wwPDB EM Validation Summary Report (i)

Nov 20, 2022 – 12:59 am GMT

PDB ID	:	6FVV
EMDB ID	:	EMD-4321
Title	:	26S proteasome, s3 state
Authors	:	Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on	:	2018-03-05
Resolution	:	5.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

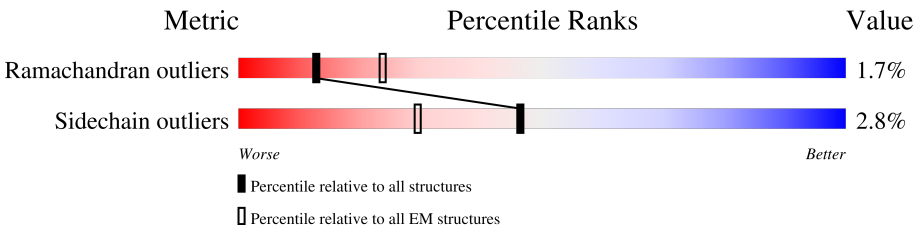
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	241	99%
1	a	241	32%, 80%, 17%
2	B	249	98%
2	b	249	40%, 82%, 16%
3	C	244	99%
3	c	244	37%, 76%, 23%
4	D	251	92%, 6%
4	d	251	38%, 80%, 18%
5	E	244	7%, 95%, 5%

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Mol	Chain	Length	Quality of chain
5	e	244	42% 78% 20%
6	F	231	97%
6	f	231	29% 74% 21%
7	G	242	96%
7	g	242	33% 74% 21% 5%
8	1	196	82% 15%
8	h	196	75% 21%
9	2	226	83% 16%
9	i	226	5% 80% 16%
10	3	204	7% 76% 22%
10	j	204	8% 77% 20%
11	4	195	79% 19%
11	k	195	7% 75% 21%
12	5	212	75% 23%
12	l	212	6% 77% 21%
13	6	222	74% 23%
13	m	222	12% 74% 23%
14	7	232	70% 25%
14	n	232	6% 76% 18% 6%
15	W	197	18% 76% 20%
16	V	289	9% 75% 21%
17	T	266	14% 81% 17%
18	X	127	73% 74% 22%
19	Y	89	46% 78% 19%
20	Z	970	59% 86% 6% 7%

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Mol	Chain	Length	Quality of chain
21	N	922	12% 81% 16%
22	S	475	15% 78% 18%
23	P	440	81% 17%
24	Q	434	7% 77% 18%
25	R	405	7% 77% 20%
26	U	304	14% 81% 17%
27	O	388	7% 76% 21%
28	H	417	23% 74% 23%
29	I	385	23% 78% 19%
30	K	394	18% 72% 23%
31	L	388	13% 77% 18%
32	M	421	21% 78% 19%
33	J	405	23% 74% 21%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 110420 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	241	1908	1214	320	366	8	0	0
1	A	241	1908	1214	320	366	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	249	1907	1214	314	376	3	0	0
2	B	249	1907	1214	314	376	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	244	1905	1201	321	380	3	0	0
3	C	244	1905	1201	321	380	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	251	1982	1235	350	393	4	0	0
4	D	237	1859	1164	325	366	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	244	1883	1176	316	384	7	0	0
5	E	244	1883	1176	316	384	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	231	1773	1114	307	348	4	0	0
6	F	231	1773	1114	307	348	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	242	1886	1199	328	355	4	0	0
7	G	242	1886	1199	328	355	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	196	1512	955	250	300	7	0	0
8	1	196	1512	955	250	300	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	226	1720	1082	298	333	7	0	0
9	2	226	1720	1082	298	333	7	0	0

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	3	204	1581	1010	258	305	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	195	1562	992	264	300	6	0	0
			Total	C	N	O	S		
11	4	195	1562	992	264	300	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	212	1644	1045	280	312	7	0	0
			Total	C	N	O	S		
12	5	212	1644	1045	280	312	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	222	1757	1115	303	335	4	0	0
			Total	C	N	O	S		
13	6	222	1757	1115	303	335	4	0	0

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	232	1816	1148	311	350	7	0	0
			Total	C	N	O	S		
14	7	229	1790	1133	306	344	7	0	0

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	W	197	1535	962	269	301	3	0	0

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	V	289	2274	1425	389	446	14	0	0

- Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	T	266	2193	1405	349	433	6	0	0

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	X	127	1033	664	169	196	4	0	0

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	Y	89	731	447	119	164	1	0	0

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	Z	906	7006	4416	1150	1410	30	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	922	7158	4536	1205	1389	28	0	0

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	S	475	3895	2488	653	739	15	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	440	3609	2297	604	698	10	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	434	3499	2225	577	681	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	405	3259	2077	535	637	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	U	304	2427	1529	414	477	7	0	0

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	O	388	3186	2051	519	608	8	0	0

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	H	417	3234	2008	578	632	16	0	0

- Molecule 29 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	I	385	3022	1899	508	598	17	0	0

- Molecule 30 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	K	394	3113	1951	548	604	10	0	0

- Molecule 31 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	L	388	3083	1942	548	581	12	0	0

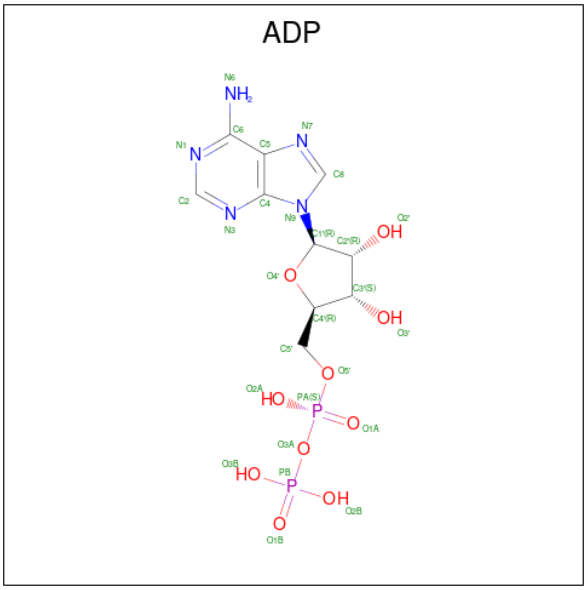
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	M	421	3285	2043	573	656	13	0	0

- Molecule 33 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	J	405	3171	1995	565	593	18	0	0

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
34	H	1	27	10	5	10	2	0

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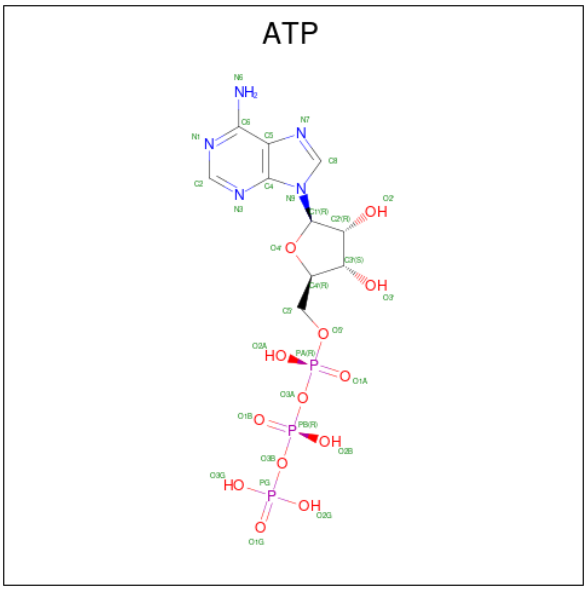
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
34	M	1	27	10	5	10	2	0

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
35	H	1	1	1	0
35	I	1	1	1	0
35	K	1	1	1	0
35	L	1	1	1	0
35	M	1	1	1	0
35	J	1	1	1	0

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	I	1	31	10	5	13	3	0
36	K	1	31	10	5	13	3	0

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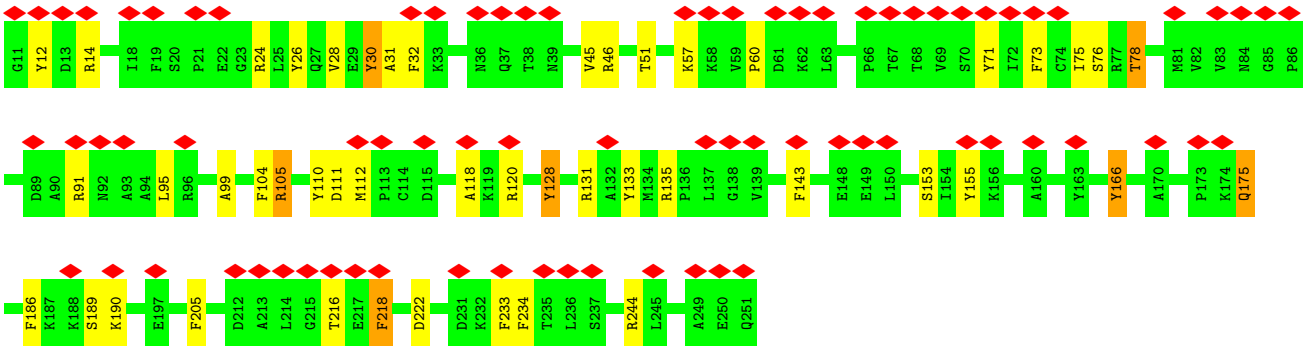
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	L	1	31	10	5	13	3	0
			Total	C	N	O	P	
36	J	1	31	10	5	13	3	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

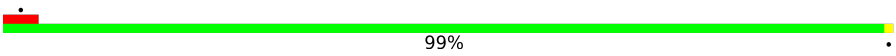
- Molecule 1: Proteasome subunit alpha type-1

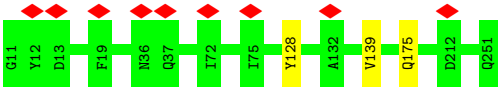
Chain a:



- Molecule 1: Proteasome subunit alpha type-1

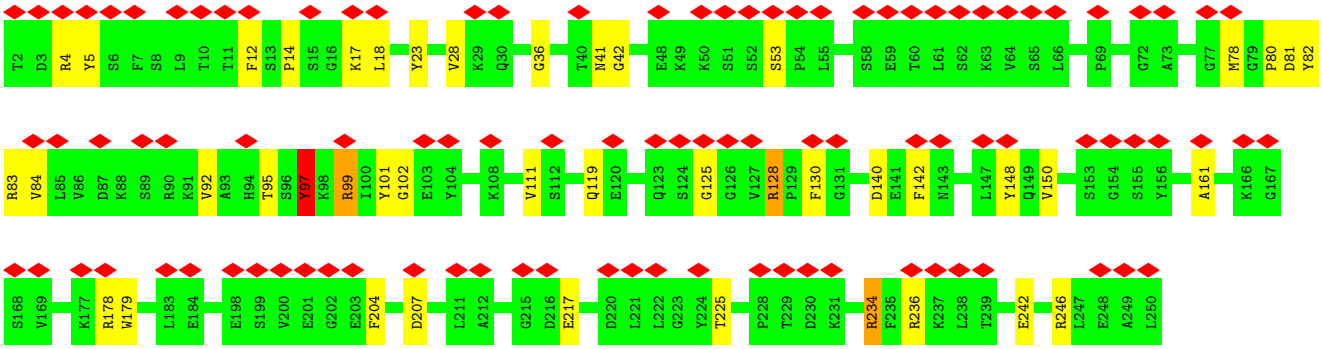
Chain A:





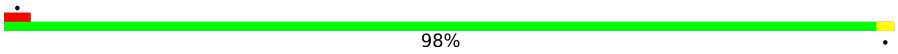
- Molecule 2: Proteasome subunit alpha type-2

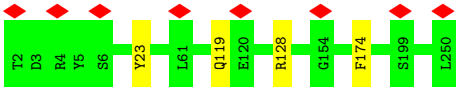
Chain b:



- Molecule 2: Proteasome subunit alpha type-2

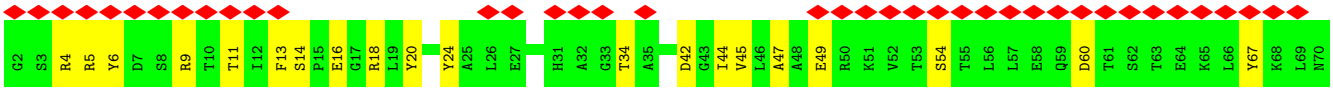
Chain B:

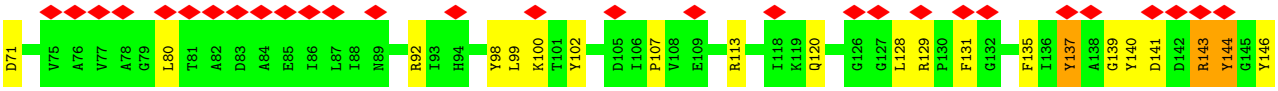


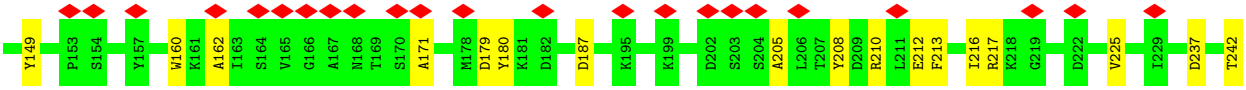


- Molecule 3: Proteasome subunit alpha type-3

Chain c:

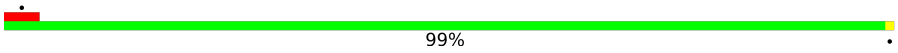


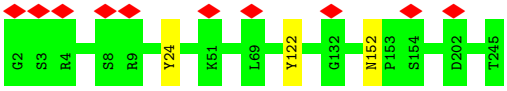




- Molecule 3: Proteasome subunit alpha type-3

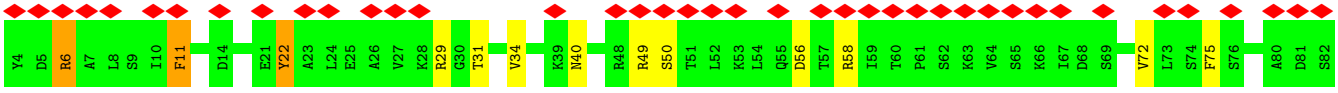
Chain C:

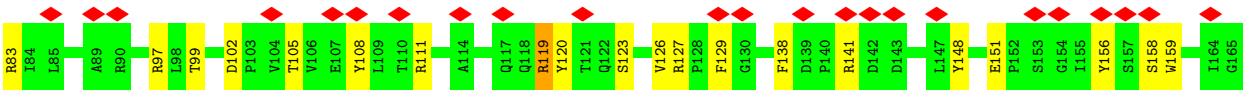


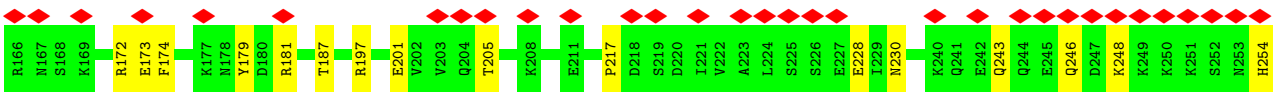


- Molecule 4: Proteasome subunit alpha type-4

Chain d:

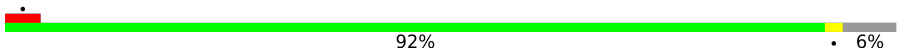


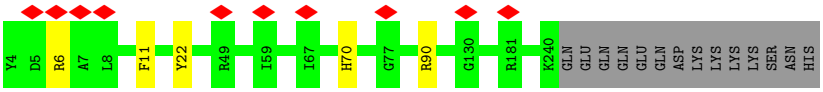




- Molecule 4: Proteasome subunit alpha type-4

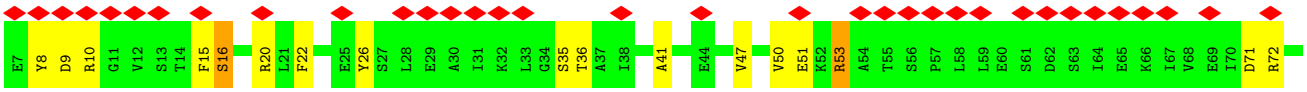
Chain D:

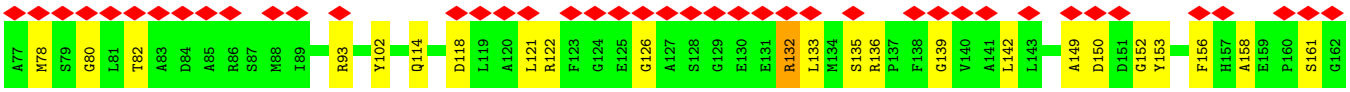


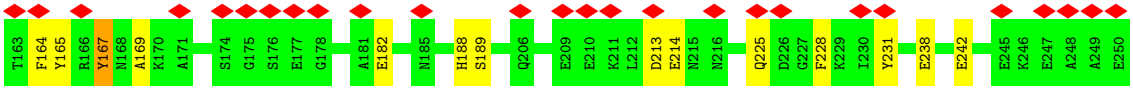


• Molecule 5: Proteasome subunit alpha type-5

Chain e:

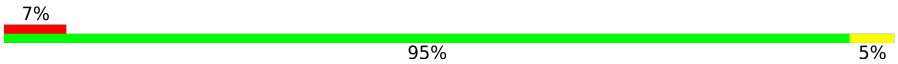


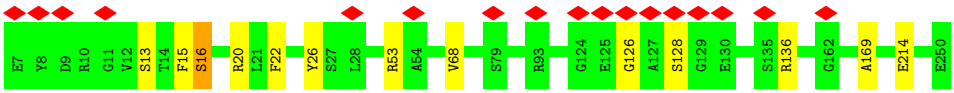




• Molecule 5: Proteasome subunit alpha type-5

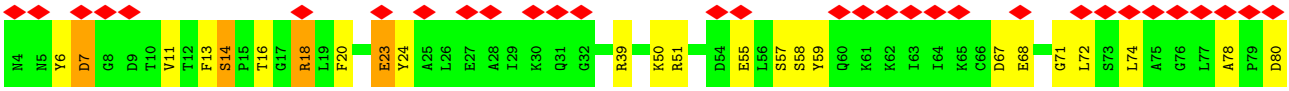
Chain E:

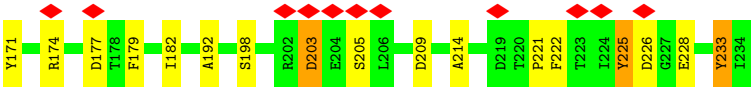




• Molecule 6: Proteasome subunit alpha type-6

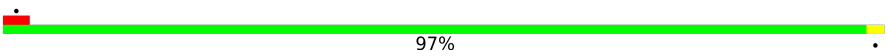
Chain f:

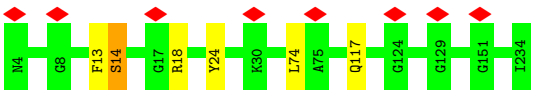




• Molecule 6: Proteasome subunit alpha type-6

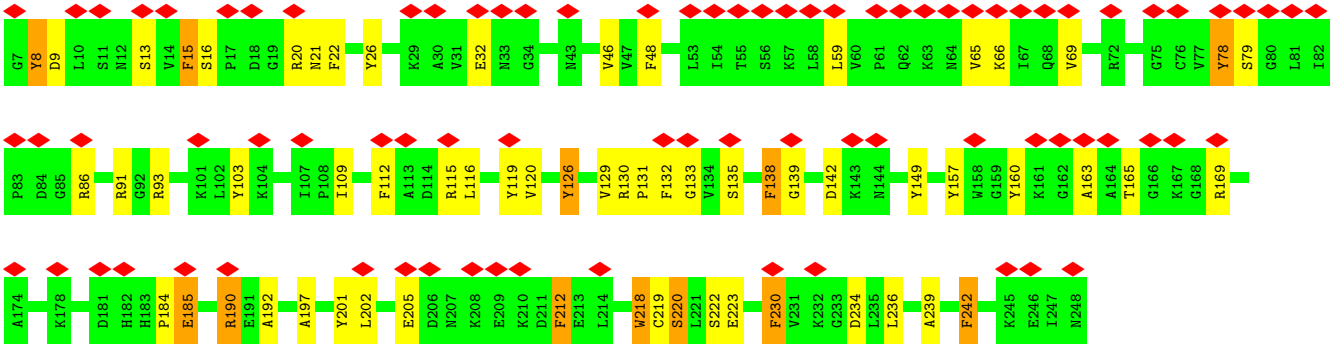
Chain F:





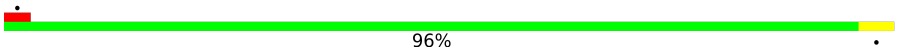
• Molecule 7: Probable proteasome subunit alpha type-7

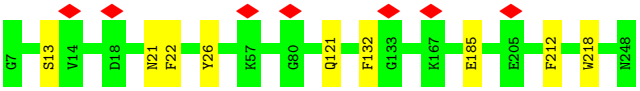
Chain g:



• Molecule 7: Probable proteasome subunit alpha type-7

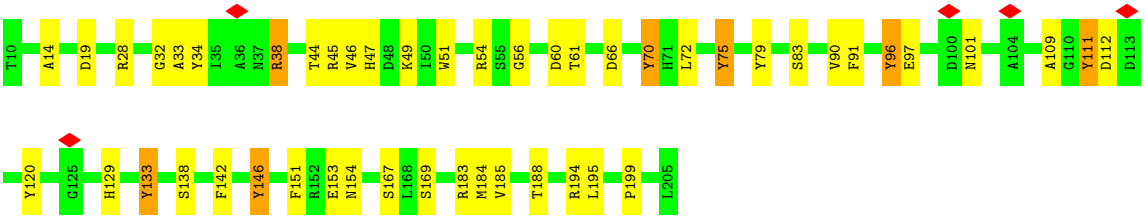
Chain G:





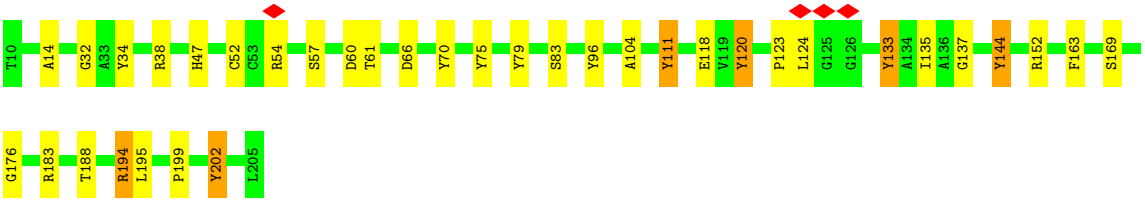
• Molecule 8: Proteasome subunit beta type-1

Chain h:



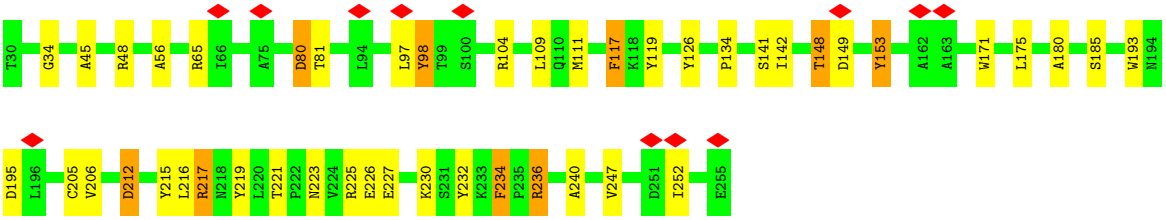
• Molecule 8: Proteasome subunit beta type-1

Chain 1:



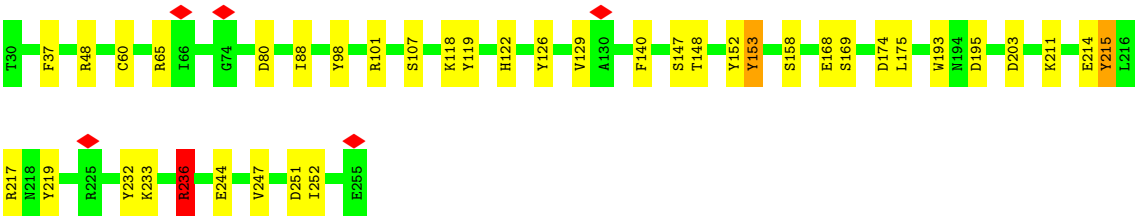
• Molecule 9: Proteasome subunit beta type-2

Chain i:



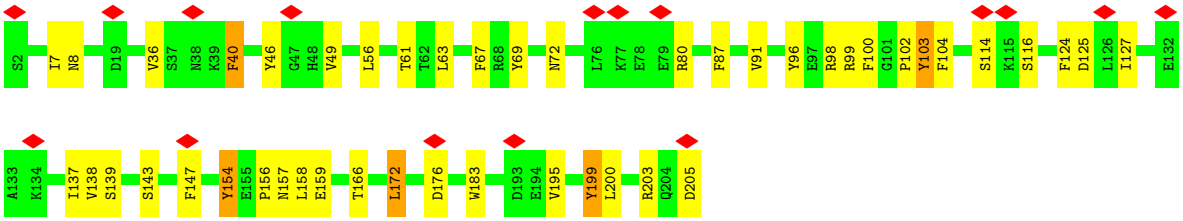
• Molecule 9: Proteasome subunit beta type-2

Chain 2:



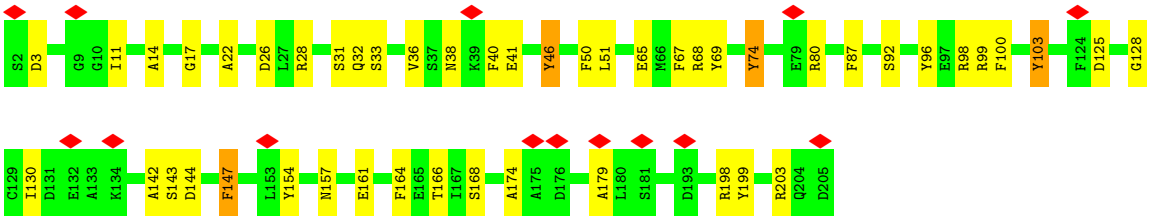
• Molecule 10: Proteasome subunit beta type-3

Chain j:



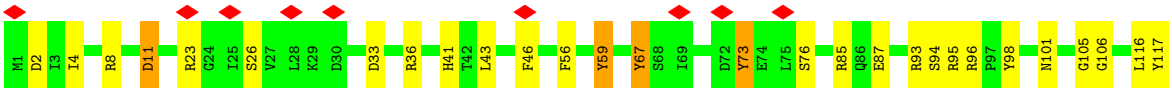
• Molecule 10: Proteasome subunit beta type-3

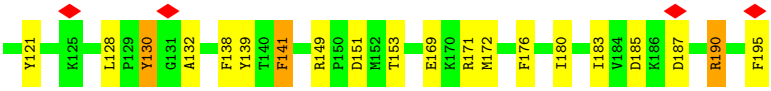
Chain 3:



• Molecule 11: Proteasome subunit beta type-4

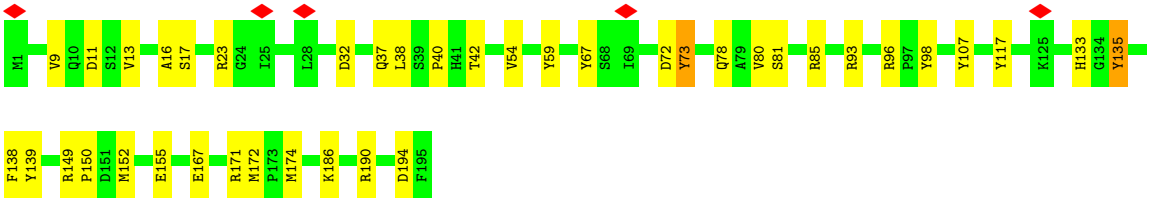
Chain k:





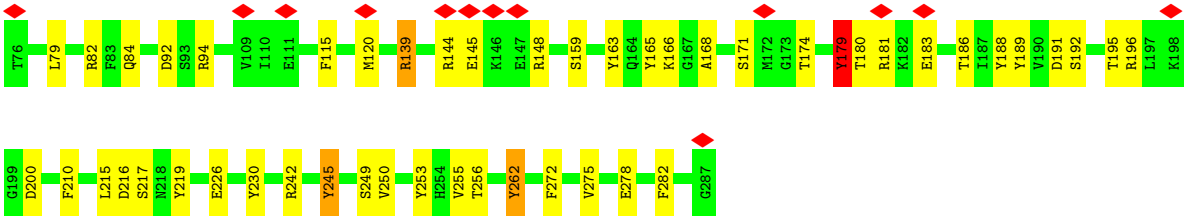
• Molecule 11: Proteasome subunit beta type-4

Chain 4:



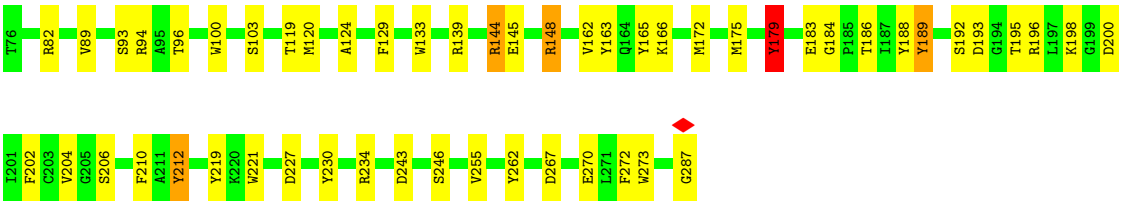
• Molecule 12: Proteasome subunit beta type-5

Chain l:



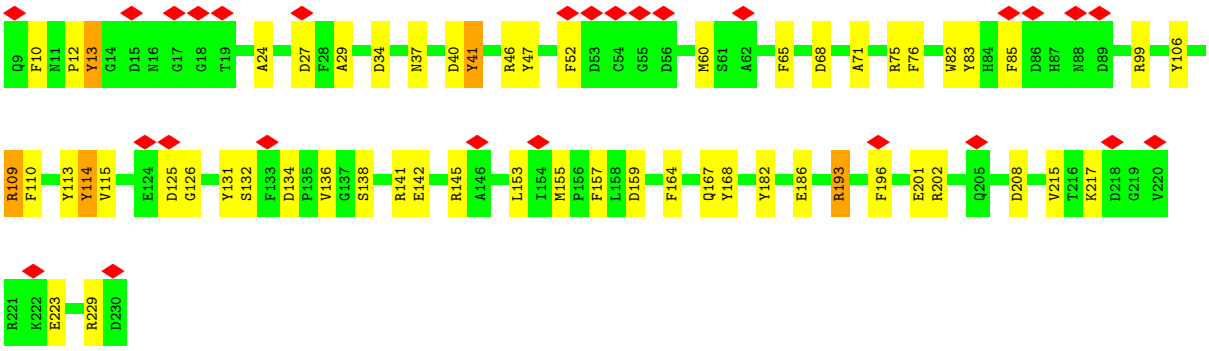
• Molecule 12: Proteasome subunit beta type-5

Chain 5:



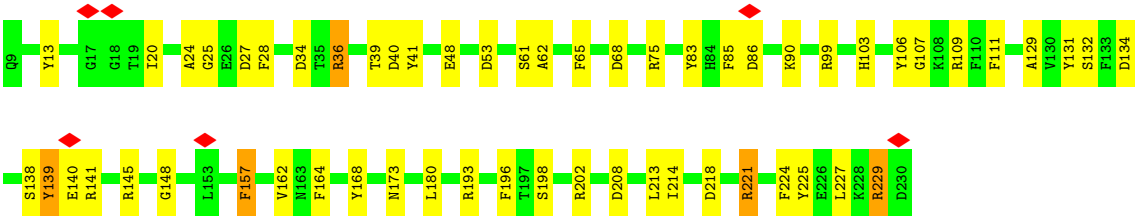
• Molecule 13: Proteasome subunit beta type-6

Chain m:



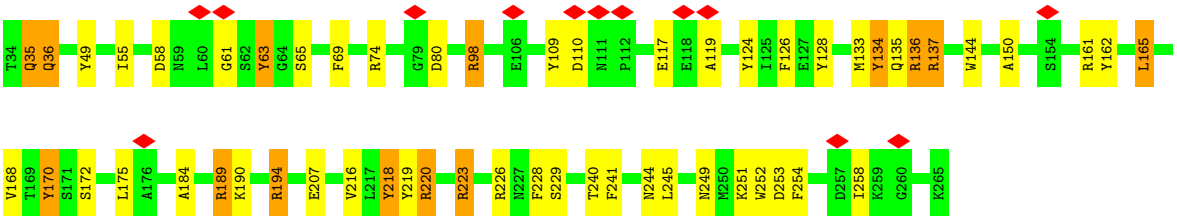
- Molecule 13: Proteasome subunit beta type-6

Chain 6:



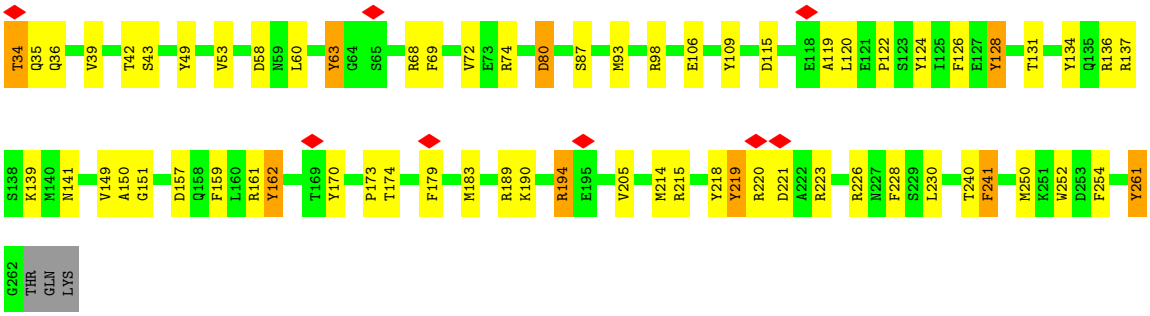
- Molecule 14: Proteasome subunit beta type-7

Chain n:



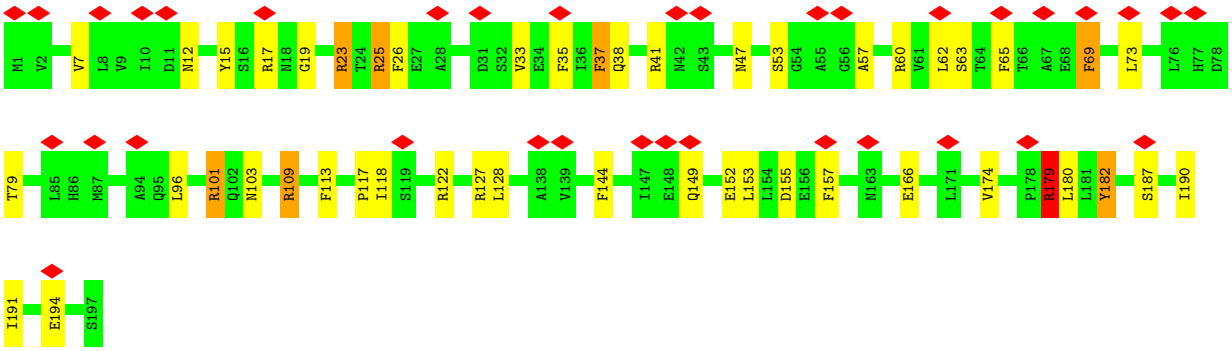
- Molecule 14: Proteasome subunit beta type-7

Chain 7:



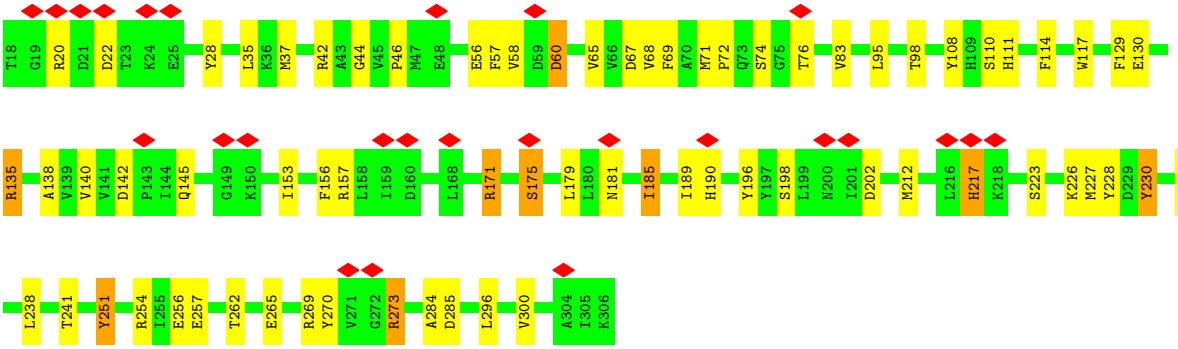
- Molecule 15: 26S proteasome regulatory subunit RPN10

Chain W:



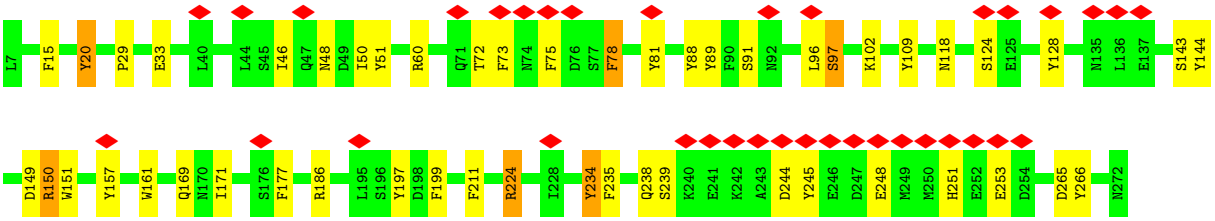
- Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



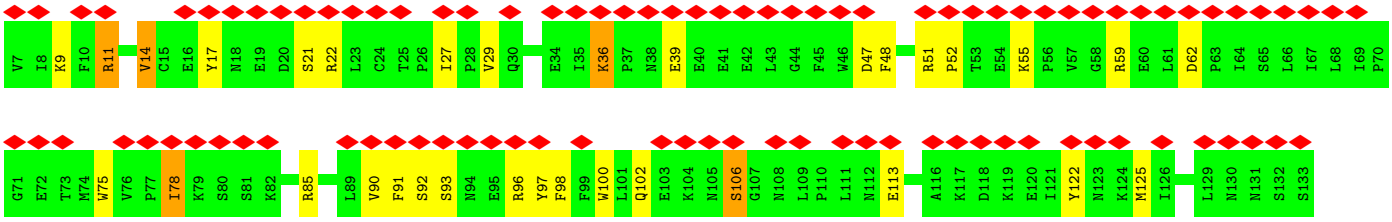
- Molecule 17: 26S proteasome regulatory subunit RPN12

Chain T:



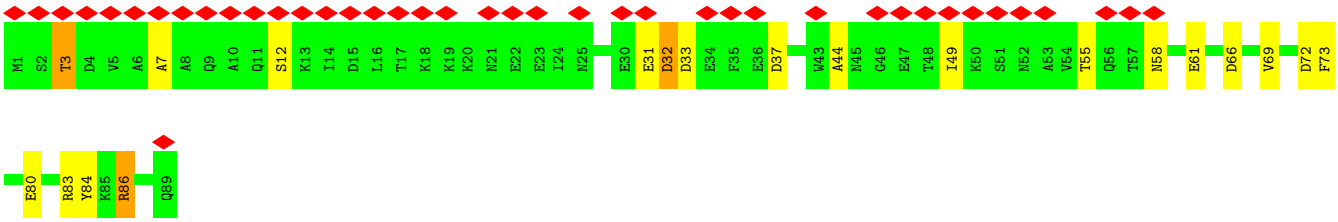
- Molecule 18: 26S proteasome regulatory subunit RPN13

Chain X:



- Molecule 19: 26S proteasome complex subunit SEM1

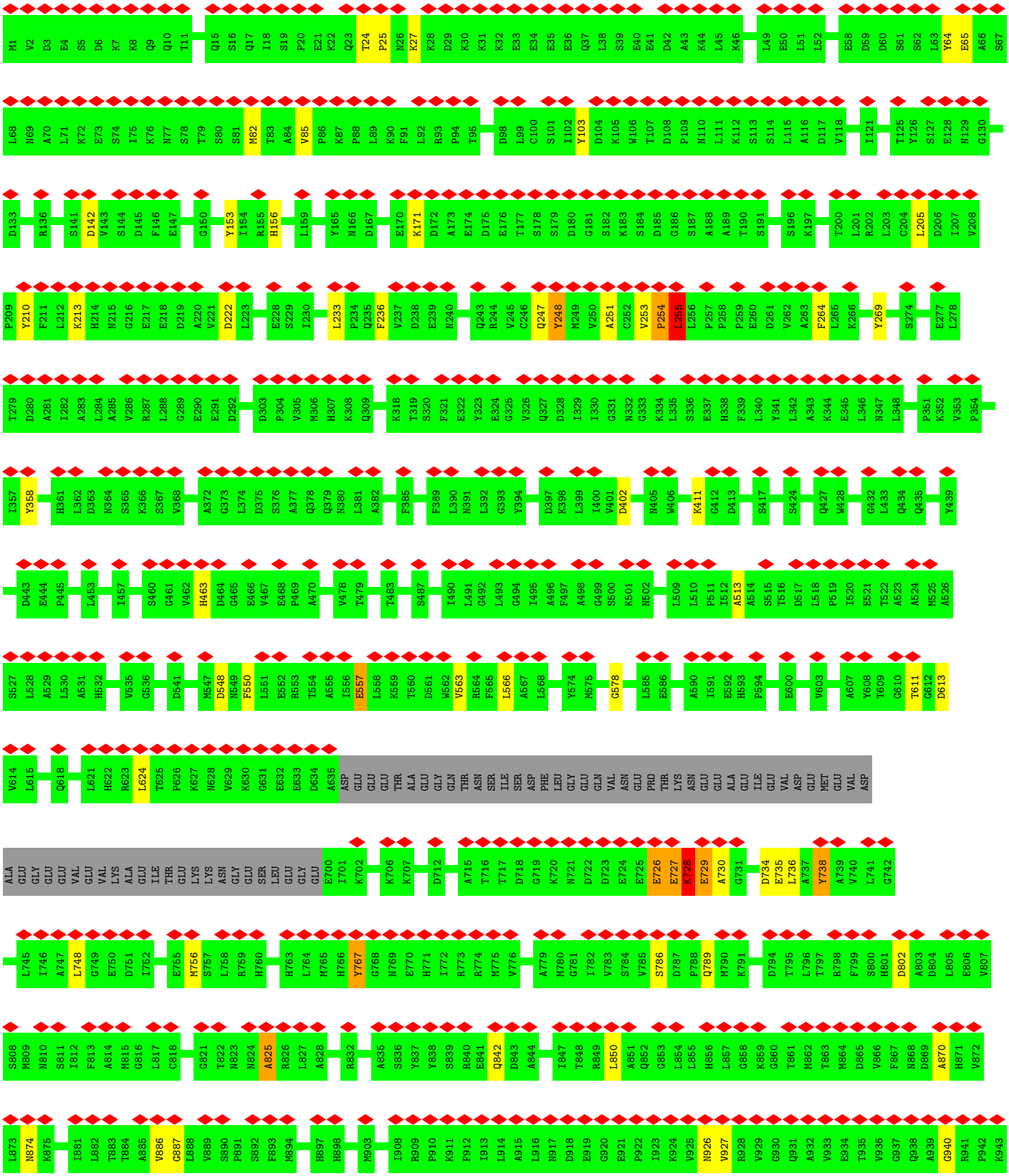
Chain Y:



- Molecule 20: 26S proteasome regulatory subunit RPN1

Chain Z:

59%
86%
6%
7%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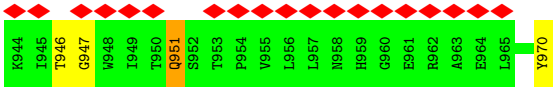
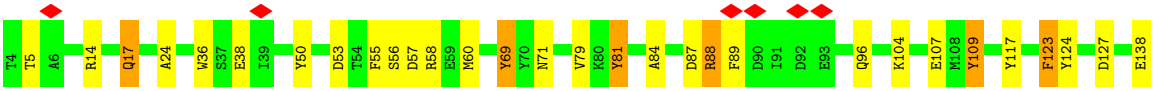
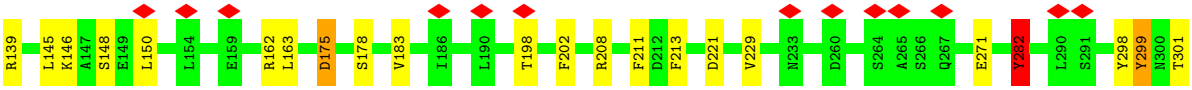
L68 N69 A70 L71 K72 E73 S74 I75 K76 N77 S78 T79 S80 S81 M82 T83 A84 V85 P86 K87 P88 L89 K90 F91 L92 R93 P94 T95 D98 L99 C100 S101 I102 Y103 D104 K105 W106 T107 D108 P109 N110 L111 K112 S113 S114 L115 A116 D117 V118 I121 T125 Y126 S127 E128 N129 G130
D133 R136 S141 D142 V143 S144 D145 F146 E147 G150 Y153 I154 R155 H156 L159 Y165 N166 D167 E170 K171 D172 A173 E174 D175 E176 T177 S178 S179 D180 G181 S182 K183 S184 D185 G186 S187 A188 A189 T190 S191 S196 K197 T200 L201 R202 L203 C204 L205 D206 I207 V208
P209 Y210 F211 L212 K213 H214 N215 G216 E217 E218 D219 A220 V221 D222 L223 E228 S229 I230 L233 P234 Q235 F236 V237 D238 E239 N240 Q243 R244 V245 C246 Q247 Y248 M249 V250 A251 C252 V253 P254 L255 L256 P257 P258 P259 E260 D261 V262 A263 F264 L265 K266 Y269 S274 E277 L278
T279 D280 A281 I282 A283 L284 A285 V286 R287 L288 G289 E290 E291 D292 D303 P304 V305 M306 H307 K308 Q309 K318 T319 S320 F321 E322 Y323 E324 G325 V326 Q327 D328 I329 I330 G331 N332 G333 K334 L335 S336 E337 H338 F339 L340 Y341 L342 A343 K344 E345 L346 N347 L348 P351 K352 V353 P354
I357 Y358 H361 L362 D363 N364 S365 K366 S367 V368 A372 G373 L374 D375 S376 A377 Q378 Q379 N380 L381 A382 F385 F389 L390 N391 L392 G393 Y394 D397 K398 L399 I400 V401 D402 N405 W406 K411 G412 D413 S417 S424 Q427 W428 G432 L433 Q434 Q435 Y439
D443 E444 P445 L453 I457 S460 G461 V462 H463 D464 G465 E466 V467 E468 P469 A470 V478 T479 T483 S487 I490 L491 G492 L493 G494 I495 A496 F497 A498 G499 S500 K501 N502 L509 L510 P511 I512 A513 A514 S515 T516 D517 L518 P519 I520 E521 T522 A523 A524 M525 A526
S527 L528 A529 L530 A531 H532 V535 G536 D541 M547 D548 N549 F550 L551 E552 R553 T554 A555 I556 E557 L558 K559 T560 D561 W562 V563 R564 F565 L566 A567 L568 Y574 M575 G578 L585 E586 A590 I591 E592 H593 P594 E600 V603 A607 Y608 T609 G610 T611 G612 D613
V614 L615 Q618 L621 H622 R623 L624 T625 P626 K627 N628 V629 K630 G631 E632 E633 D634 A635 ASP GLU GLU GLU THR ALA GLU GLY GLN THR 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 E700 I701 K702 K706 K707 D712 A715 T716 T717 D718 G719 K720 N721 D722 D723 E724 E725 E726 E727 K728 E729 A730 G731 D734 E735 L736 A737 Y738 A739 V740 L741 G742
L745 I746 A747 L748 G749 E750 D751 I752 E755 M756 S757 L758 R759 H760 H763 L764 M765 H766 Y767 G768 N769 E770 H771 I772 R773 R774 M775 V776 A779 M780 G781 I782 V783 S784 V785 S786 D787 P788 Q789 M790 K791 D794 T795 L796 T797 R798 F799 S800 H801 D802 A803 D804 L805 E806 V807
S808 M809 N810 S811 I812 F813 A814 M815 G816 L817 C818 G821 T822 N823 N824 A825 R826 L827 A828 R832 A835 S836 Y837 Y838 S839 R840 E841 Q842 D843 A844 I847 T848 R849 L850 A851 Q852 G853 L854 L855 H856 L857 G858 K859 G860 T861 M862 T863 M864 D865 V866 F867 N868 D869 A870 H871 V872
L873 N874 K875 I881 L882 T883 T884 A885 V886 G887 L888 V889 S890 P891 S892 F893 M894 H897 H898 M903 I908 R909 P910 K911 F912 I913 L914 A915 L916 N917 D918 E919 G920 E921 P922 I923 K924 V925 N926 V927 R928 V929 G930 Q931 A932 V933 E934 T935 V936 G937 Q938 A939 G940 R941 P942 K943

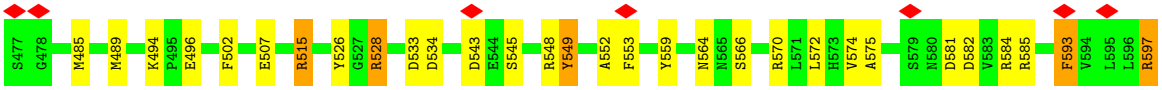


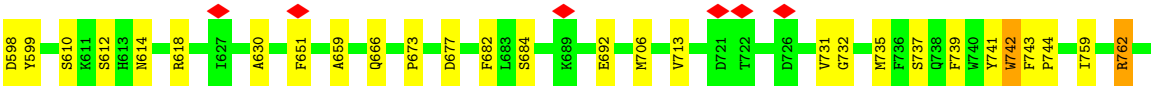
• Molecule 21: 26S proteasome regulatory subunit RPN2

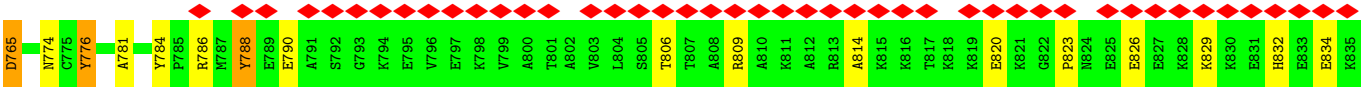
Chain N:

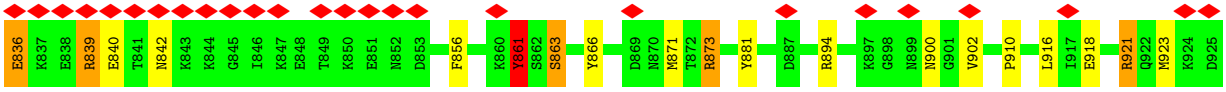






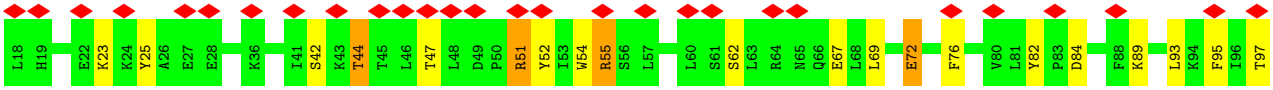


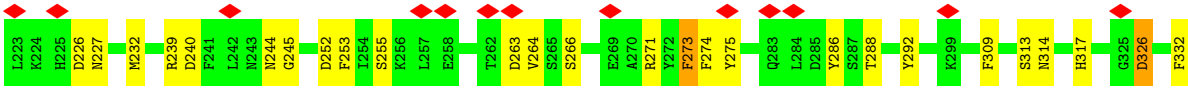


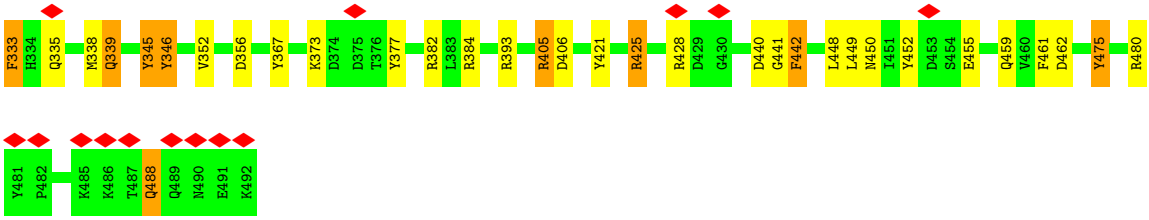


• Molecule 22: 26S proteasome regulatory subunit RPN3

Chain S:

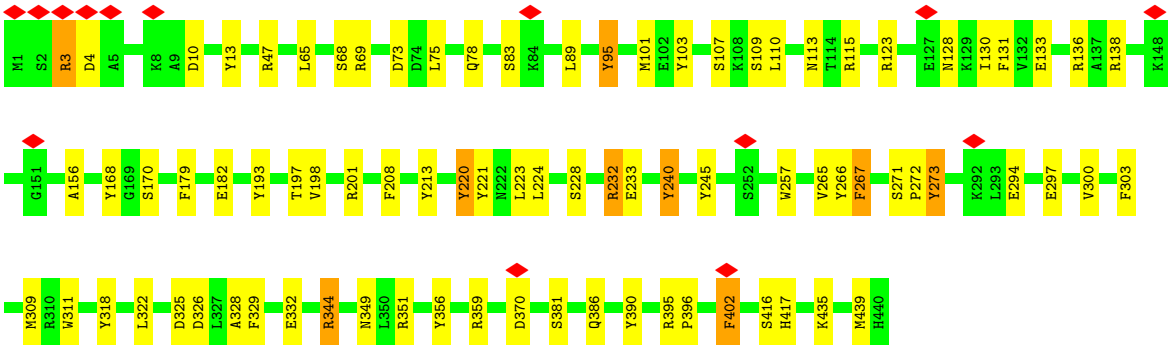






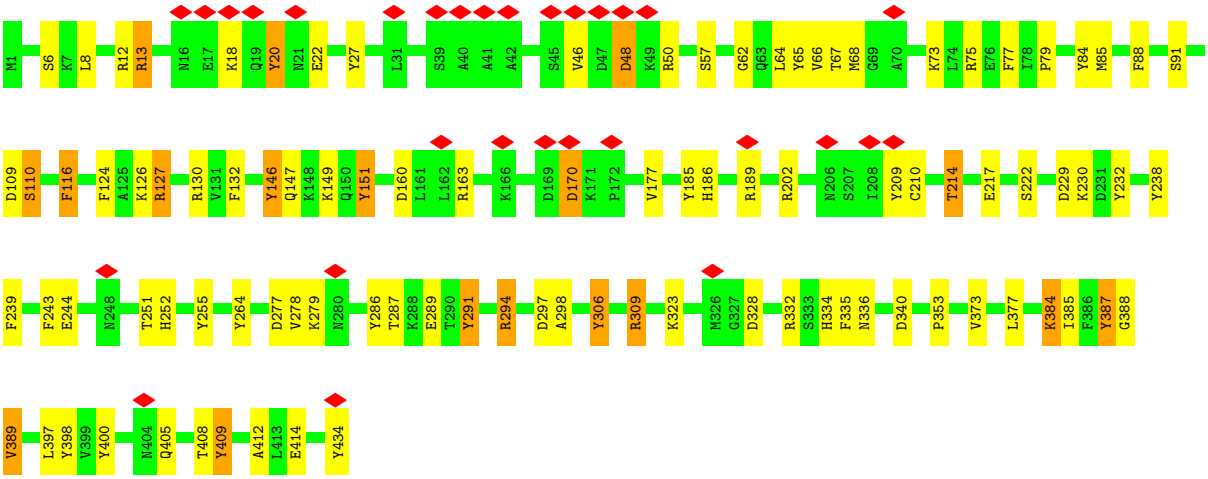
• Molecule 23: 26S proteasome regulatory subunit RPN5

Chain P:



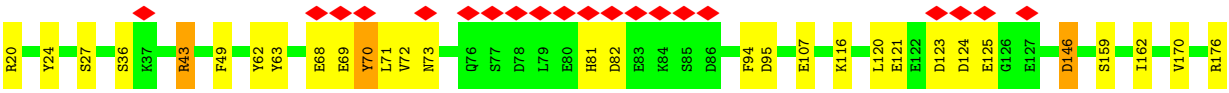
• Molecule 24: 26S proteasome regulatory subunit RPN6

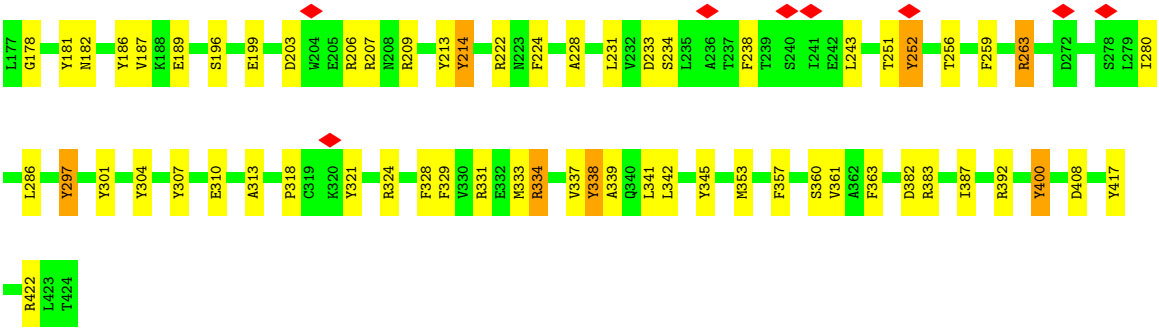
Chain Q:



• Molecule 25: 26S proteasome regulatory subunit RPN7

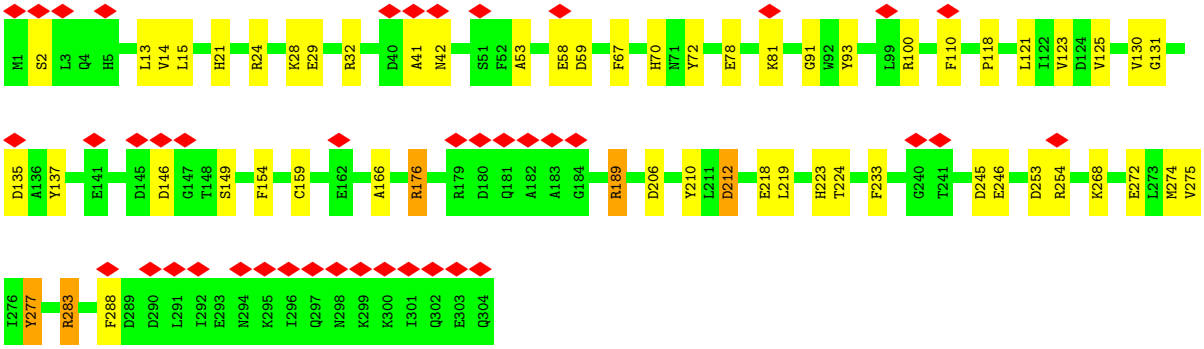
Chain R:





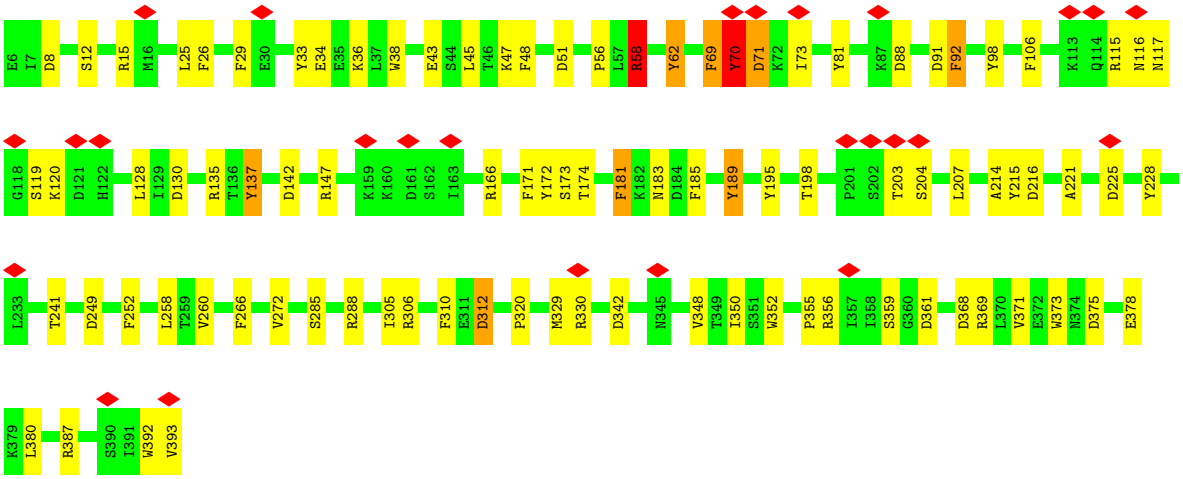
- Molecule 26: 26S proteasome regulatory subunit RPN8

Chain U:



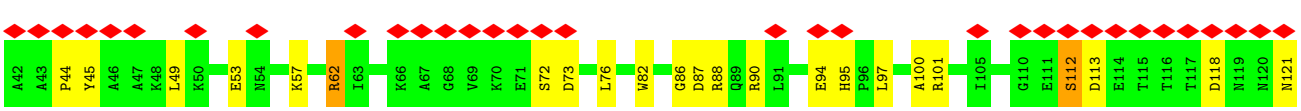
- Molecule 27: 26S proteasome regulatory subunit RPN9

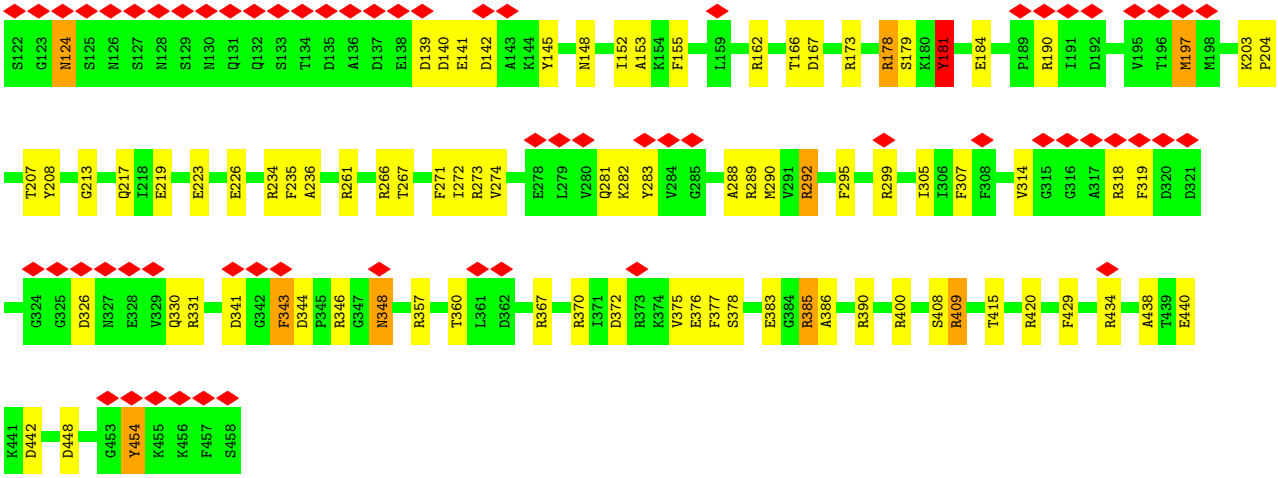
Chain O:



- Molecule 28: 26S proteasome regulatory subunit 7 homolog

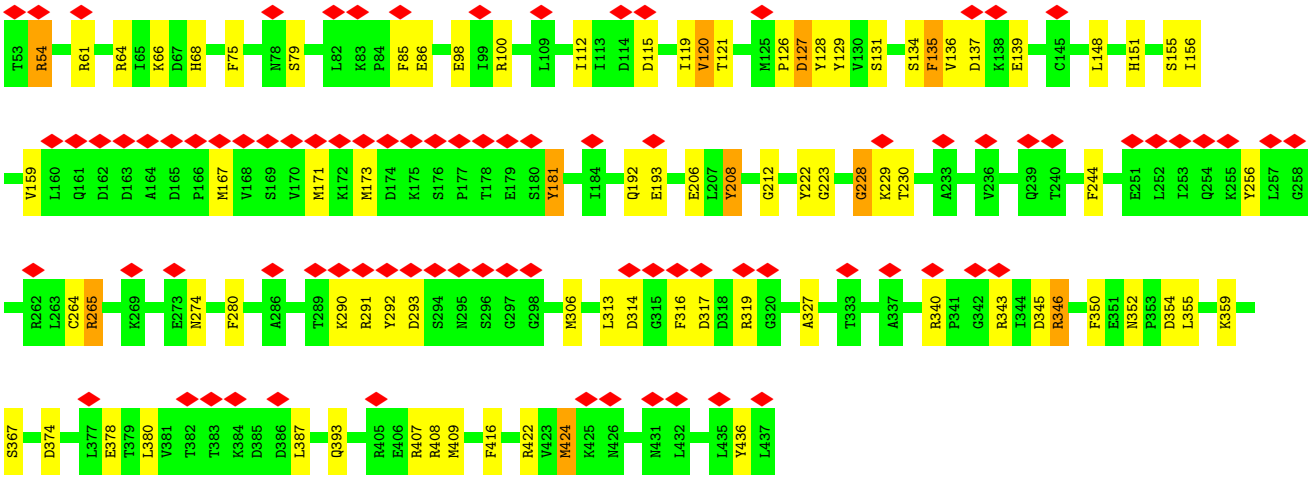
Chain H:





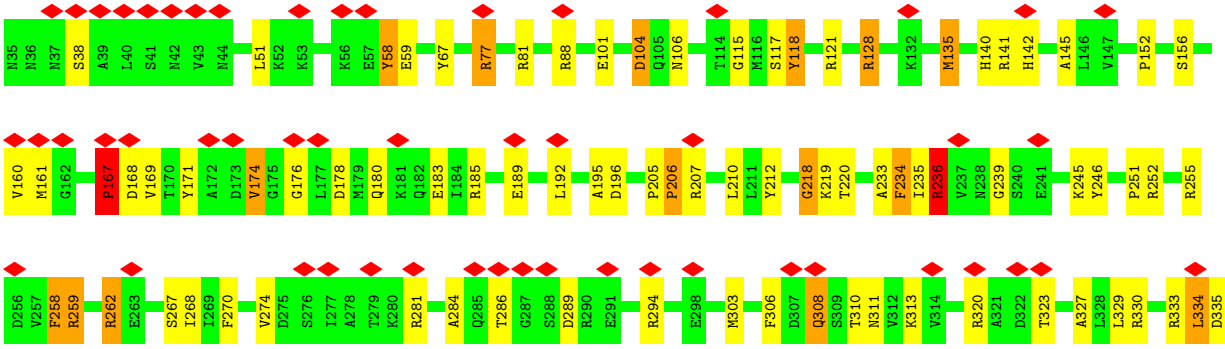
- Molecule 29: 26S proteasome regulatory subunit 4 homolog

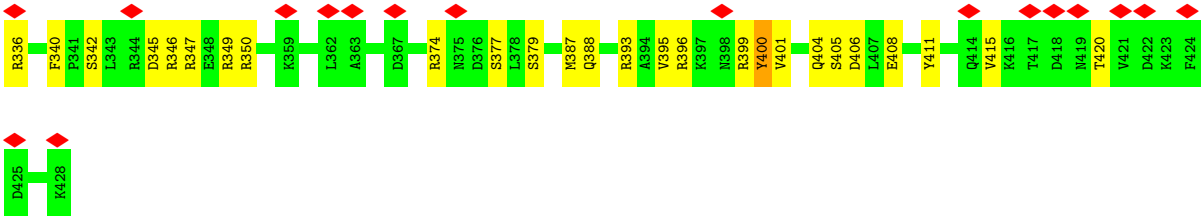
Chain I:



- Molecule 30: 26S proteasome regulatory subunit 6B homolog

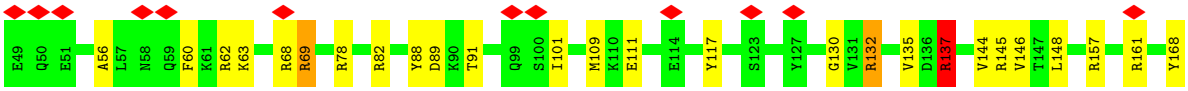
Chain K:

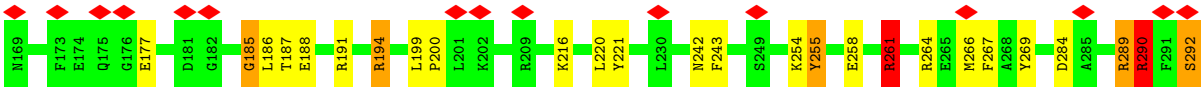


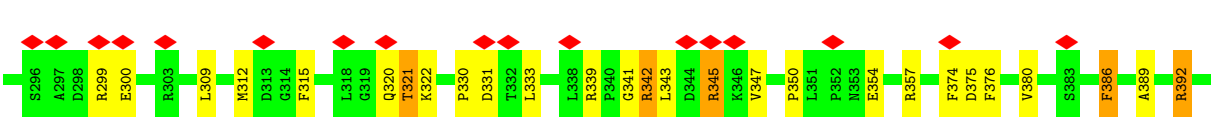


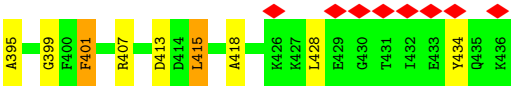
• Molecule 31: 26S proteasome subunit RPT4

Chain L:



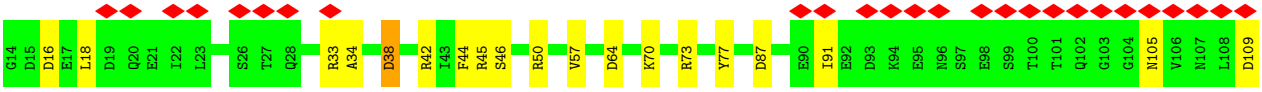


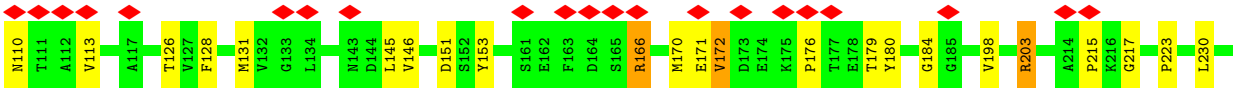


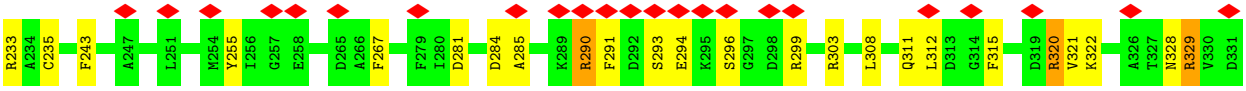


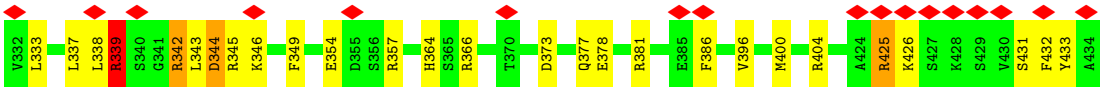
• Molecule 32: 26S proteasome regulatory subunit 6A

Chain M:



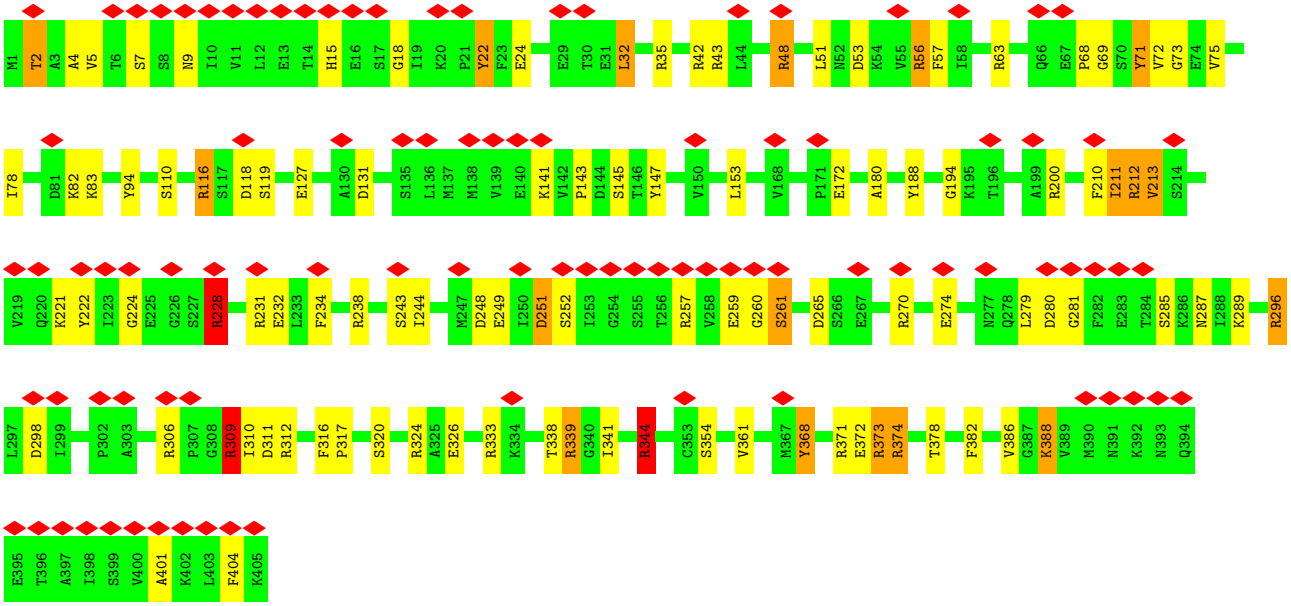






• Molecule 33: 26S proteasome regulatory subunit 8 homolog

Chain J:


M1 T2 A3 A4 V5 T6 S7 S8 N9 I10 V11 L12 E13 T14 H15 E16 S17 G18 I19 K20 P21 Y22 F23 E24 E29 T30 E31 L32 R35 R42 R43 L44 R48 L51 N52 D53 K54 V55 R56 F57 I58 R63 Q66 E67 P68 G69 S70 Y71 V72 G73 E74 V75
I78 D81 K82 K83 Y94 S110 R116 S117 D118 S119 E127 A130 D131 S135 L136 M137 M138 V139 E140 K141 V142 P143 D144 S145 T146 Y147 V150 L153 V168 P171 E172 A180 Y188 G194 K195 T196 A199 R200 F210 I211 R212 V213 S214
V219 Q220 K221 Y222 I223 G224 E225 G226 S227 R228 R231 E232 L233 F234 R238 S243 I244 M247 D248 E249 I250 D251 S252 I253 G254 S255 T256 R257 V258 E259 G260 S261 D265 S266 E267 R270 E274 N277 Q278 L279 D280 G281 F282 E283 T284 S285 K286 N287 I288 K289 R296
L297 D298 I299 P302 A303 R306 P307 G308 R309 I310 D311 R312 F316 P317 S320 R324 A325 E326 R333 K334 T338 R339 G340 I341 R344 C353 S354 V361 M367 Y368 R371 E372 R373 R374 T378 F382 V386 G387 K388 V389 M390 N391 K392 N393 Q394
E395 T396 A397 I398 S399 V400 A401 K402 L403 F404 K405

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	292279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.93	0/1946	0.97	2/2634 (0.1%)
1	a	1.71	14/1946 (0.7%)	1.88	37/2634 (1.4%)
2	B	0.91	0/1944	0.96	1/2632 (0.0%)
2	b	1.73	15/1944 (0.8%)	1.90	44/2632 (1.7%)
3	C	0.94	0/1935	0.96	4/2618 (0.2%)
3	c	1.77	20/1935 (1.0%)	2.02	58/2618 (2.2%)
4	D	0.96	0/1888	0.96	2/2557 (0.1%)
4	d	1.75	19/2012 (0.9%)	1.93	38/2718 (1.4%)
5	E	1.70	2/1909 (0.1%)	1.32	7/2571 (0.3%)
5	e	1.71	23/1909 (1.2%)	1.86	34/2571 (1.3%)
6	F	0.95	0/1800	0.97	3/2433 (0.1%)
6	f	1.76	23/1800 (1.3%)	1.99	52/2433 (2.1%)
7	G	0.93	0/1926	1.20	6/2599 (0.2%)
7	g	1.73	21/1926 (1.1%)	2.10	54/2599 (2.1%)
8	1	1.72	16/1541 (1.0%)	1.85	25/2087 (1.2%)
8	h	1.73	14/1541 (0.9%)	1.90	41/2087 (2.0%)
9	2	1.74	21/1751 (1.2%)	1.87	31/2373 (1.3%)
9	i	1.75	17/1751 (1.0%)	1.93	35/2373 (1.5%)
10	3	1.74	18/1611 (1.1%)	1.94	42/2174 (1.9%)
10	j	1.71	10/1611 (0.6%)	1.94	41/2174 (1.9%)
11	4	1.73	9/1590 (0.6%)	1.90	28/2142 (1.3%)
11	k	1.76	19/1590 (1.2%)	1.95	39/2142 (1.8%)
12	5	1.75	23/1681 (1.4%)	1.92	41/2274 (1.8%)
12	l	1.77	16/1681 (1.0%)	2.05	48/2274 (2.1%)
13	6	1.76	16/1795 (0.9%)	2.00	51/2420 (2.1%)
13	m	1.74	20/1795 (1.1%)	2.05	52/2420 (2.1%)
14	7	1.72	15/1821 (0.8%)	2.03	61/2470 (2.5%)
14	n	1.73	18/1847 (1.0%)	2.07	52/2503 (2.1%)
15	W	1.71	16/1558 (1.0%)	1.94	39/2111 (1.8%)
16	V	1.69	21/2309 (0.9%)	1.95	61/3115 (2.0%)
17	T	1.70	16/2236 (0.7%)	1.89	44/3017 (1.5%)
18	X	1.74	6/1059 (0.6%)	1.98	33/1432 (2.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	Y	1.65	4/741 (0.5%)	1.98	15/1000 (1.5%)
20	Z	1.34	16/7123 (0.2%)	1.29	62/9645 (0.6%)
21	N	1.71	48/7273 (0.7%)	1.89	159/9822 (1.6%)
22	S	1.69	32/3967 (0.8%)	1.87	81/5355 (1.5%)
23	P	1.66	25/3664 (0.7%)	1.87	71/4940 (1.4%)
24	Q	1.70	30/3556 (0.8%)	1.93	88/4787 (1.8%)
25	R	1.72	26/3314 (0.8%)	1.97	93/4469 (2.1%)
26	U	1.67	16/2461 (0.7%)	1.82	42/3327 (1.3%)
27	O	1.70	30/3247 (0.9%)	1.95	82/4380 (1.9%)
28	H	1.73	29/3282 (0.9%)	1.94	88/4423 (2.0%)
29	I	1.69	28/3059 (0.9%)	1.87	66/4115 (1.6%)
30	K	1.75	37/3156 (1.2%)	2.19	89/4261 (2.1%)
31	L	1.73	33/3128 (1.1%)	2.22	90/4201 (2.1%)
32	M	2.68	30/3323 (0.9%)	2.13	81/4478 (1.8%)
33	J	1.91	44/3212 (1.4%)	2.14	86/4316 (2.0%)
All	All	1.68	856/112094 (0.8%)	1.84	2299/151356 (1.5%)

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
1	a	0	9
2	b	0	3
3	c	0	5
4	D	0	1
4	d	0	5
5	e	0	3
6	F	0	1
6	f	0	6
7	G	0	2
7	g	0	12
8	1	0	6
8	h	0	8
9	2	0	4
9	i	0	6
10	3	0	4
10	j	0	4
11	4	0	6
11	k	0	4
12	5	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	l	0	5
13	6	0	9
13	m	0	6
14	7	0	5
14	n	0	12
15	W	0	7
16	V	0	6
17	T	0	10
18	X	0	2
19	Y	0	1
20	Z	0	9
21	N	0	24
22	S	0	18
23	P	0	16
24	Q	0	13
25	R	0	11
26	U	0	6
27	O	0	9
28	H	0	13
29	I	0	9
30	K	0	19
31	L	0	18
32	M	0	13
33	J	0	15
All	All	0	351

The worst 5 of 856 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	20	ARG	NE-CZ	62.28	2.14	1.33
32	M	433	TYR	CE2-CZ	51.52	2.05	1.38
32	M	433	TYR	CG-CD1	51.22	2.05	1.39
32	M	433	TYR	CG-CD2	50.39	2.04	1.39
32	M	433	TYR	CE1-CZ	48.44	2.01	1.38

The worst 5 of 2299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	185	GLY	O-C-N	-66.69	16.00	122.70
30	K	167	PRO	O-C-N	-47.18	47.21	122.70
33	J	211	ILE	O-C-N	-47.12	47.31	122.70
32	M	338	LEU	O-C-N	-33.56	69.00	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	728	LYS	CG-CD-CE	-29.48	23.45	111.90

There are no chirality outliers.

5 of 351 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	a	105	ARG	Sidechain
1	a	128	TYR	Sidechain
1	a	131	ARG	Sidechain
1	a	30	TYR	Sidechain
1	a	46	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	239/241 (99%)	223 (93%)	16 (7%)	0	100 100
1	a	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	19 60
2	B	247/249 (99%)	232 (94%)	15 (6%)	0	100 100
2	b	247/249 (99%)	231 (94%)	14 (6%)	2 (1%)	19 60
3	C	242/244 (99%)	232 (96%)	10 (4%)	0	100 100
3	c	242/244 (99%)	230 (95%)	12 (5%)	0	100 100
4	D	235/251 (94%)	222 (94%)	13 (6%)	0	100 100
4	d	249/251 (99%)	229 (92%)	14 (6%)	6 (2%)	6 35
5	E	242/244 (99%)	225 (93%)	11 (4%)	6 (2%)	5 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	13	50
6	F	229/231 (99%)	219 (96%)	9 (4%)	1 (0%)	34	72
6	f	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	6	37
7	G	240/242 (99%)	229 (95%)	11 (5%)	0	100	100
7	g	240/242 (99%)	229 (95%)	10 (4%)	1 (0%)	34	72
8	1	194/196 (99%)	185 (95%)	8 (4%)	1 (0%)	29	69
8	h	194/196 (99%)	177 (91%)	12 (6%)	5 (3%)	5	33
9	2	224/226 (99%)	215 (96%)	7 (3%)	2 (1%)	17	56
9	i	224/226 (99%)	206 (92%)	15 (7%)	3 (1%)	12	48
10	3	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	29	69
10	j	202/204 (99%)	185 (92%)	11 (5%)	6 (3%)	4	30
11	4	193/195 (99%)	183 (95%)	7 (4%)	3 (2%)	9	44
11	k	193/195 (99%)	176 (91%)	13 (7%)	4 (2%)	7	37
12	5	210/212 (99%)	197 (94%)	12 (6%)	1 (0%)	29	69
12	l	210/212 (99%)	195 (93%)	15 (7%)	0	100	100
13	6	220/222 (99%)	204 (93%)	12 (6%)	4 (2%)	8	41
13	m	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	11	46
14	7	227/232 (98%)	205 (90%)	18 (8%)	4 (2%)	8	41
14	n	230/232 (99%)	214 (93%)	14 (6%)	2 (1%)	17	56
15	W	195/197 (99%)	178 (91%)	11 (6%)	6 (3%)	4	30
16	V	287/289 (99%)	260 (91%)	20 (7%)	7 (2%)	6	35
17	T	264/266 (99%)	248 (94%)	14 (5%)	2 (1%)	19	60
18	X	125/127 (98%)	105 (84%)	15 (12%)	5 (4%)	3	25
19	Y	87/89 (98%)	72 (83%)	10 (12%)	5 (6%)	1	19
20	Z	902/970 (93%)	820 (91%)	59 (6%)	23 (2%)	5	34
21	N	920/922 (100%)	865 (94%)	41 (4%)	14 (2%)	10	46
22	S	473/475 (100%)	445 (94%)	19 (4%)	9 (2%)	8	39
23	P	438/440 (100%)	415 (95%)	16 (4%)	7 (2%)	9	44
24	Q	432/434 (100%)	394 (91%)	26 (6%)	12 (3%)	5	32
25	R	403/405 (100%)	388 (96%)	10 (2%)	5 (1%)	13	50
26	U	302/304 (99%)	288 (95%)	13 (4%)	1 (0%)	41	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	O	386/388 (100%)	371 (96%)	10 (3%)	5 (1%)	12	48
28	H	415/417 (100%)	364 (88%)	39 (9%)	12 (3%)	4	31
29	I	379/385 (98%)	353 (93%)	18 (5%)	8 (2%)	7	37
30	K	392/394 (100%)	353 (90%)	28 (7%)	11 (3%)	5	32
31	L	384/388 (99%)	360 (94%)	18 (5%)	6 (2%)	9	44
32	M	419/421 (100%)	376 (90%)	30 (7%)	13 (3%)	4	30
33	J	403/405 (100%)	362 (90%)	22 (6%)	19 (5%)	2	23
All	All	13911/14094 (99%)	12913 (93%)	763 (6%)	235 (2%)	13	43

