



## Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 10:04 AM JST

PDB ID : 5GJR  
EMDB ID : EMD-9512  
Title : An atomic structure of the human 26S proteasome  
Authors : Huang, X.L.; Luan, B.; Wu, J.P.; Shi, Y.G.  
Deposited on : 2016-07-01  
Resolution : 3.50 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

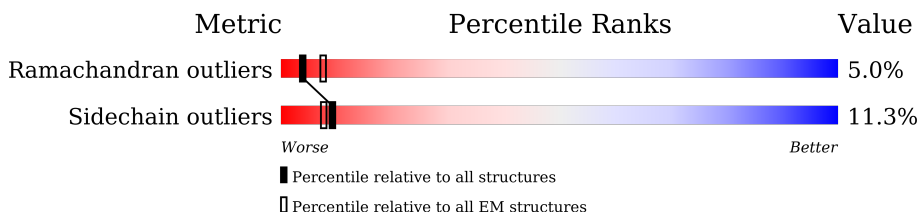
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	I	440	
1	w	440	
2	H	433	
2	v	433	
3	L	389	
3	z	389	
4	0	439	
4	M	439	
5	J	406	

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Mol	Chain	Length	Quality of chain
5	x	406	66% 19% 12% 6%
6	K	418	67% 22% 9% 6%
6	y	418	67% 22% 9% 6%
7	1	953	80% 5% 14% 40%
7	N	953	80% 5% 14% 40%
8	2	376	89% 9% 9% 54%
8	O	376	89% 9% 9% 54%
9	3	456	83% 7% 9% 22%
9	P	456	83% 7% 9% 22%
10	4	422	83% 14% 9% 33%
10	Q	422	83% 14% 9% 33%
11	5	389	82% 13% 9% 11%
11	R	389	83% 13% 9% 11%
12	6	525	75% 5% 20% 31%
12	S	525	75% 5% 20% 30%
13	7	350	64% 8% 26% 48%
13	T	350	64% 8% 26% 48%
14	8	324	76% 10% 13% 21%
14	U	324	76% 10% 13% 21%
15	9	310	70% 11% 17% 20%
15	V	310	70% 11% 17% 20%
16	AA	377	45% 6% 49% 50%
16	W	377	44% 6% 49% 50%
17	AB	70	69% 16% 16% 51%
17	Y	70	69% 16% 16% 51%


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Mol	Chain	Length	Quality of chain
18	AC	908	77% 75% 6% 19%
18	Z	908	77% 75% 6% 19%
19	B	246	92% 7%
19	h	246	94% 5%
20	C	234	95%
20	i	234	91% 7%
21	D	261	91% 5%
21	j	261	91%
22	E	248	91% 7%
22	k	248	92% 6%
23	F	241	94%
23	l	241	93%
24	G	263	87% 10%
24	m	263	85% 5% 10%
25	X	255	91% 5%
25	n	255	91% 5% 5%
26	a	239	82% 15%
26	o	239	82% 15%
27	b	277	75% 21%
27	p	277	76% 21%
28	c	205	94% 5%
28	q	205	94% 5%
29	d	201	96%
29	r	201	96%
30	e	263	75% 24%

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Mol	Chain	Length	Quality of chain
30	s	263	 <p>74% 24%</p>
31	f	241	 <p>85% 12%</p>
31	t	241	 <p>85% 12%</p>
32	g	264	 <p>77% 5% 18%</p>
32	u	264	 <p>77% 5% 18%</p>

## 2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 142753 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 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	I	359	2720	1708	465	535	12	0	0
1	w	359	2720	1708	465	535	12	0	0

- Molecule 2 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H	380	2893	1817	515	543	18	0	0
2	v	380	2893	1817	515	543	18	0	0

- Molecule 3 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	L	375	2860	1796	512	536	16	0	0
3	z	375	2860	1796	512	536	16	0	0

- Molecule 4 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	M	376	2858	1802	496	545	15	0	0
4	0	376	2858	1802	496	545	15	0	0

- Molecule 5 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	J	358	2820	1780	506	518	16	0	0
5	x	358	2820	1780	506	518	16	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	K	380	3039	1923	524	579	13	0	0
6	y	380	3039	1923	524	579	13	0	0

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	821	5449	3491	931	1009	18	0	0
7	1	821	5449	3491	931	1009	18	0	0

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	372	2369	1515	405	438	11	0	0
8	2	372	2375	1521	405	438	11	0	0

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	P	413	2832	1821	489	516	6	0	0
9	3	413	2831	1820	489	516	6	0	0

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	Q	421	2956	1866	512	569	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	4	421	Total	C	N	O	S	0	0
			2956	1866	512	569	9		

- Molecule 11 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	376	Total	C	N	O	S	0	0
			2767	1794	461	504	8		
11	5	376	Total	C	N	O	S	0	0
			2770	1796	461	504	9		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	S	421	Total	C	N	O	S	0	0
			2723	1737	484	499	3		
12	6	421	Total	C	N	O	S	0	0
			2732	1741	487	501	3		

- Molecule 13 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	T	258	Total	C	N	O	S	0	0
			1699	1099	280	315	5		
13	7	258	Total	C	N	O	S	0	0
			1699	1099	280	315	5		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	283	Total	C	N	O	S	0	0
			2131	1370	369	388	4		
14	8	283	Total	C	N	O	S	0	0
			2131	1370	369	388	4		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	257	Total	C	N	O	S	0	0
			2011	1276	341	377	17		
15	9	257	Total	C	N	O	S	0	0
			2009	1274	341	377	17		



- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	193	Total	C	N	O	S	0	0
			1300	818	228	250	4		
16	AA	193	Total	C	N	O	S	0	0
			1300	818	228	250	4		

- Molecule 17 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Y	59	Total	C	N	O	0	0
			316	191	60	65		
17	AB	59	Total	C	N	O	0	0
			316	191	60	65		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Z	732	Total	C	N	O	0	0
			3608	2144	732	732		
18	AC	732	Total	C	N	O	0	0
			3608	2144	732	732		

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	B	244	Total	C	N	O	S	0	0
			1845	1171	309	352	13		
19	h	244	Total	C	N	O	S	0	0
			1853	1177	311	352	13		

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	C	231	Total	C	N	O	S	0	0
			1737	1106	289	336	6		
20	i	231	Total	C	N	O	S	0	0
			1744	1112	290	336	6		

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	D	250	Total	C	N	O	S	0	0
			1916	1206	330	372	8		
21	j	250	Total	C	N	O	S	0	0
			1913	1203	330	372	8		

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	E	243	Total	C	N	O	S	0	0
			1724	1068	312	339	5		
22	k	243	Total	C	N	O	S	0	0
			1691	1051	309	327	4		

- Molecule 23 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	F	234	Total	C	N	O	S	0	0
			1766	1108	290	357	11		
23	l	234	Total	C	N	O	S	0	0
			1726	1107	291	317	11		

- Molecule 24 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	G	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
24	m	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	243	Total	C	N	O	S	0	0
			1873	1189	317	356	11		
25	n	243	Total	C	N	O	S	0	0
			1873	1189	317	356	11		

- Molecule 26 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	o	202	Total	C	N	O	S	0	0
			1509	945	258	294	12		

- Molecule 27 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
27	p	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 28 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
28	q	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 29 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
29	r	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 30 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
30	s	201	Total	C	N	O	S	0	0
			1551	977	273	292	9		

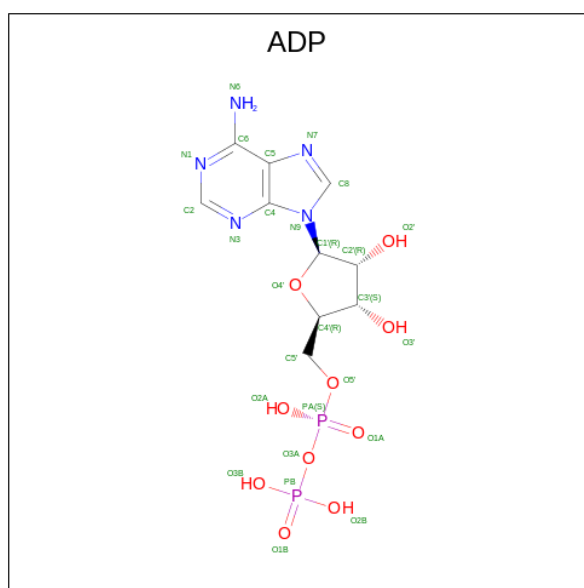
- Molecule 31 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		
31	t	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

- Molecule 32 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	g	216	Total 1672	C 1055	N 286	O 319	S 12	0	0
32	u	217	Total 1678	C 1058	N 290	O 318	S 12	0	0

- Molecule 33 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	
33	I	1	Total 27	C 10	N 5	O 10	P 2	0
33	H	1	Total 27	C 10	N 5	O 10	P 2	0
33	L	1	Total 27	C 10	N 5	O 10	P 2	0
33	M	1	Total 27	C 10	N 5	O 10	P 2	0
33	J	1	Total 27	C 10	N 5	O 10	P 2	0
33	K	1	Total 27	C 10	N 5	O 10	P 2	0
33	v	1	Total 27	C 10	N 5	O 10	P 2	0
33	w	1	Total 27	C 10	N 5	O 10	P 2	0

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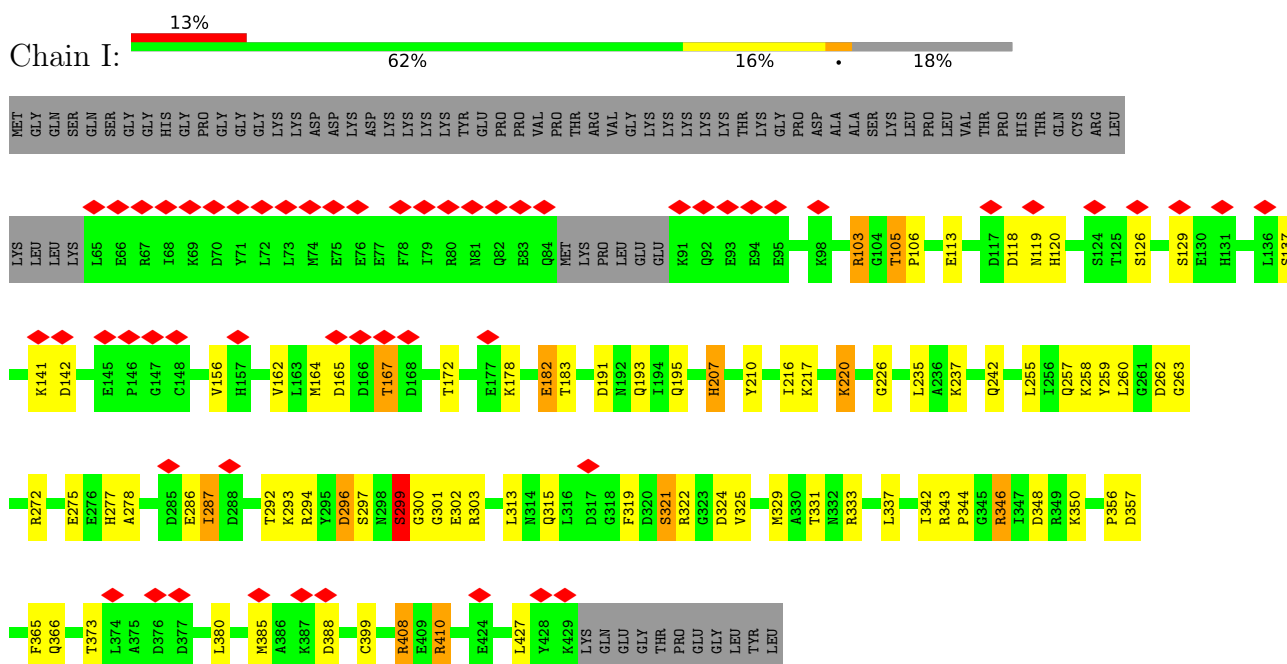
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
33	x	1	Total 27	10	5	10	2	0
33	y	1	Total 27	10	5	10	2	0
33	z	1	Total 27	10	5	10	2	0
33	0	1	Total 27	10	5	10	2	0

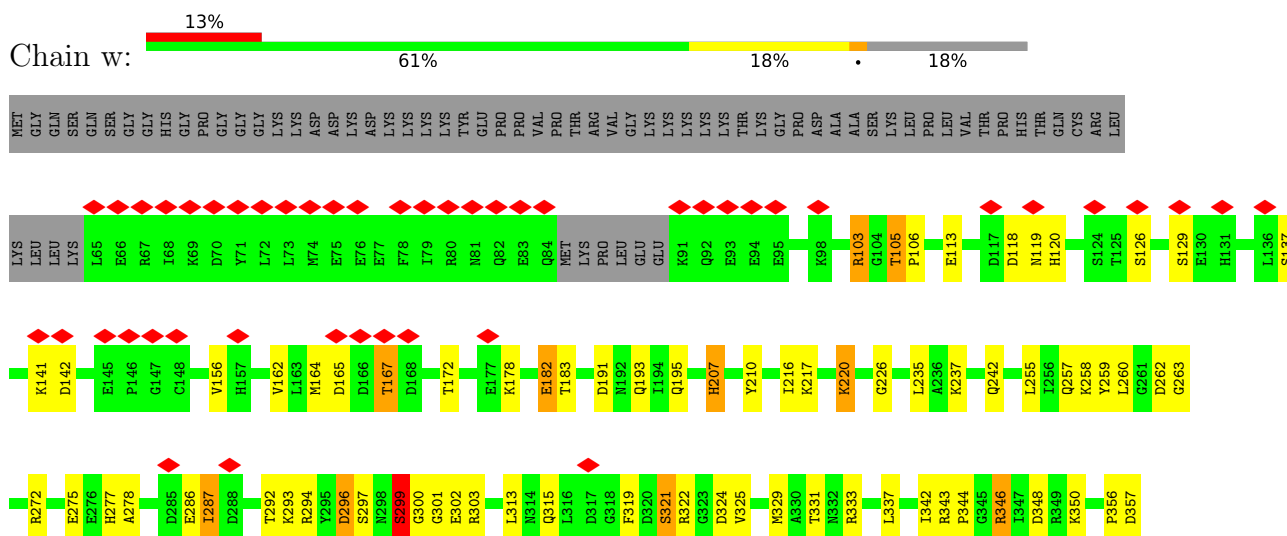
### 3 Residue-property plots i

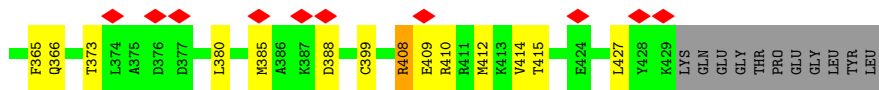
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S protease regulatory subunit 4

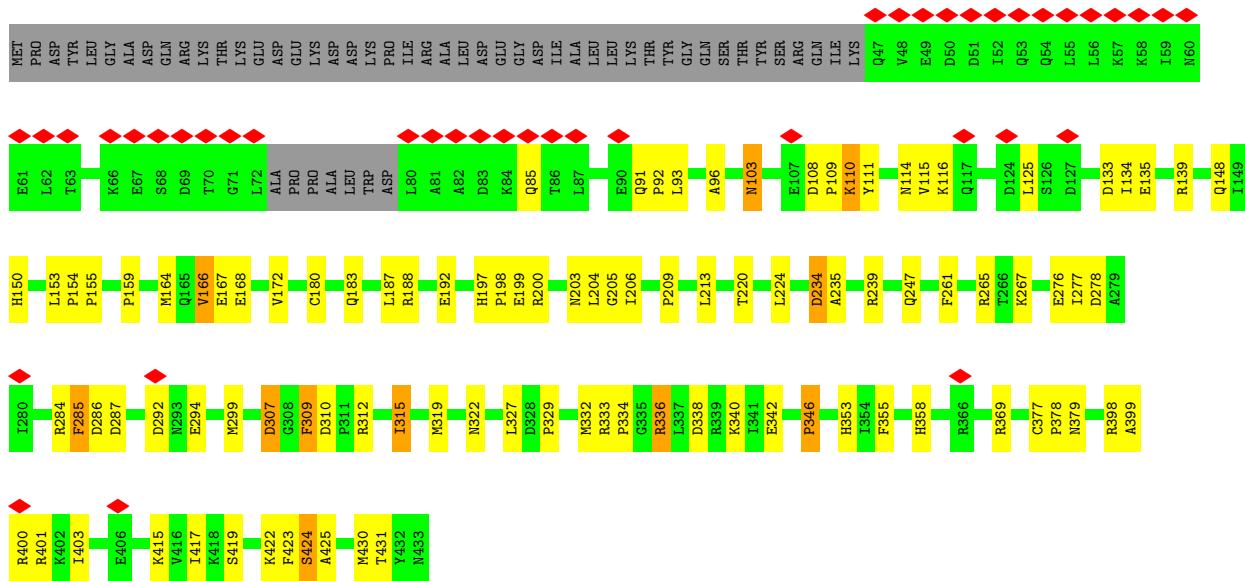


• Molecule 1: 26S protease regulatory subunit 4

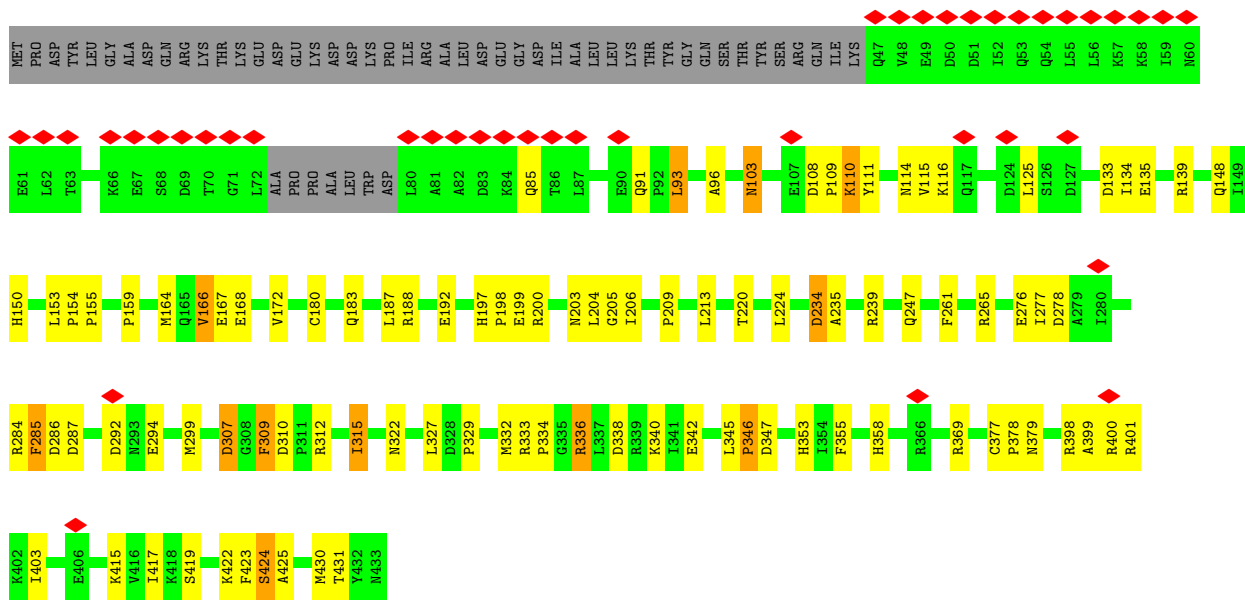




• Molecule 2: 26S protease regulatory subunit 7



• Molecule 2: 26S protease regulatory subunit 7



• Molecule 3: 26S protease regulatory subunit 10B

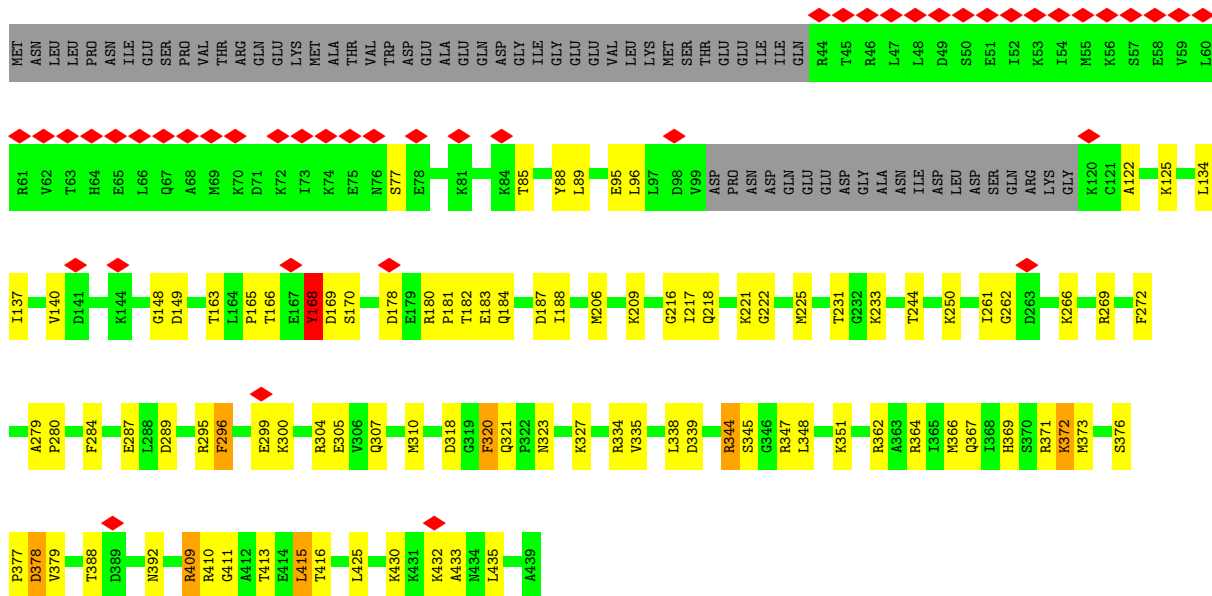




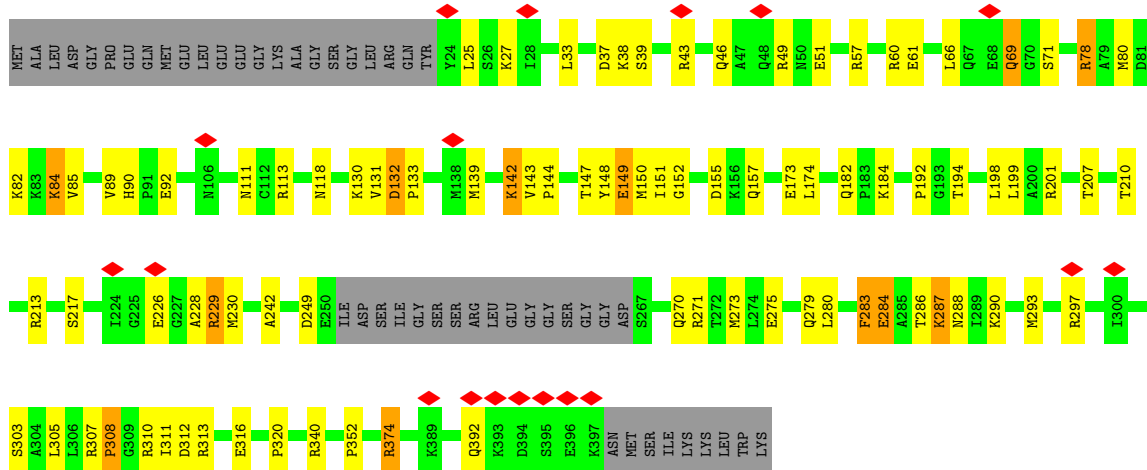




• Molecule 4: 26S protease regulatory subunit 6A

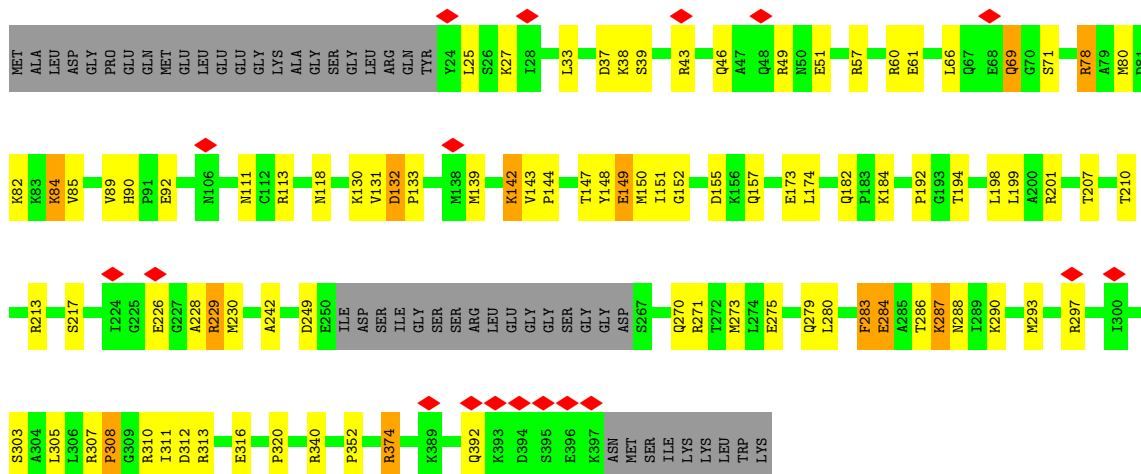


• Molecule 5: 26S protease regulatory subunit 8

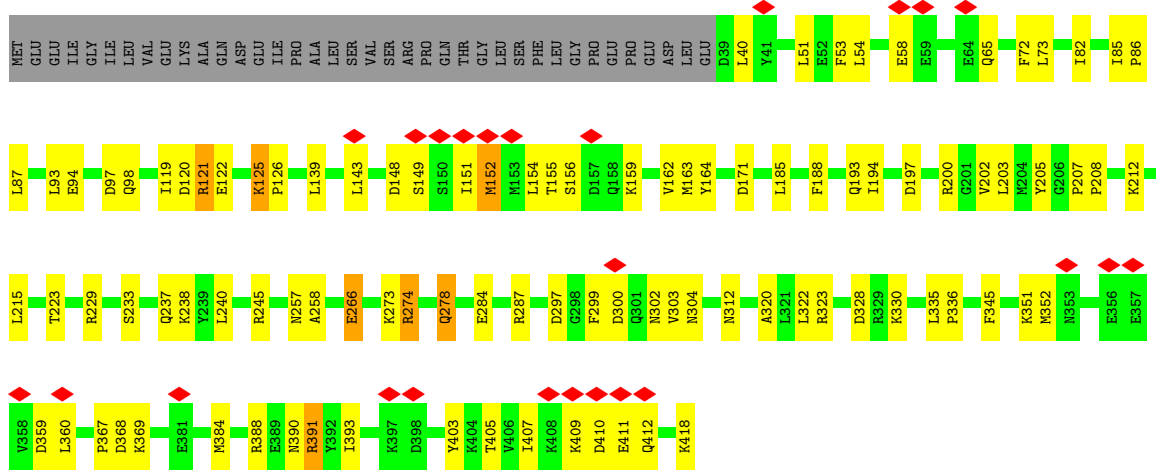


• Molecule 5: 26S protease regulatory subunit 8

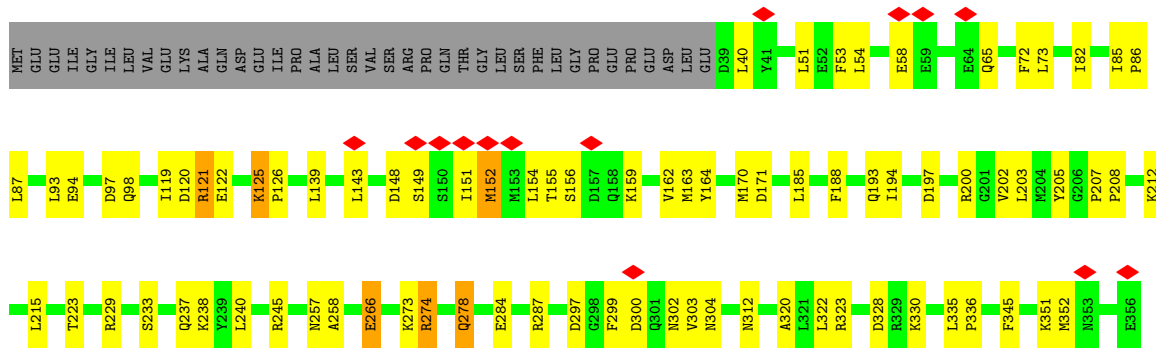


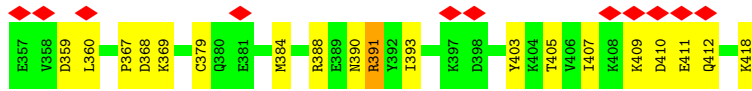


• Molecule 6: 26S protease regulatory subunit 6B

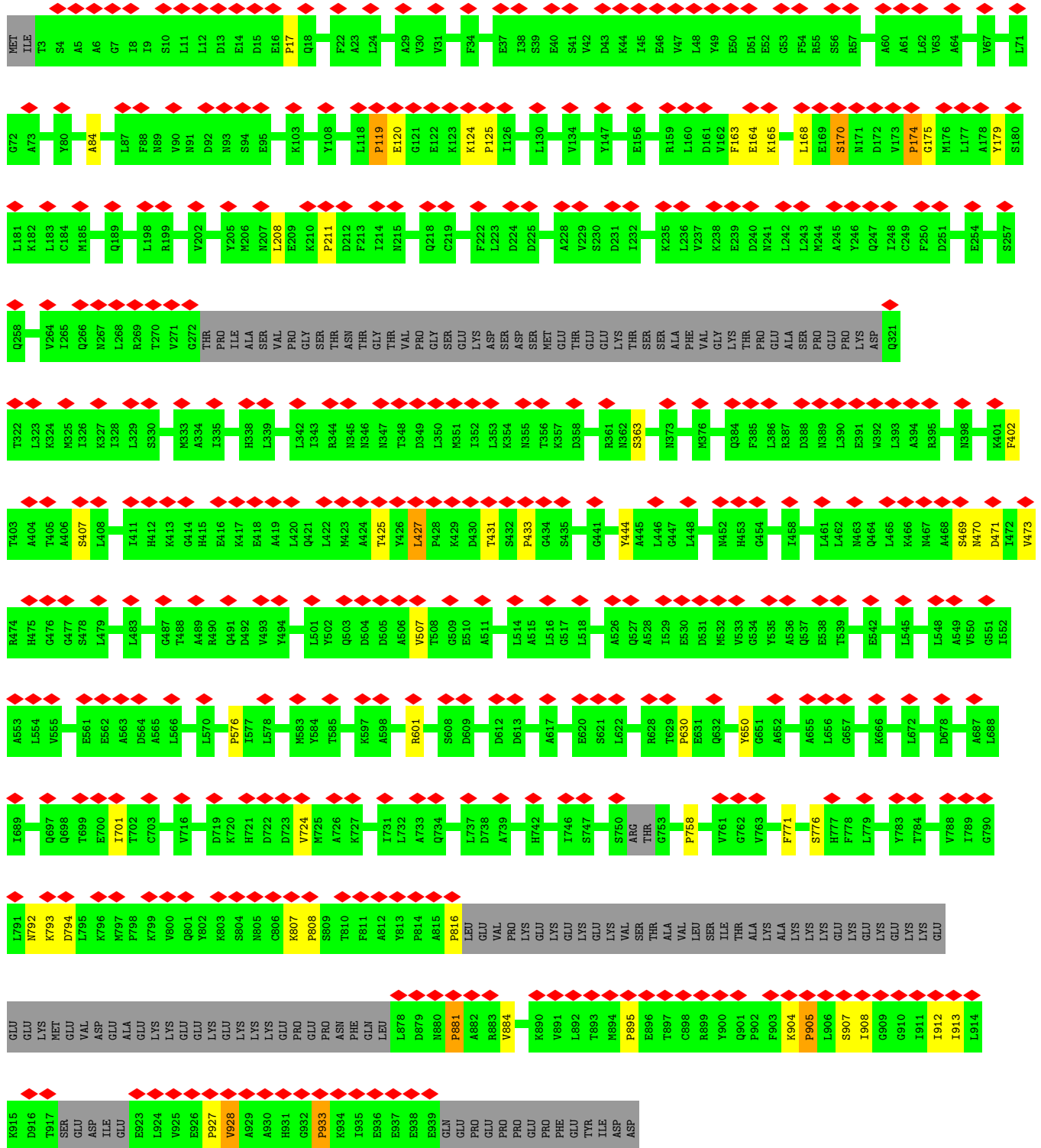
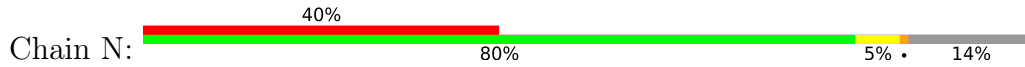


