Full wwPDB EM Validation Report (i)

Mar 13, 2024 – 01:56 PM JST

PDB ID	:	3JCO
EMDB ID	:	EMD-6574
Title	:	Structure of yeast 26S proteasome in M1 state derived from Titan dataset
Authors	:	Luan, B.; Huang, X.L.; Wu, J.P.; Shi, Y.G.; Wang, F.
Deposited on	:	2016-01-06
Resolution	:	4.80 Å(reported)
Based on initial model	:	4CR4

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:

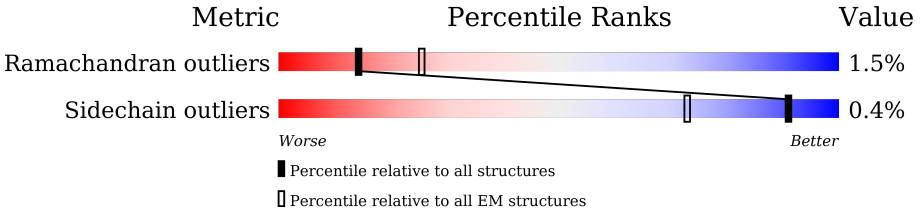
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.80 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	1	241	• 92% 8%
1	8	241	5% 92% 8%
2	2	266	• 87% 12%
2	9	266	• 87% 12%
3	3	215	7% 94% • 5%
3	h	215	6% 95% 5%
4	4	261	• 85% 15%
4	i	261	• 85% 15%
5	5	205	• 99%

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Mol	Chain	Length	Quality of chain
5	j	205	99%
6	6	198	5%, 97%
6	k	198	7%, 97%
7	7	287	73%, 26%
7	l	287	73%, 26%
8	A	252	7%, 96%
8	a	252	11%, 95%
9	B	250	7%, 100%
9	b	250	22%, 100%
10	C	258	5%, 93%, 5%
10	c	258	20%, 93%, 5%
11	D	254	6%, 95%, 5%
11	d	254	15%, 95%, 5%
12	E	260	7%, 92%, 7%
12	e	260	8%, 92%, 7%
13	F	234	98%
13	f	234	5%, 98%
14	G	288	83%, 15%
14	g	288	9%, 83%, 15%
15	H	467	38%, 73%, 24%
16	I	437	59%, 73%, 26%
17	J	405	71%, 89%, 8%
18	K	428	54%, 82%, 16%
19	L	437	43%, 81%, 18%
20	M	434	43%, 80%, 18%

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Mol	Chain	Length	Quality of chain
21	N	945	87% 10%
22	O	393	8% 85% 9%
23	P	445	7% 87% 9%
24	Q	434	24% 96%
25	R	429	10% 85% 8% 7%
26	S	523	9% 76% 8% 16%
27	T	274	9% 95%
28	U	338	5% 70% 25%
29	V	306	7% 73% 6% 20%
30	W	268	6% 68% 5% 26%
31	X	156	71% 74% 6% 19%
32	Y	89	7% 34% 62%
33	Z	993	53% 75% 23%

2 Entry composition (i)

There are 33 unique types of molecules in this entry. The entry contains 104317 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 beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	222	1757	1115	303	335	4	0	0
1	8	222	1757	1115	303	335	4	0	0

- Molecule 2 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	233	1824	1154	312	351	7	0	0
2	9	233	1824	1154	312	351	7	0	0

- Molecule 3 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	205	1574	995	261	311	7	0	0
3	h	205	1574	995	261	311	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	222	1684	1061	293	323	7	0	0
4	i	222	1684	1061	293	323	7	0	0

- Molecule 5 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	5	204	1581	1010	258	305	8	0	0
5	j	204	1581	1010	258	305	8	0	0

- Molecule 6 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	198	1585	1005	269	305	6	0	0
6	k	198	1585	1005	269	305	6	0	0

- Molecule 7 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	7	212	1644	1045	280	312	7	0	0
7	l	212	1644	1045	280	312	7	0	0

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	A	243	1921	1221	322	370	8	0	0
8	a	243	1921	1221	322	370	8	0	0

- Molecule 9 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	B	250	1915	1219	315	377	4	0	0
9	b	250	1915	1219	315	377	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	C	244	1904	1201	321	379	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	c	244	1904	1201	321	379	3	0	0

- Molecule 11 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D	241	1890	1181	331	374	4	0	0
11	d	241	1890	1181	331	374	4	0	0

- Molecule 12 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E	242	1861	1162	314	378	7	0	0
12	e	242	1861	1162	314	378	7	0	0

- Molecule 13 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	F	233	1795	1129	312	350	4	0	0
13	f	233	1795	1129	312	350	4	0	0

- Molecule 14 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	G	244	1896	1205	330	357	4	0	0
14	g	244	1896	1205	330	357	4	0	0

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	H	356	2771	1744	496	516	15	0	0

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	I	325	2513	1573	424	503	13	0	0

- Molecule 17 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	J	373	2928	1837	527	547	17	0	0

- Molecule 18 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	K	361	2849	1788	506	545	10	0	0

- Molecule 19 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	358	2829	1782	501	534	12	0	0

- Molecule 20 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	M	357	2754	1723	473	548	10	0	0

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	849	6562	4174	1099	1261	28	0	0

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	O	376	3083	1991	497	586	9	0	0

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	431	3470	2210	585	667	8	0	0

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	431	3471	2205	574	676	16	0	0

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	400	3218	2051	527	630	10	0	0

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	439	3357	2136	569	635	17	0	0

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	T	267	2201	1410	350	435	6	0	0

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	U	254	2034	1291	350	387	6	0	0

- Molecule 29 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	V	245	1912	1206	322	371	13	0	0

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	W	197	1534	962	269	300	3	0	0

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	X	127	1032	664	169	195	4	0	0

- Molecule 32 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	Y	34	243	146	45	52	0	0

- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

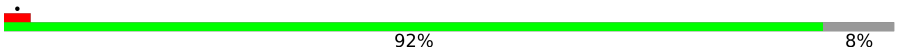
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	Z	763	5894	3744	966	1156	28	0	0

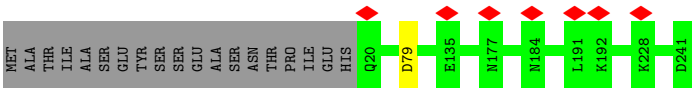
3 Residue-property plots (i)

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 beta type-6

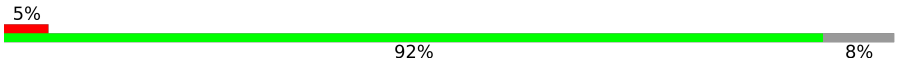
Chain 1:

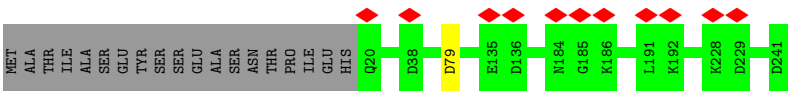




• Molecule 1: Proteasome subunit beta type-6

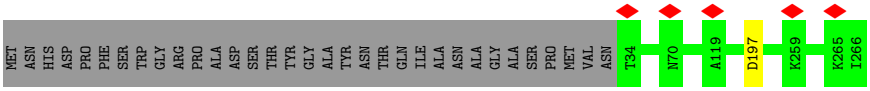
Chain 8:





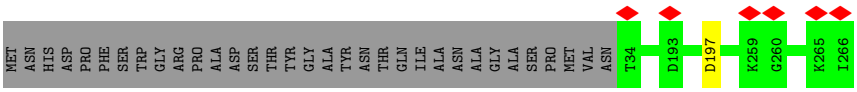
• Molecule 2: Proteasome subunit beta type-7

Chain 2:



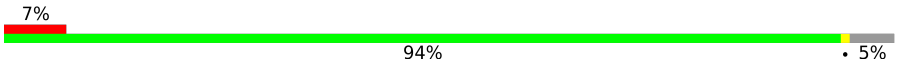
• Molecule 2: Proteasome subunit beta type-7

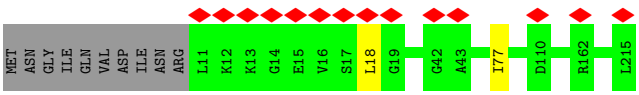
Chain 9:



• Molecule 3: Proteasome subunit beta type-1

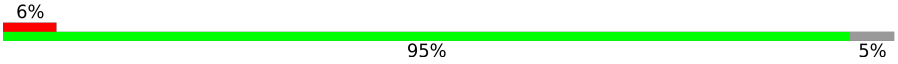
Chain 3:

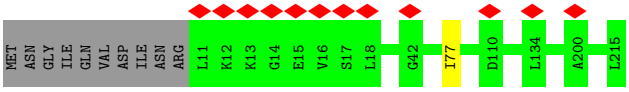




• Molecule 3: Proteasome subunit beta type-1

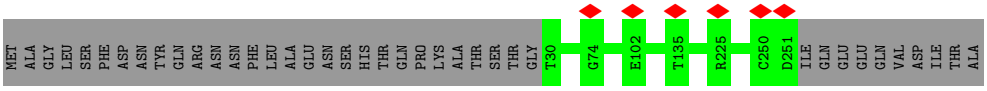
Chain h:





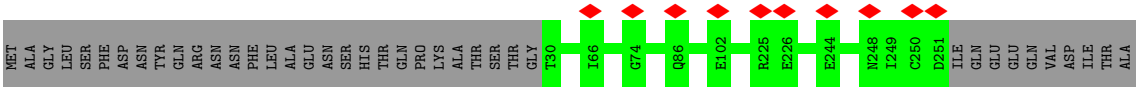
• Molecule 4: Proteasome subunit beta type-2

Chain 4:



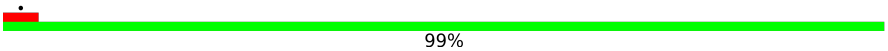
• Molecule 4: Proteasome subunit beta type-2

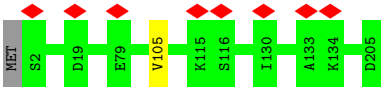
Chain i:



• Molecule 5: Proteasome subunit beta type-3

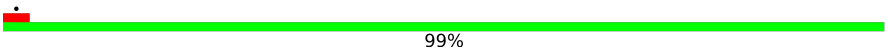
Chain 5:

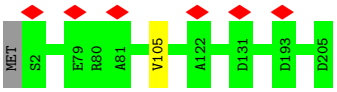




• Molecule 5: Proteasome subunit beta type-3

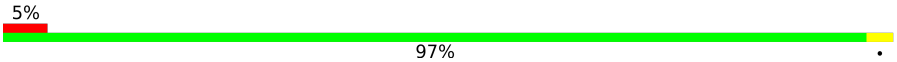
Chain j:

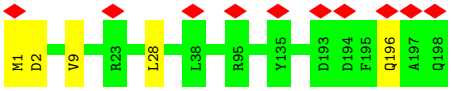




• Molecule 6: Proteasome subunit beta type-4

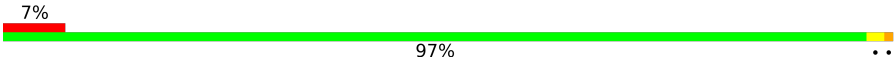
Chain 6:

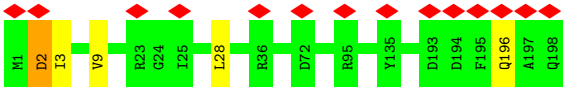




• Molecule 6: Proteasome subunit beta type-4

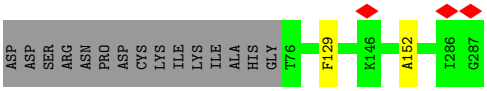
Chain k:





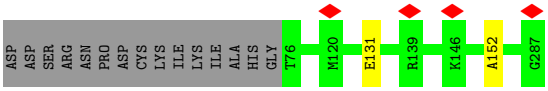
• Molecule 7: Proteasome subunit beta type-5

Chain 7:



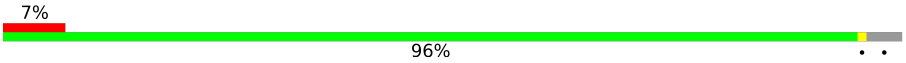
• Molecule 7: Proteasome subunit beta type-5

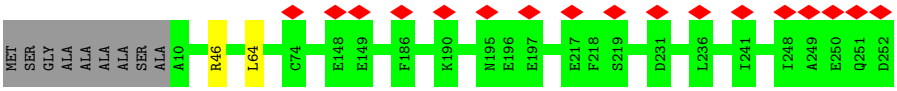
Chain l:



• Molecule 8: Proteasome subunit alpha type-1

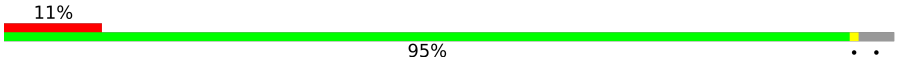
Chain A:

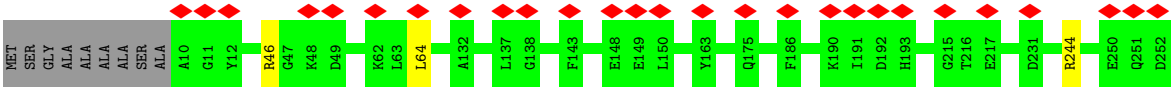




• Molecule 8: Proteasome subunit alpha type-1

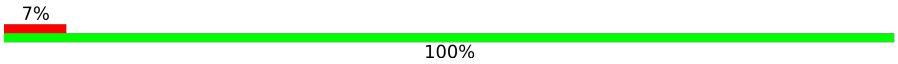
Chain a:

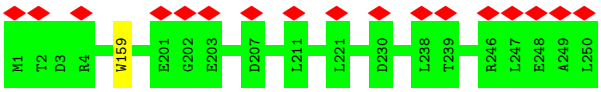




• Molecule 9: Proteasome subunit alpha type-2

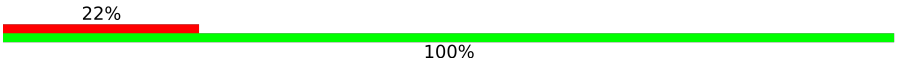
Chain B:

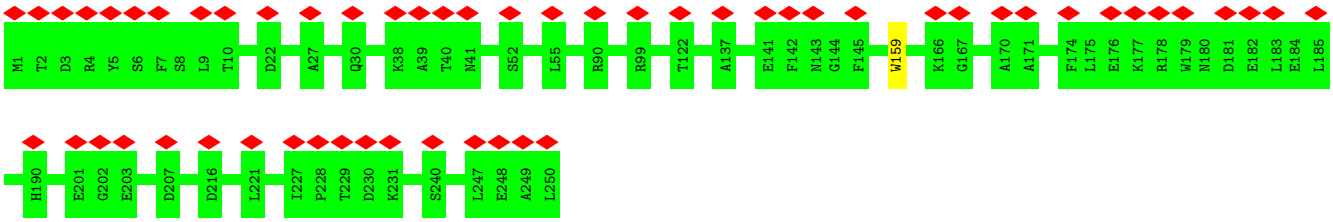




• Molecule 9: Proteasome subunit alpha type-2

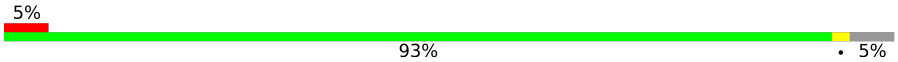
Chain b:

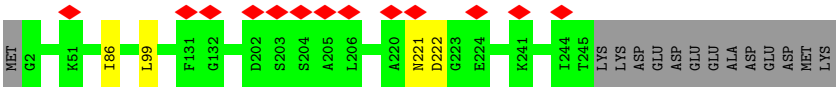




• Molecule 10: Proteasome subunit alpha type-3

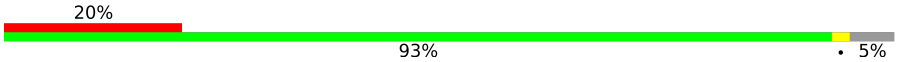
Chain C:

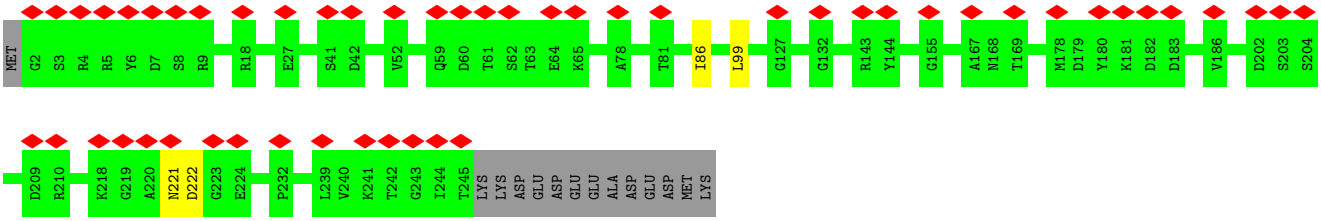




• Molecule 10: Proteasome subunit alpha type-3

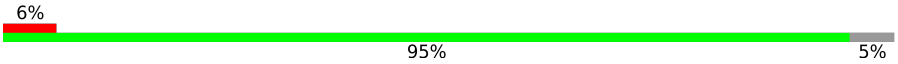
Chain c:

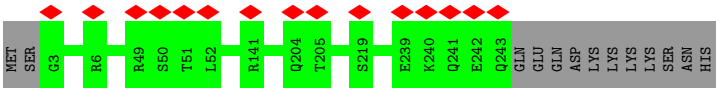




• Molecule 11: Proteasome subunit alpha type-4

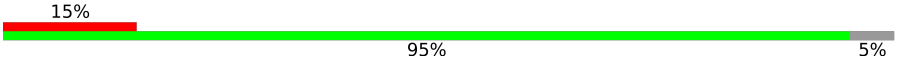
Chain D:

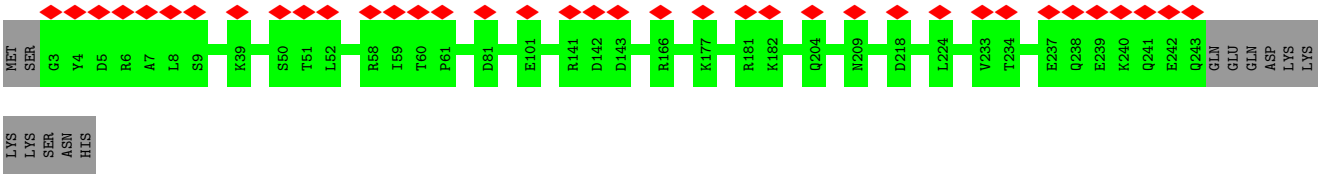




• Molecule 11: Proteasome subunit alpha type-4

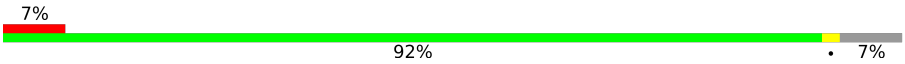
Chain d:

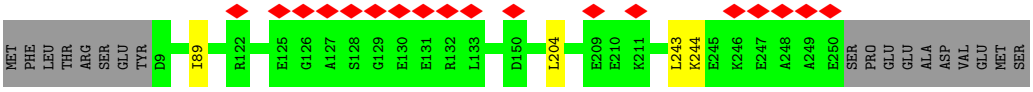




• Molecule 12: Proteasome subunit alpha type-5

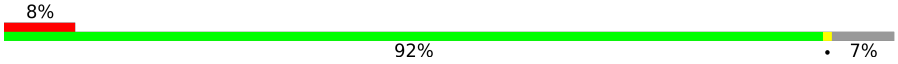
Chain E:

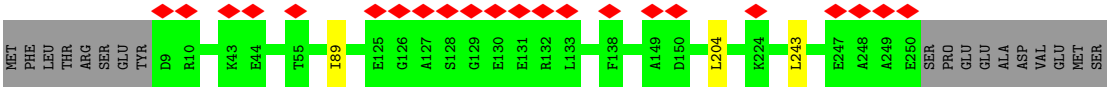




- Molecule 12: Proteasome subunit alpha type-5

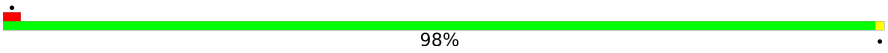
Chain e:

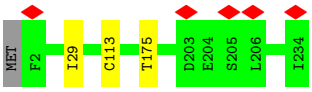




- Molecule 13: Proteasome subunit alpha type-6

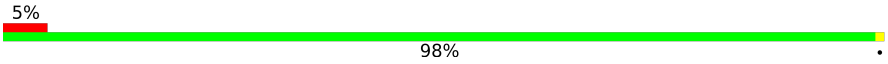
Chain F:

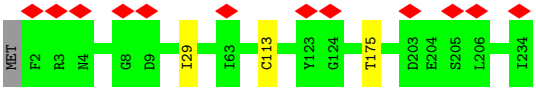




- Molecule 13: Proteasome subunit alpha type-6

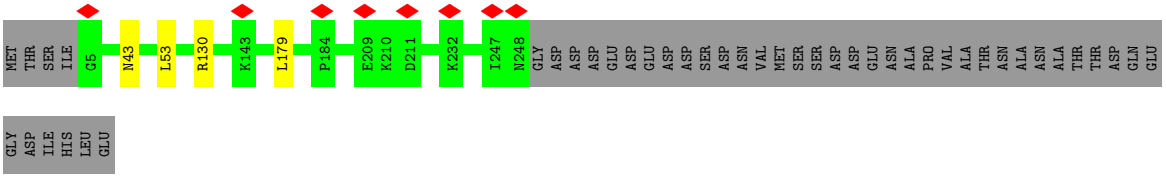
Chain f:





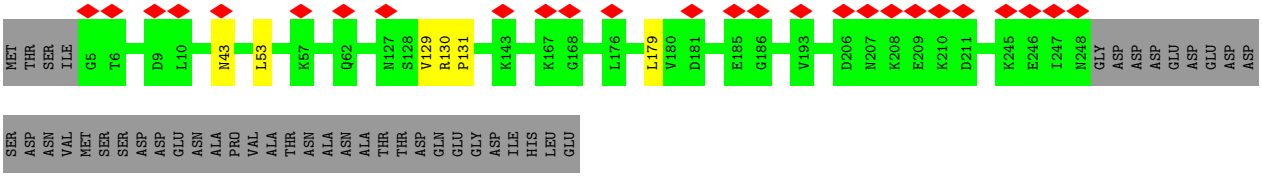
- Molecule 14: Probable proteasome subunit alpha type-7

Chain G:



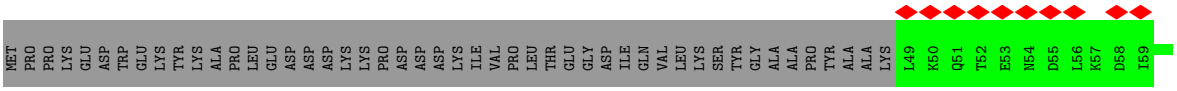
- Molecule 14: Probable proteasome subunit alpha type-7

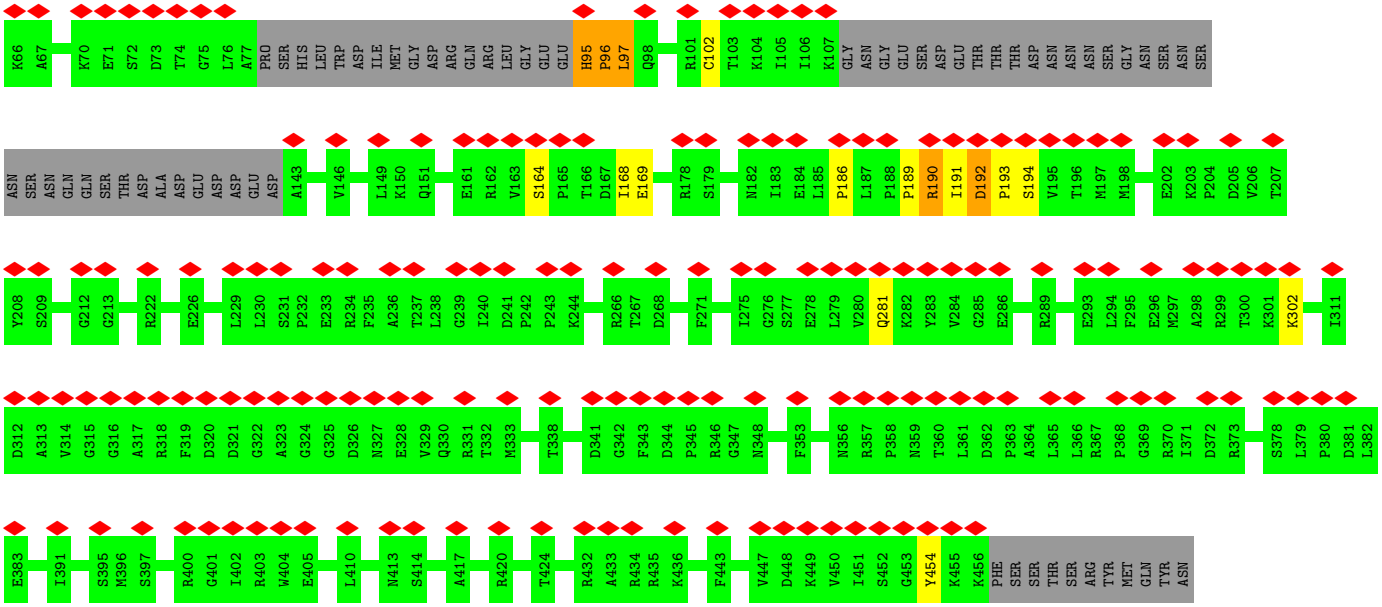
Chain g:



- Molecule 15: 26S protease regulatory subunit 7 homolog

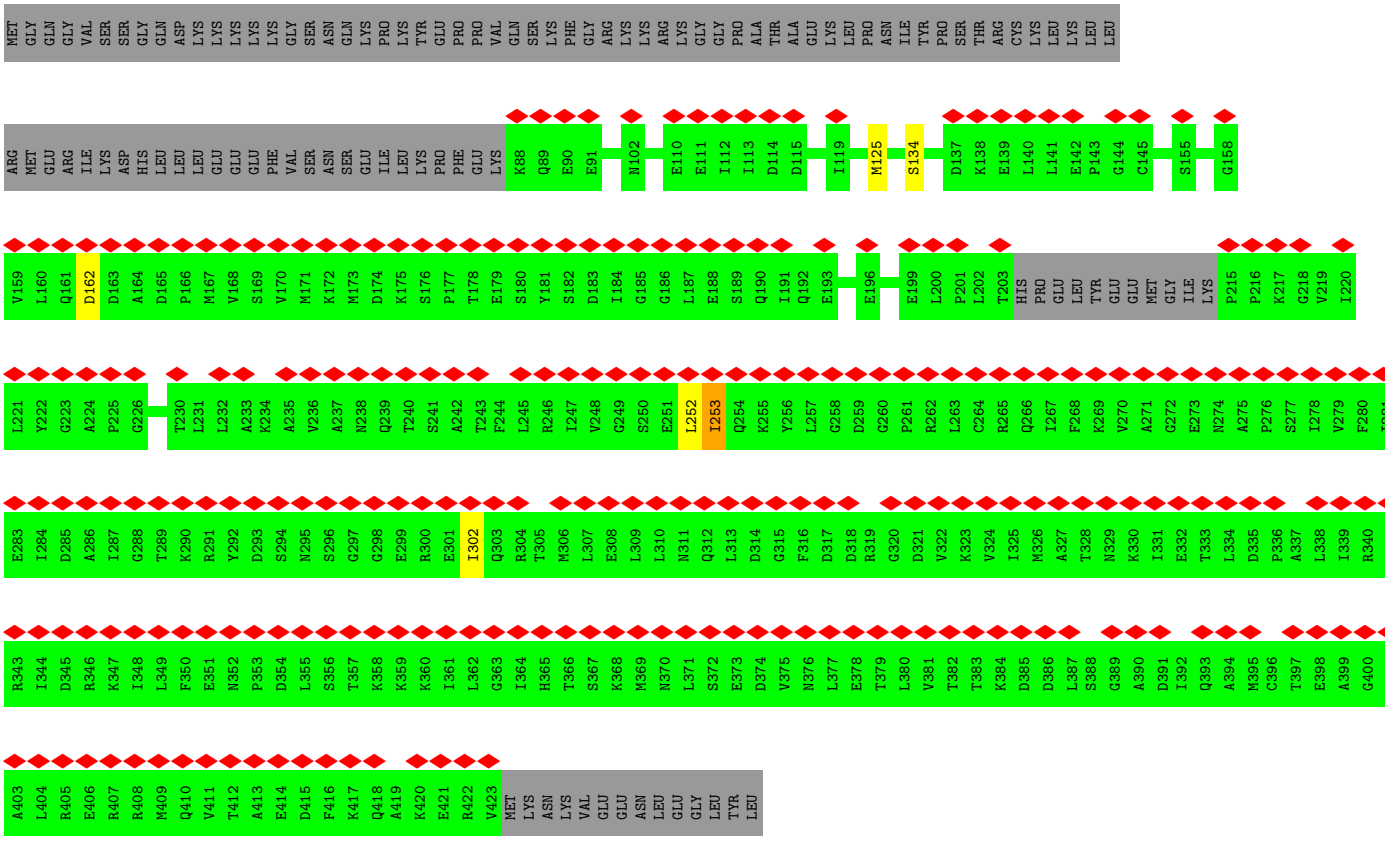
Chain H:





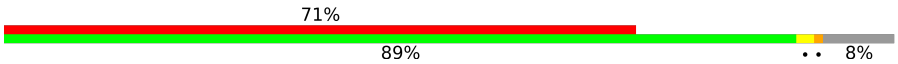
- Molecule 16: 26S protease regulatory subunit 4 homolog

Chain I:



- Molecule 17: 26S protease regulatory subunit 8 homolog

Chain J:



MET THR ALA ALA VAL THR SER SER ASN ILE VAL LEU GLU THR HIS GLU SER GLY ILE LYS PRO TYR PHE E24 K37 T38 V41 V55 Q66 E67 P68 G69 I76 V79 S80 D81 K82 E91 K100 D101 I102 N103 V104 K105 D106 L107 S110 D118 S119

E127 N128 K129 A130 D131 P132 L133 V134 S135 L136 M137 M138 V139 E140 K141 V142 P143 D144 S145 T146 Y147 D148 M149 V150 G151 G152 L153 T154 K155 Q156 I157 K158 E159 I160 K161 E162 V163 I164 E165 L166 P167 V168 K169 H170 P171 E172 L173 F174 E175 S176 L177 G178 I179 A180 Q181 P182 K183 G184 V185 I186

L187 Y188 G189 P190 P191 G192 T193 G194 K195 T196 L197 L198 A199 R200 A201 V202 A203 H204 H205 T206 D207 C208 K209 F210 I211 R212 V213 S214 G215 A216 E217 L218 V219 Q220 K221 Y222 I223 G224 E225 G226 S227 R228 M229 V230 R231 E232 L233 F234 V235 M236 A237 R238 E239 H240 A241 P242 S243 I244 I245 F246

M247 D248 E249 I250 D251 S252 I253 G254 S255 T256 R257 V258 E259 G260 S261 G262 G263 G264 D265 S266 E267 V268 Q269 R270 T271 M272 L273 E274 L275 L276 N277 Q278 L279 D280 G281 F282 E283 T284 S285 K286 N287 I288 K289 I290 I291 M292 A293 T294 N295 R296 L297 D298 I299 L300 D301 P302 A303 L304 L305 R306

P307 G308 R309 I310 D311 R312 K313 I314 E315 F316 P317 P318 P319 S320 V321 A322 A325 E326 I327 L328 R329 I330 H331 S332 R333 K334 M335 N336 L337 T338 R339 G340 I341 N342 L343 R344 K345 V346 A347 E348 K349 M350 N351 G352 C353 S354 G355 A356 D357 V358 K359 G360 V361 C362 T363 E364 A365 G366 M367

Y368 A369 L370 R371 E372 R373 R374 I375 H376 V377 T378 Q379 E380 D381 F382 E383 L384 A385 V386 G387 K388 V389 M390 N391 K392 N393 Q394 E395 T396 ALA ILE SER VAL ALA LYS LEU PHE LYS