5 of 235 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	31	THR
4	d	50	SER
6	f	14	SER
5	E	16	SER
13	6	27	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/206 (100%)	204 (99%)	2 (1%)	76	86
1	a	206/206 (100%)	201 (98%)	5 (2%)	49	69
2	B	208/208 (100%)	205 (99%)	3 (1%)	67	81
2	b	208/208 (100%)	203 (98%)	5 (2%)	49	69
3	C	203/203 (100%)	202 (100%)	1 (0%)	88	93
3	c	203/203 (100%)	199 (98%)	4 (2%)	55	73
4	D	210/224 (94%)	207 (99%)	3 (1%)	67	81
4	d	224/224 (100%)	217 (97%)	7 (3%)	40	62
5	E	200/200 (100%)	196 (98%)	4 (2%)	55	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	e	200/200 (100%)	192 (96%)	8 (4%)	31	56
6	F	190/190 (100%)	188 (99%)	2 (1%)	73	85
6	f	190/190 (100%)	181 (95%)	9 (5%)	26	52
7	G	200/200 (100%)	196 (98%)	4 (2%)	55	73
7	g	200/200 (100%)	189 (94%)	11 (6%)	21	48
8	1	162/162 (100%)	157 (97%)	5 (3%)	40	62
8	h	162/162 (100%)	159 (98%)	3 (2%)	57	75
9	2	185/185 (100%)	180 (97%)	5 (3%)	44	65
9	i	185/185 (100%)	178 (96%)	7 (4%)	33	57
10	3	172/172 (100%)	168 (98%)	4 (2%)	50	70
10	j	172/172 (100%)	168 (98%)	4 (2%)	50	70
11	4	173/173 (100%)	168 (97%)	5 (3%)	42	64
11	k	173/173 (100%)	170 (98%)	3 (2%)	60	78
12	5	169/169 (100%)	166 (98%)	3 (2%)	59	77
12	l	169/169 (100%)	161 (95%)	8 (5%)	26	52
13	6	185/185 (100%)	182 (98%)	3 (2%)	62	79
13	m	185/185 (100%)	178 (96%)	7 (4%)	33	57
14	7	195/198 (98%)	186 (95%)	9 (5%)	27	53
14	n	198/198 (100%)	188 (95%)	10 (5%)	24	50
15	W	171/171 (100%)	165 (96%)	6 (4%)	36	60
16	V	253/253 (100%)	249 (98%)	4 (2%)	62	79
17	T	249/249 (100%)	243 (98%)	6 (2%)	49	69
18	X	116/116 (100%)	112 (97%)	4 (3%)	37	60
19	Y	81/81 (100%)	78 (96%)	3 (4%)	34	58
20	Z	773/828 (93%)	746 (96%)	27 (4%)	36	60
21	N	776/776 (100%)	758 (98%)	18 (2%)	50	70
22	S	447/447 (100%)	433 (97%)	14 (3%)	40	62
23	P	412/412 (100%)	405 (98%)	7 (2%)	60	78
24	Q	391/391 (100%)	380 (97%)	11 (3%)	43	65
25	R	356/356 (100%)	350 (98%)	6 (2%)	60	78
26	U	277/277 (100%)	268 (97%)	9 (3%)	39	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	O	363/363 (100%)	348 (96%)	15 (4%)	30	55
28	H	352/352 (100%)	343 (97%)	9 (3%)	46	67
29	I	342/342 (100%)	329 (96%)	13 (4%)	33	57
30	K	346/346 (100%)	329 (95%)	17 (5%)	25	51
31	L	332/332 (100%)	321 (97%)	11 (3%)	38	61
32	M	364/364 (100%)	357 (98%)	7 (2%)	57	75
33	J	352/352 (100%)	339 (96%)	13 (4%)	34	58
All	All	12086/12158 (99%)	11742 (97%)	344 (3%)	46	65

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	P	435	LYS
29	I	112	ILE
24	Q	170	ASP
27	O	58	ARG
30	K	161	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 120 such sidechains are listed below:

Mol	Chain	Res	Type
17	T	123	HIS
31	L	189	GLN
21	N	613	HIS
31	L	67	HIS
33	J	123	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)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	ATP	L	501	35	26,33,33	1.30	3 (11%)	31,52,52	1.61	5 (16%)
36	ATP	J	501	35	26,33,33	1.21	3 (11%)	31,52,52	1.91	6 (19%)
36	ATP	I	501	35	26,33,33	1.37	3 (11%)	31,52,52	1.61	6 (19%)
36	ATP	K	501	35	26,33,33	1.37	3 (11%)	31,52,52	1.61	6 (19%)
34	ADP	H	501	35	24,29,29	1.27	3 (12%)	29,45,45	2.41	6 (20%)
34	ADP	M	501	35	24,29,29	2.00	6 (25%)	29,45,45	2.33	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	L	501	35	-	5/18/38/38	0/3/3/3
36	ATP	J	501	35	-	4/18/38/38	0/3/3/3
36	ATP	I	501	35	-	5/18/38/38	0/3/3/3
36	ATP	K	501	35	-	4/18/38/38	0/3/3/3
34	ADP	H	501	35	-	4/12/32/32	0/3/3/3
34	ADP	M	501	35	-	4/12/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	M	501	ADP	C4-N3	-5.43	1.28	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	M	501	ADP	O4'-C4'	4.85	1.55	1.45
36	L	501	ATP	C2-N3	4.26	1.39	1.32
36	K	501	ATP	C2-N3	4.26	1.39	1.32
36	I	501	ATP	C2-N3	4.25	1.38	1.32

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	M	501	ADP	PA-O3A-PB	10.20	167.84	132.83
34	H	501	ADP	PA-O3A-PB	8.49	161.96	132.83
36	J	501	ATP	PB-O3B-PG	5.53	151.80	132.83
36	J	501	ATP	PA-O3A-PB	5.00	149.97	132.83
34	H	501	ADP	N3-C2-N1	4.95	136.41	128.68

There are no chirality outliers.

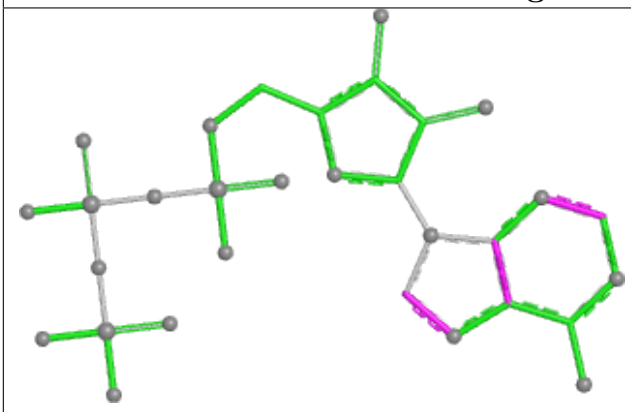
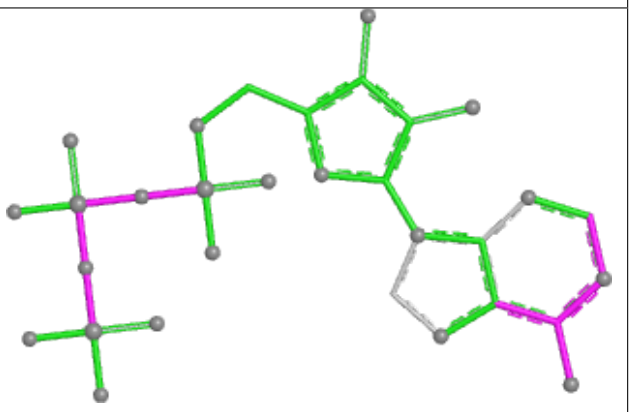
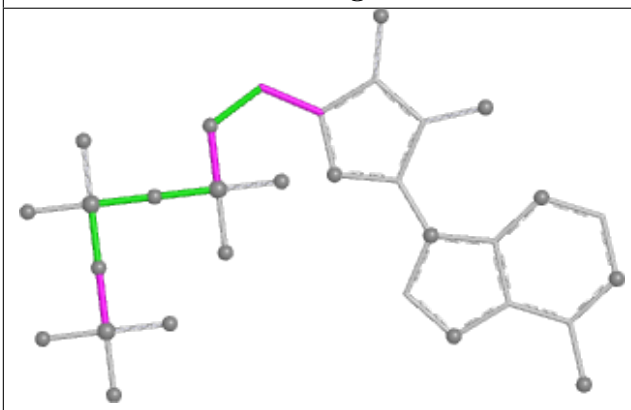
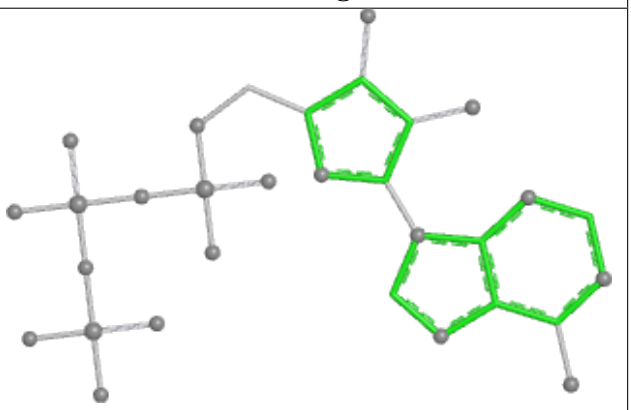
5 of 26 torsion outliers are listed below:

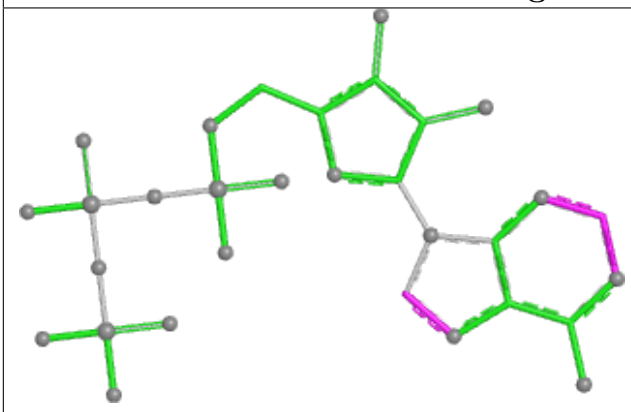
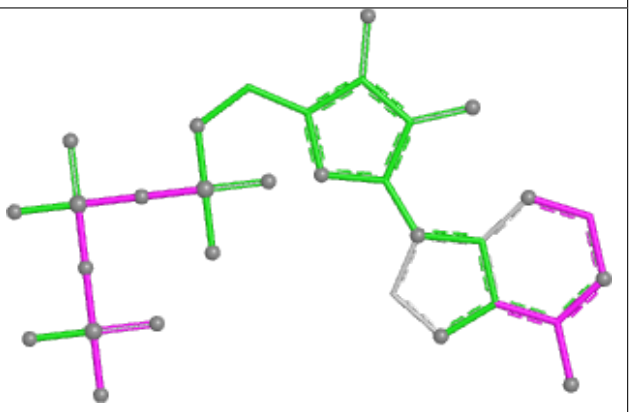
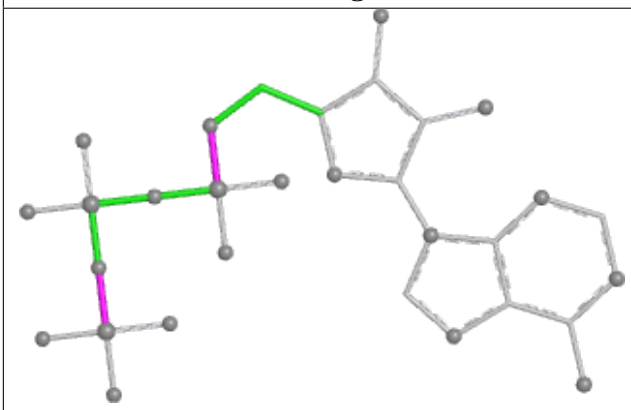
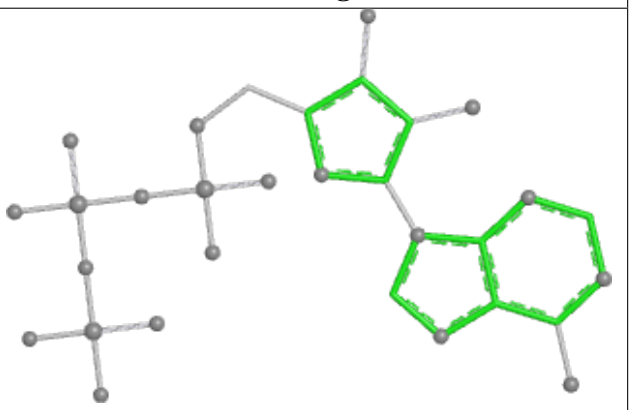
Mol	Chain	Res	Type	Atoms
34	H	501	ADP	C5'-O5'-PA-O2A
34	H	501	ADP	C5'-O5'-PA-O3A
34	M	501	ADP	C5'-O5'-PA-O1A
36	I	501	ATP	PB-O3B-PG-O2G
36	K	501	ATP	PB-O3B-PG-O2G

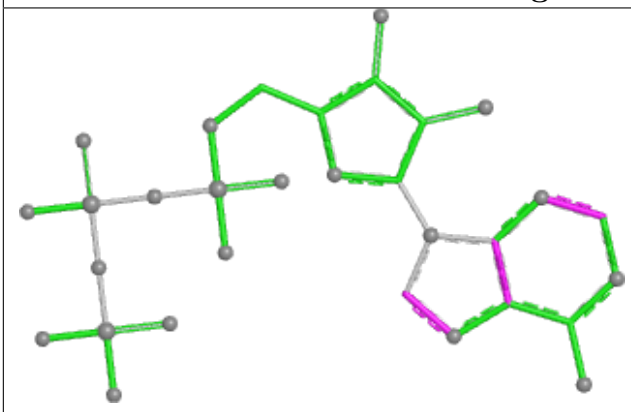
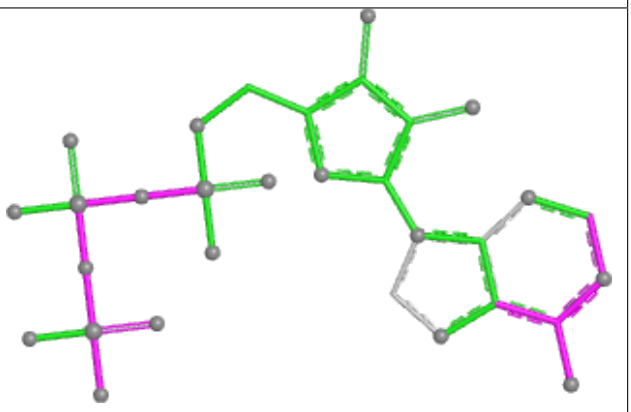
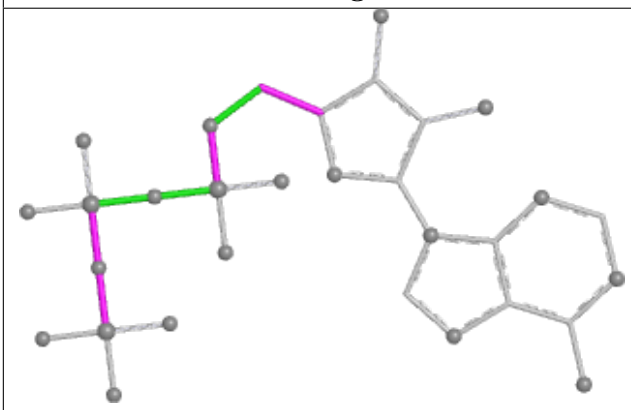
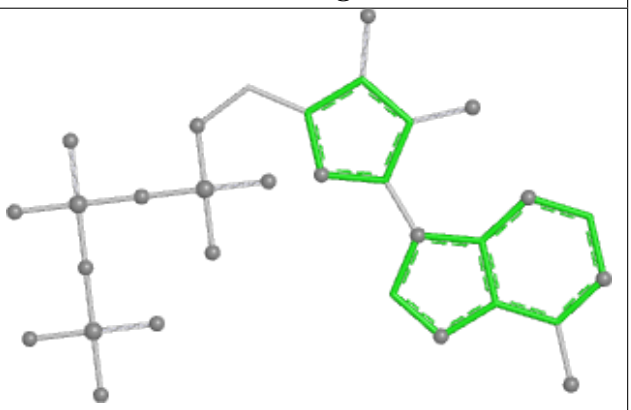
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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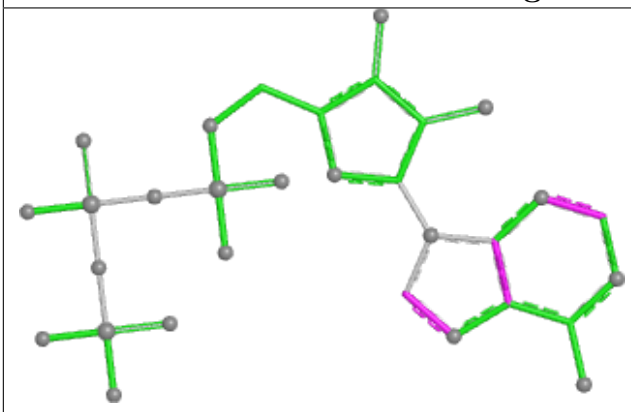
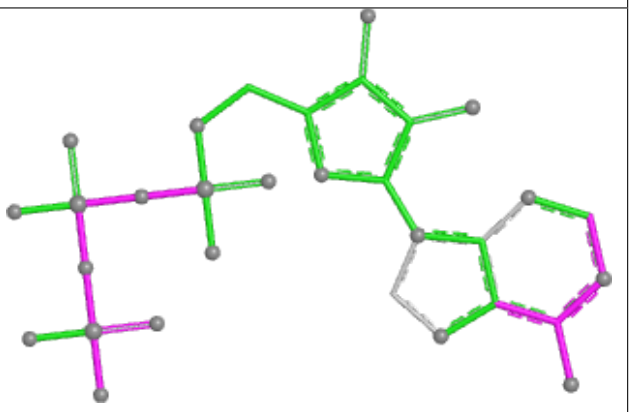
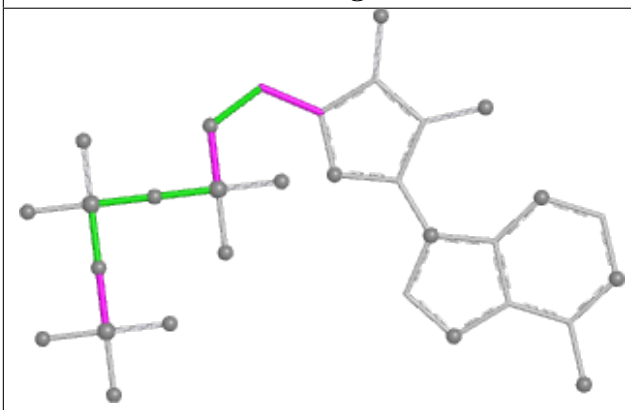
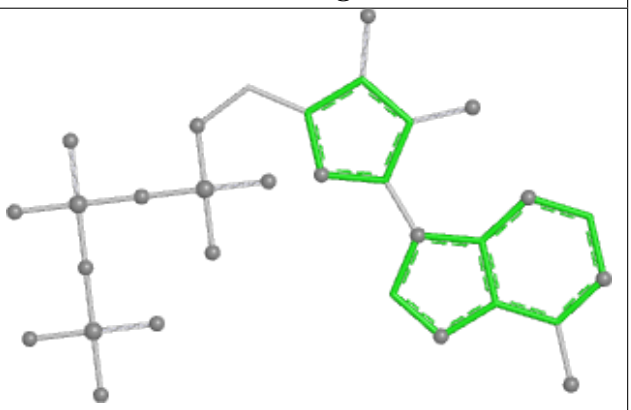
 Bond lengths	 Bond angles
 Torsions	 Rings

