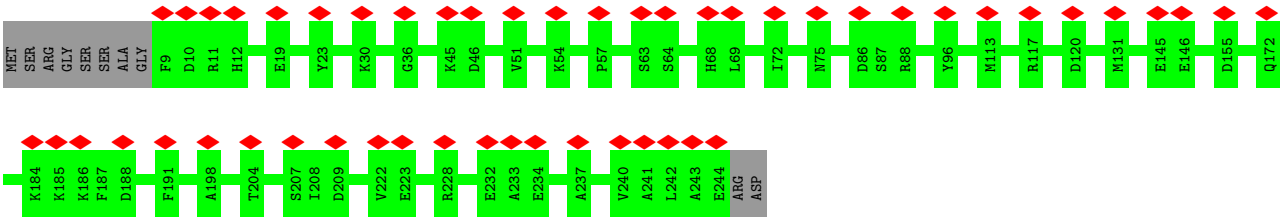
3 Residue-property plots (i)

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-6

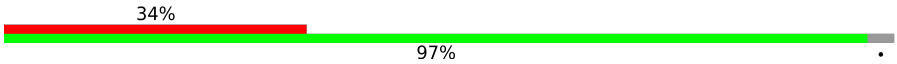
Chain L:

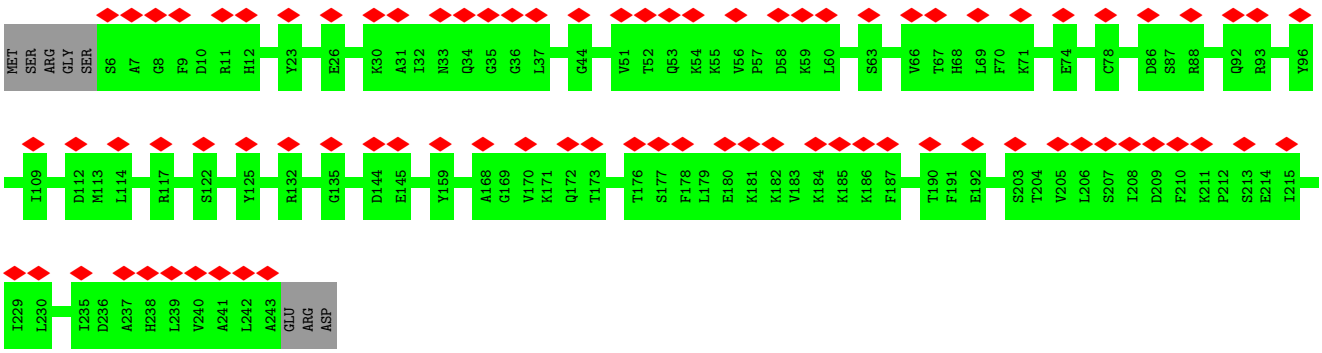




• Molecule 1: Proteasome subunit alpha type-6

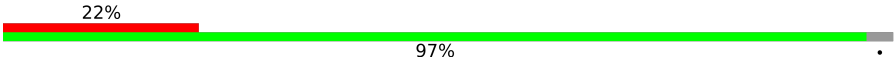
Chain e:

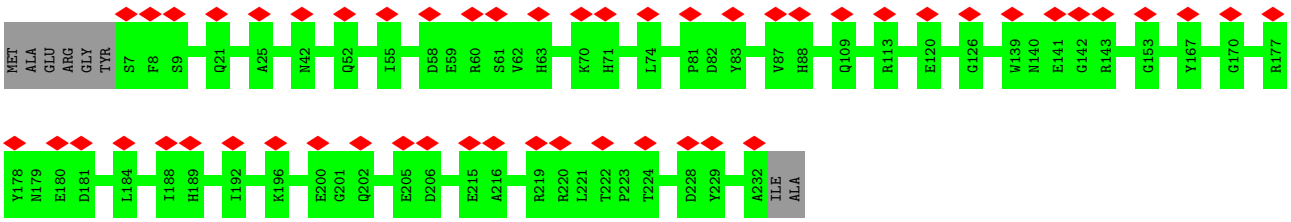




• Molecule 2: Proteasome subunit alpha type-2

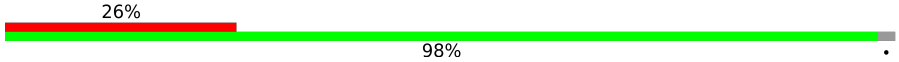
Chain M:

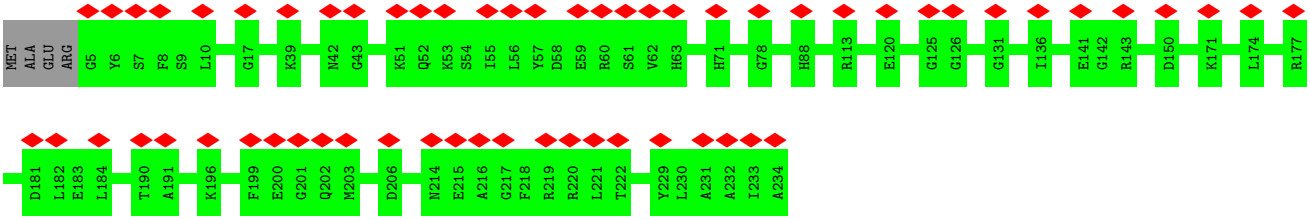




- Molecule 2: Proteasome subunit alpha type-2

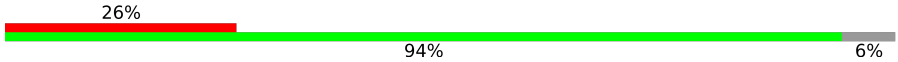
Chain f:

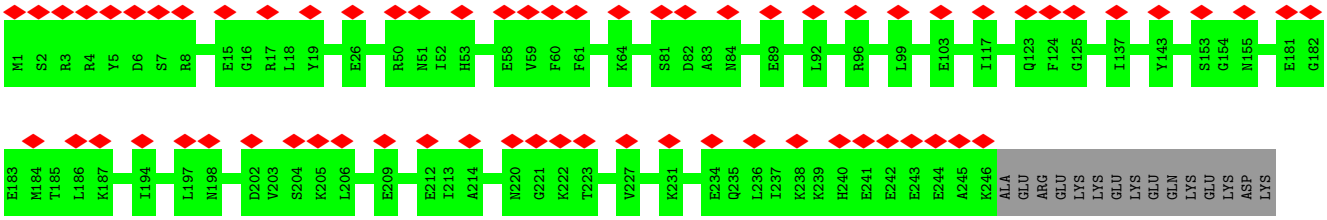




- Molecule 3: Proteasome subunit alpha type-4

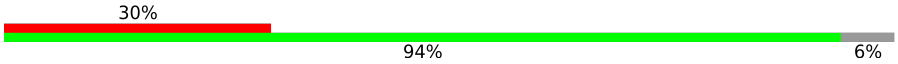
Chain N:

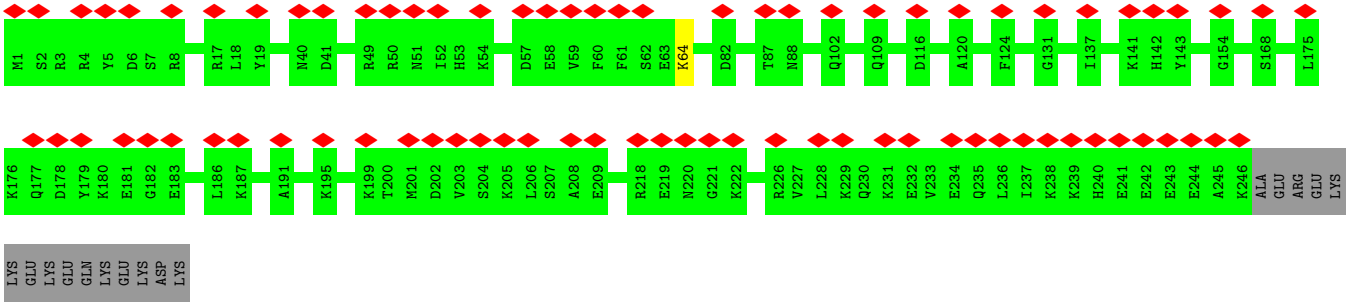




- Molecule 3: Proteasome subunit alpha type-4

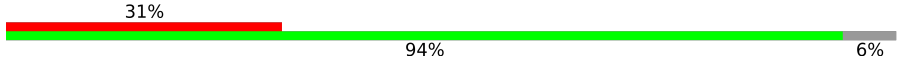
Chain g:

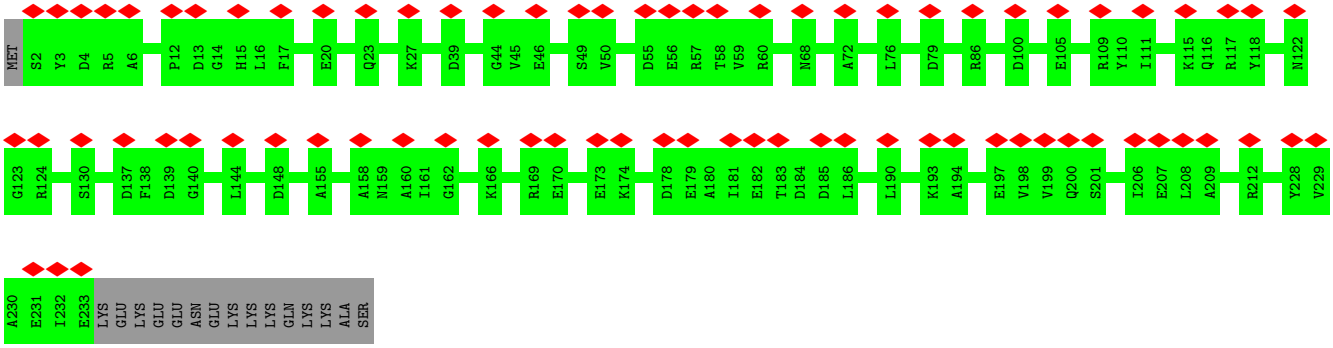




- Molecule 4: Proteasome subunit alpha type-7

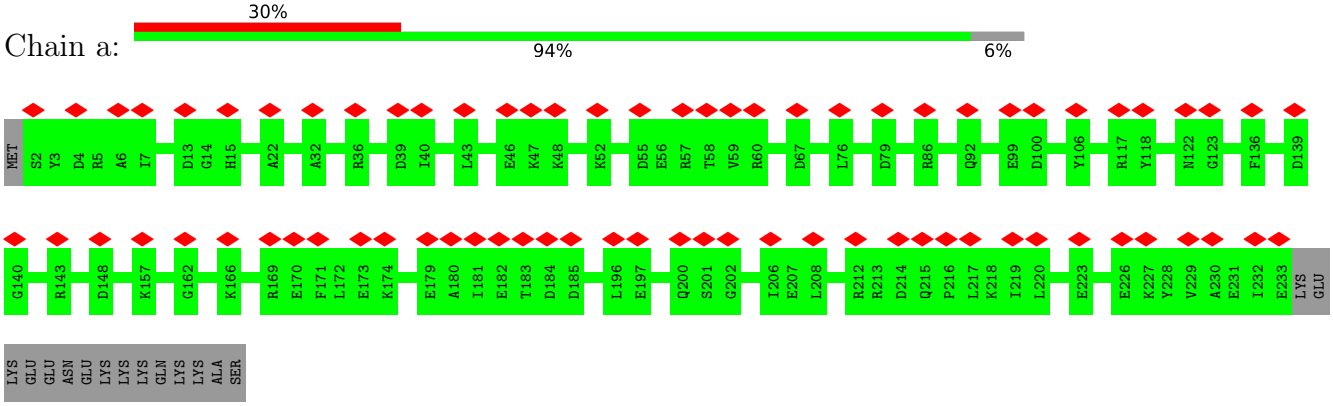
Chain O:





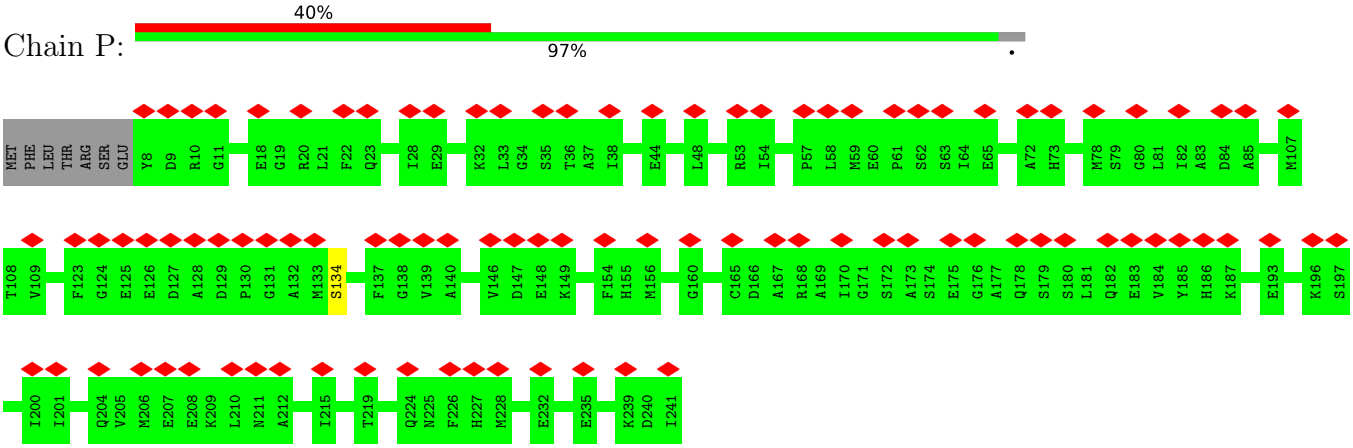
• Molecule 4: Proteasome subunit alpha type-7

Chain a:



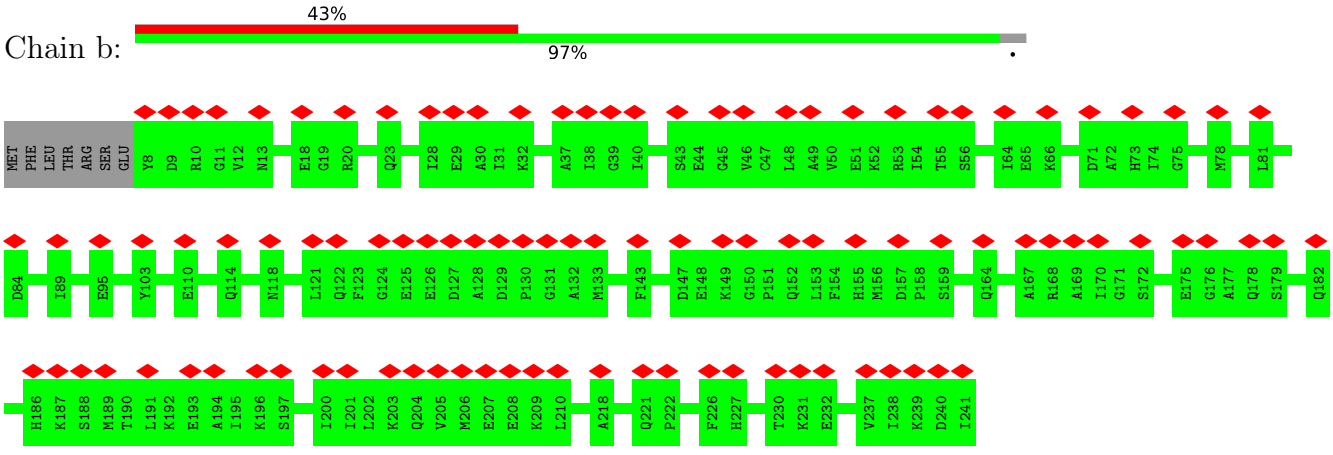
• Molecule 5: Proteasome subunit alpha type-5

Chain P:



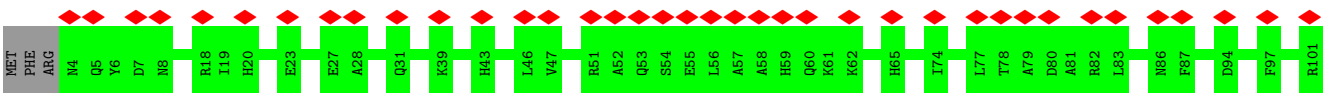
• Molecule 5: Proteasome subunit alpha type-5

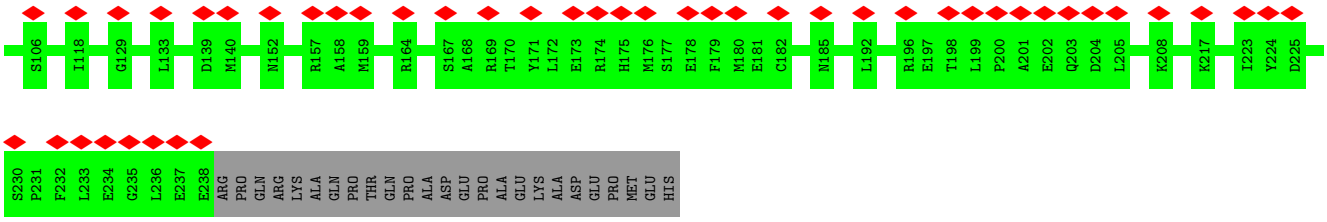
Chain b:



• Molecule 6: Proteasome subunit alpha type-1

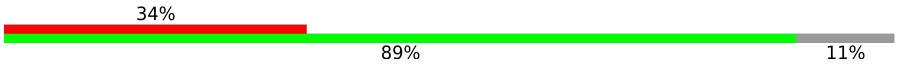
Chain Q:

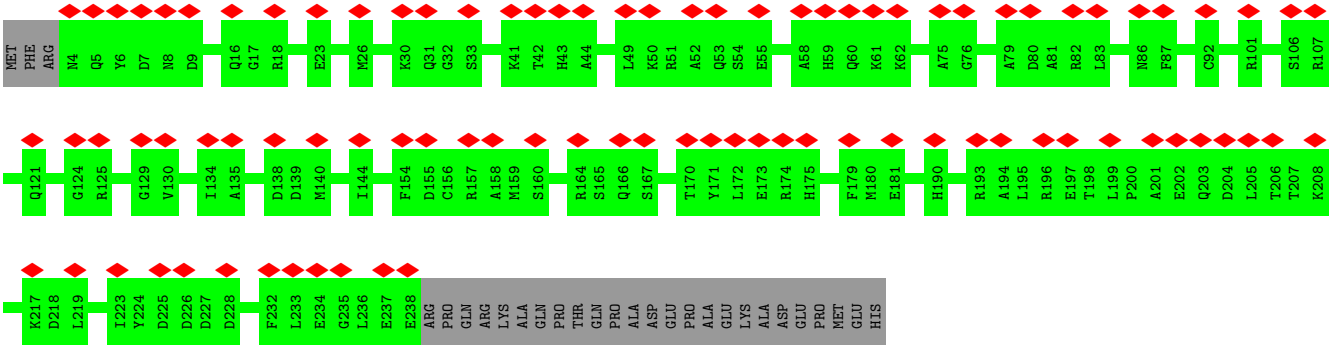




• Molecule 6: Proteasome subunit alpha type-1

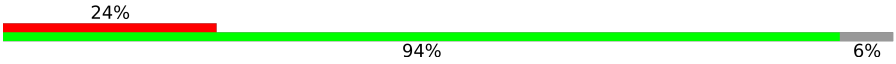
Chain c:

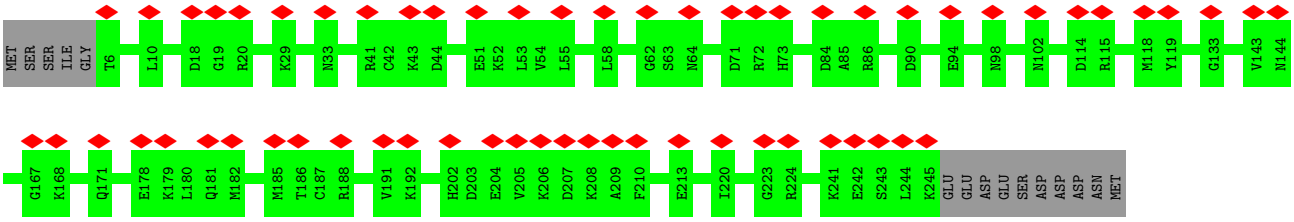




• Molecule 7: Proteasome subunit alpha type-3

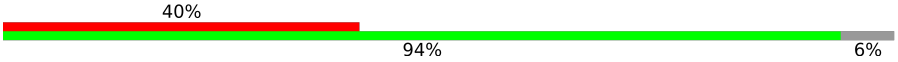
Chain R:

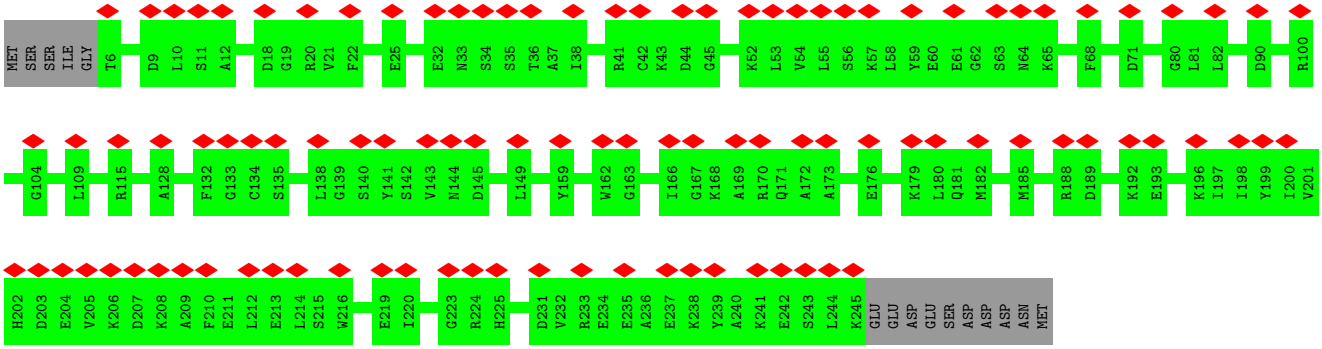




• Molecule 7: Proteasome subunit alpha type-3

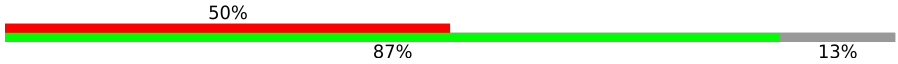
Chain d:

