Full wwPDB EM Validation Report

Jul 12, 2022 – 11:01 pm BST

PDB ID	:	7QO6
EMDB ID	:	EMD-14085
Title	:	26S proteasome Rpt1-RK -Ubp6-UbVS complex in the s2 state
Authors	:	Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsasser, S.; Geng, T.T.; Cheng, T.C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.
Deposited on	:	2021-12-23
Resolution	:	6.30 Å(reported)

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

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

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

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

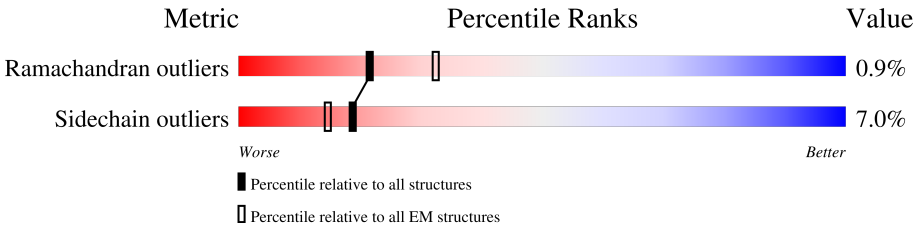
EMDB validation analysis	:	0.0.1.dev8
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.30 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	252	15% 81% 12%
1	a	252	80% 81% 13%
2	B	250	23% 80% 20%
2	b	250	90% 80% 20%
3	C	258	19% 78% 14% 5%
3	c	258	76% 78% 14% 5%
4	D	254	15% 91% 7%
4	d	254	70% 90% 7%
5	E	260	20% 80% 15%

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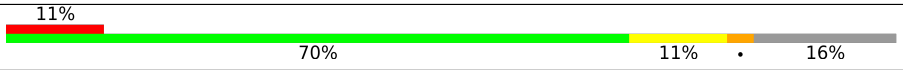
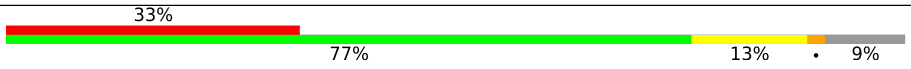
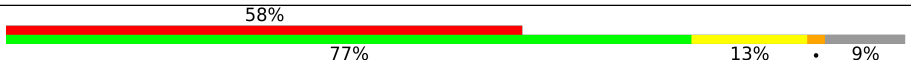
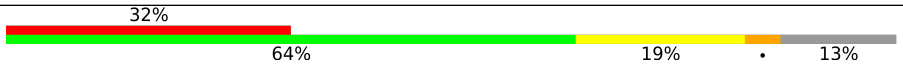
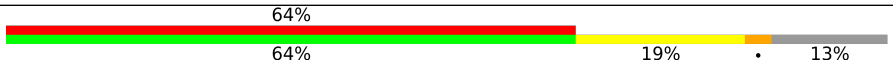
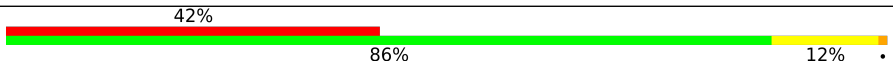
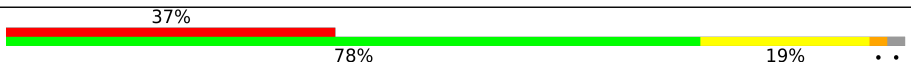
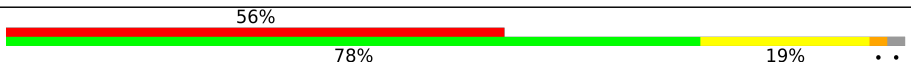
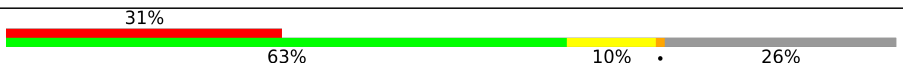
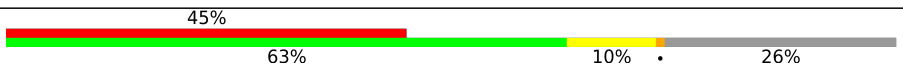
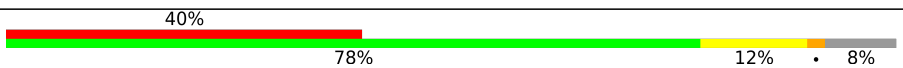
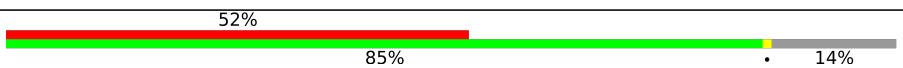
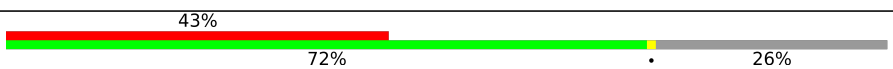
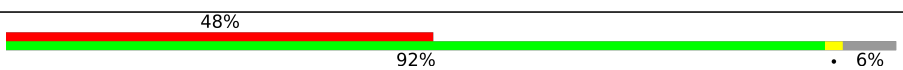
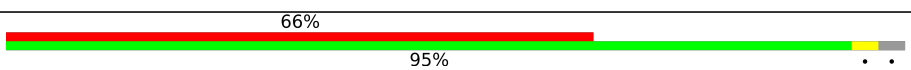
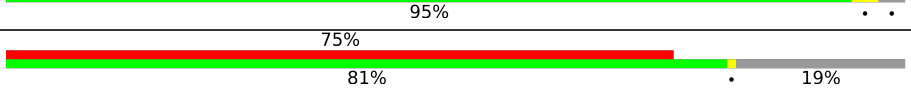
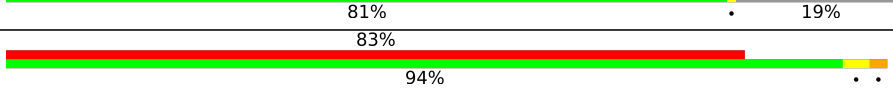
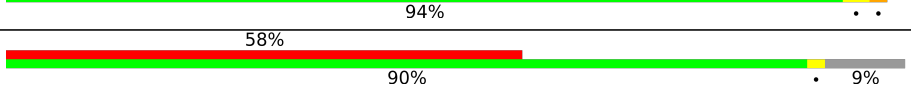
Mol	Chain	Length	Quality of chain
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	1	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	W	268	
16	V	306	
17	T	274	
18	X	156	
19	Y	89	
20	Z	993	

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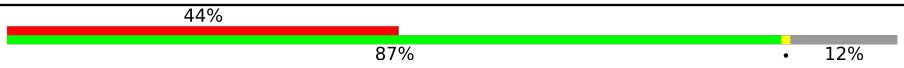
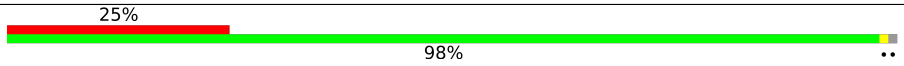
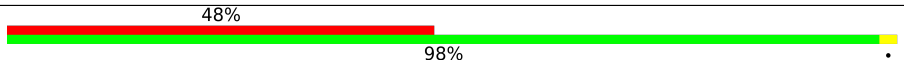
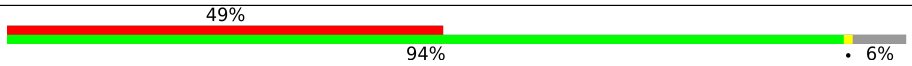
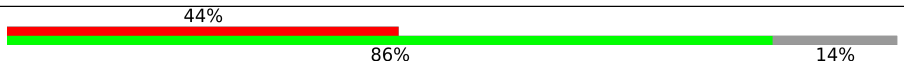
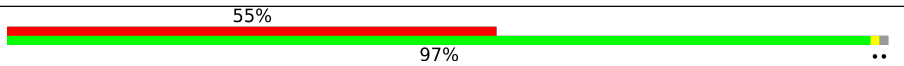
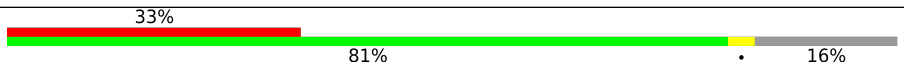
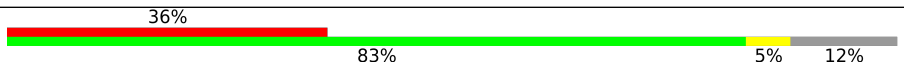
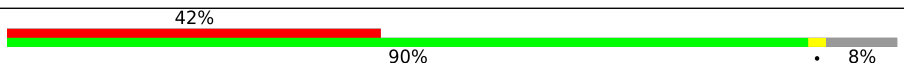
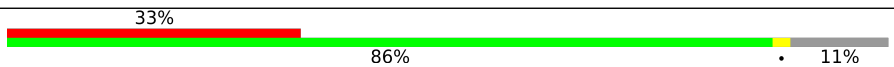
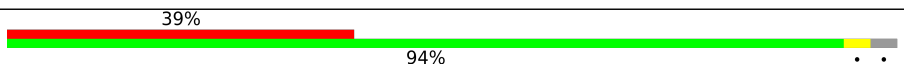
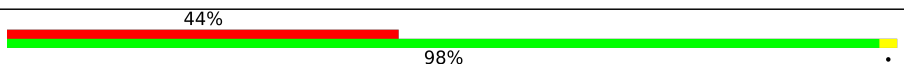
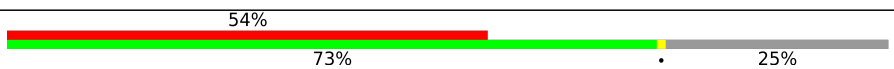
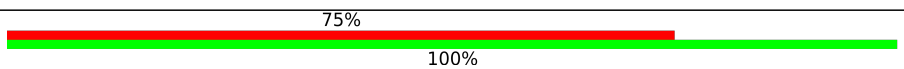
Mol	Chain	Length	Quality of chain
21	N	945	
22	S	523	
23	P	445	
24	Q	434	
25	R	429	
26	U	338	
27	O	393	
28	H	467	
29	I	437	
30	K	428	
31	L	437	
32	M	434	
33	J	405	
34	8	499	
35	9	76	

2 Entry composition (i)

There are 38 unique types of molecules in this entry. The entry contains 112930 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 BJ4_G0020160.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	242	Total	C	N	O	S	0	0
			1912	1217	321	366	8		
1	A	242	Total	C	N	O	S	0	0
			1912	1217	321	366	8		

- Molecule 2 is a protein called HLJ1_G0039880.mRNA.1.CDS.1.

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

- Molecule 3 is a protein called BJ4_G0021480.mRNA.1.CDS.1.

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

- Molecule 4 is a protein called HLJ1_G0048980.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		
4	D	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		

- Molecule 5 is a protein called EM14S01-3B_G0035190.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	249	Total	C	N	O	S	0	0
			1925	1204	324	390	7		
5	E	249	Total	C	N	O	S	0	0
			1925	1204	324	390	7		

- Molecule 6 is a protein called BJ4_G0043800.mRNA.1.CDS.1.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

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

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

- Molecule 9 is a protein called Proteasome endopeptidase complex.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

- Molecule 10 is a protein called Proteasome endopeptidase complex.

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

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

- Molecule 11 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

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

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

- Molecule 13 is a protein called HLJ1_G0013750.mRNA.1.CDS.1.

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

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

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

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

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

- Molecule 16 is a protein called 26S proteasome regulatory subunit RPN11.