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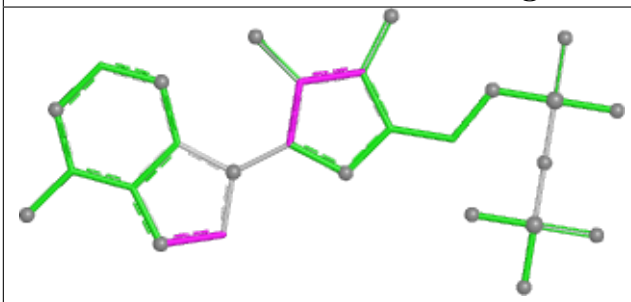
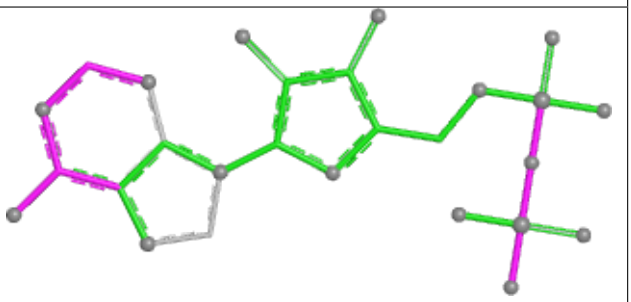
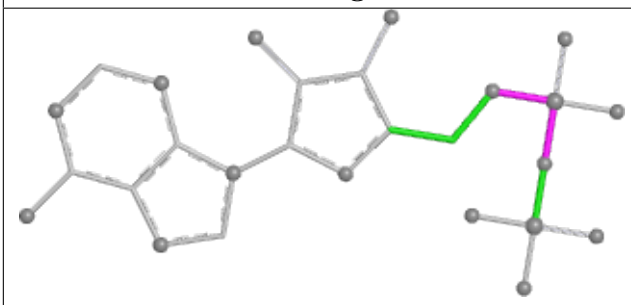
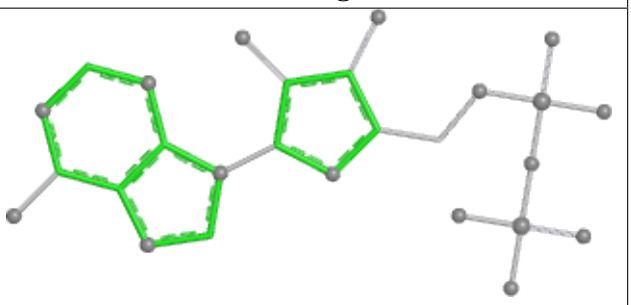
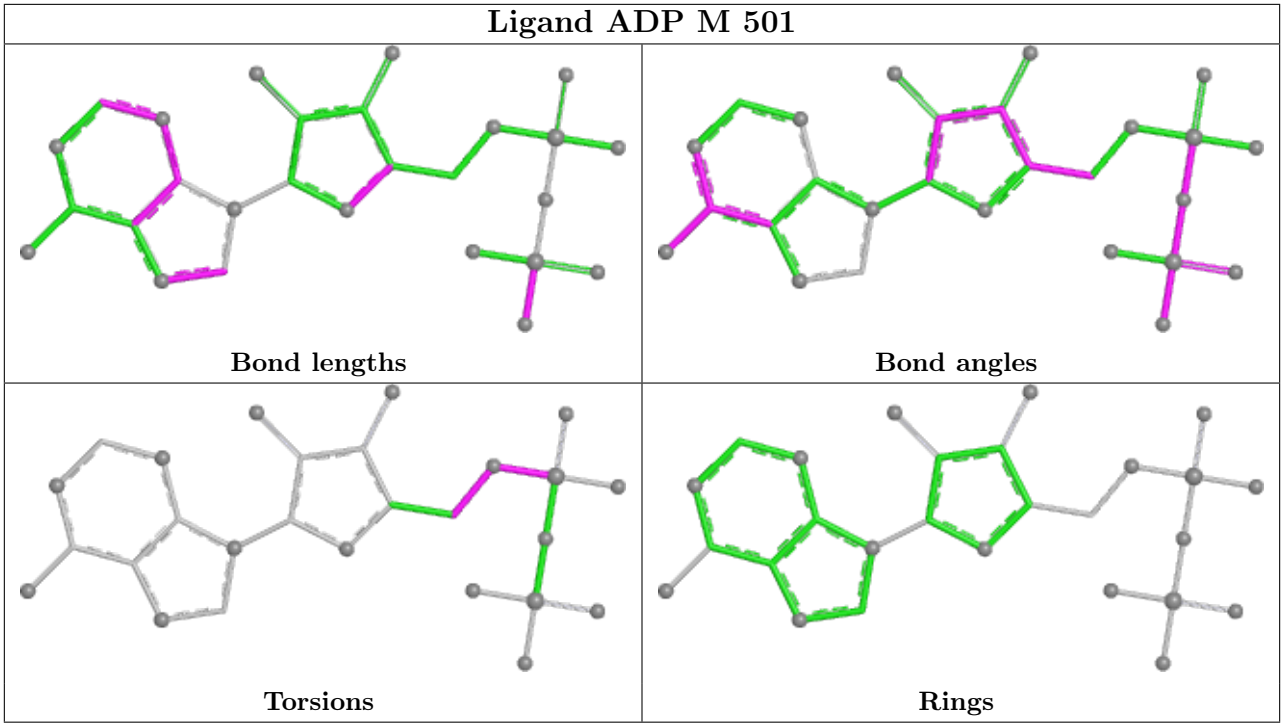
 Bond lengths	 Bond angles
 Torsions	 Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	I	2
32	M	2
33	J	2
31	L	1
30	K	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	180:PHE	C	181:ASP	N	2.67
1	I	183:ASP	C	184:ILE	N	2.58
1	I	186:GLY	C	187:LEU	N	2.56
1	M	338:LEU	C	339:ARG	N	1.69
1	J	212:ARG	C	213:VAL	N	1.68

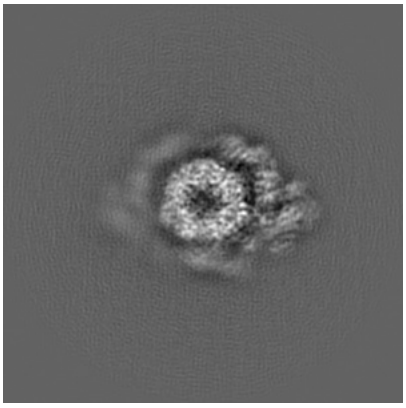
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4321. These allow visual inspection of the internal detail of the map and identification of artifacts.

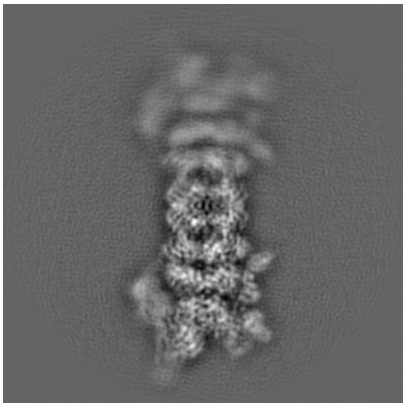
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

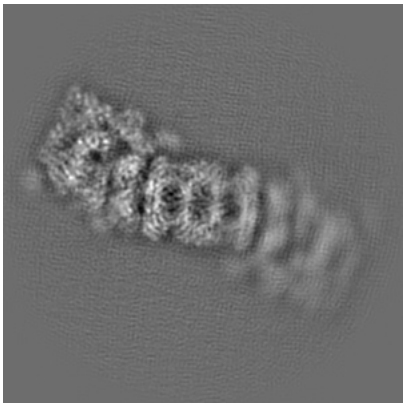
6.1.1 Primary map



X



Y

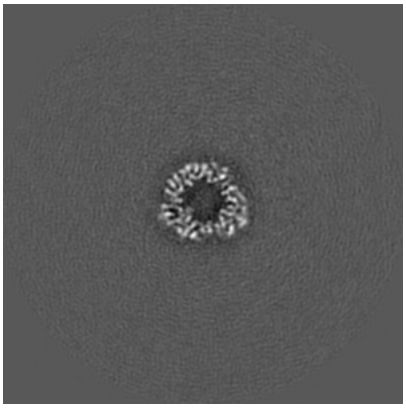


Z

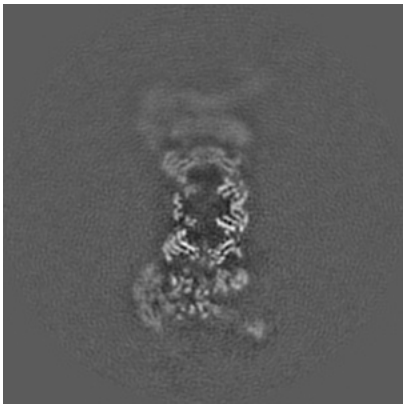
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

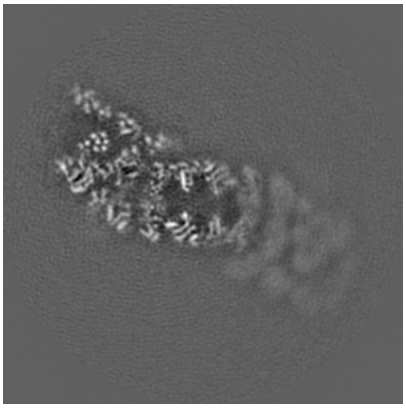
6.2.1 Primary map



X Index: 192



Y Index: 192

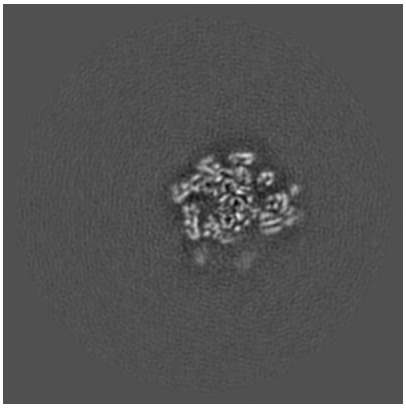


Z Index: 192

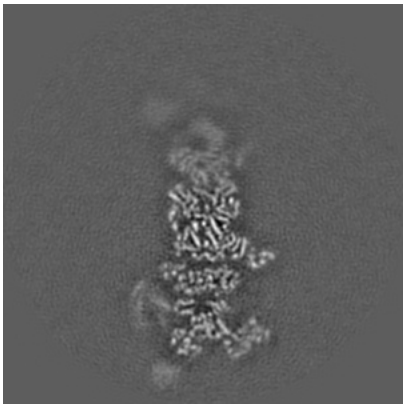
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

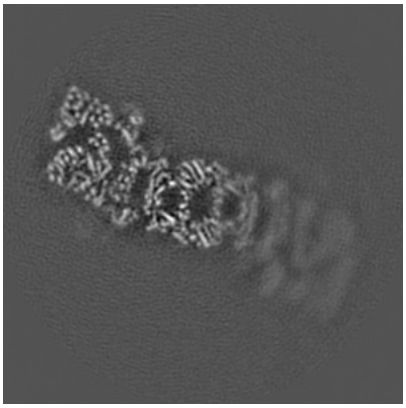
6.3.1 Primary map



X Index: 122



Y Index: 213



Z Index: 182

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

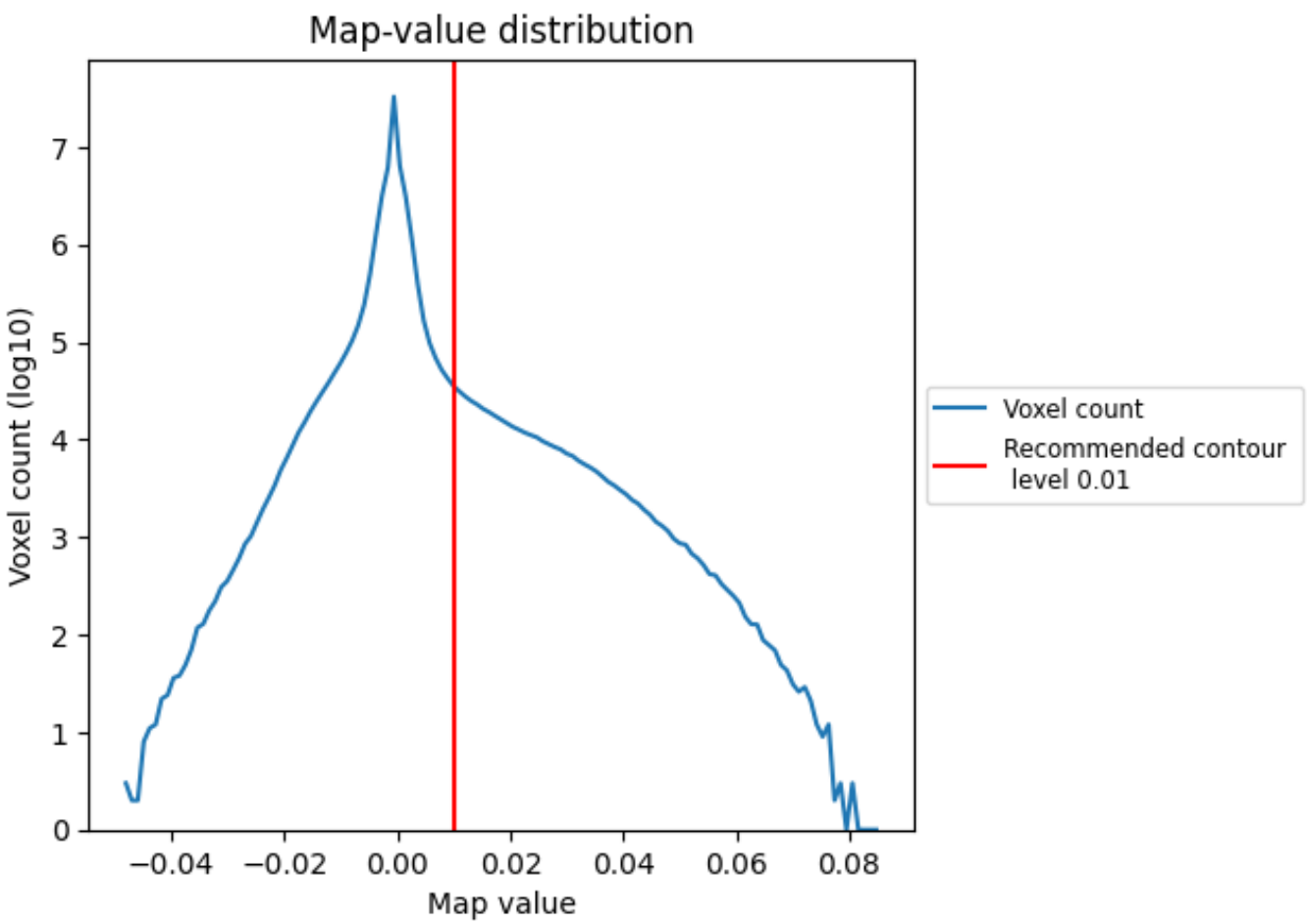
6.5 Mask visualisation (i)