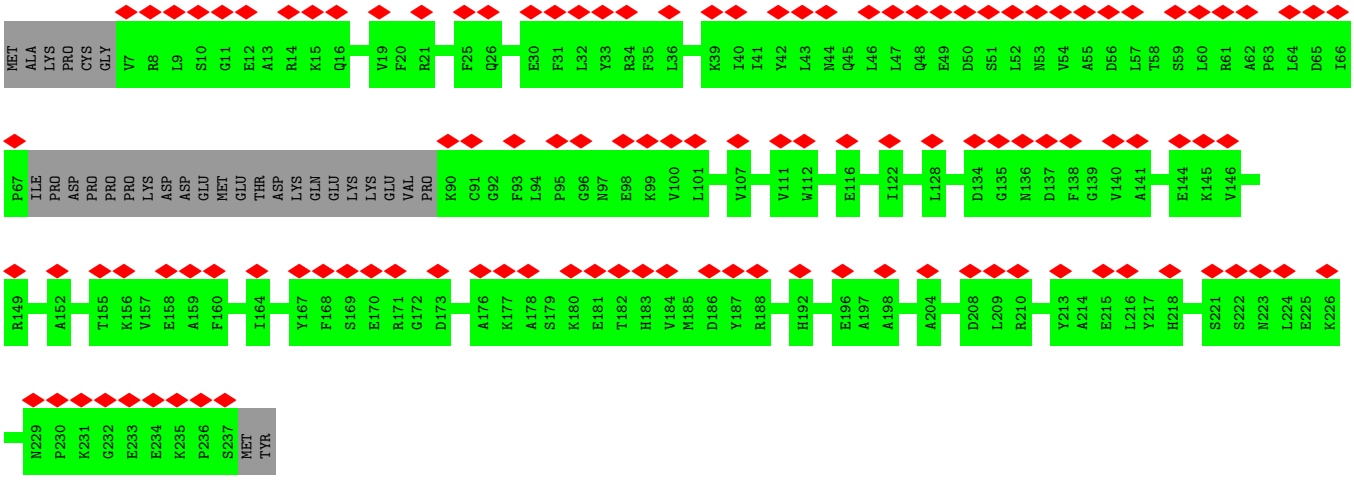




• Molecule 8: Proteasome activator complex subunit 2

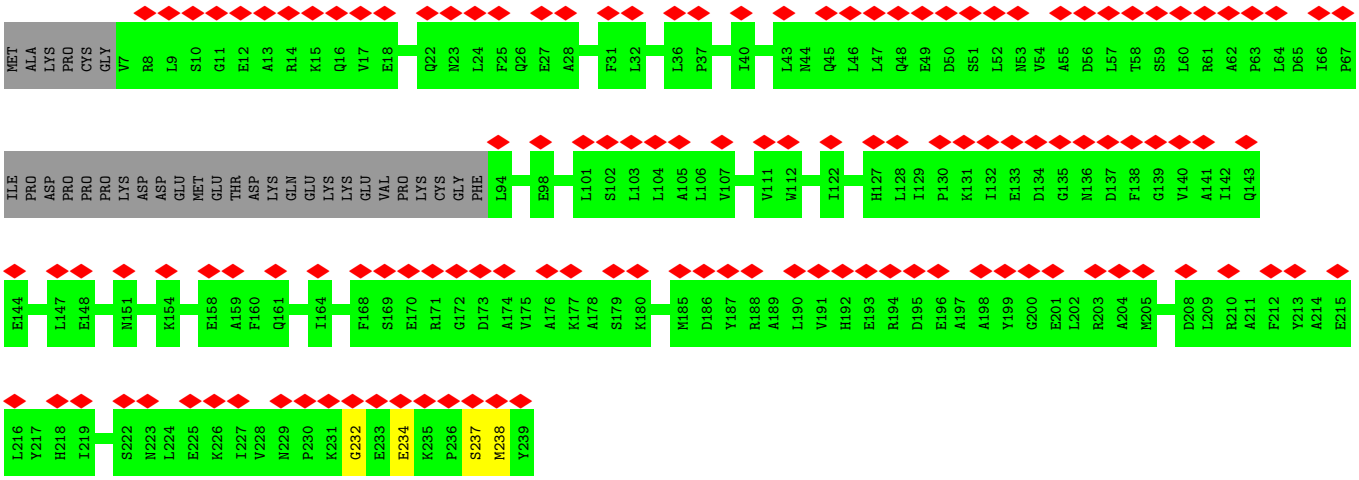
Chain A:





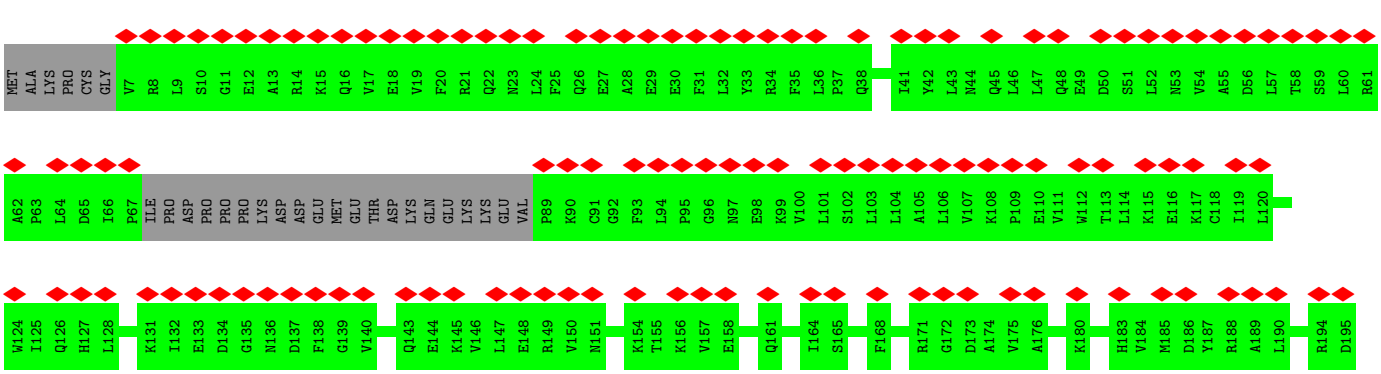
• Molecule 8: Proteasome activator complex subunit 2

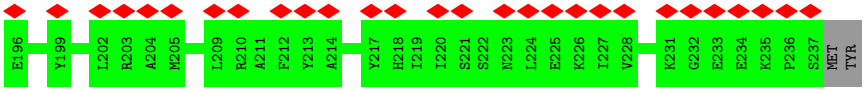
Chain D:



• Molecule 8: Proteasome activator complex subunit 2

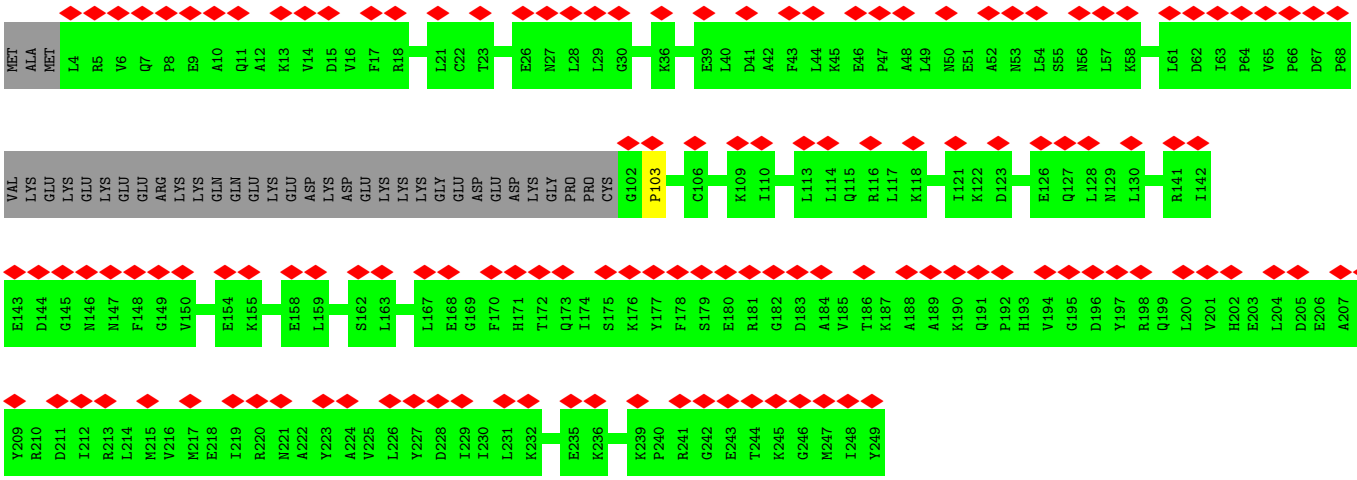
Chain F:





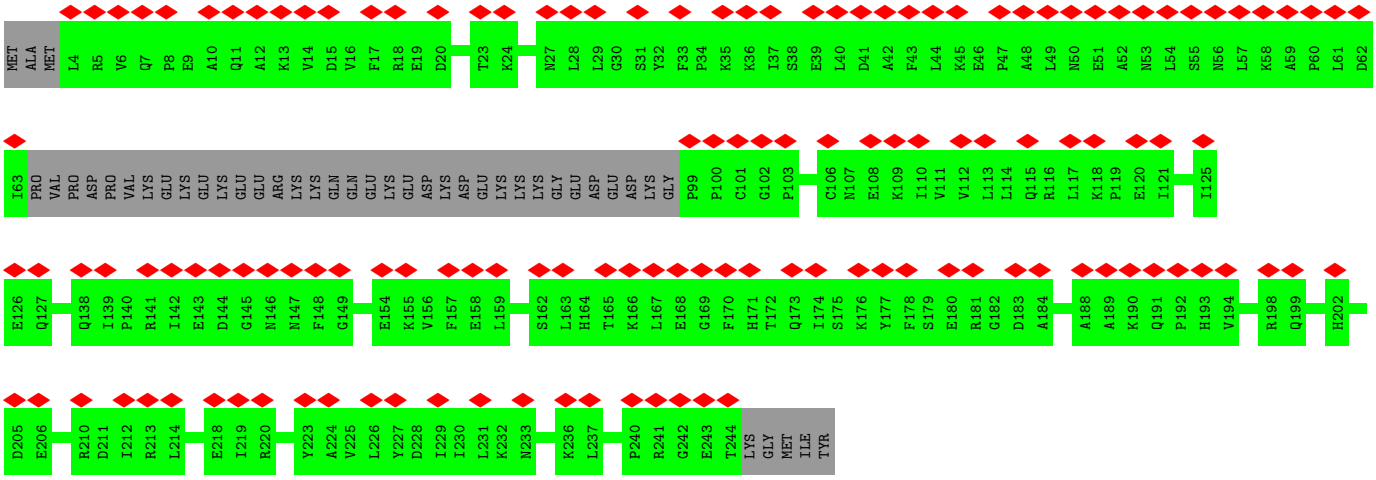
• Molecule 9: Proteasome activator complex subunit 1

Chain B:



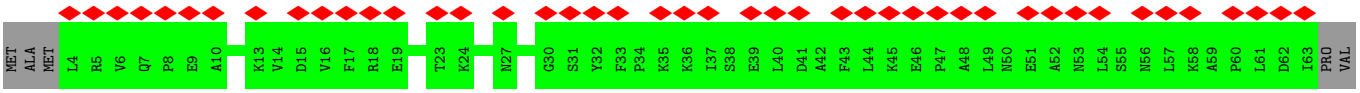
• Molecule 9: Proteasome activator complex subunit 1

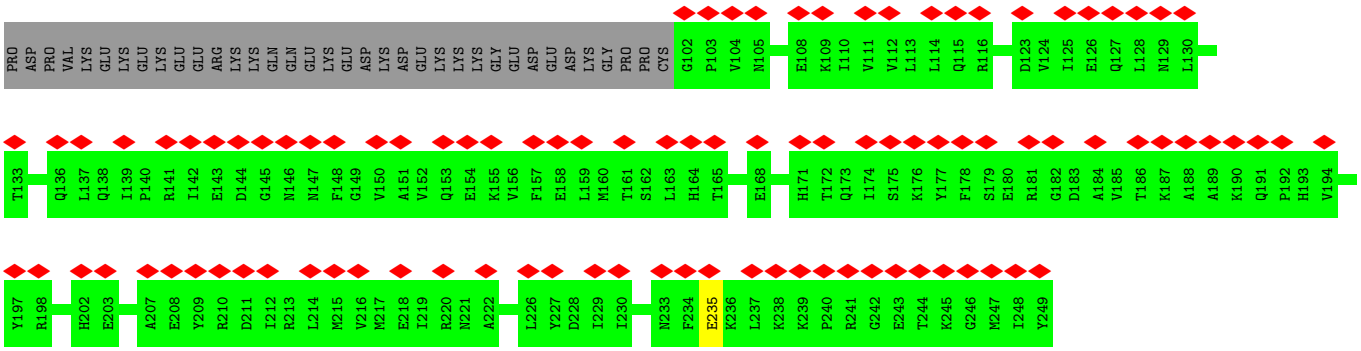
Chain C:



• Molecule 9: Proteasome activator complex subunit 1

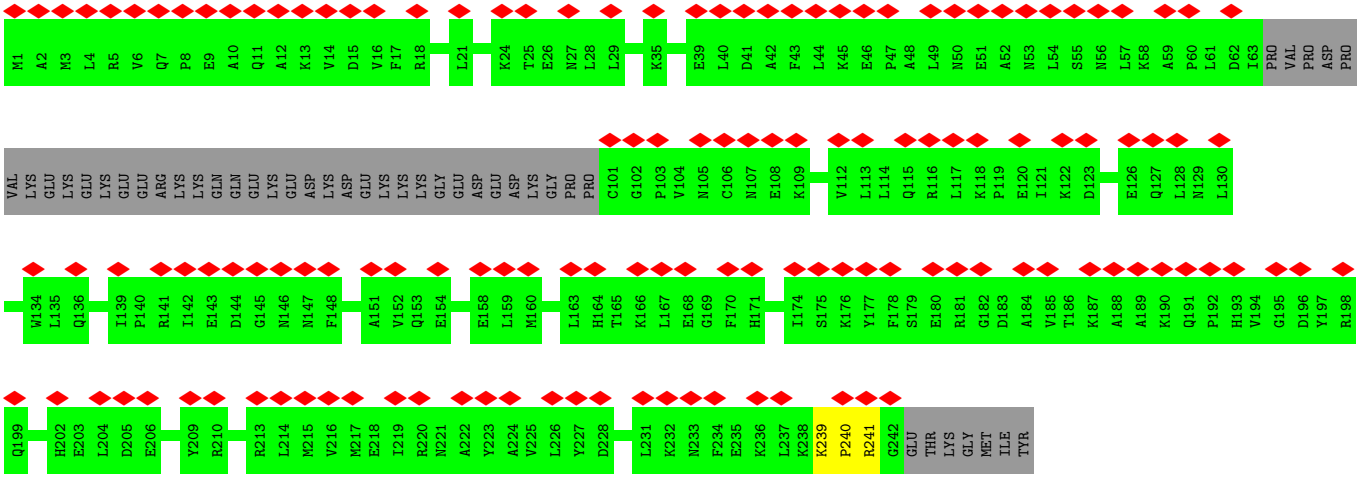
Chain E:





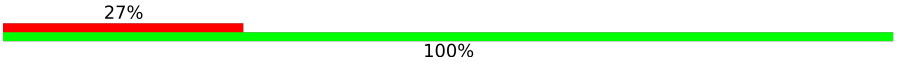
• Molecule 9: Proteasome activator complex subunit 1

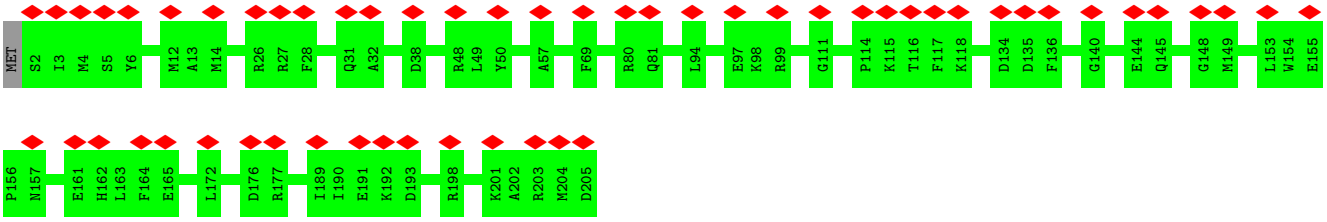
Chain G:



• Molecule 10: Proteasome subunit beta type-3

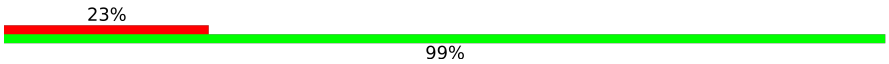
Chain H:

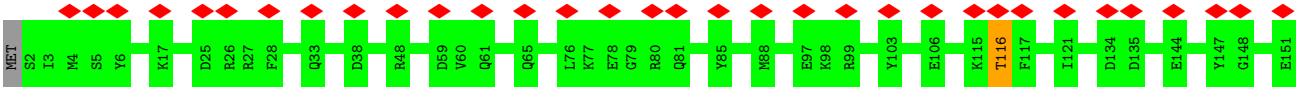


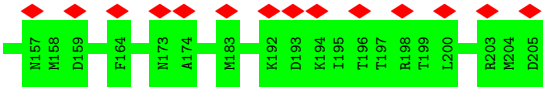


• Molecule 10: Proteasome subunit beta type-3

Chain S:

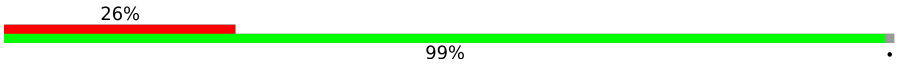


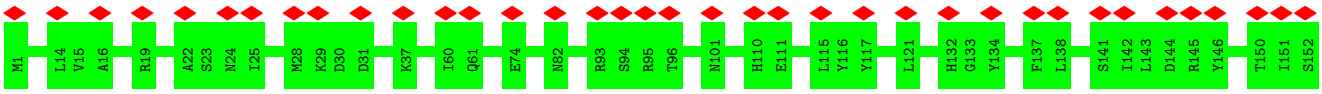


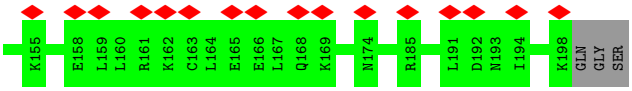


• Molecule 11: Proteasome subunit beta type-2

Chain I:

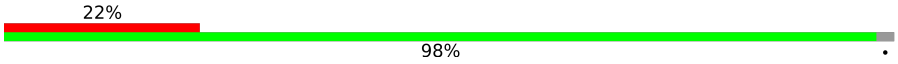


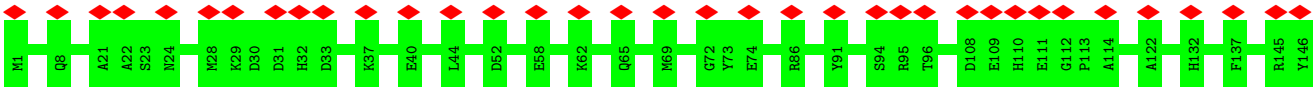


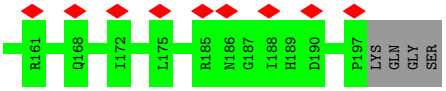


• Molecule 11: Proteasome subunit beta type-2

Chain T:

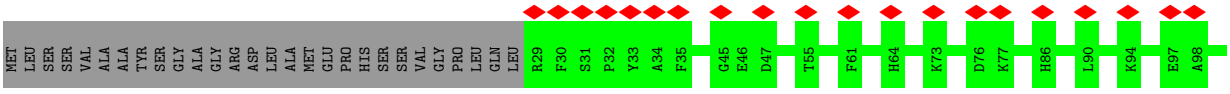


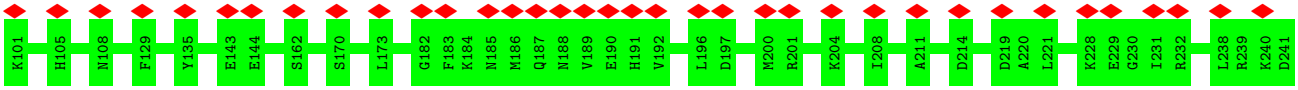




• Molecule 12: Proteasome subunit beta type-1

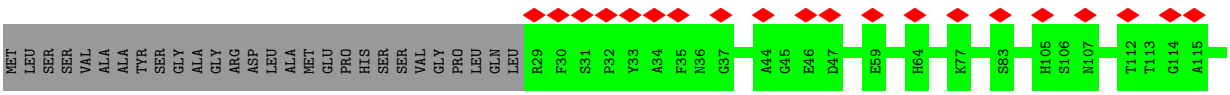
Chain J:

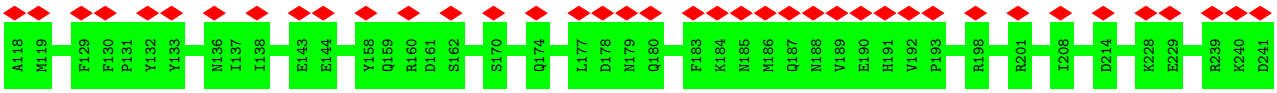




• Molecule 12: Proteasome subunit beta type-1

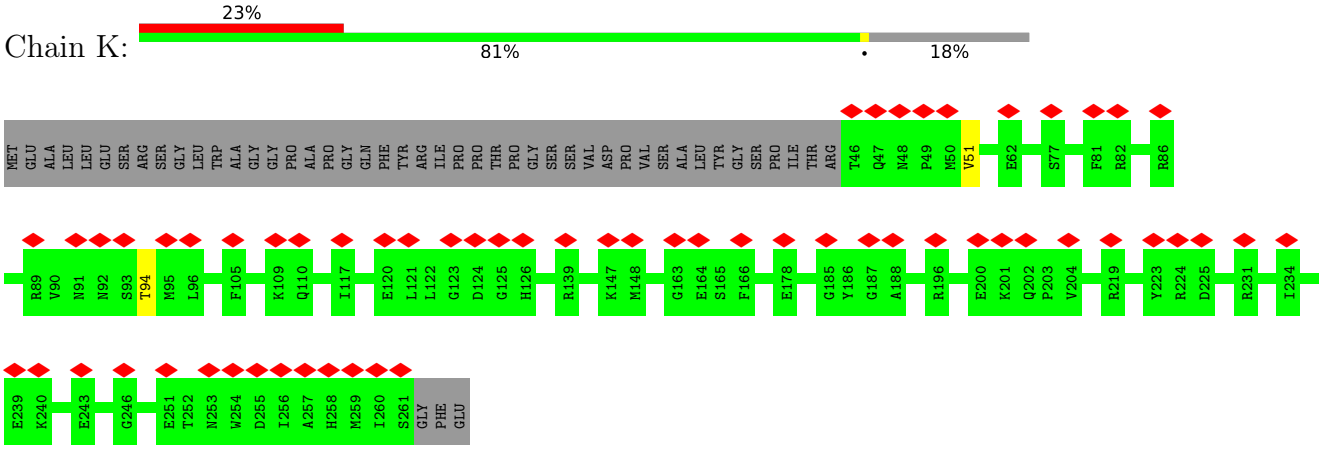
Chain U:





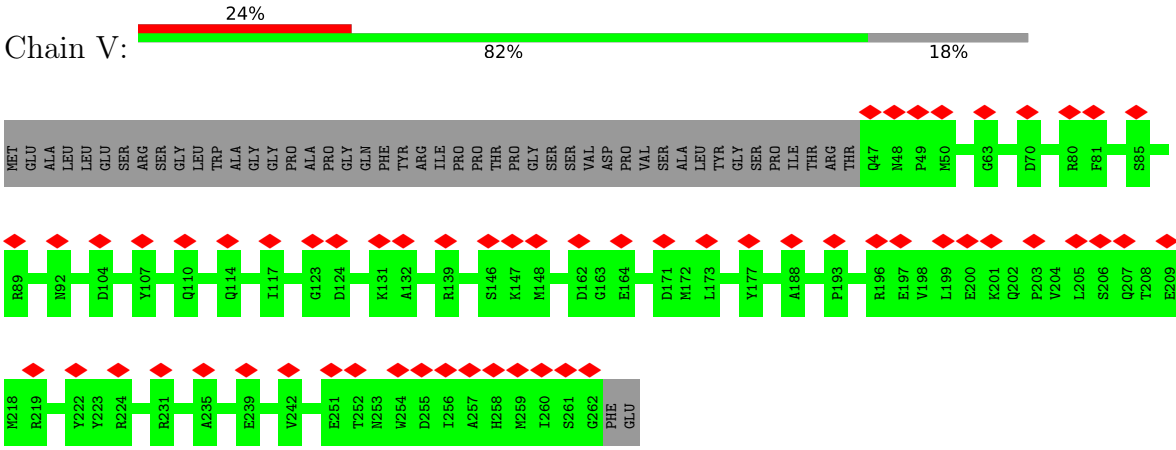
• Molecule 13: Proteasome subunit beta type-4