- Molecule 18: 26S protease regulatory subunit 6B homolog

Chain K: 54% 82% 16%

MET GLU GLU LEU GLY ILE VAL THR PRO VAL GLU LYS ALA VAL GLU GLU LYS PRO ALA VAL LYS SER TYR ALA SER LEU LEU ALA GLN LEU ASN GLY THR VAL ASN ASN ASN SER ALA LEU SER ASN VAL ASN SER ASP ILE Y48 F49 R88 P102 I103 D104 Q105 T114 T125

L126 D127 R128 E129 P133 H142 V147 D148 I149 L150 P151 P152 D153 S154 D155 S156 S157 I158 S159 V160 M161 G162 E163 N164 E165 K166 P167 D168 V169 T170 Y171 A172 D173 V174 G175 G176 L177 D178 M179 Q180 K181 Q182 E183 I184 R185 E186 A187 V188 E189 L190 P191 L192 V193 Q194 ALA ASP LEU

TYR GLU GLN ILE GLY ILE ASP P205 P206 R207 G208 V209 L210 L211 Y212 G213 G218 L222 V223 V226 A227 N228 S229 T230 K231 A232 A233 F234 I235 R236 V237 N238 G239 S240 E241 F242 V243 H244 K245 Y246 L247 G248 E249 G250 P251 R252 R255 F258 R259 L260 A261 R262 E263 N264 A265

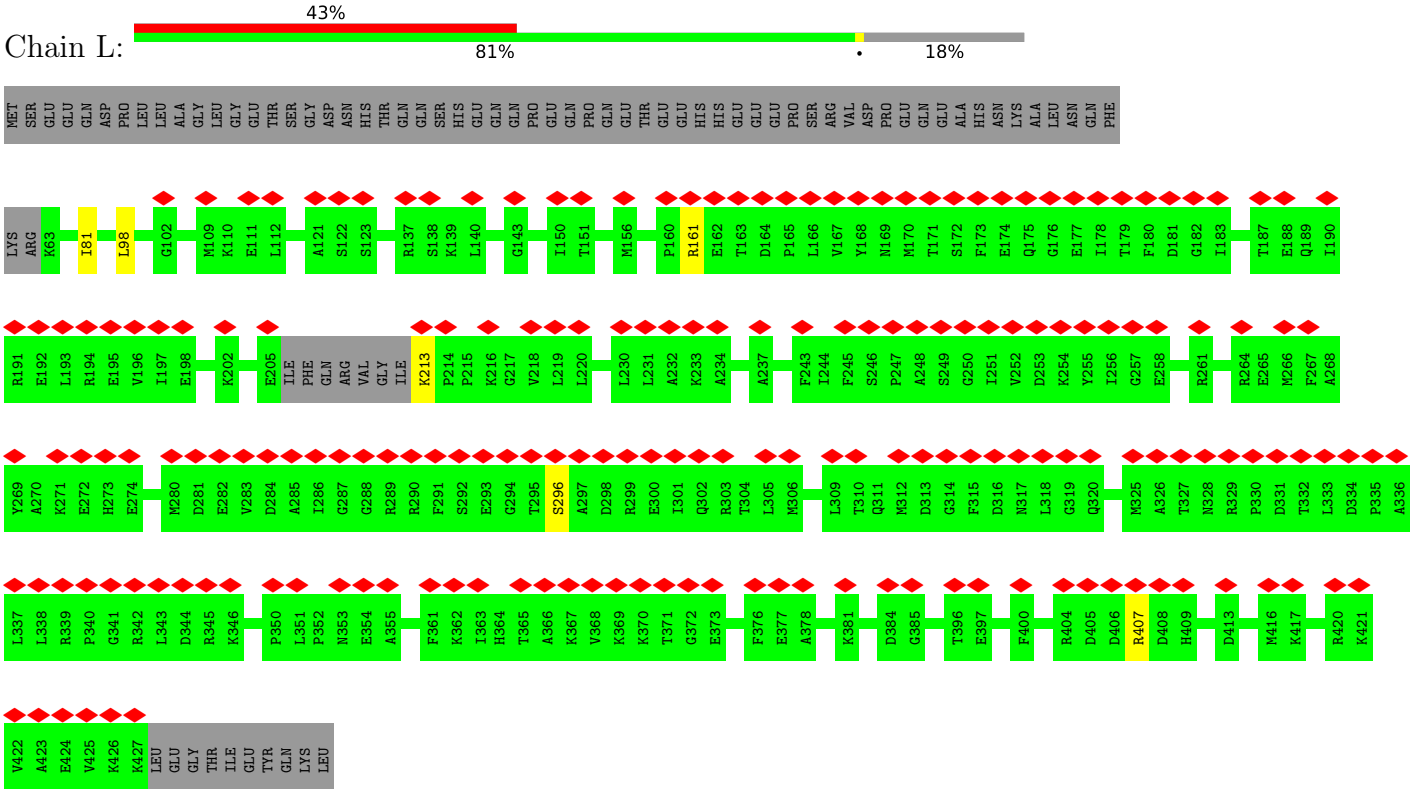
P266 S267 I268 D272 E273 V274 D275 S276 I277 A278 T279 K280 R281 F282 D283 A284 Q285 T286 G287 S288 D289 R290 E291 V292 Q293 R294 I295 L296 I297 E298 L299 L300 T301 Q302 M303 D304 G305 F306 D307 Q308 S309 T310 N311 V312 K313 V314 I315 M316 A317 T318 N319 R320 A321 D322 T323 L324 D325 P326 A327

L328 L329 R330 P331 G332 R333 L334 D335 R336 K337 I338 P341 S342 L343 R344 D345 R346 R349 R350 L351 I352 F353 G354 T355 I356 A357 S358 K359 M360 S361 L362 A363 P364 E365 A366 D367 L368 D369 S370 L371 I372 I373 R374 N375 D376 S377 L378 S379 I383 A384 A385 Q388 E389 A390 G391 L392

R393 A394 V395 R396 K397 N398 R399 Y400 L403 Q404 S405 D406 L407 E408 E409 A410 Y411 A412 T413 Q414 V415 K416 T417 D418 ASN THR VAL ASP LYS PHE ASP PHE TYR LYS

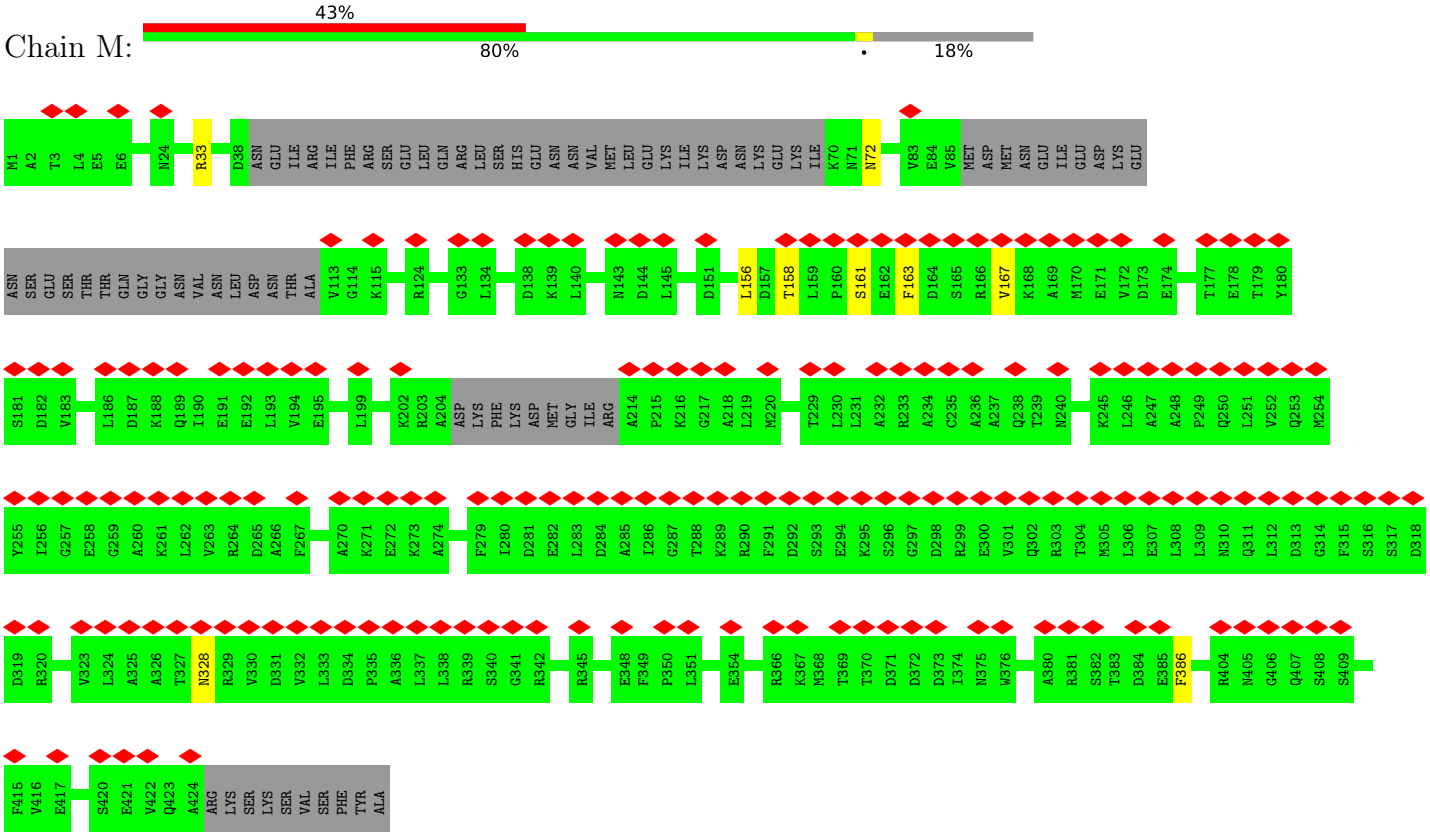
- Molecule 19: 26S protease subunit RPT4

Chain L:



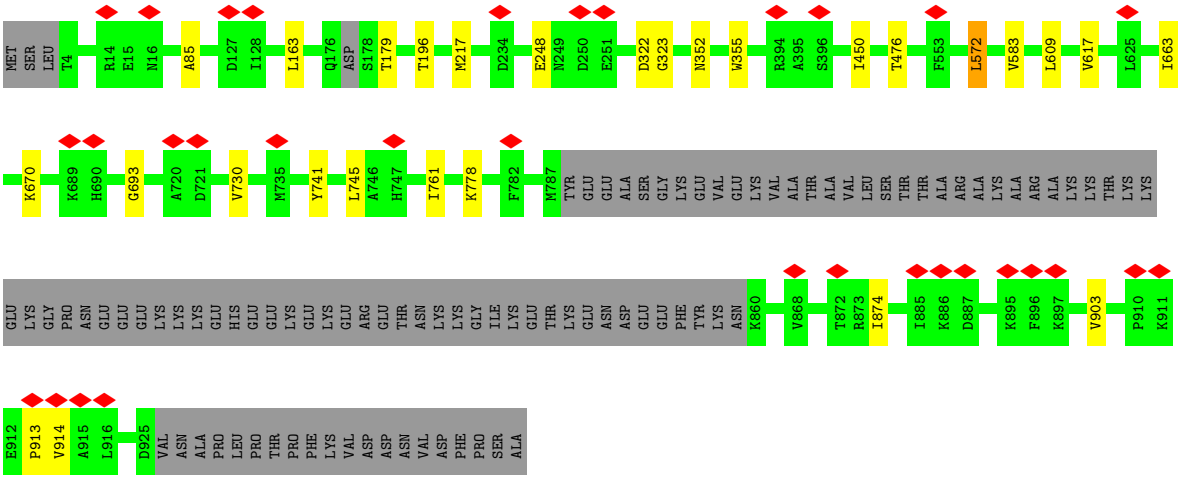
- Molecule 20: 26S protease regulatory subunit 6A

Chain M:



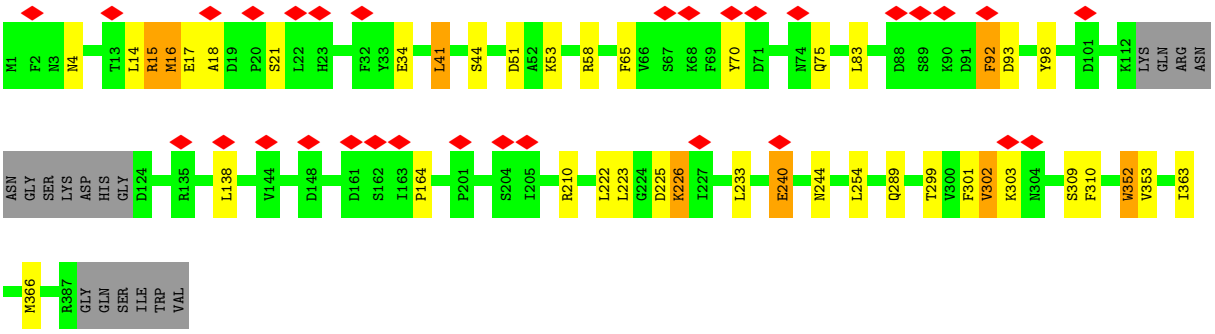
- Molecule 21: 26S proteasome regulatory subunit RPN2

Chain N:



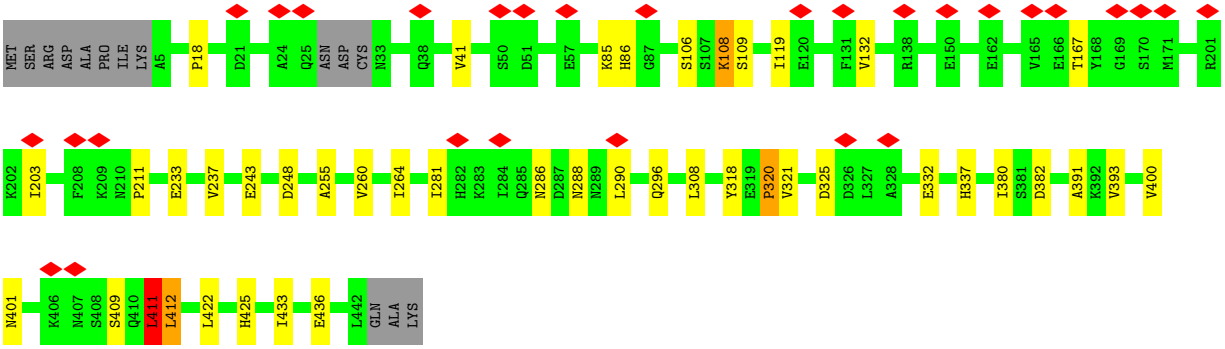
- Molecule 22: 26S proteasome regulatory subunit RPN9

Chain O:



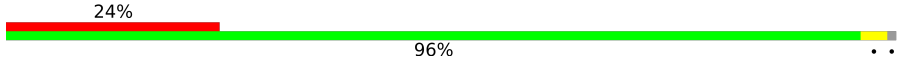
- Molecule 23: 26S proteasome regulatory subunit RPN5

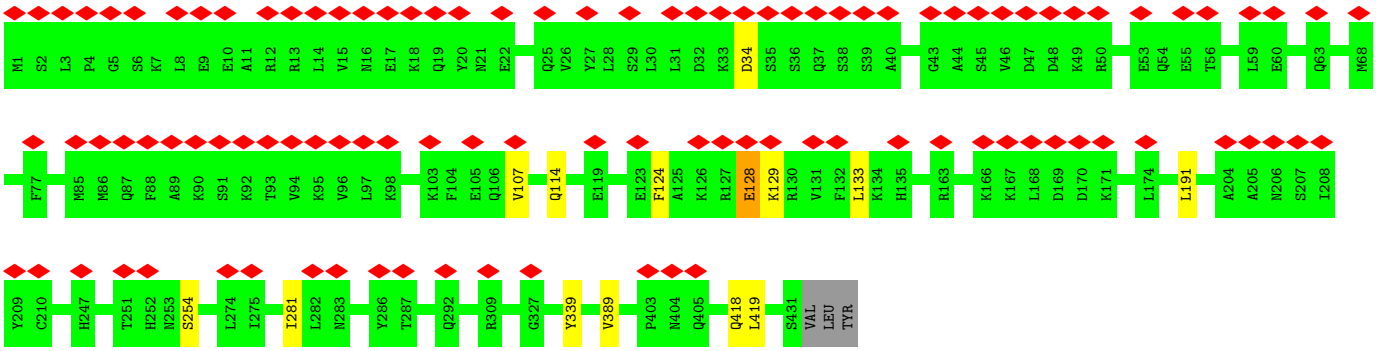
Chain P:



- Molecule 24: 26S proteasome regulatory subunit RPN6

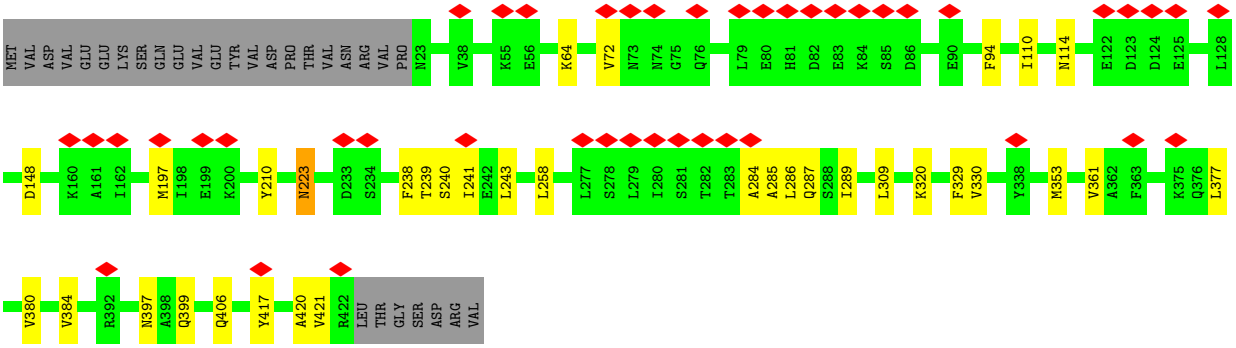
Chain Q:





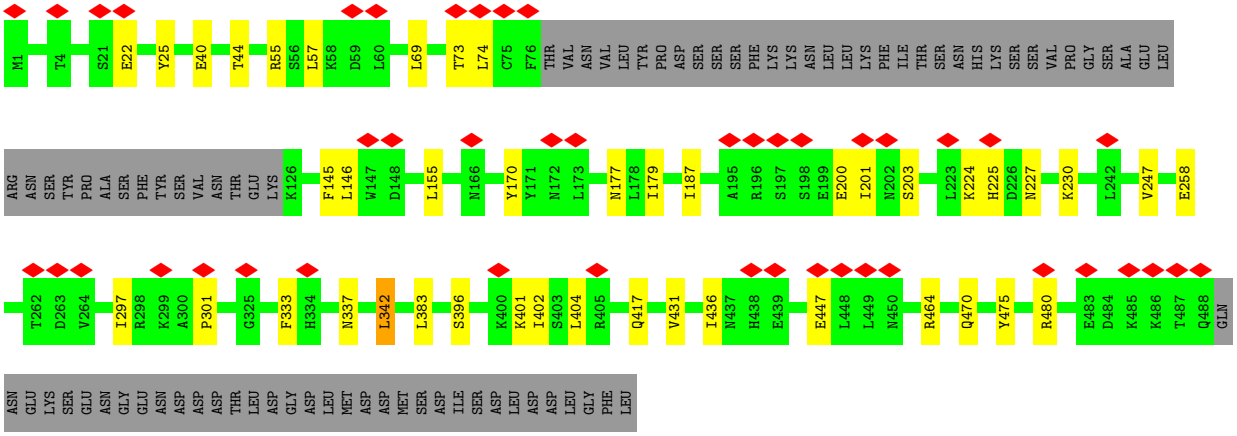
- Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R:



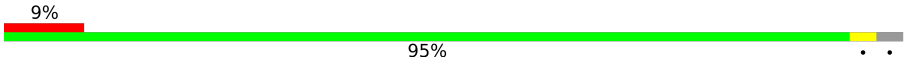
- Molecule 26: 26S proteasome regulatory subunit RPN3

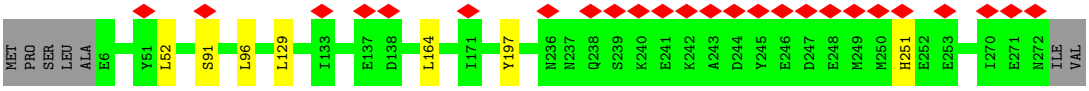
Chain S:



- Molecule 27: 26S proteasome regulatory subunit RPN12

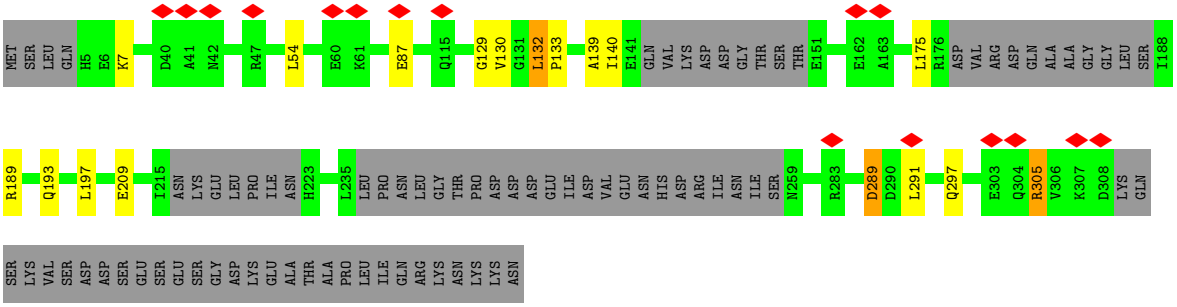
Chain T:





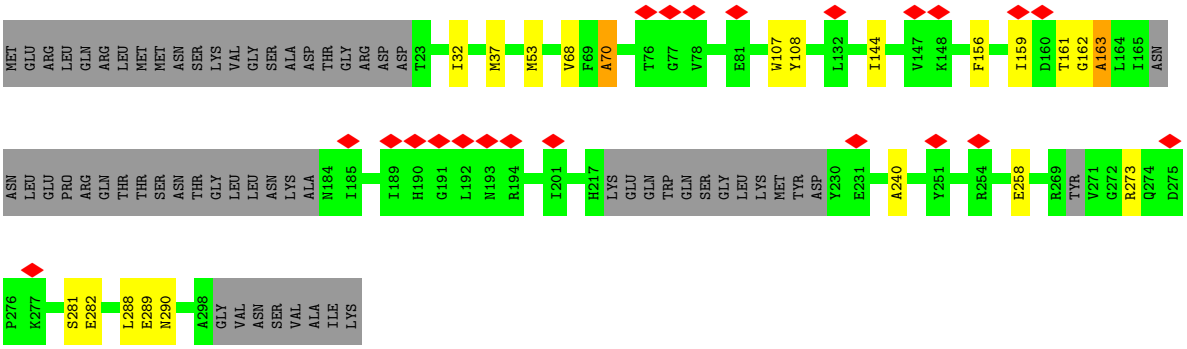
• Molecule 28: 26S proteasome regulatory subunit RPN8

Chain U:



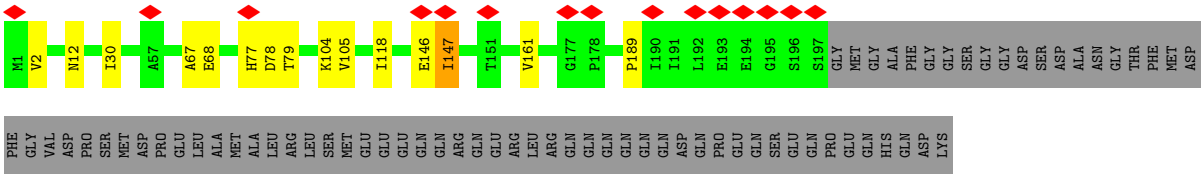
• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



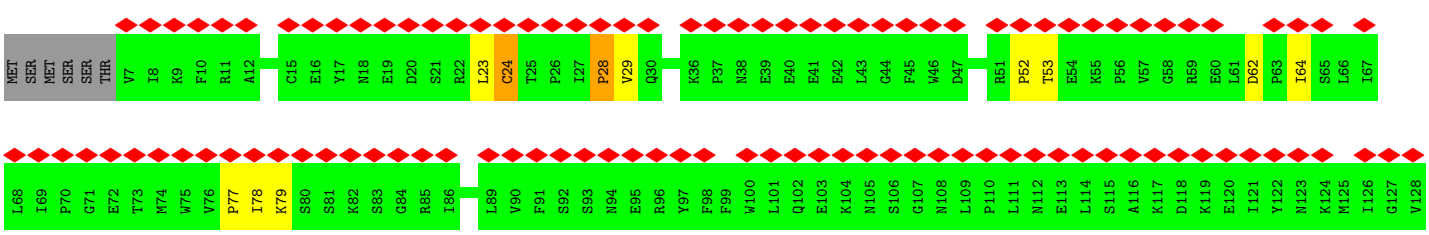
• Molecule 30: 26S proteasome regulatory subunit RPN10

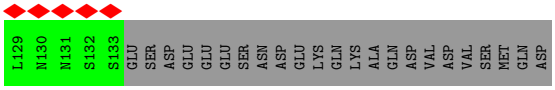
Chain W:



• Molecule 31: 26S proteasome regulatory subunit RPN13

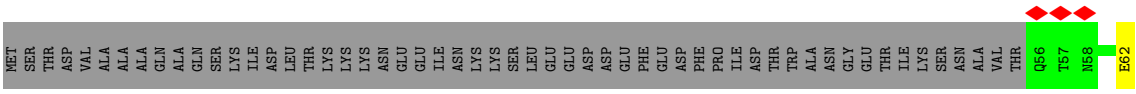
Chain X:

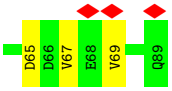




• Molecule 32: 26S proteasome complex subunit SEM1

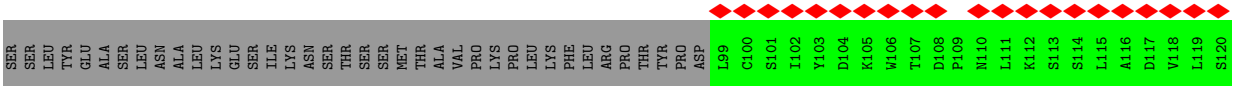
Chain Y:

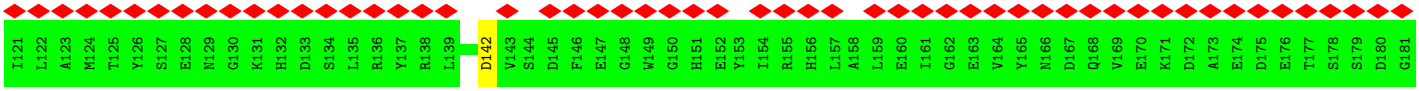


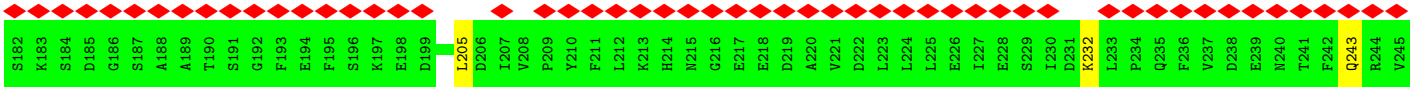


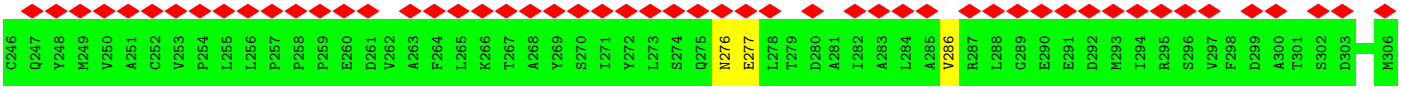
• Molecule 33: 26S proteasome regulatory subunit RPN1

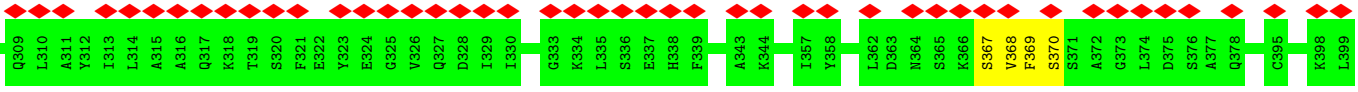
Chain Z:

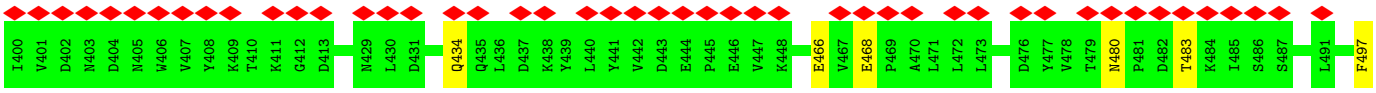


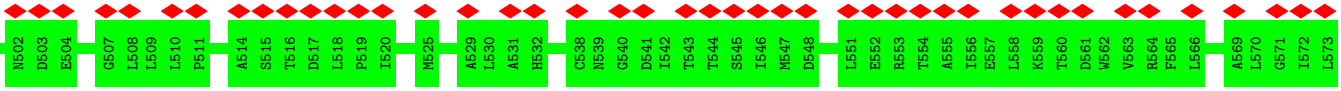


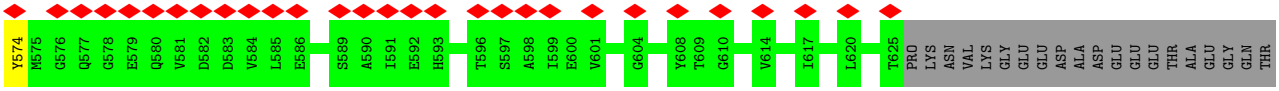












ASN SER ILE SER ASP PHE LEU GLY GLU GLN VAL ASN GLU PRO THR LYS ASN GLU GLU ALA GLU ILE GLU VAL ASP GLU MET GLU VAL ASP ALA GLU GLY GLU GLU GLU VAL GLU VAL LYS ALA GLU ILE THR GLU LYS LYS ASN GLY GLU SER LEU GLU GLY GLU GLU ILE LYS SER GLU GLU

LYS LYS GLY LYS SER SER ASP LYS ASP ALA THR THR ASP GLY LYS ASN ASP ASP GLU GLU GLU GLU LYS GLU ALA GLY ILE VAL ASP GLU L736 I743 A744 L745 I746 A747 L748 G749 E750 D751 I752 G753 K754 E755 M756 S757 L758 R759 H760 H763 H766 Y767 G768 N769 E770 R774

M780 G781 I782 V785 S786 D787 P788 Q789 M790 K791 V792 F793 D794 T795 L796 T797 R798 F799 S800 H801 D802 A803 D804 L805 E806 M809 N810 S811 I812 F813 A814 M815 G816 L817 C818 G819 A820 N823 N824 A825 R826 L827 A828 Q829 L830 L831 R832 Q833 L834 A835 S836 Y837 Y838 S839 R840 E841

Q842 D843 A844 L845 F846 I847 T848 R849 Q852 G853 H856 K859 M864 D865 V866 F867 N868 D869 A870 H871 V872 L873 T877 L878 A879 S880 I881 L882 T883 T884 A885 L888 V889 S890 P891 S892 F893 M894 L895 K896 H897 H898 Q899 L900 F901 Y902 M903 L904 N905 I908 R909 P910 K911

F912 I913 L914 A915 L916 N917 D918 E919 I923 K924 V925 N926 V927 R928 V929 G930 Q931 ALA VAL GLU THR VAL GLY GLN ALA GLY ARG PRO LYS LYS ILE THR GLY TRP ILE THR GLN SER THR P954 V955 L956 L957 N958 H959 G960 E961 R962 A963 E964 L965 E966 T967 D968 E969 Y970 I971 S972 Y973