• Molecule 6: 26S protease regulatory subunit 6B

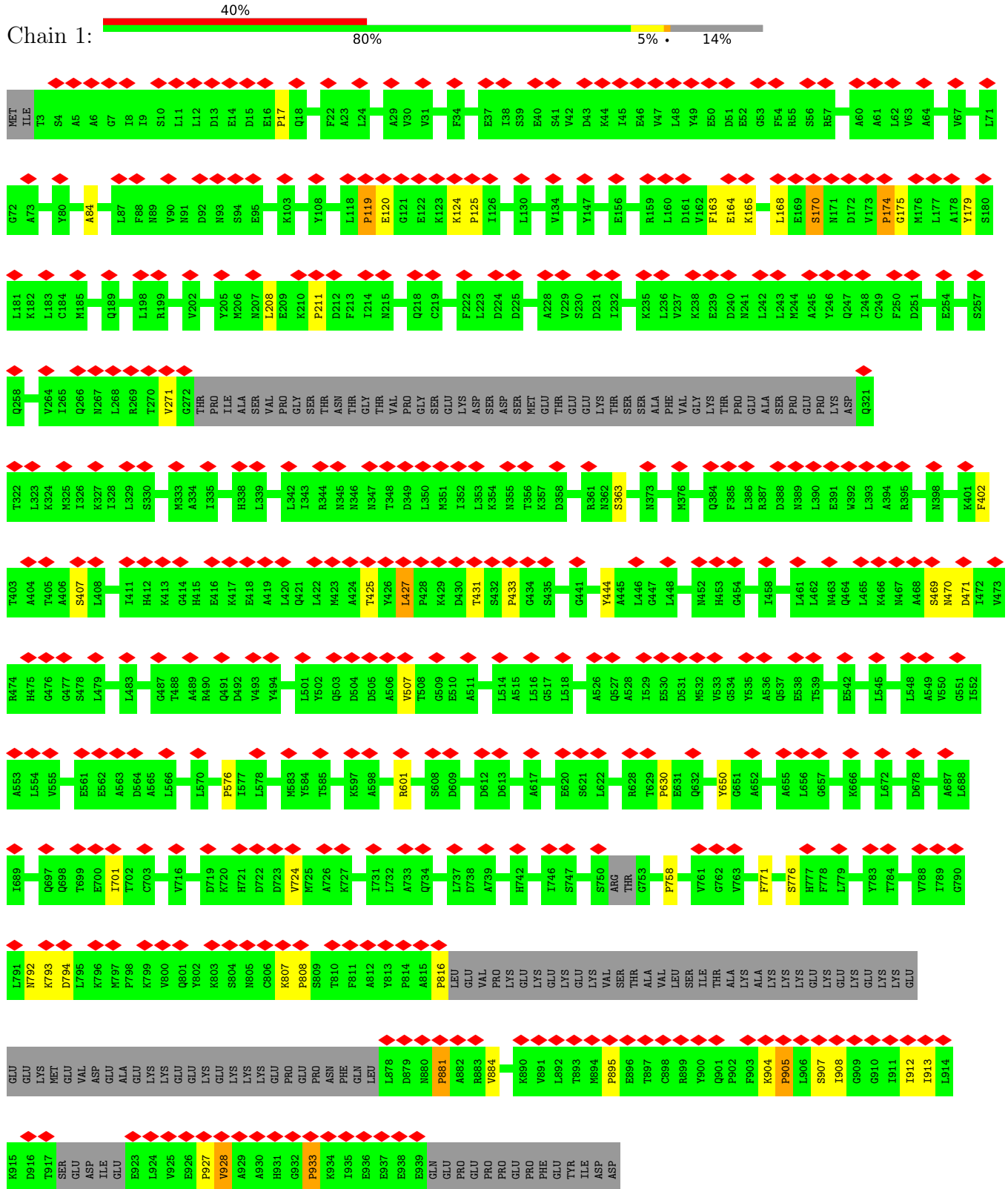




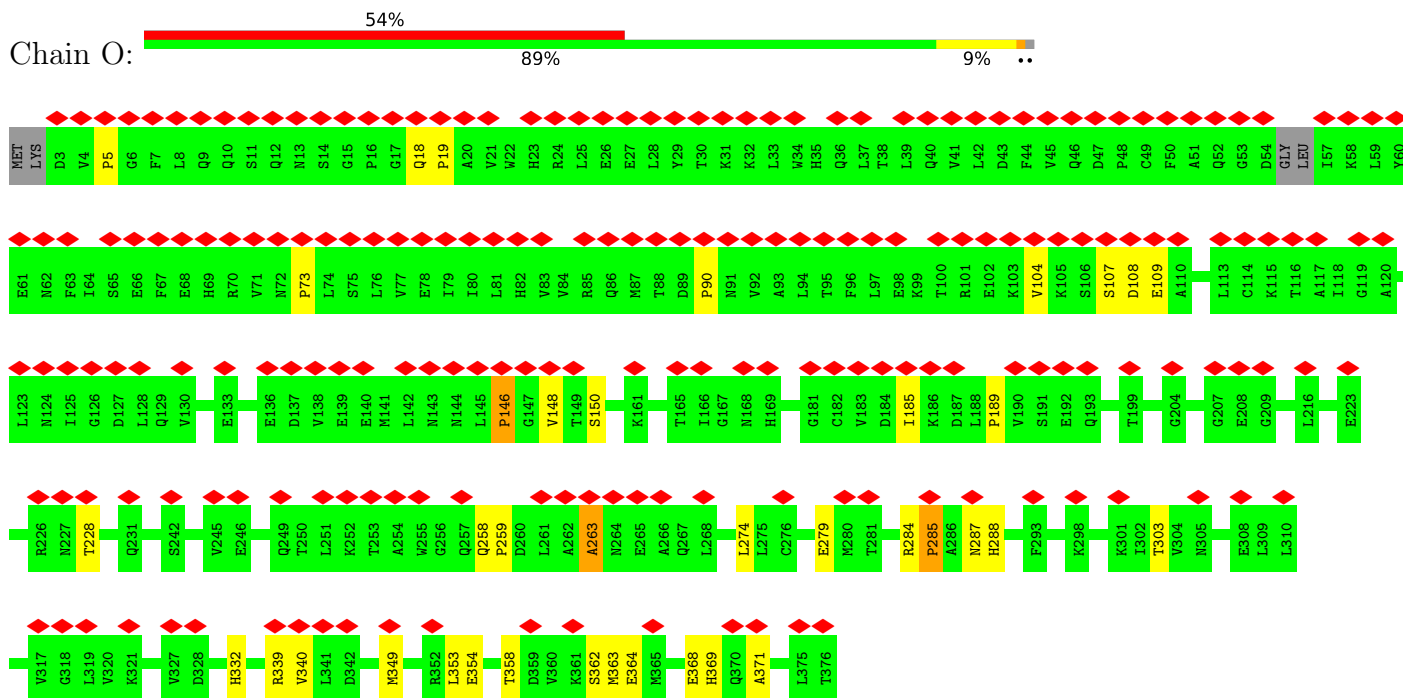
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1



• Molecule 7: 26S proteasome non-ATPase regulatory subunit 1



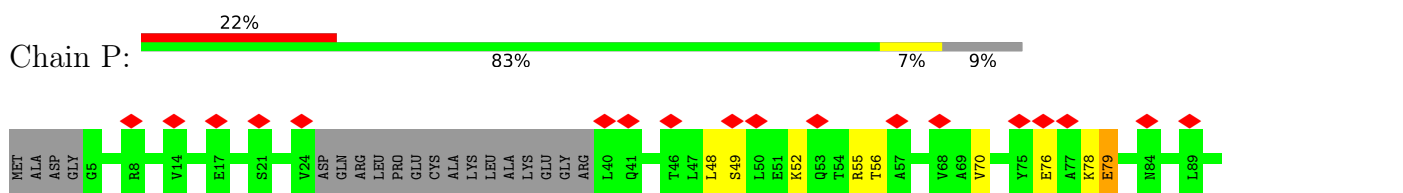
• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

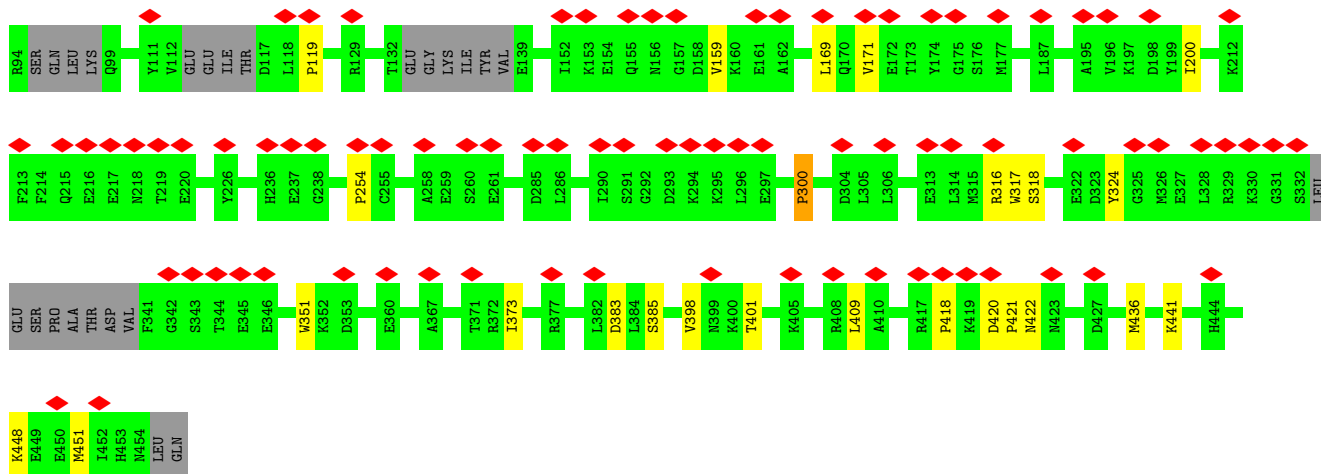


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 13

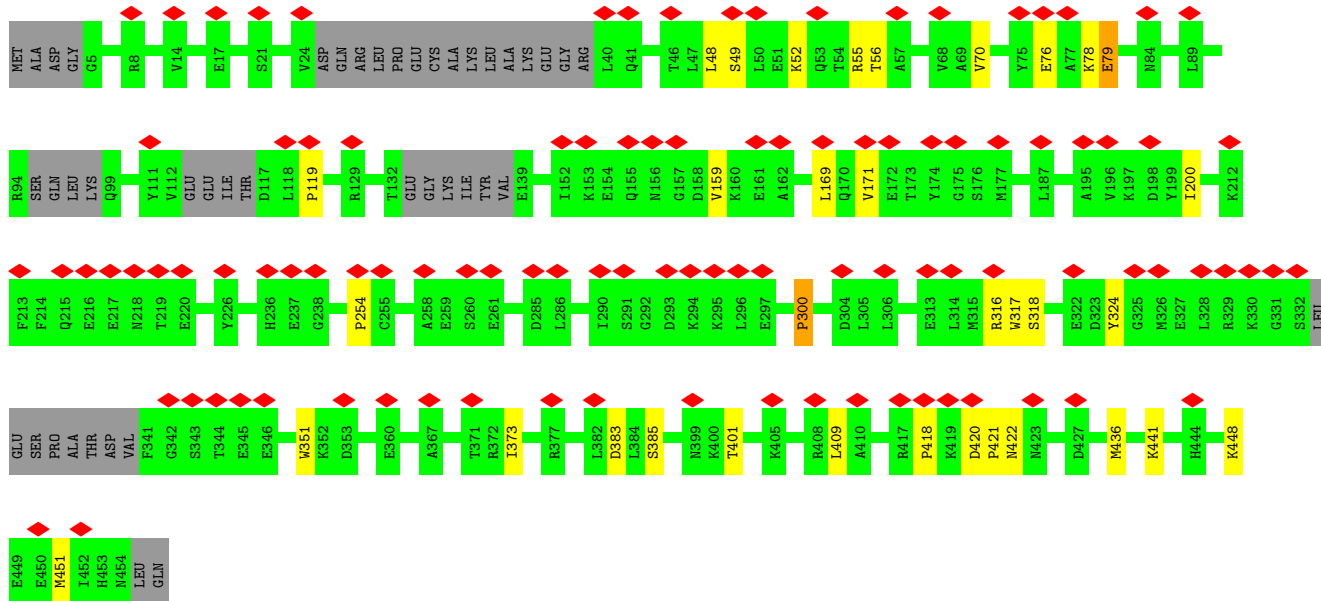
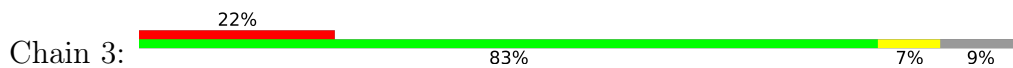


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

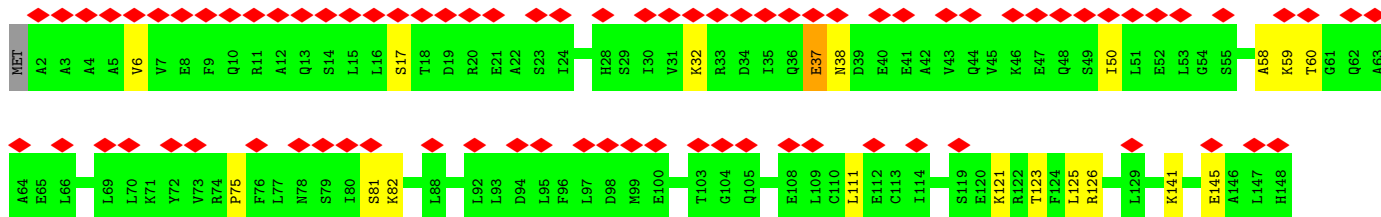
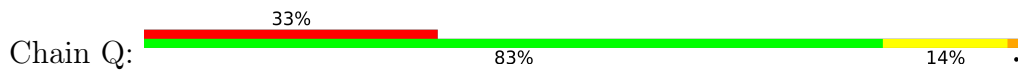


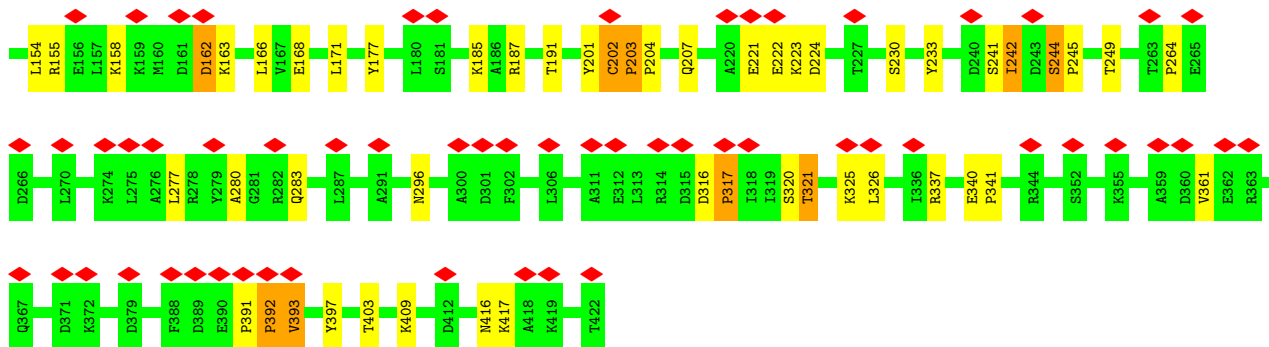


• Molecule 9: 26S proteasome non-ATPase regulatory subunit 12

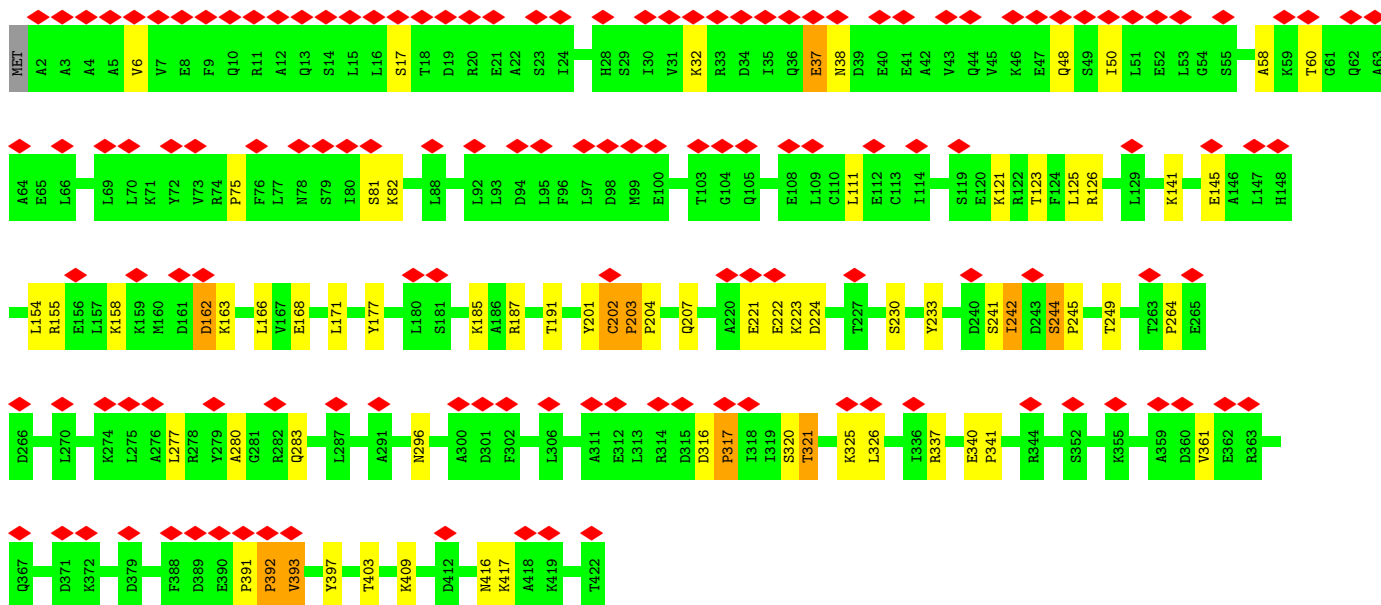
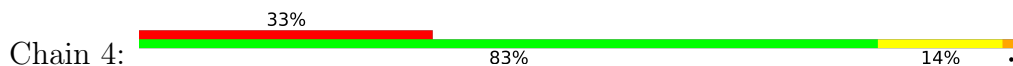


• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11

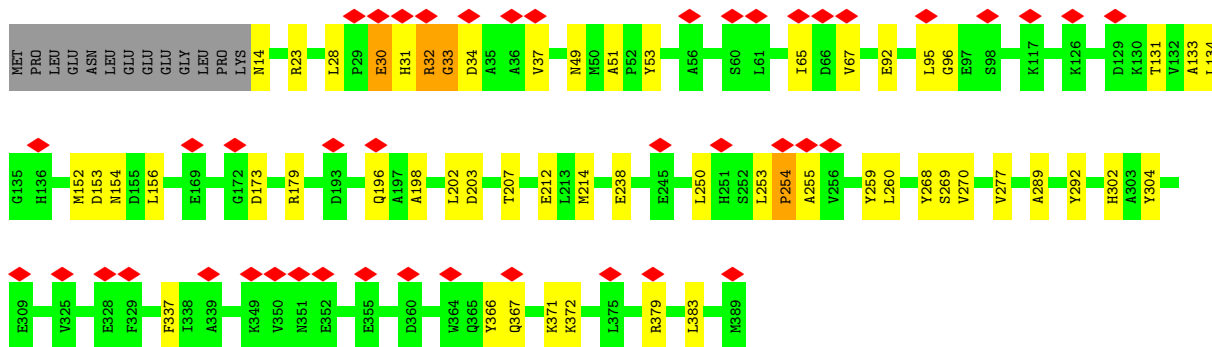
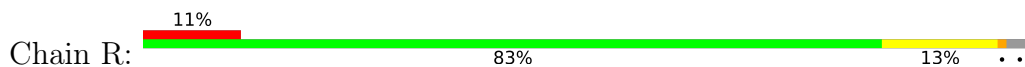




• Molecule 10: 26S proteasome non-ATPase regulatory subunit 11

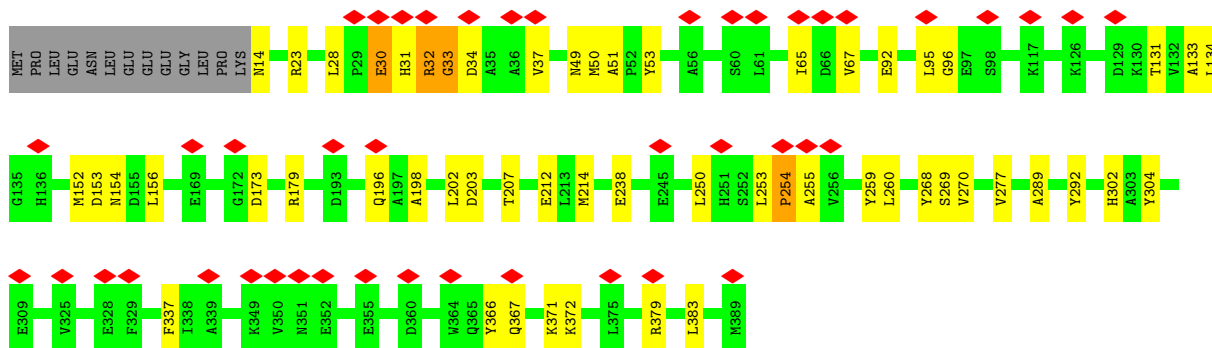


• Molecule 11: 26S proteasome non-ATPase regulatory subunit 6



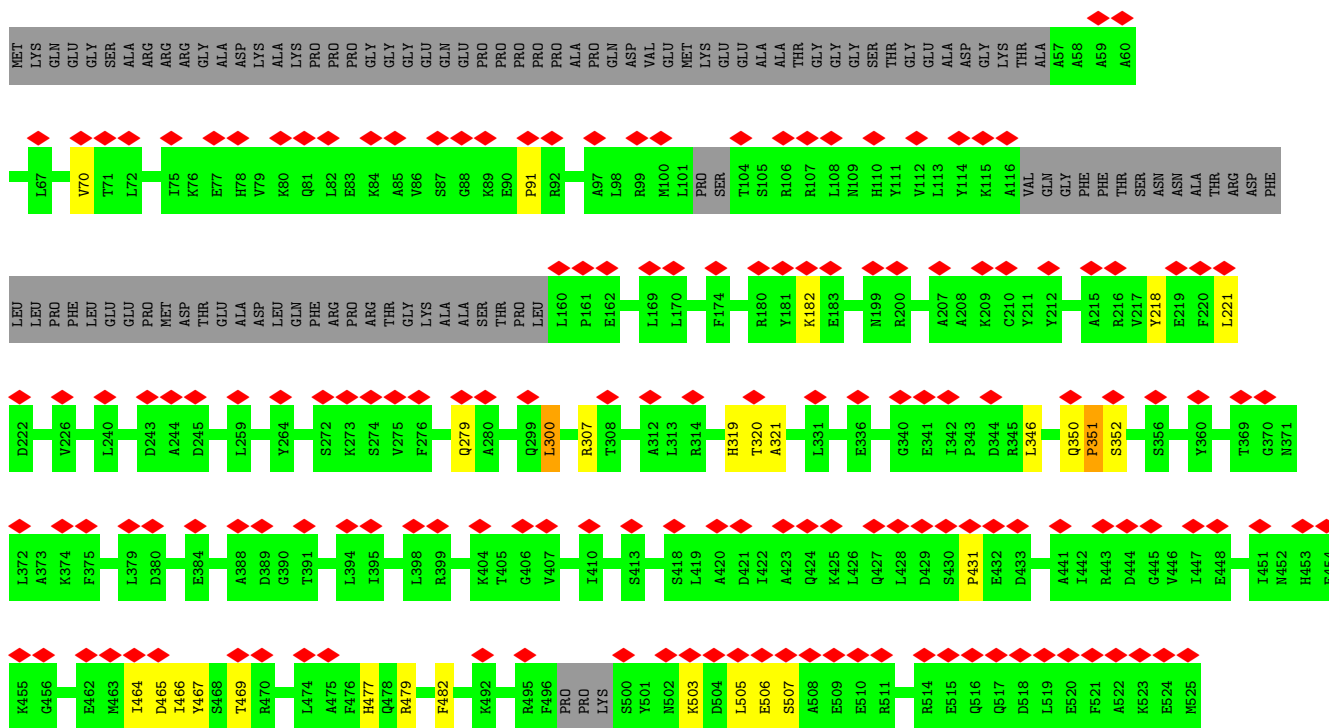
• Molecule 11: 26S proteasome non-ATPase regulatory subunit 6

Chain 5: 11% 82% 13%



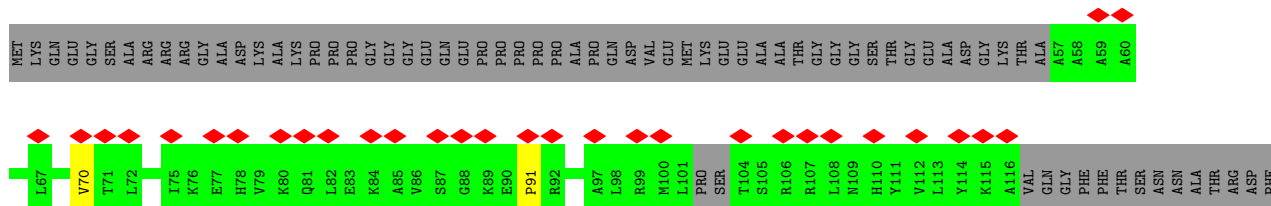
- Molecule 12: 26S proteasome non-ATPase regulatory subunit 3

Chain S: 30% 75% 5% 20%

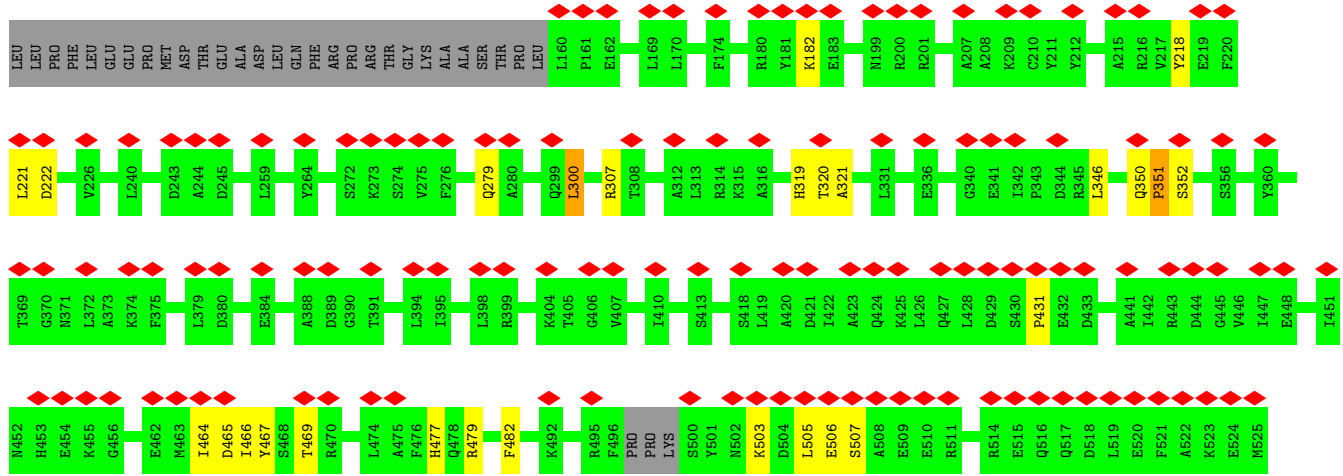


- Molecule 12: 26S proteasome non-ATPase regulatory subunit 3

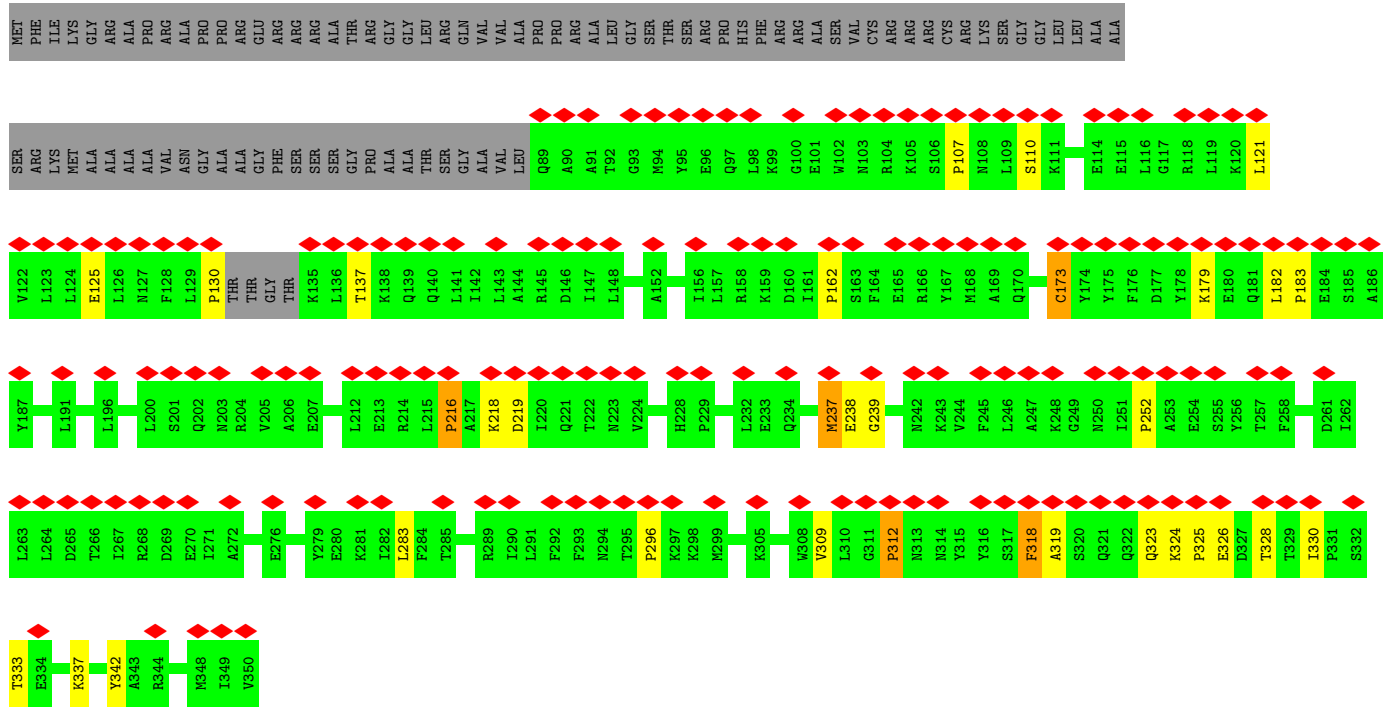
Chain 6: 31% 75% 5% 20%



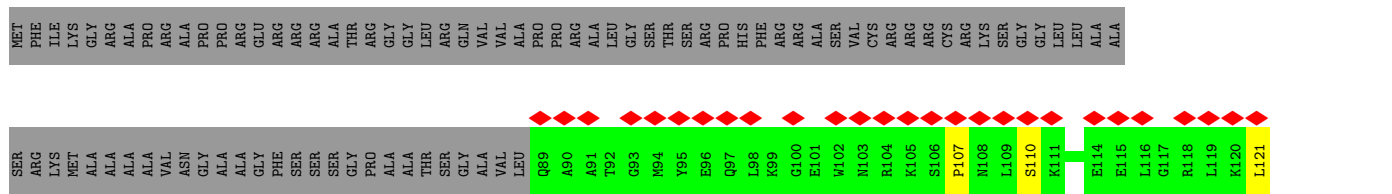


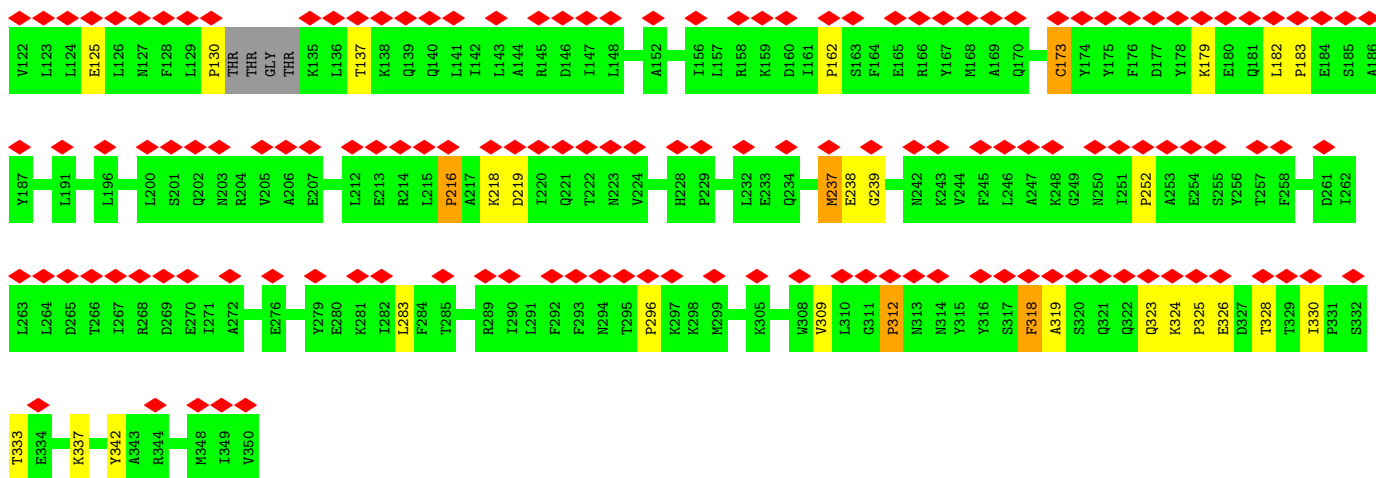


• Molecule 13: 26S proteasome non-ATPase regulatory subunit 8

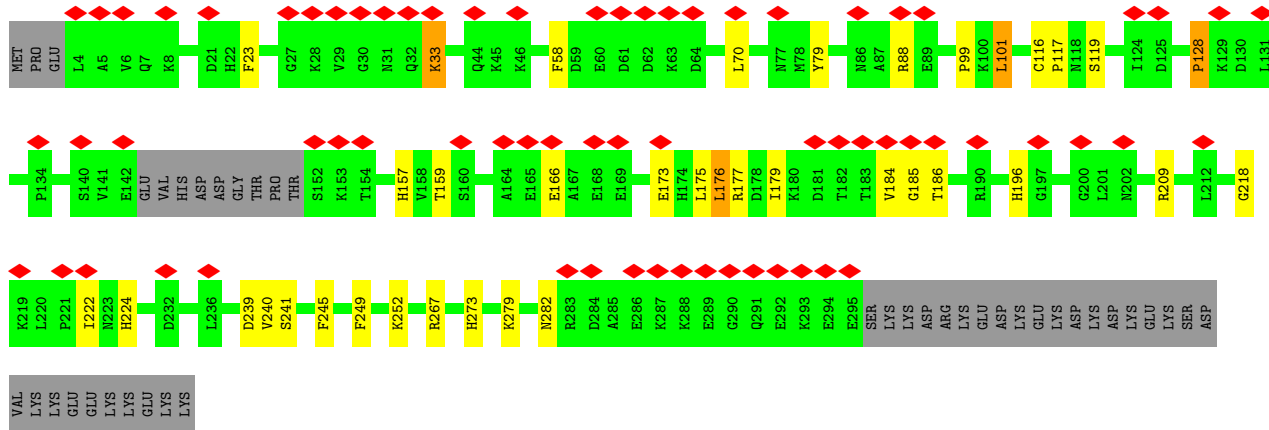
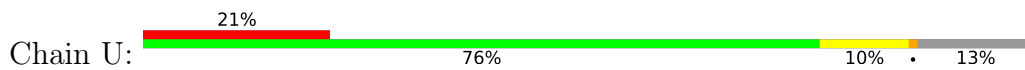