Chain K:



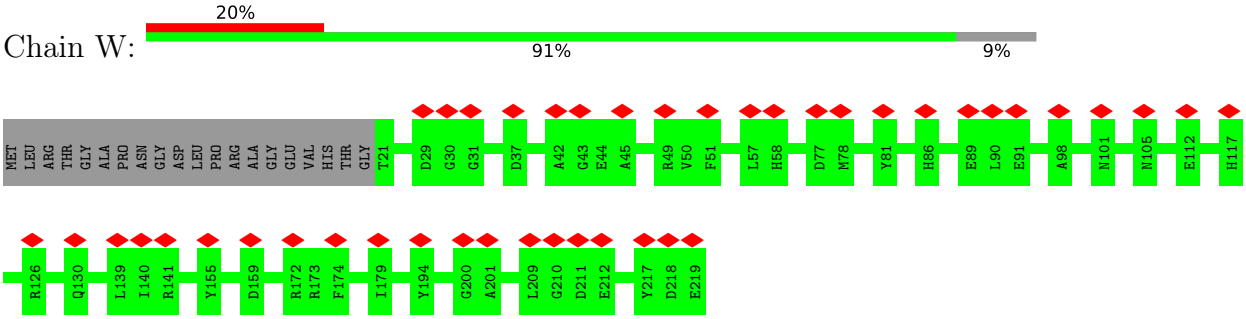
• Molecule 13: Proteasome subunit beta type-4

Chain V:



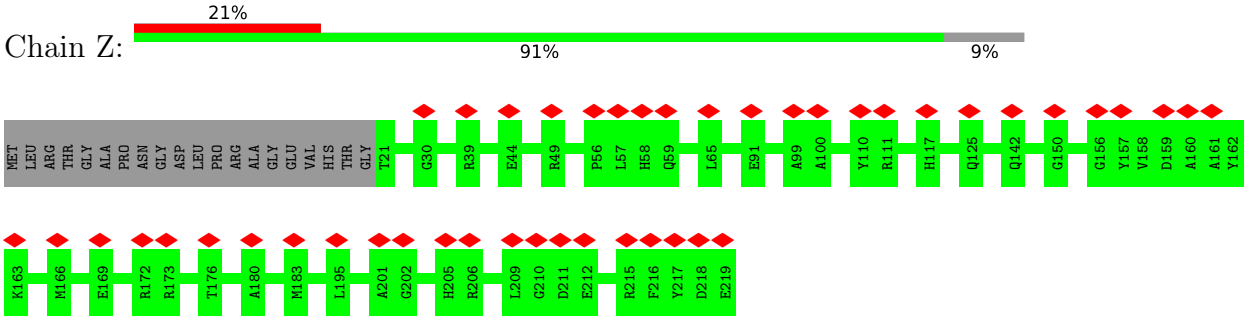
• Molecule 14: Proteasome subunit beta type-9

Chain W:



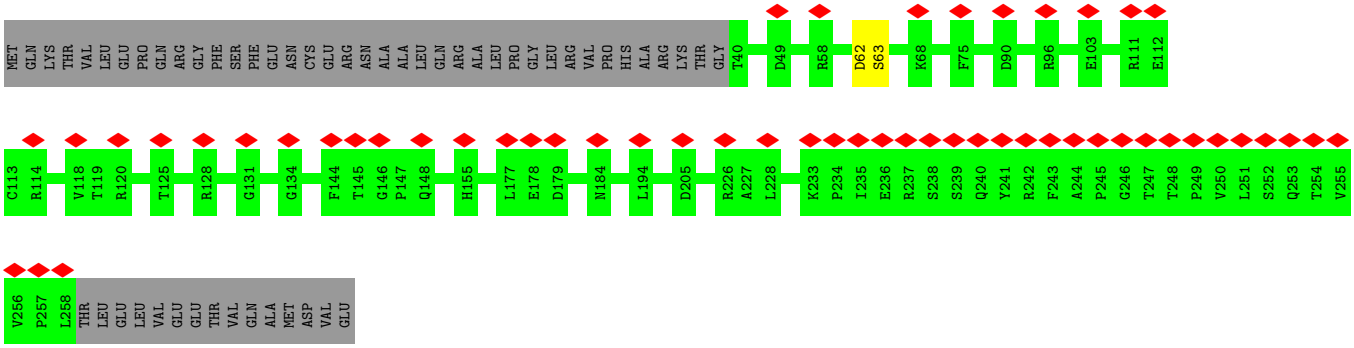
• Molecule 14: Proteasome subunit beta type-9

Chain Z:



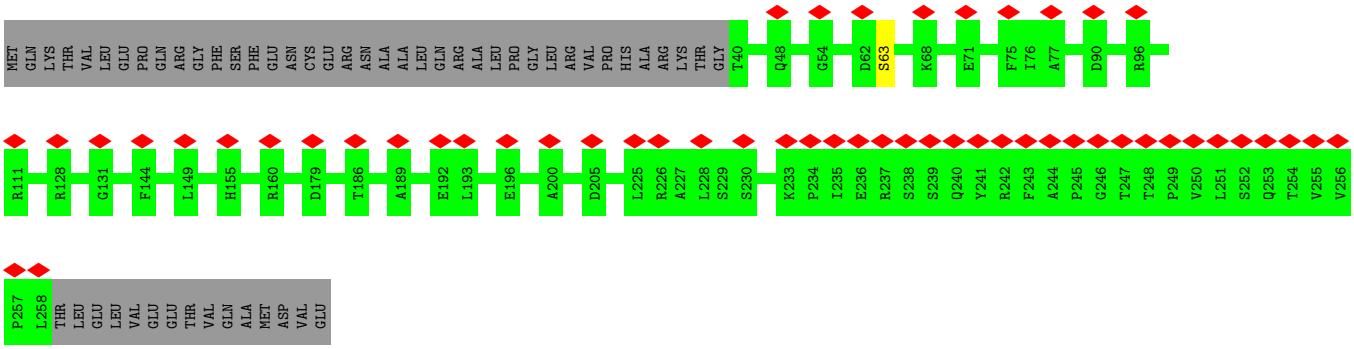
• Molecule 15: Proteasome subunit beta type-10

Chain X:



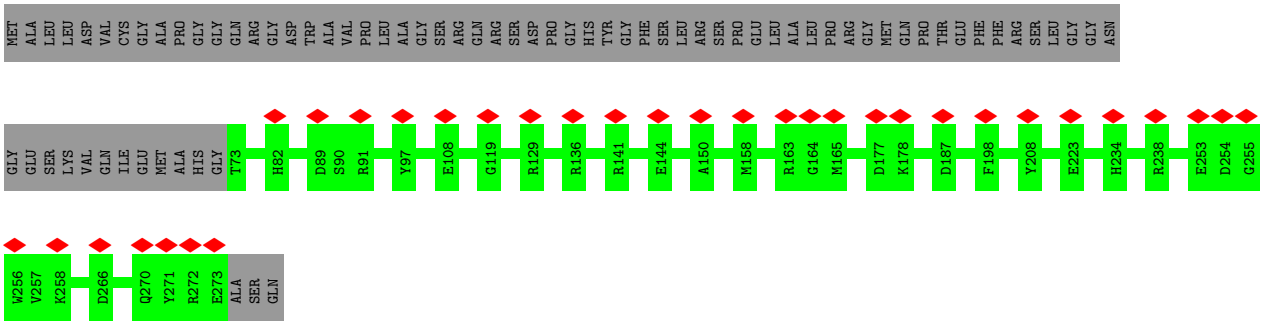
• Molecule 15: Proteasome subunit beta type-10

Chain 1:



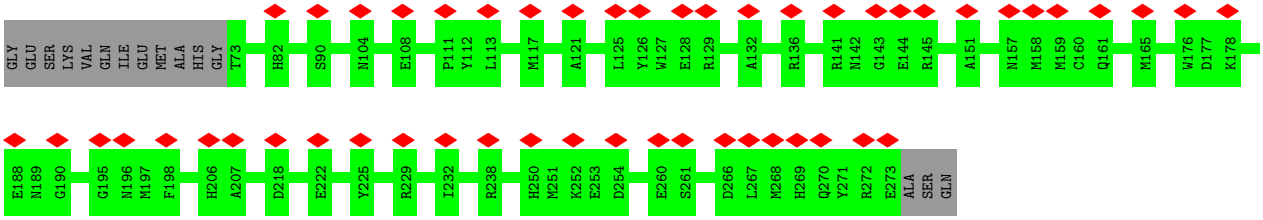
• Molecule 16: Proteasome subunit beta type-8

Chain Y:



• Molecule 16: Proteasome subunit beta type-8

Chain 2:


GLY GLU SER LYS VAL GLN ILE GLU MET ALA HIS GLY T73
H82
S90
N104
E108
P111 Y112
L113
M117
A121
L125 Y126 W127 E128 R129
A132
R136
R141 N142 G143 E144 R145
A151
N157 M158 M159 C160 Q161
M165
W176 D177 K178

E188 N189 G190
G195 N196 M197 F198
H206 A207
D218
E222
Y225
R229
I232
R238
H250 M251 K252 E253 D254
E260 S261
D266 L267 M268 H269 Q270 Y271 R272 E273
ALA SER GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45030	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	38	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	2.322	Depositor
Minimum map value	-1.426	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.619	Depositor
Map size (Å)	337.408, 337.408, 337.408	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.318, 1.318, 1.318	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	L	0.24	0/1884	0.41	0/2548
1	e	0.23	0/1890	0.41	0/2556
2	M	0.24	0/1801	0.40	0/2440
2	f	0.24	0/1832	0.41	0/2481
3	N	0.24	0/1966	0.40	0/2648
3	g	0.24	0/1966	0.42	0/2648
4	O	0.23	0/1851	0.43	0/2501
4	a	0.23	0/1851	0.42	0/2501
5	P	0.24	0/1818	0.42	0/2455
5	b	0.23	0/1818	0.40	0/2455
6	Q	0.23	0/1880	0.41	0/2541
6	c	0.23	0/1880	0.43	0/2541
7	R	0.24	0/1914	0.39	0/2578
7	d	0.24	0/1914	0.41	0/2578
8	A	0.24	0/1714	0.36	0/2315
8	D	0.23	0/1708	0.35	0/2308
8	F	0.23	0/1726	0.37	0/2331
9	B	0.25	0/1751	0.36	0/2366
9	C	0.23	0/1692	0.36	0/2285
9	E	0.24	0/1713	0.37	0/2309
9	G	0.23	0/1681	0.37	0/2267
10	H	0.24	0/1623	0.45	0/2188
10	S	0.25	0/1623	0.44	0/2188
11	I	0.24	0/1627	0.42	0/2201
11	T	0.24	0/1618	0.42	0/2190
12	J	0.24	0/1676	0.43	0/2258
12	U	0.24	0/1676	0.43	0/2258
13	K	0.23	0/1718	0.43	0/2324
13	V	0.24	0/1715	0.45	0/2319
14	W	0.24	0/1529	0.41	0/2071
14	Z	0.24	0/1529	0.42	0/2071
15	1	0.25	0/1637	0.45	0/2225
15	X	0.25	0/1637	0.44	0/2225
16	2	0.24	0/1592	0.43	0/2145

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
16	Y	0.25	0/1592	0.41	0/2145
All	All	0.24	0/61042	0.41	0/82460

There are no bond length outliers.

There are no bond angle outliers.