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

- Molecule 17 is a protein called EM14S01-3B_G0050020.mRNA.1.CDS.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	266	Total	C	N	O	S	0	0
			2192	1405	349	432	6		

- Molecule 18 is a protein called HLJ1_G0030700.mRNA.1.CDS.1.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	906	Total	C	N	O	S	0	0
			7005	4416	1150	1409	30		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	832	Total	C	N	O	S	0	0
			6418	4078	1077	1238	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	440	Total	C	N	O	S	0	0
			3608	2297	604	697	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	434	Total	C	N	O	S	0	0
			3499	2225	577	681	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	405	Total	C	N	O	S	0	0
			3258	2077	535	636	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	290	Total	C	N	O	S	0	0
			2306	1454	392	453	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	391	Total	C	N	O	S	0	0
			3064	1927	551	569	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ARG	SER	variant	UNP A0A6A5PV22
H	166	LYS	THR	variant	UNP A0A6A5PV22

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I	384	Total	C	N	O	S	0	0
			3015	1895	507	596	17		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	388	Total	C	N	O	S	0	0
			3082	1942	548	580	12		

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

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

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

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

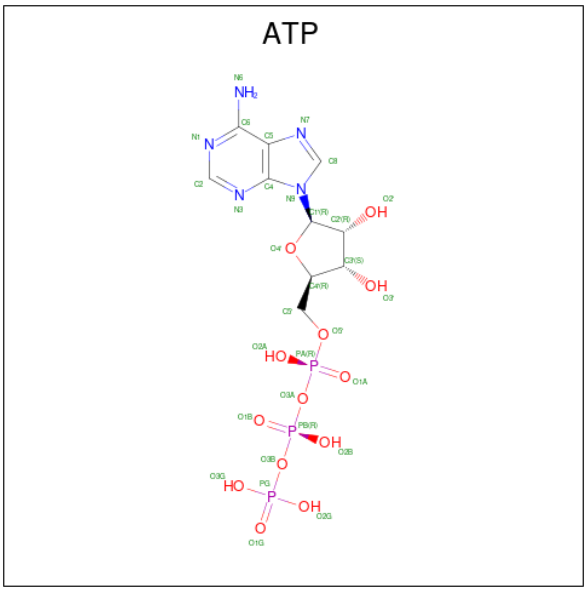
- Molecule 34 is a protein called Ubiquitin carboxyl-terminal hydrolase.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	372	Total	C	N	O	S	0	0
			3034	1918	521	583	12		

- Molecule 35 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

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



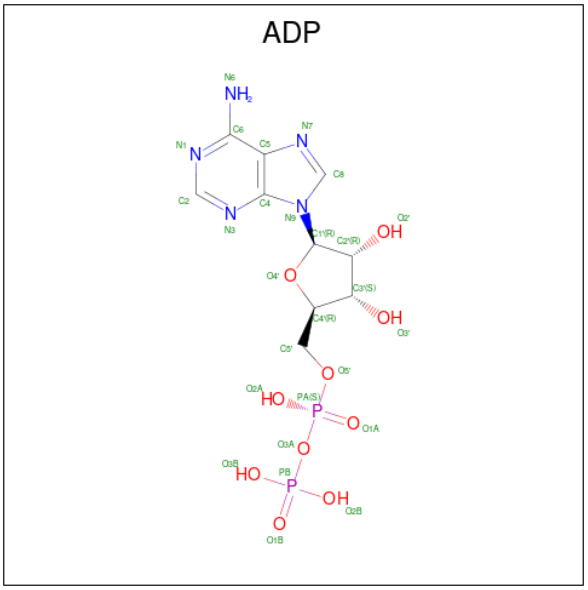
Mol	Chain	Residues	Atoms					AltConf
36	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

$C_{10}H_{15}N_5O_{10}P_2$).



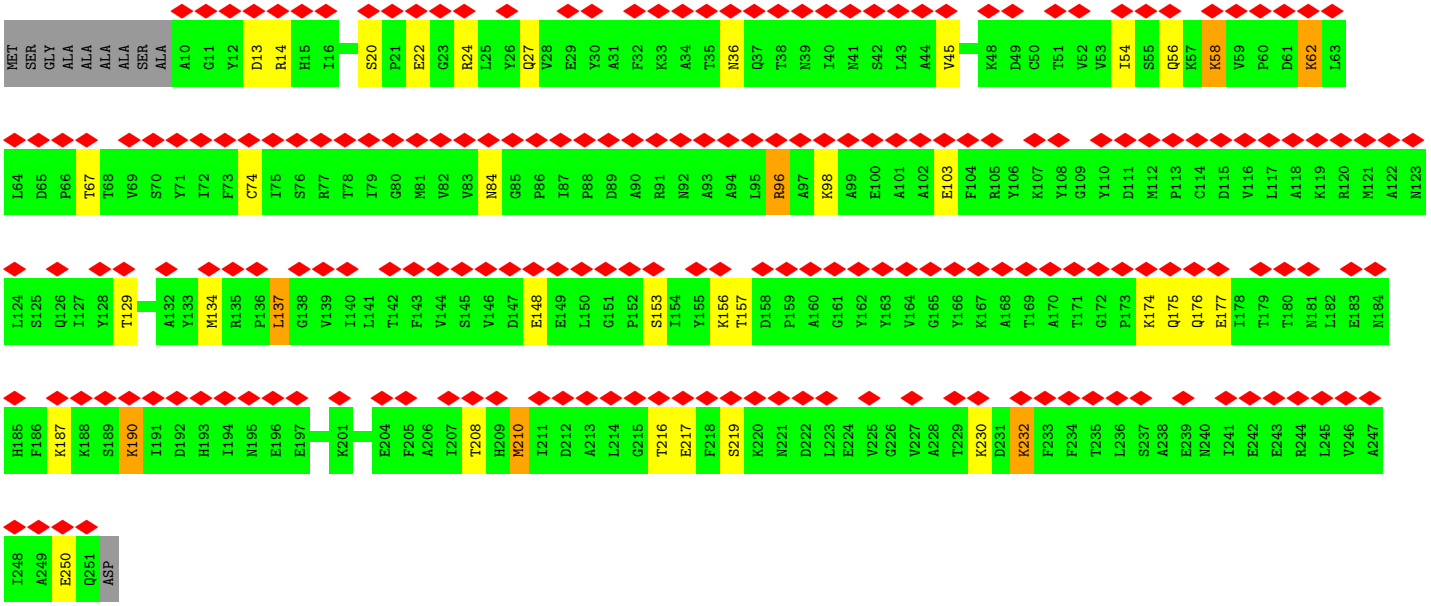
Mol	Chain	Residues	Atoms					AltConf
38	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

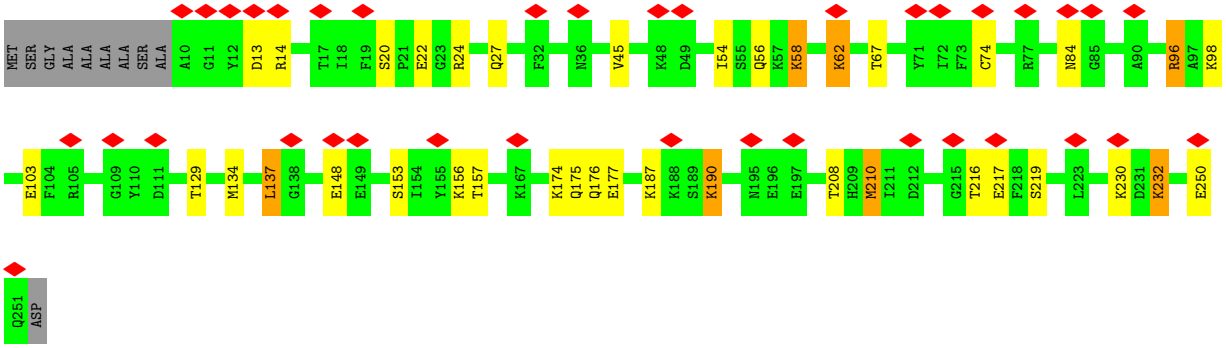
• Molecule 1: BJ4_G0020160.mRNA.1.CDS.1

Chain a:



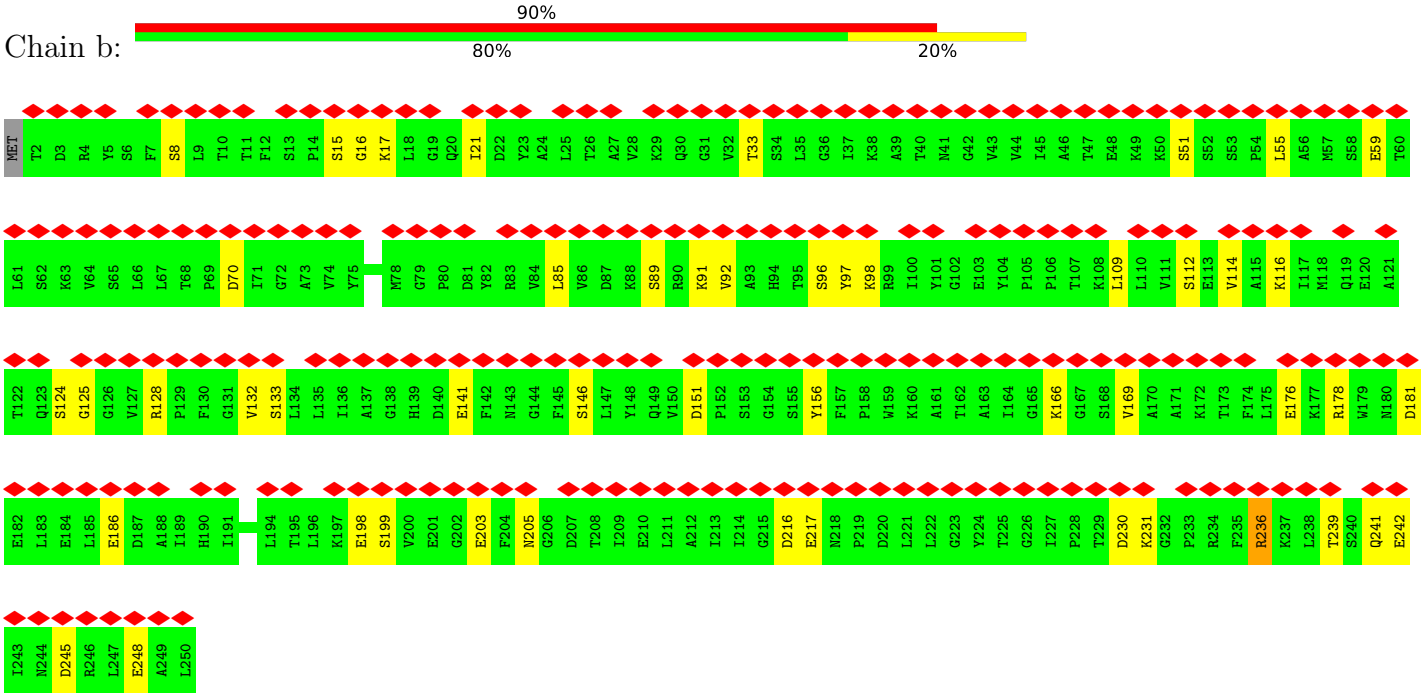
• Molecule 1: BJ4_G0020160.mRNA.1.CDS.1

Chain A:



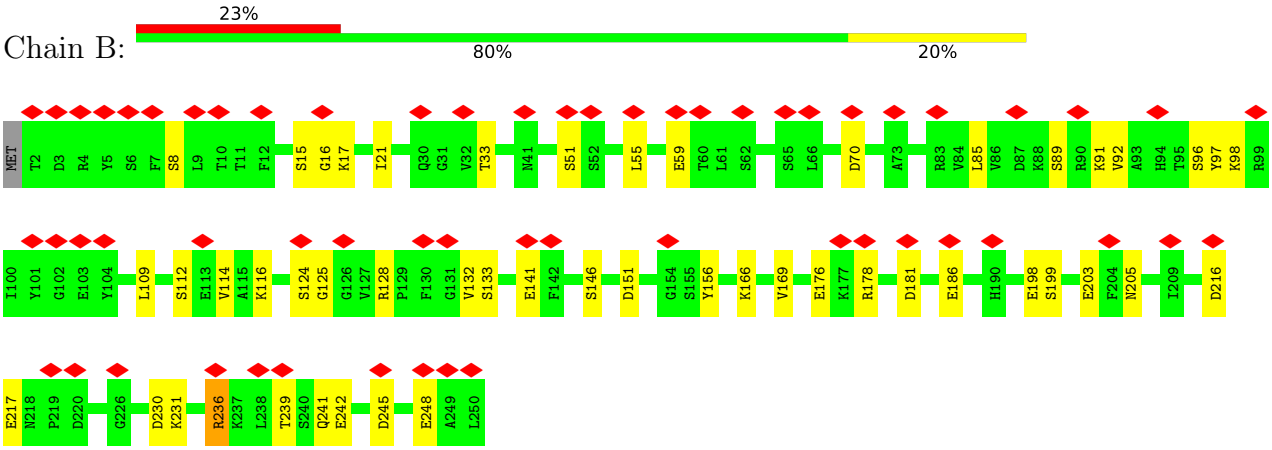
• Molecule 2: HLJ1_G0039880.mRNA.1.CDS.1