• Molecule 13: 26S proteasome non-ATPase regulatory subunit 8

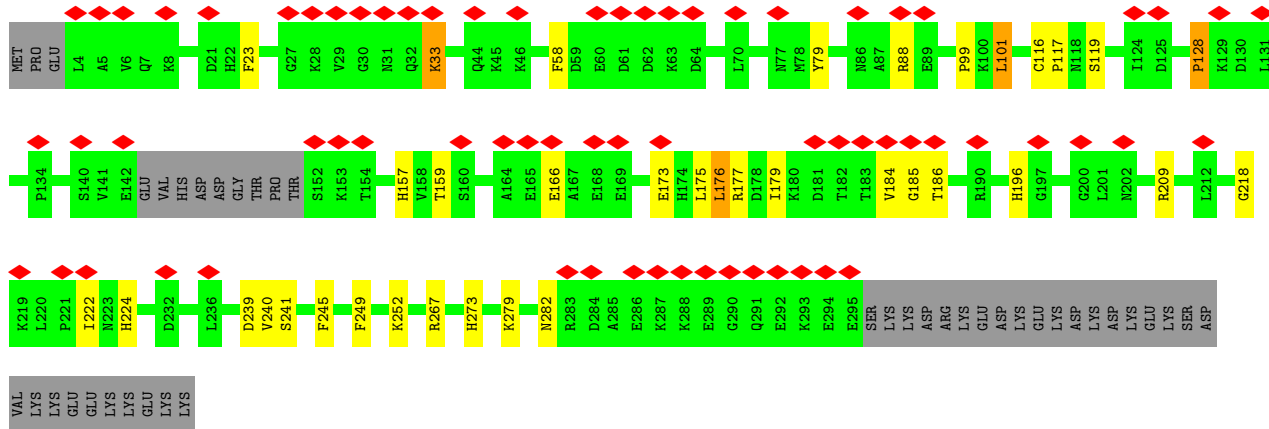
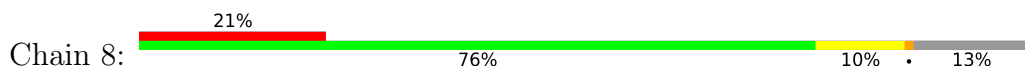




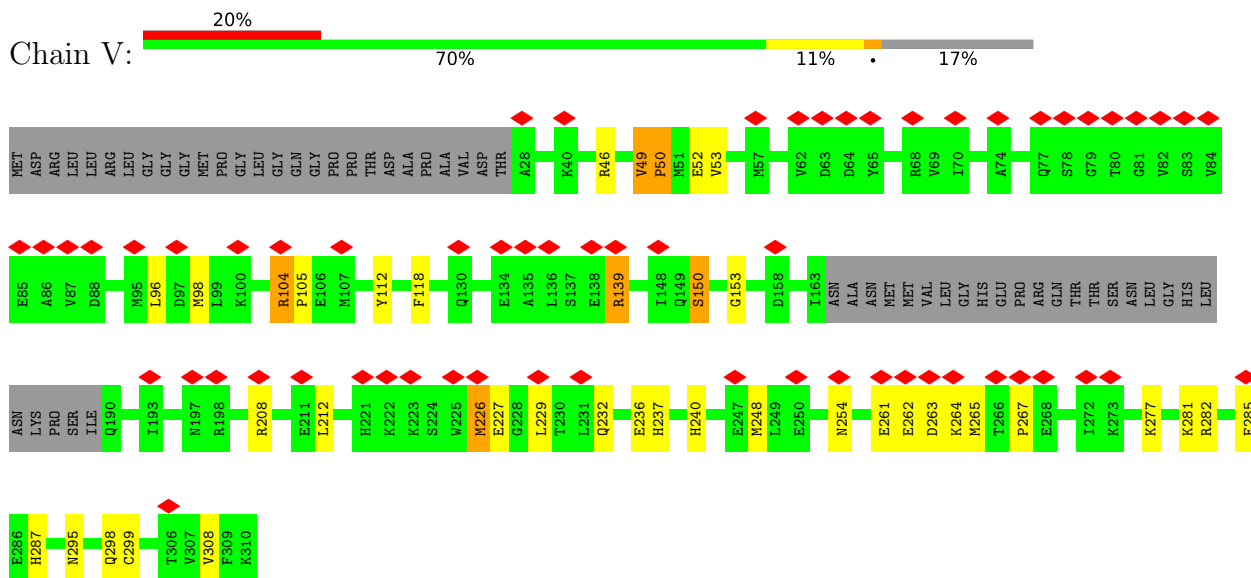
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 7



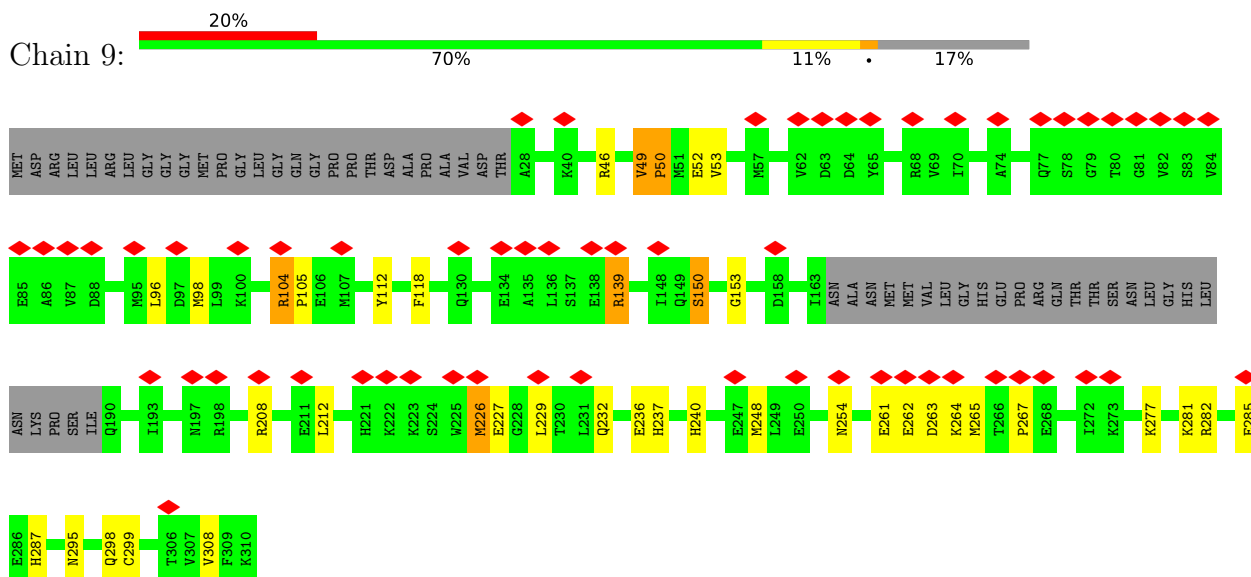
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 7



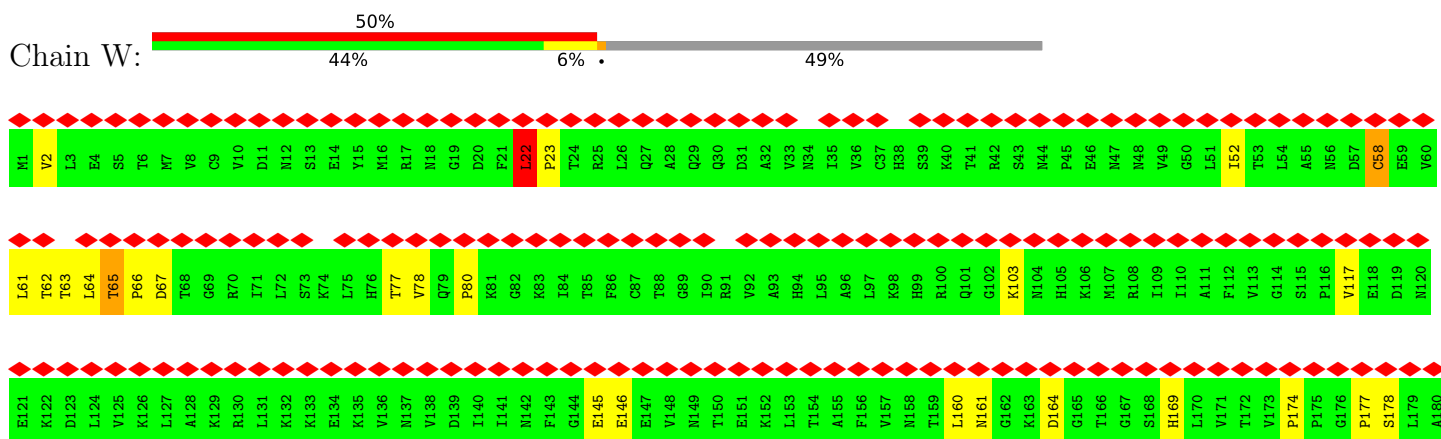
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

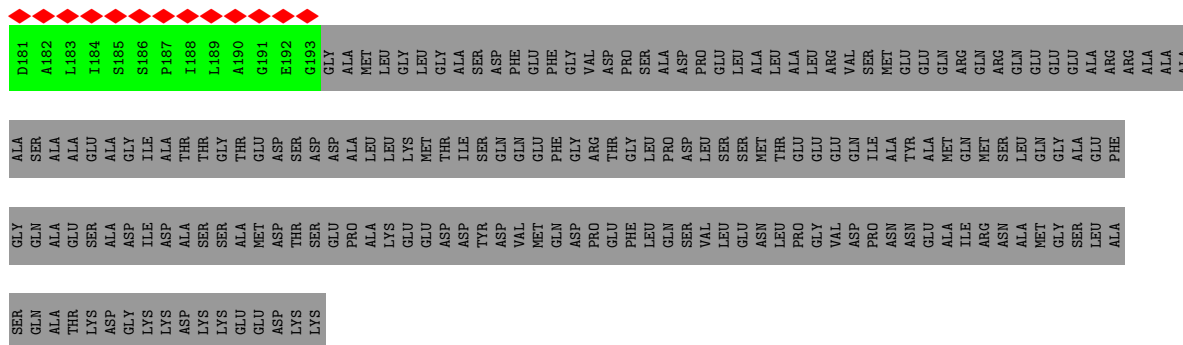


• Molecule 15: 26S proteasome non-ATPase regulatory subunit 14

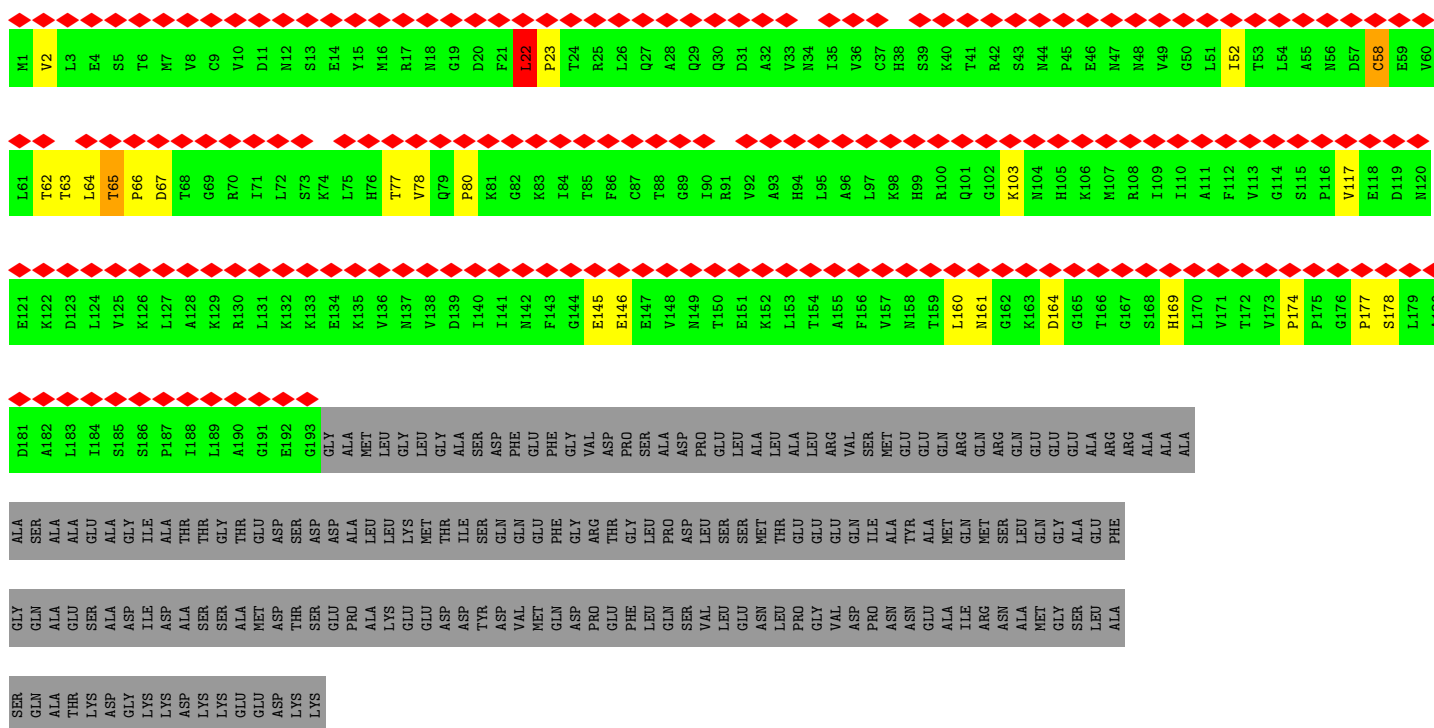


• Molecule 16: 26S proteasome non-ATPase regulatory subunit 4

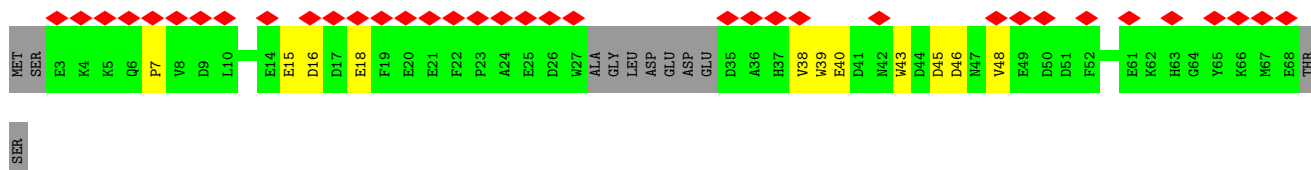




• Molecule 16: 26S proteasome non-ATPase regulatory subunit 4

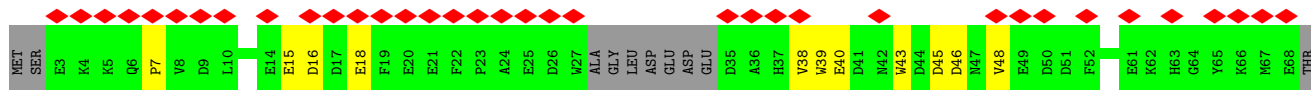


• Molecule 17: 26S proteasome complex subunit DSS1

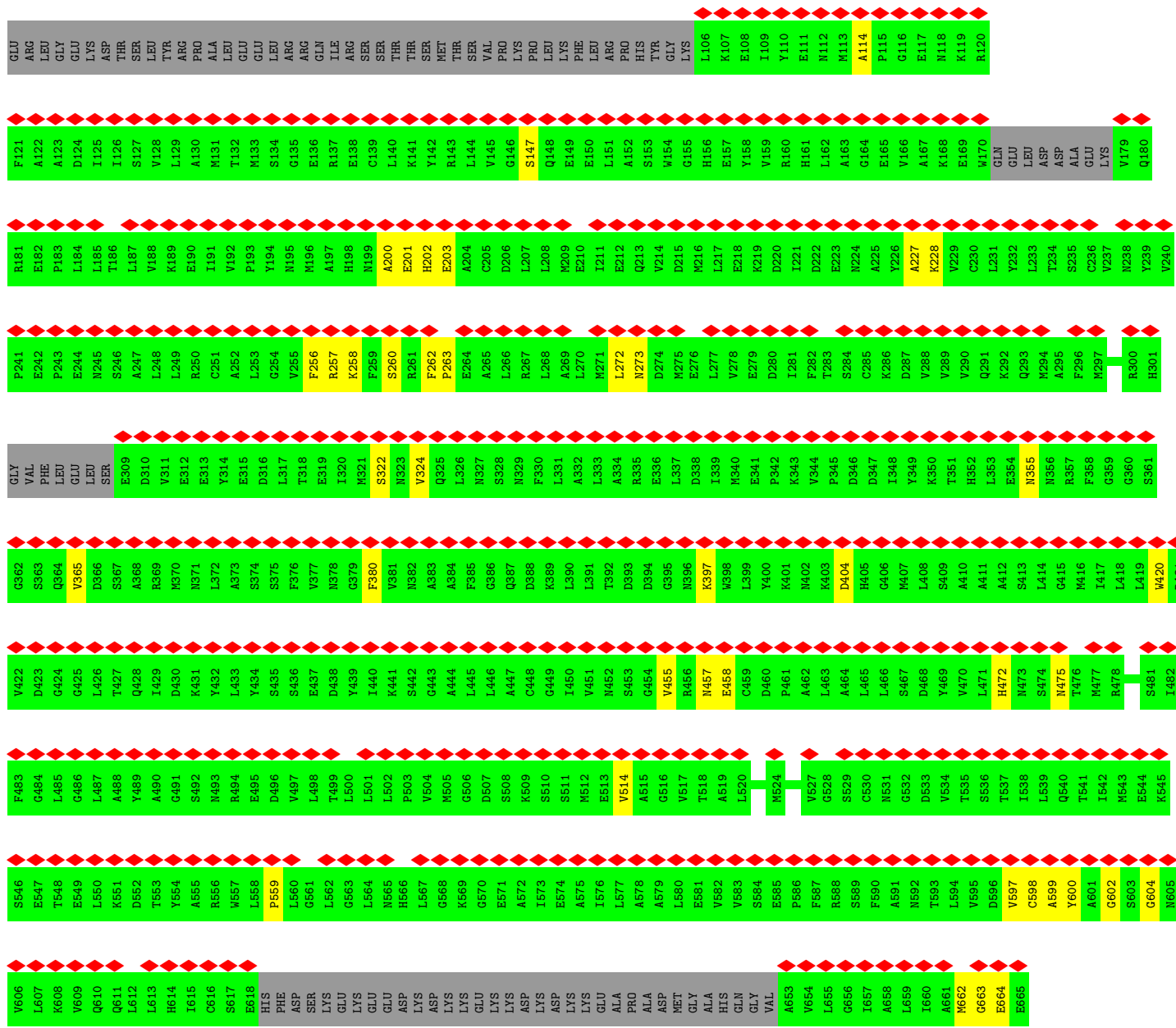
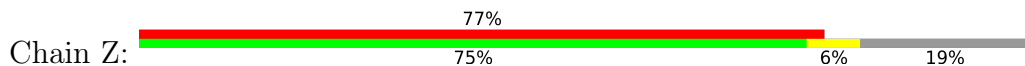


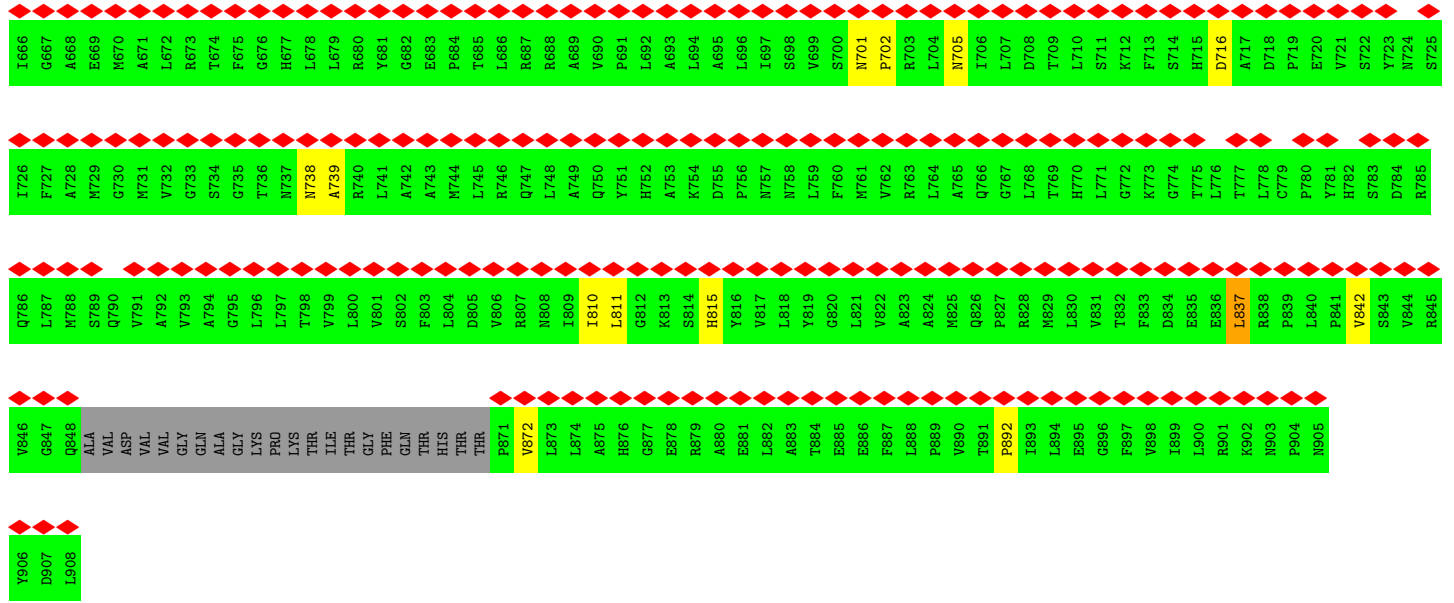
• Molecule 17: 26S proteasome complex subunit DSS1



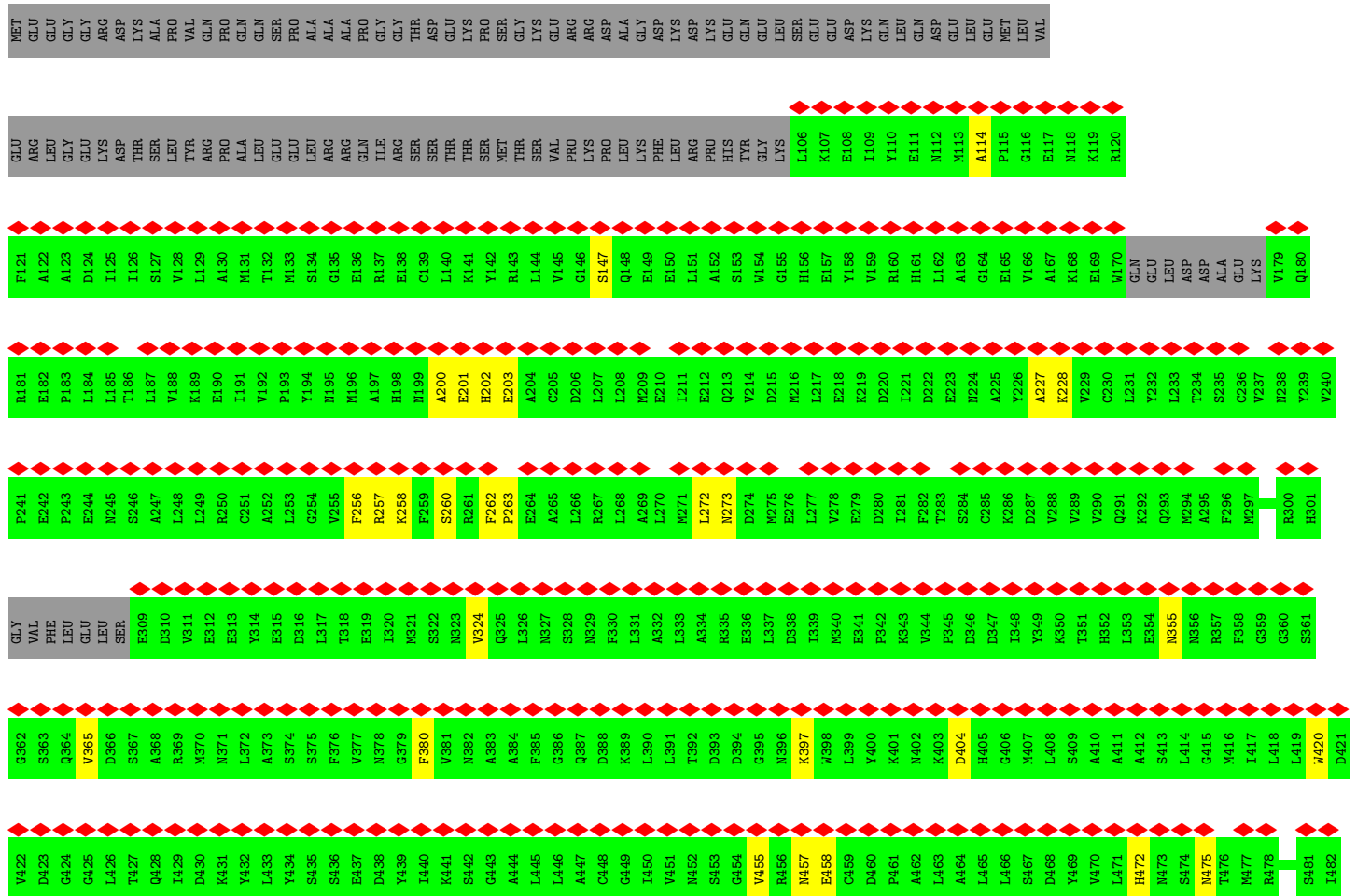
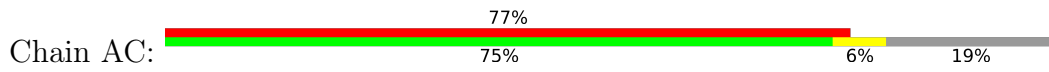


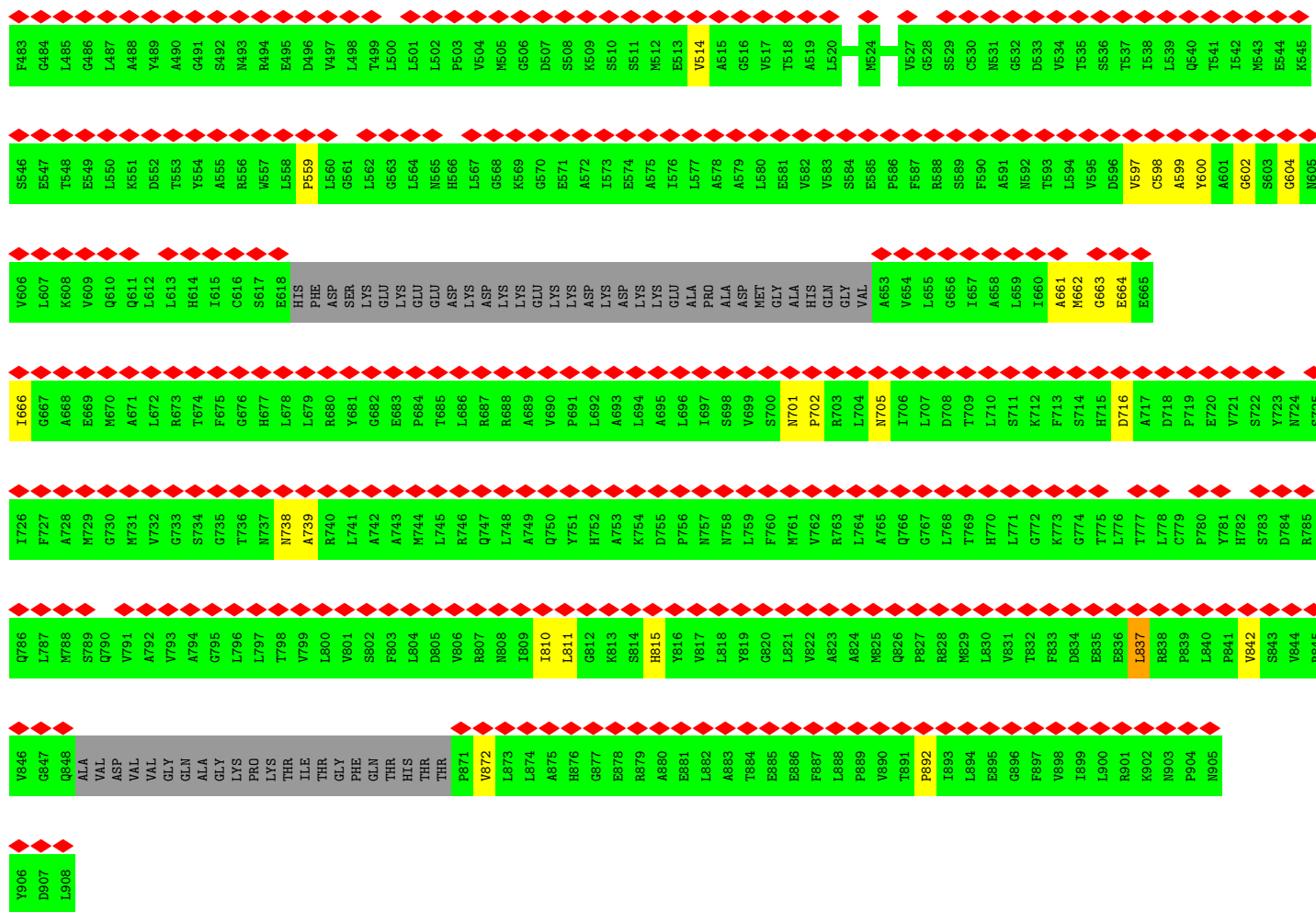
• Molecule 18: 26S proteasome non-ATPase regulatory subunit 2





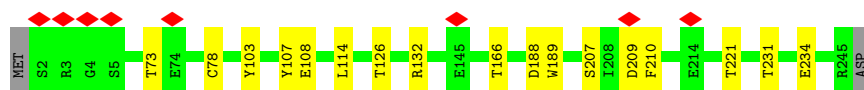
● Molecule 18: 26S proteasome non-ATPase regulatory subunit 2





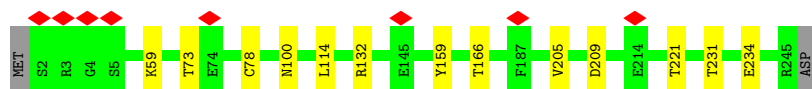
- Molecule 19: Proteasome subunit alpha type-6

Chain B: 92% 7%



- Molecule 19: Proteasome subunit alpha type-6

Chain h: 94% 5%

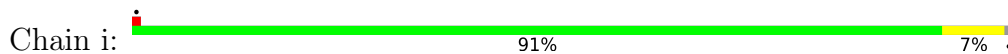


- Molecule 20: Proteasome subunit alpha type-2

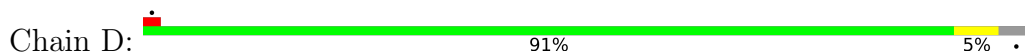
Chain C: 95%



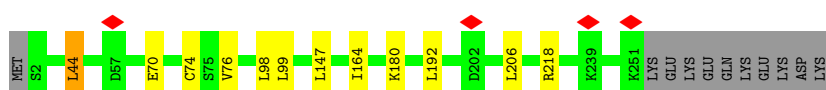
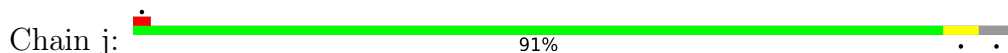
• Molecule 20: Proteasome subunit alpha type-2



• Molecule 21: Proteasome subunit alpha type-4



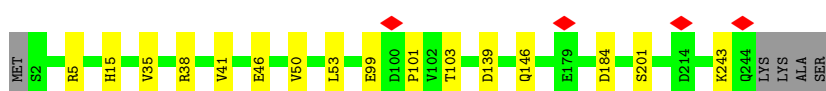
• Molecule 21: Proteasome subunit alpha type-4



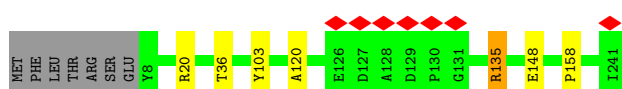
• Molecule 22: Proteasome subunit alpha type-7



• Molecule 22: Proteasome subunit alpha type-7

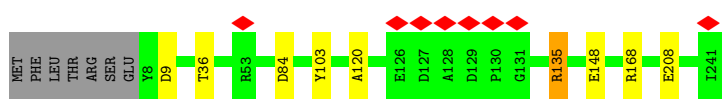
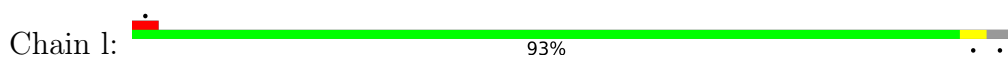


• Molecule 23: Proteasome subunit alpha type-5

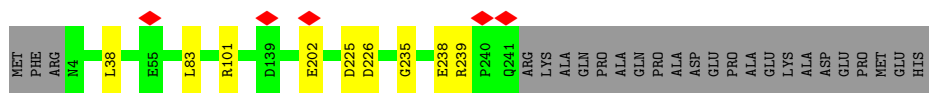
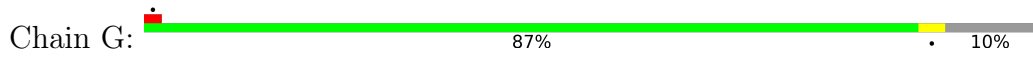


• Molecule 23: Proteasome subunit alpha type-5

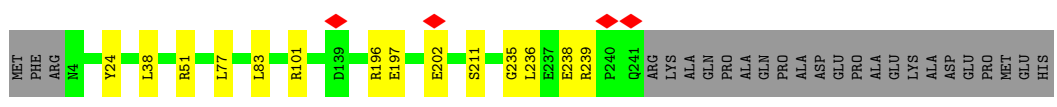
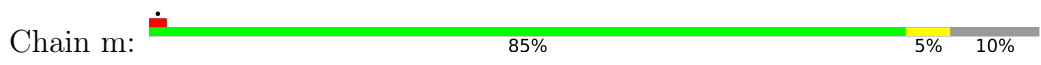




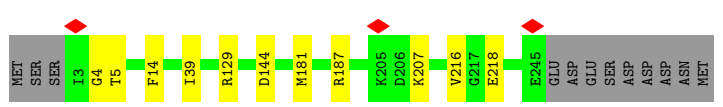
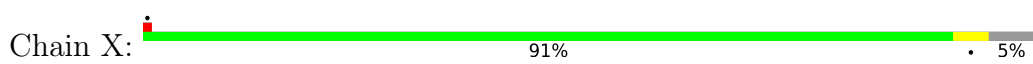
• Molecule 24: Proteasome subunit alpha type-1



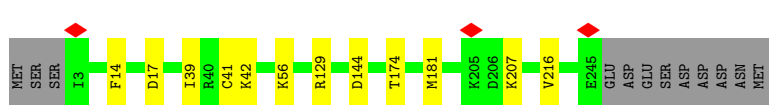
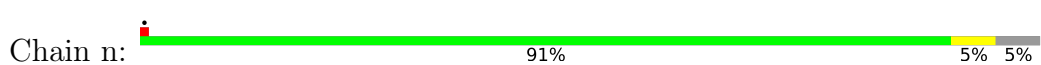
• Molecule 24: Proteasome subunit alpha type-1