T974 S975 H976 I977 E978 G979 V980 V981 I982 L983 K984 K985 N986 P987 D988 Y989 R990 E991 E992 E993

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	81782	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	each micrograph	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	2.5	Depositor
Magnification	75000	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.230	Depositor
Minimum map value	-0.079	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0796	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.1, 2.1, 2.1	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	1	0.62	0/1795	0.67	0/2420
1	8	0.61	0/1795	0.67	0/2420
2	2	0.62	0/1855	0.67	0/2514
2	9	0.62	0/1855	0.67	0/2514
3	3	0.64	0/1603	0.66	0/2168
3	h	0.64	0/1603	0.67	0/2168
4	4	0.59	0/1715	0.67	0/2326
4	i	0.59	0/1715	0.67	0/2326
5	5	0.60	0/1611	0.64	0/2174
5	j	0.60	0/1611	0.64	0/2174
6	6	0.60	0/1613	0.69	1/2173 (0.0%)
6	k	0.60	0/1613	0.69	1/2173 (0.0%)
7	7	0.60	0/1681	0.67	0/2274
7	l	0.61	0/1681	0.67	0/2274
8	A	0.60	0/1959	0.69	1/2652 (0.0%)
8	a	0.61	0/1959	0.71	2/2652 (0.1%)
9	B	0.56	1/1952 (0.1%)	0.64	0/2642
9	b	0.56	1/1952 (0.1%)	0.64	0/2642
10	C	0.56	0/1934	0.63	0/2618
10	c	0.56	0/1934	0.63	0/2618
11	D	0.57	0/1919	0.64	0/2598
11	d	0.57	0/1919	0.64	0/2598
12	E	0.57	0/1886	0.67	0/2541
12	e	0.58	0/1886	0.69	1/2541 (0.0%)
13	F	0.57	0/1823	0.68	0/2463
13	f	0.57	0/1823	0.68	0/2463
14	G	0.60	0/1936	0.67	3/2614 (0.1%)
14	g	0.60	1/1936 (0.1%)	0.67	3/2614 (0.1%)
15	H	0.51	1/2810 (0.0%)	0.70	2/3780 (0.1%)
16	I	0.41	0/2543	0.63	1/3429 (0.0%)
17	J	0.50	2/2964 (0.1%)	0.68	3/3981 (0.1%)
18	K	0.49	1/2887 (0.0%)	0.69	0/3894
19	L	0.48	0/2870	0.65	1/3858 (0.0%)
20	M	0.44	0/2785	0.66	2/3763 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
21	N	0.55	1/6670 (0.0%)	0.69	4/9023 (0.0%)
22	O	0.63	0/3142	0.87	6/4241 (0.1%)
23	P	0.64	0/3520	0.82	6/4752 (0.1%)
24	Q	0.59	1/3527 (0.0%)	0.68	2/4748 (0.0%)
25	R	0.61	0/3272	0.75	2/4412 (0.0%)
26	S	0.54	0/3410	0.78	3/4621 (0.1%)
27	T	0.58	0/2244	0.73	2/3029 (0.1%)
28	U	0.56	0/2059	0.78	5/2774 (0.2%)
29	V	0.57	1/1939 (0.1%)	0.81	2/2613 (0.1%)
30	W	0.49	0/1557	0.72	0/2111
31	X	0.48	1/1058 (0.1%)	0.68	1/1432 (0.1%)
32	Y	0.62	0/244	0.82	0/328
33	Z	0.37	1/6001 (0.0%)	0.61	1/8141 (0.0%)
All	All	0.56	12/106066 (0.0%)	0.69	55/143284 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	6	0	1
6	k	0	1
8	A	0	1
8	a	0	1
10	C	0	1
10	c	0	1
13	F	0	1
13	f	0	1
15	H	0	10
16	I	0	2
17	J	0	3
18	K	0	4
19	L	0	4
20	M	0	4
21	N	0	11
22	O	0	22
23	P	0	17
24	Q	0	8
25	R	0	8
26	S	0	16
27	T	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
28	U	0	8
29	V	0	6
30	W	0	8
31	X	0	6
32	Y	0	2
33	Z	0	5
All	All	0	156

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	V	107	TRP	CB-CG	-6.56	1.38	1.50
21	N	355	TRP	CB-CG	-5.89	1.39	1.50
24	Q	339	TYR	CE1-CZ	-5.77	1.31	1.38
9	B	159	TRP	CB-CG	-5.74	1.40	1.50
18	K	362	LEU	C-N	-5.73	1.20	1.34
9	b	159	TRP	CB-CG	-5.71	1.40	1.50
33	Z	468	GLU	C-N	-5.47	1.23	1.34
14	g	131	PRO	N-CD	5.26	1.55	1.47
15	H	96	PRO	N-CD	5.16	1.55	1.47
17	J	319	PRO	N-CD	5.11	1.55	1.47
17	J	318	PRO	N-CD	5.09	1.54	1.47
31	X	62	ASP	C-N	-5.01	1.24	1.34

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	S	155	LEU	CA-CB-CG	-10.11	92.05	115.30
25	R	309	LEU	CA-CB-CG	-9.51	93.44	115.30
23	P	412	LEU	CA-CB-CG	8.47	134.79	115.30
29	V	107	TRP	CB-CA-C	-8.08	94.25	110.40
29	V	70	ALA	C-N-CA	-7.60	102.71	121.70
24	Q	419	LEU	CA-CB-CG	-7.39	98.31	115.30
8	a	244	ARG	NE-CZ-NH1	-7.35	116.63	120.30
28	U	175	LEU	CA-CB-CG	6.69	130.69	115.30
22	O	225	ASP	CB-CG-OD1	6.38	124.04	118.30
20	M	158	THR	C-N-CA	-6.36	105.79	121.70
15	H	97	LEU	CB-CG-CD1	-6.34	100.23	111.00
22	O	254	LEU	CA-CB-CG	-6.29	100.83	115.30
26	S	402	ILE	N-CA-C	-6.26	94.11	111.00
17	J	316	PHE	C-N-CD	6.15	141.31	128.40
16	I	162	ASP	CB-CG-OD1	6.11	123.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	L	98	LEU	CA-CB-CG	-6.10	101.27	115.30
12	e	243	LEU	CA-CB-CG	6.09	129.31	115.30
14	G	130	ARG	C-N-CD	6.03	141.06	128.40
6	k	28	LEU	CA-CB-CG	-6.02	101.45	115.30
6	6	28	LEU	CA-CB-CG	-6.01	101.48	115.30
14	g	179	LEU	CA-CB-CG	-5.90	101.73	115.30
24	Q	191	LEU	CA-CB-CG	-5.90	101.73	115.30
14	G	179	LEU	CA-CB-CG	-5.89	101.76	115.30
21	N	609	LEU	CA-CB-CG	-5.84	101.87	115.30
22	O	352	TRP	C-N-CA	5.81	136.23	121.70
23	P	18	PRO	N-CA-CB	5.74	110.18	103.30
22	O	41	LEU	CB-CG-CD1	-5.66	101.39	111.00
23	P	422	LEU	CA-CB-CG	-5.64	102.32	115.30
22	O	222	LEU	CA-CB-CG	-5.64	102.33	115.30
14	g	130	ARG	C-N-CD	5.58	140.13	128.40
22	O	240	GLU	N-CA-C	5.57	126.04	111.00
21	N	163	LEU	CA-CB-CG	-5.48	102.70	115.30
28	U	289	ASP	N-CA-C	5.44	125.70	111.00
26	S	383	LEU	CA-CB-CG	-5.44	102.80	115.30
17	J	318	PRO	C-N-CD	5.41	139.76	128.40
27	T	129	LEU	CA-CB-CG	5.41	127.74	115.30
25	R	243	LEU	CA-CB-CG	-5.41	102.87	115.30
23	P	290	LEU	CA-CB-CG	5.38	127.67	115.30
20	M	156	LEU	CA-CB-CG	-5.33	103.03	115.30
33	Z	827	LEU	CB-CG-CD2	-5.27	102.04	111.00
14	g	53	LEU	CA-CB-CG	-5.27	103.19	115.30
14	G	53	LEU	CA-CB-CG	-5.26	103.20	115.30
23	P	401	ASN	C-N-CA	-5.26	108.56	121.70
8	a	46	ARG	NE-CZ-NH1	-5.25	117.67	120.30
8	A	46	ARG	NE-CZ-NH1	-5.24	117.68	120.30
21	N	745	LEU	CA-CB-CG	-5.21	103.31	115.30
28	U	54	LEU	CA-CB-CG	-5.18	103.39	115.30
15	H	95	HIS	C-N-CD	5.14	139.19	128.40
23	P	411	LEU	CA-CB-CG	5.11	127.05	115.30
28	U	289	ASP	C-N-CA	5.10	134.45	121.70
17	J	317	PRO	C-N-CD	5.10	139.10	128.40
31	X	53	THR	N-CA-C	-5.08	97.27	111.00
21	N	572	LEU	CA-CB-CG	-5.08	103.62	115.30
28	U	289	ASP	CB-CA-C	5.06	120.52	110.40
27	T	164	LEU	CA-CB-CG	-5.04	103.72	115.30

There are no chirality outliers.

All (156) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	6	196	GLN	Peptide
8	A	64	LEU	Peptide
10	C	221	ASN	Peptide
13	F	175	THR	Peptide
15	H	102	CYS	Peptide
15	H	164	SER	Peptide
15	H	169	GLU	Peptide
15	H	189	PRO	Peptide
15	H	190	ARG	Peptide
15	H	192	ASP	Peptide
15	H	193	PRO	Peptide
15	H	281	GLN	Peptide
15	H	302	LYS	Peptide
15	H	97	LEU	Peptide
16	I	125	MET	Peptide
16	I	134	SER	Peptide
17	J	257	ARG	Peptide
17	J	37	LYS	Peptide
17	J	38	THR	Peptide
18	K	151	PRO	Peptide
18	K	154	SER	Peptide
18	K	158	ILE	Peptide
18	K	318	THR	Peptide
19	L	161	ARG	Peptide
19	L	213	LYS	Peptide
19	L	296	SER	Peptide
19	L	407	ARG	Peptide
20	M	161	SER	Peptide
20	M	328	ASN	Peptide
20	M	386	PHE	Peptide
20	M	72	ASN	Peptide
21	N	196	THR	Peptide
21	N	217	MET	Peptide
21	N	248	GLU	Peptide
21	N	322	ASP	Peptide
21	N	323	GLY	Peptide
21	N	352	ASN	Peptide
21	N	663	ILE	Peptide
21	N	670	LYS	Peptide
21	N	693	GLY	Peptide
21	N	730	VAL	Peptide
21	N	778	LYS	Peptide

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Mol	Chain	Res	Type	Group
22	O	15	ARG	Peptide
22	O	16	MET	Peptide
22	O	164	PRO	Peptide
22	O	17	GLU	Peptide
22	O	21	SER	Peptide
22	O	223	LEU	Peptide
22	O	226	LYS	Peptide
22	O	240	GLU	Peptide
22	O	244	ASN	Peptide
22	O	299	THR	Peptide
22	O	301	PHE	Peptide
22	O	302	VAL	Peptide
22	O	309	SER	Peptide
22	O	310	PHE	Peptide
22	O	34	GLU	Peptide
22	O	41	LEU	Peptide
22	O	51	ASP	Peptide
22	O	53	LYS	Peptide
22	O	58	ARG	Peptide
22	O	75	GLN	Peptide
22	O	92	PHE	Peptide
22	O	98	TYR	Peptide
23	P	203	ILE	Peptide
23	P	211	PRO	Peptide
23	P	233	GLU	Peptide
23	P	248	ASP	Peptide
23	P	286	ASN	Peptide
23	P	308	LEU	Peptide
23	P	318	TYR	Peptide
23	P	320	PRO	Peptide
23	P	321	VAL	Peptide
23	P	325	ASP	Peptide
23	P	332	GLU	Peptide
23	P	391	ALA	Peptide
23	P	393	VAL	Peptide
23	P	400	VAL	Peptide
23	P	409	SER	Peptide
23	P	411	LEU	Peptide
23	P	86	HIS	Peptide
24	Q	107	VAL	Peptide
24	Q	124	PHE	Peptide
24	Q	128	GLU	Peptide

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Mol	Chain	Res	Type	Group
24	Q	129	LYS	Peptide
24	Q	133	LEU	Peptide
24	Q	254	SER	Peptide
24	Q	34	ASP	Peptide
24	Q	418	GLN	Peptide
25	R	223	ASN	Peptide
25	R	238	PHE	Peptide
25	R	240	SER	Peptide
25	R	329	PHE	Peptide
25	R	377	LEU	Peptide
25	R	380	VAL	Peptide
25	R	397	ASN	Peptide
25	R	94	PHE	Peptide
26	S	145	PHE	Peptide
26	S	146	LEU	Peptide
26	S	170	TYR	Peptide
26	S	200	GLU	Peptide
26	S	203	SER	Peptide
26	S	224	LYS	Peptide
26	S	227	ASN	Peptide
26	S	247	VAL	Peptide
26	S	258	GLU	Peptide
26	S	333	PHE	Peptide
26	S	337	ASN	Peptide
26	S	342	LEU	Peptide
26	S	401	LYS	Peptide
26	S	417	GLN	Peptide
26	S	436	ILE	Peptide
26	S	480	ARG	Peptide
27	T	197	TYR	Peptide
27	T	52	LEU	Peptide
27	T	91	SER	Peptide
27	T	96	LEU	Peptide
28	U	129	GLY	Peptide
28	U	132	LEU	Peptide
28	U	193	GLN	Peptide
28	U	197	LEU	Peptide
28	U	289	ASP	Peptide
28	U	305	ARG	Peptide
28	U	7	LYS	Peptide
28	U	87	GLU	Peptide
29	V	156	PHE	Peptide

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Mol	Chain	Res	Type	Group
29	V	161	THR	Peptide
29	V	162	GLY	Peptide
29	V	163	ALA	Peptide
29	V	273	ARG	Peptide
29	V	70	ALA	Peptide
30	W	104	LYS	Peptide
30	W	12	ASN	Peptide
30	W	146	GLU	Peptide
30	W	147	ILE	Peptide
30	W	161	VAL	Peptide
30	W	189	PRO	Peptide
30	W	2	VAL	Peptide
30	W	77	HIS	Peptide
31	X	23	LEU	Peptide
31	X	24	CYS	Peptide
31	X	28	PRO	Peptide
31	X	52	PRO	Peptide
31	X	77	PRO	Peptide
31	X	79	LYS	Peptide
32	Y	62	GLU	Peptide
32	Y	65	ASP	Peptide
33	Z	142	ASP	Peptide
33	Z	205	LEU	Peptide
33	Z	276	ASN	Peptide
33	Z	497	PHE	Peptide
33	Z	574	TYR	Peptide
8	a	64	LEU	Peptide
10	c	221	ASN	Peptide
13	f	175	THR	Peptide
6	k	196	GLN	Peptide