Chain b:



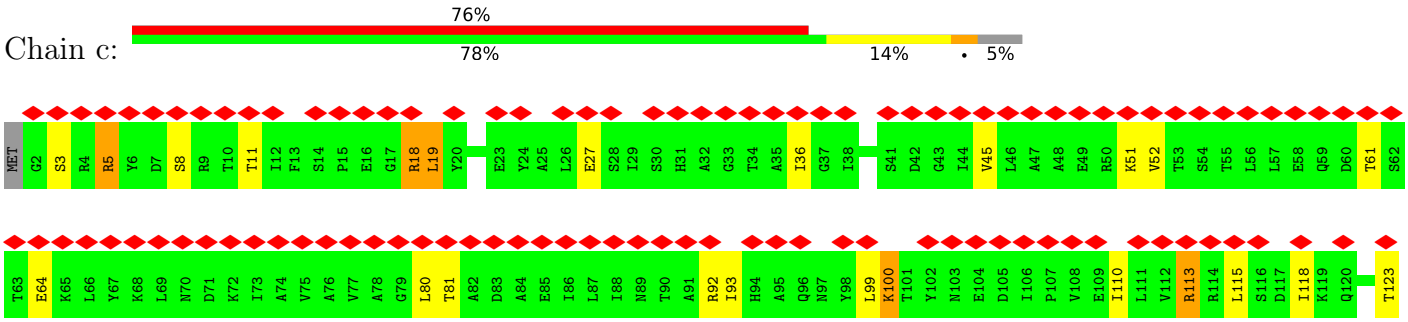
• Molecule 2: HLJ1_G0039880.mRNA.1.CDS.1

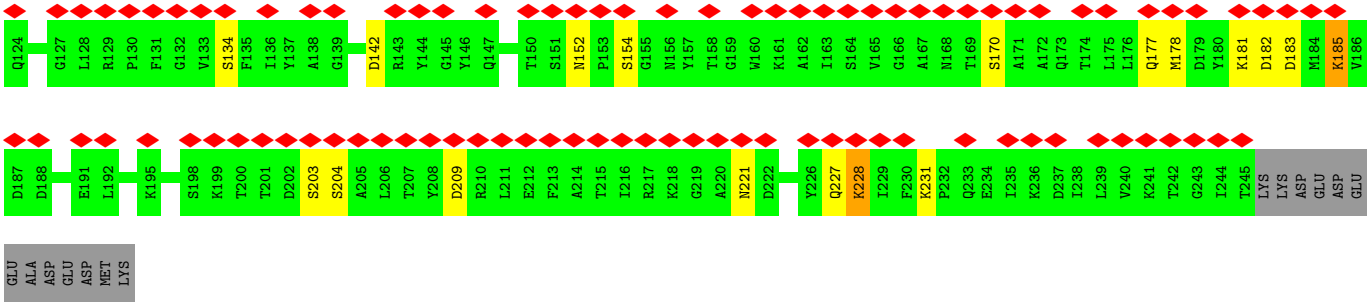
Chain B:



• Molecule 3: BJ4_G0021480.mRNA.1.CDS.1

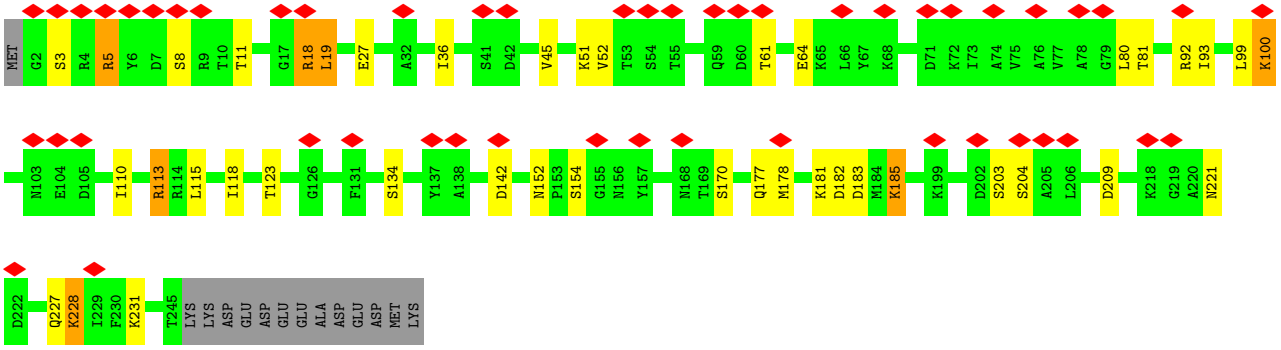
Chain c:





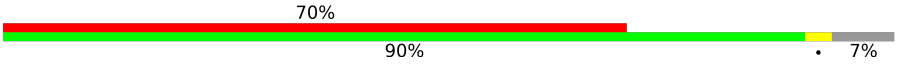
• Molecule 3: BJ4_G0021480.mRNA.1.CDS.1

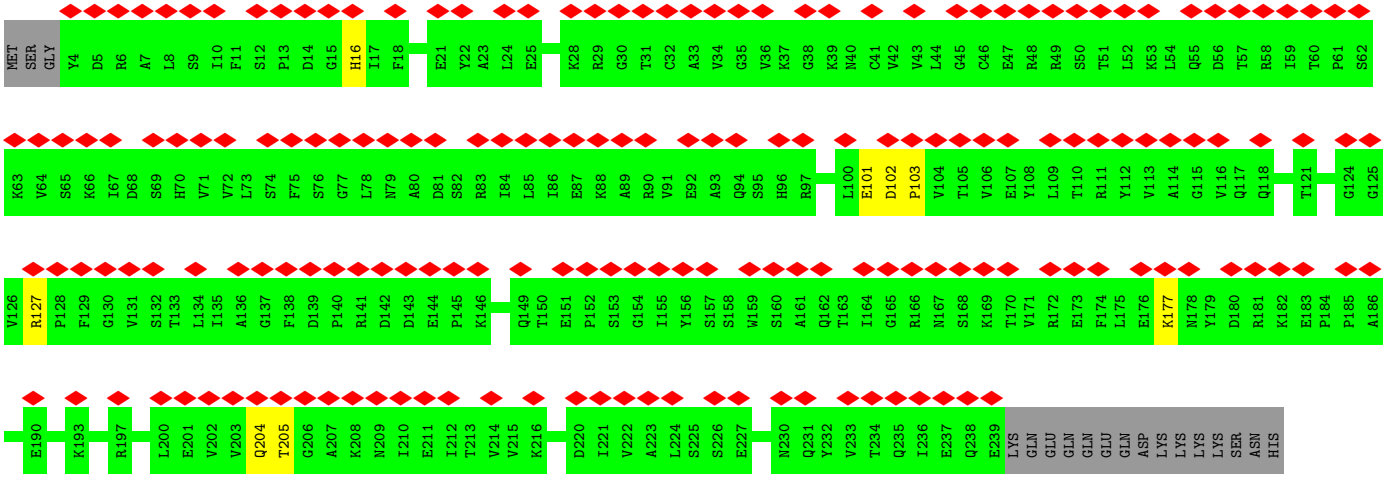
Chain C:



• Molecule 4: HLJ1_G0048980.mRNA.1.CDS.1

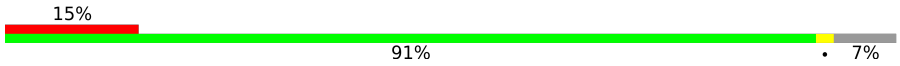
Chain d:

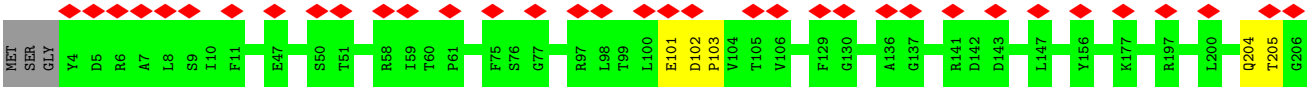


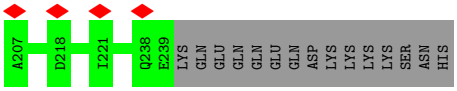


• Molecule 4: HLJ1_G0048980.mRNA.1.CDS.1

Chain D:

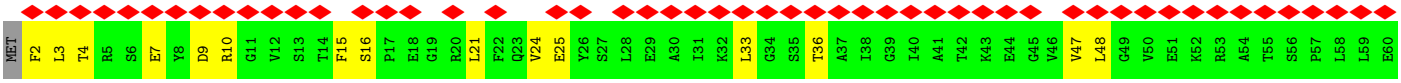


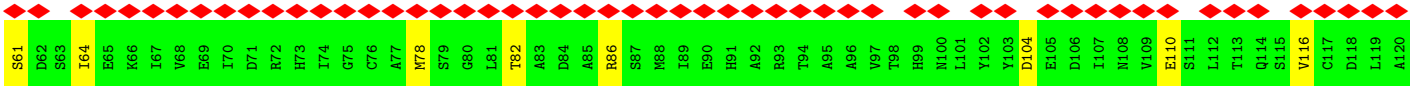


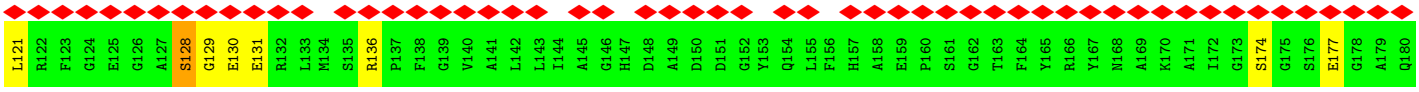


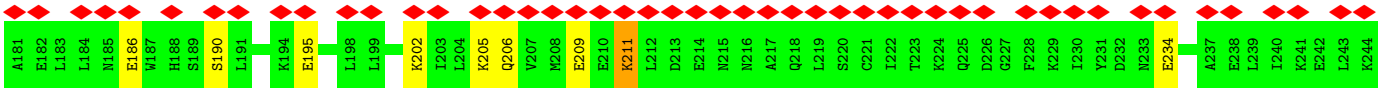
• Molecule 5: EM14S01-3B_G0035190.mRNA.1.CDS.1

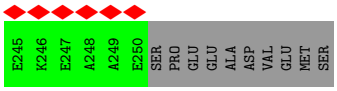
Chain e:





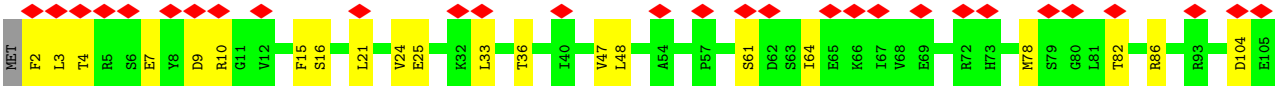


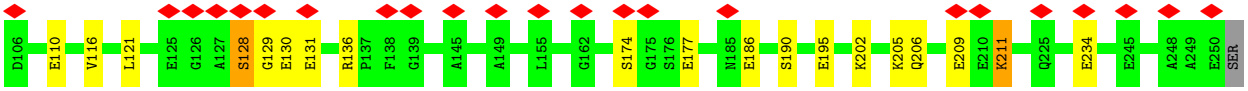




• Molecule 5: EM14S01-3B_G0035190.mRNA.1.CDS.1

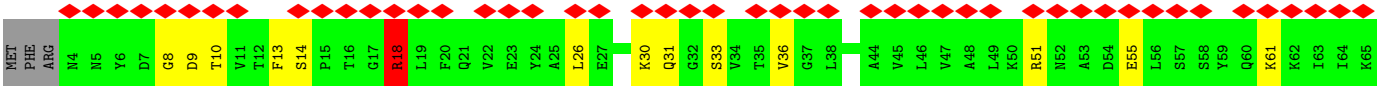
Chain E:

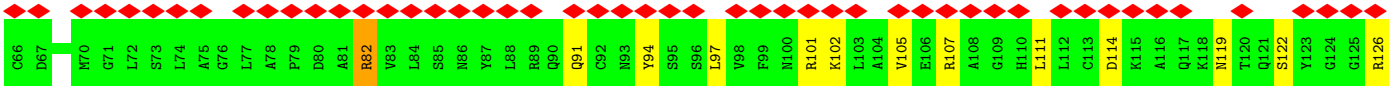


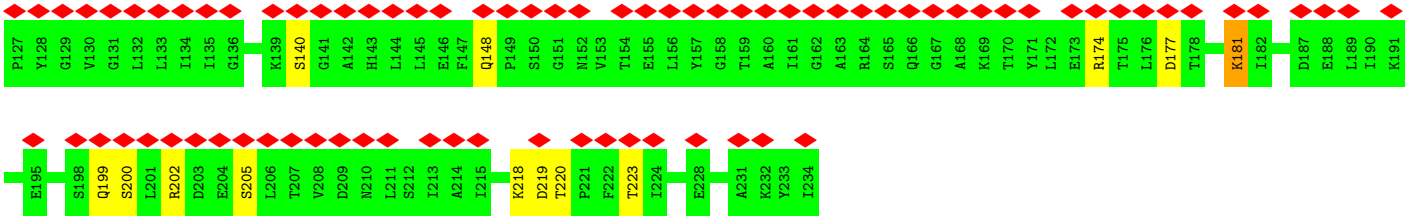


• Molecule 6: BJ4_G0043800.mRNA.1.CDS.1

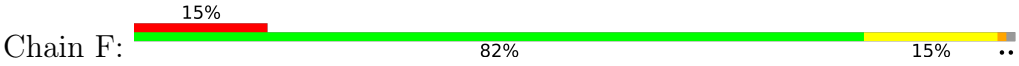
Chain f:







• Molecule 6: BJ4_G0043800.mRNA.1.CDS.1

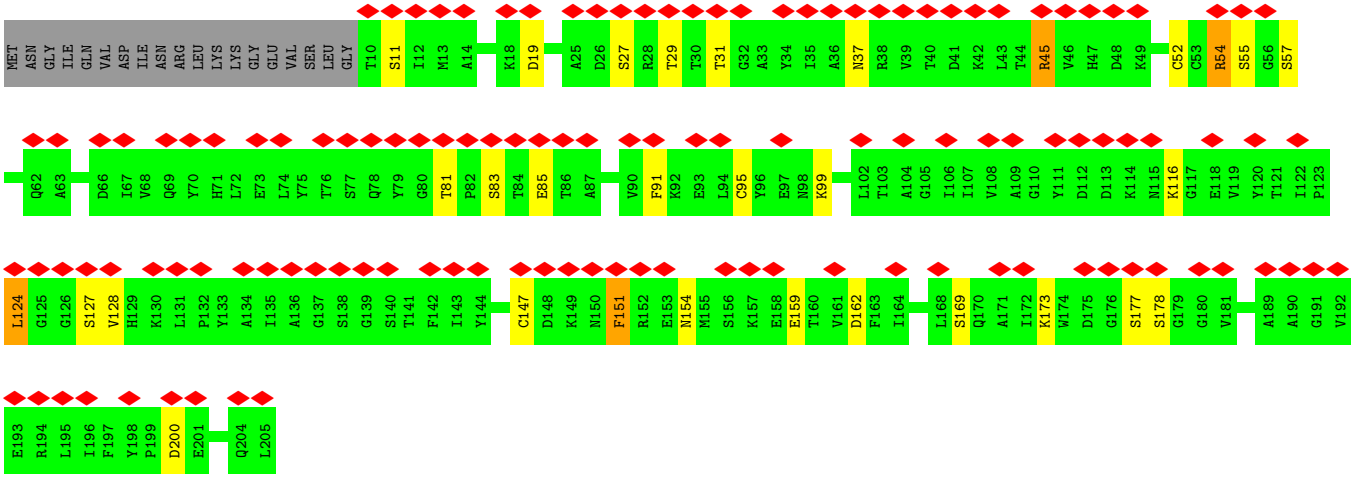


• Molecule 7: Probable proteasome subunit alpha type-7

• Molecule 7: Probable proteasome subunit alpha type-7

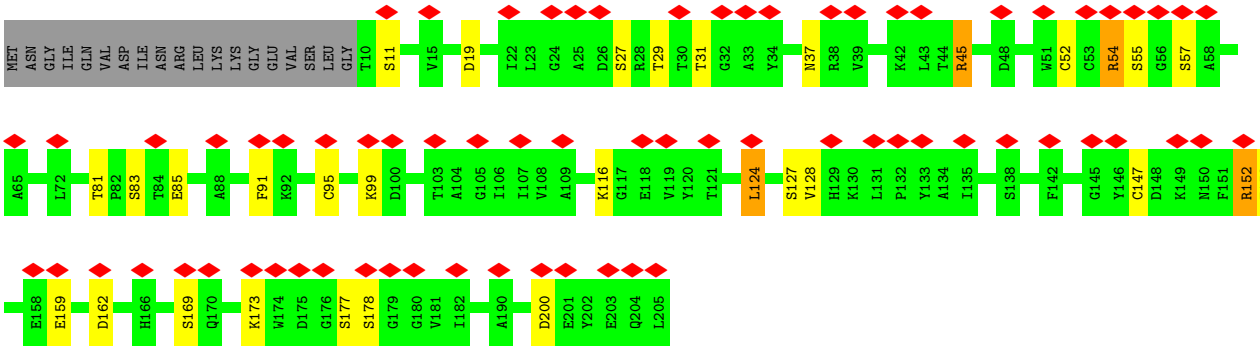
• Molecule 8: Proteasome subunit beta type-1

Chain h:



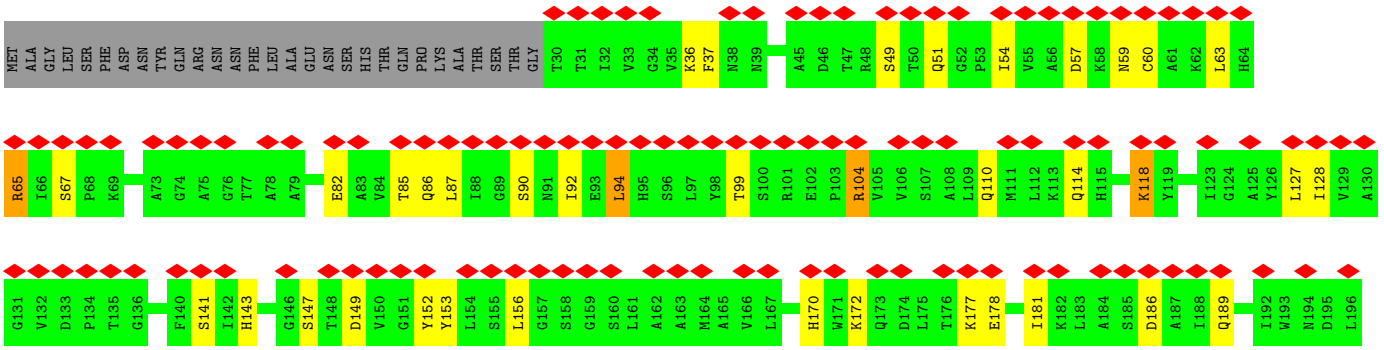
• Molecule 8: Proteasome subunit beta type-1

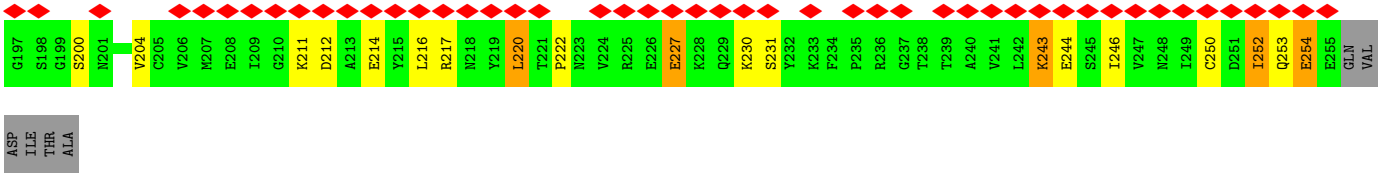
Chain 1:



• Molecule 9: Proteasome endopeptidase complex

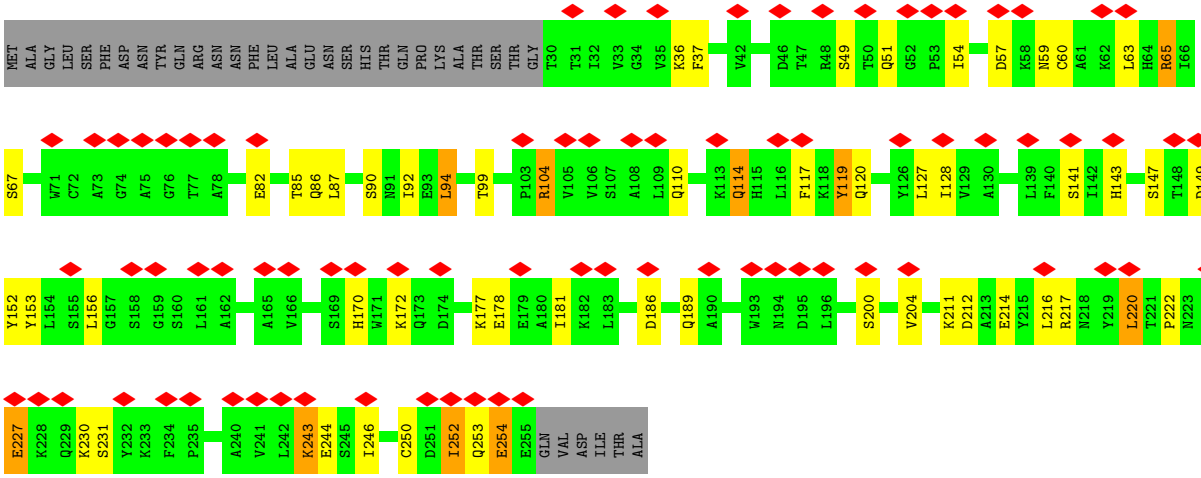
Chain i:





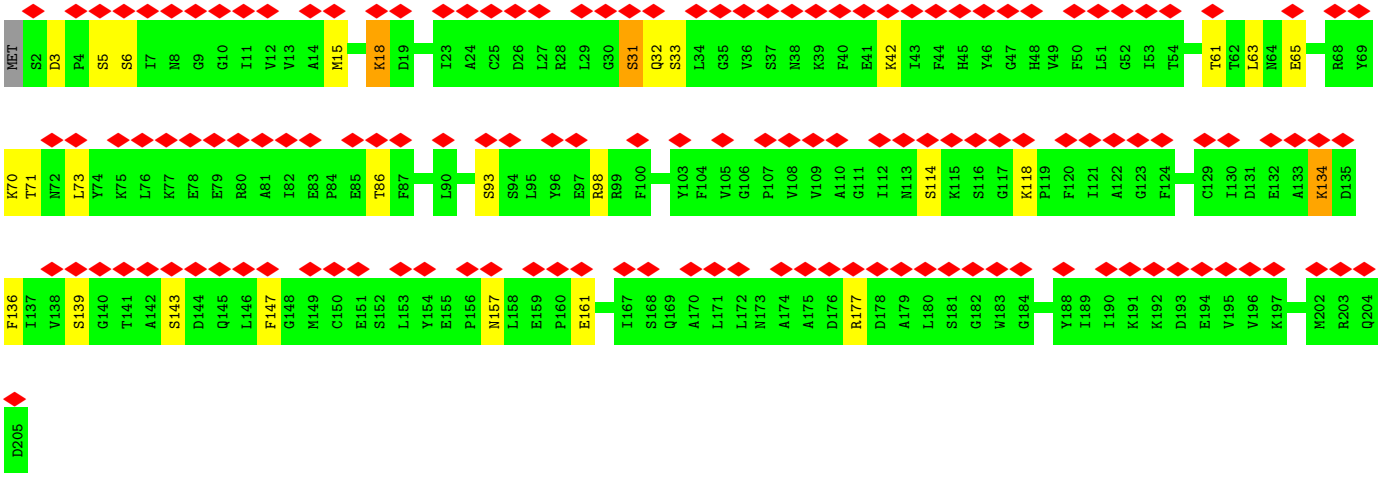
• Molecule 9: Proteasome endopeptidase complex