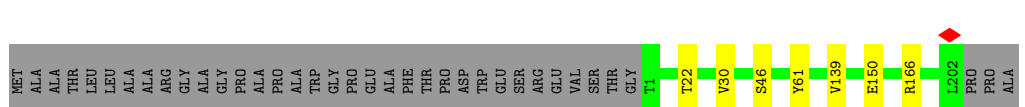
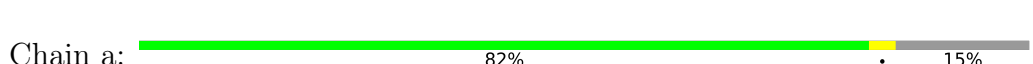
• Molecule 25: Proteasome subunit alpha type-3



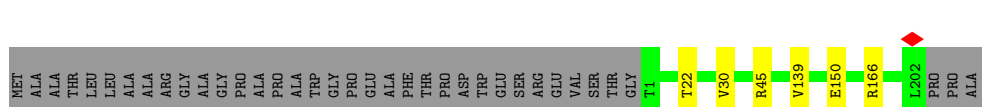
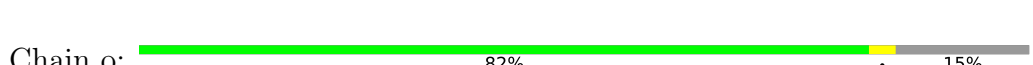
• Molecule 25: Proteasome subunit alpha type-3



• Molecule 26: Proteasome subunit beta type-6

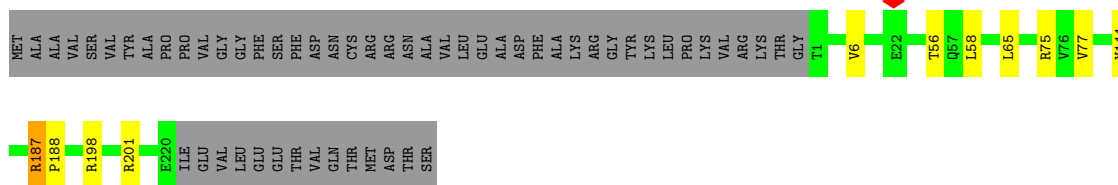


• Molecule 26: Proteasome subunit beta type-6



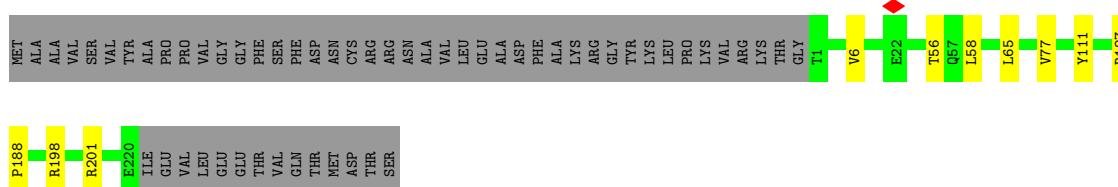
- Molecule 27: Proteasome subunit beta type-7

Chain b:  75% 21%



- Molecule 27: Proteasome subunit beta type-7

Chain p:  76% 21%



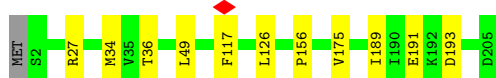
- Molecule 28: Proteasome subunit beta type-3

Chain c:  94% 5%



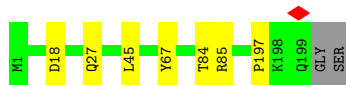
- Molecule 28: Proteasome subunit beta type-3

Chain q:  94% 5%



- Molecule 29: Proteasome subunit beta type-2

Chain d:  96%

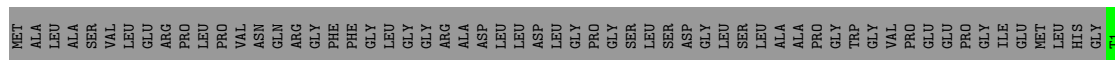


- Molecule 29: Proteasome subunit beta type-2

Chain r:  96%



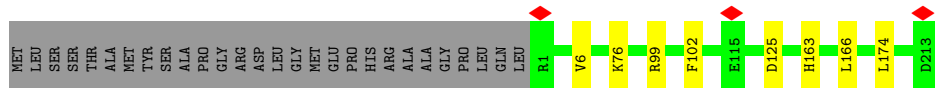
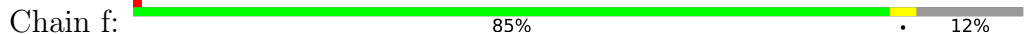
• Molecule 30: Proteasome subunit beta type-5



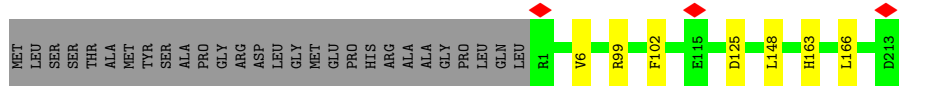
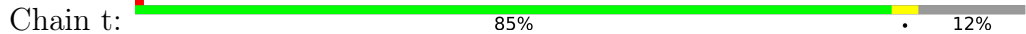
• Molecule 30: Proteasome subunit beta type-5



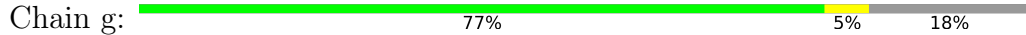
• Molecule 31: Proteasome subunit beta type-1



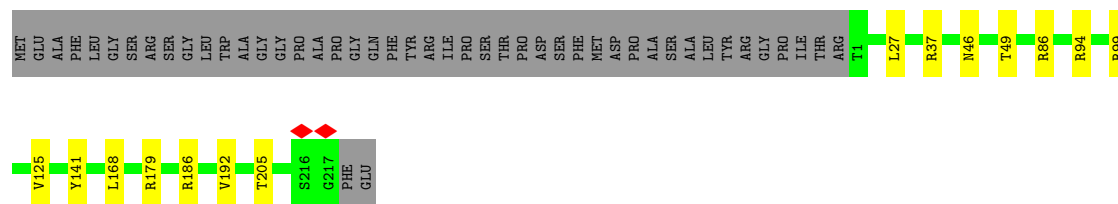
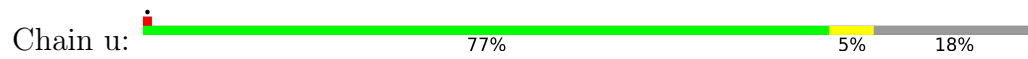
• Molecule 31: Proteasome subunit beta type-1



• Molecule 32: Proteasome subunit beta type-4



• Molecule 32: Proteasome subunit beta type-4



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	165699	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 ( $e^-/\text{\AA}^2$ )	37	Depositor
Minimum defocus (nm)	1.6	Depositor
Maximum defocus (nm)	2.6	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.258	Depositor
Minimum map value	-0.127	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0336	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	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

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	I	0.66	2/2756 (0.1%)	1.09	7/3727 (0.2%)
1	w	0.66	2/2756 (0.1%)	1.09	7/3727 (0.2%)
2	H	0.76	3/2939 (0.1%)	0.96	9/3970 (0.2%)
2	v	0.76	2/2939 (0.1%)	0.97	11/3970 (0.3%)
3	L	0.66	0/2904	0.80	5/3924 (0.1%)
3	z	0.65	0/2904	0.79	4/3924 (0.1%)
4	0	0.65	0/2896	0.81	6/3912 (0.2%)
4	M	0.65	0/2896	0.81	6/3912 (0.2%)
5	J	0.59	0/2857	0.75	3/3844 (0.1%)
5	x	0.59	0/2857	0.75	3/3844 (0.1%)
6	K	0.61	0/3089	0.80	3/4168 (0.1%)
6	y	0.61	0/3089	0.80	3/4168 (0.1%)
7	1	0.41	0/5506	0.60	1/7425 (0.0%)
7	N	0.41	0/5506	0.60	1/7425 (0.0%)
8	2	0.43	0/2390	0.65	2/3215 (0.1%)
8	O	0.43	0/2383	0.65	2/3206 (0.1%)
9	3	0.45	0/2860	0.67	3/3860 (0.1%)
9	P	0.45	0/2861	0.67	3/3861 (0.1%)
10	4	0.49	2/2989 (0.1%)	0.63	6/4054 (0.1%)
10	Q	0.48	1/2989 (0.0%)	0.63	6/4054 (0.1%)
11	5	0.48	0/2820	0.65	3/3815 (0.1%)
11	R	0.48	0/2817	0.65	3/3812 (0.1%)
12	6	0.41	0/2754	0.59	3/3728 (0.1%)
12	S	0.41	0/2745	0.58	2/3717 (0.1%)
13	7	0.41	0/1713	0.63	4/2306 (0.2%)
13	T	0.41	0/1713	0.63	4/2306 (0.2%)
14	8	0.46	0/2167	0.60	0/2936
14	U	0.46	0/2167	0.60	0/2936
15	9	0.47	0/2045	0.73	2/2760 (0.1%)
15	V	0.47	0/2047	0.72	2/2763 (0.1%)
16	AA	0.44	0/1312	0.76	4/1769 (0.2%)
16	W	0.44	0/1312	0.76	4/1769 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AB	0.43	0/315	0.74	1/433 (0.2%)
17	Y	0.43	0/315	0.74	1/433 (0.2%)
18	AC	0.32	0/3603	0.55	1/5005 (0.0%)
18	Z	0.32	0/3603	0.55	1/5005 (0.0%)
19	B	0.75	0/1878	0.74	0/2549
19	h	0.81	0/1886	0.77	0/2557
20	C	0.85	1/1773 (0.1%)	0.78	1/2409 (0.0%)
20	i	0.86	1/1780 (0.1%)	0.79	1/2417 (0.0%)
21	D	1.13	4/1946 (0.2%)	0.85	6/2633 (0.2%)
21	j	1.39	3/1943 (0.2%)	0.83	6/2629 (0.2%)
22	E	0.77	0/1748	0.77	0/2386
22	k	0.78	0/1716	0.80	1/2347 (0.0%)
23	F	0.78	1/1794 (0.1%)	0.79	1/2430 (0.0%)
23	l	0.80	1/1753 (0.1%)	0.83	2/2346 (0.1%)
24	G	0.75	0/1885	0.77	0/2552
24	m	0.77	1/1885 (0.1%)	0.79	0/2552
25	X	0.83	2/1908 (0.1%)	0.76	0/2575
25	n	0.81	1/1908 (0.1%)	0.76	0/2575
26	a	0.88	5/1535 (0.3%)	0.86	4/2078 (0.2%)
26	o	0.86	3/1535 (0.2%)	0.87	4/2078 (0.2%)
27	b	0.79	1/1670 (0.1%)	0.84	3/2265 (0.1%)
27	p	0.80	1/1670 (0.1%)	0.82	2/2265 (0.1%)
28	c	0.87	0/1614	0.85	1/2177 (0.0%)
28	q	0.87	0/1614	0.85	1/2177 (0.0%)
29	d	0.87	1/1603 (0.1%)	0.83	0/2174
29	r	0.87	1/1603 (0.1%)	0.83	0/2174
30	e	0.92	0/1579	0.85	1/2134 (0.0%)
30	s	0.91	0/1582	0.84	1/2138 (0.0%)
31	f	0.85	0/1674	0.81	0/2257
31	t	0.85	0/1674	0.81	1/2257 (0.0%)
32	g	0.90	2/1705 (0.1%)	0.86	4/2312 (0.2%)
32	u	0.89	2/1711 (0.1%)	0.85	4/2319 (0.2%)
All	All	0.66	43/144386 (0.0%)	0.76	170/195445 (0.1%)

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	I	0	4
1	w	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	H	0	1
2	v	0	1
3	L	0	3
3	z	0	3
4	0	0	3
4	M	0	3
5	J	0	1
5	x	0	1
6	K	0	2
6	y	0	2
7	1	0	3
7	N	0	3
8	2	0	1
8	O	0	1
9	3	0	2
9	P	0	2
10	4	0	7
10	Q	0	7
11	5	0	9
11	R	0	9
13	7	0	2
13	T	0	2
14	8	0	1
14	U	0	1
15	9	0	3
15	V	0	3
16	AA	0	8
16	W	0	8
17	AB	0	2
17	Y	0	2
18	AC	0	7
18	Z	0	7
27	b	0	2
All	All	0	120

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	j	70	GLU	CD-OE1	44.40	1.74	1.25
21	D	70	GLU	CD-OE1	23.09	1.51	1.25
21	D	70	GLU	CD-OE2	22.37	1.50	1.25
21	j	70	GLU	CD-OE2	18.38	1.45	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	D	70	GLU	CG-CD	13.41	1.72	1.51
21	j	70	GLU	CG-CD	13.30	1.72	1.51
32	g	179	ARG	CZ-NH1	9.58	1.45	1.33
32	u	179	ARG	CZ-NH1	8.86	1.44	1.33
32	g	179	ARG	NE-CZ	7.49	1.42	1.33
10	4	48	GLN	C-N	7.39	1.51	1.34
10	Q	163	LYS	N-CA	-7.03	1.32	1.46
10	4	163	LYS	N-CA	-7.03	1.32	1.46
27	p	111	TYR	CE2-CZ	-6.94	1.29	1.38
32	u	179	ARG	NE-CZ	6.52	1.41	1.33
2	H	336	ARG	CD-NE	-6.43	1.35	1.46
2	v	336	ARG	CD-NE	-6.43	1.35	1.46
26	o	166	ARG	NE-CZ	6.30	1.41	1.33
26	a	166	ARG	NE-CZ	6.20	1.41	1.33
20	C	12	PHE	CG-CD2	-6.20	1.29	1.38
26	a	61	TYR	CB-CG	6.18	1.60	1.51
20	i	12	PHE	CG-CD2	-6.08	1.29	1.38
26	a	61	TYR	CG-CD1	5.89	1.46	1.39
2	v	346	PRO	N-CD	5.89	1.56	1.47
26	o	166	ARG	CZ-NH1	5.86	1.40	1.33
25	X	218	GLU	CD-OE2	5.78	1.32	1.25
26	o	166	ARG	CD-NE	5.69	1.56	1.46
26	a	166	ARG	CZ-NH1	5.66	1.40	1.33
1	I	142	ASP	CB-CG	5.58	1.63	1.51
1	w	142	ASP	CB-CG	5.58	1.63	1.51
25	n	14	PHE	CG-CD2	-5.57	1.30	1.38
27	b	111	TYR	CE2-CZ	-5.54	1.31	1.38
2	H	346	PRO	N-CD	5.53	1.55	1.47
25	X	14	PHE	CG-CD2	-5.38	1.30	1.38
21	D	70	GLU	CB-CG	5.28	1.62	1.52
23	F	103	TYR	CG-CD2	-5.22	1.32	1.39
1	I	142	ASP	CG-OD1	5.14	1.37	1.25
1	w	142	ASP	CG-OD1	5.14	1.37	1.25
26	a	166	ARG	CD-NE	5.11	1.55	1.46
29	r	67	TYR	CE1-CZ	-5.11	1.31	1.38
2	H	92	PRO	N-CD	5.10	1.54	1.47
23	l	103	TYR	CG-CD2	-5.07	1.32	1.39
24	m	24	TYR	CE1-CZ	-5.06	1.31	1.38
29	d	67	TYR	CE1-CZ	-5.02	1.32	1.38

All (170) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	142	ASP	CB-CG-OD1	34.78	149.61	118.30
1	w	142	ASP	CB-CG-OD1	34.78	149.61	118.30
1	I	142	ASP	CB-CG-OD2	-25.59	95.27	118.30
1	w	142	ASP	CB-CG-OD2	-25.59	95.27	118.30
2	H	336	ARG	NE-CZ-NH1	-19.14	110.73	120.30
2	v	336	ARG	NE-CZ-NH1	-19.14	110.73	120.30
6	K	200	ARG	NE-CZ-NH2	-15.05	112.77	120.30
6	y	200	ARG	NE-CZ-NH2	-15.05	112.77	120.30
26	a	166	ARG	NE-CZ-NH1	14.49	127.55	120.30
26	o	166	ARG	NE-CZ-NH1	14.05	127.33	120.30
15	V	139	ARG	NE-CZ-NH2	-13.90	113.35	120.30
15	9	139	ARG	NE-CZ-NH2	-13.90	113.35	120.30
6	K	200	ARG	NE-CZ-NH1	13.86	127.23	120.30
6	y	200	ARG	NE-CZ-NH1	13.86	127.23	120.30
9	P	420	ASP	C-N-CD	-13.65	90.58	120.60
9	3	420	ASP	C-N-CD	-13.65	90.58	120.60
32	g	179	ARG	NE-CZ-NH2	-12.65	113.97	120.30
28	q	27	ARG	NE-CZ-NH2	-11.46	114.57	120.30
32	g	179	ARG	NE-CZ-NH1	11.28	125.94	120.30
32	u	179	ARG	NE-CZ-NH2	-10.97	114.82	120.30
28	c	27	ARG	NE-CZ-NH2	-10.84	114.88	120.30
2	H	336	ARG	NE-CZ-NH2	10.64	125.62	120.30
2	v	336	ARG	NE-CZ-NH2	10.64	125.62	120.30
15	V	139	ARG	NE-CZ-NH1	10.13	125.36	120.30
15	9	139	ARG	NE-CZ-NH1	10.13	125.36	120.30
4	M	168	TYR	CB-CA-C	-10.01	90.39	110.40
4	0	168	TYR	CB-CA-C	-10.01	90.39	110.40
32	u	179	ARG	NE-CZ-NH1	9.60	125.10	120.30
16	W	52	ILE	CB-CA-C	-8.84	93.92	111.60
16	AA	52	ILE	CB-CA-C	-8.84	93.92	111.60
1	I	263	GLY	C-N-CD	-8.72	101.42	120.60
1	w	263	GLY	C-N-CD	-8.72	101.42	120.60
2	H	336	ARG	CD-NE-CZ	8.62	135.66	123.60
2	v	336	ARG	CD-NE-CZ	8.62	135.66	123.60
21	j	99	LEU	CB-CG-CD1	-8.38	96.76	111.00
21	D	99	LEU	CB-CG-CD1	-8.38	96.76	111.00
2	H	315	ILE	N-CA-C	-8.24	88.74	111.00
2	v	315	ILE	N-CA-C	-8.24	88.74	111.00
8	O	263	ALA	N-CA-C	7.67	131.71	111.00
8	2	263	ALA	N-CA-C	7.67	131.71	111.00
27	b	58	LEU	CB-CG-CD1	-7.60	98.08	111.00
1	I	325	VAL	N-CA-C	-7.46	90.84	111.00
1	w	325	VAL	N-CA-C	-7.46	90.84	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	169	ASP	N-CA-C	7.39	130.95	111.00
4	0	169	ASP	N-CA-C	7.39	130.95	111.00
3	L	148	VAL	CB-CA-C	7.38	125.41	111.40
3	z	148	VAL	CB-CA-C	7.38	125.41	111.40
16	W	58	CYS	CA-CB-SG	-7.21	101.02	114.00
16	AA	58	CYS	CA-CB-SG	-7.21	101.02	114.00
27	p	58	LEU	CB-CG-CD1	-7.20	98.77	111.00
21	j	70	GLU	CG-CD-OE2	7.16	132.62	118.30
23	l	135	ARG	NE-CZ-NH2	-6.82	116.89	120.30
10	Q	397	TYR	CB-CG-CD1	6.72	125.03	121.00
10	4	397	TYR	CB-CG-CD1	6.72	125.03	121.00
4	M	169	ASP	N-CA-CB	-6.62	98.68	110.60
4	0	169	ASP	N-CA-CB	-6.62	98.68	110.60
27	p	65	LEU	CB-CG-CD1	-6.61	99.76	111.00
1	I	346	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	w	346	ARG	NE-CZ-NH1	6.59	123.60	120.30
11	R	33	GLY	N-CA-C	-6.55	96.72	113.10
11	5	33	GLY	N-CA-C	-6.55	96.72	113.10
13	T	173	CYS	CA-CB-SG	-6.53	102.24	114.00
13	7	173	CYS	CA-CB-SG	-6.53	102.24	114.00
23	l	135	ARG	NE-CZ-NH1	6.53	123.56	120.30
10	Q	75	PRO	N-CA-CB	6.53	111.13	103.30
10	4	75	PRO	N-CA-CB	6.53	111.13	103.30
18	Z	201	GLU	N-CA-CB	-6.51	98.88	110.60
18	AC	201	GLU	N-CA-CB	-6.51	98.88	110.60
4	M	320	PHE	CB-CG-CD1	-6.51	116.25	120.80
4	0	320	PHE	CB-CG-CD1	-6.51	116.25	120.80
23	F	135	ARG	NE-CZ-NH2	-6.47	117.07	120.30
21	j	70	GLU	CG-CD-OE1	-6.36	105.57	118.30
3	L	356	ARG	NE-CZ-NH1	6.29	123.45	120.30
3	z	356	ARG	NE-CZ-NH1	6.29	123.45	120.30
27	b	65	LEU	CB-CG-CD1	-6.25	100.38	111.00
5	J	311	ILE	N-CA-C	-6.23	94.18	111.00
5	x	311	ILE	N-CA-C	-6.23	94.18	111.00
13	T	121	LEU	CB-CG-CD2	-6.19	100.47	111.00
13	7	121	LEU	CB-CG-CD2	-6.19	100.47	111.00
2	H	224	LEU	CB-CG-CD1	-6.19	100.48	111.00
2	v	224	LEU	CB-CG-CD1	-6.19	100.48	111.00
12	S	91	PRO	N-CA-CB	6.18	110.72	103.30
12	6	91	PRO	N-CA-CB	6.18	110.72	103.30
1	I	216	ILE	CB-CA-C	6.17	123.94	111.60
1	w	216	ILE	CB-CA-C	6.17	123.94	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	g	125	VAL	CG1-CB-CG2	-6.15	101.06	110.90
32	u	125	VAL	CG1-CB-CG2	-6.12	101.10	110.90
32	g	27	LEU	CB-CG-CD1	-6.06	100.70	111.00
7	N	427	LEU	C-N-CD	6.03	141.07	128.40
7	1	427	LEU	C-N-CD	6.03	141.07	128.40
3	L	318	GLY	C-N-CD	6.01	141.03	128.40
16	W	65	THR	N-CA-C	5.98	127.15	111.00
16	AA	65	THR	N-CA-C	5.98	127.15	111.00
4	M	320	PHE	CB-CG-CD2	5.96	124.97	120.80
4	0	320	PHE	CB-CG-CD2	5.96	124.97	120.80
2	v	91	GLN	C-N-CD	5.92	140.83	128.40
4	M	269	ARG	NE-CZ-NH2	5.90	123.25	120.30
4	0	269	ARG	NE-CZ-NH2	5.90	123.25	120.30
21	D	98	LEU	CB-CG-CD1	-5.87	101.01	111.00
21	j	98	LEU	CB-CG-CD1	-5.87	101.02	111.00
30	e	14	VAL	CG1-CB-CG2	-5.87	101.52	110.90
13	T	252	PRO	N-CA-CB	5.86	110.33	103.30
13	7	252	PRO	N-CA-CB	5.86	110.33	103.30
2	H	91	GLN	C-N-CD	5.82	140.62	128.40
32	u	27	LEU	CB-CG-CD1	-5.81	101.12	111.00
2	v	346	PRO	CA-N-CD	-5.79	103.39	111.50
10	Q	203	PRO	CA-N-CD	-5.79	103.39	111.50
10	4	203	PRO	CA-N-CD	-5.79	103.39	111.50
11	R	383	LEU	CB-CG-CD1	5.77	120.81	111.00
11	5	383	LEU	CB-CG-CD1	5.77	120.81	111.00
21	j	44	LEU	CA-CB-CG	5.76	128.56	115.30
9	P	324	TYR	CA-C-N	5.76	127.71	116.20
9	3	324	TYR	CA-C-N	5.76	127.71	116.20
2	v	346	PRO	N-CA-C	5.74	127.02	112.10
2	H	336	ARG	CG-CD-NE	5.73	123.83	111.80
2	v	336	ARG	CG-CD-NE	5.73	123.83	111.80
26	o	166	ARG	CD-NE-CZ	5.71	131.59	123.60
26	a	166	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
6	K	215	LEU	CB-CG-CD1	-5.66	101.39	111.00
6	y	215	LEU	CB-CG-CD1	-5.66	101.39	111.00
21	D	44	LEU	CA-CB-CG	5.65	128.29	115.30
30	s	14	VAL	CG1-CB-CG2	-5.65	101.86	110.90
2	H	155	PRO	CA-C-N	-5.64	104.80	117.20
2	v	155	PRO	CA-C-N	-5.64	104.80	117.20
26	o	45	ARG	NE-CZ-NH2	-5.62	117.49	120.30
8	O	332	HIS	N-CA-C	-5.60	95.88	111.00
8	2	332	HIS	N-CA-C	-5.60	95.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Q	162	ASP	C-N-CA	-5.55	107.81	121.70
10	4	162	ASP	C-N-CA	-5.55	107.81	121.70
20	i	127	ARG	NE-CZ-NH2	-5.54	117.53	120.30
26	a	166	ARG	CD-NE-CZ	5.49	131.29	123.60
9	P	79	GLU	N-CA-CB	-5.47	100.75	110.60
9	3	79	GLU	N-CA-CB	-5.47	100.75	110.60
13	T	283	LEU	CA-CB-CG	-5.47	102.72	115.30
13	7	283	LEU	CA-CB-CG	-5.47	102.72	115.30
21	D	70	GLU	CG-CD-OE2	5.44	129.18	118.30
22	k	53	LEU	CB-CG-CD2	-5.44	101.76	111.00
26	a	61	TYR	CB-CG-CD1	5.42	124.25	121.00
20	C	127	ARG	NE-CZ-NH2	-5.39	117.60	120.30
17	Y	7	PRO	N-CA-CB	5.33	109.70	103.30
17	AB	7	PRO	N-CA-CB	5.33	109.70	103.30
10	Q	162	ASP	CA-C-N	-5.31	105.52	117.20
10	4	162	ASP	CA-C-N	-5.31	105.52	117.20
26	o	166	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
2	H	261	PHE	CB-CA-C	5.28	120.95	110.40
2	v	261	PHE	CB-CA-C	5.28	120.95	110.40
5	J	374	ARG	NE-CZ-NH1	5.24	122.92	120.30
11	R	96	GLY	N-CA-C	-5.24	100.00	113.10
5	x	374	ARG	NE-CZ-NH1	5.24	122.92	120.30
11	5	96	GLY	N-CA-C	-5.24	100.00	113.10
12	6	222	ASP	CB-CG-OD2	5.21	122.99	118.30
10	Q	203	PRO	C-N-CD	5.20	139.33	128.40
10	4	203	PRO	C-N-CD	5.20	139.33	128.40
27	b	75	ARG	NE-CZ-NH1	5.19	122.89	120.30
12	S	465	ASP	CB-CG-OD2	5.18	122.97	118.30
12	6	465	ASP	CB-CG-OD2	5.18	122.97	118.30
21	D	147	LEU	CB-CG-CD1	-5.18	102.19	111.00
5	J	374	ARG	NE-CZ-NH2	-5.12	117.74	120.30
5	x	374	ARG	NE-CZ-NH2	-5.12	117.74	120.30
21	j	147	LEU	CB-CG-CD1	-5.11	102.32	111.00
3	L	294	ARG	NE-CZ-NH1	5.10	122.85	120.30
16	W	22	LEU	CA-CB-CG	-5.10	103.57	115.30
3	z	294	ARG	NE-CZ-NH1	5.10	122.85	120.30
16	AA	22	LEU	CA-CB-CG	-5.10	103.57	115.30
21	D	70	GLU	CG-CD-OE1	-5.08	108.14	118.30
1	I	226	GLY	C-N-CD	5.06	139.03	128.40
1	w	226	GLY	C-N-CD	5.06	139.03	128.40
31	t	148	LEU	CB-CG-CD2	-5.05	102.42	111.00
3	L	50	LEU	N-CA-C	5.03	124.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	z	50	LEU	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

All (120) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	0	279	ALA	Mainchain,Peptide
4	0	362	ARG	Sidechain
7	1	208	LEU	Peptide
7	1	724	VAL	Peptide
7	1	807	LYS	Peptide
8	2	285	PRO	Peptide
9	3	78	LYS	Mainchain,Peptide
10	4	162	ASP	Peptide
10	4	202	CYS	Mainchain,Peptide
10	4	32	LYS	Mainchain,Peptide
10	4	37	GLU	Mainchain,Peptide
11	5	14	ASN	Mainchain,Peptide
11	5	30	GLU	Mainchain,Peptide
11	5	32	ARG	Mainchain,Peptide
11	5	33	GLY	Peptide
11	5	95	LEU	Mainchain,Peptide
13	7	318	PHE	Mainchain,Peptide
14	8	239	ASP	Peptide
15	9	112	TYR	Peptide
15	9	49	VAL	Mainchain,Peptide
16	AA	103	LYS	Peptide
16	AA	145	GLU	Peptide
16	AA	146	GLU	Peptide
16	AA	160	LEU	Peptide
16	AA	161	ASN	Peptide
16	AA	2	VAL	Peptide
16	AA	22	LEU	Mainchain,Peptide
17	AB	16	ASP	Peptide
17	AB	43	TRP	Peptide
18	AC	147	SER	Peptide
18	AC	200	ALA	Mainchain,Peptide
18	AC	260	SER	Mainchain,Peptide
18	AC	355	ASN	Peptide
18	AC	837	LEU	Peptide
2	H	336	ARG	Sidechain
1	I	105	THR	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	I	137	SER	Peptide
1	I	299	SER	Mainchain,Peptide
5	J	242	ALA	Peptide
6	K	149	SER	Mainchain,Peptide
3	L	226	GLN	Mainchain,Peptide
3	L	244	SER	Peptide
4	M	279	ALA	Mainchain,Peptide
4	M	362	ARG	Sidechain
7	N	208	LEU	Peptide
7	N	724	VAL	Peptide
7	N	807	LYS	Peptide
8	O	285	PRO	Peptide
9	P	78	LYS	Mainchain,Peptide
10	Q	162	ASP	Peptide
10	Q	202	CYS	Mainchain,Peptide
10	Q	32	LYS	Mainchain,Peptide
10	Q	37	GLU	Mainchain,Peptide
11	R	14	ASN	Mainchain,Peptide
11	R	30	GLU	Mainchain,Peptide
11	R	32	ARG	Mainchain,Peptide
11	R	33	GLY	Peptide
11	R	95	LEU	Mainchain,Peptide
13	T	318	PHE	Mainchain,Peptide
14	U	239	ASP	Peptide
15	V	112	TYR	Peptide
15	V	49	VAL	Mainchain,Peptide
16	W	103	LYS	Peptide
16	W	145	GLU	Peptide
16	W	146	GLU	Peptide
16	W	160	LEU	Peptide
16	W	161	ASN	Peptide
16	W	2	VAL	Peptide
16	W	22	LEU	Mainchain,Peptide
17	Y	16	ASP	Peptide
17	Y	43	TRP	Peptide
18	Z	147	SER	Peptide
18	Z	200	ALA	Mainchain,Peptide
18	Z	260	SER	Mainchain,Peptide
18	Z	355	ASN	Peptide
18	Z	837	LEU	Peptide
27	b	187	ARG	Mainchain,Peptide
2	v	336	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	w	105	THR	Peptide
1	w	137	SER	Peptide
1	w	299	SER	Mainchain,Peptide
5	x	242	ALA	Peptide
6	y	149	SER	Mainchain,Peptide
3	z	226	GLN	Mainchain,Peptide
3	z	244	SER	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	I	355/440 (81%)	255 (72%)	72 (20%)	28 (8%)	1	10
1	w	355/440 (81%)	255 (72%)	71 (20%)	29 (8%)	1	9
2	H	376/433 (87%)	248 (66%)	91 (24%)	37 (10%)	0	7
2	v	376/433 (87%)	249 (66%)	88 (23%)	39 (10%)	0	7
3	L	373/389 (96%)	264 (71%)	72 (19%)	37 (10%)	0	7
3	z	373/389 (96%)	263 (70%)	73 (20%)	37 (10%)	0	7
4	0	372/439 (85%)	255 (68%)	74 (20%)	43 (12%)	0	5
4	M	372/439 (85%)	255 (68%)	74 (20%)	43 (12%)	0	5
5	J	354/406 (87%)	255 (72%)	66 (19%)	33 (9%)	0	8
5	x	354/406 (87%)	255 (72%)	66 (19%)	33 (9%)	0	8
6	K	378/418 (90%)	266 (70%)	70 (18%)	42 (11%)	0	6
6	y	378/418 (90%)	266 (70%)	70 (18%)	42 (11%)	0	6
7	1	811/953 (85%)	607 (75%)	176 (22%)	28 (4%)	3	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	N	811/953 (85%)	607 (75%)	176 (22%)	28 (4%)	3	27
8	2	368/376 (98%)	287 (78%)	61 (17%)	20 (5%)	2	17
8	O	368/376 (98%)	287 (78%)	61 (17%)	20 (5%)	2	17
9	3	401/456 (88%)	338 (84%)	51 (13%)	12 (3%)	4	30
9	P	401/456 (88%)	338 (84%)	51 (13%)	12 (3%)	4	30
10	4	419/422 (99%)	331 (79%)	58 (14%)	30 (7%)	1	11
10	Q	419/422 (99%)	330 (79%)	58 (14%)	31 (7%)	1	11
11	5	374/389 (96%)	295 (79%)	54 (14%)	25 (7%)	1	13
11	R	374/389 (96%)	295 (79%)	54 (14%)	25 (7%)	1	13
12	6	413/525 (79%)	354 (86%)	42 (10%)	17 (4%)	3	23
12	S	413/525 (79%)	354 (86%)	42 (10%)	17 (4%)	3	23
13	7	254/350 (73%)	195 (77%)	43 (17%)	16 (6%)	1	14
13	T	254/350 (73%)	195 (77%)	43 (17%)	16 (6%)	1	14
14	8	279/324 (86%)	222 (80%)	42 (15%)	15 (5%)	2	17
14	U	279/324 (86%)	222 (80%)	42 (15%)	15 (5%)	2	17
15	9	253/310 (82%)	209 (83%)	32 (13%)	12 (5%)	2	20
15	V	253/310 (82%)	209 (83%)	32 (13%)	12 (5%)	2	20
16	AA	191/377 (51%)	145 (76%)	35 (18%)	11 (6%)	1	16
16	W	191/377 (51%)	145 (76%)	35 (18%)	11 (6%)	1	16
17	AB	55/70 (79%)	37 (67%)	10 (18%)	8 (14%)	0	3
17	Y	55/70 (79%)	37 (67%)	10 (18%)	8 (14%)	0	3
18	AC	722/908 (80%)	557 (77%)	116 (16%)	49 (7%)	1	13
18	Z	722/908 (80%)	558 (77%)	116 (16%)	48 (7%)	1	13
19	B	242/246 (98%)	230 (95%)	8 (3%)	4 (2%)	9	42
19	h	242/246 (98%)	229 (95%)	13 (5%)	0	100	100
20	C	229/234 (98%)	204 (89%)	23 (10%)	2 (1%)	17	56
20	i	229/234 (98%)	206 (90%)	21 (9%)	2 (1%)	17	56
21	D	248/261 (95%)	234 (94%)	13 (5%)	1 (0%)	34	72
21	j	248/261 (95%)	236 (95%)	11 (4%)	1 (0%)	34	72
22	E	241/248 (97%)	221 (92%)	15 (6%)	5 (2%)	7	38
22	k	241/248 (97%)	221 (92%)	15 (6%)	5 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	F	232/241 (96%)	217 (94%)	13 (6%)	2 (1%)	17	56
23	l	232/241 (96%)	214 (92%)	17 (7%)	1 (0%)	34	72
24	G	236/263 (90%)	224 (95%)	9 (4%)	3 (1%)	12	48
24	m	236/263 (90%)	224 (95%)	9 (4%)	3 (1%)	12	48
25	X	241/255 (94%)	234 (97%)	4 (2%)	3 (1%)	13	50
25	n	241/255 (94%)	235 (98%)	4 (2%)	2 (1%)	19	58
26	a	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	29	68
26	o	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	29	68
27	b	218/277 (79%)	209 (96%)	8 (4%)	1 (0%)	29	68
27	p	218/277 (79%)	208 (95%)	8 (4%)	2 (1%)	17	56
28	c	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15	54
28	q	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15	54
29	d	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	29	68
29	r	197/201 (98%)	187 (95%)	9 (5%)	1 (0%)	29	68
30	e	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
30	s	199/263 (76%)	195 (98%)	4 (2%)	0	100	100
31	f	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
31	t	211/241 (88%)	203 (96%)	8 (4%)	0	100	100
32	g	214/264 (81%)	203 (95%)	10 (5%)	1 (0%)	29	68
32	u	215/264 (81%)	206 (96%)	8 (4%)	1 (0%)	29	68
All	All	19717/22846 (86%)	16137 (82%)	2604 (13%)	976 (5%)	4	19