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	L	234/246 (95%)	220 (94%)	14 (6%)	0	100	100
1	e	236/246 (96%)	217 (92%)	19 (8%)	0	100	100
2	M	224/234 (96%)	217 (97%)	7 (3%)	0	100	100
2	f	228/234 (97%)	220 (96%)	8 (4%)	0	100	100
3	N	244/261 (94%)	234 (96%)	10 (4%)	0	100	100
3	g	244/261 (94%)	226 (93%)	17 (7%)	1 (0%)	34	71
4	O	230/248 (93%)	220 (96%)	10 (4%)	0	100	100
4	a	230/248 (93%)	218 (95%)	12 (5%)	0	100	100
5	P	232/241 (96%)	218 (94%)	14 (6%)	0	100	100
5	b	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
6	Q	233/263 (89%)	217 (93%)	16 (7%)	0	100	100
6	c	233/263 (89%)	224 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	R	238/255 (93%)	230 (97%)	8 (3%)	0	100	100
7	d	238/255 (93%)	227 (95%)	11 (5%)	0	100	100
8	A	205/239 (86%)	204 (100%)	1 (0%)	0	100	100
8	D	203/239 (85%)	193 (95%)	9 (4%)	1 (0%)	29	67
8	F	206/239 (86%)	202 (98%)	4 (2%)	0	100	100
9	B	209/249 (84%)	202 (97%)	6 (3%)	1 (0%)	29	67
9	C	202/249 (81%)	198 (98%)	4 (2%)	0	100	100
9	E	204/249 (82%)	194 (95%)	9 (4%)	1 (0%)	29	67
9	G	201/249 (81%)	194 (96%)	4 (2%)	3 (2%)	10	44
10	H	202/205 (98%)	188 (93%)	14 (7%)	0	100	100
10	S	202/205 (98%)	185 (92%)	16 (8%)	1 (0%)	29	67
11	I	196/201 (98%)	186 (95%)	10 (5%)	0	100	100
11	T	195/201 (97%)	183 (94%)	12 (6%)	0	100	100
12	J	211/241 (88%)	198 (94%)	13 (6%)	0	100	100
12	U	211/241 (88%)	197 (93%)	14 (7%)	0	100	100
13	K	214/264 (81%)	206 (96%)	7 (3%)	1 (0%)	29	67
13	V	214/264 (81%)	203 (95%)	11 (5%)	0	100	100
14	W	197/219 (90%)	185 (94%)	12 (6%)	0	100	100
14	Z	197/219 (90%)	191 (97%)	6 (3%)	0	100	100
15	1	217/273 (80%)	203 (94%)	13 (6%)	1 (0%)	29	67
15	X	217/273 (80%)	199 (92%)	17 (8%)	1 (0%)	29	67
16	2	199/276 (72%)	186 (94%)	13 (6%)	0	100	100
16	Y	199/276 (72%)	185 (93%)	14 (7%)	0	100	100
All	All	7577/8567 (88%)	7194 (95%)	372 (5%)	11 (0%)	54	84

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	232	GLY
15	1	63	SER
15	X	63	SER
9	G	240	PRO
9	G	241	ARG
10	S	116	THR

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Mol	Chain	Res	Type
9	B	103	PRO
9	E	235	GLU
3	g	64	LYS
9	G	239	LYS
13	K	51	VAL

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	L	203/210 (97%)	203 (100%)	0	100	100
1	e	203/210 (97%)	203 (100%)	0	100	100
2	M	186/191 (97%)	186 (100%)	0	100	100
2	f	188/191 (98%)	188 (100%)	0	100	100
3	N	207/221 (94%)	207 (100%)	0	100	100
3	g	207/221 (94%)	207 (100%)	0	100	100
4	O	196/211 (93%)	196 (100%)	0	100	100
4	a	196/211 (93%)	196 (100%)	0	100	100
5	P	196/203 (97%)	195 (100%)	1 (0%)	88	93
5	b	196/203 (97%)	196 (100%)	0	100	100
6	Q	201/225 (89%)	201 (100%)	0	100	100
6	c	201/225 (89%)	201 (100%)	0	100	100
7	R	198/212 (93%)	198 (100%)	0	100	100
7	d	198/212 (93%)	198 (100%)	0	100	100
8	A	183/212 (86%)	183 (100%)	0	100	100
8	D	183/212 (86%)	180 (98%)	3 (2%)	62	78
8	F	185/212 (87%)	185 (100%)	0	100	100
9	B	191/224 (85%)	191 (100%)	0	100	100
9	C	185/224 (83%)	185 (100%)	0	100	100
9	E	186/224 (83%)	186 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	G	183/224 (82%)	183 (100%)	0	100	100
10	H	174/175 (99%)	174 (100%)	0	100	100
10	S	174/175 (99%)	173 (99%)	1 (1%)	86	92
11	I	169/171 (99%)	169 (100%)	0	100	100
11	T	168/171 (98%)	168 (100%)	0	100	100
12	J	177/198 (89%)	177 (100%)	0	100	100
12	U	177/198 (89%)	177 (100%)	0	100	100
13	K	178/215 (83%)	177 (99%)	1 (1%)	86	92
13	V	177/215 (82%)	177 (100%)	0	100	100
14	W	153/167 (92%)	153 (100%)	0	100	100
14	Z	153/167 (92%)	153 (100%)	0	100	100
15	1	170/216 (79%)	170 (100%)	0	100	100
15	X	170/216 (79%)	169 (99%)	1 (1%)	86	92
16	2	166/222 (75%)	166 (100%)	0	100	100
16	Y	166/222 (75%)	166 (100%)	0	100	100
All	All	6444/7206 (89%)	6437 (100%)	7 (0%)	93	97

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	P	134	SER
8	D	234	GLU
8	D	237	SER
8	D	238	MET
13	K	94	THR
10	S	116	THR
15	X	62	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	24	GLN
1	L	53	GLN
1	L	123	GLN
1	L	150	GLN
2	M	119	GLN

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Mol	Chain	Res	Type
3	N	146	GLN
3	N	155	ASN
4	O	18	GLN
4	O	94	HIS
4	O	175	ASN
4	O	205	ASN
5	P	23	GLN
6	Q	16	GLN
8	D	136	ASN
9	E	136	GLN
9	E	164	HIS
9	G	7	GLN
9	G	199	GLN
4	a	18	GLN
4	a	94	HIS
4	a	116	GLN
5	b	99	HIS
5	b	164	GLN
7	d	144	ASN
3	g	100	GLN
3	g	146	GLN
3	g	240	HIS
10	H	7	ASN
10	H	33	GLN
12	J	86	HIS
12	J	105	HIS
12	J	107	ASN
12	J	185	ASN
13	K	126	HIS
10	S	188	HIS
12	U	105	HIS
12	U	107	ASN
12	U	108	ASN
13	V	91	ASN
13	V	126	HIS
15	X	61	ASN
15	X	191	GLN
16	Y	234	HIS
16	Y	237	HIS
16	Y	269	HIS
14	Z	86	HIS
16	2	110	ASN

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Mol	Chain	Res	Type
16	2	206	HIS
16	2	234	HIS
16	2	247	ASN

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)

There are no ligands in this entry.

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.

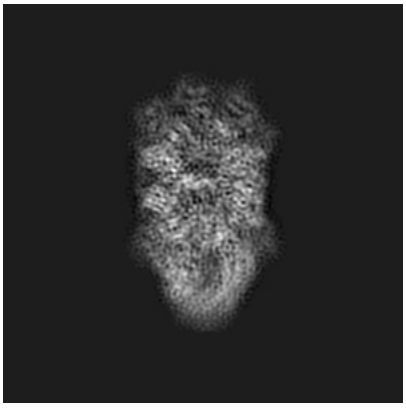
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-30824. These allow visual inspection of the internal detail of the map and identification of artifacts.

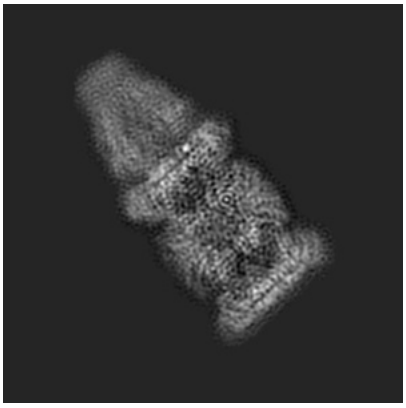
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

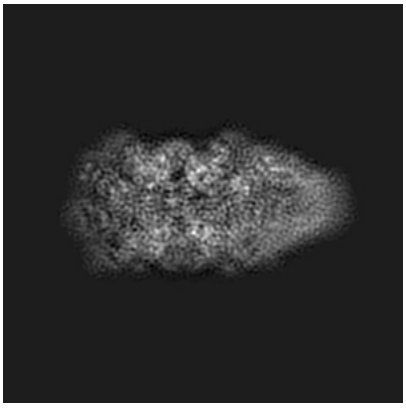
6.1.1 Primary map



X



Y



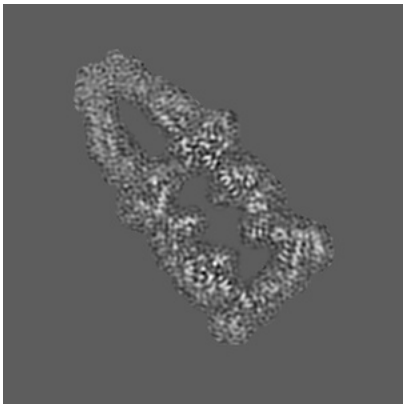
Z

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

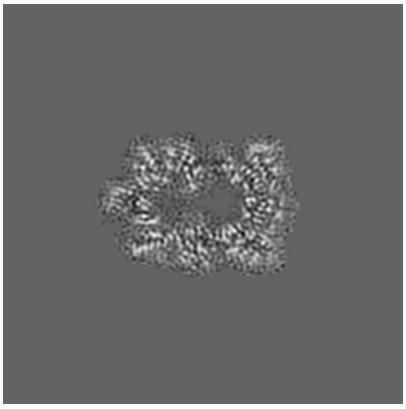
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128



Y Index: 128



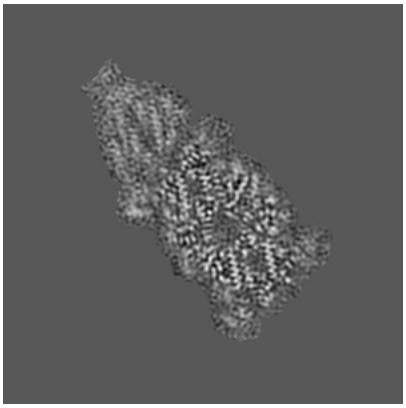
Z Index: 128

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

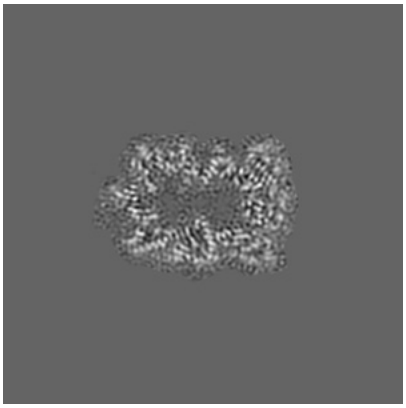
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 120



Y Index: 109

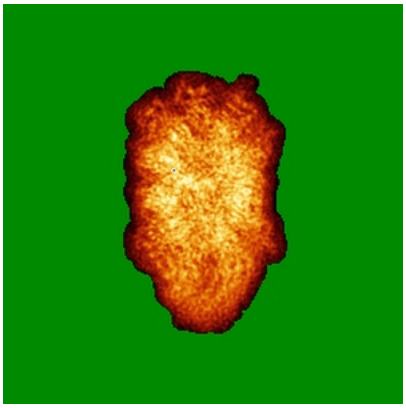


Z Index: 130

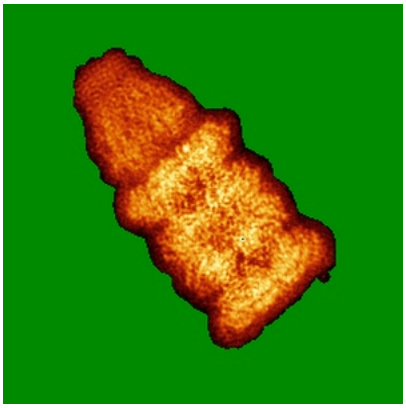
The images above show the largest variance slices of the map in three orthogonal directions.