Chain 2:



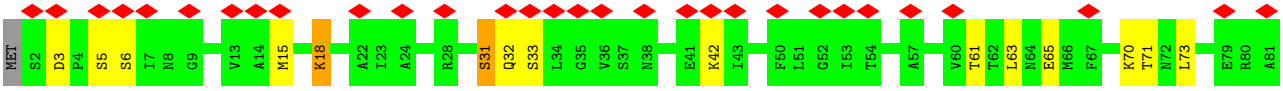
• Molecule 10: Proteasome endopeptidase complex

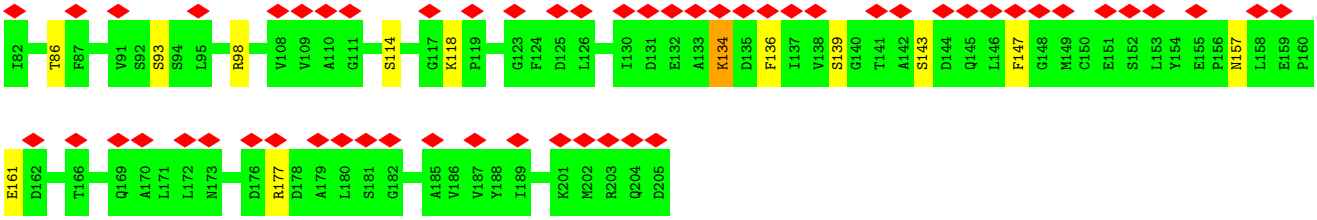
Chain j:



• Molecule 10: Proteasome endopeptidase complex

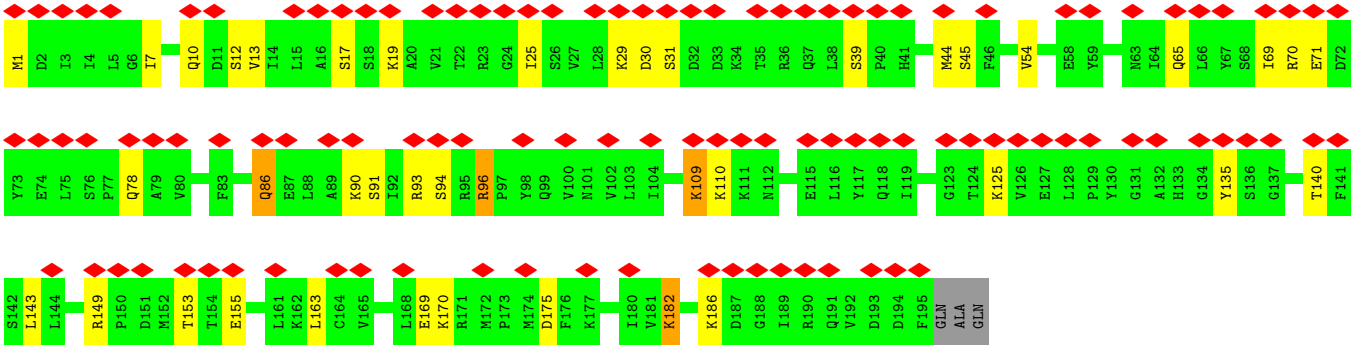
Chain 3:





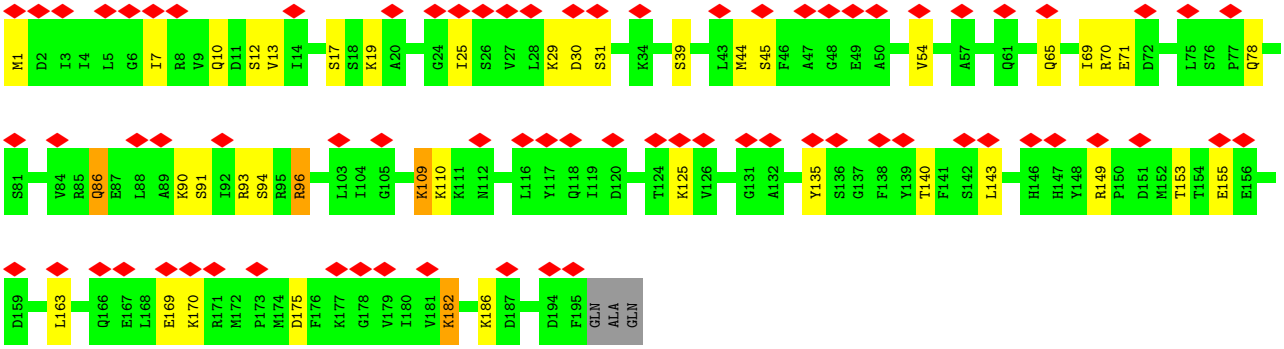
• Molecule 11: Proteasome subunit beta

Chain k:



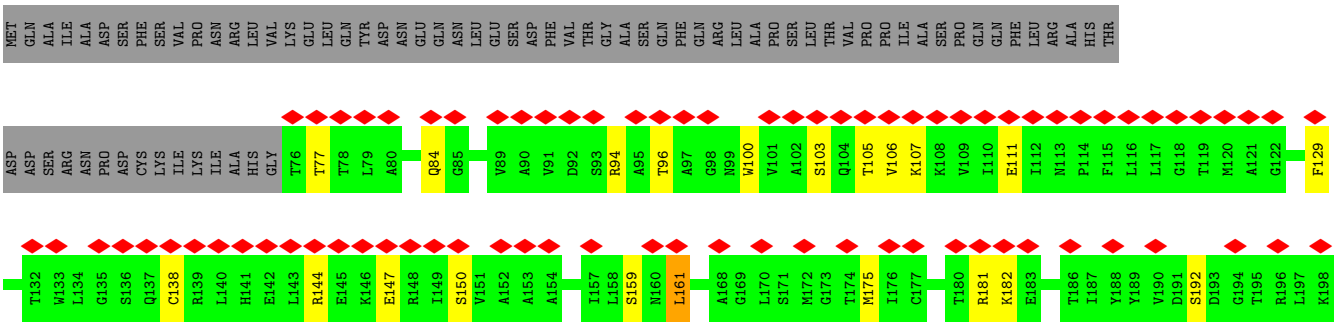
• Molecule 11: Proteasome subunit beta

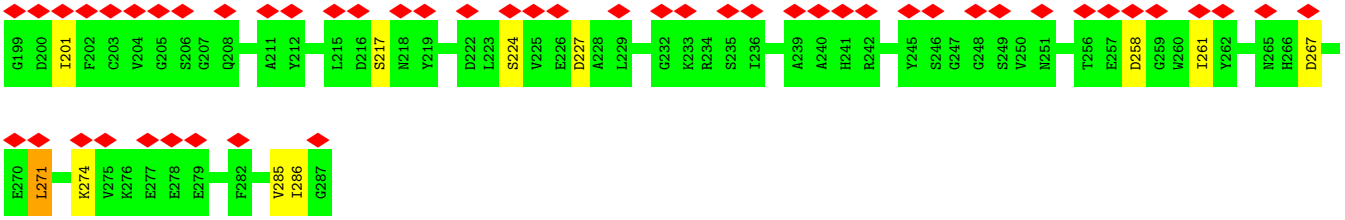
Chain 4:



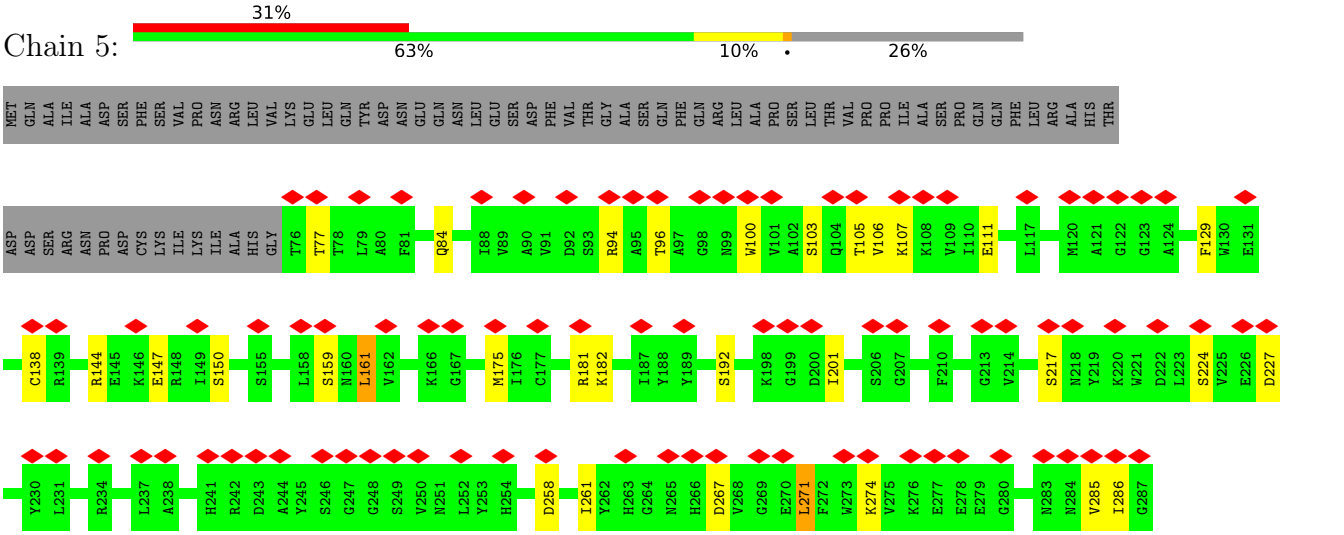
• Molecule 12: Proteasome subunit beta type-5

Chain l:

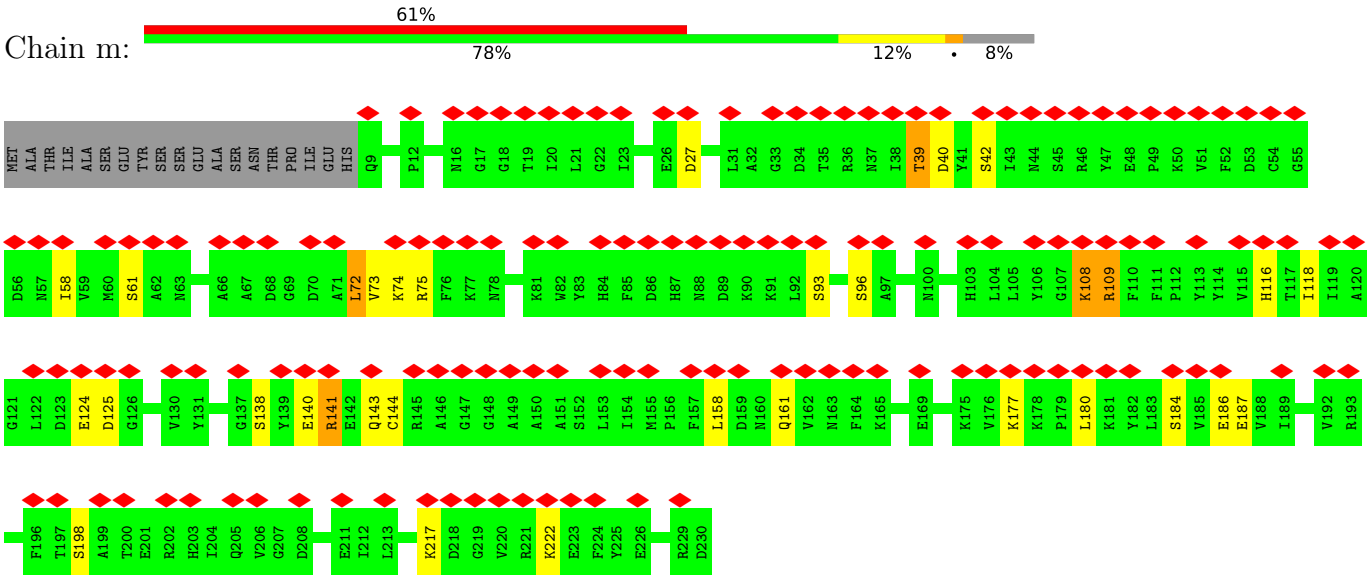




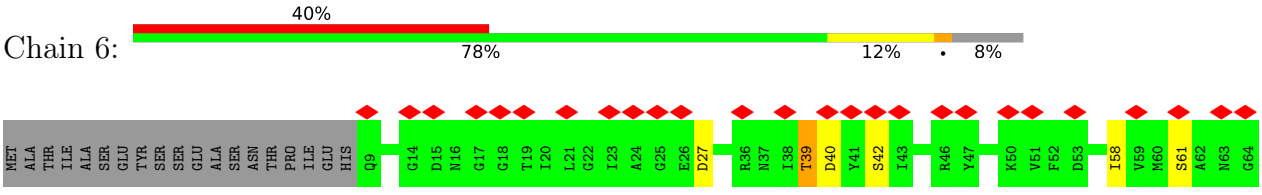
• Molecule 12: Proteasome subunit beta type-5