All (976) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	165	ASP
1	I	207	HIS
1	I	220	LYS
1	I	277	HIS
1	I	278	ALA
1	I	292	THR
1	I	297	SER
1	I	321	SER
1	I	356	PRO
1	I	357	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	380	LEU
2	H	108	ASP
2	H	109	PRO
2	H	110	LYS
2	H	115	VAL
2	H	154	PRO
2	H	167	GLU
2	H	234	ASP
2	H	285	PHE
2	H	286	ASP
2	H	307	ASP
2	H	417	ILE
2	H	424	SER
3	L	85	ARG
3	L	88	ASP
3	L	109	ARG
3	L	114	GLU
3	L	139	SER
3	L	194	ASN
3	L	206	LYS
3	L	237	ALA
3	L	324	GLY
3	L	358	ASP
4	M	137	ILE
4	M	140	VAL
4	M	168	TYR
4	M	184	GLN
4	M	218	GLN
4	M	244	THR
4	M	261	ILE
4	M	345	SER
4	M	378	ASP
4	M	413	THR
4	M	415	LEU
4	M	433	ALA
5	J	89	VAL
5	J	90	HIS
5	J	92	GLU
5	J	131	VAL
5	J	149	GLU
5	J	150	MET
5	J	151	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	J	152	GLY
5	J	229	ARG
5	J	284	GLU
5	J	288	ASN
5	J	310	ARG
5	J	352	PRO
6	K	85	ILE
6	K	97	ASP
6	K	119	ILE
6	K	120	ASP
6	K	122	GLU
6	K	125	LYS
6	K	151	ILE
6	K	152	MET
6	K	155	THR
6	K	162	VAL
6	K	223	THR
6	K	258	ALA
6	K	273	LYS
6	K	274	ARG
6	K	278	GLN
6	K	300	ASP
6	K	336	PRO
6	K	360	LEU
6	K	367	PRO
6	K	393	ILE
6	K	409	LYS
6	K	410	ASP
6	K	411	GLU
6	K	412	GLN
7	N	164	GLU
7	N	170	SER
7	N	701	ILE
7	N	792	ASN
7	N	793	LYS
7	N	881	PRO
7	N	905	PRO
7	N	933	PRO
8	O	146	PRO
8	O	263	ALA
8	O	284	ARG
8	O	285	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	O	288	HIS
8	O	369	HIS
8	O	371	ALA
9	P	169	LEU
9	P	300	PRO
9	P	409	LEU
10	Q	58	ALA
10	Q	60	THR
10	Q	121	LYS
10	Q	141	LYS
10	Q	201	TYR
10	Q	203	PRO
10	Q	204	PRO
10	Q	277	LEU
10	Q	280	ALA
10	Q	317	PRO
10	Q	391	PRO
10	Q	393	VAL
11	R	28	LEU
11	R	34	ASP
11	R	131	THR
11	R	254	PRO
11	R	268	TYR
11	R	269	SER
11	R	289	ALA
12	S	218	TYR
12	S	279	GLN
12	S	321	ALA
12	S	346	LEU
12	S	351	PRO
12	S	464	ILE
12	S	466	ILE
12	S	505	LEU
12	S	507	SER
13	T	216	PRO
13	T	312	PRO
13	T	319	ALA
13	T	323	GLN
13	T	325	PRO
14	U	117	PRO
14	U	128	PRO
14	U	222	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	U	240	VAL
14	U	241	SER
15	V	52	GLU
15	V	226	MET
16	W	62	THR
16	W	65	THR
16	W	66	PRO
16	W	67	ASP
16	W	78	VAL
17	Y	38	VAL
17	Y	45	ASP
17	Y	46	ASP
17	Y	48	VAL
18	Z	203	GLU
18	Z	228	LYS
18	Z	256	PHE
18	Z	257	ARG
18	Z	258	LYS
18	Z	272	LEU
18	Z	273	ASN
18	Z	324	VAL
18	Z	404	ASP
18	Z	457	ASN
18	Z	662	MET
18	Z	664	GLU
18	Z	701	ASN
18	Z	705	ASN
18	Z	810	ILE
18	Z	815	HIS
18	Z	837	LEU
18	Z	892	PRO
20	C	40	ALA
20	C	198	PHE
22	E	50	VAL
23	F	120	ALA
25	X	207	LYS
28	c	156	PRO
20	i	40	ALA
22	k	50	VAL
25	n	207	LYS
28	q	156	PRO
2	v	108	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	v	109	PRO
2	v	110	LYS
2	v	115	VAL
2	v	154	PRO
2	v	167	GLU
2	v	234	ASP
2	v	285	PHE
2	v	286	ASP
2	v	307	ASP
2	v	346	PRO
2	v	417	ILE
2	v	424	SER
1	w	165	ASP
1	w	207	HIS
1	w	220	LYS
1	w	277	HIS
1	w	278	ALA
1	w	292	THR
1	w	297	SER
1	w	321	SER
1	w	356	PRO
1	w	357	ASP
1	w	380	LEU
5	x	89	VAL
5	x	90	HIS
5	x	92	GLU
5	x	131	VAL
5	x	149	GLU
5	x	150	MET
5	x	151	ILE
5	x	152	GLY
5	x	229	ARG
5	x	284	GLU
5	x	288	ASN
5	x	310	ARG
5	x	352	PRO
6	y	85	ILE
6	y	97	ASP
6	y	119	ILE
6	y	120	ASP
6	y	122	GLU
6	y	125	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	y	151	ILE
6	y	152	MET
6	y	155	THR
6	y	162	VAL
6	y	223	THR
6	y	258	ALA
6	y	273	LYS
6	y	274	ARG
6	y	278	GLN
6	y	300	ASP
6	y	336	PRO
6	y	360	LEU
6	y	367	PRO
6	y	393	ILE
6	y	409	LYS
6	y	410	ASP
6	y	411	GLU
6	y	412	GLN
3	z	85	ARG
3	z	88	ASP
3	z	109	ARG
3	z	114	GLU
3	z	139	SER
3	z	194	ASN
3	z	206	LYS
3	z	237	ALA
3	z	324	GLY
3	z	358	ASP
4	0	137	ILE
4	0	140	VAL
4	0	168	TYR
4	0	184	GLN
4	0	218	GLN
4	0	244	THR
4	0	261	ILE
4	0	345	SER
4	0	378	ASP
4	0	413	THR
4	0	415	LEU
4	0	433	ALA
7	1	164	GLU
7	1	170	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	1	701	ILE
7	1	792	ASN
7	1	793	LYS
7	1	881	PRO
7	1	905	PRO
7	1	933	PRO
8	2	146	PRO
8	2	263	ALA
8	2	284	ARG
8	2	285	PRO
8	2	288	HIS
8	2	369	HIS
8	2	371	ALA
9	3	169	LEU
9	3	300	PRO
9	3	409	LEU
10	4	58	ALA
10	4	121	LYS
10	4	141	LYS
10	4	201	TYR
10	4	203	PRO
10	4	204	PRO
10	4	277	LEU
10	4	280	ALA
10	4	317	PRO
10	4	391	PRO
10	4	393	VAL
11	5	28	LEU
11	5	34	ASP
11	5	131	THR
11	5	254	PRO
11	5	268	TYR
11	5	269	SER
11	5	289	ALA
12	6	218	TYR
12	6	279	GLN
12	6	321	ALA
12	6	346	LEU
12	6	351	PRO
12	6	464	ILE
12	6	505	LEU
12	6	507	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	7	216	PRO
13	7	312	PRO
13	7	319	ALA
13	7	323	GLN
13	7	325	PRO
14	8	117	PRO
14	8	128	PRO
14	8	222	ILE
14	8	240	VAL
14	8	241	SER
15	9	52	GLU
15	9	226	MET
16	AA	62	THR
16	AA	65	THR
16	AA	66	PRO
16	AA	67	ASP
16	AA	78	VAL
17	AB	38	VAL
17	AB	45	ASP
17	AB	46	ASP
17	AB	48	VAL
18	AC	203	GLU
18	AC	228	LYS
18	AC	256	PHE
18	AC	257	ARG
18	AC	258	LYS
18	AC	272	LEU
18	AC	273	ASN
18	AC	324	VAL
18	AC	404	ASP
18	AC	457	ASN
18	AC	662	MET
18	AC	664	GLU
18	AC	701	ASN
18	AC	705	ASN
18	AC	810	ILE
18	AC	815	HIS
18	AC	837	LEU
18	AC	892	PRO
1	I	119	ASN
1	I	167	THR
1	I	296	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	300	GLY
2	H	103	ASN
2	H	133	ASP
2	H	166	VAL
2	H	205	GLY
2	H	206	ILE
2	H	235	ALA
2	H	292	ASP
2	H	378	PRO
2	H	399	ALA
3	L	131	SER
3	L	208	ILE
3	L	244	SER
3	L	254	GLN
3	L	357	ALA
4	M	85	THR
4	M	165	PRO
4	M	216	GLY
4	M	217	ILE
4	M	222	GLY
4	M	287	GLU
4	M	300	LYS
4	M	371	ARG
4	M	372	LYS
4	M	392	ASN
4	M	409	ARG
4	M	411	GLY
4	M	432	LYS
5	J	84	LYS
5	J	148	TYR
5	J	287	LYS
6	K	126	PRO
6	K	156	SER
6	K	299	PHE
6	K	303	VAL
6	K	304	ASN
6	K	368	ASP
6	K	391	ARG
7	N	120	GLU
7	N	174	PRO
7	N	175	GLY
7	N	427	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	N	776	SER
7	N	908	ILE
8	O	104	VAL
8	O	107	SER
8	O	109	GLU
8	O	148	VAL
8	O	150	SER
8	O	287	ASN
9	P	56	THR
9	P	316	ARG
10	Q	37	GLU
10	Q	242	ILE
10	Q	321	THR
10	Q	392	PRO
11	R	31	HIS
11	R	32	ARG
11	R	37	VAL
11	R	49	ASN
11	R	133	ALA
12	S	319	HIS
12	S	506	GLU
13	T	238	GLU
13	T	239	GLY
13	T	318	PHE
13	T	324	LYS
14	U	99	PRO
14	U	101	LEU
14	U	176	LEU
14	U	186	THR
14	U	218	GLY
14	U	224	HIS
15	V	53	VAL
15	V	153	GLY
17	Y	18	GLU
17	Y	40	GLU
18	Z	365	VAL
18	Z	455	VAL
18	Z	514	VAL
18	Z	599	ALA
18	Z	600	TYR
18	Z	663	GLY
22	E	101	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
24	G	238	GLU
25	X	4	GLY
27	b	188	PRO
28	c	117	PHE
22	k	46	GLU
22	k	101	PRO
24	m	197	GLU
28	q	117	PHE
2	v	93	LEU
2	v	103	ASN
2	v	133	ASP
2	v	166	VAL
2	v	205	GLY
2	v	206	ILE
2	v	235	ALA
2	v	292	ASP
2	v	345	LEU
2	v	378	PRO
2	v	399	ALA
1	w	119	ASN
1	w	167	THR
1	w	296	ASP
1	w	300	GLY
1	w	408	ARG
1	w	409	GLU
5	x	84	LYS
5	x	148	TYR
5	x	287	LYS
6	y	126	PRO
6	y	156	SER
6	y	299	PHE
6	y	303	VAL
6	y	304	ASN
6	y	368	ASP
6	y	391	ARG
3	z	131	SER
3	z	208	ILE
3	z	244	SER
3	z	254	GLN
3	z	357	ALA
4	0	85	THR
4	0	165	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	0	216	GLY
4	0	217	ILE
4	0	222	GLY
4	0	287	GLU
4	0	300	LYS
4	0	371	ARG
4	0	372	LYS
4	0	392	ASN
4	0	409	ARG
4	0	411	GLY
4	0	432	LYS
7	1	120	GLU
7	1	174	PRO
7	1	175	GLY
7	1	427	LEU
7	1	776	SER
7	1	908	ILE
8	2	104	VAL
8	2	107	SER
8	2	109	GLU
8	2	148	VAL
8	2	150	SER
8	2	287	ASN
9	3	56	THR
9	3	316	ARG
10	4	37	GLU
10	4	60	THR
10	4	242	ILE
10	4	321	THR
10	4	392	PRO
11	5	31	HIS
11	5	32	ARG
11	5	37	VAL
11	5	49	ASN
11	5	133	ALA
12	6	319	HIS
12	6	466	ILE
12	6	506	GLU
13	7	238	GLU
13	7	239	GLY
13	7	318	PHE
13	7	324	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	8	99	PRO
14	8	101	LEU
14	8	176	LEU
14	8	186	THR
14	8	218	GLY
14	8	224	HIS
15	9	53	VAL
15	9	153	GLY
17	AB	18	GLU
17	AB	40	GLU
18	AC	365	VAL
18	AC	455	VAL
18	AC	514	VAL
18	AC	599	ALA
18	AC	600	TYR
18	AC	663	GLY
18	AC	666	ILE
1	I	103	ARG
1	I	106	PRO
1	I	172	THR
1	I	191	ASP
1	I	217	LYS
1	I	410	ARG
1	I	427	LEU
2	H	116	LYS
2	H	139	ARG
2	H	197	HIS
2	H	209	PRO
2	H	310	ASP
2	H	346	PRO
3	L	138	LEU
3	L	192	ASP
3	L	193	CYS
3	L	241	ARG
3	L	247	THR
3	L	339	ASN
4	M	122	ALA
4	M	180	ARG
4	M	280	PRO
4	M	296	PHE
4	M	344	ARG
4	M	347	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	M	373	MET
4	M	377	PRO
4	M	379	VAL
4	M	410	ARG
5	J	27	LYS
5	J	37	ASP
5	J	78	ARG
5	J	133	PRO
5	J	228	ALA
5	J	308	PRO
5	J	312	ASP
6	K	121	ARG
6	K	320	ALA
6	K	390	ASN
6	K	407	ILE
7	N	119	PRO
7	N	163	PHE
7	N	771	PHE
7	N	884	VAL
7	N	907	SER
8	O	258	GLN
8	O	259	PRO
9	P	76	GLU
10	Q	17	SER
10	Q	38	ASN
10	Q	59	LYS
10	Q	123	THR
10	Q	202	CYS
10	Q	245	PRO
10	Q	320	SER
11	R	51	ALA
12	S	503	LYS
13	T	237	MET
14	U	33	LYS
15	V	104	ARG
15	V	150	SER
16	W	77	THR
17	Y	39	TRP
18	Z	227	ALA
18	Z	397	LYS
18	Z	420	TRP
18	Z	458	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	Z	472	HIS
18	Z	598	CYS
18	Z	738	ASN
18	Z	739	ALA
18	Z	811	LEU
19	B	188	ASP
19	B	189	TRP
19	B	210	PHE
22	E	46	GLU
22	E	201	SER
24	G	226	ASP
24	G	235	GLY
32	g	46	ASN
20	i	202	MET
22	k	201	SER
23	l	120	ALA
24	m	235	GLY
27	p	187	ARG
32	u	46	ASN
2	v	116	LYS
2	v	139	ARG
2	v	197	HIS
2	v	209	PRO
2	v	310	ASP
1	w	103	ARG
1	w	106	PRO
1	w	172	THR
1	w	191	ASP
1	w	217	LYS
1	w	427	LEU
5	x	27	LYS
5	x	37	ASP
5	x	78	ARG
5	x	133	PRO
5	x	228	ALA
5	x	308	PRO
5	x	312	ASP
6	y	121	ARG
6	y	320	ALA
6	y	390	ASN
6	y	407	ILE
3	z	138	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	z	192	ASP
3	z	193	CYS
3	z	241	ARG
3	z	247	THR
3	z	339	ASN
4	0	122	ALA
4	0	180	ARG
4	0	280	PRO
4	0	296	PHE
4	0	344	ARG
4	0	347	ARG
4	0	373	MET
4	0	377	PRO
4	0	379	VAL
4	0	410	ARG
7	1	119	PRO
7	1	163	PHE
7	1	771	PHE
7	1	884	VAL
7	1	907	SER
8	2	258	GLN
8	2	259	PRO
9	3	76	GLU
10	4	17	SER
10	4	38	ASN
10	4	123	THR
10	4	202	CYS
10	4	245	PRO
10	4	320	SER
11	5	51	ALA
12	6	503	LYS
13	7	237	MET
14	8	33	LYS
15	9	104	ARG
15	9	150	SER
16	AA	77	THR
17	AB	39	TRP
18	AC	227	ALA
18	AC	397	LYS
18	AC	420	TRP
18	AC	458	GLU
18	AC	472	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	AC	598	CYS
18	AC	738	ASN
18	AC	739	ALA
18	AC	811	LEU
1	I	182	GLU
2	H	134	ILE
2	H	172	VAL
2	H	192	GLU
2	H	425	ALA
3	L	130	VAL
3	L	152	PRO
3	L	234	GLU
3	L	366	ASP
3	L	383	LYS
4	M	321	GLN
5	J	66	LEU
5	J	69	GLN
5	J	283	PHE
6	K	266	GLU
7	N	470	ASN
7	N	912	ILE
7	N	927	PRO
8	O	108	ASP
9	P	79	GLU
9	P	385	SER
9	P	418	PRO
9	P	421	PRO
10	Q	81	SER
11	R	30	GLU
11	R	156	LEU
11	R	255	ALA
12	S	221	LEU
12	S	300	LEU
12	S	350	GLN
13	T	125	GLU
13	T	179	LYS
13	T	219	ASP
13	T	326	GLU
15	V	49	VAL
15	V	263	ASP
16	W	64	LEU
18	Z	202	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	Z	262	PHE
18	Z	475	ASN
18	Z	597	VAL
18	Z	716	ASP
18	Z	842	VAL
19	B	207	SER
21	D	206	LEU
21	j	206	LEU
24	m	238	GLU
27	p	188	PRO
2	v	134	ILE
2	v	172	VAL
2	v	192	GLU
2	v	425	ALA
1	w	182	GLU
5	x	66	LEU
5	x	69	GLN
5	x	283	PHE
6	y	266	GLU
3	z	130	VAL
3	z	152	PRO
3	z	234	GLU
3	z	366	ASP
3	z	383	LYS
4	0	321	GLN
7	1	470	ASN
7	1	912	ILE
7	1	927	PRO
8	2	108	ASP
9	3	79	GLU
9	3	385	SER
9	3	418	PRO
9	3	421	PRO
10	4	81	SER
11	5	30	GLU
11	5	156	LEU
11	5	255	ALA
12	6	221	LEU
12	6	300	LEU
12	6	350	GLN
13	7	125	GLU
13	7	179	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	7	219	ASP
13	7	326	GLU
15	9	49	VAL
15	9	263	ASP
16	AA	64	LEU
18	AC	202	HIS
18	AC	262	PHE
18	AC	475	ASN
18	AC	597	VAL
18	AC	716	ASP
18	AC	842	VAL
1	I	299	SER
2	H	85	GLN
2	H	96	ALA
2	H	198	PRO
2	H	309	PHE
3	L	266	GLY
3	L	296	ASP
4	M	77	SER
4	M	148	GLY
4	M	376	SER
5	J	142	LYS
5	J	297	ARG
6	K	257	ASN
7	N	904	LYS
7	N	928	VAL
8	O	228	THR
10	Q	6	VAL
10	Q	224	ASP
10	Q	340	GLU
11	R	152	MET
11	R	153	ASP
11	R	154	ASN
11	R	198	ALA
11	R	253	LEU
13	T	328	THR
14	U	179	ILE
16	W	164	ASP
16	W	177	PRO
17	Y	15	GLU
18	Z	114	ALA
18	Z	322	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
18	Z	602	GLY
22	E	243	LYS
2	v	85	GLN
2	v	96	ALA
2	v	198	PRO
2	v	309	PHE
1	w	299	SER
5	x	142	LYS
5	x	297	ARG
6	y	257	ASN
3	z	266	GLY
3	z	296	ASP
4	0	77	SER
4	0	148	GLY
4	0	376	SER
7	1	904	LYS
7	1	928	VAL
8	2	228	THR
10	4	6	VAL
10	4	224	ASP
10	4	340	GLU
11	5	152	MET
11	5	153	ASP
11	5	154	ASN
11	5	198	ALA
11	5	253	LEU
13	7	328	THR
14	8	179	ILE
16	AA	164	ASP
16	AA	177	PRO
17	AB	15	GLU
18	AC	114	ALA
18	AC	602	GLY
18	AC	661	ALA
1	I	408	ARG
3	L	116	ASP
3	L	319	PRO
3	L	337	GLY
6	K	86	PRO
6	K	197	ASP
6	K	208	PRO
7	N	84	ALA

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	O	340	VAL
10	Q	244	SER
10	Q	341	PRO
11	R	53	TYR
12	S	182	LYS
14	U	119	SER
15	V	232	GLN
18	Z	263	PRO
18	Z	380	PHE
18	Z	559	PRO
22	k	243	LYS
6	y	86	PRO
6	y	197	ASP
6	y	208	PRO
3	z	116	ASP
3	z	319	PRO
3	z	337	GLY
7	1	84	ALA
8	2	340	VAL
10	4	244	SER
10	4	341	PRO
11	5	53	TYR
12	6	182	LYS
14	8	119	SER
15	9	232	GLN
18	AC	263	PRO
18	AC	380	PHE
18	AC	559	PRO
3	L	128	GLY
4	M	181	PRO
4	M	335	VAL
5	J	144	PRO
5	J	320	PRO
12	S	70	VAL
13	T	330	ILE
16	W	22	LEU
18	Z	604	GLY
29	r	197	PRO
5	x	144	PRO
5	x	320	PRO
3	z	128	GLY
4	0	181	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	0	335	VAL
12	6	70	VAL
13	7	330	ILE
16	AA	22	LEU
18	AC	604	GLY
3	L	126	ASP
5	J	192	PRO
6	K	207	PRO
8	O	18	GLN
9	P	171	VAL
10	Q	361	VAL
14	U	185	GLY
16	W	117	VAL
29	d	197	PRO
1	w	414	VAL
5	x	192	PRO
6	y	207	PRO
3	z	126	ASP
8	2	18	GLN
9	3	171	VAL
10	4	361	VAL
14	8	185	GLY
16	AA	117	VAL
1	I	301	GLY
2	H	159	PRO
2	H	333	ARG
3	L	115	VAL
3	L	240	GLY
4	M	262	GLY
7	N	913	ILE
8	O	185	ILE
10	Q	50	ILE
11	R	65	ILE
11	R	67	VAL
26	a	30	VAL
25	n	216	VAL
26	o	30	VAL
2	v	159	PRO
2	v	333	ARG
1	w	301	GLY
3	z	115	VAL
3	z	240	GLY

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	0	262	GLY
7	1	913	ILE
8	2	185	ILE
10	4	50	ILE
11	5	65	ILE
11	5	67	VAL
1	I	287	ILE
1	I	343	ARG
5	J	182	GLN
6	K	194	ILE
7	N	507	VAL
15	V	50	PRO
15	V	267	PRO
18	Z	702	PRO
18	Z	872	VAL
23	F	158	PRO
25	X	216	VAL
1	w	287	ILE
1	w	343	ARG
5	x	182	GLN
6	y	194	ILE
7	1	507	VAL
15	9	50	PRO
15	9	267	PRO
18	AC	702	PRO
18	AC	872	VAL
3	L	292	PRO
3	L	363	VAL
4	M	188	ILE
5	J	132	ASP
7	N	124	LYS
9	P	200	ILE
11	R	277	VAL
15	V	308	VAL
5	x	132	ASP
3	z	292	PRO
3	z	363	VAL
4	0	188	ILE
7	1	124	LYS
9	3	200	ILE
11	5	277	VAL
15	9	308	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	291/385 (76%)	229 (79%)	62 (21%)	1	5
1	w	291/385 (76%)	227 (78%)	64 (22%)	1	5
2	H	298/372 (80%)	232 (78%)	66 (22%)	1	5
2	v	297/372 (80%)	232 (78%)	65 (22%)	1	5
3	L	298/341 (87%)	233 (78%)	65 (22%)	1	5
3	z	298/341 (87%)	233 (78%)	65 (22%)	1	5
4	0	296/379 (78%)	240 (81%)	56 (19%)	1	8
4	M	296/379 (78%)	240 (81%)	56 (19%)	1	8
5	J	310/352 (88%)	244 (79%)	66 (21%)	1	5
5	x	310/352 (88%)	244 (79%)	66 (21%)	1	5
6	K	333/366 (91%)	272 (82%)	61 (18%)	1	8
6	y	333/366 (91%)	270 (81%)	63 (19%)	1	8
7	1	376/816 (46%)	344 (92%)	32 (8%)	10	39
7	N	376/816 (46%)	344 (92%)	32 (8%)	10	39
8	2	142/336 (42%)	124 (87%)	18 (13%)	4	22
8	O	141/336 (42%)	123 (87%)	18 (13%)	4	22
9	3	201/416 (48%)	181 (90%)	20 (10%)	7	32
9	P	202/416 (49%)	181 (90%)	21 (10%)	7	31
10	4	250/362 (69%)	210 (84%)	40 (16%)	2	14
10	Q	249/362 (69%)	209 (84%)	40 (16%)	2	14
11	5	229/344 (67%)	202 (88%)	27 (12%)	5	25
11	R	228/344 (66%)	202 (89%)	26 (11%)	5	26
12	6	164/452 (36%)	153 (93%)	11 (7%)	16	48
12	S	163/452 (36%)	152 (93%)	11 (7%)	16	48
13	7	108/294 (37%)	91 (84%)	17 (16%)	2	15
13	T	109/294 (37%)	92 (84%)	17 (16%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	8	211/295 (72%)	186 (88%)	25 (12%)	5	25
14	U	212/295 (72%)	186 (88%)	26 (12%)	4	23
15	9	218/268 (81%)	187 (86%)	31 (14%)	3	19
15	V	219/268 (82%)	188 (86%)	31 (14%)	3	19
16	AA	111/312 (36%)	104 (94%)	7 (6%)	18	51
16	W	111/312 (36%)	103 (93%)	8 (7%)	14	45
17	AB	6/63 (10%)	6 (100%)	0	100	100
17	Y	6/63 (10%)	6 (100%)	0	100	100
19	B	193/210 (92%)	180 (93%)	13 (7%)	16	48
19	h	195/210 (93%)	182 (93%)	13 (7%)	16	48
20	C	175/191 (92%)	170 (97%)	5 (3%)	42	71
20	i	177/191 (93%)	164 (93%)	13 (7%)	14	45
21	D	194/221 (88%)	186 (96%)	8 (4%)	30	63
21	j	193/221 (87%)	186 (96%)	7 (4%)	35	66
22	E	152/211 (72%)	140 (92%)	12 (8%)	12	41
22	k	142/211 (67%)	132 (93%)	10 (7%)	15	46
23	F	190/203 (94%)	186 (98%)	4 (2%)	53	79
23	l	191/203 (94%)	184 (96%)	7 (4%)	34	65
24	G	198/224 (88%)	192 (97%)	6 (3%)	41	71
24	m	198/224 (88%)	188 (95%)	10 (5%)	24	57
25	X	193/212 (91%)	187 (97%)	6 (3%)	40	70
25	n	193/212 (91%)	184 (95%)	9 (5%)	26	60
26	a	155/181 (86%)	151 (97%)	4 (3%)	46	74
26	o	155/181 (86%)	152 (98%)	3 (2%)	57	80
27	b	177/228 (78%)	171 (97%)	6 (3%)	37	68
27	p	177/228 (78%)	172 (97%)	5 (3%)	43	72
28	c	172/174 (99%)	164 (95%)	8 (5%)	26	60
28	q	172/174 (99%)	164 (95%)	8 (5%)	26	60
29	d	164/171 (96%)	159 (97%)	5 (3%)	41	71
29	r	164/171 (96%)	160 (98%)	4 (2%)	49	76
30	e	153/202 (76%)	149 (97%)	4 (3%)	46	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	s	154/202 (76%)	149 (97%)	5 (3%)	39	69
31	f	175/199 (88%)	167 (95%)	8 (5%)	27	61
31	t	175/199 (88%)	169 (97%)	6 (3%)	37	68
32	g	175/215 (81%)	167 (95%)	8 (5%)	27	61
32	u	175/215 (81%)	165 (94%)	10 (6%)	20	53
All	All	12610/17990 (70%)	11190 (89%)	1420 (11%)	9	27