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

7 Map analysis (i)

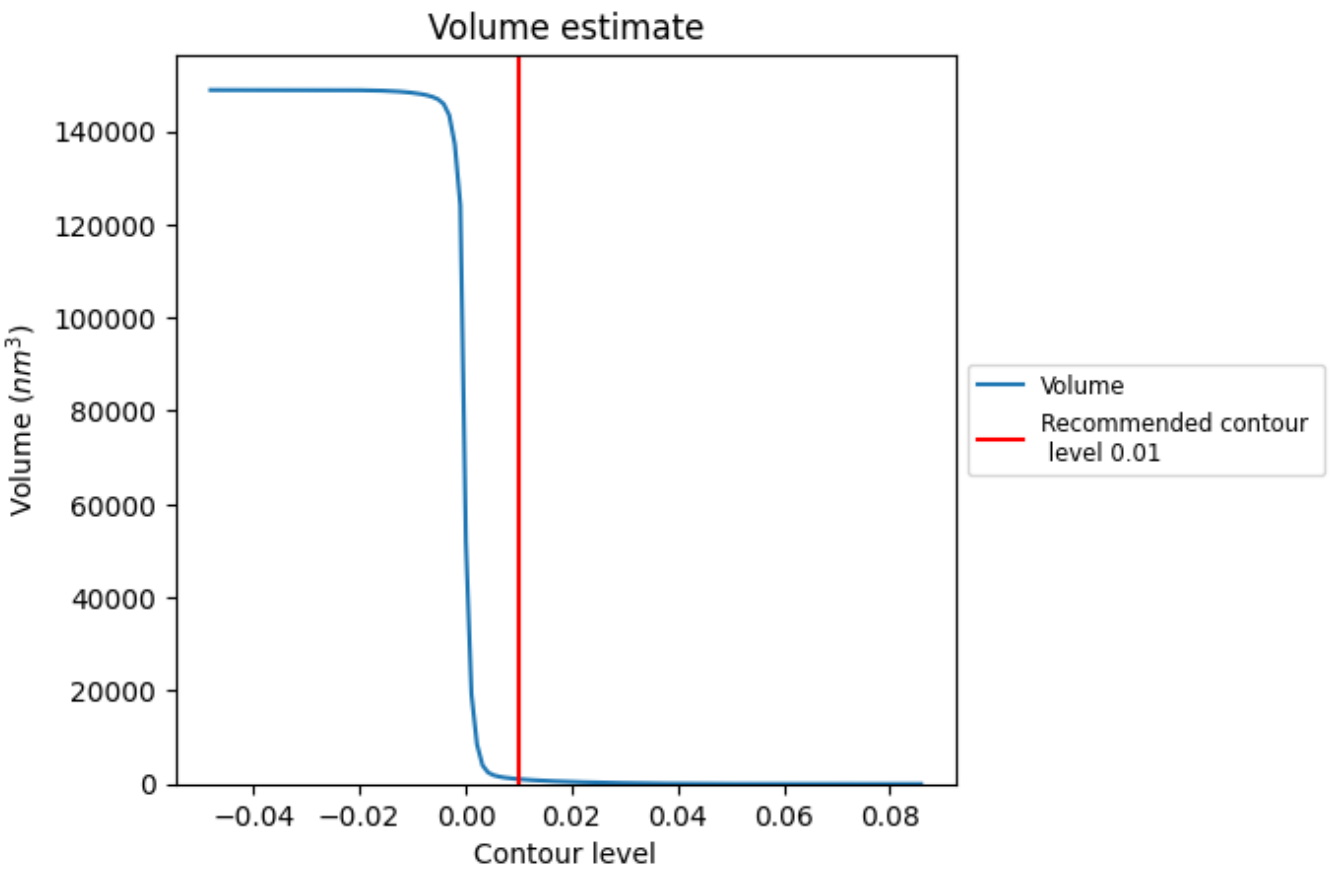
This section contains the results of statistical analysis of the map.

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.

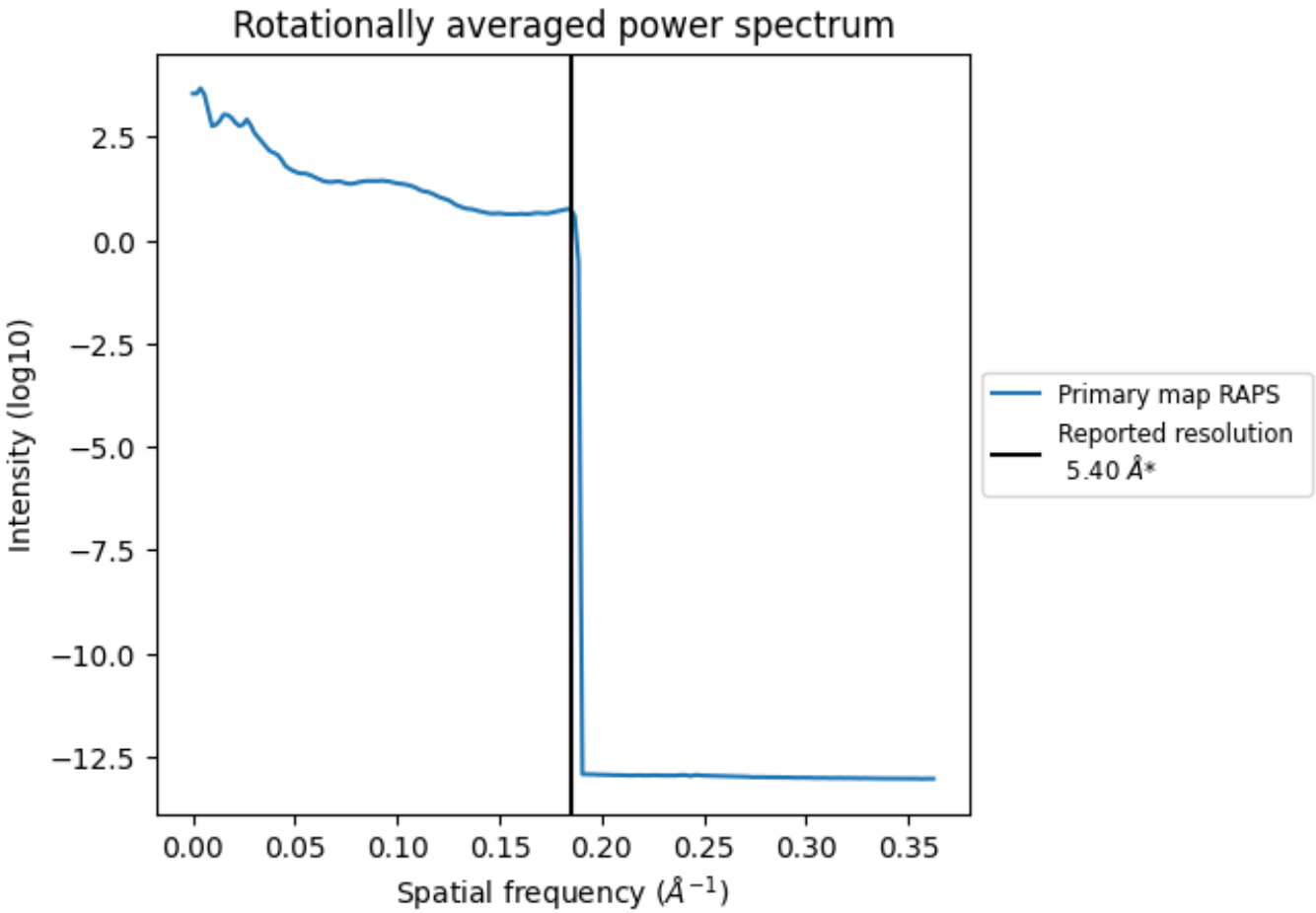
7.2 Volume estimate (i)



The volume at the recommended contour level is 1039 nm^3; this corresponds to an approximate mass of 938 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 0.185 Å^{-1}

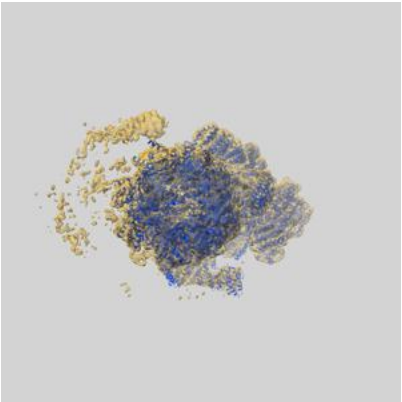
8 Fourier-Shell correlation (i)

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

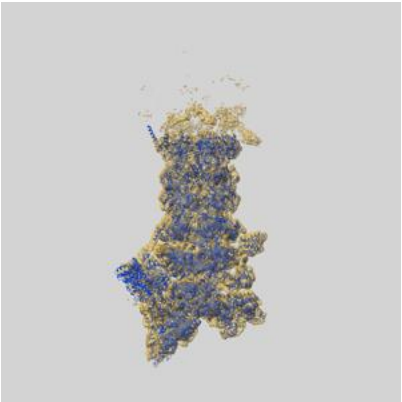
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4321 and PDB model 6FVV. Per-residue inclusion information can be found in section 3 on page 13.

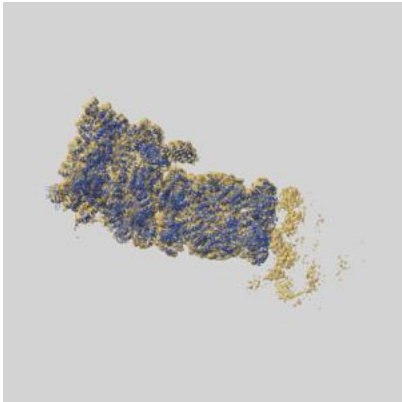
9.1 Map-model overlay (i)



X



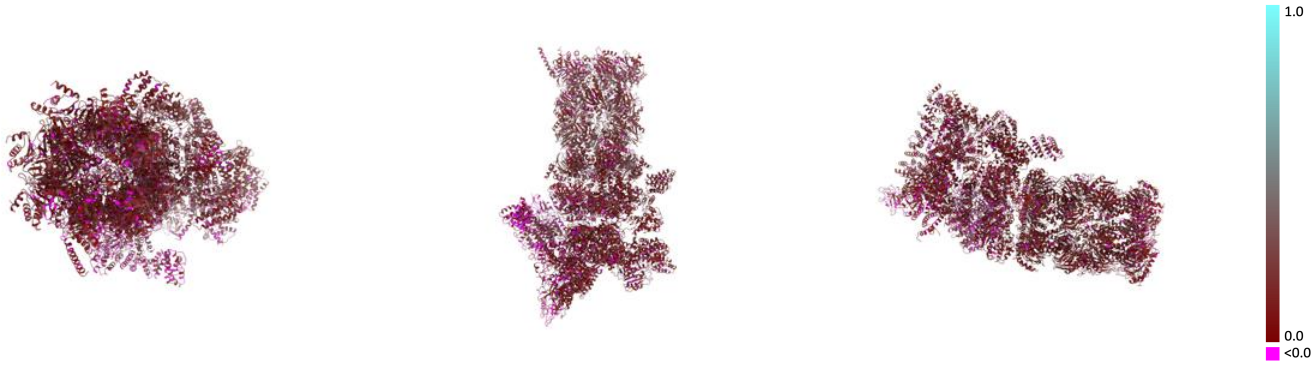
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

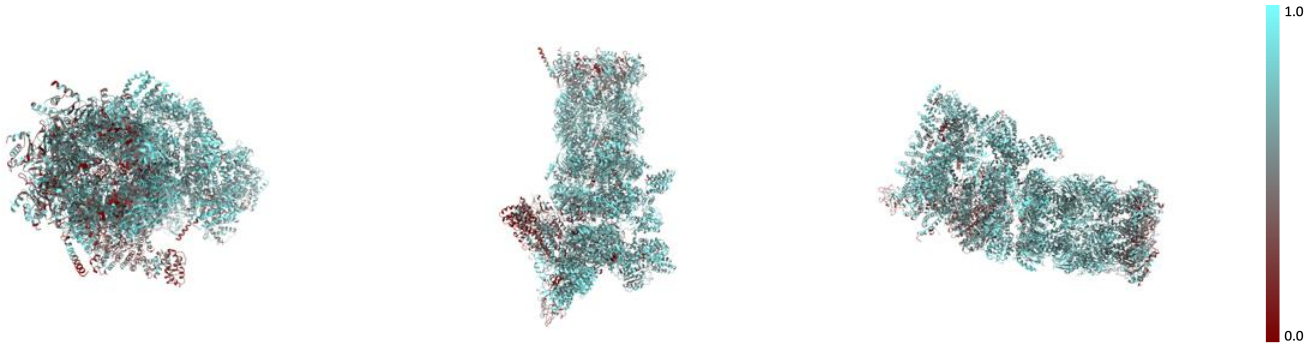
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

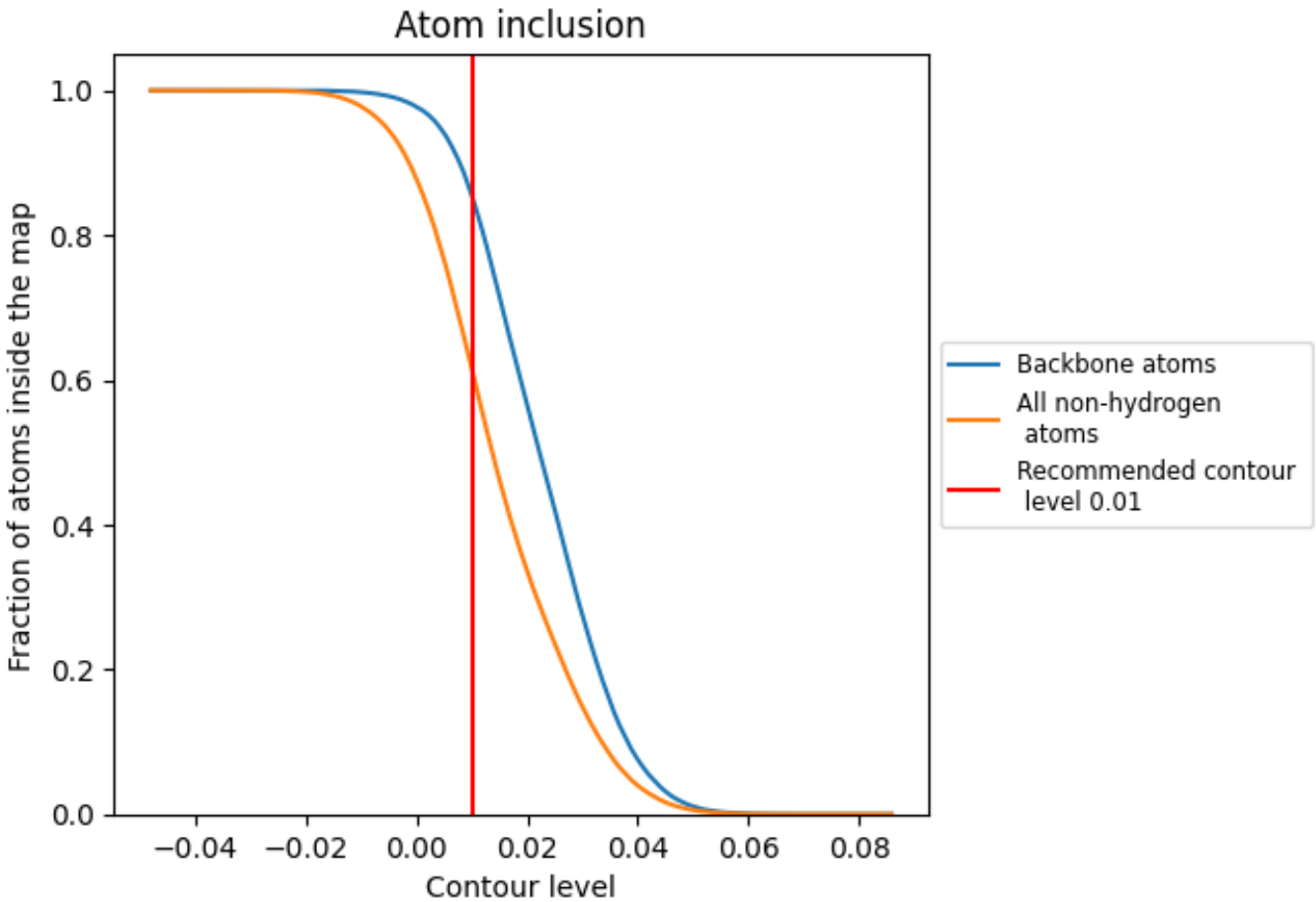
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 61% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6137	0.1490
1	0.7305	0.1860
2	0.7209	0.1970
3	0.6851	0.1880
4	0.7142	0.1830
5	0.7396	0.1850
6	0.7096	0.1840
7	0.7228	0.1830
A	0.7003	0.1800
B	0.6814	0.1950
C	0.6883	0.1850
D	0.7001	0.1870
E	0.6742	0.1750
F	0.7096	0.1830
G	0.7101	0.1820
H	0.5848	0.1240
I	0.5764	0.1380
J	0.5794	0.1250
K	0.5986	0.1410
L	0.6451	0.1490
M	0.5988	0.1300
N	0.6509	0.1540
O	0.6891	0.1520
P	0.7388	0.1520
Q	0.6927	0.1450
R	0.6898	0.1450
S	0.6218	0.1380
T	0.6385	0.1340
U	0.6133	0.1490
V	0.6502	0.1610
W	0.6015	0.1360
X	0.2613	0.0510
Y	0.4136	0.0670
Z	0.3348	0.0590
a	0.5005	0.1460

Continued on next page...

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Chain	Atom inclusion	Q-score
b	0.4422	0.1550
c	0.4705	0.1370
d	0.4515	0.1300
e	0.4498	0.1420
f	0.5227	0.1570
g	0.5167	0.1430
h	0.6954	0.1650
i	0.6779	0.1790
j	0.6600	0.1750
k	0.6763	0.1760
l	0.6874	0.1680
m	0.6527	0.1690
n	0.6639	0.1710