wwPDB EM Validation Summary Report ⓘ

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

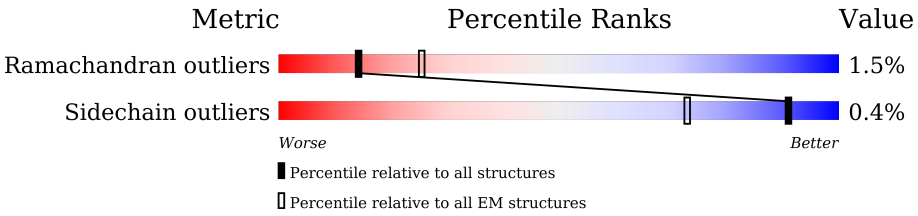
EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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
1	1	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
1	8	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

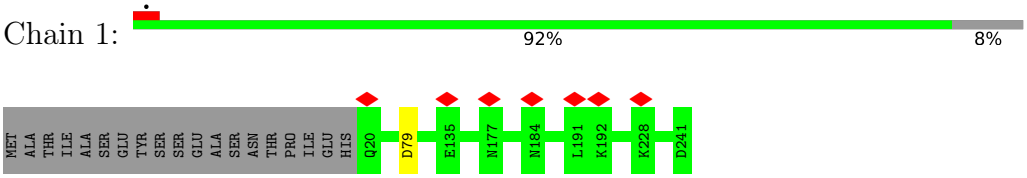
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN1.

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

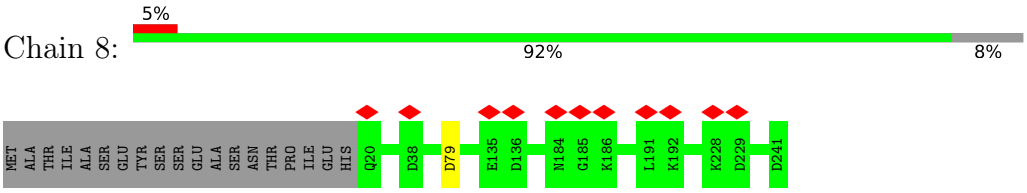
3 Residue-property plots (i)

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.

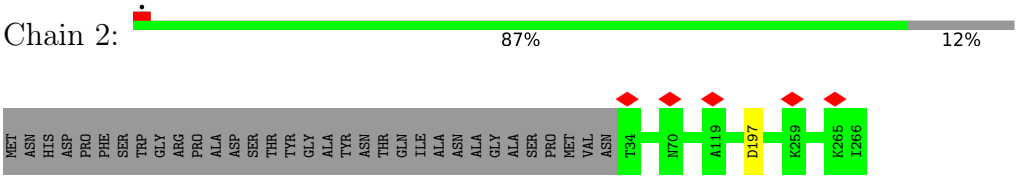
• Molecule 1: Proteasome subunit beta type-6



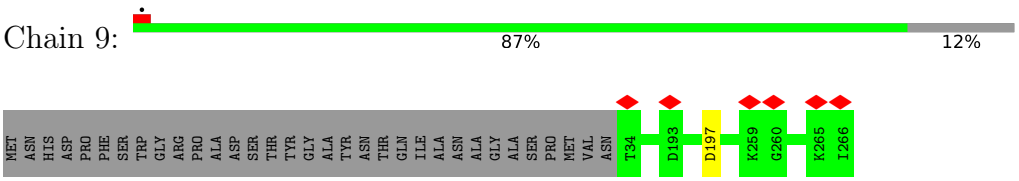
• Molecule 1: Proteasome subunit beta type-6



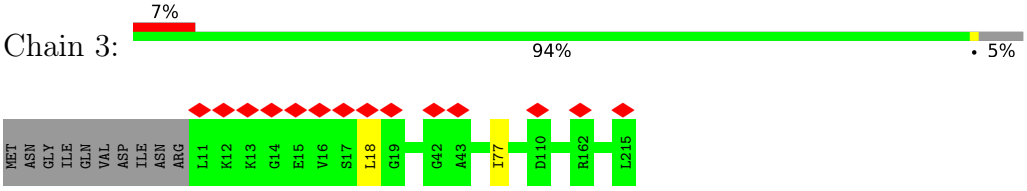
• Molecule 2: Proteasome subunit beta type-7



• Molecule 2: Proteasome subunit beta type-7

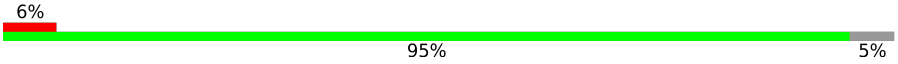


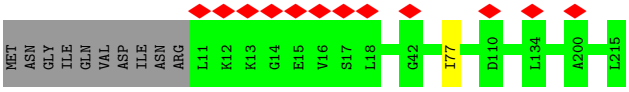
• Molecule 3: Proteasome subunit beta type-1



• Molecule 3: Proteasome subunit beta type-1

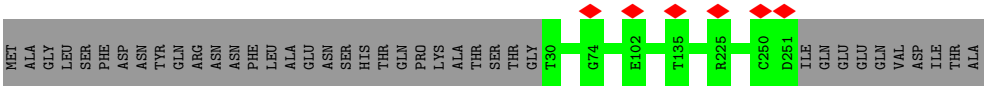
Chain h:





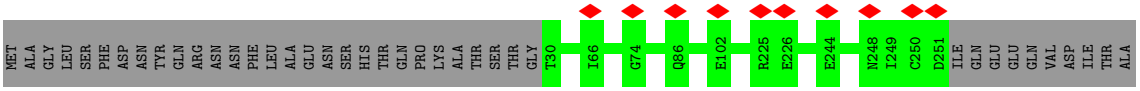
• Molecule 4: Proteasome subunit beta type-2

Chain 4:



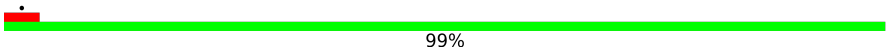
• Molecule 4: Proteasome subunit beta type-2

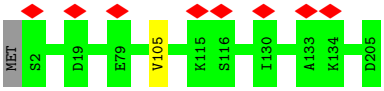
Chain i:



• Molecule 5: Proteasome subunit beta type-3

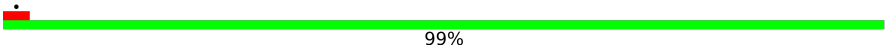
Chain 5:

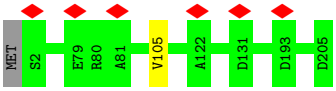




• Molecule 5: Proteasome subunit beta type-3

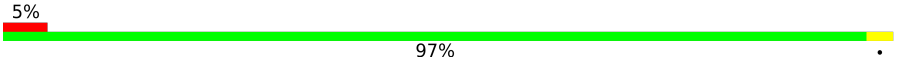
Chain j:

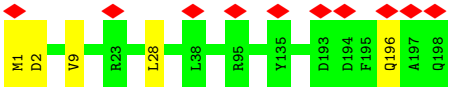




• Molecule 6: Proteasome subunit beta type-4

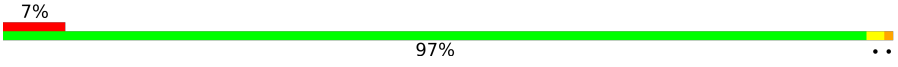
Chain 6:

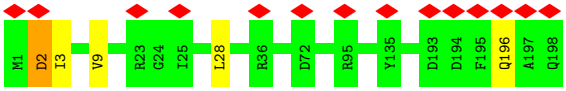




• Molecule 6: Proteasome subunit beta type-4

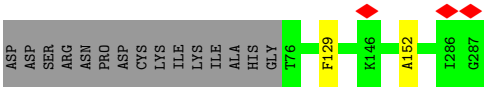
Chain k:





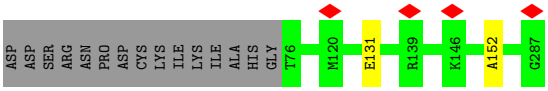
• Molecule 7: Proteasome subunit beta type-5

Chain 7:



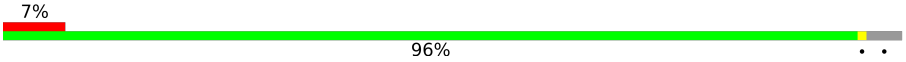
• Molecule 7: Proteasome subunit beta type-5

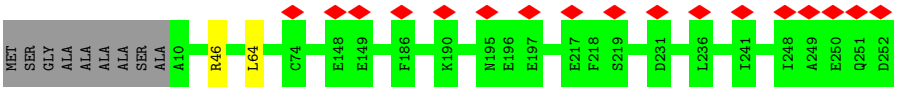
Chain l:



• Molecule 8: Proteasome subunit alpha type-1

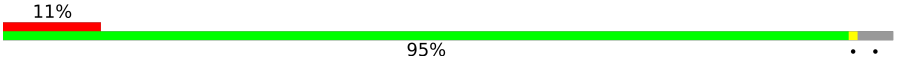
Chain A:

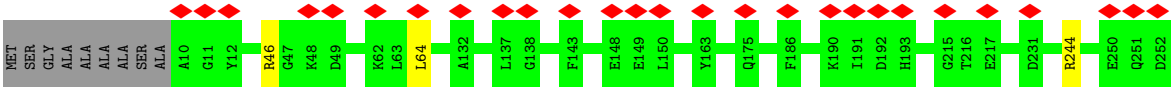




• Molecule 8: Proteasome subunit alpha type-1

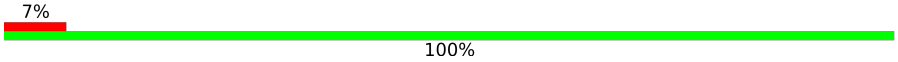
Chain a:

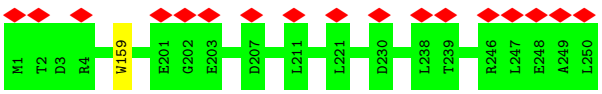




• Molecule 9: Proteasome subunit alpha type-2

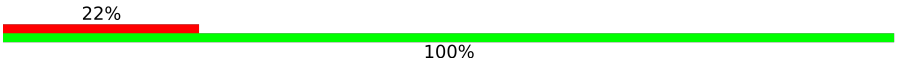
Chain B:

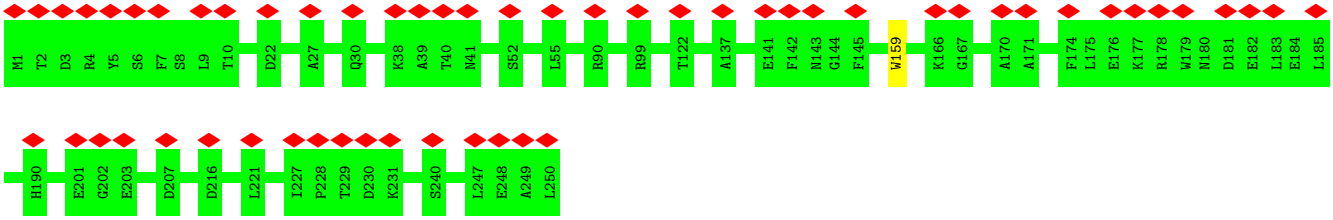




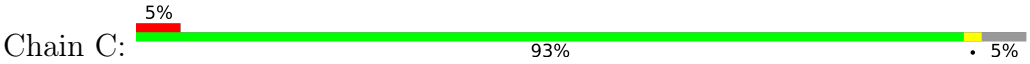
• Molecule 9: Proteasome subunit alpha type-2

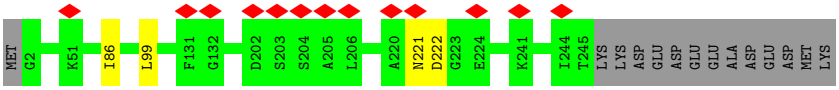
Chain b:



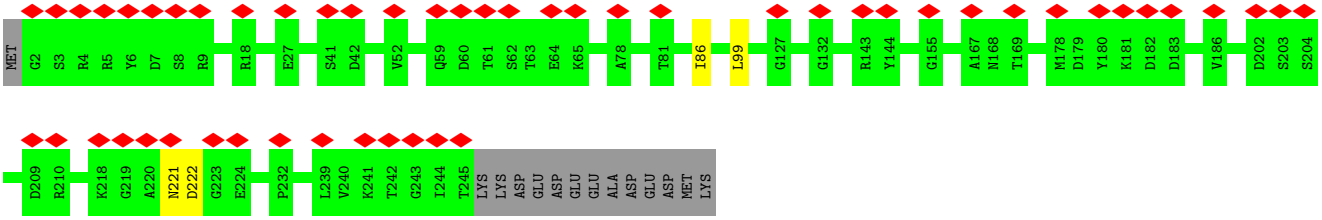


• Molecule 10: Proteasome subunit alpha type-3

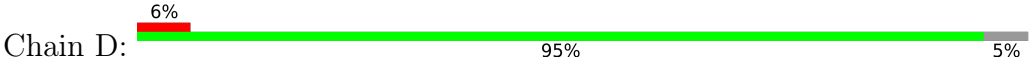


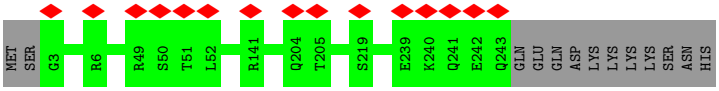


• Molecule 10: Proteasome subunit alpha type-3

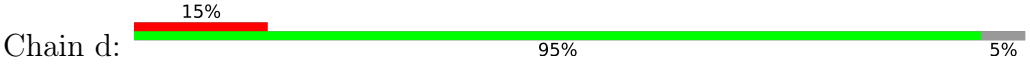


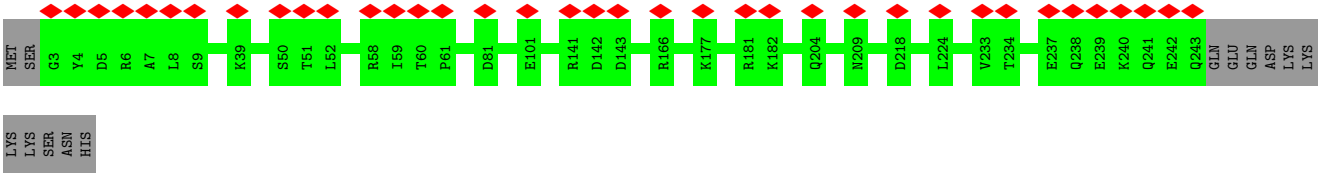
• Molecule 11: Proteasome subunit alpha type-4



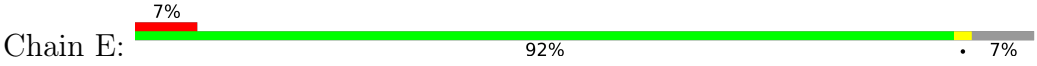


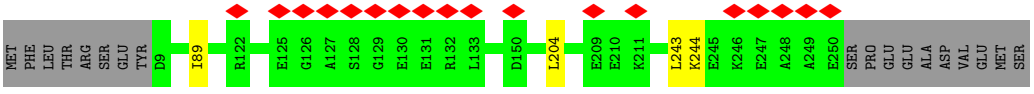
• Molecule 11: Proteasome subunit alpha type-4





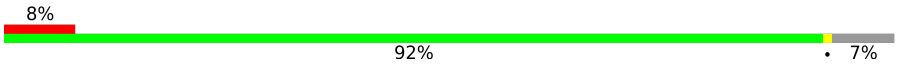
• Molecule 12: Proteasome subunit alpha type-5

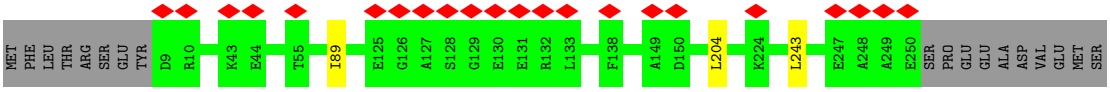




• Molecule 12: Proteasome subunit alpha type-5

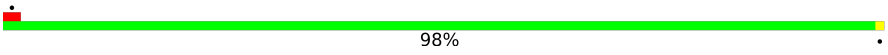
Chain e:

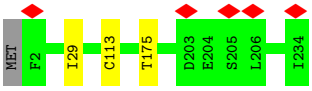




• Molecule 13: Proteasome subunit alpha type-6

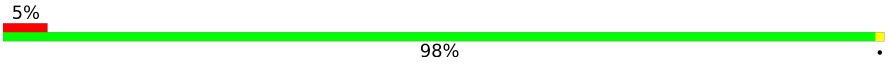
Chain F:

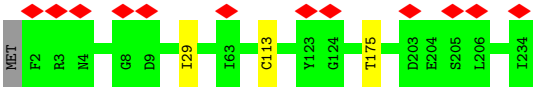




• Molecule 13: Proteasome subunit alpha type-6

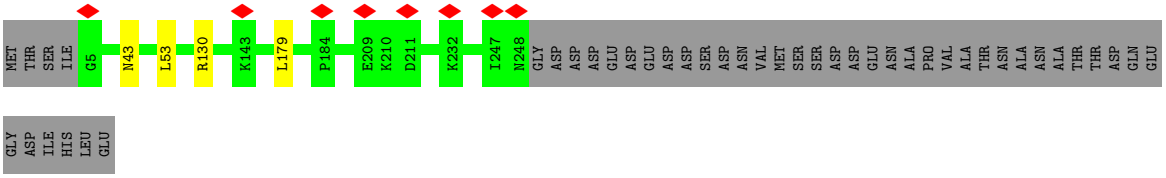
Chain f:





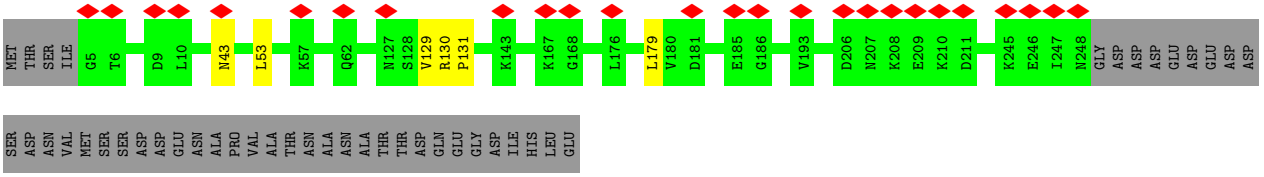
• Molecule 14: Probable proteasome subunit alpha type-7

Chain G:



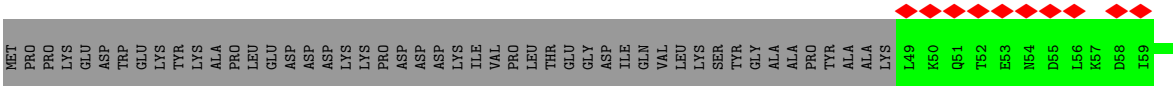
• Molecule 14: Probable proteasome subunit alpha type-7

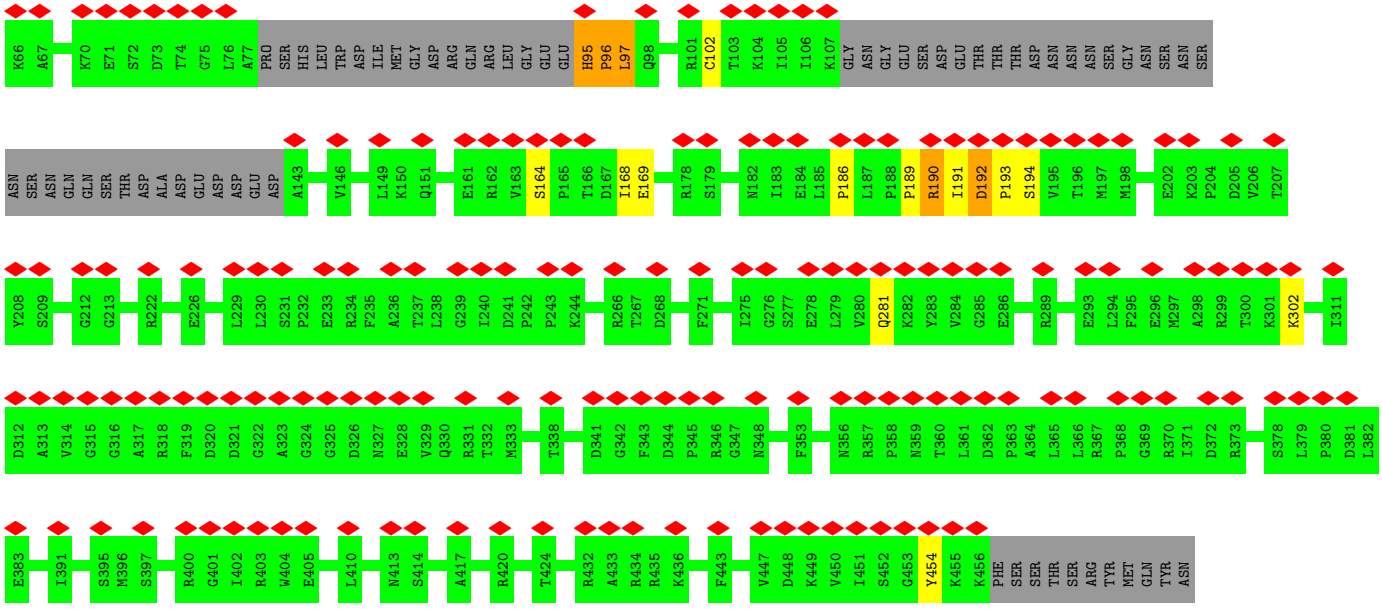
Chain g:



• Molecule 15: 26S protease regulatory subunit 7 homolog

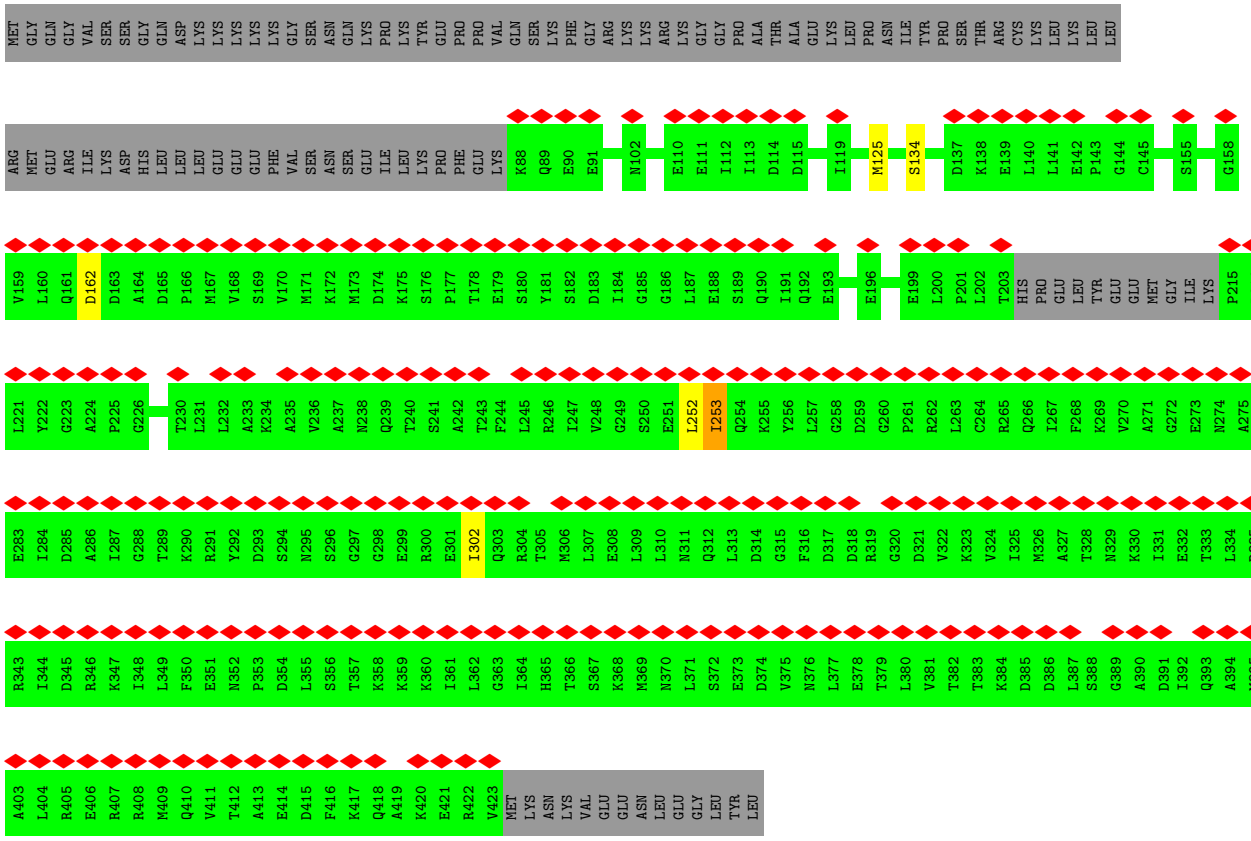
Chain H:





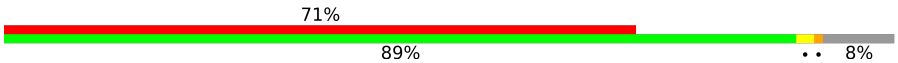
• Molecule 16: 26S protease regulatory subunit 4 homolog

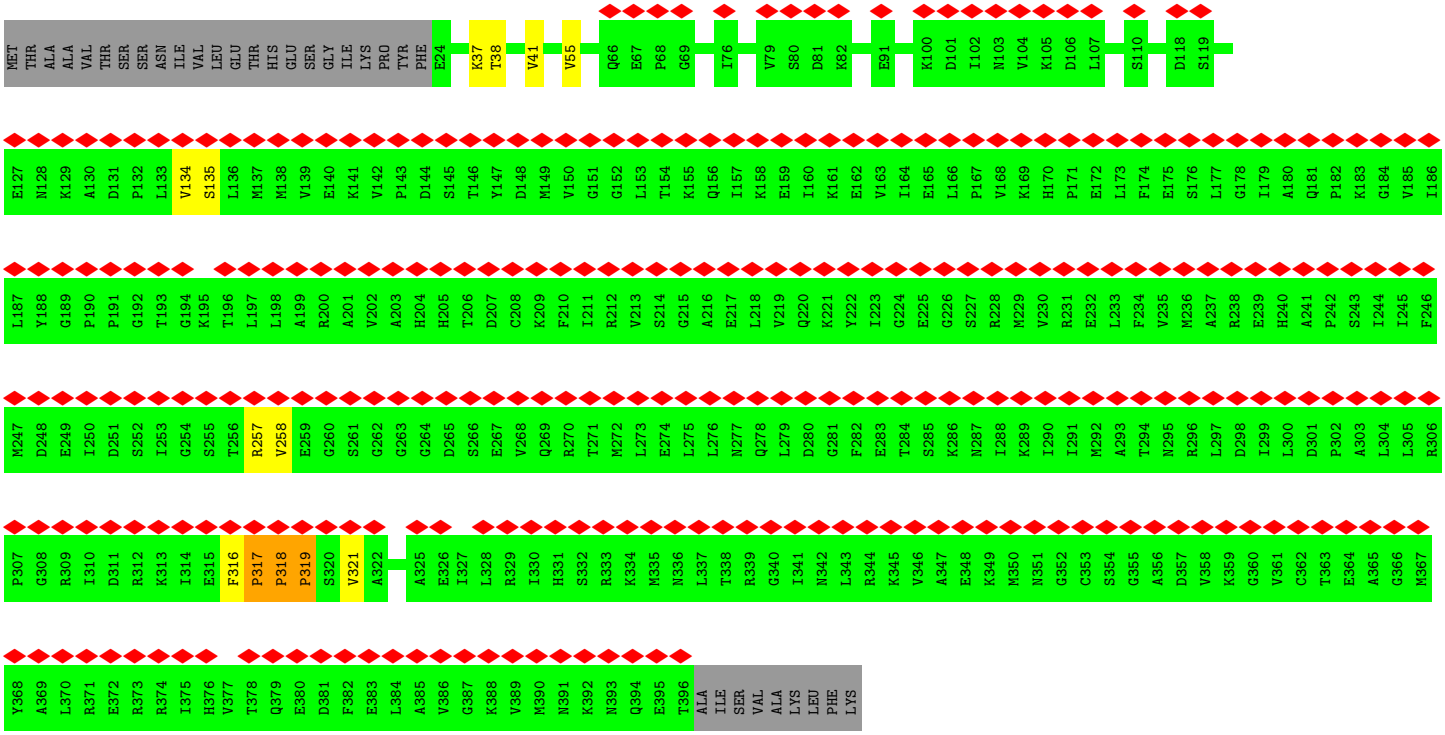
Chain I:



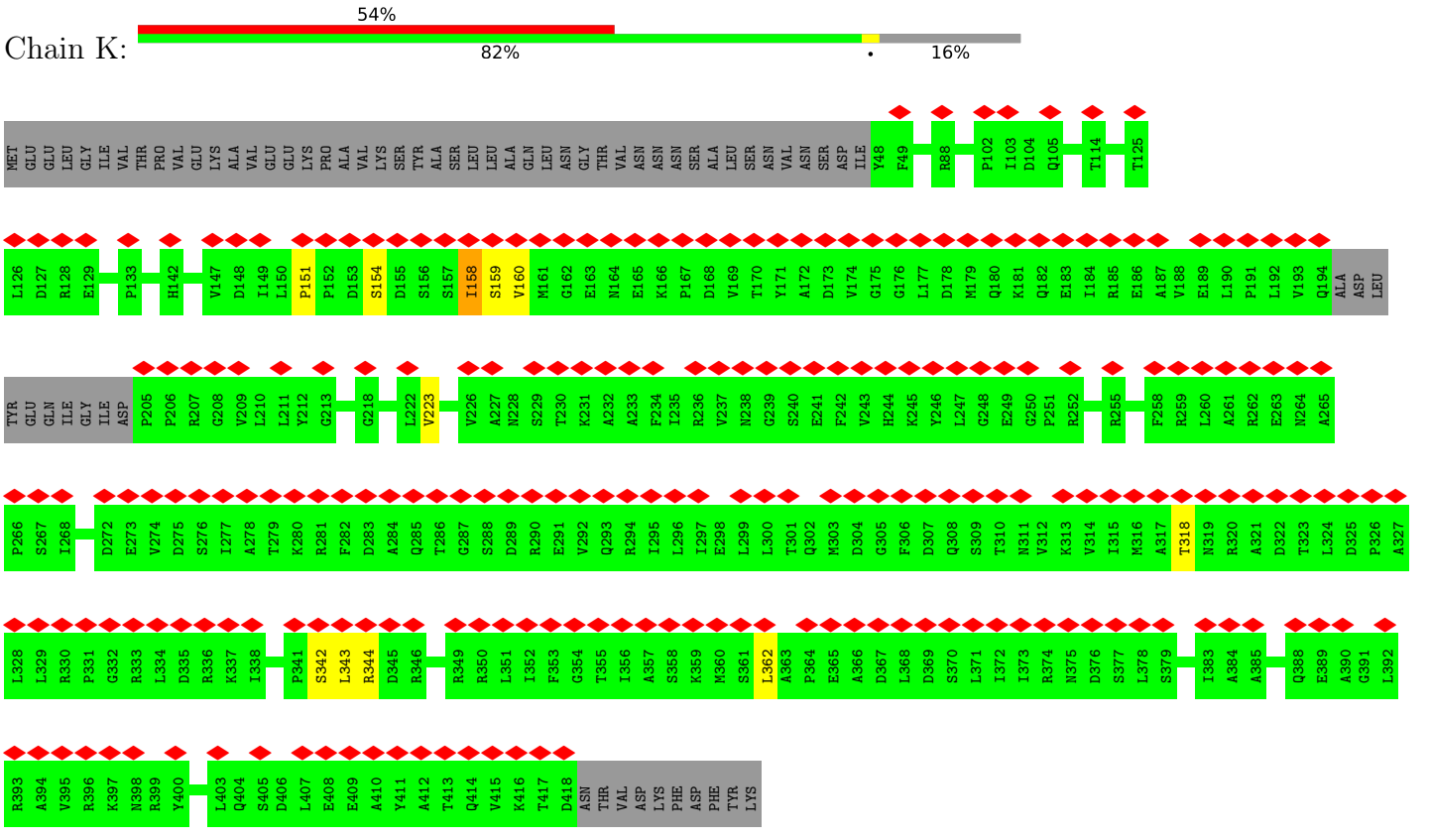
• Molecule 17: 26S protease regulatory subunit 8 homolog

Chain J:



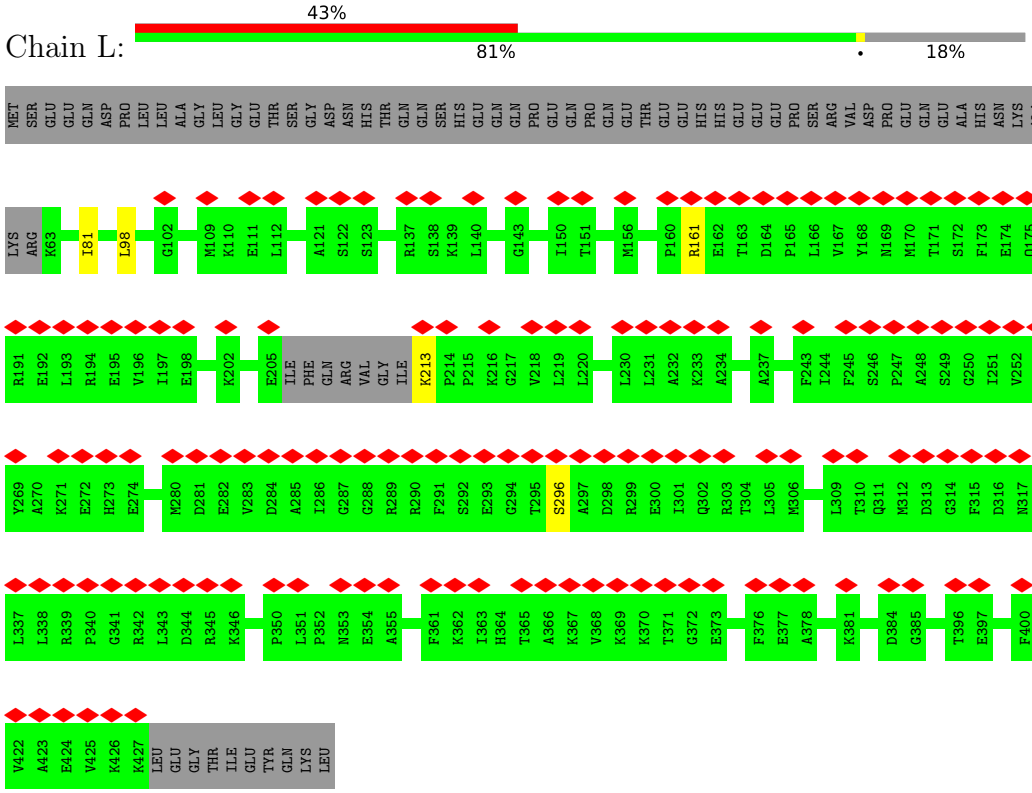


• Molecule 18: 26S protease regulatory subunit 6B homolog



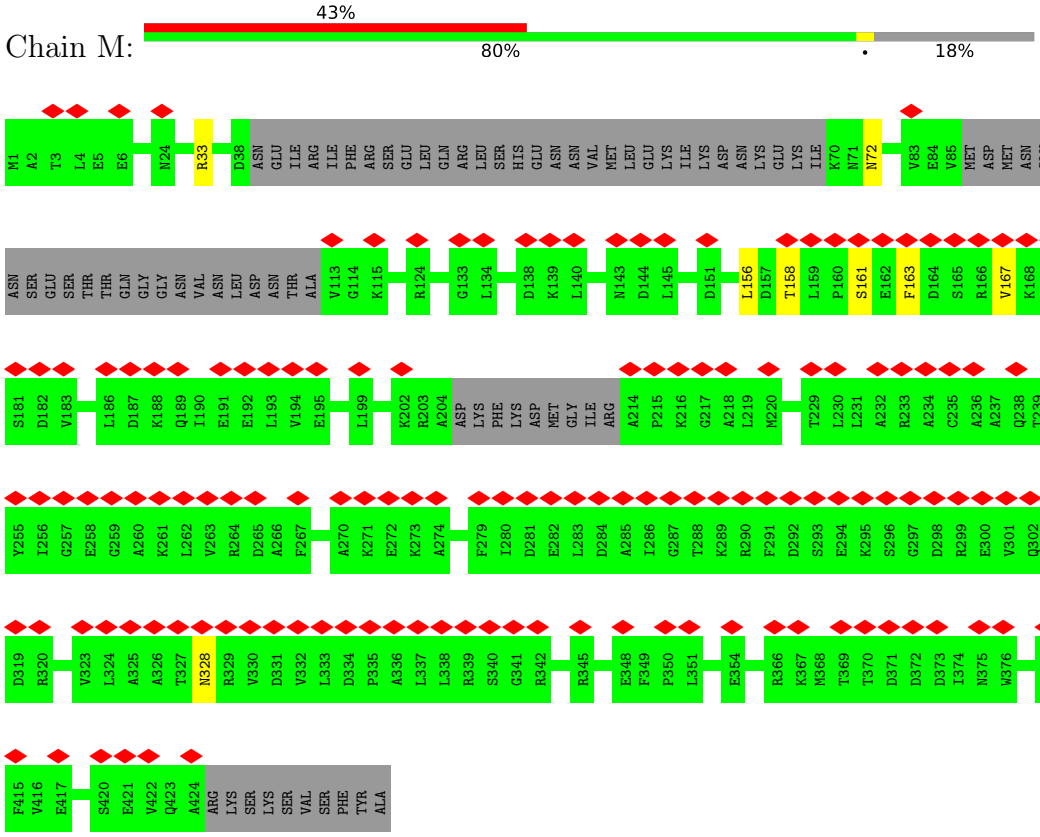
• Molecule 19: 26S protease subunit RPT4

Chain L:



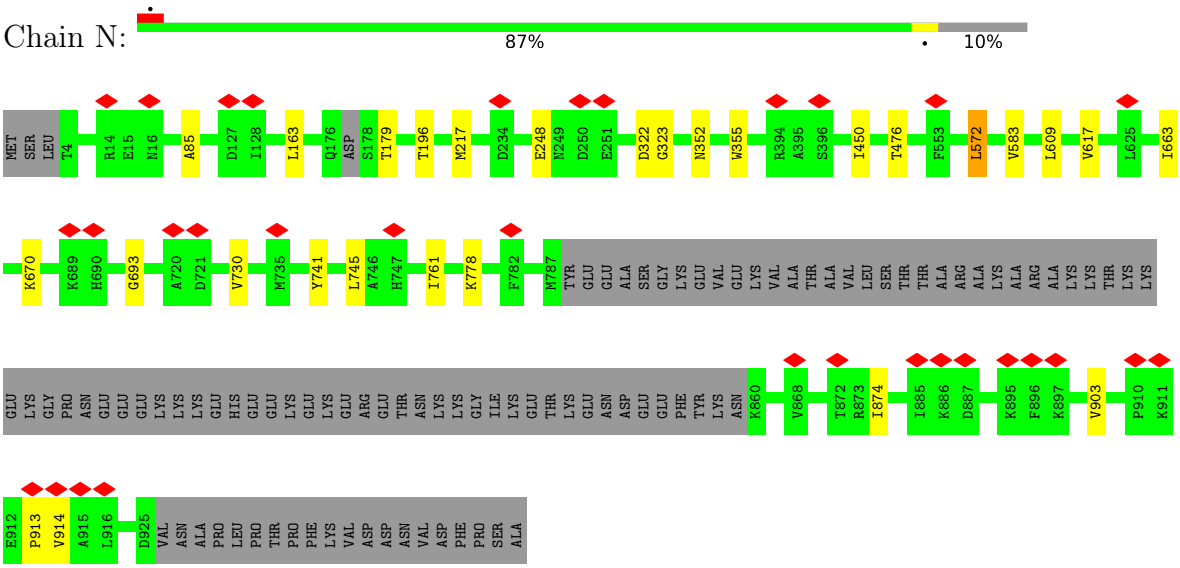
• Molecule 20: 26S protease regulatory subunit 6A

Chain M:



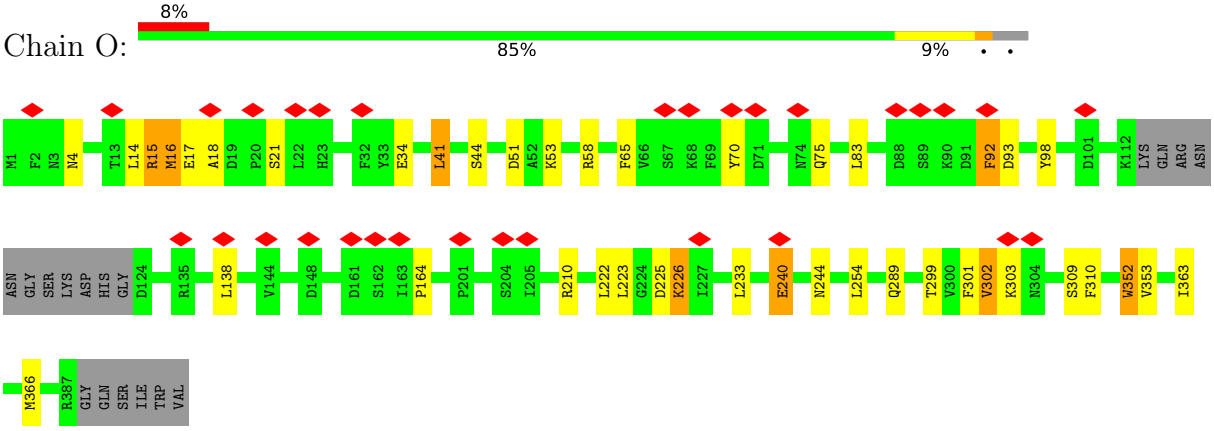
• Molecule 21: 26S proteasome regulatory subunit RPN2

Chain N:



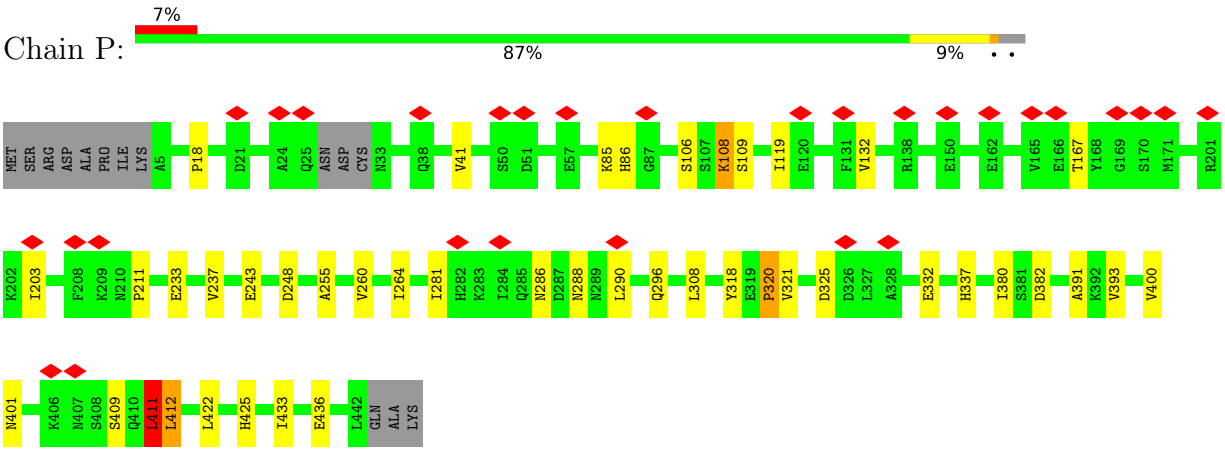
• Molecule 22: 26S proteasome regulatory subunit RPN9

Chain O:



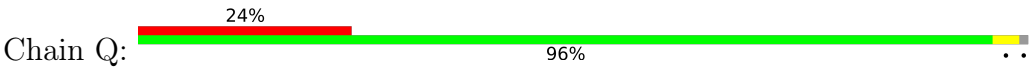
• Molecule 23: 26S proteasome regulatory subunit RPN5

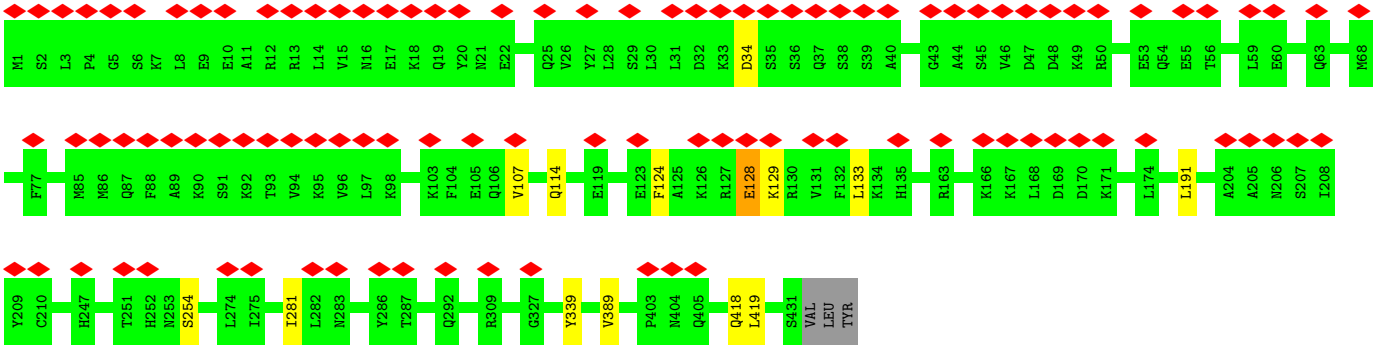
Chain P:



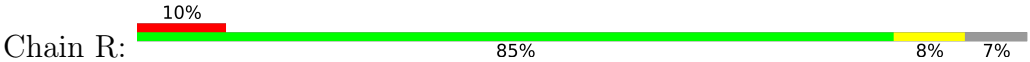
• Molecule 24: 26S proteasome regulatory subunit RPN6