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	1	220/241 (91%)	202 (92%)	17 (8%)	1 (0%)	29	68
1	8	220/241 (91%)	202 (92%)	17 (8%)	1 (0%)	29	68
2	2	231/266 (87%)	210 (91%)	21 (9%)	0	100	100
2	9	231/266 (87%)	210 (91%)	21 (9%)	0	100	100
3	3	203/215 (94%)	180 (89%)	22 (11%)	1 (0%)	29	68
3	h	203/215 (94%)	179 (88%)	23 (11%)	1 (0%)	29	68
4	4	220/261 (84%)	206 (94%)	14 (6%)	0	100	100
4	i	220/261 (84%)	206 (94%)	14 (6%)	0	100	100
5	5	202/205 (98%)	185 (92%)	16 (8%)	1 (0%)	29	68
5	j	202/205 (98%)	185 (92%)	16 (8%)	1 (0%)	29	68
6	6	196/198 (99%)	175 (89%)	19 (10%)	2 (1%)	15	53
6	k	196/198 (99%)	174 (89%)	19 (10%)	3 (2%)	10	46
7	7	210/287 (73%)	188 (90%)	20 (10%)	2 (1%)	15	53
7	l	210/287 (73%)	190 (90%)	19 (9%)	1 (0%)	29	68
8	A	241/252 (96%)	220 (91%)	21 (9%)	0	100	100
8	a	241/252 (96%)	220 (91%)	21 (9%)	0	100	100
9	B	248/250 (99%)	225 (91%)	23 (9%)	0	100	100
9	b	248/250 (99%)	225 (91%)	23 (9%)	0	100	100
10	C	242/258 (94%)	220 (91%)	19 (8%)	3 (1%)	13	50
10	c	242/258 (94%)	220 (91%)	19 (8%)	3 (1%)	13	50
11	D	239/254 (94%)	215 (90%)	24 (10%)	0	100	100
11	d	239/254 (94%)	215 (90%)	24 (10%)	0	100	100
12	E	240/260 (92%)	215 (90%)	23 (10%)	2 (1%)	19	59
12	e	240/260 (92%)	215 (90%)	23 (10%)	2 (1%)	19	59
13	F	231/234 (99%)	210 (91%)	19 (8%)	2 (1%)	17	56
13	f	231/234 (99%)	210 (91%)	19 (8%)	2 (1%)	17	56
14	G	242/288 (84%)	216 (89%)	25 (10%)	1 (0%)	34	72
14	g	242/288 (84%)	216 (89%)	24 (10%)	2 (1%)	19	59
15	H	350/467 (75%)	286 (82%)	56 (16%)	8 (2%)	6	36
16	I	321/437 (74%)	286 (89%)	33 (10%)	2 (1%)	25	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	J	371/405 (92%)	332 (90%)	31 (8%)	8 (2%)	6	37
18	K	357/428 (83%)	306 (86%)	45 (13%)	6 (2%)	9	43
19	L	354/437 (81%)	302 (85%)	51 (14%)	1 (0%)	41	76
20	M	349/434 (80%)	306 (88%)	40 (12%)	3 (1%)	17	56
21	N	843/945 (89%)	656 (78%)	174 (21%)	13 (2%)	10	46
22	O	372/393 (95%)	250 (67%)	103 (28%)	19 (5%)	2	22
23	P	427/445 (96%)	305 (71%)	99 (23%)	23 (5%)	2	21
24	Q	429/434 (99%)	350 (82%)	76 (18%)	3 (1%)	22	62
25	R	398/429 (93%)	281 (71%)	94 (24%)	23 (6%)	1	20
26	S	435/523 (83%)	313 (72%)	103 (24%)	19 (4%)	2	24
27	T	265/274 (97%)	190 (72%)	74 (28%)	1 (0%)	34	72
28	U	244/338 (72%)	198 (81%)	39 (16%)	7 (3%)	4	31
29	V	237/306 (78%)	176 (74%)	53 (22%)	8 (3%)	3	29
30	W	195/268 (73%)	157 (80%)	30 (15%)	8 (4%)	3	25
31	X	125/156 (80%)	94 (75%)	26 (21%)	5 (4%)	3	25
32	Y	32/89 (36%)	21 (66%)	9 (28%)	2 (6%)	1	18
33	Z	757/993 (76%)	665 (88%)	80 (11%)	12 (2%)	9	44
All	All	13191/15139 (87%)	11208 (85%)	1781 (14%)	202 (2%)	14	46

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
16	I	253	ILE
17	J	321	VAL
18	K	342	SER
18	K	344	ARG
25	R	239	THR
25	R	284	ALA
25	R	285	ALA
25	R	286	LEU
26	S	25	TYR
26	S	40	GLU
26	S	44	THR
26	S	55	ARG
26	S	201	ILE
26	S	301	PRO

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Mol	Chain	Res	Type
26	S	431	VAL
28	U	139	ALA
28	U	140	ILE
30	W	67	ALA
30	W	105	VAL
31	X	64	ILE
31	X	78	ILE
6	k	2	ASP
6	k	3	ILE
10	C	222	ASP
18	K	158	ILE
18	K	160	VAL
21	N	761	ILE
22	O	16	MET
22	O	302	VAL
23	P	108	LYS
23	P	109	SER
23	P	425	HIS
25	R	289	ILE
26	S	57	LEU
26	S	73	THR
29	V	68	VAL
29	V	159	ILE
29	V	290	ASN
31	X	24	CYS
33	Z	368	VAL
33	Z	370	SER
10	c	222	ASP
14	g	129	VAL
6	6	2	ASP
20	M	163	PHE
21	N	741	TYR
21	N	874	ILE
22	O	15	ARG
22	O	92	PHE
22	O	93	ASP
22	O	226	LYS
22	O	233	LEU
22	O	303	LYS
22	O	352	TRP
22	O	366	MET
23	P	85	LYS

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Mol	Chain	Res	Type
23	P	411	LEU
25	R	353	MET
26	S	470	GLN
28	U	209	GLU
29	V	163	ALA
33	Z	466	GLU
7	7	129	PHE
14	G	43	ASN
15	H	454	TYR
17	J	135	SER
17	J	318	PRO
17	J	319	PRO
18	K	159	SER
21	N	572	LEU
21	N	903	VAL
22	O	18	ALA
22	O	44	SER
22	O	65	PHE
22	O	70	TYR
22	O	289	GLN
23	P	243	GLU
23	P	288	ASN
23	P	412	LEU
25	R	64	LYS
25	R	223	ASN
25	R	241	ILE
25	R	287	GLN
25	R	420	ALA
25	R	421	VAL
26	S	177	ASN
26	S	230	LYS
27	T	251	HIS
28	U	130	VAL
28	U	305	ARG
29	V	240	ALA
30	W	68	GLU
30	W	79	THR
30	W	147	ILE
31	X	29	VAL
32	Y	67	VAL
33	Z	277	GLU
33	Z	483	THR

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Mol	Chain	Res	Type
33	Z	802	ASP
14	g	43	ASN
7	7	152	ALA
10	C	99	LEU
15	H	186	PRO
15	H	190	ARG
15	H	194	SER
17	J	317	PRO
21	N	179	THR
21	N	476	THR
21	N	913	PRO
22	O	210	ARG
23	P	132	VAL
23	P	167	THR
23	P	382	ASP
23	P	436	GLU
25	R	197	MET
25	R	210	TYR
25	R	320	LYS
25	R	399	GLN
26	S	69	LEU
26	S	74	LEU
10	c	99	LEU
7	l	152	ALA
1	1	79	ASP
3	3	77	ILE
1	8	79	ASP
12	E	204	LEU
13	F	113	CYS
20	M	33	ARG
21	N	85	ALA
22	O	83	LEU
22	O	353	VAL
23	P	41	VAL
23	P	255	ALA
23	P	296	GLN
24	Q	114	GLN
24	Q	128	GLU
25	R	114	ASN
25	R	258	LEU
26	S	225	HIS
26	S	342	LEU

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Mol	Chain	Res	Type
26	S	404	LEU
26	S	447	GLU
29	V	282	GLU
30	W	78	ASP
33	Z	232	LYS
33	Z	243	GLN
33	Z	434	GLN
12	e	204	LEU
13	f	113	CYS
15	H	192	ASP
16	I	302	ILE
17	J	55	VAL
17	J	134	VAL
21	N	450	ILE
21	N	914	VAL
23	P	237	VAL
23	P	320	PRO
25	R	72	VAL
25	R	384	VAL
28	U	132	LEU
28	U	133	PRO
30	W	30	ILE
31	X	28	PRO
33	Z	925	VAL
3	h	77	ILE
10	C	86	ILE
15	H	168	ILE
19	L	81	ILE
20	M	167	VAL
21	N	617	VAL
23	P	119	ILE
23	P	281	ILE
26	S	187	ILE
32	Y	69	VAL
10	c	86	ILE
15	H	191	ILE
17	J	41	VAL
21	N	583	VAL
23	P	260	VAL
23	P	264	ILE
23	P	433	ILE
25	R	330	VAL

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Mol	Chain	Res	Type
25	R	361	VAL
29	V	32	ILE
29	V	144	ILE
30	W	118	ILE
33	Z	286	VAL
5	5	105	VAL
6	6	9	VAL
13	F	29	ILE
18	K	223	VAL
22	O	363	ILE
23	P	380	ILE
24	Q	281	ILE
25	R	110	ILE
33	Z	480	ASN
13	f	29	ILE
5	j	105	VAL
6	k	9	VAL
12	E	89	ILE
15	H	96	PRO
12	e	89	ILE

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	1	185/201 (92%)	185 (100%)	0	100	100
1	8	185/201 (92%)	185 (100%)	0	100	100
2	2	199/224 (89%)	198 (100%)	1 (0%)	88	93
2	9	199/224 (89%)	198 (100%)	1 (0%)	88	93
3	3	168/178 (94%)	167 (99%)	1 (1%)	86	92
3	h	168/178 (94%)	168 (100%)	0	100	100
4	4	181/214 (85%)	181 (100%)	0	100	100
4	i	181/214 (85%)	181 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	5	172/173 (99%)	172 (100%)	0	100	100
5	j	172/173 (99%)	172 (100%)	0	100	100
6	6	175/175 (100%)	174 (99%)	1 (1%)	86	92
6	k	175/175 (100%)	174 (99%)	1 (1%)	86	92
7	7	169/235 (72%)	169 (100%)	0	100	100
7	l	169/235 (72%)	168 (99%)	1 (1%)	86	92
8	A	207/210 (99%)	207 (100%)	0	100	100
8	a	207/210 (99%)	207 (100%)	0	100	100
9	B	209/209 (100%)	209 (100%)	0	100	100
9	b	209/209 (100%)	209 (100%)	0	100	100
10	C	203/216 (94%)	203 (100%)	0	100	100
10	c	203/216 (94%)	203 (100%)	0	100	100
11	D	213/226 (94%)	213 (100%)	0	100	100
11	d	213/226 (94%)	213 (100%)	0	100	100
12	E	198/215 (92%)	196 (99%)	2 (1%)	76	86
12	e	198/215 (92%)	198 (100%)	0	100	100
13	F	192/193 (100%)	192 (100%)	0	100	100
13	f	192/193 (100%)	192 (100%)	0	100	100
14	G	201/239 (84%)	201 (100%)	0	100	100
14	g	201/239 (84%)	201 (100%)	0	100	100
15	H	301/399 (75%)	300 (100%)	1 (0%)	92	95
16	I	284/385 (74%)	282 (99%)	2 (1%)	84	90
17	J	325/352 (92%)	324 (100%)	1 (0%)	92	95
18	K	316/374 (84%)	315 (100%)	1 (0%)	92	95
19	L	306/377 (81%)	306 (100%)	0	100	100
20	M	303/375 (81%)	303 (100%)	0	100	100
21	N	713/797 (90%)	713 (100%)	0	100	100
22	O	350/368 (95%)	347 (99%)	3 (1%)	78	87
23	P	384/415 (92%)	381 (99%)	3 (1%)	81	89
24	Q	388/391 (99%)	387 (100%)	1 (0%)	92	95
25	R	351/379 (93%)	348 (99%)	3 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	S	342/489 (70%)	336 (98%)	6 (2%)	59	77
27	T	250/256 (98%)	250 (100%)	0	100	100
28	U	228/308 (74%)	225 (99%)	3 (1%)	69	82
29	V	211/268 (79%)	204 (97%)	7 (3%)	38	61
30	W	171/230 (74%)	171 (100%)	0	100	100
31	X	116/144 (81%)	116 (100%)	0	100	100
32	Y	18/81 (22%)	18 (100%)	0	100	100
33	Z	645/850 (76%)	643 (100%)	2 (0%)	92	95
All	All	11346/13054 (87%)	11305 (100%)	41 (0%)	91	94

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	197	ASP
3	3	18	LEU
6	6	1	MET
2	9	197	ASP
12	E	243	LEU
12	E	244	LYS
15	H	95	HIS
16	I	252	LEU
16	I	253	ILE
17	J	258	VAL
18	K	343	LEU
22	O	4	ASN
22	O	14	LEU
22	O	138	LEU
23	P	106	SER
23	P	108	LYS
23	P	337	HIS
24	Q	389	VAL
25	R	148	ASP
25	R	406	GLN
25	R	417	TYR
26	S	22	GLU
26	S	179	ILE
26	S	297	ILE
26	S	396	SER
26	S	464	ARG

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Mol	Chain	Res	Type
26	S	475	TYR
28	U	189	ARG
28	U	291	LEU
28	U	297	GLN
29	V	37	MET
29	V	53	MET
29	V	108	TYR
29	V	258	GLU
29	V	281	SER
29	V	288	LEU
29	V	289	GLU
33	Z	367	SER
33	Z	369	PHE
6	k	2	ASP
7	l	131	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (275) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	113	GLN
1	1	154	GLN
2	2	35	GLN
2	2	36	GLN
2	2	51	ASN
2	2	70	ASN
2	2	95	HIS
2	2	227	ASN
2	2	246	GLN
3	3	164	ASN
3	3	176	HIS
3	3	180	GLN
4	4	86	GLN
4	4	91	ASN
4	4	110	GLN
4	4	115	HIS
4	4	122	HIS
4	4	173	GLN
5	5	72	ASN
5	5	89	GLN
6	6	37	GLN
6	6	112	ASN
6	6	118	GLN

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Mol	Chain	Res	Type
6	6	146	HIS
6	6	198	GLN
7	7	141	HIS
7	7	251	ASN
1	8	113	GLN
1	8	154	GLN
2	9	35	GLN
2	9	36	GLN
2	9	51	ASN
2	9	70	ASN
2	9	94	GLN
2	9	95	HIS
2	9	227	ASN
2	9	246	GLN
8	A	123	ASN
8	A	130	GLN
8	A	175	GLN
8	A	176	GLN
8	A	181	ASN
10	C	21	GLN
10	C	31	HIS
10	C	59	GLN
10	C	94	HIS
10	C	96	GLN
10	C	124	GLN
10	C	173	GLN
10	C	177	GLN
11	D	16	HIS
11	D	19	GLN
11	D	70	HIS
11	D	94	GLN
11	D	162	GLN
11	D	204	GLN
11	D	235	GLN
12	E	23	GLN
12	E	91	HIS
12	E	114	GLN
12	E	147	HIS
12	E	233	ASN
13	F	69	HIS
13	F	93	ASN
13	F	119	ASN

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Mol	Chain	Res	Type
13	F	121	GLN
13	F	148	GLN
13	F	199	GLN
14	G	23	GLN
14	G	90	ASN
14	G	170	GLN
14	G	195	GLN
14	G	237	GLN
15	H	265	ASN
15	H	339	GLN
16	I	274	ASN
16	I	295	ASN
16	I	303	GLN
17	J	47	GLN
17	J	49	ASN
17	J	52	ASN
17	J	111	GLN
17	J	128	ASN
17	J	156	GLN
17	J	205	HIS
17	J	331	HIS
17	J	379	GLN
17	J	393	ASN
18	K	182	GLN
18	K	264	ASN
18	K	285	GLN
18	K	302	GLN
18	K	375	ASN
18	K	404	GLN
19	L	67	HIS
19	L	80	ASN
19	L	103	GLN
19	L	133	ASN
20	M	71	ASN
20	M	74	GLN
20	M	311	GLN
20	M	359	GLN
20	M	364	HIS
20	M	375	ASN
20	M	405	ASN
21	N	182	ASN
21	N	226	ASN

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Mol	Chain	Res	Type
21	N	231	ASN
21	N	300	ASN
21	N	305	ASN
21	N	308	ASN
21	N	340	HIS
21	N	378	ASN
21	N	666	GLN
21	N	688	ASN
21	N	716	GLN
21	N	870	ASN
21	N	899	ASN
21	N	922	GLN
22	O	4	ASN
22	O	5	HIS
22	O	75	GLN
22	O	107	GLN
22	O	212	GLN
22	O	236	HIS
22	O	244	ASN
22	O	304	ASN
22	O	323	ASN
22	O	362	GLN
22	O	374	ASN
23	P	38	GLN
23	P	88	GLN
23	P	210	ASN
23	P	242	GLN
23	P	288	ASN
23	P	296	GLN
23	P	342	GLN
23	P	349	ASN
23	P	440	HIS
24	Q	19	GLN
24	Q	63	GLN
24	Q	114	GLN
24	Q	186	HIS
24	Q	226	HIS
24	Q	253	ASN
24	Q	283	ASN
24	Q	308	ASN
24	Q	336	ASN
24	Q	361	HIS

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Mol	Chain	Res	Type
24	Q	379	GLN
24	Q	420	ASN
25	R	23	ASN
25	R	100	ASN
25	R	114	ASN
25	R	136	ASN
25	R	340	GLN
25	R	366	ASN
25	R	399	GLN
26	S	20	HIS
26	S	159	ASN
26	S	177	ASN
26	S	235	ASN
26	S	243	ASN
26	S	280	ASN
26	S	314	ASN
26	S	339	GLN
26	S	458	GLN
27	T	17	ASN
27	T	37	ASN
27	T	94	HIS
27	T	123	HIS
27	T	127	GLN
27	T	135	ASN
27	T	204	ASN
27	T	238	GLN
27	T	258	ASN
27	T	272	ASN
28	U	26	GLN
28	U	192	ASN
28	U	223	HIS
28	U	230	GLN
28	U	259	ASN
28	U	260	ASN
28	U	280	ASN
28	U	298	ASN
28	U	302	GLN
29	V	64	ASN
29	V	102	GLN
29	V	111	HIS
29	V	184	ASN
29	V	190	HIS

Continued on next page...