All (1420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	103	ARG
1	I	105	THR
1	I	113	GLU
1	I	118	ASP
1	I	120	HIS
1	I	126	SER
1	I	129	SER
1	I	141	LYS
1	I	156	VAL
1	I	162	VAL
1	I	164	MET
1	I	167	THR
1	I	178	LYS
1	I	182	GLU
1	I	183	THR
1	I	193	GLN
1	I	195	GLN
1	I	207	HIS
1	I	210	TYR
1	I	220	LYS
1	I	235	LEU
1	I	237	LYS
1	I	242	GLN
1	I	255	LEU
1	I	257	GLN
1	I	258	LYS
1	I	259	TYR
1	I	260	LEU
1	I	262	ASP
1	I	272	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	275	GLU
1	I	286	GLU
1	I	287	ILE
1	I	293	LYS
1	I	294	ARG
1	I	296	ASP
1	I	299	SER
1	I	302	GLU
1	I	303	ARG
1	I	313	LEU
1	I	315	GLN
1	I	319	PHE
1	I	321	SER
1	I	322	ARG
1	I	324	ASP
1	I	329	MET
1	I	331	THR
1	I	333	ARG
1	I	337	LEU
1	I	342	ILE
1	I	344	PRO
1	I	346	ARG
1	I	348	ASP
1	I	350	LYS
1	I	365	PHE
1	I	366	GLN
1	I	373	THR
1	I	385	MET
1	I	388	ASP
1	I	399	CYS
1	I	408	ARG
1	I	410	ARG
2	H	93	LEU
2	H	103	ASN
2	H	110	LYS
2	H	111	TYR
2	H	114	ASN
2	H	125	LEU
2	H	135	GLU
2	H	148	GLN
2	H	150	HIS
2	H	153	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	164	MET
2	H	166	VAL
2	H	168	GLU
2	H	180	CYS
2	H	183	GLN
2	H	187	LEU
2	H	188	ARG
2	H	199	GLU
2	H	200	ARG
2	H	203	ASN
2	H	204	LEU
2	H	213	LEU
2	H	220	THR
2	H	234	ASP
2	H	239	ARG
2	H	247	GLN
2	H	265	ARG
2	H	267	LYS
2	H	276	GLU
2	H	277	ILE
2	H	278	ASP
2	H	284	ARG
2	H	285	PHE
2	H	287	ASP
2	H	294	GLU
2	H	299	MET
2	H	307	ASP
2	H	309	PHE
2	H	312	ARG
2	H	315	ILE
2	H	319	MET
2	H	322	ASN
2	H	327	LEU
2	H	329	PRO
2	H	332	MET
2	H	334	PRO
2	H	338	ASP
2	H	340	LYS
2	H	342	GLU
2	H	353	HIS
2	H	355	PHE
2	H	358	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	369	ARG
2	H	377	CYS
2	H	379	ASN
2	H	398	ARG
2	H	400	ARG
2	H	401	ARG
2	H	403	ILE
2	H	415	LYS
2	H	419	SER
2	H	422	LYS
2	H	423	PHE
2	H	424	SER
2	H	430	MET
2	H	431	THR
3	L	86	GLN
3	L	87	LEU
3	L	96	THR
3	L	97	ARG
3	L	105	LEU
3	L	108	MET
3	L	109	ARG
3	L	113	ARG
3	L	114	GLU
3	L	116	ASP
3	L	118	LEU
3	L	120	TYR
3	L	122	MET
3	L	123	SER
3	L	129	ASN
3	L	132	TYR
3	L	134	GLU
3	L	138	LEU
3	L	153	LEU
3	L	158	LEU
3	L	159	PHE
3	L	183	LEU
3	L	193	CYS
3	L	196	LEU
3	L	197	LYS
3	L	200	SER
3	L	202	SER
3	L	206	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	L	216	ARG
3	L	225	HIS
3	L	226	GLN
3	L	234	GLU
3	L	235	ILE
3	L	238	ILE
3	L	241	ARG
3	L	242	ARG
3	L	244	SER
3	L	245	GLU
3	L	247	THR
3	L	251	ARG
3	L	254	GLN
3	L	255	ARG
3	L	257	LEU
3	L	260	LEU
3	L	261	LEU
3	L	267	PHE
3	L	268	ASP
3	L	271	HIS
3	L	272	ARG
3	L	281	ARG
3	L	283	ASP
3	L	307	GLN
3	L	322	LYS
3	L	334	LEU
3	L	344	ARG
3	L	356	ARG
3	L	358	ASP
3	L	361	PHE
3	L	363	VAL
3	L	364	GLN
3	L	367	PHE
3	L	368	MET
3	L	372	ARG
3	L	383	LYS
3	L	385	ASP
4	M	88	TYR
4	M	89	LEU
4	M	95	GLU
4	M	96	LEU
4	M	125	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	M	134	LEU
4	M	149	ASP
4	M	163	THR
4	M	166	THR
4	M	168	TYR
4	M	170	SER
4	M	178	ASP
4	M	182	THR
4	M	183	GLU
4	M	187	ASP
4	M	206	MET
4	M	209	LYS
4	M	221	LYS
4	M	225	MET
4	M	231	THR
4	M	233	LYS
4	M	250	LYS
4	M	266	LYS
4	M	272	PHE
4	M	284	PHE
4	M	289	ASP
4	M	295	ARG
4	M	296	PHE
4	M	299	GLU
4	M	304	ARG
4	M	305	GLU
4	M	307	GLN
4	M	310	MET
4	M	318	ASP
4	M	320	PHE
4	M	323	ASN
4	M	327	LYS
4	M	334	ARG
4	M	338	LEU
4	M	339	ASP
4	M	344	ARG
4	M	348	LEU
4	M	351	LYS
4	M	364	ARG
4	M	366	MET
4	M	367	GLN
4	M	369	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	M	372	LYS
4	M	378	ASP
4	M	388	THR
4	M	409	ARG
4	M	415	LEU
4	M	416	THR
4	M	425	LEU
4	M	430	LYS
4	M	435	LEU
5	J	25	LEU
5	J	33	LEU
5	J	38	LYS
5	J	39	SER
5	J	43	ARG
5	J	46	GLN
5	J	49	ARG
5	J	51	GLU
5	J	57	ARG
5	J	60	ARG
5	J	61	GLU
5	J	69	GLN
5	J	71	SER
5	J	78	ARG
5	J	80	MET
5	J	82	LYS
5	J	84	LYS
5	J	85	VAL
5	J	111	ASN
5	J	113	ARG
5	J	118	ASN
5	J	130	LYS
5	J	132	ASP
5	J	139	MET
5	J	142	LYS
5	J	143	VAL
5	J	147	THR
5	J	149	GLU
5	J	155	ASP
5	J	157	GLN
5	J	173	GLU
5	J	174	LEU
5	J	184	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	J	194	THR
5	J	198	LEU
5	J	199	LEU
5	J	201	ARG
5	J	207	THR
5	J	210	THR
5	J	213	ARG
5	J	217	SER
5	J	226	GLU
5	J	229	ARG
5	J	230	MET
5	J	249	ASP
5	J	270	GLN
5	J	271	ARG
5	J	273	MET
5	J	275	GLU
5	J	279	GLN
5	J	280	LEU
5	J	283	PHE
5	J	284	GLU
5	J	286	THR
5	J	287	LYS
5	J	290	LYS
5	J	293	MET
5	J	303	SER
5	J	305	LEU
5	J	307	ARG
5	J	308	PRO
5	J	313	ARG
5	J	316	GLU
5	J	340	ARG
5	J	374	ARG
5	J	392	GLN
6	K	40	LEU
6	K	51	LEU
6	K	53	PHE
6	K	54	LEU
6	K	58	GLU
6	K	65	GLN
6	K	72	PHE
6	K	73	LEU
6	K	82	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	K	87	LEU
6	K	93	LEU
6	K	94	GLU
6	K	98	GLN
6	K	121	ARG
6	K	125	LYS
6	K	139	LEU
6	K	143	LEU
6	K	148	ASP
6	K	152	MET
6	K	154	LEU
6	K	159	LYS
6	K	163	MET
6	K	164	TYR
6	K	171	ASP
6	K	185	LEU
6	K	188	PHE
6	K	193	GLN
6	K	202	VAL
6	K	203	LEU
6	K	205	TYR
6	K	212	LYS
6	K	229	ARG
6	K	233	SER
6	K	237	GLN
6	K	238	LYS
6	K	240	LEU
6	K	245	ARG
6	K	266	GLU
6	K	274	ARG
6	K	278	GLN
6	K	284	GLU
6	K	287	ARG
6	K	297	ASP
6	K	302	ASN
6	K	312	ASN
6	K	322	LEU
6	K	323	ARG
6	K	328	ASP
6	K	330	LYS
6	K	335	LEU
6	K	345	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	K	351	LYS
6	K	352	MET
6	K	359	ASP
6	K	369	LYS
6	K	384	MET
6	K	388	ARG
6	K	391	ARG
6	K	403	TYR
6	K	405	THR
6	K	418	LYS
7	N	17	PRO
7	N	119	PRO
7	N	125	PRO
7	N	165	LYS
7	N	168	LEU
7	N	170	SER
7	N	174	PRO
7	N	179	TYR
7	N	211	PRO
7	N	363	SER
7	N	402	PHE
7	N	407	SER
7	N	425	THR
7	N	431	THR
7	N	433	PRO
7	N	444	TYR
7	N	469	SER
7	N	471	ASP
7	N	473	VAL
7	N	576	PRO
7	N	601	ARG
7	N	630	PRO
7	N	650	TYR
7	N	758	PRO
7	N	794	ASP
7	N	808	PRO
7	N	816	PRO
7	N	881	PRO
7	N	895	PRO
7	N	905	PRO
7	N	928	VAL
7	N	933	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
8	O	5	PRO
8	O	19	PRO
8	O	73	PRO
8	O	90	PRO
8	O	146	PRO
8	O	189	PRO
8	O	274	LEU
8	O	279	GLU
8	O	303	THR
8	O	339	ARG
8	O	349	MET
8	O	353	LEU
8	O	354	GLU
8	O	358	THR
8	O	362	SER
8	O	363	MET
8	O	364	GLU
8	O	368	GLU
9	P	48	LEU
9	P	49	SER
9	P	52	LYS
9	P	55	ARG
9	P	70	VAL
9	P	119	PRO
9	P	159	VAL
9	P	254	PRO
9	P	300	PRO
9	P	317	TRP
9	P	318	SER
9	P	351	TRP
9	P	373	ILE
9	P	383	ASP
9	P	398	VAL
9	P	401	THR
9	P	422	ASN
9	P	436	MET
9	P	441	LYS
9	P	448	LYS
9	P	451	MET
10	Q	82	LYS
10	Q	111	LEU
10	Q	125	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	Q	126	ARG
10	Q	145	GLU
10	Q	154	LEU
10	Q	155	ARG
10	Q	158	LYS
10	Q	166	LEU
10	Q	168	GLU
10	Q	171	LEU
10	Q	177	TYR
10	Q	185	LYS
10	Q	187	ARG
10	Q	191	THR
10	Q	207	GLN
10	Q	221	GLU
10	Q	222	GLU
10	Q	223	LYS
10	Q	230	SER
10	Q	233	TYR
10	Q	241	SER
10	Q	242	ILE
10	Q	244	SER
10	Q	249	THR
10	Q	264	PRO
10	Q	283	GLN
10	Q	296	ASN
10	Q	316	ASP
10	Q	317	PRO
10	Q	321	THR
10	Q	325	LYS
10	Q	326	LEU
10	Q	337	ARG
10	Q	392	PRO
10	Q	393	VAL
10	Q	403	THR
10	Q	409	LYS
10	Q	416	ASN
10	Q	417	LYS
11	R	23	ARG
11	R	92	GLU
11	R	134	LEU
11	R	173	ASP
11	R	179	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	R	196	GLN
11	R	202	LEU
11	R	203	ASP
11	R	207	THR
11	R	212	GLU
11	R	214	MET
11	R	238	GLU
11	R	250	LEU
11	R	254	PRO
11	R	259	TYR
11	R	260	LEU
11	R	270	VAL
11	R	292	TYR
11	R	302	HIS
11	R	304	TYR
11	R	337	PHE
11	R	366	TYR
11	R	367	GLN
11	R	371	LYS
11	R	372	LYS
11	R	379	ARG
12	S	300	LEU
12	S	307	ARG
12	S	320	THR
12	S	351	PRO
12	S	352	SER
12	S	431	PRO
12	S	467	TYR
12	S	469	THR
12	S	477	HIS
12	S	479	ARG
12	S	482	PHE
13	T	107	PRO
13	T	110	SER
13	T	130	PRO
13	T	137	THR
13	T	162	PRO
13	T	173	CYS
13	T	182	LEU
13	T	183	PRO
13	T	216	PRO
13	T	218	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	T	237	MET
13	T	296	PRO
13	T	309	VAL
13	T	312	PRO
13	T	333	THR
13	T	337	LYS
13	T	342	TYR
14	U	23	PHE
14	U	33	LYS
14	U	58	PHE
14	U	70	LEU
14	U	79	TYR
14	U	88	ARG
14	U	101	LEU
14	U	116	CYS
14	U	128	PRO
14	U	157	HIS
14	U	159	THR
14	U	166	GLU
14	U	173	GLU
14	U	175	LEU
14	U	176	LEU
14	U	177	ARG
14	U	184	VAL
14	U	196	HIS
14	U	209	ARG
14	U	245	PHE
14	U	249	PHE
14	U	252	LYS
14	U	267	ARG
14	U	273	HIS
14	U	279	LYS
14	U	282	ASN
15	V	46	ARG
15	V	50	PRO
15	V	96	LEU
15	V	98	MET
15	V	104	ARG
15	V	105	PRO
15	V	118	PHE
15	V	139	ARG
15	V	150	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
15	V	208	ARG
15	V	212	LEU
15	V	226	MET
15	V	227	GLU
15	V	229	LEU
15	V	236	GLU
15	V	237	HIS
15	V	240	HIS
15	V	248	MET
15	V	254	ASN
15	V	261	GLU
15	V	262	GLU
15	V	264	LYS
15	V	265	MET
15	V	277	LYS
15	V	281	LYS
15	V	282	ARG
15	V	285	GLU
15	V	287	HIS
15	V	295	ASN
15	V	298	GLN
15	V	299	CYS
16	W	23	PRO
16	W	58	CYS
16	W	61	LEU
16	W	63	THR
16	W	80	PRO
16	W	169	HIS
16	W	174	PRO
16	W	178	SER
19	B	73	THR
19	B	78	CYS
19	B	103	TYR
19	B	107	TYR
19	B	108	GLU
19	B	114	LEU
19	B	126	THR
19	B	132	ARG
19	B	166	THR
19	B	209	ASP
19	B	221	THR
19	B	231	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	B	234	GLU
20	C	74	VAL
20	C	132	SER
20	C	162	MET
20	C	178	ASN
20	C	189	THR
21	D	44	LEU
21	D	74	CYS
21	D	76	VAL
21	D	164	ILE
21	D	180	LYS
21	D	192	LEU
21	D	197	LEU
21	D	218	ARG
22	E	5	ARG
22	E	15	HIS
22	E	35	VAL
22	E	38	ARG
22	E	41	VAL
22	E	43	LEU
22	E	56	GLU
22	E	99	GLU
22	E	103	THR
22	E	139	ASP
22	E	146	GLN
22	E	184	ASP
23	F	20	ARG
23	F	36	THR
23	F	135	ARG
23	F	148	GLU
24	G	38	LEU
24	G	83	LEU
24	G	101	ARG
24	G	202	GLU
24	G	225	ASP
24	G	239	ARG
25	X	5	THR
25	X	39	ILE
25	X	129	ARG
25	X	144	ASP
25	X	181	MET
25	X	187	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	a	22	THR
26	a	46	SER
26	a	139	VAL
26	a	150	GLU
27	b	6	VAL
27	b	56	THR
27	b	77	VAL
27	b	187	ARG
27	b	198	ARG
27	b	201	ARG
28	c	34	MET
28	c	36	THR
28	c	49	LEU
28	c	126	LEU
28	c	175	VAL
28	c	189	ILE
28	c	191	GLU
28	c	193	ASP
29	d	18	ASP
29	d	27	GLN
29	d	45	LEU
29	d	84	THR
29	d	85	ARG
30	e	8	PHE
30	e	87	VAL
30	e	115	ASP
30	e	138	VAL
31	f	6	VAL
31	f	76	LYS
31	f	99	ARG
31	f	102	PHE
31	f	125	ASP
31	f	163	HIS
31	f	166	LEU
31	f	174	LEU
32	g	37	ARG
32	g	49	THR
32	g	86	ARG
32	g	94	ARG
32	g	141	TYR
32	g	168	LEU
32	g	192	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
32	g	205	THR
19	h	59	LYS
19	h	73	THR
19	h	78	CYS
19	h	100	ASN
19	h	114	LEU
19	h	132	ARG
19	h	159	TYR
19	h	166	THR
19	h	205	VAL
19	h	209	ASP
19	h	221	THR
19	h	231	THR
19	h	234	GLU
20	i	51	GLN
20	i	52	LYS
20	i	74	VAL
20	i	87	HIS
20	i	132	SER
20	i	178	ASN
20	i	182	GLU
20	i	183	LEU
20	i	192	LEU
20	i	195	LYS
20	i	198	PHE
20	i	201	GLN
20	i	227	ASP
21	j	44	LEU
21	j	74	CYS
21	j	76	VAL
21	j	164	ILE
21	j	180	LYS
21	j	192	LEU
21	j	218	ARG
22	k	5	ARG
22	k	15	HIS
22	k	35	VAL
22	k	38	ARG
22	k	41	VAL
22	k	99	GLU
22	k	103	THR
22	k	139	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
22	k	146	GLN
22	k	184	ASP
23	l	9	ASP
23	l	36	THR
23	l	84	ASP
23	l	135	ARG
23	l	148	GLU
23	l	168	ARG
23	l	208	GLU
24	m	38	LEU
24	m	51	ARG
24	m	77	LEU
24	m	83	LEU
24	m	101	ARG
24	m	196	ARG
24	m	202	GLU
24	m	211	SER
24	m	236	LEU
24	m	239	ARG
25	n	17	ASP
25	n	39	ILE
25	n	41	CYS
25	n	42	LYS
25	n	56	LYS
25	n	129	ARG
25	n	144	ASP
25	n	174	THR
25	n	181	MET
26	o	22	THR
26	o	139	VAL
26	o	150	GLU
27	p	6	VAL
27	p	56	THR
27	p	77	VAL
27	p	198	ARG
27	p	201	ARG
28	q	34	MET
28	q	36	THR
28	q	49	LEU
28	q	126	LEU
28	q	175	VAL
28	q	189	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
28	q	191	GLU
28	q	193	ASP
29	r	27	GLN
29	r	45	LEU
29	r	84	THR
29	r	85	ARG
30	s	8	PHE
30	s	73	ARG
30	s	87	VAL
30	s	115	ASP
30	s	138	VAL
31	t	6	VAL
31	t	99	ARG
31	t	102	PHE
31	t	125	ASP
31	t	163	HIS
31	t	166	LEU
32	u	37	ARG
32	u	49	THR
32	u	86	ARG
32	u	94	ARG
32	u	99	ARG
32	u	141	TYR
32	u	168	LEU
32	u	186	ARG
32	u	192	VAL
32	u	205	THR
2	v	93	LEU
2	v	103	ASN
2	v	110	LYS
2	v	111	TYR
2	v	114	ASN
2	v	125	LEU
2	v	135	GLU
2	v	148	GLN
2	v	150	HIS
2	v	153	LEU
2	v	164	MET
2	v	166	VAL
2	v	168	GLU
2	v	180	CYS
2	v	183	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	v	187	LEU
2	v	188	ARG
2	v	199	GLU
2	v	200	ARG
2	v	203	ASN
2	v	204	LEU
2	v	213	LEU
2	v	220	THR
2	v	234	ASP
2	v	239	ARG
2	v	247	GLN
2	v	265	ARG
2	v	276	GLU
2	v	277	ILE
2	v	278	ASP
2	v	284	ARG
2	v	285	PHE
2	v	287	ASP
2	v	294	GLU
2	v	299	MET
2	v	307	ASP
2	v	309	PHE
2	v	312	ARG
2	v	315	ILE
2	v	322	ASN
2	v	327	LEU
2	v	329	PRO
2	v	332	MET
2	v	334	PRO
2	v	338	ASP
2	v	340	LYS
2	v	342	GLU
2	v	347	ASP
2	v	353	HIS
2	v	355	PHE
2	v	358	HIS
2	v	369	ARG
2	v	377	CYS
2	v	379	ASN
2	v	398	ARG
2	v	400	ARG
2	v	401	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	v	403	ILE
2	v	415	LYS
2	v	419	SER
2	v	422	LYS
2	v	423	PHE
2	v	424	SER
2	v	430	MET
2	v	431	THR
1	w	103	ARG
1	w	105	THR
1	w	113	GLU
1	w	118	ASP
1	w	120	HIS
1	w	126	SER
1	w	129	SER
1	w	141	LYS
1	w	156	VAL
1	w	162	VAL
1	w	164	MET
1	w	167	THR
1	w	178	LYS
1	w	182	GLU
1	w	183	THR
1	w	193	GLN
1	w	195	GLN
1	w	207	HIS
1	w	210	TYR
1	w	220	LYS
1	w	235	LEU
1	w	237	LYS
1	w	242	GLN
1	w	255	LEU
1	w	257	GLN
1	w	258	LYS
1	w	259	TYR
1	w	260	LEU
1	w	262	ASP
1	w	272	ARG
1	w	275	GLU
1	w	286	GLU
1	w	287	ILE
1	w	293	LYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	w	294	ARG
1	w	296	ASP
1	w	299	SER
1	w	302	GLU
1	w	303	ARG
1	w	313	LEU
1	w	315	GLN
1	w	319	PHE
1	w	321	SER
1	w	322	ARG
1	w	324	ASP
1	w	329	MET
1	w	331	THR
1	w	333	ARG
1	w	337	LEU
1	w	342	ILE
1	w	344	PRO
1	w	346	ARG
1	w	348	ASP
1	w	350	LYS
1	w	365	PHE
1	w	366	GLN
1	w	373	THR
1	w	385	MET
1	w	388	ASP
1	w	399	CYS
1	w	408	ARG
1	w	410	ARG
1	w	412	MET
1	w	415	THR
5	x	25	LEU
5	x	33	LEU
5	x	38	LYS
5	x	39	SER
5	x	43	ARG
5	x	46	GLN
5	x	49	ARG
5	x	51	GLU
5	x	57	ARG
5	x	60	ARG
5	x	61	GLU
5	x	69	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	x	71	SER
5	x	78	ARG
5	x	80	MET
5	x	82	LYS
5	x	84	LYS
5	x	85	VAL
5	x	111	ASN
5	x	113	ARG
5	x	118	ASN
5	x	130	LYS
5	x	132	ASP
5	x	139	MET
5	x	142	LYS
5	x	143	VAL
5	x	147	THR
5	x	149	GLU
5	x	155	ASP
5	x	157	GLN
5	x	173	GLU
5	x	174	LEU
5	x	184	LYS
5	x	194	THR
5	x	198	LEU
5	x	199	LEU
5	x	201	ARG
5	x	207	THR
5	x	210	THR
5	x	213	ARG
5	x	217	SER
5	x	226	GLU
5	x	229	ARG
5	x	230	MET
5	x	249	ASP
5	x	270	GLN
5	x	271	ARG
5	x	273	MET
5	x	275	GLU
5	x	279	GLN
5	x	280	LEU
5	x	283	PHE
5	x	284	GLU
5	x	286	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	x	287	LYS
5	x	290	LYS
5	x	293	MET
5	x	303	SER
5	x	305	LEU
5	x	307	ARG
5	x	308	PRO
5	x	313	ARG
5	x	316	GLU
5	x	340	ARG
5	x	374	ARG
5	x	392	GLN
6	y	40	LEU
6	y	51	LEU
6	y	53	PHE
6	y	54	LEU
6	y	58	GLU
6	y	65	GLN
6	y	72	PHE
6	y	73	LEU
6	y	82	ILE
6	y	87	LEU
6	y	93	LEU
6	y	94	GLU
6	y	98	GLN
6	y	121	ARG
6	y	125	LYS
6	y	139	LEU
6	y	143	LEU
6	y	148	ASP
6	y	152	MET
6	y	154	LEU
6	y	159	LYS
6	y	163	MET
6	y	164	TYR
6	y	170	MET
6	y	171	ASP
6	y	185	LEU
6	y	188	PHE
6	y	193	GLN
6	y	202	VAL
6	y	203	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	y	205	TYR
6	y	212	LYS
6	y	229	ARG
6	y	233	SER
6	y	237	GLN
6	y	238	LYS
6	y	240	LEU
6	y	245	ARG
6	y	266	GLU
6	y	274	ARG
6	y	278	GLN
6	y	284	GLU
6	y	287	ARG
6	y	297	ASP
6	y	302	ASN
6	y	312	ASN
6	y	322	LEU
6	y	323	ARG
6	y	328	ASP
6	y	330	LYS
6	y	335	LEU
6	y	345	PHE
6	y	351	LYS
6	y	352	MET
6	y	359	ASP
6	y	369	LYS
6	y	379	CYS
6	y	384	MET
6	y	388	ARG
6	y	391	ARG
6	y	403	TYR
6	y	405	THR
6	y	418	LYS
3	z	86	GLN
3	z	87	LEU
3	z	96	THR
3	z	97	ARG
3	z	105	LEU
3	z	108	MET
3	z	109	ARG
3	z	113	ARG
3	z	114	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	z	116	ASP
3	z	118	LEU
3	z	120	TYR
3	z	122	MET
3	z	123	SER
3	z	129	ASN
3	z	132	TYR
3	z	134	GLU
3	z	138	LEU
3	z	153	LEU
3	z	158	LEU
3	z	159	PHE
3	z	183	LEU
3	z	193	CYS
3	z	196	LEU
3	z	197	LYS
3	z	200	SER
3	z	202	SER
3	z	206	LYS
3	z	216	ARG
3	z	225	HIS
3	z	226	GLN
3	z	234	GLU
3	z	235	ILE
3	z	238	ILE
3	z	241	ARG
3	z	242	ARG
3	z	244	SER
3	z	245	GLU
3	z	247	THR
3	z	251	ARG
3	z	254	GLN
3	z	255	ARG
3	z	257	LEU
3	z	260	LEU
3	z	261	LEU
3	z	267	PHE
3	z	268	ASP
3	z	271	HIS
3	z	272	ARG
3	z	281	ARG
3	z	283	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	z	307	GLN
3	z	322	LYS
3	z	334	LEU
3	z	344	ARG
3	z	356	ARG
3	z	358	ASP
3	z	361	PHE
3	z	363	VAL
3	z	364	GLN
3	z	367	PHE
3	z	368	MET
3	z	372	ARG
3	z	383	LYS
3	z	385	ASP
4	0	88	TYR
4	0	89	LEU
4	0	95	GLU
4	0	96	LEU
4	0	125	LYS
4	0	134	LEU
4	0	149	ASP
4	0	163	THR
4	0	166	THR
4	0	168	TYR
4	0	170	SER
4	0	178	ASP
4	0	182	THR
4	0	183	GLU
4	0	187	ASP
4	0	206	MET
4	0	209	LYS
4	0	221	LYS
4	0	225	MET
4	0	231	THR
4	0	233	LYS
4	0	250	LYS
4	0	266	LYS
4	0	272	PHE
4	0	284	PHE
4	0	289	ASP
4	0	295	ARG
4	0	296	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	0	299	GLU
4	0	304	ARG
4	0	305	GLU
4	0	307	GLN
4	0	310	MET
4	0	318	ASP
4	0	320	PHE
4	0	323	ASN
4	0	327	LYS
4	0	334	ARG
4	0	338	LEU
4	0	339	ASP
4	0	344	ARG
4	0	348	LEU
4	0	351	LYS
4	0	364	ARG
4	0	366	MET
4	0	367	GLN
4	0	369	HIS
4	0	372	LYS
4	0	378	ASP
4	0	388	THR
4	0	409	ARG
4	0	415	LEU
4	0	416	THR
4	0	425	LEU
4	0	430	LYS
4	0	435	LEU
7	1	17	PRO
7	1	119	PRO
7	1	125	PRO
7	1	165	LYS
7	1	168	LEU
7	1	170	SER
7	1	174	PRO
7	1	179	TYR
7	1	211	PRO
7	1	271	VAL
7	1	363	SER
7	1	402	PHE
7	1	407	SER
7	1	425	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
7	1	431	THR
7	1	433	PRO
7	1	444	TYR
7	1	469	SER
7	1	471	ASP
7	1	576	PRO
7	1	601	ARG
7	1	630	PRO
7	1	650	TYR
7	1	758	PRO
7	1	794	ASP
7	1	808	PRO
7	1	816	PRO
7	1	881	PRO
7	1	895	PRO
7	1	905	PRO
7	1	928	VAL
7	1	933	PRO
8	2	5	PRO
8	2	19	PRO
8	2	73	PRO
8	2	90	PRO
8	2	146	PRO
8	2	189	PRO
8	2	274	LEU
8	2	279	GLU
8	2	303	THR
8	2	339	ARG
8	2	349	MET
8	2	353	LEU
8	2	354	GLU
8	2	358	THR
8	2	362	SER
8	2	363	MET
8	2	364	GLU
8	2	368	GLU
9	3	48	LEU
9	3	49	SER
9	3	52	LYS
9	3	55	ARG
9	3	70	VAL
9	3	119	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
9	3	159	VAL
9	3	254	PRO
9	3	300	PRO
9	3	317	TRP
9	3	318	SER
9	3	351	TRP
9	3	373	ILE
9	3	383	ASP
9	3	401	THR
9	3	422	ASN
9	3	436	MET
9	3	441	LYS
9	3	448	LYS
9	3	451	MET
10	4	82	LYS
10	4	111	LEU
10	4	125	LEU
10	4	126	ARG
10	4	145	GLU
10	4	154	LEU
10	4	155	ARG
10	4	158	LYS
10	4	166	LEU
10	4	168	GLU
10	4	171	LEU
10	4	177	TYR
10	4	185	LYS
10	4	187	ARG
10	4	191	THR
10	4	207	GLN
10	4	221	GLU
10	4	222	GLU
10	4	223	LYS
10	4	230	SER
10	4	233	TYR
10	4	241	SER
10	4	242	ILE
10	4	244	SER
10	4	249	THR
10	4	264	PRO
10	4	283	GLN
10	4	296	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
10	4	316	ASP
10	4	317	PRO
10	4	321	THR
10	4	325	LYS
10	4	326	LEU
10	4	337	ARG
10	4	392	PRO
10	4	393	VAL
10	4	403	THR
10	4	409	LYS
10	4	416	ASN
10	4	417	LYS
11	5	23	ARG
11	5	50	MET
11	5	92	GLU
11	5	134	LEU
11	5	173	ASP
11	5	179	ARG
11	5	196	GLN
11	5	202	LEU
11	5	203	ASP
11	5	207	THR
11	5	212	GLU
11	5	214	MET
11	5	238	GLU
11	5	250	LEU
11	5	254	PRO
11	5	259	TYR
11	5	260	LEU
11	5	270	VAL
11	5	292	TYR
11	5	302	HIS
11	5	304	TYR
11	5	337	PHE
11	5	366	TYR
11	5	367	GLN
11	5	371	LYS
11	5	372	LYS
11	5	379	ARG
12	6	300	LEU
12	6	307	ARG
12	6	320	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
12	6	351	PRO
12	6	352	SER
12	6	431	PRO
12	6	467	TYR
12	6	469	THR
12	6	477	HIS
12	6	479	ARG
12	6	482	PHE
13	7	107	PRO
13	7	110	SER
13	7	130	PRO
13	7	137	THR
13	7	162	PRO
13	7	173	CYS
13	7	182	LEU
13	7	183	PRO
13	7	216	PRO
13	7	218	LYS
13	7	237	MET
13	7	296	PRO
13	7	309	VAL
13	7	312	PRO
13	7	333	THR
13	7	337	LYS
13	7	342	TYR
14	8	23	PHE
14	8	33	LYS
14	8	58	PHE
14	8	79	TYR
14	8	88	ARG
14	8	101	LEU
14	8	116	CYS
14	8	128	PRO
14	8	157	HIS
14	8	159	THR
14	8	166	GLU
14	8	173	GLU
14	8	175	LEU
14	8	176	LEU
14	8	177	ARG
14	8	184	VAL
14	8	196	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
14	8	209	ARG
14	8	245	PHE
14	8	249	PHE
14	8	252	LYS
14	8	267	ARG
14	8	273	HIS
14	8	279	LYS
14	8	282	ASN
15	9	46	ARG
15	9	50	PRO
15	9	96	LEU
15	9	98	MET
15	9	104	ARG
15	9	105	PRO
15	9	118	PHE
15	9	139	ARG
15	9	150	SER
15	9	208	ARG
15	9	212	LEU
15	9	226	MET
15	9	227	GLU
15	9	229	LEU
15	9	236	GLU
15	9	237	HIS
15	9	240	HIS
15	9	248	MET
15	9	254	ASN
15	9	261	GLU
15	9	262	GLU
15	9	264	LYS
15	9	265	MET
15	9	277	LYS
15	9	281	LYS
15	9	282	ARG
15	9	285	GLU
15	9	287	HIS
15	9	295	ASN
15	9	298	GLN
15	9	299	CYS
16	AA	23	PRO
16	AA	58	CYS
16	AA	63	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
16	AA	80	PRO
16	AA	169	HIS
16	AA	174	PRO
16	AA	178	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (221) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	120	HIS
1	I	181	GLN
1	I	193	GLN
1	I	207	HIS
1	I	241	ASN
1	I	298	ASN
1	I	314	ASN
1	I	315	GLN
1	I	332	ASN
2	H	114	ASN
2	H	148	GLN
2	H	203	ASN
2	H	247	GLN
2	H	293	ASN
2	H	305	GLN
2	H	322	ASN
3	L	51	GLN
3	L	75	ASN
3	L	124	HIS
3	L	226	GLN
3	L	262	ASN
3	L	316	HIS
4	M	315	ASN
4	M	323	ASN
4	M	333	ASN
4	M	380	ASN
4	M	436	GLN
5	J	36	ASN
5	J	69	GLN
5	J	118	ASN
5	J	157	GLN
5	J	171	HIS
5	J	206	HIS
5	J	270	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	J	279	GLN
5	J	337	ASN
5	J	380	GLN
6	K	67	ASN
6	K	74	HIS
6	K	99	ASN
6	K	110	ASN
6	K	173	GLN
6	K	175	GLN
6	K	221	HIS
6	K	222	HIS
6	K	237	GLN
6	K	257	ASN
6	K	286	GLN
6	K	302	ASN
6	K	304	ASN
6	K	312	ASN
7	N	259	GLN
7	N	345	ASN
7	N	347	ASN
7	N	412	HIS
7	N	596	ASN
7	N	645	ASN
7	N	697	GLN
7	N	880	ASN
8	O	273	GLN
9	P	288	HIS
9	P	361	HIS
9	P	423	ASN
9	P	440	ASN
9	P	444	HIS
9	P	454	ASN
10	Q	148	HIS
10	Q	152	GLN
10	Q	170	GLN
10	Q	207	GLN
10	Q	218	HIS
10	Q	334	ASN
11	R	136	HIS
11	R	178	ASN
11	R	280	GLN
11	R	291	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	R	344	HIS
11	R	363	ASN
12	S	299	GLN
12	S	326	GLN
12	S	473	GLN
14	U	12	HIS
14	U	22	HIS
14	U	96	HIS
14	U	102	HIS
14	U	109	ASN
14	U	223	ASN
14	U	254	ASN
14	U	273	HIS
14	U	278	ASN
15	V	77	GLN
15	V	101	GLN
15	V	210	ASN
15	V	221	HIS
15	V	241	ASN
15	V	295	ASN
15	V	298	GLN
16	W	18	ASN
16	W	44	ASN
16	W	101	GLN
16	W	142	ASN
16	W	169	HIS
19	B	75	ASN
19	B	100	ASN
20	C	201	GLN
21	D	142	HIS
22	E	54	GLN
23	F	182	GLN
24	G	5	GLN
24	G	166	GLN
26	a	66	HIS
28	c	173	ASN
29	d	71	ASN
30	e	38	ASN
31	f	146	GLN
32	g	81	HIS
19	h	53	GLN
19	h	100	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
26	o	66	HIS
28	q	173	ASN
29	r	71	ASN
30	s	38	ASN
31	t	146	GLN
32	u	81	HIS
2	v	114	ASN
2	v	148	GLN
2	v	203	ASN
2	v	247	GLN
2	v	293	ASN
2	v	305	GLN
2	v	322	ASN
1	w	120	HIS
1	w	181	GLN
1	w	193	GLN
1	w	207	HIS
1	w	241	ASN
1	w	298	ASN
1	w	314	ASN
1	w	315	GLN
1	w	332	ASN
5	x	36	ASN
5	x	69	GLN
5	x	118	ASN
5	x	171	HIS
5	x	206	HIS
5	x	270	GLN
5	x	337	ASN
5	x	380	GLN
6	y	67	ASN
6	y	74	HIS
6	y	99	ASN
6	y	110	ASN
6	y	173	GLN
6	y	175	GLN
6	y	221	HIS
6	y	222	HIS
6	y	237	GLN
6	y	257	ASN
6	y	286	GLN
6	y	302	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	y	304	ASN
6	y	312	ASN
3	z	51	GLN
3	z	75	ASN
3	z	124	HIS
3	z	226	GLN
3	z	262	ASN
3	z	316	HIS
4	0	315	ASN
4	0	333	ASN
4	0	380	ASN
4	0	436	GLN
7	1	259	GLN
7	1	345	ASN
7	1	347	ASN
7	1	596	ASN
7	1	645	ASN
7	1	697	GLN
7	1	880	ASN
8	2	273	GLN
9	3	288	HIS
9	3	361	HIS
9	3	423	ASN
9	3	440	ASN
9	3	444	HIS
9	3	454	ASN
10	4	148	HIS
10	4	152	GLN
10	4	170	GLN
10	4	207	GLN
10	4	218	HIS
10	4	334	ASN
11	5	136	HIS
11	5	178	ASN
11	5	280	GLN
11	5	291	HIS
11	5	344	HIS
11	5	363	ASN
12	6	299	GLN
12	6	473	GLN
14	8	12	HIS
14	8	22	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
14	8	72	HIS
14	8	96	HIS
14	8	102	HIS
14	8	223	ASN
14	8	254	ASN
14	8	273	HIS
14	8	278	ASN
15	9	77	GLN
15	9	101	GLN
15	9	210	ASN
15	9	221	HIS
15	9	241	ASN
15	9	295	ASN
15	9	298	GLN
16	AA	18	ASN
16	AA	44	ASN
16	AA	101	GLN
16	AA	142	ASN
16	AA	169	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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
33	ADP	0	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.59	4 (13%)
33	ADP	v	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)
33	ADP	z	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
33	ADP	H	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.52	4 (13%)
33	ADP	K	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)
33	ADP	w	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.51	4 (13%)
33	ADP	x	501	-	24,29,29	0.90	1 (4%)	29,45,45	1.59	4 (13%)
33	ADP	I	501	-	24,29,29	0.97	1 (4%)	29,45,45	1.51	4 (13%)
33	ADP	J	501	-	24,29,29	0.90	1 (4%)	29,45,45	1.59	4 (13%)
33	ADP	M	501	-	24,29,29	0.92	1 (4%)	29,45,45	1.59	4 (13%)
33	ADP	L	401	-	24,29,29	0.94	1 (4%)	29,45,45	1.42	4 (13%)
33	ADP	y	501	-	24,29,29	0.95	1 (4%)	29,45,45	1.45	4 (13%)