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

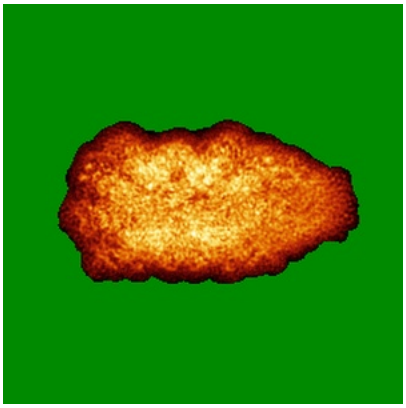
6.4.1 Primary map



X



Y

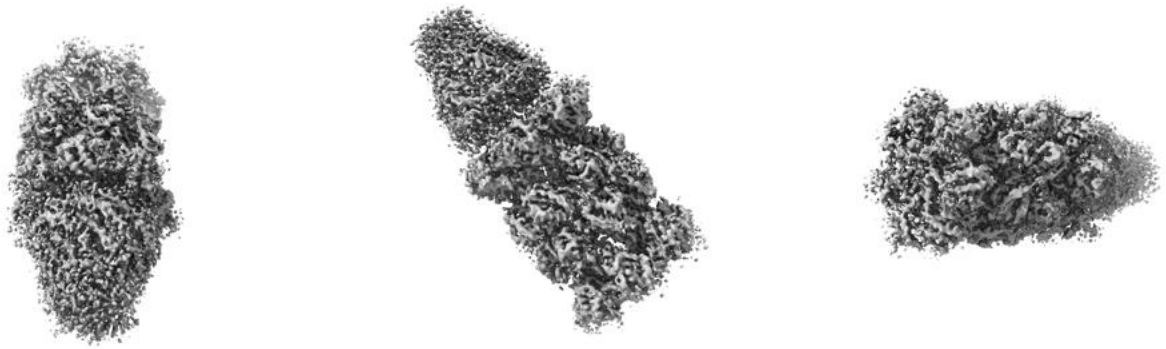


Z

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 0.619. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

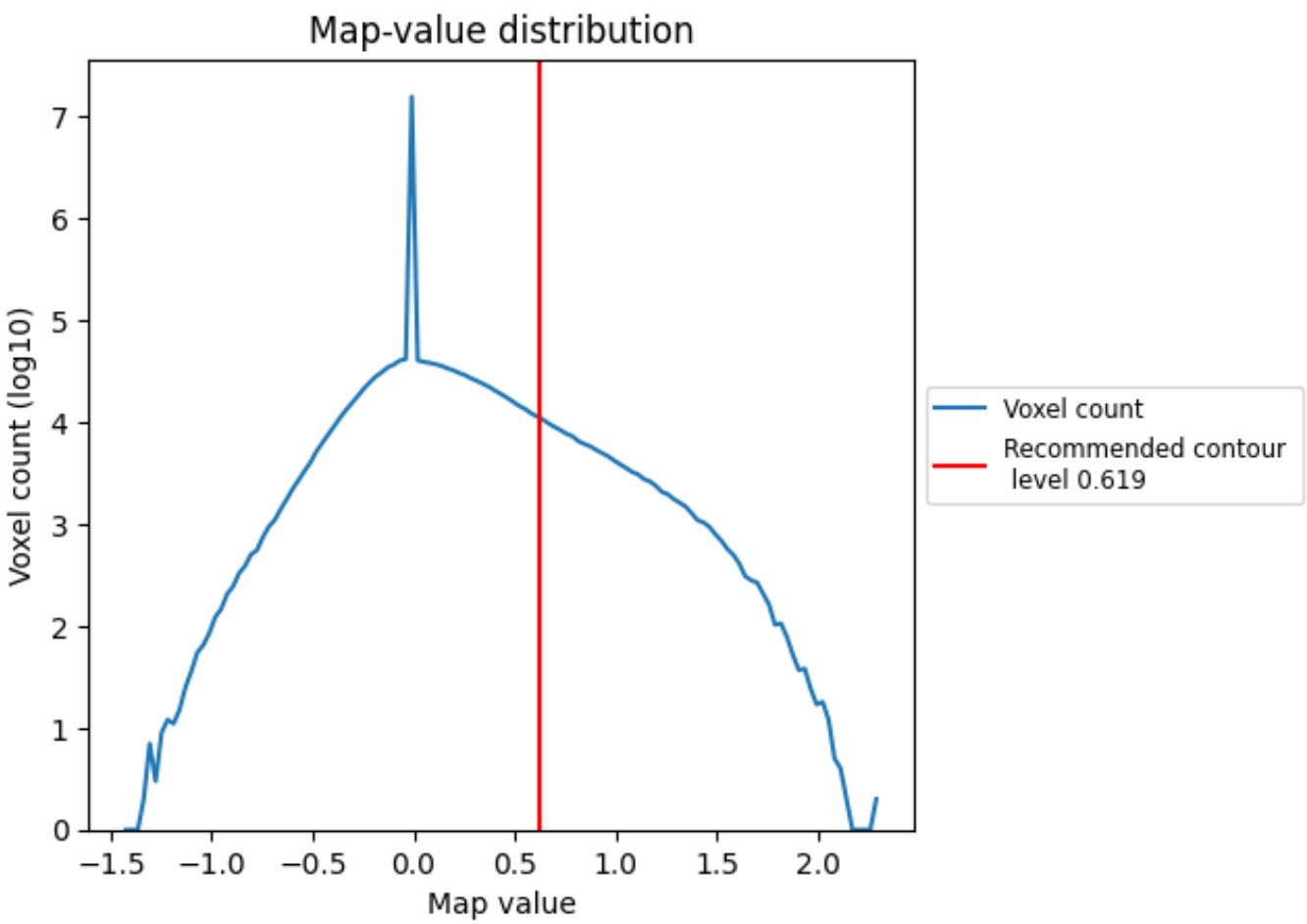
6.6 Mask visualisation (i)

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

7 Map analysis (i)

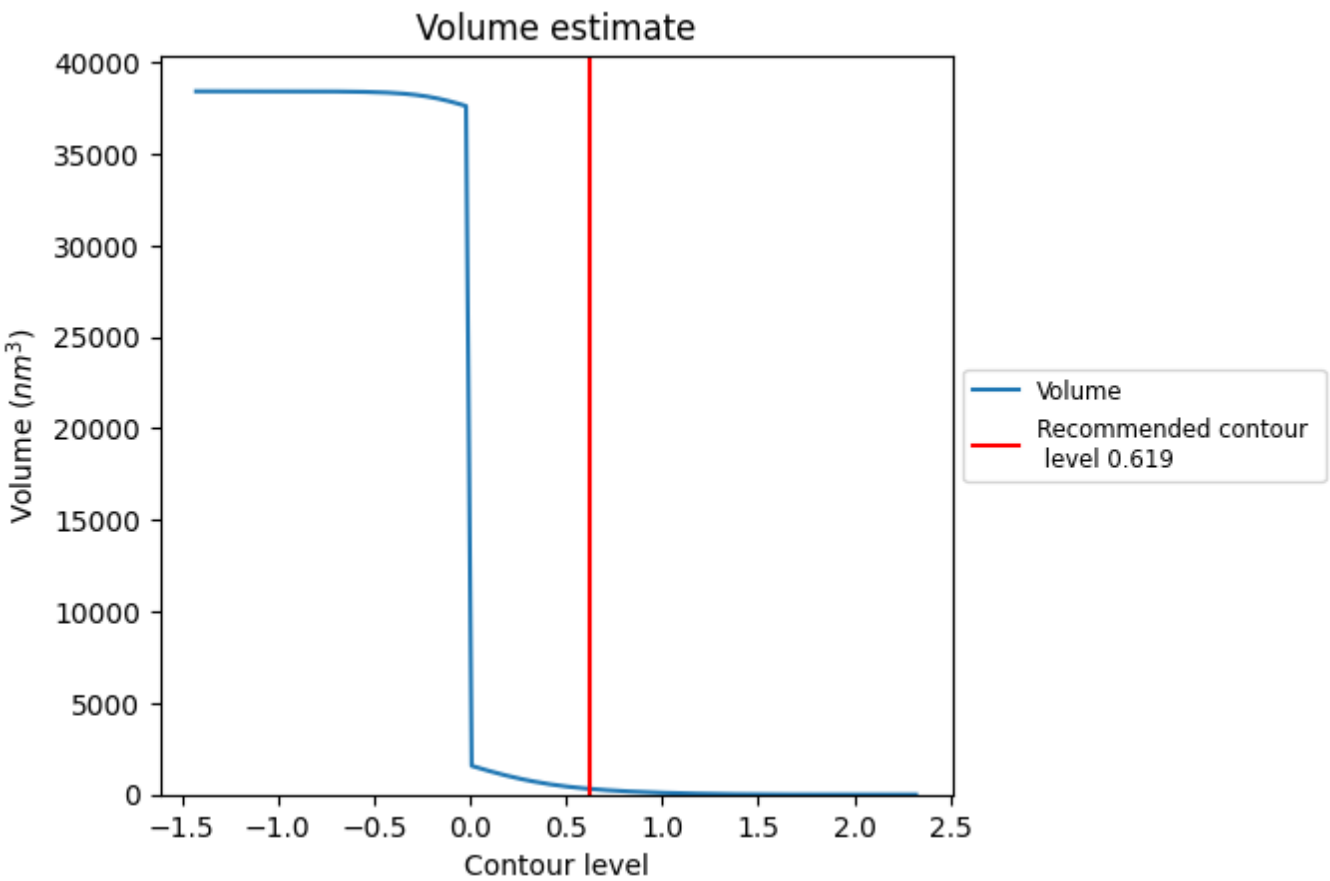
This section contains the results of statistical analysis of the map.

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.