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Mol	Chain	Res	Type
29	V	193	ASN
29	V	215	ASN
29	V	217	HIS
29	V	250	GLN
29	V	291	ASN
30	W	29	GLN
30	W	38	GLN
30	W	42	ASN
30	W	92	GLN
30	W	95	GLN
30	W	106	GLN
30	W	143	ASN
30	W	149	GLN
31	X	105	ASN
32	Y	88	ASN
33	Z	132	HIS
33	Z	156	HIS
33	Z	235	GLN
33	Z	317	GLN
33	Z	327	GLN
33	Z	364	ASN
33	Z	380	ASN
33	Z	396	ASN
33	Z	435	GLN
33	Z	475	GLN
33	Z	760	HIS
33	Z	789	GLN
33	Z	801	HIS
33	Z	833	GLN
33	Z	856	HIS
33	Z	897	HIS
8	a	175	GLN
8	a	176	GLN
8	a	181	ASN
9	b	119	GLN
10	c	21	GLN
10	c	31	HIS
10	c	94	HIS
10	c	96	GLN
10	c	173	GLN
10	c	177	GLN
11	d	16	HIS

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Mol	Chain	Res	Type
11	d	19	GLN
11	d	70	HIS
11	d	94	GLN
11	d	162	GLN
11	d	204	GLN
11	d	235	GLN
12	e	91	HIS
12	e	114	GLN
12	e	147	HIS
12	e	233	ASN
13	f	69	HIS
13	f	93	ASN
13	f	117	GLN
13	f	119	ASN
13	f	148	GLN
13	f	199	GLN
14	g	23	GLN
14	g	90	ASN
14	g	170	GLN
14	g	195	GLN
14	g	237	GLN
3	h	160	ASN
3	h	164	ASN
3	h	176	HIS
3	h	180	GLN
4	i	86	GLN
4	i	91	ASN
4	i	115	HIS
4	i	122	HIS
4	i	173	GLN
4	i	194	ASN
5	j	72	ASN
5	j	89	GLN
6	k	37	GLN
6	k	55	GLN
6	k	112	ASN
6	k	118	GLN
6	k	146	HIS
6	k	198	GLN
7	l	141	HIS
7	l	251	ASN
7	l	283	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.

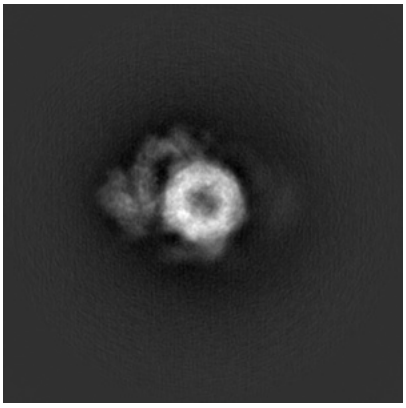
6 Map visualisation (i)

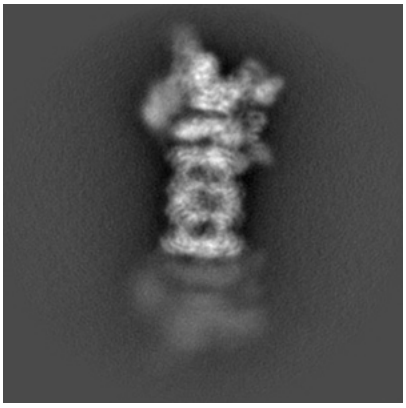
This section contains visualisations of the EMDB entry EMD-6574. These allow visual inspection of the internal detail of the map and identification of artifacts.

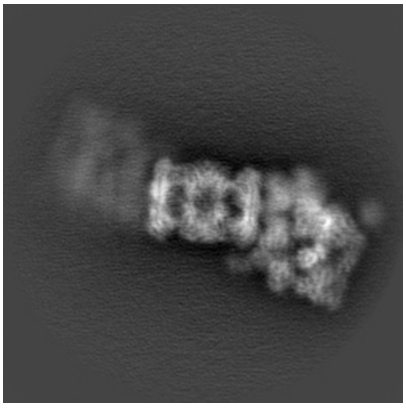
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

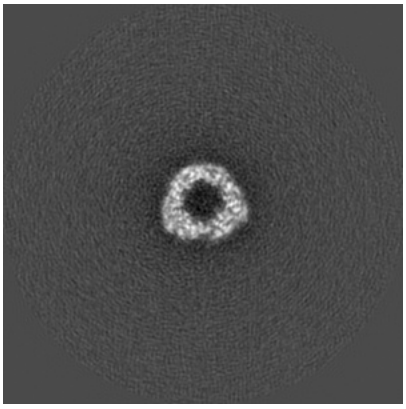

Y

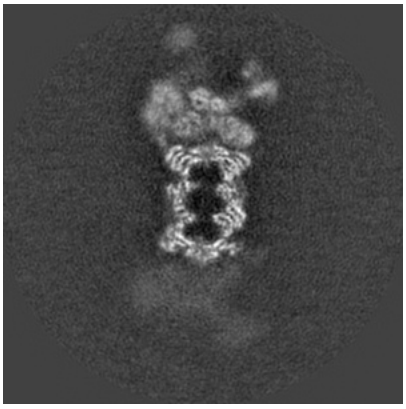

Z

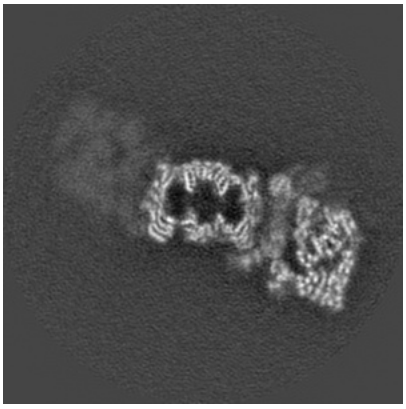
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 128

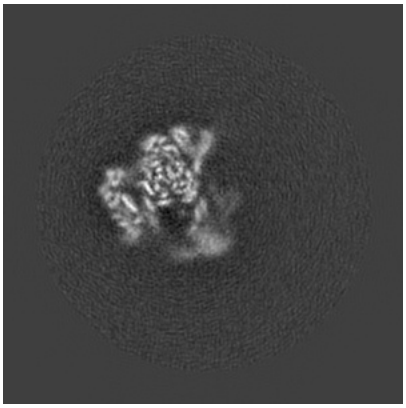

Y Index: 128


Z Index: 128

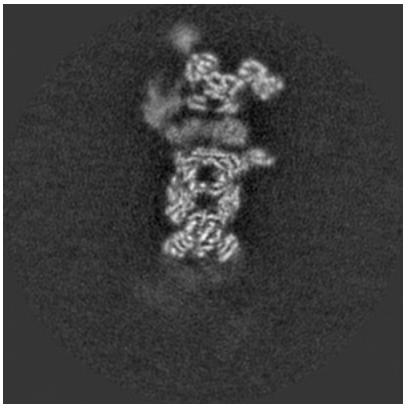
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

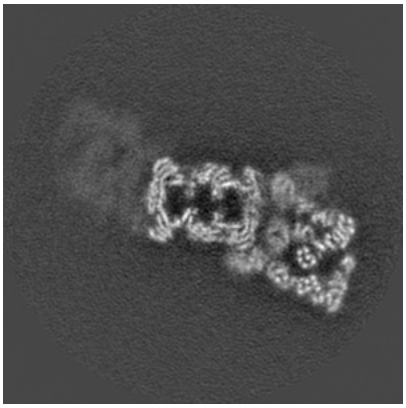
6.3.1 Primary map



X Index: 200



Y Index: 117

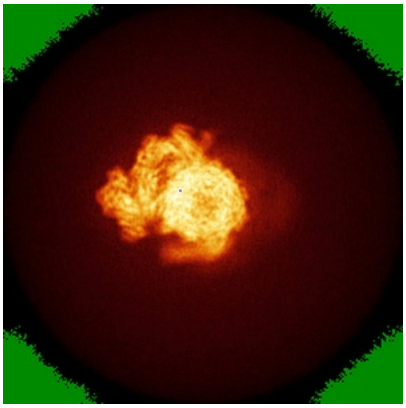


Z Index: 132

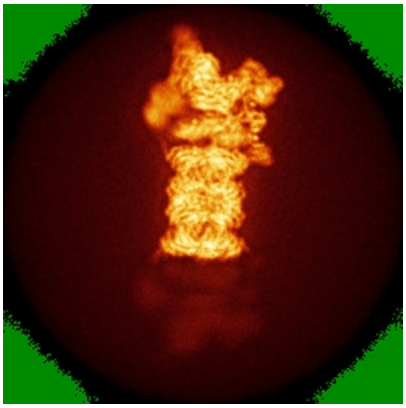
The images above show the largest variance slices of the map in three orthogonal directions.

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

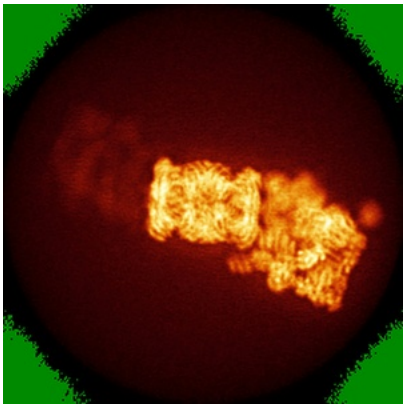
6.4.1 Primary map



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 0.0796. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

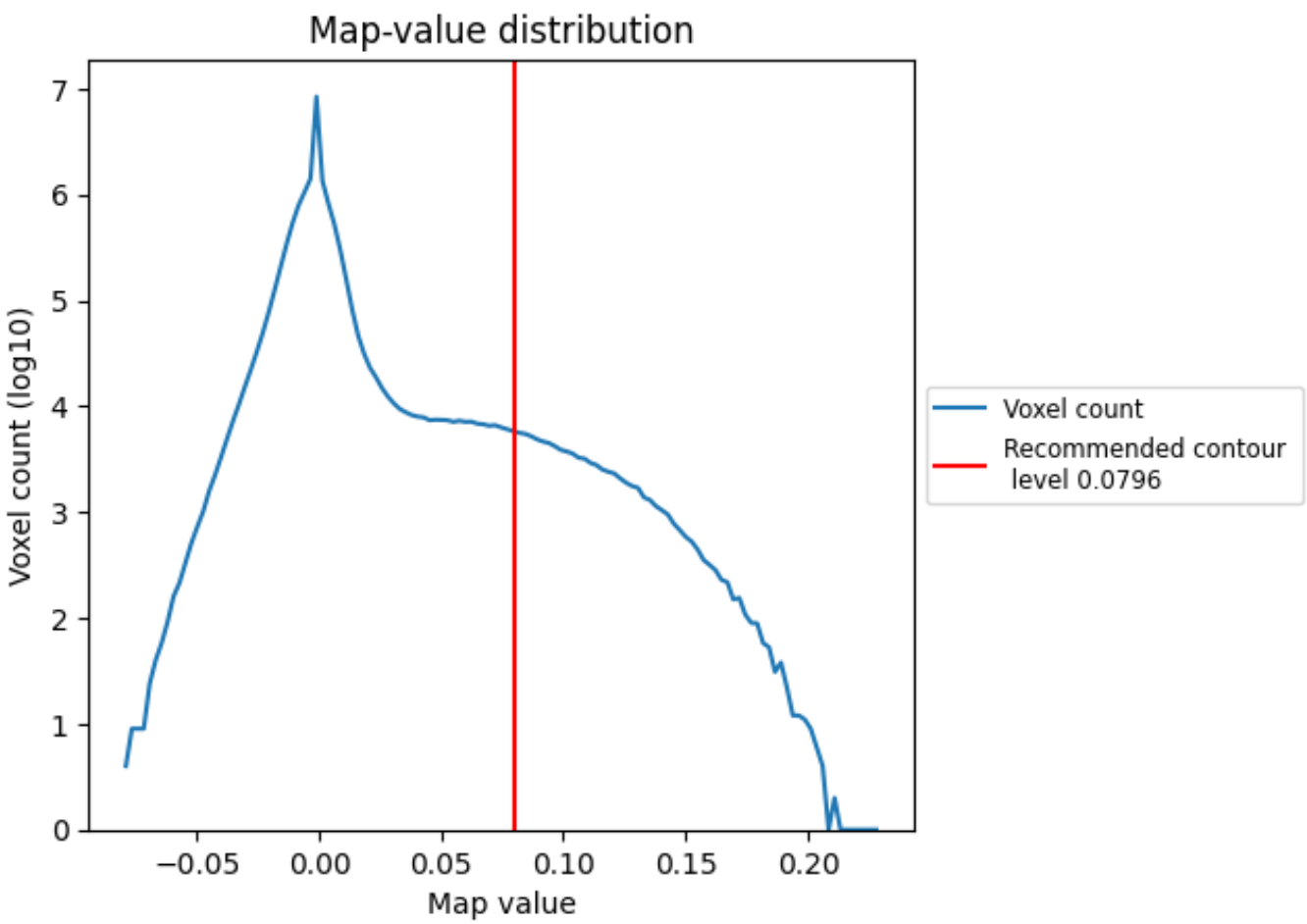
6.6 Mask visualisation (i)

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

7 Map analysis (i)

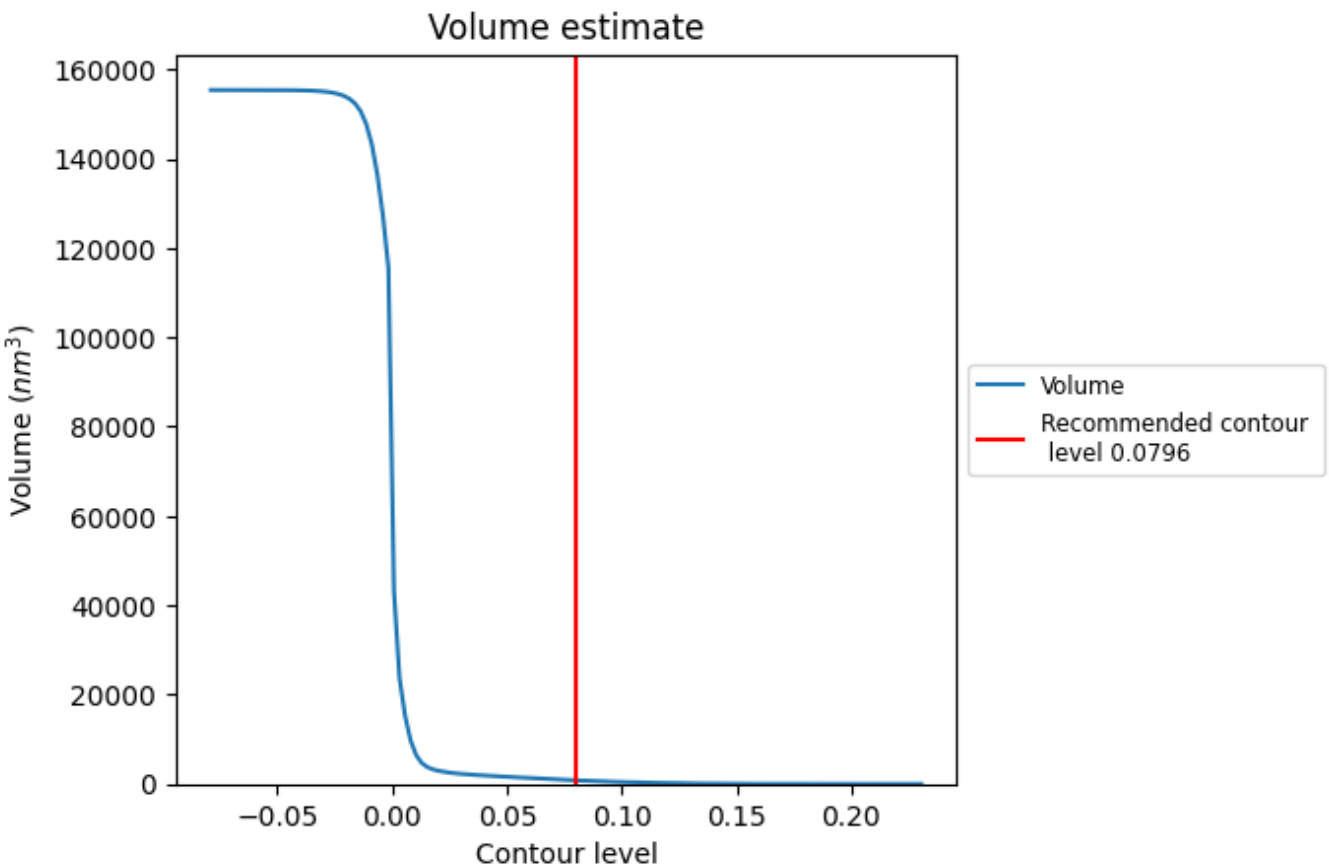
This section contains the results of statistical analysis of the map.