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
33	ADP	0	501	-	-	3/12/32/32	0/3/3/3
33	ADP	v	501	-	-	1/12/32/32	0/3/3/3
33	ADP	z	401	-	-	1/12/32/32	0/3/3/3
33	ADP	H	501	-	-	1/12/32/32	0/3/3/3
33	ADP	K	501	-	-	5/12/32/32	0/3/3/3
33	ADP	w	501	-	-	3/12/32/32	0/3/3/3
33	ADP	x	501	-	-	4/12/32/32	0/3/3/3
33	ADP	I	501	-	-	3/12/32/32	0/3/3/3
33	ADP	J	501	-	-	4/12/32/32	0/3/3/3
33	ADP	M	501	-	-	3/12/32/32	0/3/3/3
33	ADP	L	401	-	-	1/12/32/32	0/3/3/3
33	ADP	y	501	-	-	5/12/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	I	501	ADP	C5-C4	2.53	1.47	1.40
33	w	501	ADP	C5-C4	2.53	1.47	1.40
33	H	501	ADP	C5-C4	2.52	1.47	1.40
33	v	501	ADP	C5-C4	2.52	1.47	1.40
33	L	401	ADP	C5-C4	2.36	1.47	1.40
33	z	401	ADP	C5-C4	2.36	1.47	1.40
33	K	501	ADP	C5-C4	2.36	1.47	1.40
33	y	501	ADP	C5-C4	2.36	1.47	1.40
33	M	501	ADP	C5-C4	2.26	1.46	1.40
33	0	501	ADP	C5-C4	2.26	1.46	1.40
33	J	501	ADP	C5-C4	2.20	1.46	1.40
33	x	501	ADP	C5-C4	2.20	1.46	1.40

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	501	ADP	PA-O3A-PB	-4.55	117.22	132.83
33	x	501	ADP	PA-O3A-PB	-4.55	117.22	132.83
33	M	501	ADP	PA-O3A-PB	-4.47	117.47	132.83
33	0	501	ADP	PA-O3A-PB	-4.47	117.47	132.83
33	L	401	ADP	PA-O3A-PB	-3.60	120.46	132.83
33	z	401	ADP	PA-O3A-PB	-3.60	120.46	132.83
33	H	501	ADP	PA-O3A-PB	-3.60	120.47	132.83
33	v	501	ADP	PA-O3A-PB	-3.60	120.47	132.83
33	I	501	ADP	PA-O3A-PB	-3.59	120.50	132.83
33	w	501	ADP	PA-O3A-PB	-3.59	120.50	132.83
33	I	501	ADP	C3'-C2'-C1'	3.56	106.33	100.98
33	w	501	ADP	C3'-C2'-C1'	3.56	106.33	100.98
33	H	501	ADP	C3'-C2'-C1'	3.54	106.31	100.98
33	v	501	ADP	C3'-C2'-C1'	3.54	106.31	100.98
33	K	501	ADP	PA-O3A-PB	-3.54	120.67	132.83
33	y	501	ADP	PA-O3A-PB	-3.54	120.67	132.83
33	M	501	ADP	N3-C2-N1	-3.29	123.54	128.68
33	0	501	ADP	N3-C2-N1	-3.29	123.54	128.68
33	H	501	ADP	N3-C2-N1	-3.24	123.62	128.68
33	v	501	ADP	N3-C2-N1	-3.24	123.62	128.68
33	J	501	ADP	N3-C2-N1	-3.23	123.63	128.68
33	x	501	ADP	N3-C2-N1	-3.23	123.63	128.68
33	L	401	ADP	N3-C2-N1	-3.19	123.69	128.68
33	z	401	ADP	N3-C2-N1	-3.19	123.69	128.68
33	K	501	ADP	N3-C2-N1	-3.17	123.72	128.68
33	y	501	ADP	N3-C2-N1	-3.17	123.72	128.68
33	I	501	ADP	N3-C2-N1	-3.17	123.73	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	w	501	ADP	N3-C2-N1	-3.17	123.73	128.68
33	J	501	ADP	C3'-C2'-C1'	3.16	105.73	100.98
33	x	501	ADP	C3'-C2'-C1'	3.16	105.73	100.98
33	M	501	ADP	C3'-C2'-C1'	3.05	105.57	100.98
33	0	501	ADP	C3'-C2'-C1'	3.05	105.57	100.98
33	K	501	ADP	C3'-C2'-C1'	2.84	105.26	100.98
33	y	501	ADP	C3'-C2'-C1'	2.84	105.26	100.98
33	K	501	ADP	C4-C5-N7	-2.77	106.52	109.40
33	y	501	ADP	C4-C5-N7	-2.77	106.52	109.40
33	I	501	ADP	C4-C5-N7	-2.73	106.55	109.40
33	w	501	ADP	C4-C5-N7	-2.73	106.55	109.40
33	H	501	ADP	C4-C5-N7	-2.71	106.58	109.40
33	v	501	ADP	C4-C5-N7	-2.71	106.58	109.40
33	L	401	ADP	C3'-C2'-C1'	2.68	105.01	100.98
33	z	401	ADP	C3'-C2'-C1'	2.68	105.01	100.98
33	J	501	ADP	C4-C5-N7	-2.47	106.83	109.40
33	x	501	ADP	C4-C5-N7	-2.47	106.83	109.40
33	M	501	ADP	C4-C5-N7	-2.44	106.85	109.40
33	0	501	ADP	C4-C5-N7	-2.44	106.85	109.40
33	L	401	ADP	C4-C5-N7	-2.42	106.88	109.40
33	z	401	ADP	C4-C5-N7	-2.42	106.88	109.40

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	M	501	ADP	C5'-O5'-PA-O1A
33	M	501	ADP	C5'-O5'-PA-O2A
33	J	501	ADP	C5'-O5'-PA-O3A
33	K	501	ADP	C5'-O5'-PA-O1A
33	K	501	ADP	C5'-O5'-PA-O2A
33	x	501	ADP	C5'-O5'-PA-O3A
33	y	501	ADP	C5'-O5'-PA-O1A
33	y	501	ADP	C5'-O5'-PA-O2A
33	0	501	ADP	C5'-O5'-PA-O1A
33	0	501	ADP	C5'-O5'-PA-O2A
33	K	501	ADP	O4'-C4'-C5'-O5'
33	y	501	ADP	O4'-C4'-C5'-O5'
33	J	501	ADP	C3'-C4'-C5'-O5'
33	x	501	ADP	C3'-C4'-C5'-O5'
33	J	501	ADP	O4'-C4'-C5'-O5'
33	x	501	ADP	O4'-C4'-C5'-O5'

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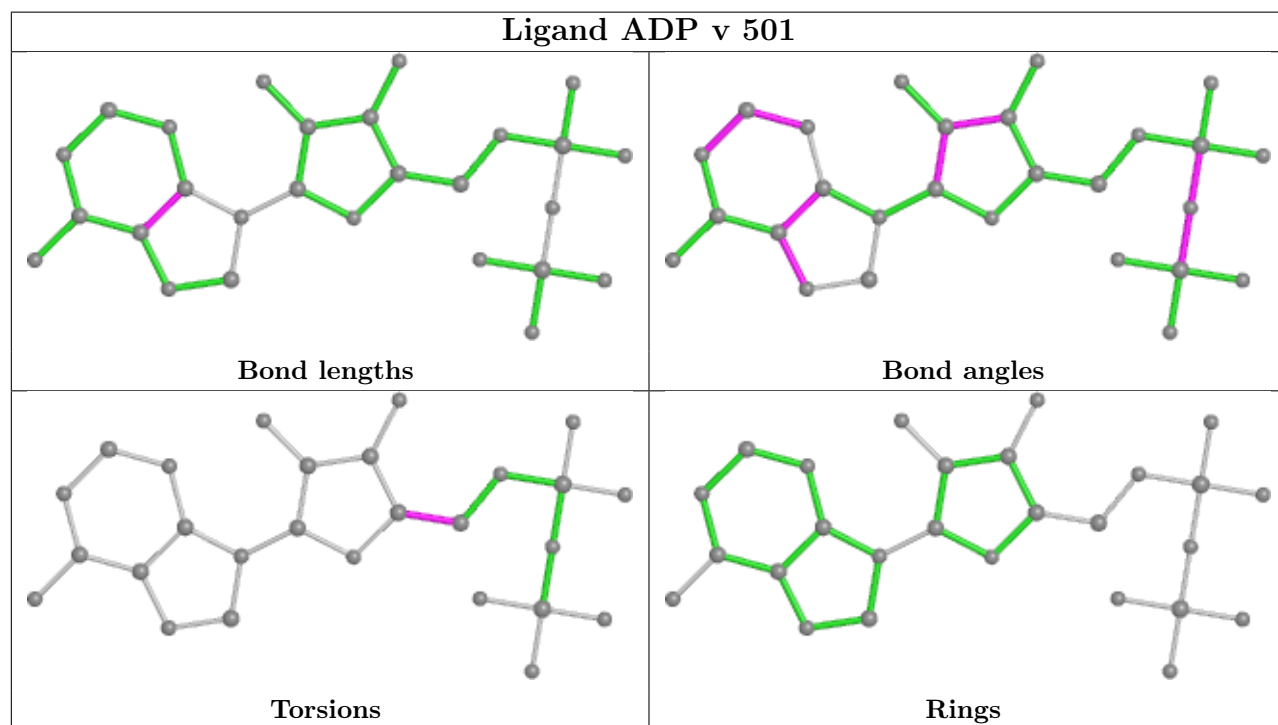
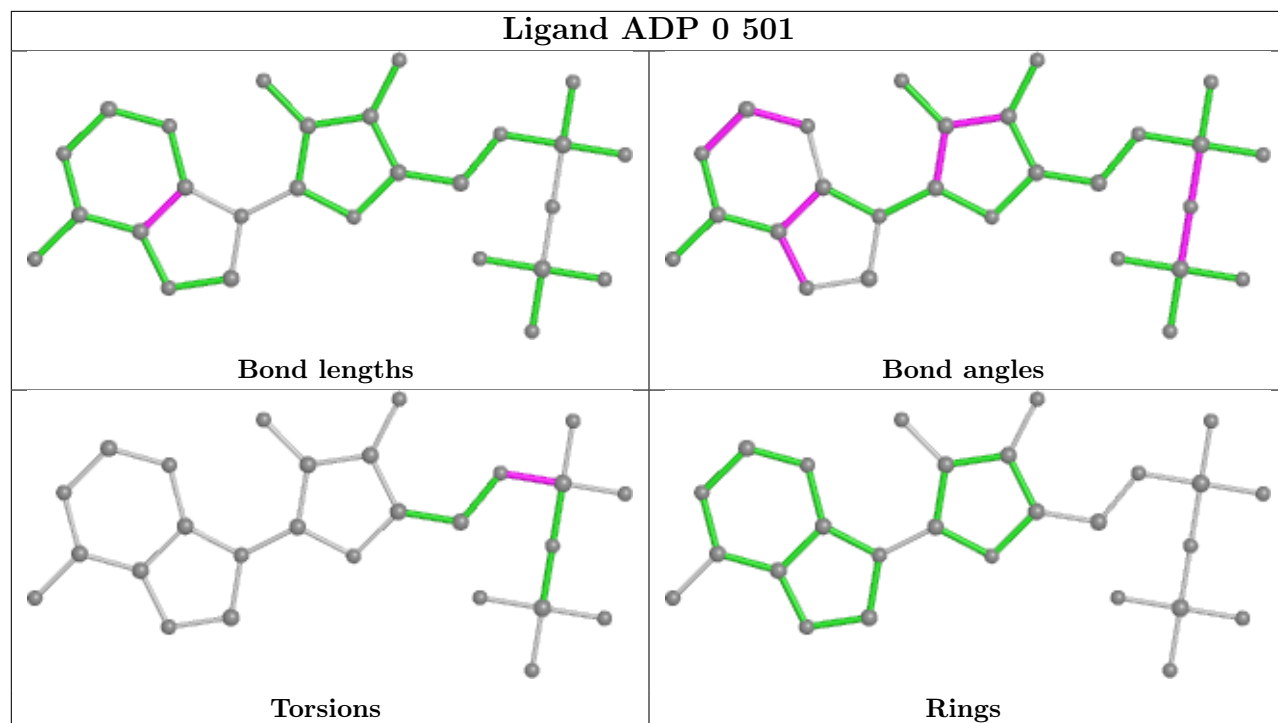
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Mol	Chain	Res	Type	Atoms
33	K	501	ADP	C3'-C4'-C5'-O5'
33	y	501	ADP	C3'-C4'-C5'-O5'
33	H	501	ADP	O4'-C4'-C5'-O5'
33	v	501	ADP	O4'-C4'-C5'-O5'
33	M	501	ADP	C5'-O5'-PA-O3A
33	0	501	ADP	C5'-O5'-PA-O3A
33	I	501	ADP	PB-O3A-PA-O2A
33	w	501	ADP	PB-O3A-PA-O2A
33	J	501	ADP	C5'-O5'-PA-O1A
33	x	501	ADP	C5'-O5'-PA-O1A
33	I	501	ADP	O4'-C4'-C5'-O5'
33	w	501	ADP	O4'-C4'-C5'-O5'
33	L	401	ADP	C5'-O5'-PA-O3A
33	K	501	ADP	C5'-O5'-PA-O3A
33	y	501	ADP	C5'-O5'-PA-O3A
33	z	401	ADP	C5'-O5'-PA-O3A
33	I	501	ADP	PB-O3A-PA-O1A
33	w	501	ADP	PB-O3A-PA-O1A

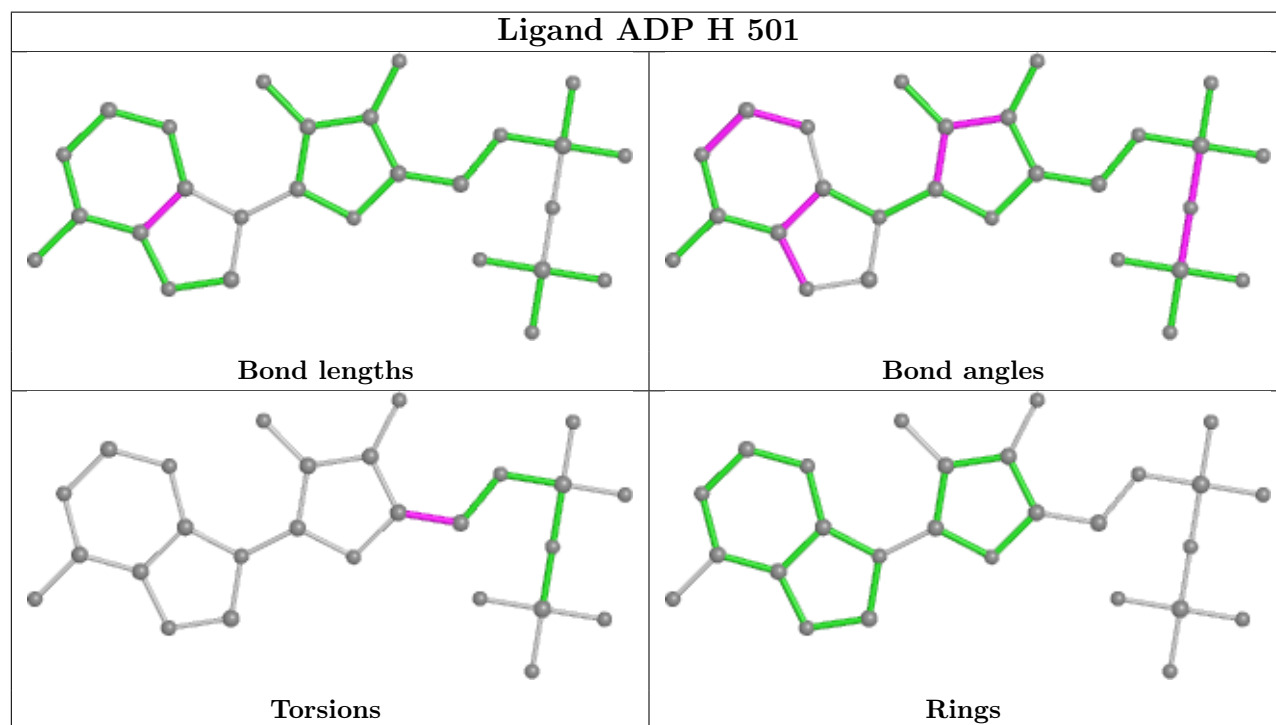
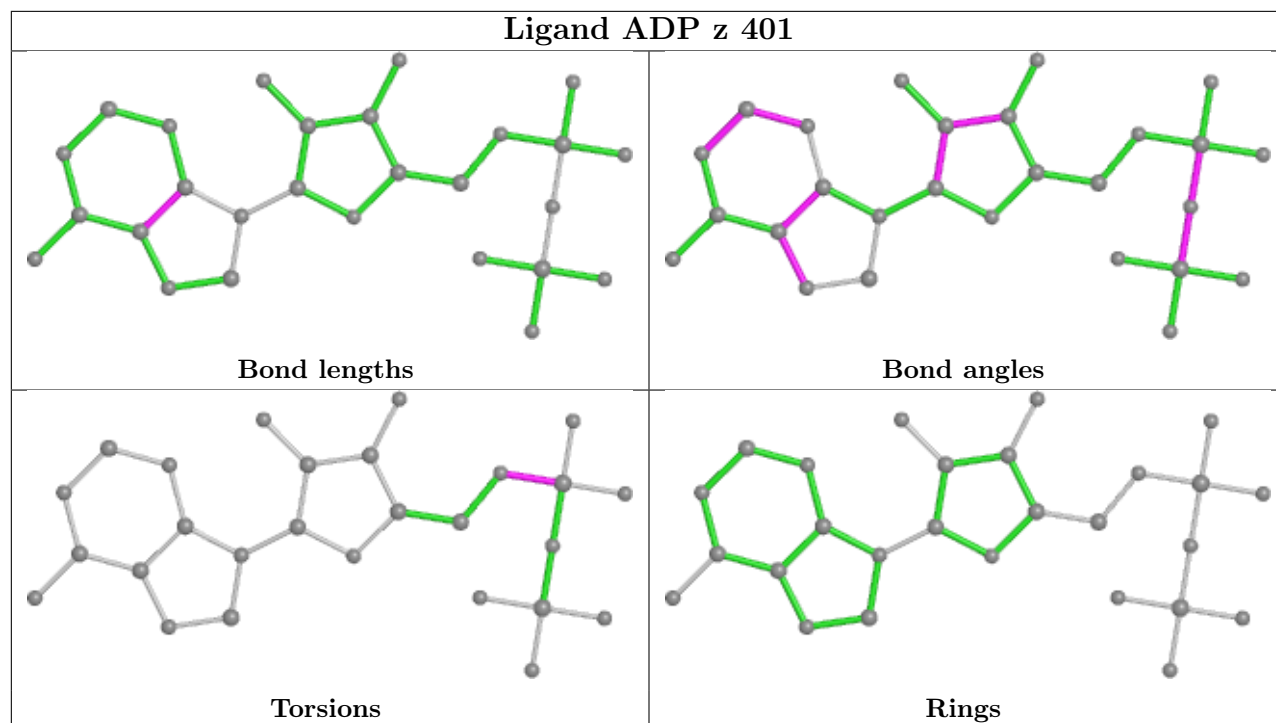
There are no ring outliers.

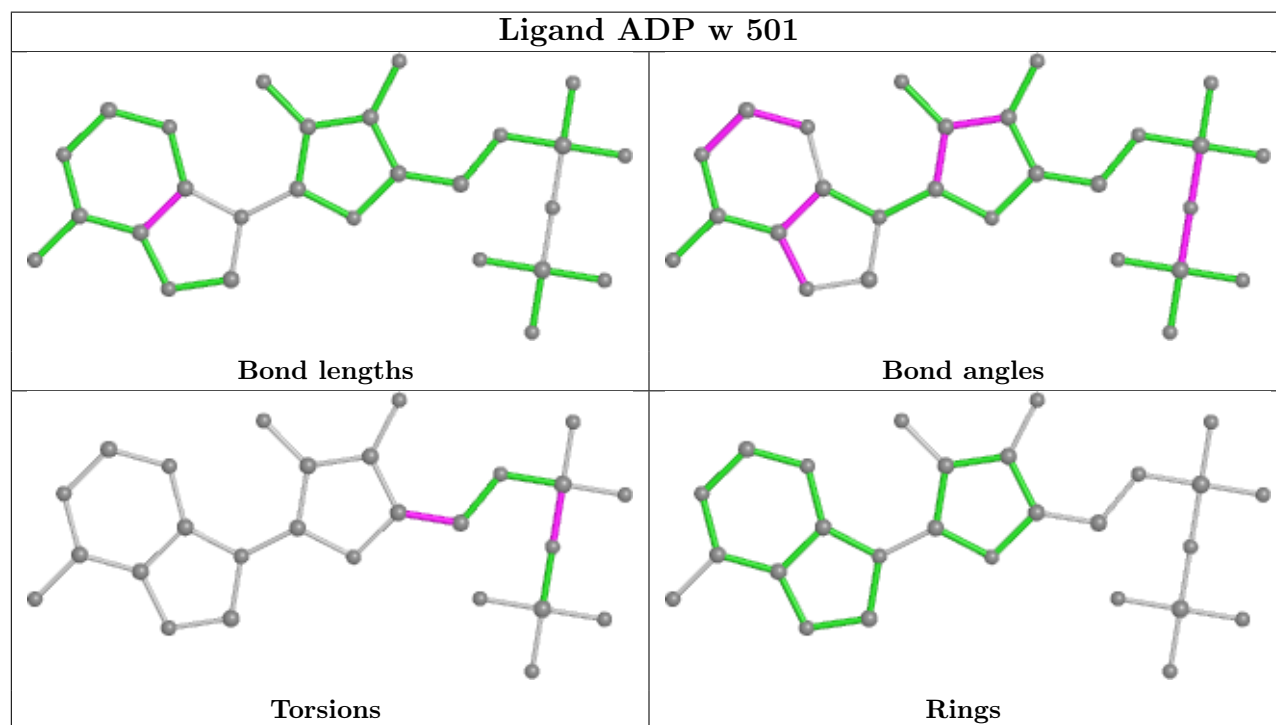
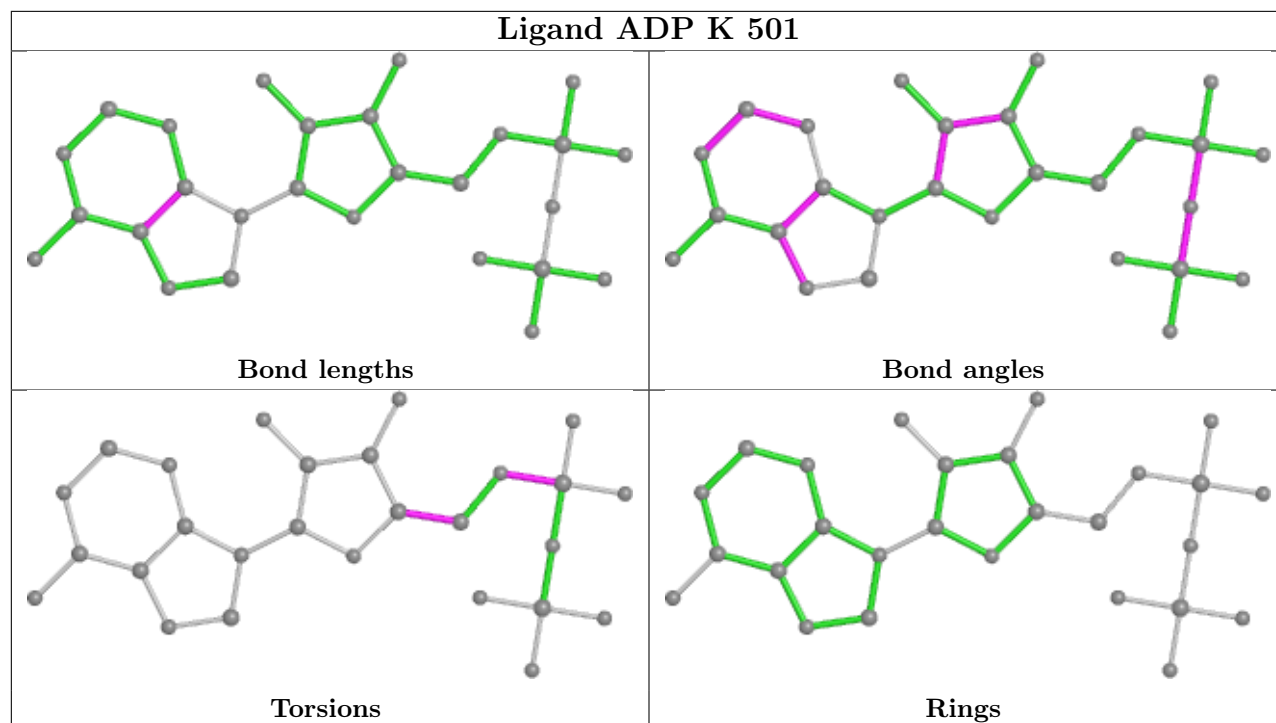
No monomer is involved in short contacts.

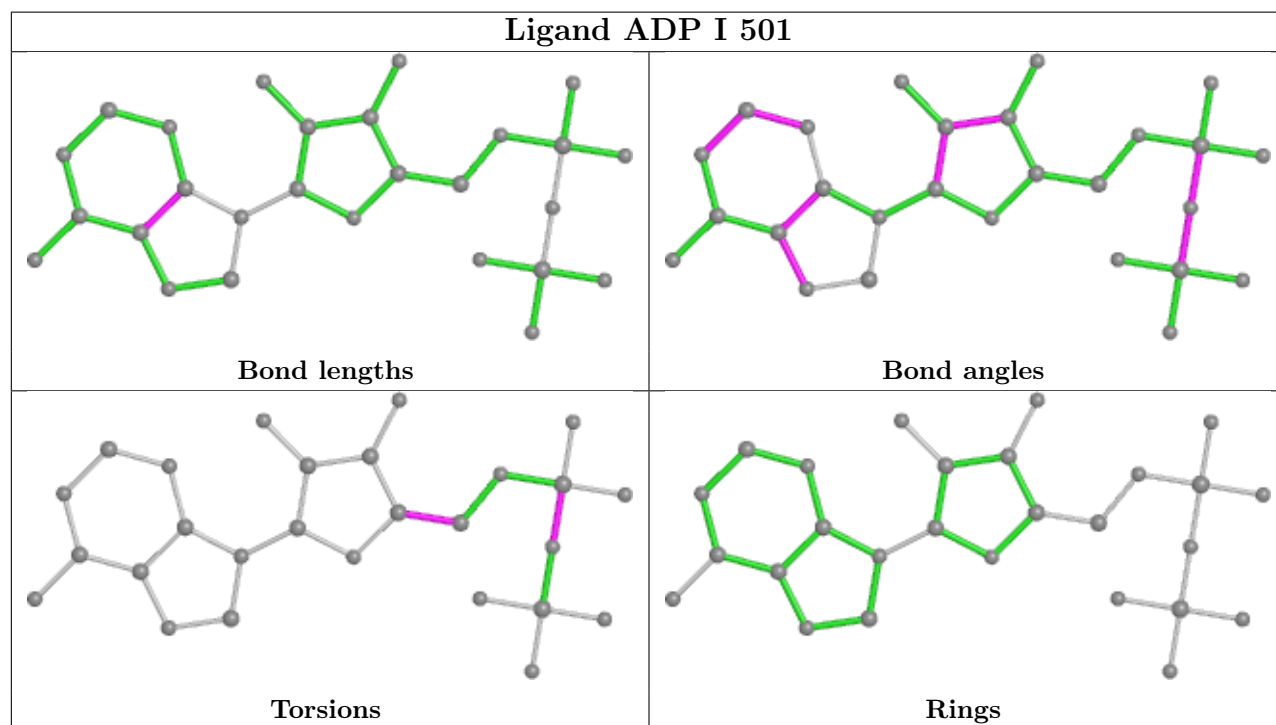
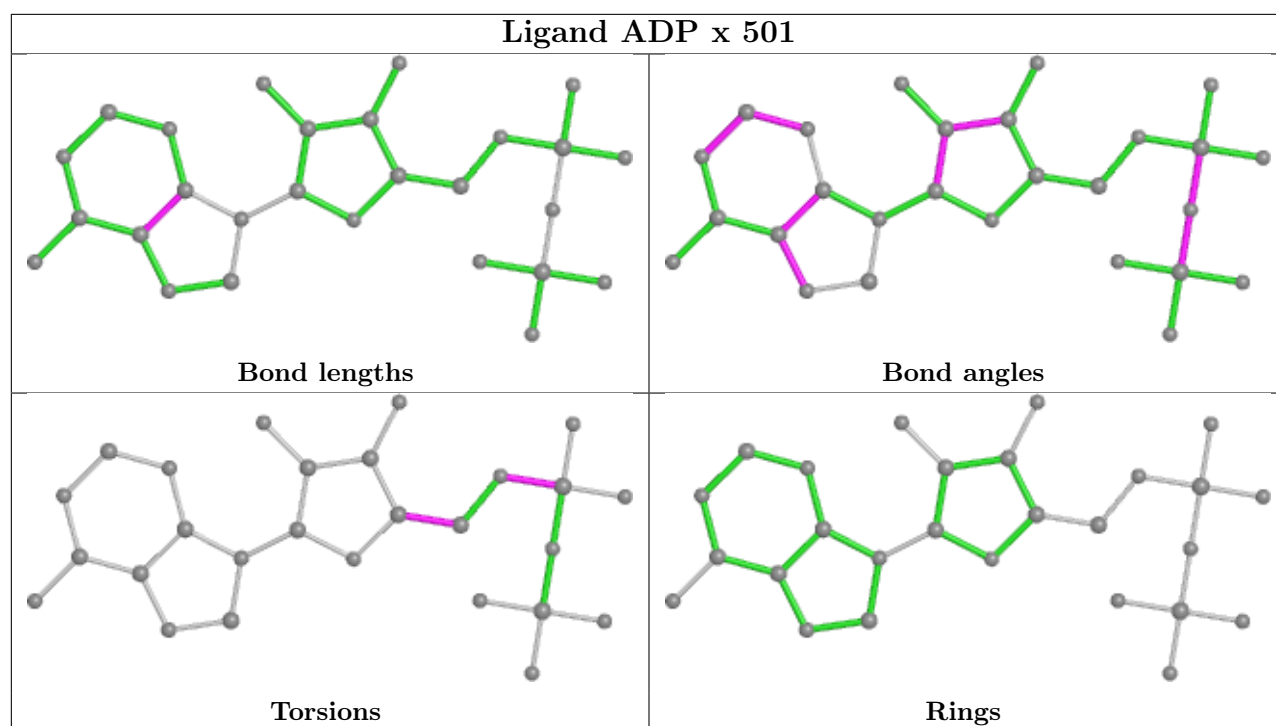
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

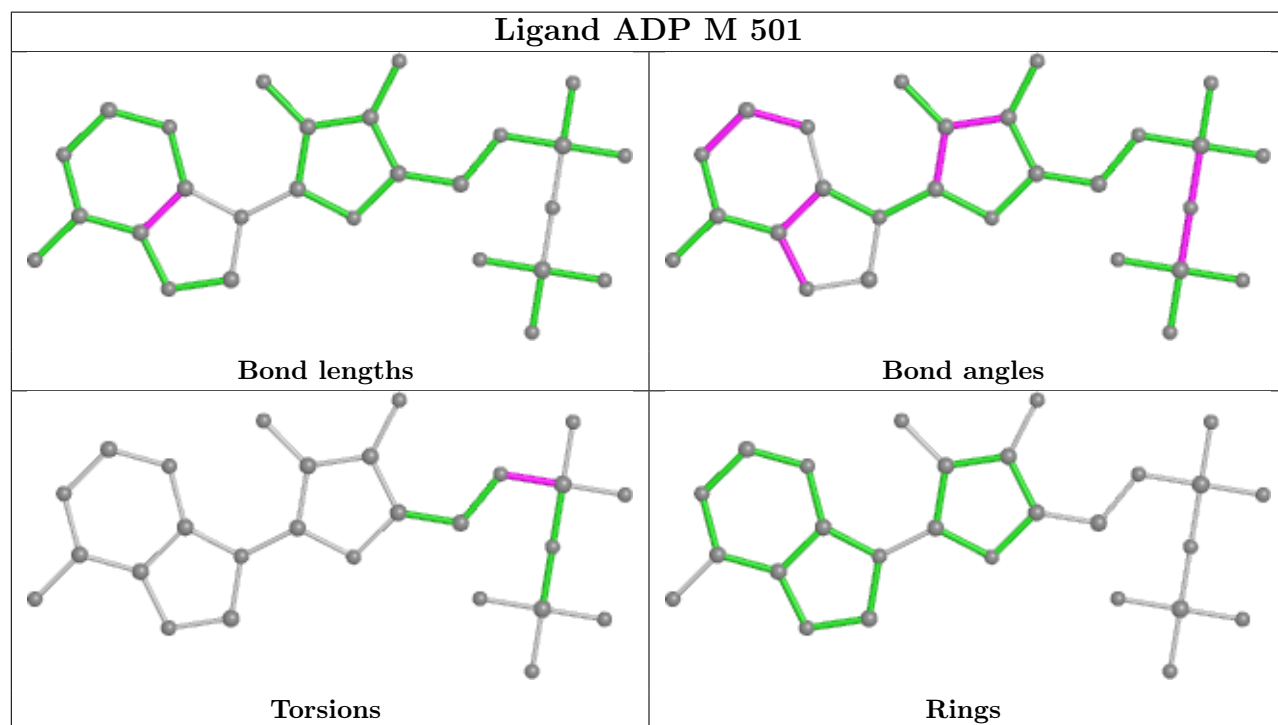
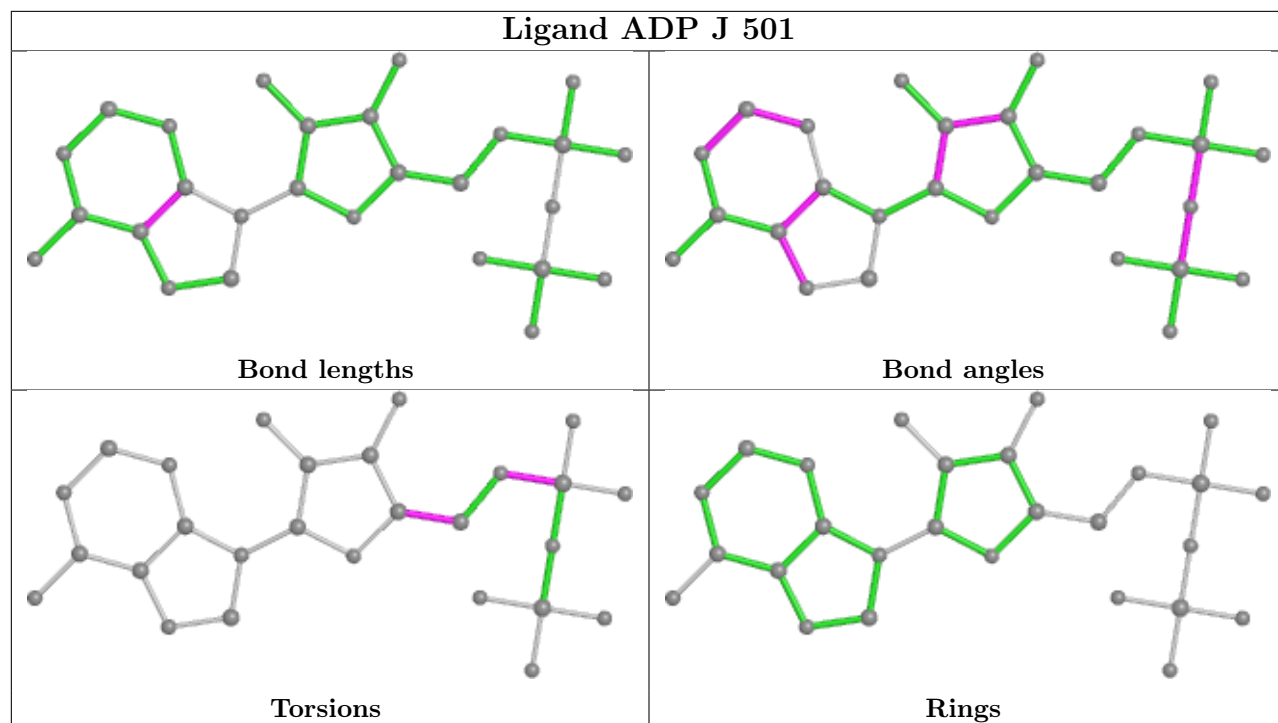