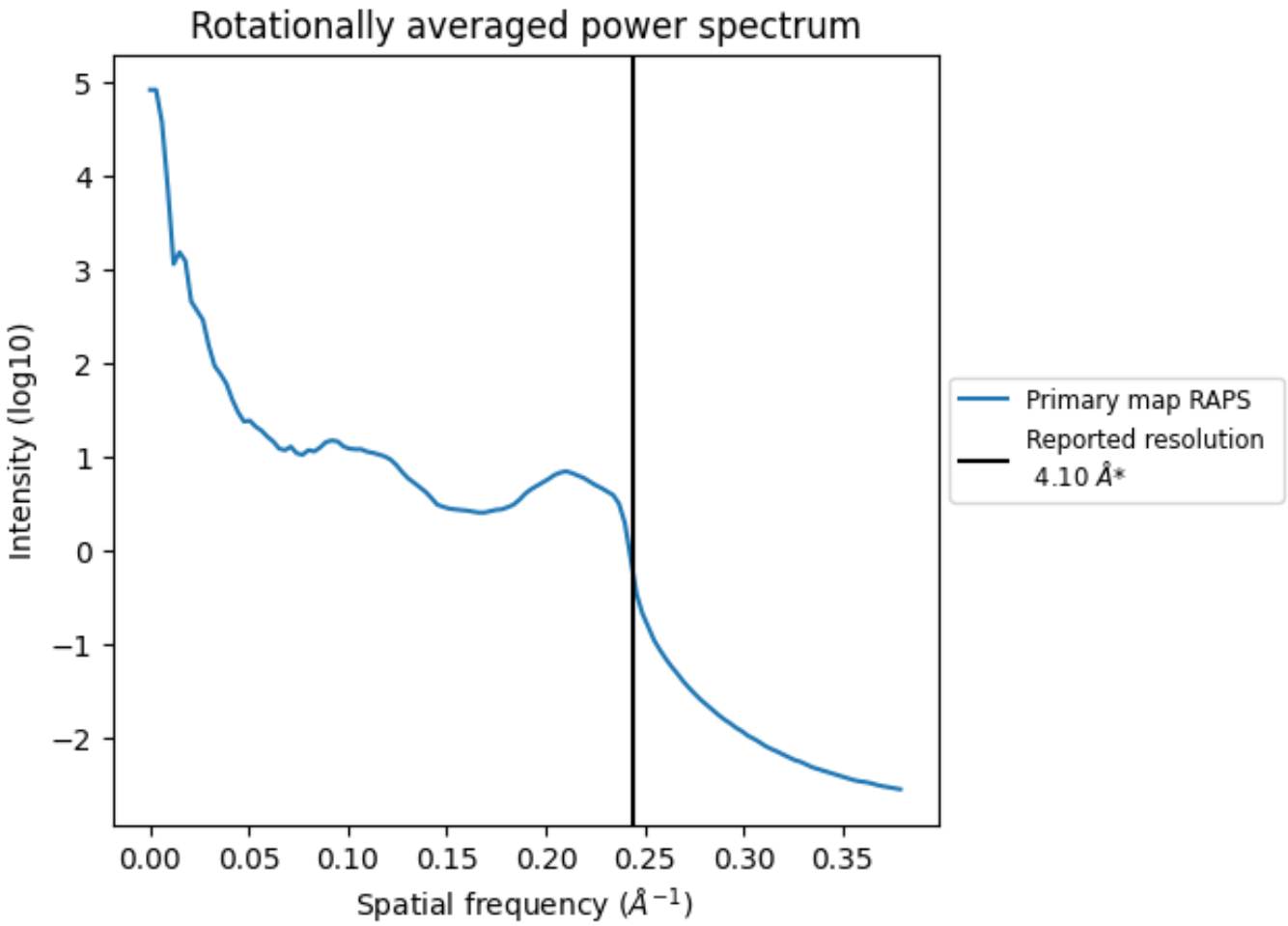
7.2 Volume estimate (i)



The volume at the recommended contour level is 315 nm^3; this corresponds to an approximate mass of 285 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 0.244 Å^{-1}

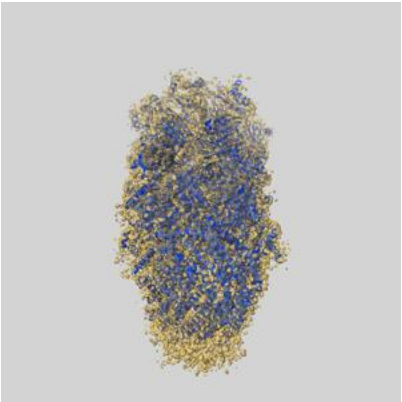
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

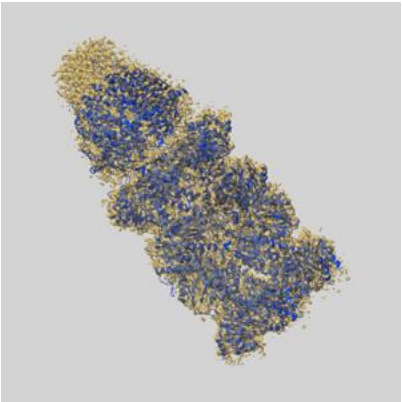
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-30824 and PDB model 7DR6. Per-residue inclusion information can be found in section 3 on page 9.

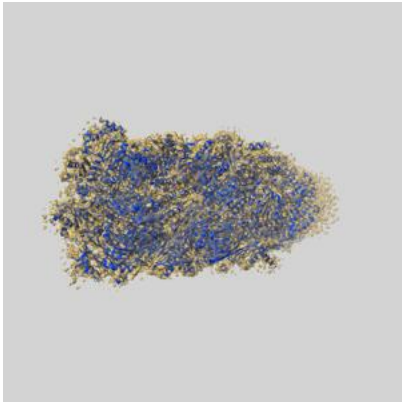
9.1 Map-model overlay (i)



X



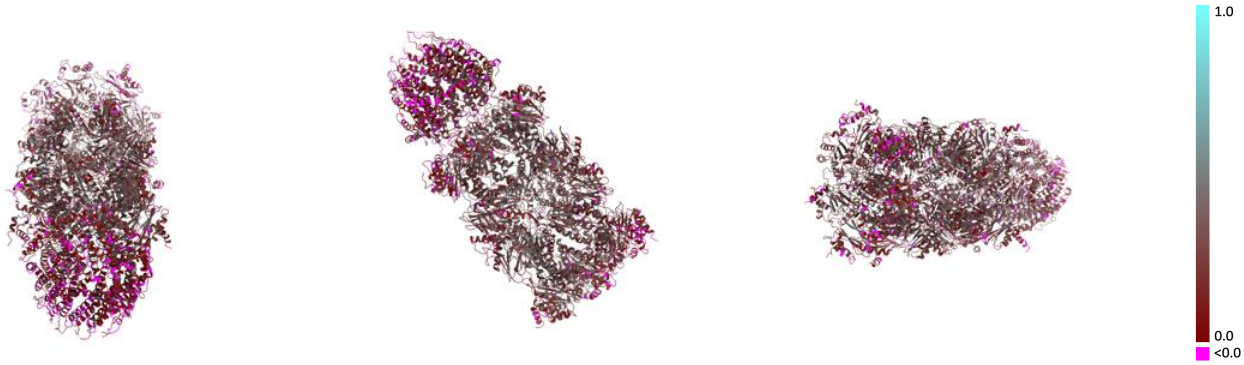
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.619 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.

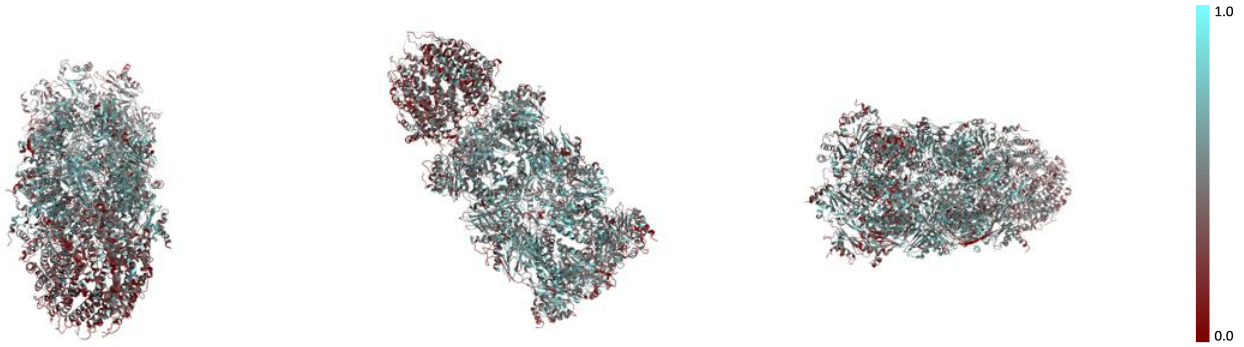
9.2 Q-score mapped to coordinate model (i)



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.

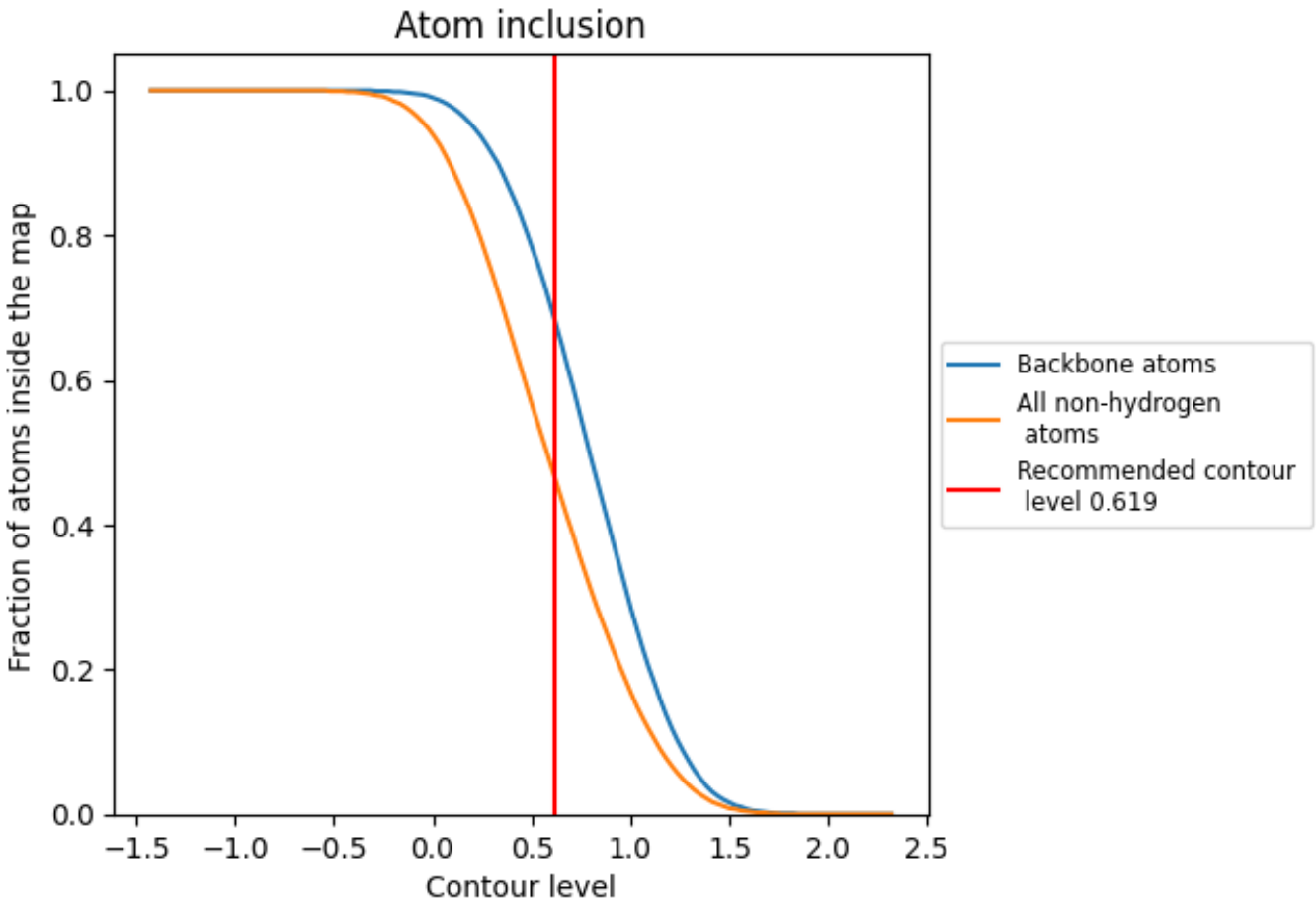
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.619).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 46% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.619) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4640	0.2400
1	0.5170	0.2920
2	0.5310	0.2430
A	0.3710	0.1670
B	0.3290	0.1390
C	0.3180	0.1130
D	0.3310	0.1600
E	0.2950	0.1240
F	0.2720	0.0870
G	0.3160	0.1060
H	0.5310	0.3120
I	0.5090	0.2890
J	0.5110	0.2890
K	0.4960	0.2680
L	0.5200	0.2840
M	0.5310	0.2810
N	0.4950	0.2640
O	0.4830	0.2330
P	0.4240	0.1750
Q	0.4840	0.2320
R	0.5150	0.2770
S	0.5300	0.3110
T	0.5300	0.2860
U	0.4910	0.2600
V	0.5050	0.2960
W	0.5490	0.3100
X	0.5140	0.3000
Y	0.5570	0.3170
Z	0.5510	0.2920
a	0.4880	0.2780
b	0.4300	0.2190
c	0.4610	0.2200
d	0.4300	0.1920
e	0.4500	0.2300
f	0.5120	0.2870
g	0.4920	0.2890