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.

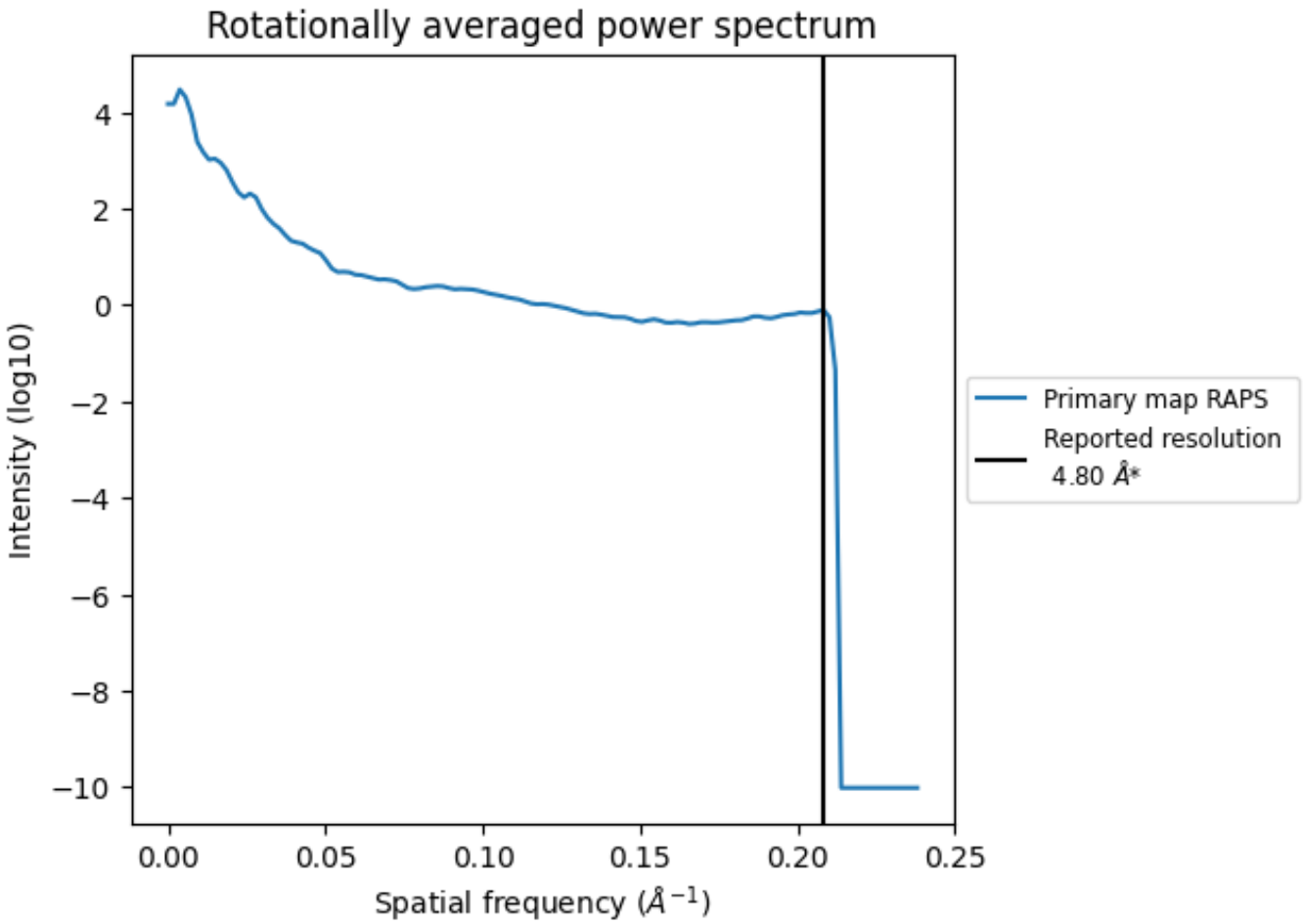
7.2 Volume estimate (i)



The volume at the recommended contour level is 826 nm^3; this corresponds to an approximate mass of 746 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 0.208 Å^{-1}

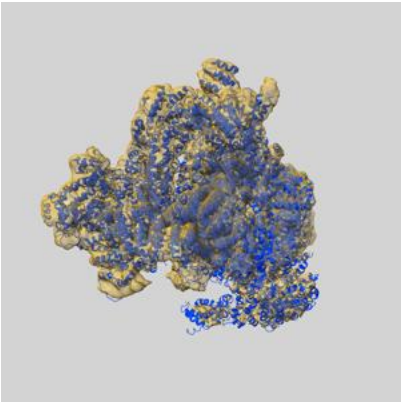
8 Fourier-Shell correlation (i)

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

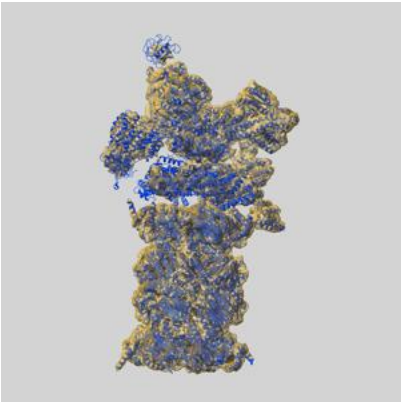
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6574 and PDB model 3JCO. Per-residue inclusion information can be found in section 3 on page 11.

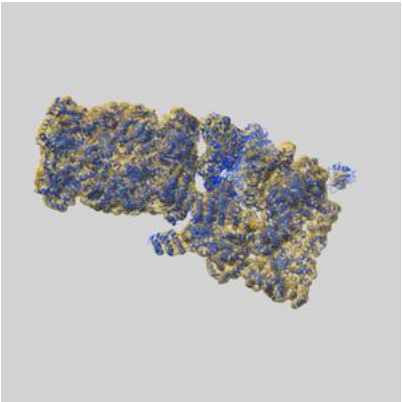
9.1 Map-model overlay (i)



X



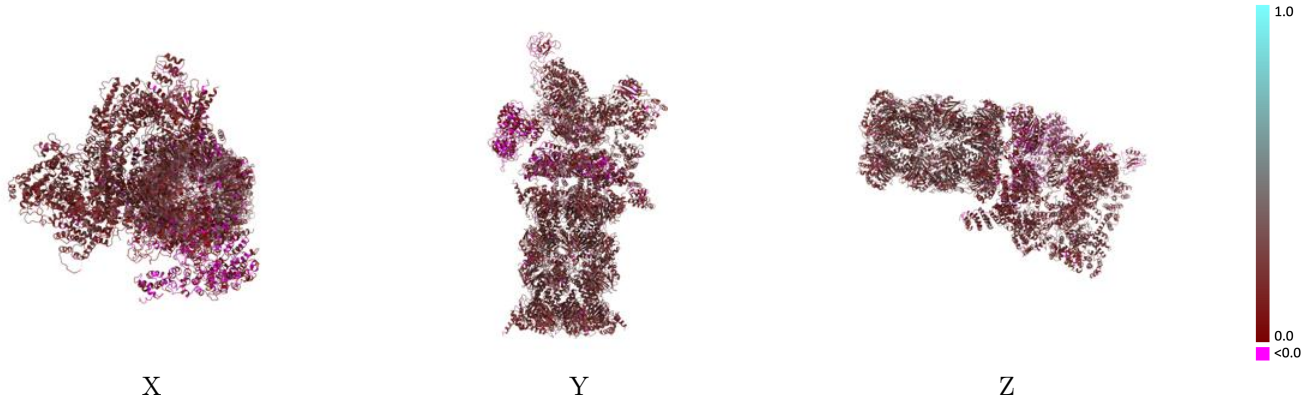
Y



Z

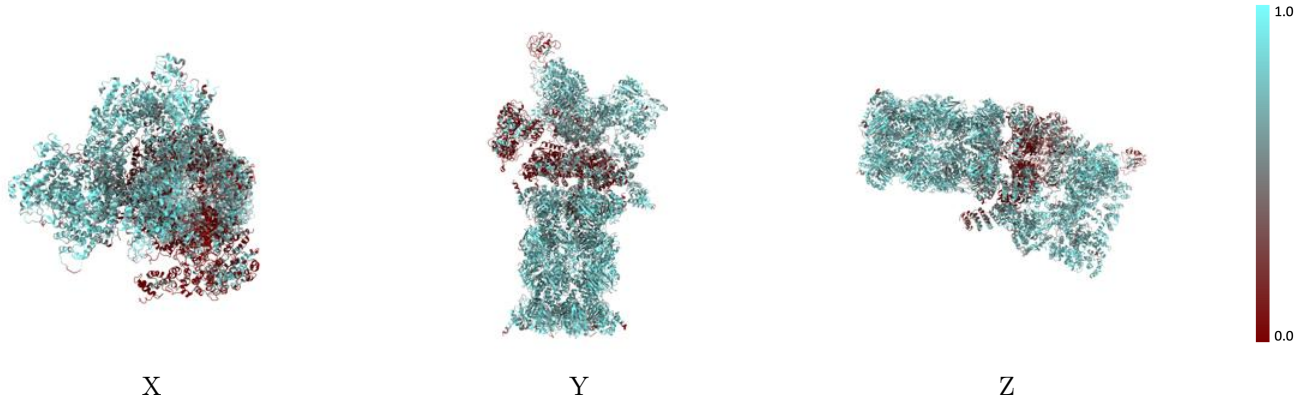
The images above show the 3D surface view of the map at the recommended contour level 0.0796 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



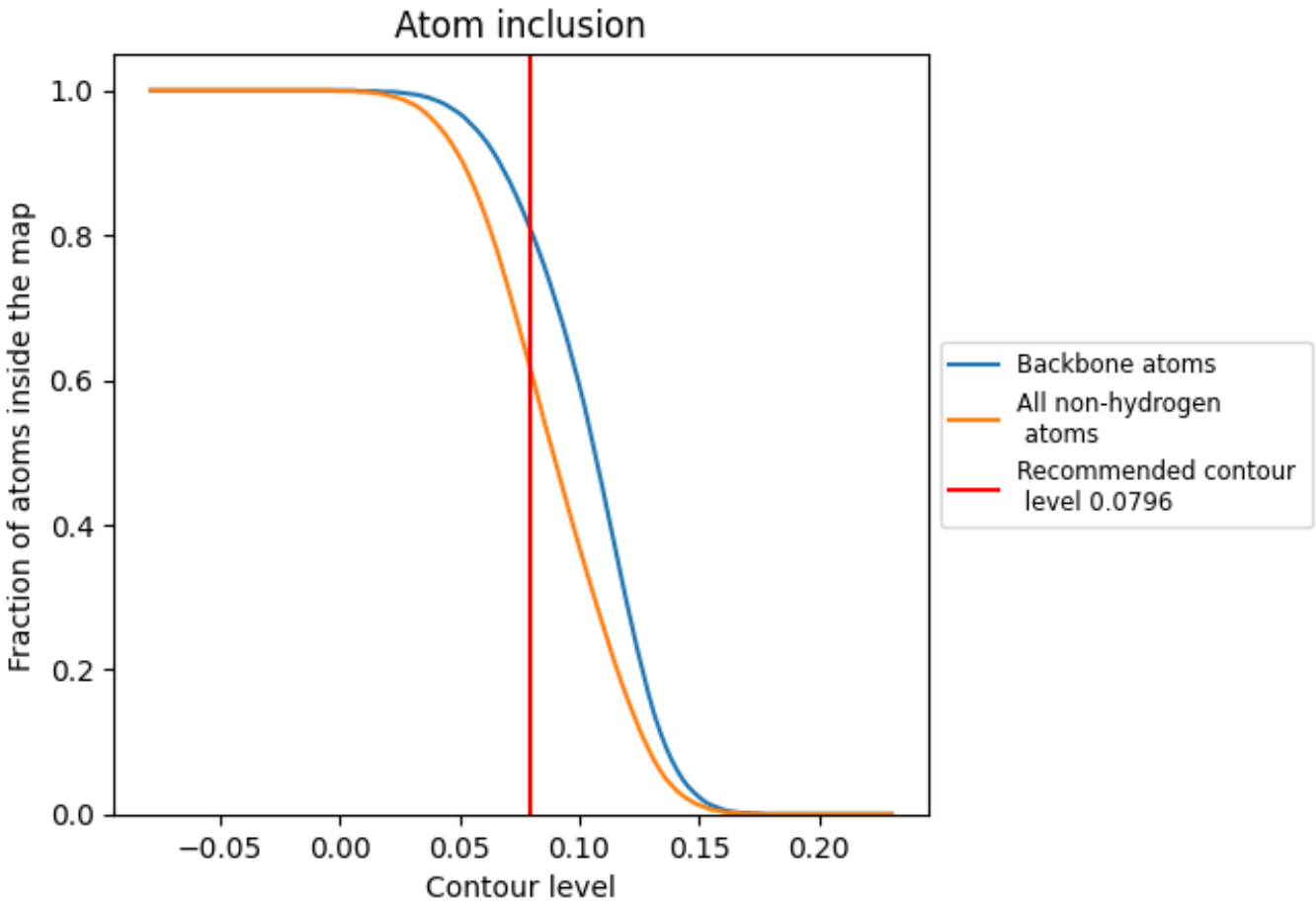
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0796).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 62% 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 (0.0796) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6150	0.1970
1	0.7600	0.2350
2	0.7590	0.2410
3	0.7480	0.2260
4	0.7700	0.2470
5	0.7450	0.2370
6	0.7400	0.2460
7	0.7870	0.2420
8	0.7450	0.2370
9	0.7690	0.2520
A	0.7390	0.2260
B	0.7170	0.2290
C	0.7310	0.2230
D	0.7380	0.2270
E	0.7170	0.2180
F	0.7710	0.2260
G	0.7640	0.2280
H	0.4060	0.1470
I	0.1910	0.1290
J	0.1750	0.1340
K	0.2910	0.1550
L	0.3850	0.1530
M	0.3830	0.1410
N	0.7290	0.2100
O	0.7200	0.1850
P	0.7060	0.1950
Q	0.5650	0.1860
R	0.6670	0.1940
S	0.7030	0.1980
T	0.6840	0.1910
U	0.6970	0.2230
V	0.6860	0.2170
W	0.7470	0.1710
X	0.1390	0.0830
Y	0.6850	0.2300

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Chain	Atom inclusion	Q-score
Z	0.2790	0.0830
a	0.6550	0.2270
b	0.5630	0.2210
c	0.5780	0.2030
d	0.6210	0.2070
e	0.6690	0.2200
f	0.7220	0.2280
g	0.6890	0.2260
h	0.7570	0.2380
i	0.7460	0.2500
j	0.7390	0.2330
k	0.7170	0.2370
l	0.7920	0.2390