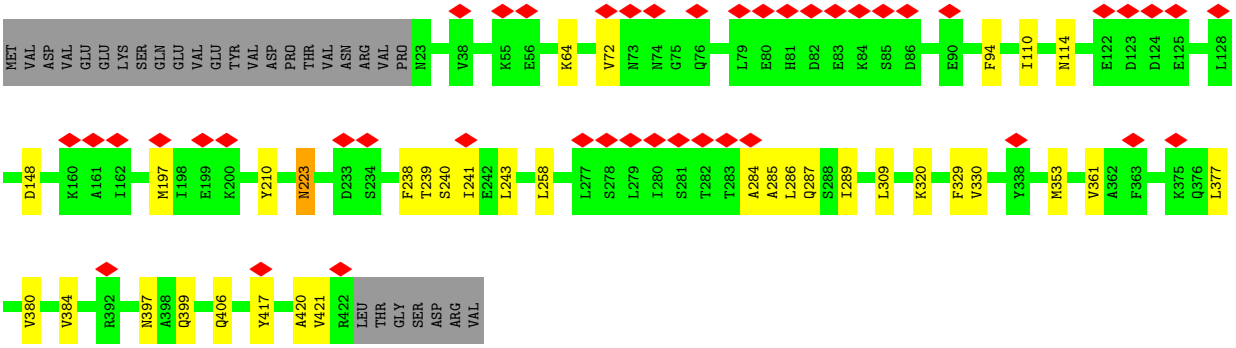
Chain Q:



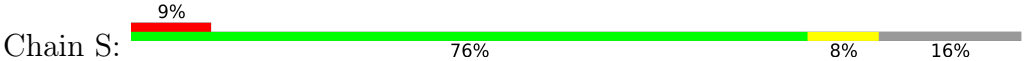


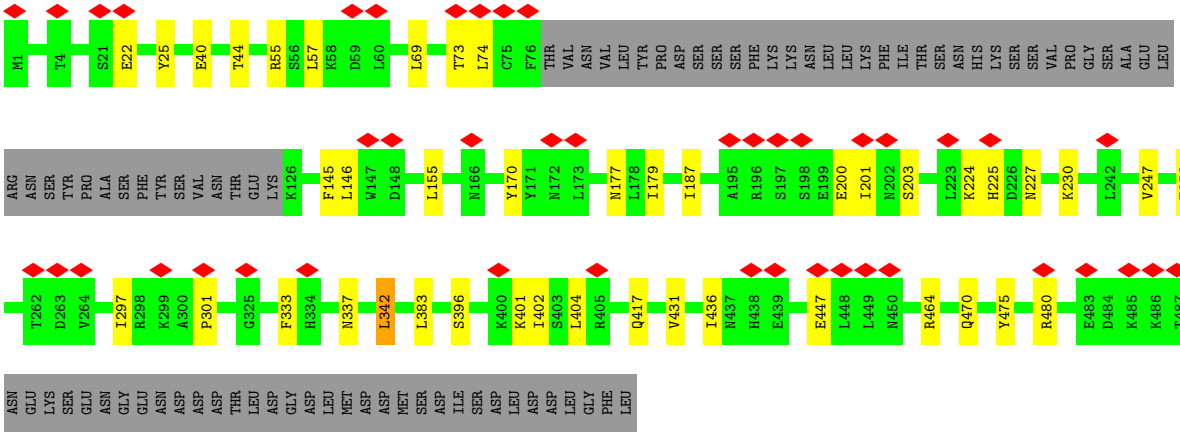
• Molecule 25: 26S proteasome regulatory subunit RPN7



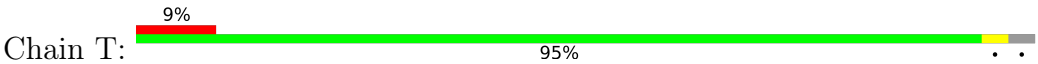


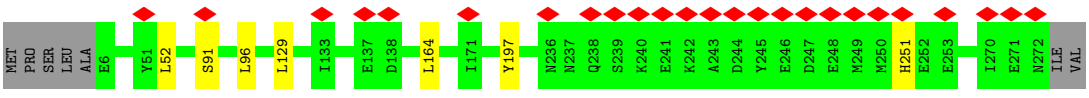
• Molecule 26: 26S proteasome regulatory subunit RPN3





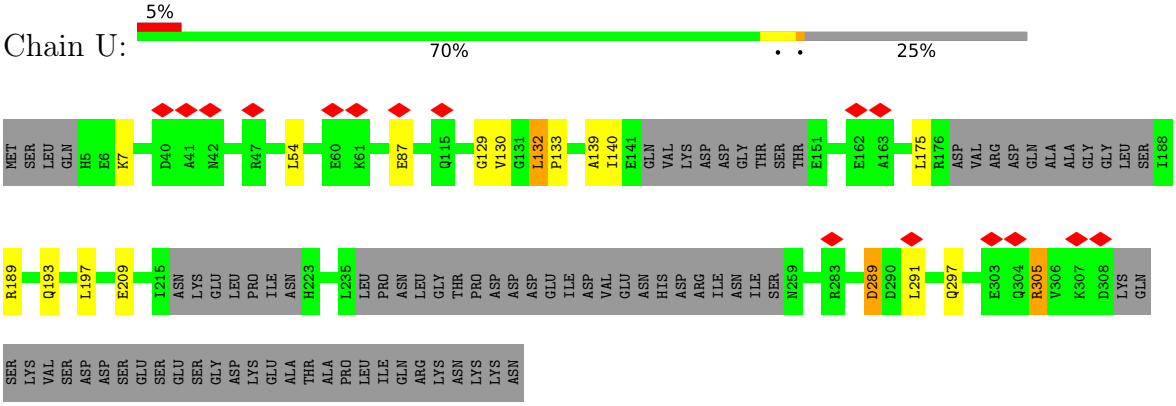
• Molecule 27: 26S proteasome regulatory subunit RPN12





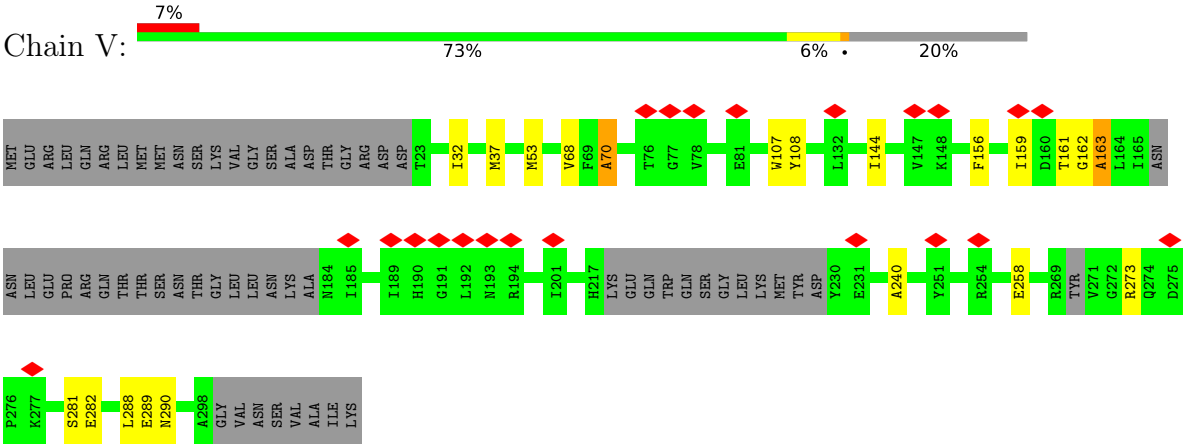
• Molecule 28: 26S proteasome regulatory subunit RPN8

Chain U:



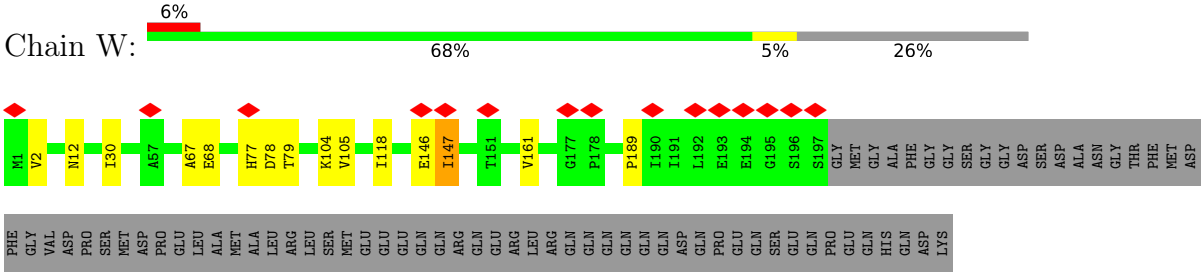
• Molecule 29: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



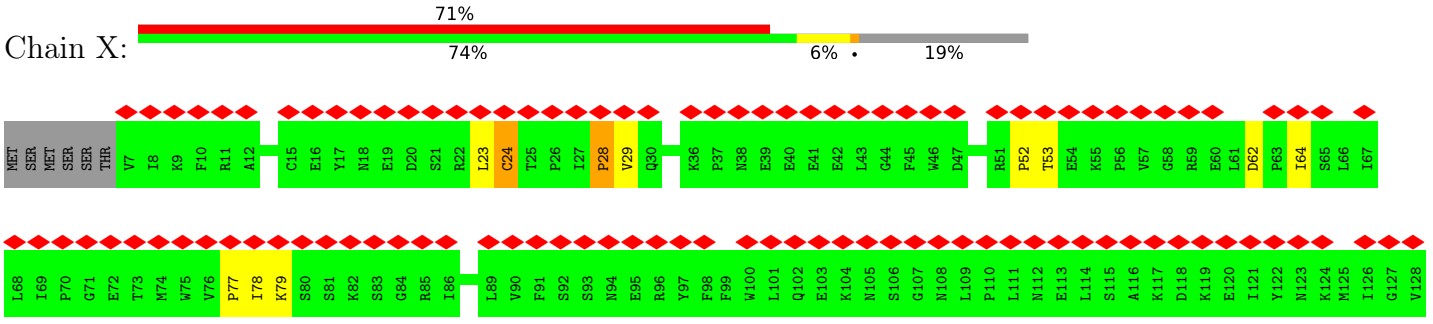
• Molecule 30: 26S proteasome regulatory subunit RPN10

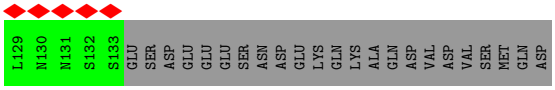
Chain W:



• Molecule 31: 26S proteasome regulatory subunit RPN13

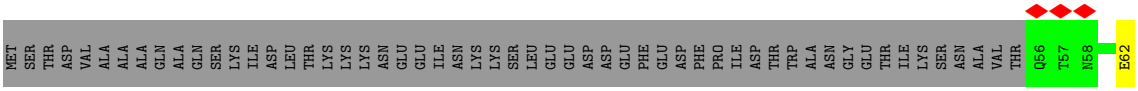
Chain X:

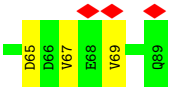




• Molecule 32: 26S proteasome complex subunit SEM1

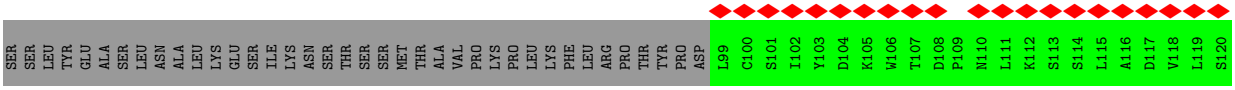
Chain Y:

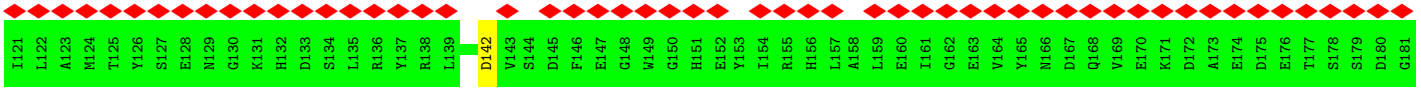


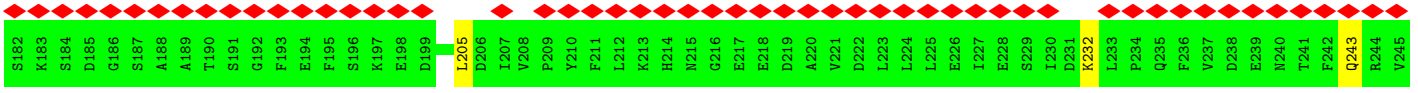


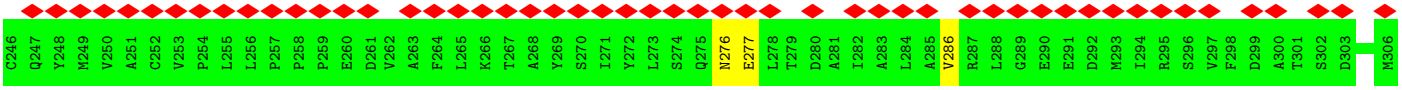
• Molecule 33: 26S proteasome regulatory subunit RPN1

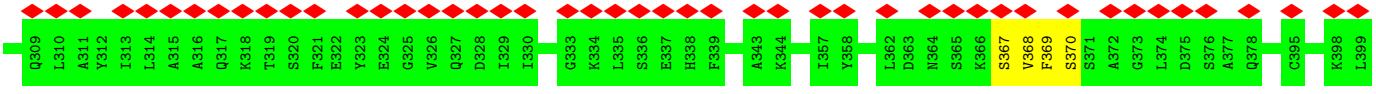
Chain Z:

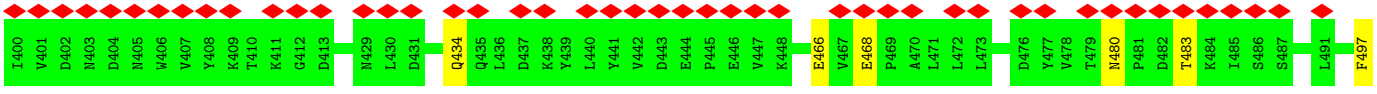


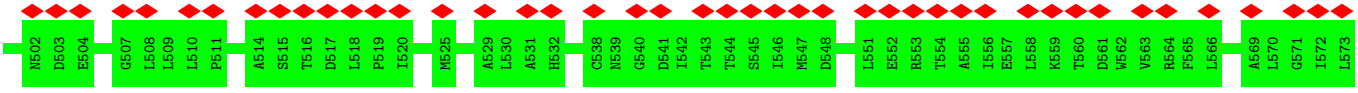


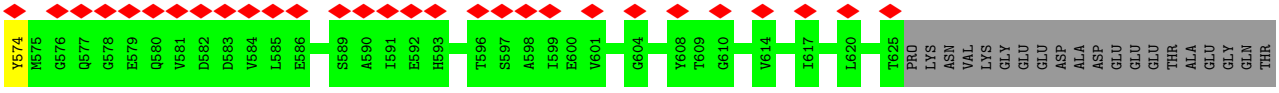


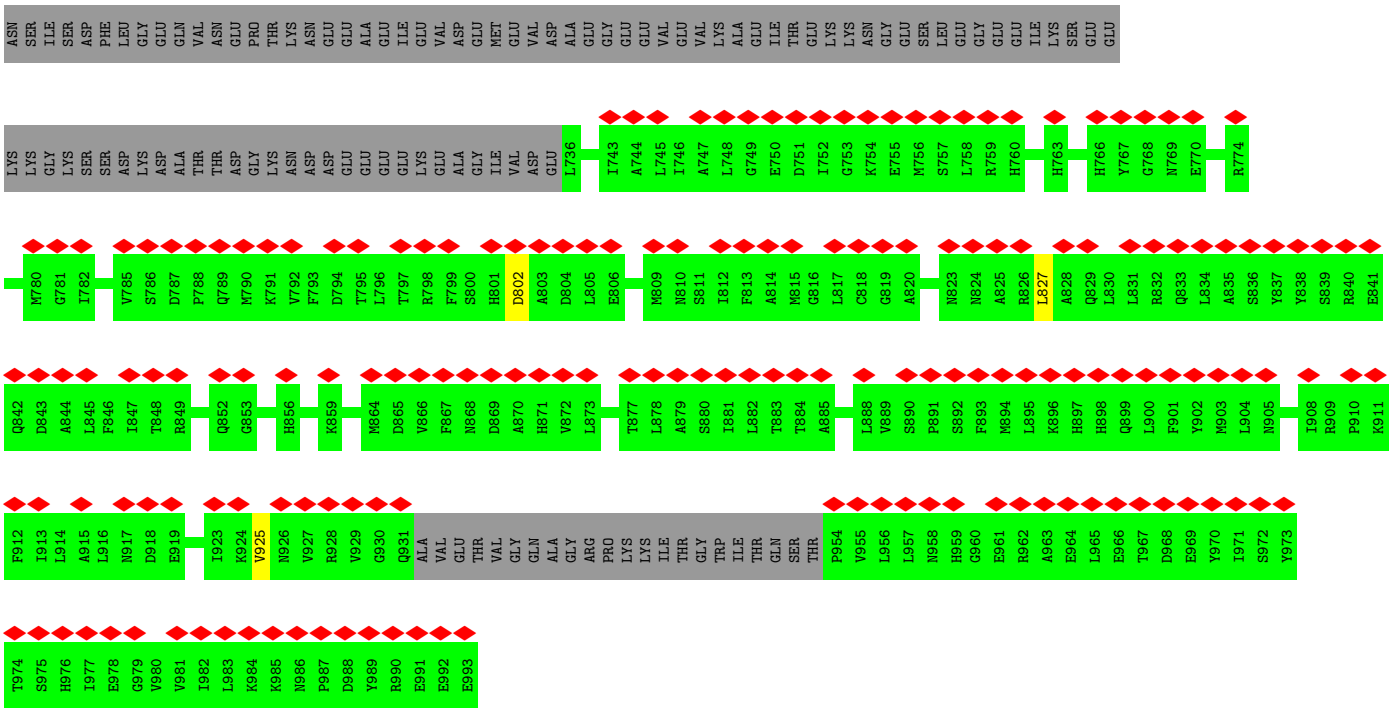











ASN SER ILE SER ASP PHE LEU GLY GLU GLN VAL ASN GLU PRO THR LYS ASN GLU GLU ALA GLU ILE GLU VAL ASP GLU MET GLU VAL ASP ALA GLU GLY GLU GLU VAL GLU VAL LYS ALA GLU ILE THR GLU LYS LYS ASN GLY GLU SER LEU GLU GLY GLU GLU ILE LYS SER GLU GLU
LYS LYS GLY LYS SER SER ASP LYS ASP ALA THR THR ASP GLY LYS ASN 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 P893 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

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 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	97	LEU	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

5 of 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

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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
28	U	291	LEU
29	V	288	LEU
28	U	297	GLN
29	V	108	TYR
33	Z	367	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 275 such sidechains are listed below:

Mol	Chain	Res	Type
10	c	177	GLN
11	d	235	GLN
4	i	115	HIS
19	L	133	ASN
19	L	67	HIS

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.

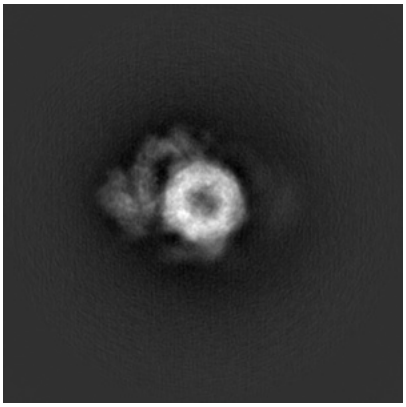
6 Map visualisation

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.

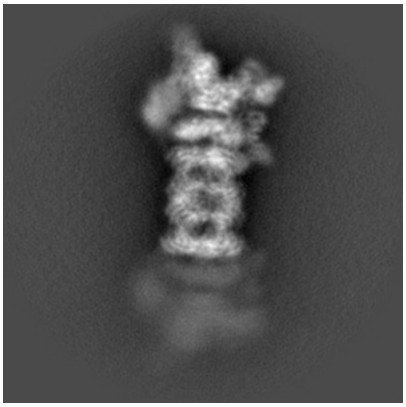
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

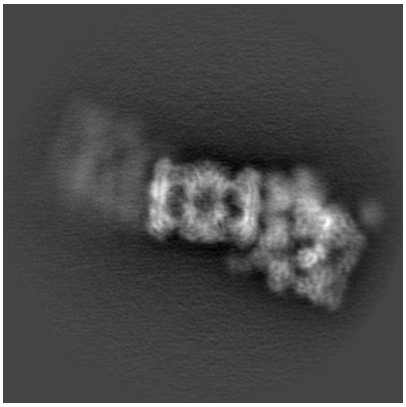
6.1.1 Primary map



X



Y

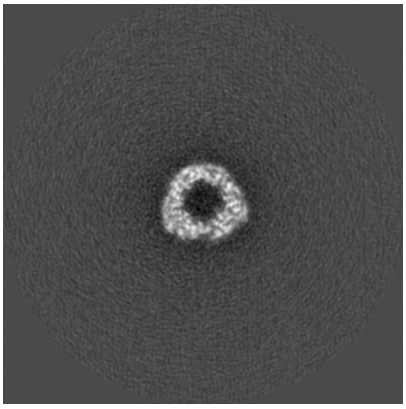


Z

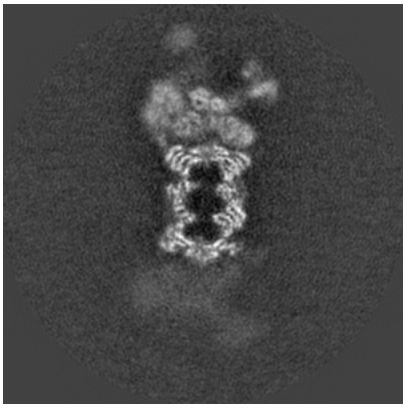
The images above show the map projected in three orthogonal directions.