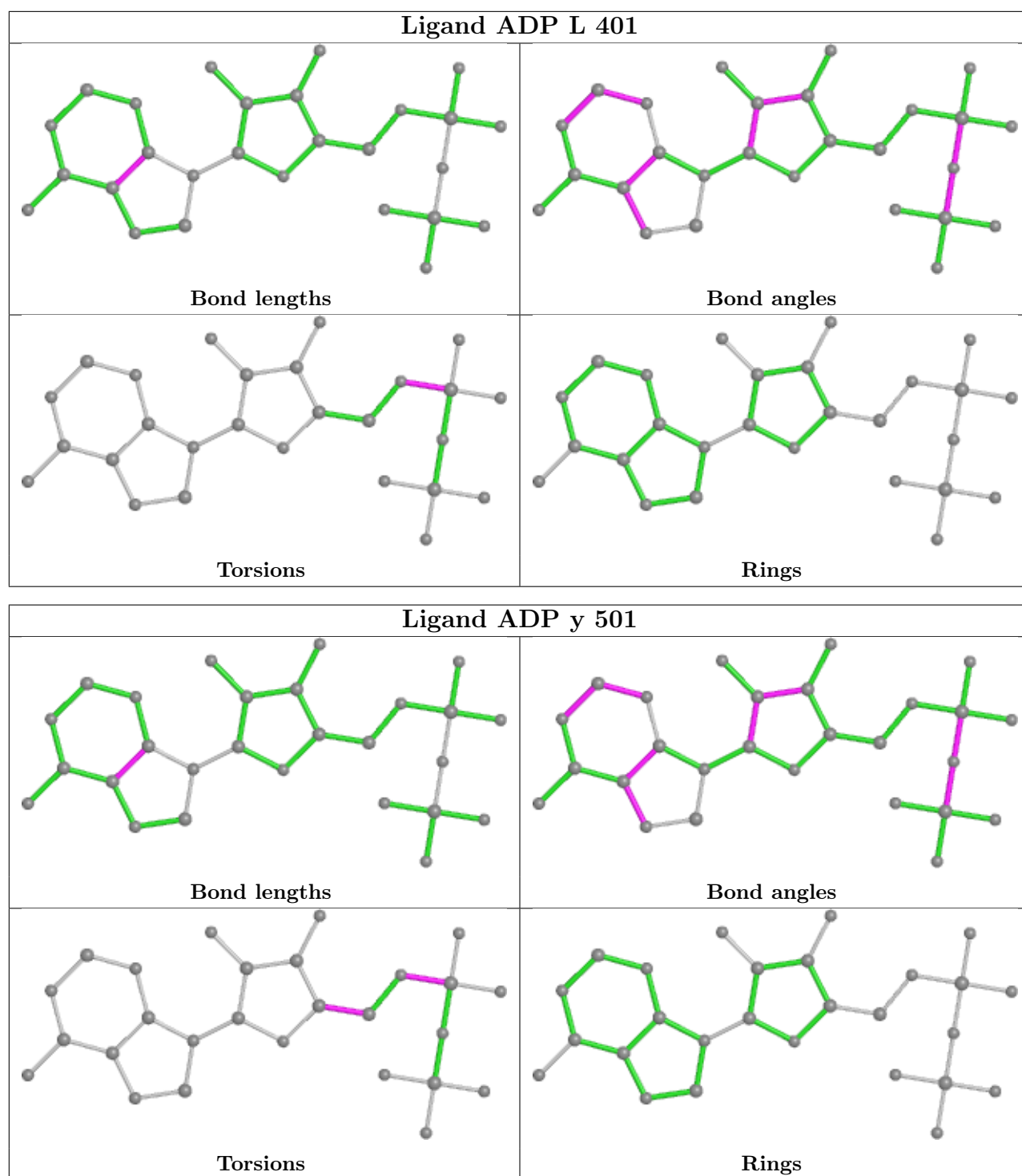












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

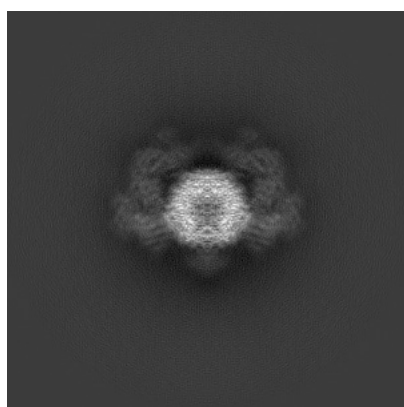
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9512. These allow visual inspection of the internal detail of the map and identification of artifacts.

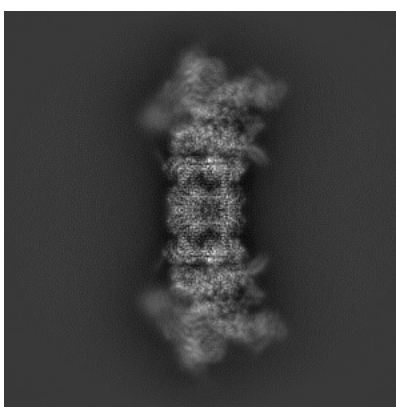
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

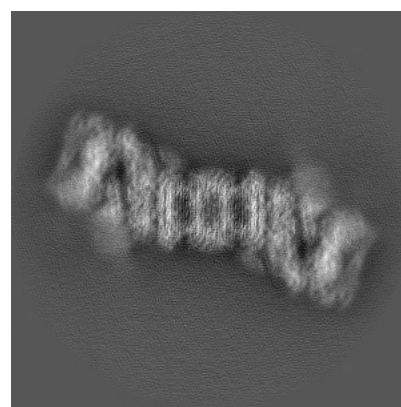
#### 6.1.1 Primary map



X



Y

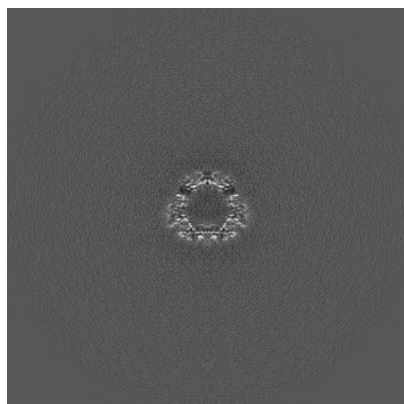


Z

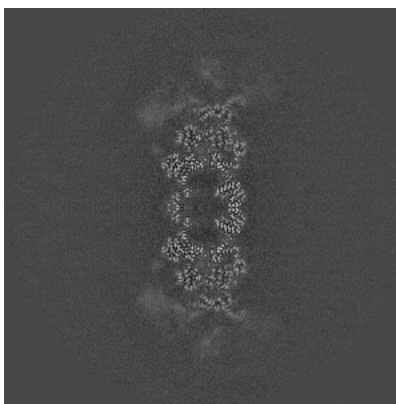
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

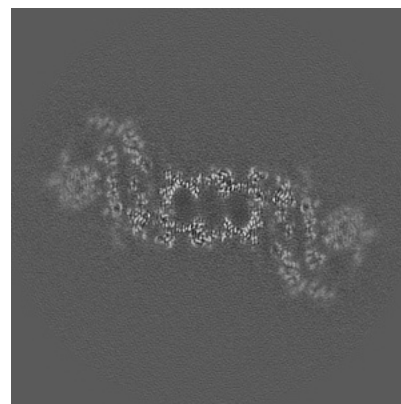
#### 6.2.1 Primary map



X Index: 256



Y Index: 256

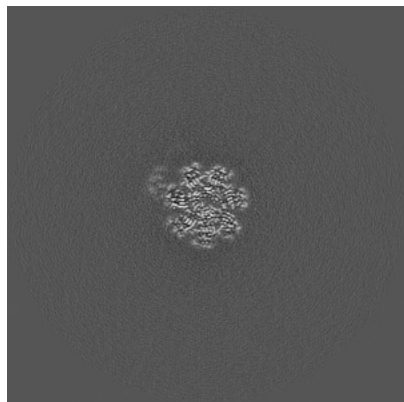


Z Index: 256

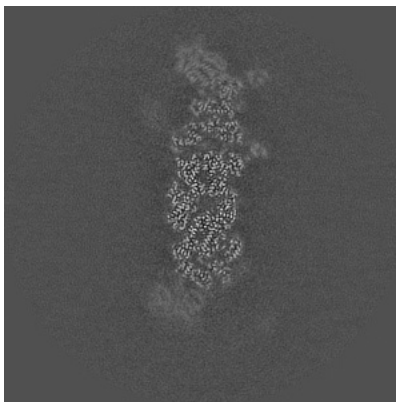
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

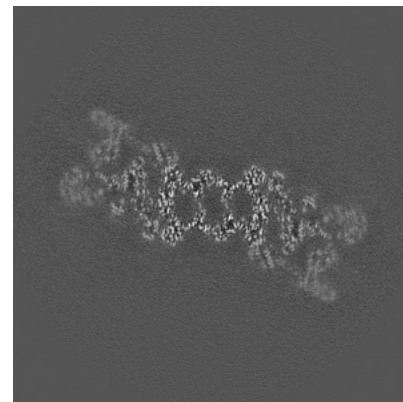
### 6.3.1 Primary map



X Index: 309



Y Index: 233



Z Index: 270

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

## 6.4 Orthogonal surface views [i](#)

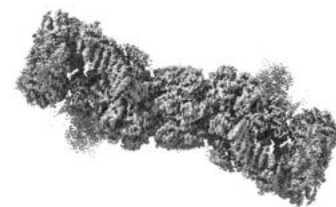
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0336. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



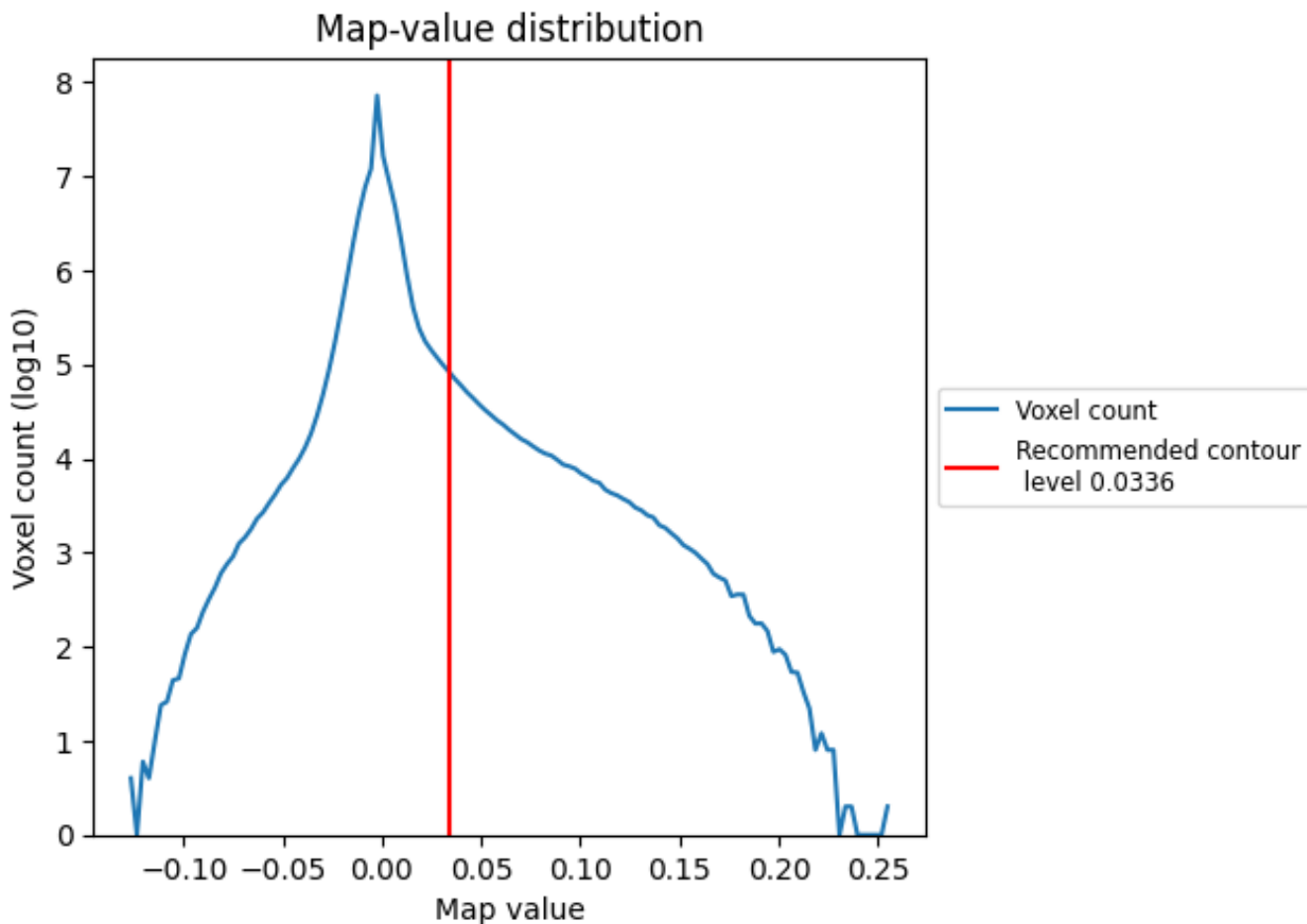
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

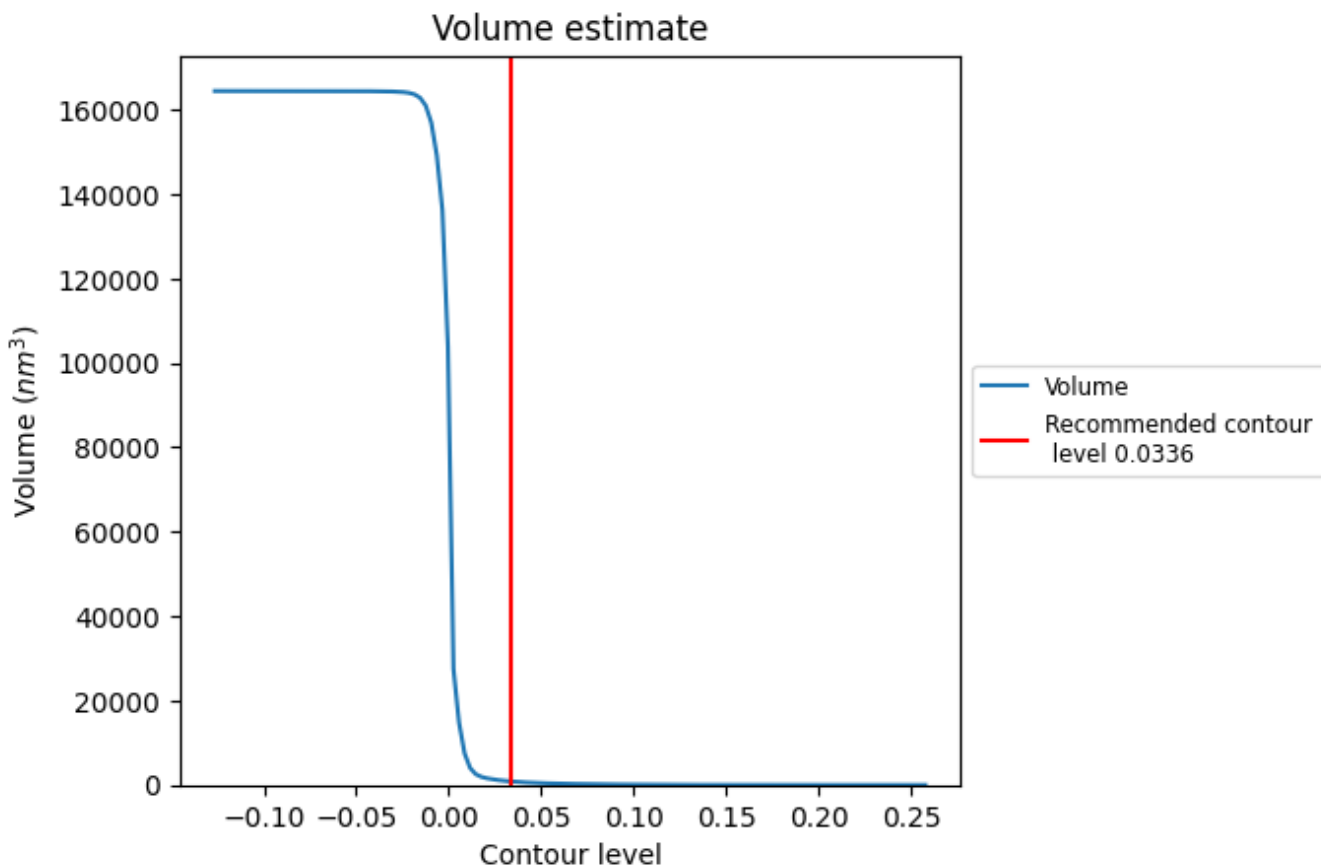
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

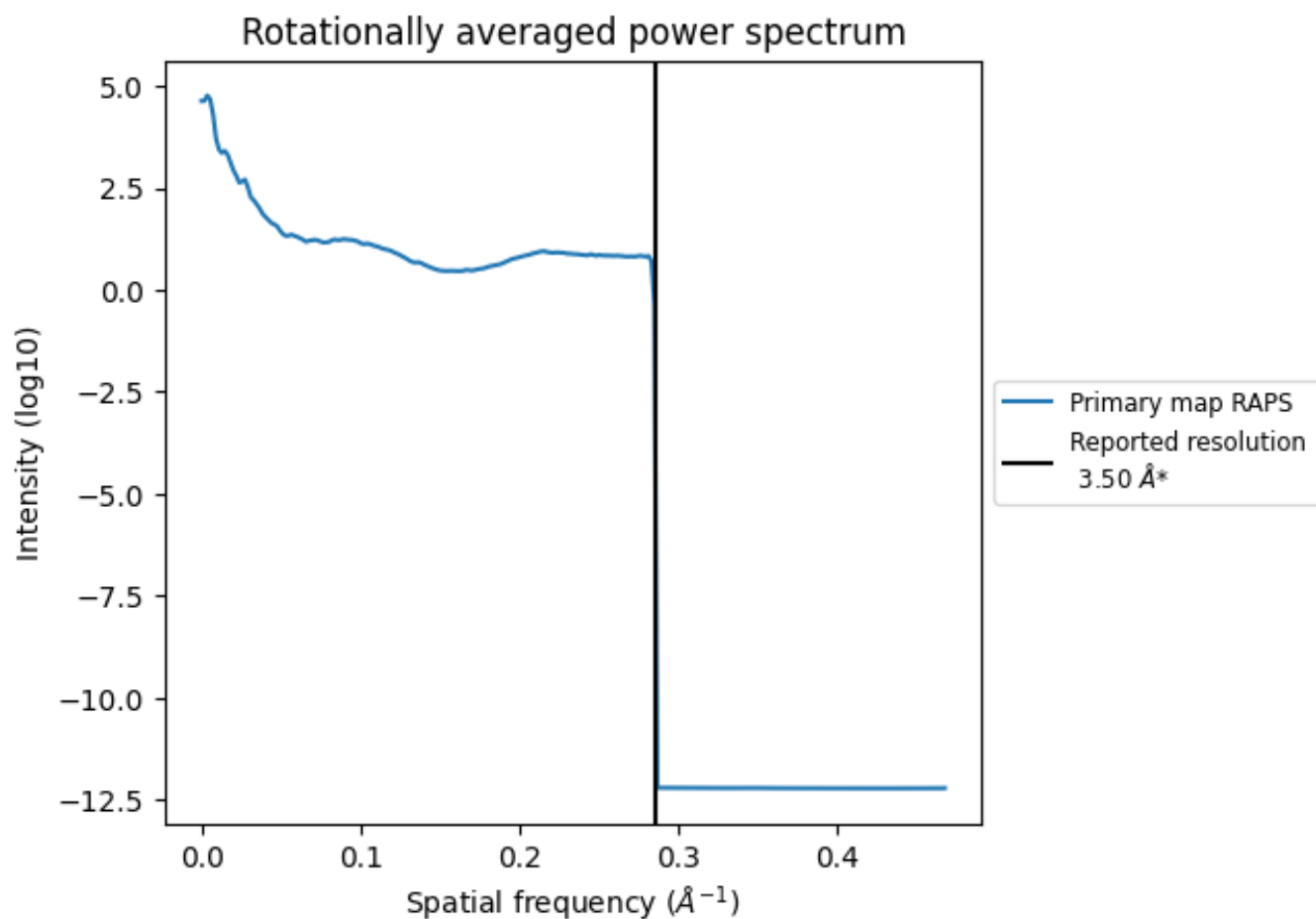
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 841  $\text{nm}^3$ ; this corresponds to an approximate mass of 760 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 0.286 Å<sup>-1</sup>

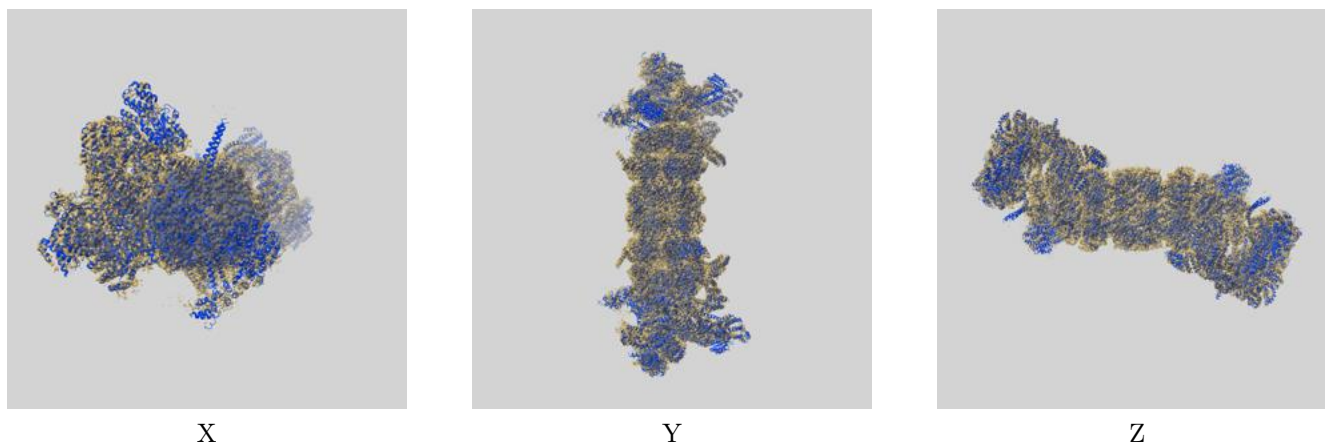
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

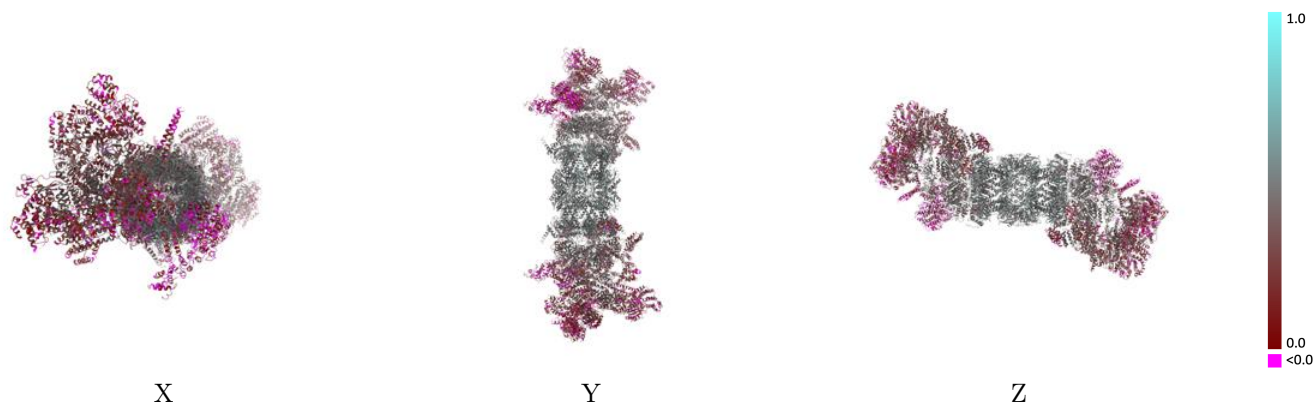
This section contains information regarding the fit between EMDB map EMD-9512 and PDB model 5GJR. Per-residue inclusion information can be found in section 3 on page 14.

### 9.1 Map-model overlay [i](#)



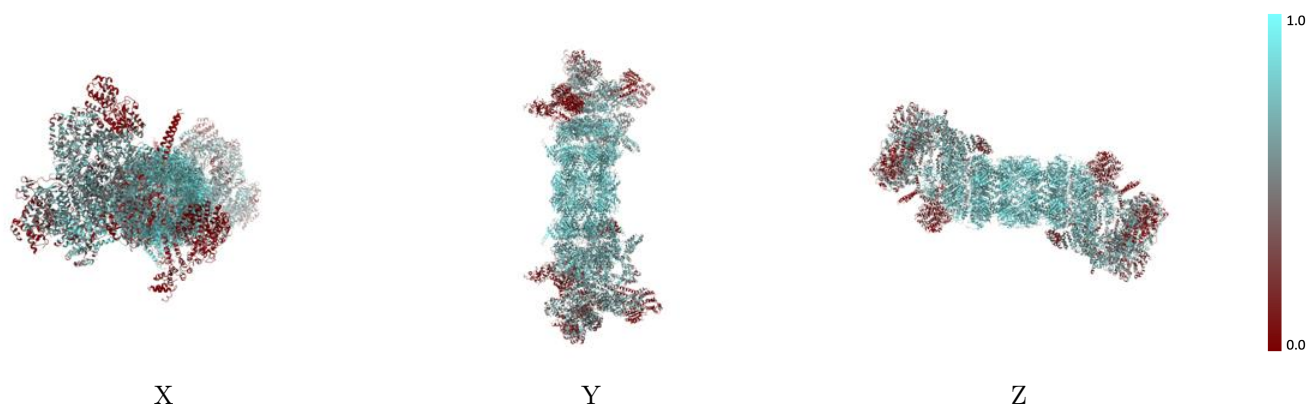
The images above show the 3D surface view of the map at the recommended contour level 0.0336 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



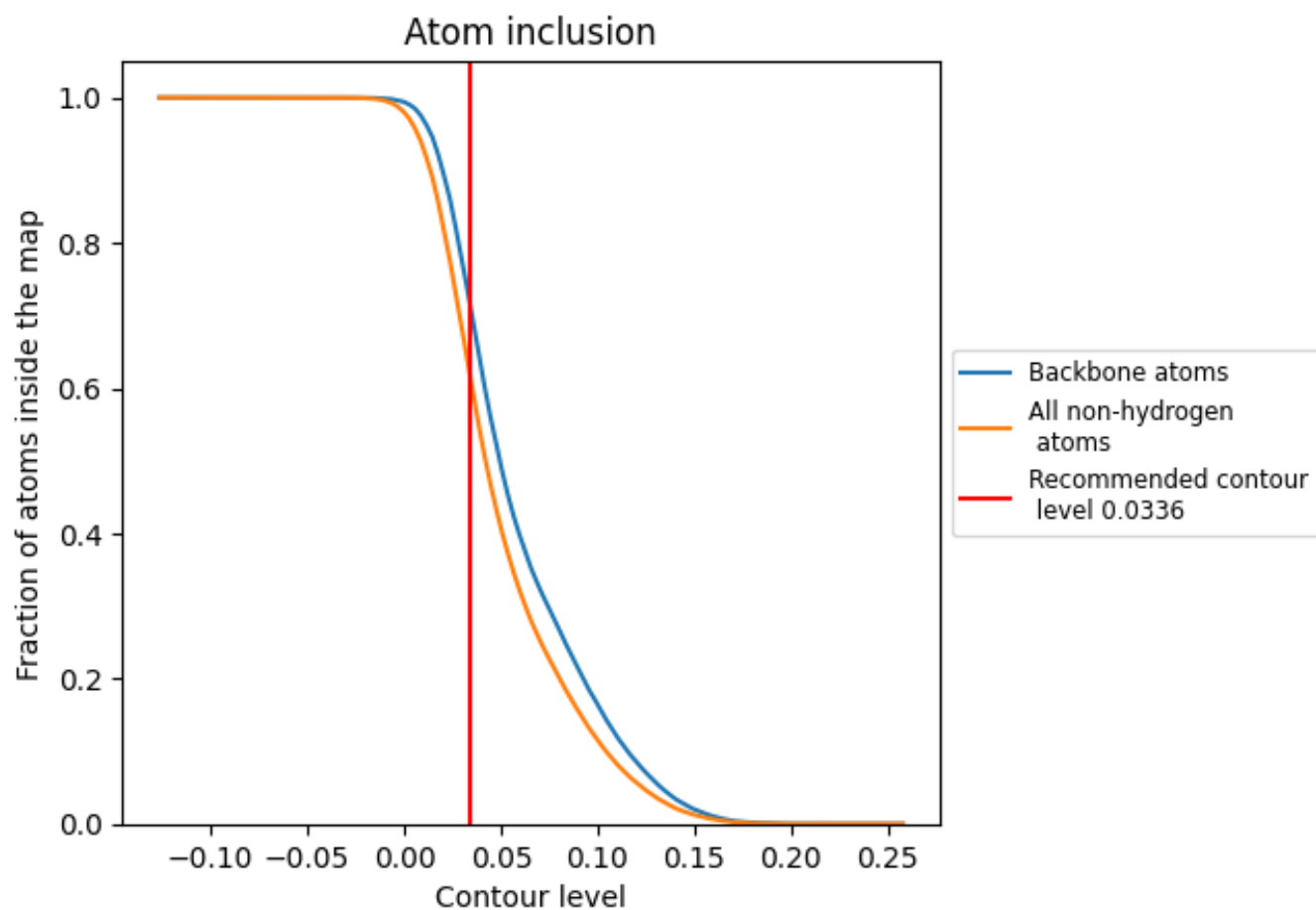
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0336).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 72% 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 (0.0336) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6228	 0.3580
0	 0.7066	 0.4190
1	 0.4272	 0.1720
2	 0.4059	 0.2280
3	 0.5741	 0.2790
4	 0.5242	 0.3320
5	 0.6562	 0.3430
6	 0.5056	 0.2500
7	 0.3209	 0.1730
8	 0.5413	 0.3120
9	 0.5616	 0.3400
AA	 0.0837	 0.1490
AB	 0.3513	 0.2790
AC	 0.0757	 0.0730
B	 0.8099	 0.4750
C	 0.8198	 0.4900
D	 0.7971	 0.4650
E	 0.8203	 0.4670
F	 0.7902	 0.4770
G	 0.8107	 0.4780
H	 0.7034	 0.4060
I	 0.6543	 0.3830
J	 0.6919	 0.3980
K	 0.6744	 0.3960
L	 0.6907	 0.3930
M	 0.7066	 0.4190
N	 0.4278	 0.1710
O	 0.4070	 0.2280
P	 0.5739	 0.2800
Q	 0.5238	 0.3330
R	 0.6562	 0.3420
S	 0.5069	 0.2500
T	 0.3209	 0.1720
U	 0.5418	 0.3150
V	 0.5615	 0.3400



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Chain	Atom inclusion	Q-score
W	 0.0837	 0.1470
X	 0.8021	 0.4730
Y	 0.3513	 0.2760
Z	 0.0757	 0.0720
a	 0.8348	 0.4930
b	 0.8271	 0.4920
c	 0.8376	 0.4950
d	 0.8391	 0.4920
e	 0.8538	 0.4970
f	 0.8358	 0.4880
g	 0.8452	 0.4940
h	 0.8058	 0.4770
i	 0.8223	 0.4870
j	 0.7979	 0.4650
k	 0.8355	 0.4740
l	 0.7942	 0.4800
m	 0.8163	 0.4790
n	 0.7993	 0.4740
o	 0.8362	 0.4930
p	 0.8271	 0.4930
q	 0.8376	 0.4970
r	 0.8404	 0.4920
s	 0.8548	 0.4950
t	 0.8340	 0.4880
u	 0.8444	 0.4940
v	 0.7051	 0.4080
w	 0.6532	 0.3820
x	 0.6922	 0.3990
y	 0.6748	 0.3960
z	 0.6907	 0.3930