6.2 Central slices

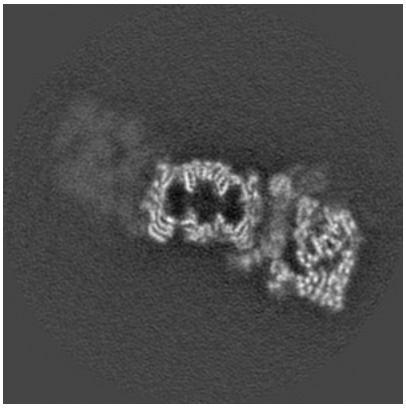
6.2.1 Primary map



X Index: 128



Y Index: 128

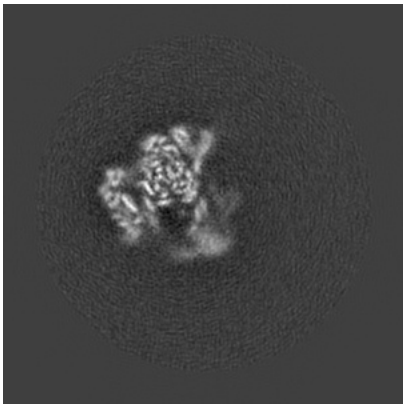


Z Index: 128

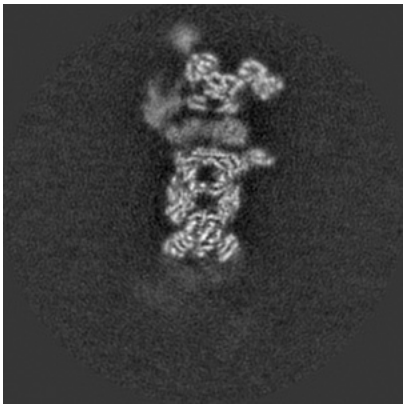
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

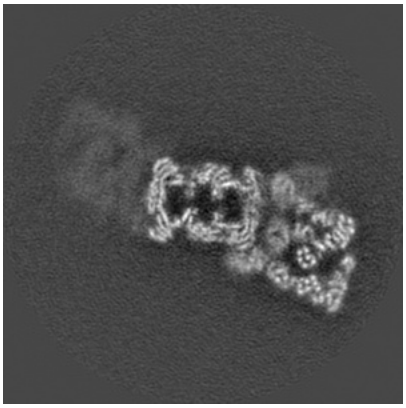
6.3.1 Primary map



X Index: 200



Y Index: 117

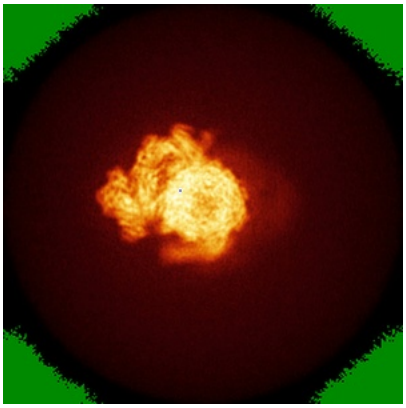


Z Index: 132

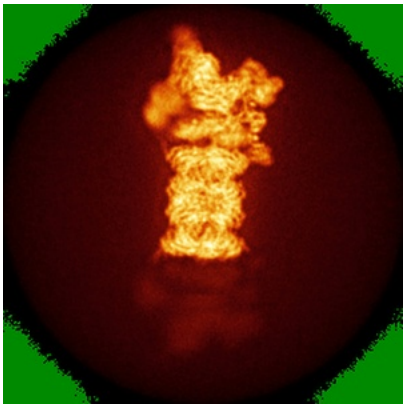
The images above show the largest variance slices of the map in three orthogonal directions.

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

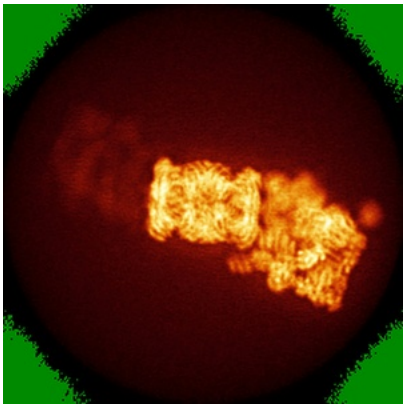
6.4.1 Primary map



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.

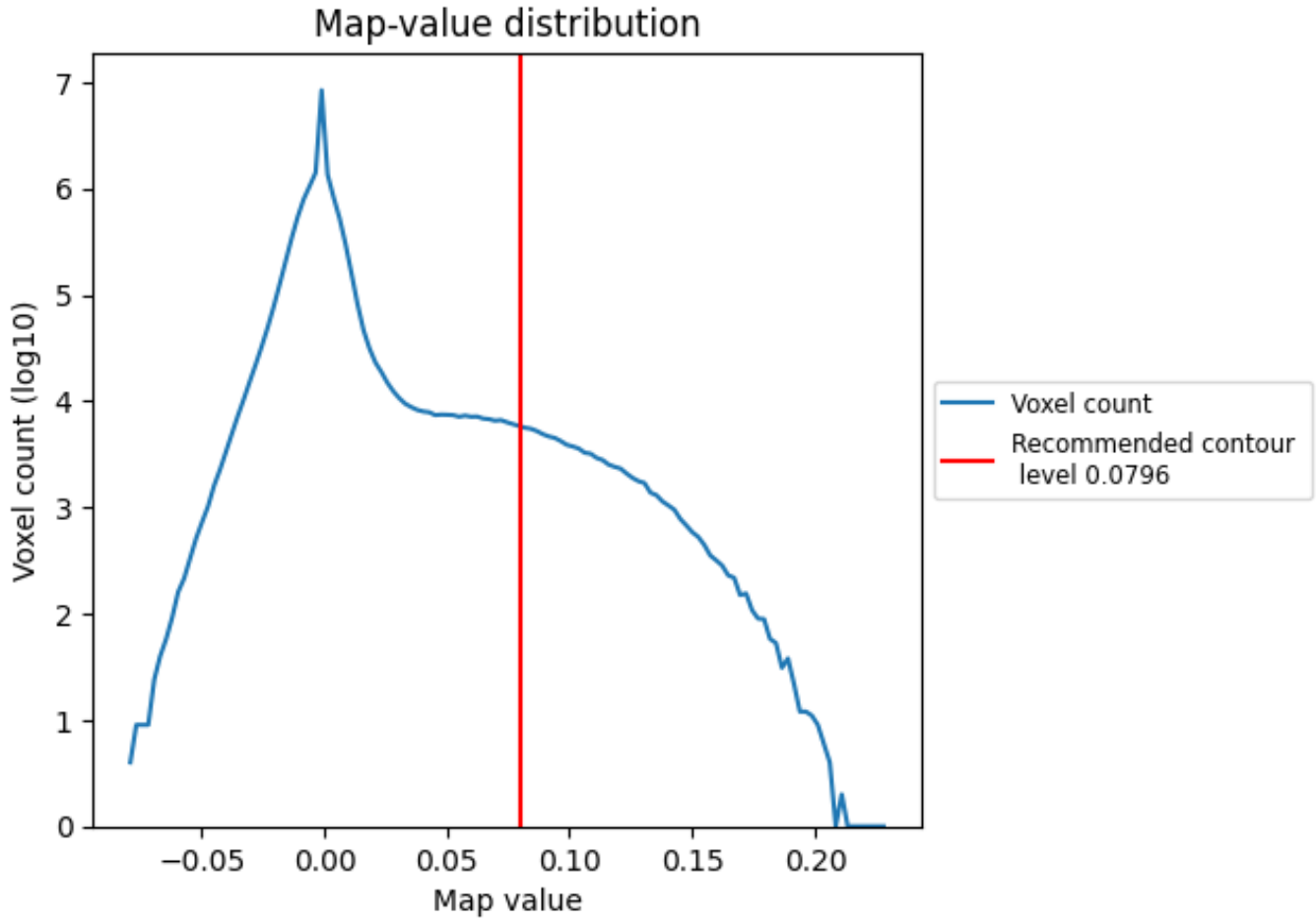
6.6 Mask visualisation (i)

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

7 Map analysis

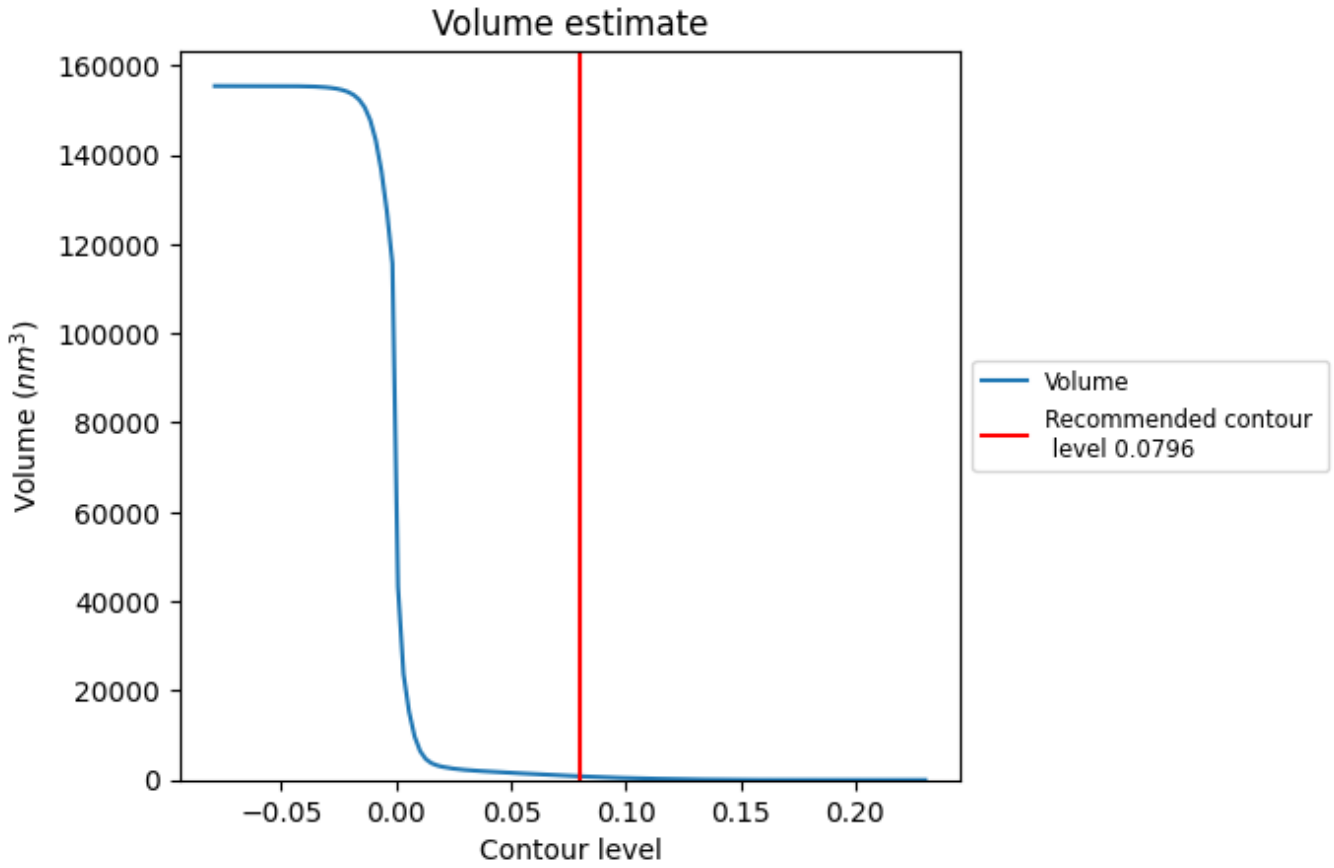
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

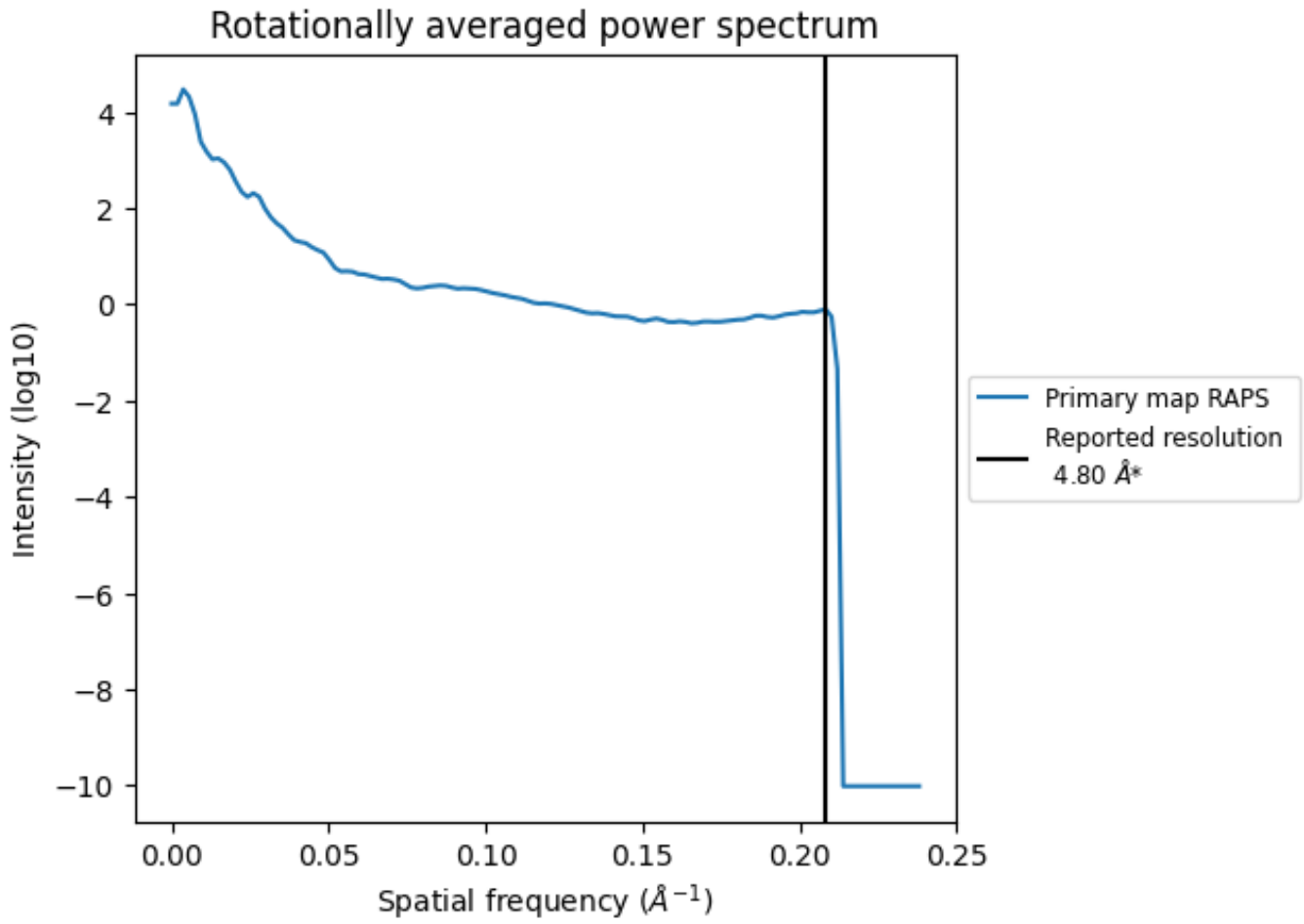
7.2 Volume estimate (i)



The volume at the recommended contour level is 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}

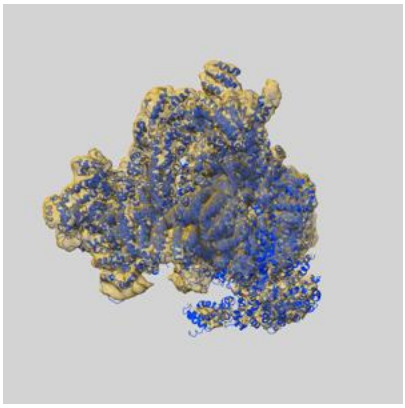
8 Fourier-Shell correlation (i)

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

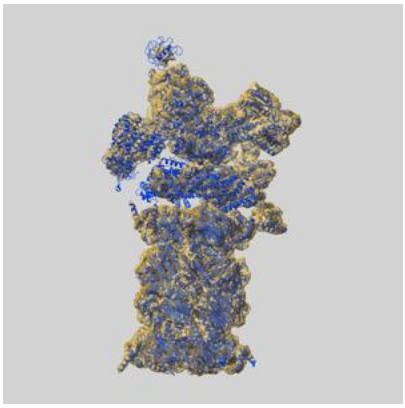
9 Map-model fit

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.

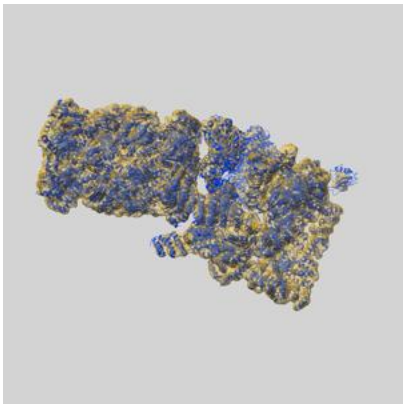
9.1 Map-model overlay



X



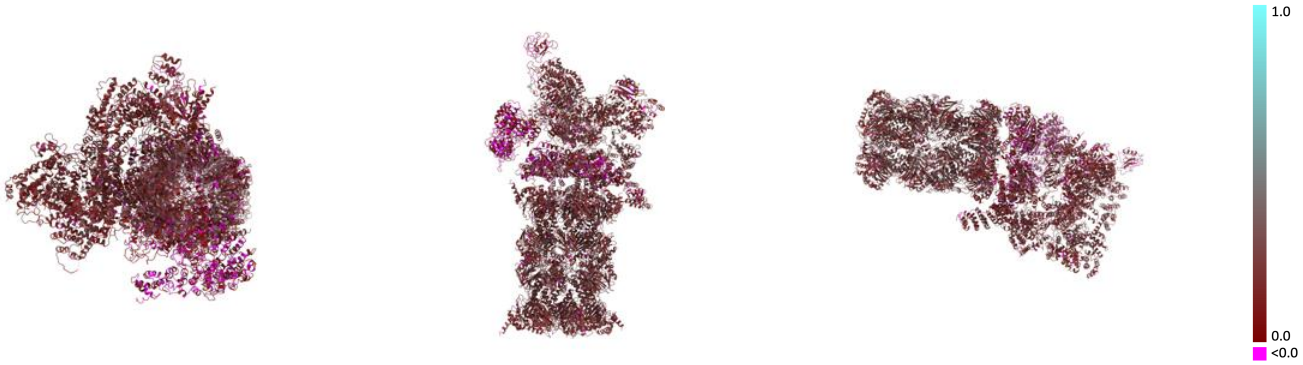
Y



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.

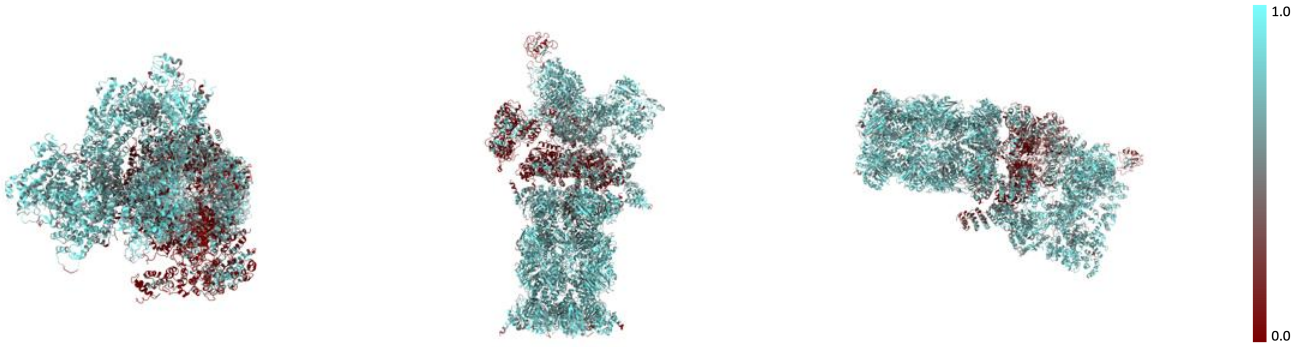
9.2 Q-score mapped to coordinate model



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.

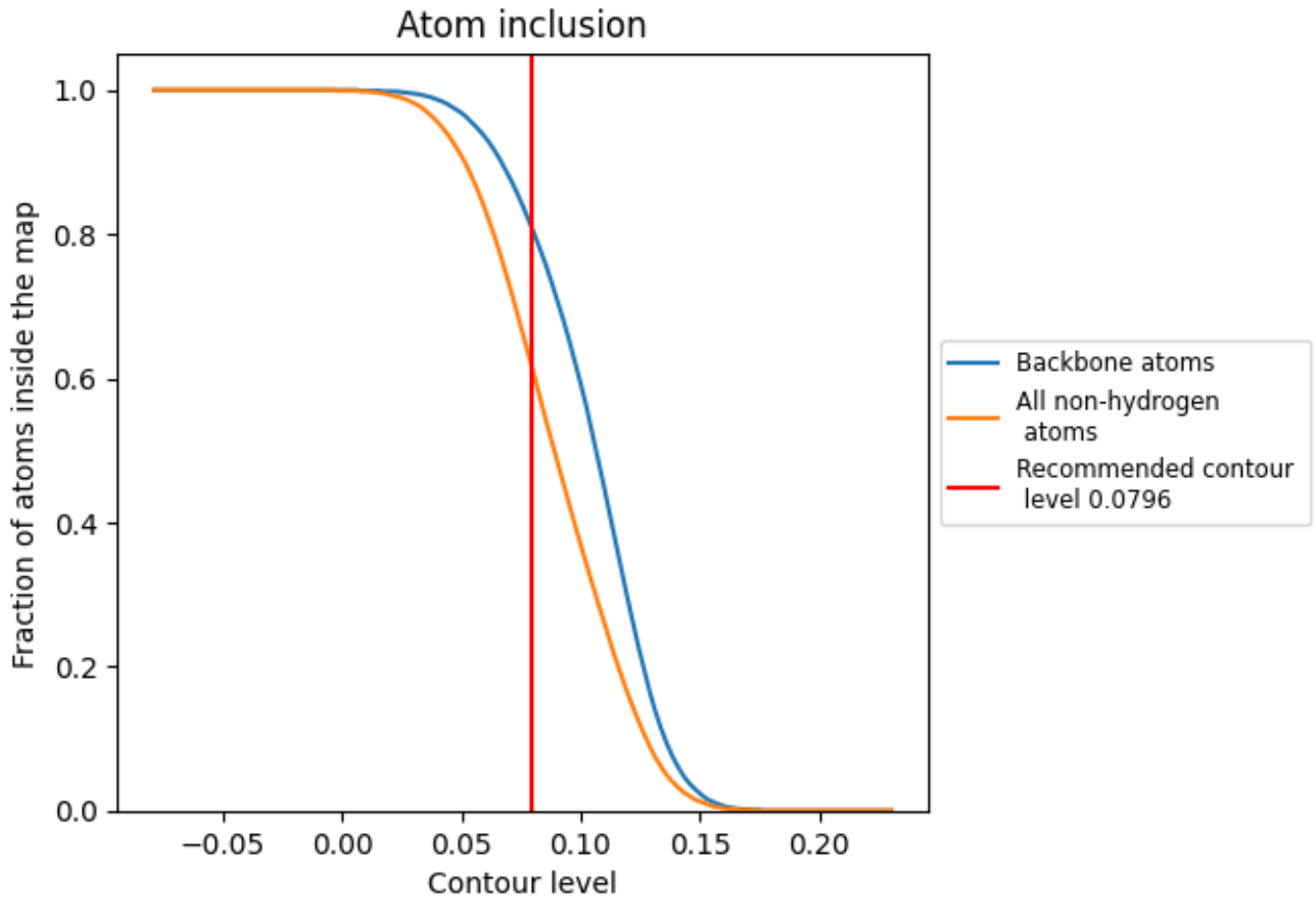
9.3 Atom inclusion mapped to coordinate model



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 (0.0796).

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

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