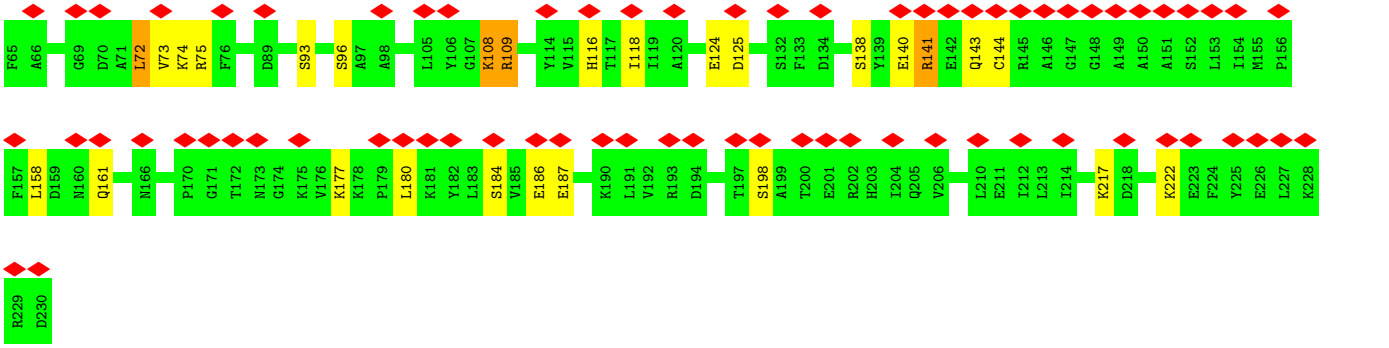


• Molecule 13: HLJ1_G0013750.mRNA.1.CDS.1

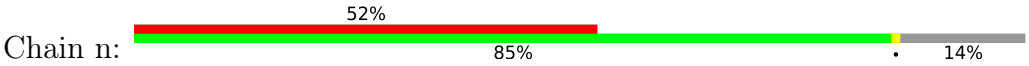


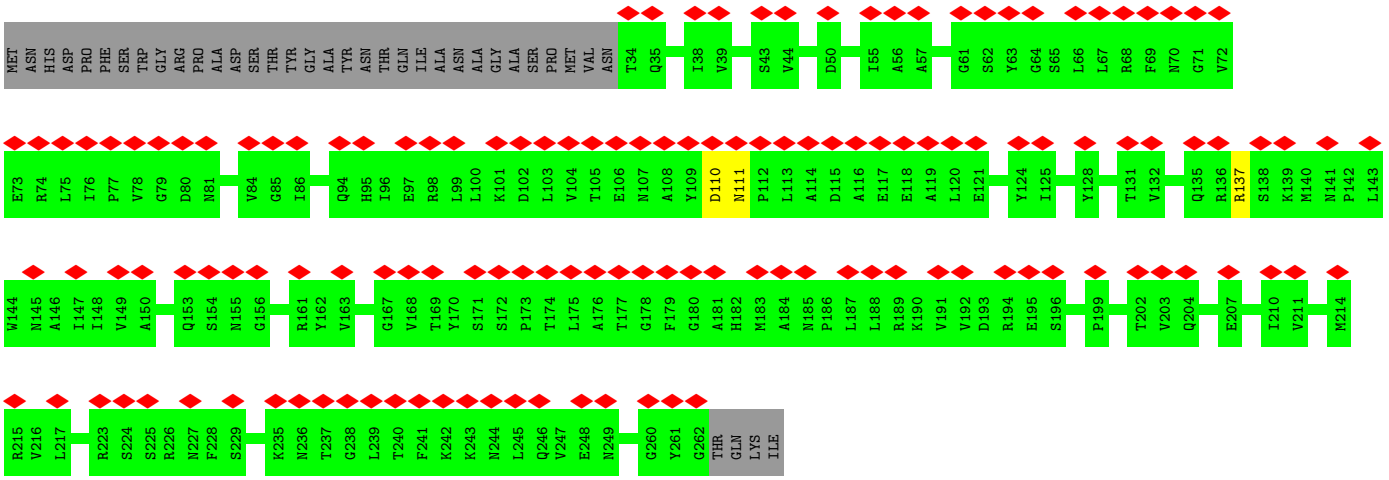
• Molecule 13: HLJ1_G0013750.mRNA.1.CDS.1



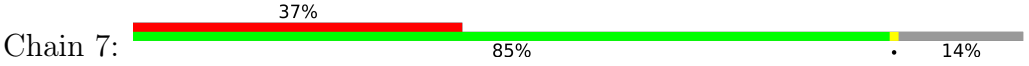


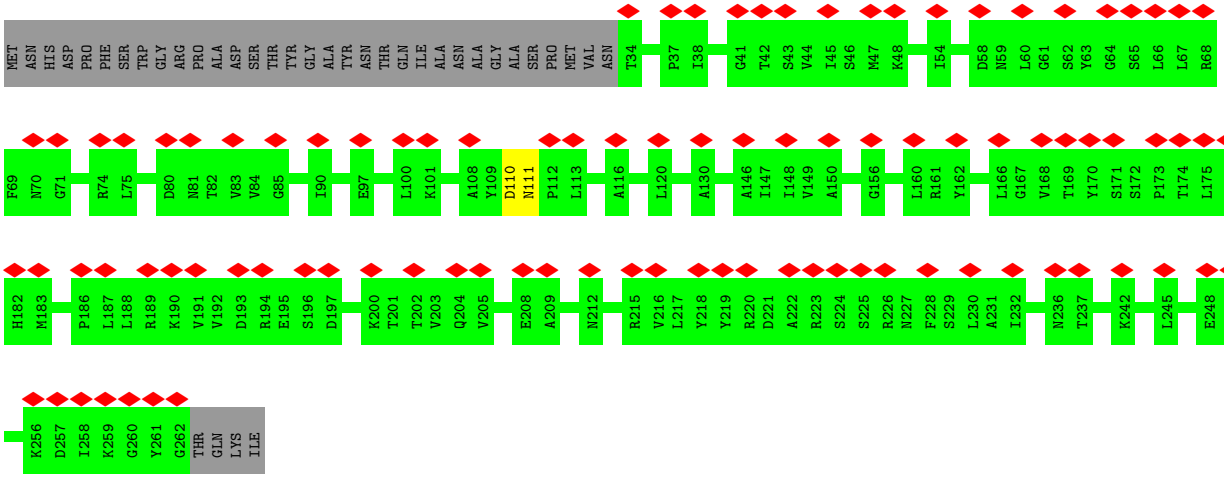
• Molecule 14: Proteasome subunit beta type-7





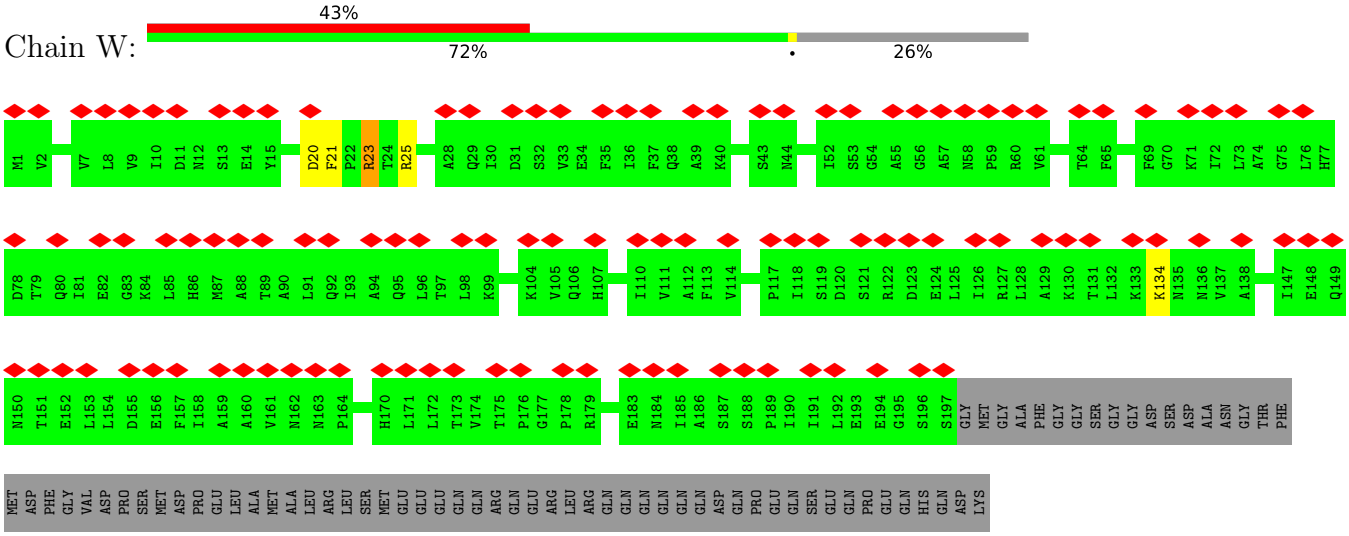
• Molecule 14: Proteasome subunit beta type-7





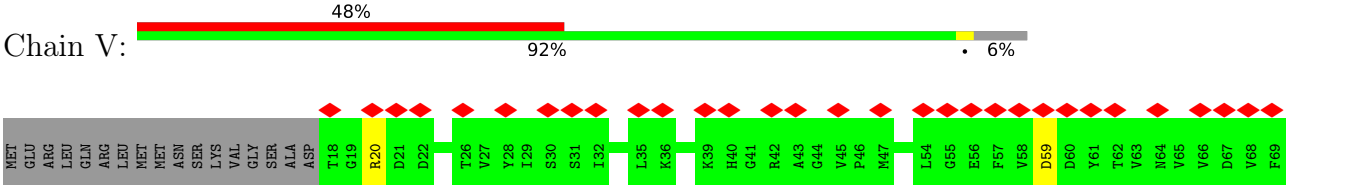
• Molecule 15: 26S proteasome regulatory subunit RPN10

Chain W:



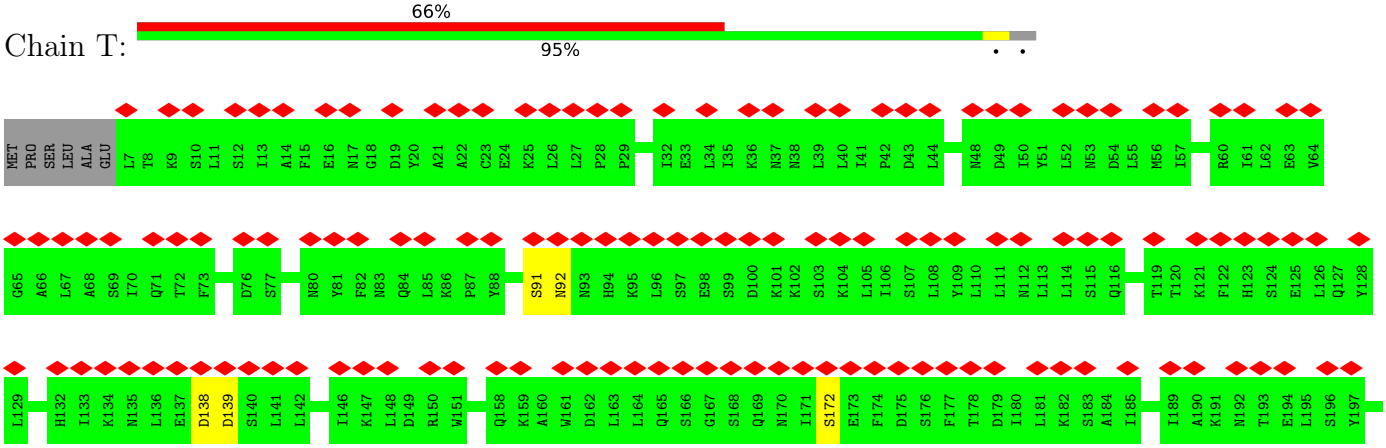
• Molecule 16: 26S proteasome regulatory subunit RPN11

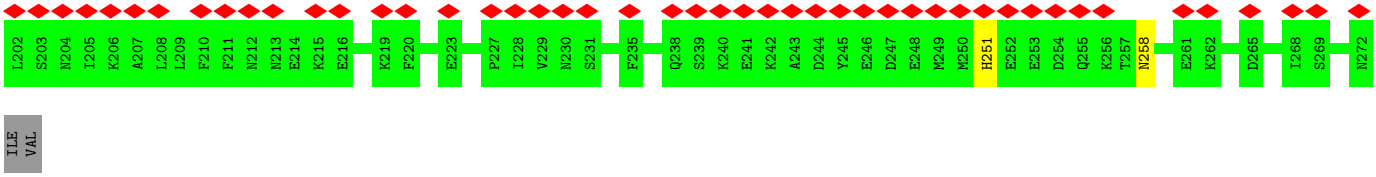
Chain V:



• Molecule 17: EM14S01-3B_G0050020.mRNA.1.CDS.1

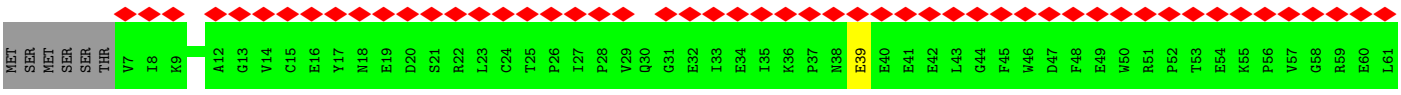
Chain T:

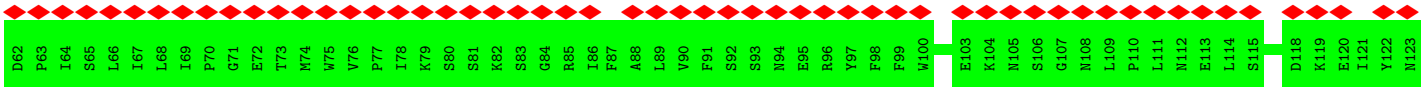


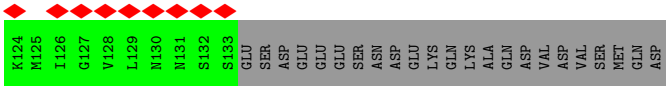


• Molecule 18: HLJ1_G0030700.mRNA.1.CDS.1

Chain X:

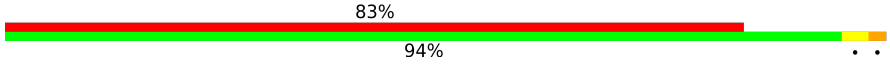


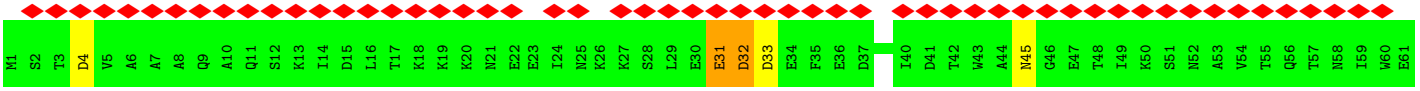


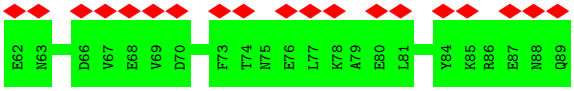


• Molecule 19: 26S proteasome complex subunit SEM1

Chain Y:

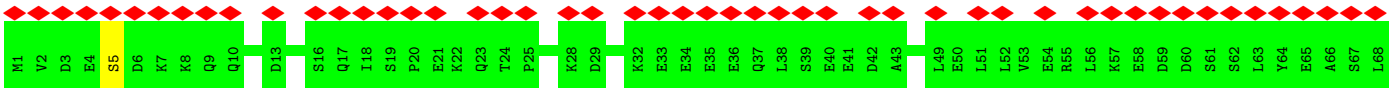


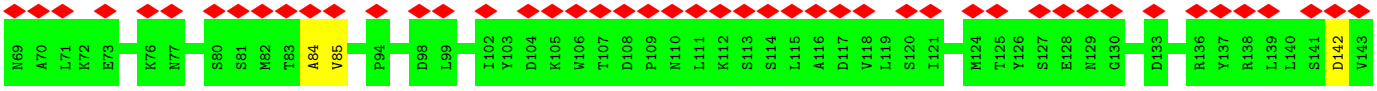


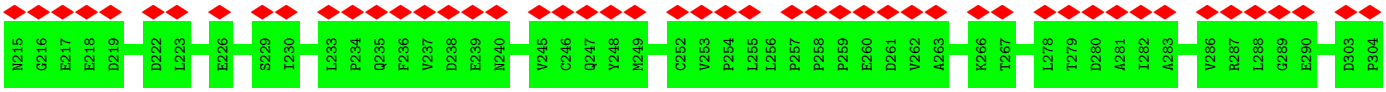


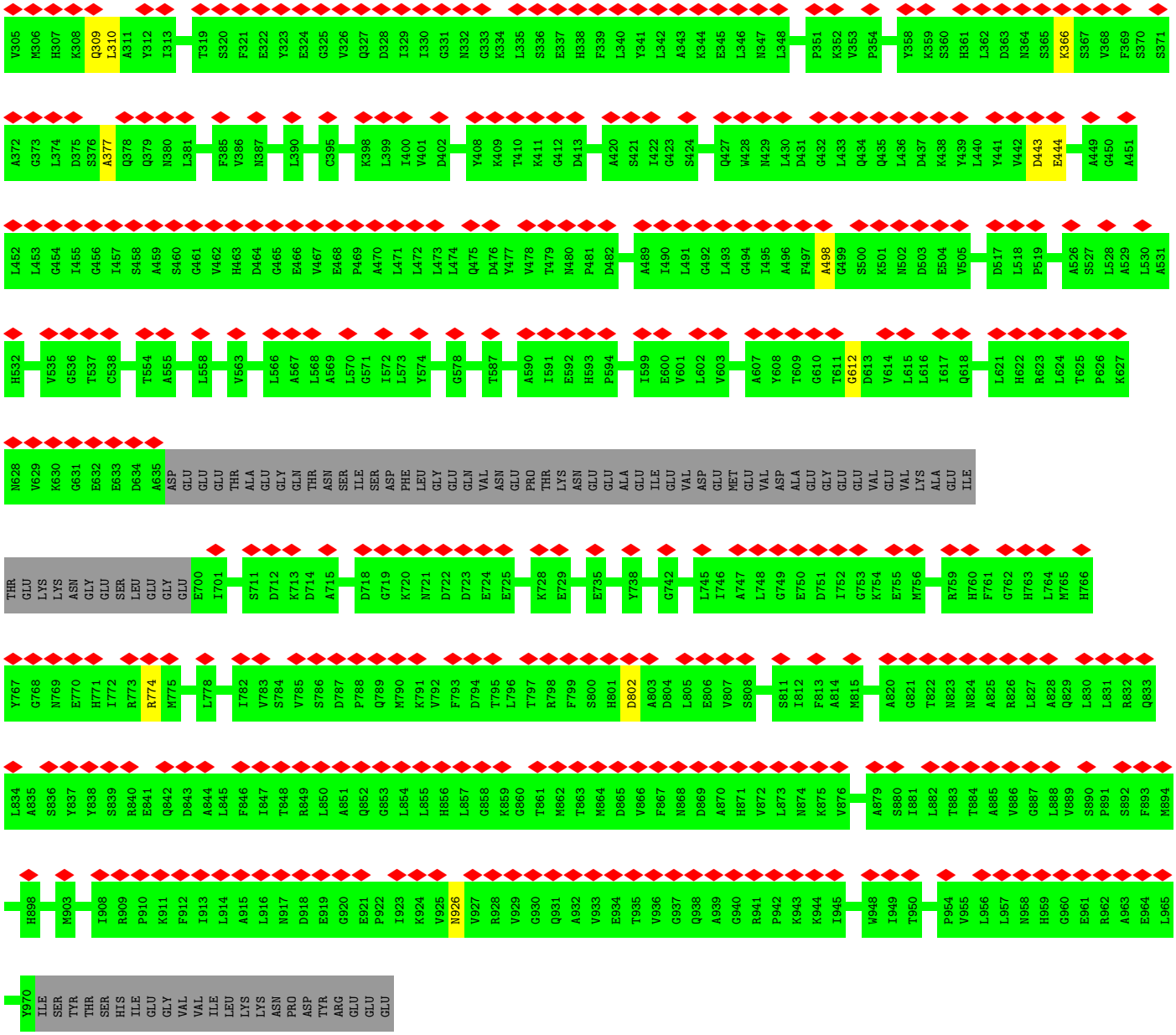
• Molecule 20: 26S proteasome regulatory subunit RPN1

Chain Z:



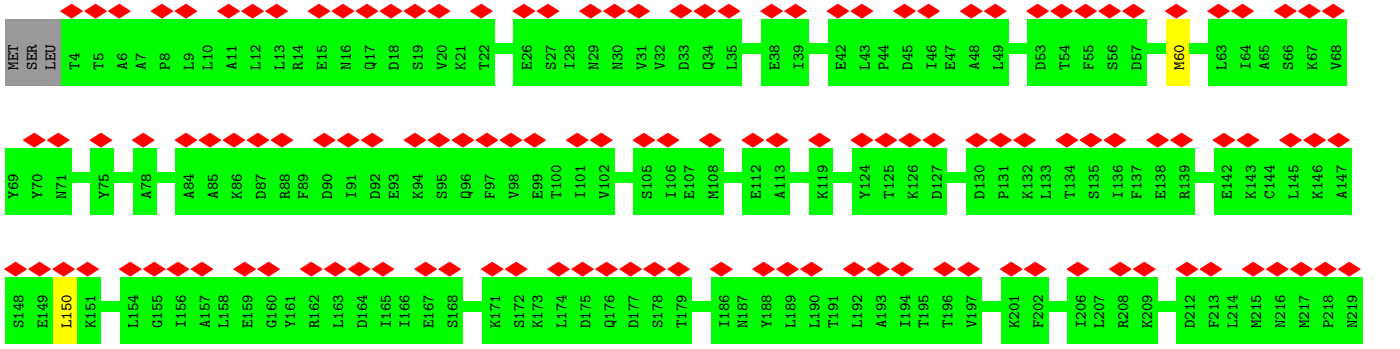


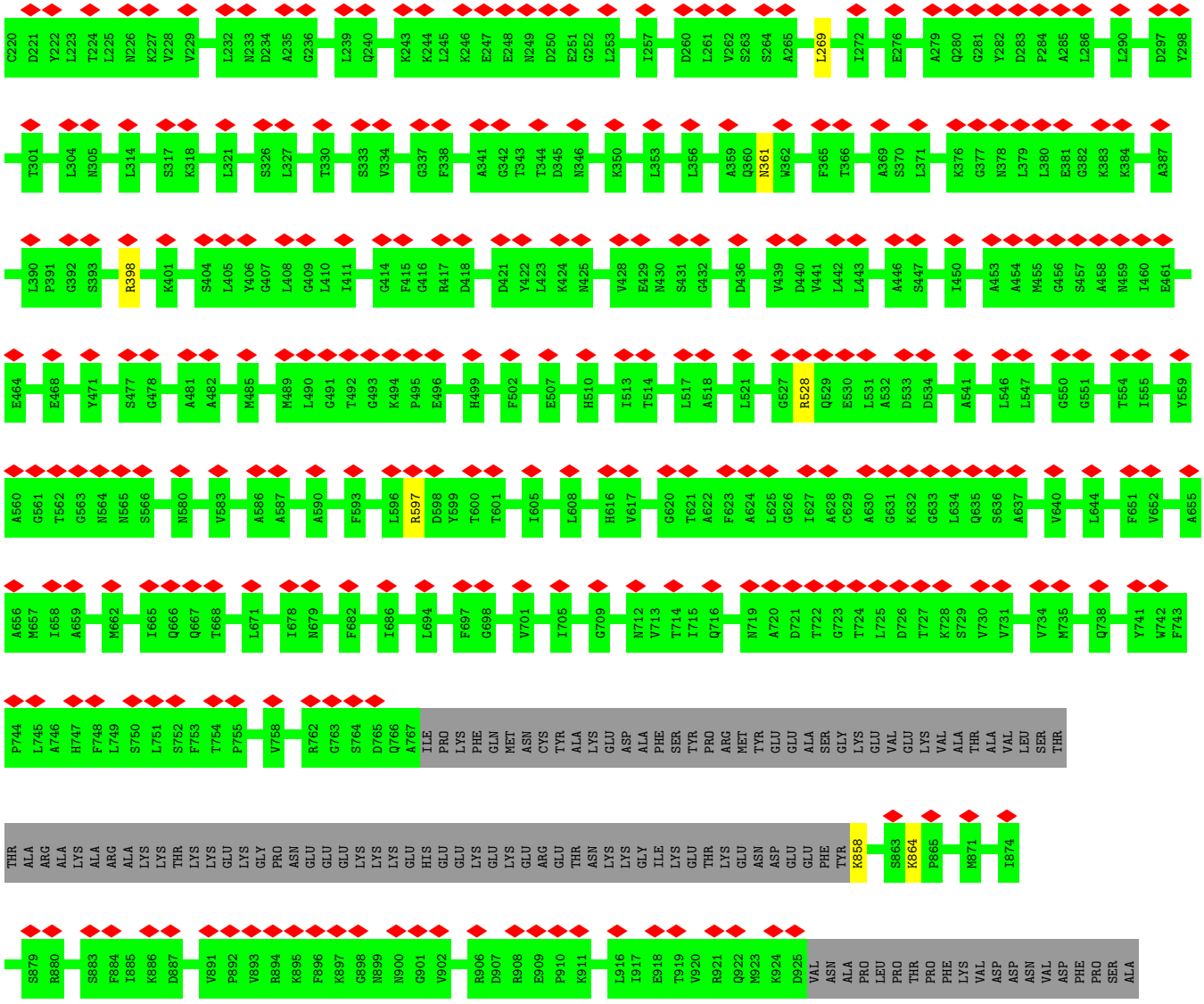




• Molecule 21: 26S proteasome regulatory subunit RPN2

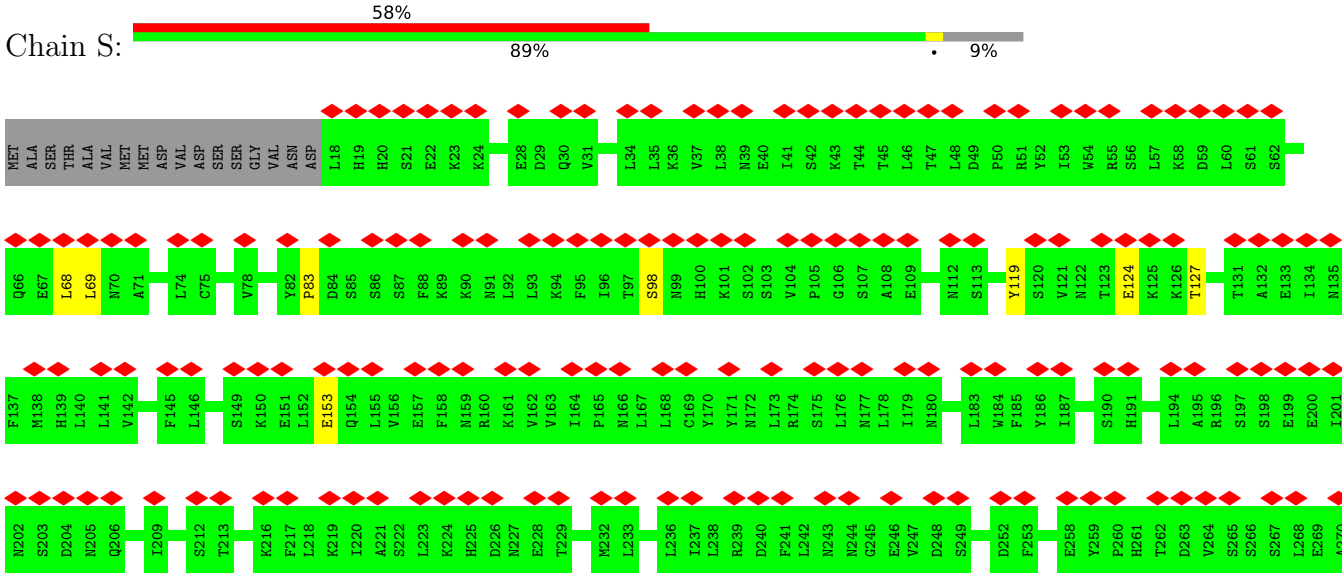
Chain N:

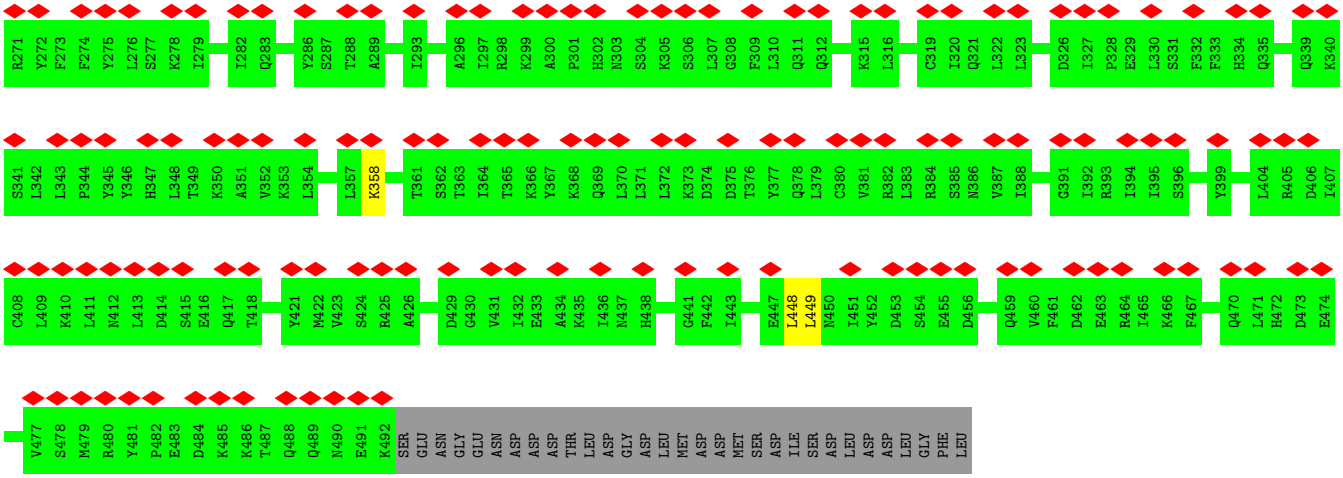




• Molecule 22: 26S proteasome regulatory subunit RPN3

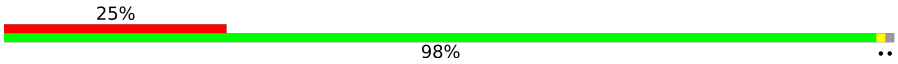
Chain S:

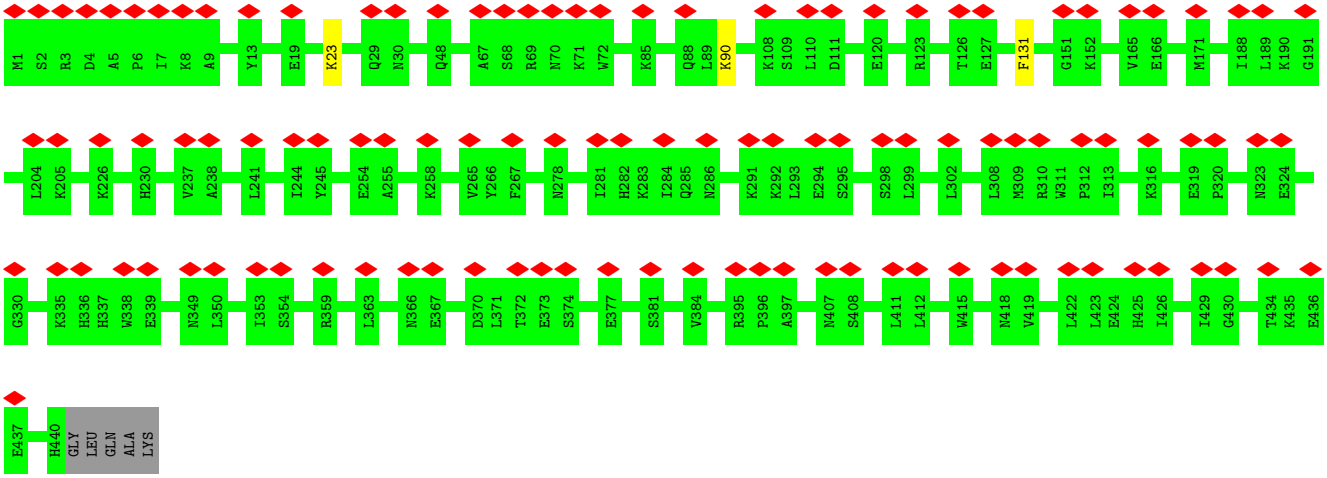




• Molecule 23: 26S proteasome regulatory subunit RPN5

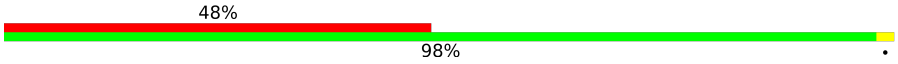
Chain P:

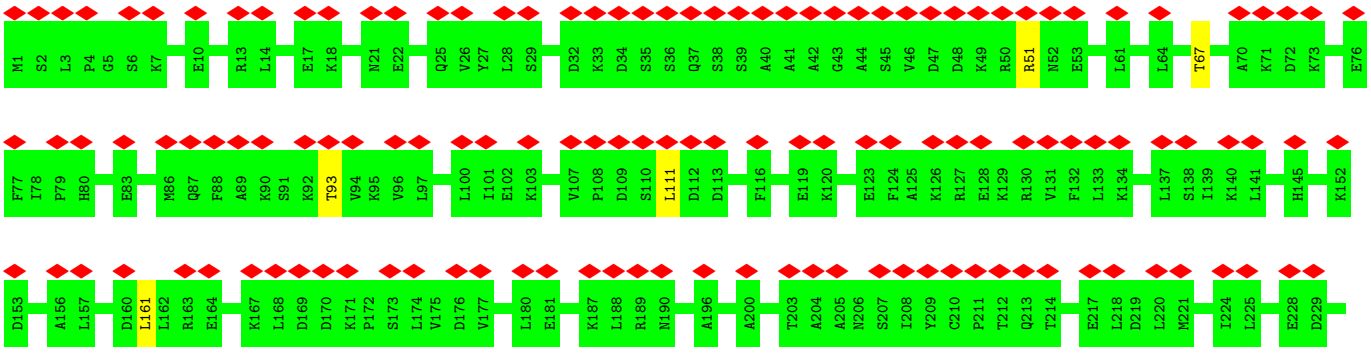


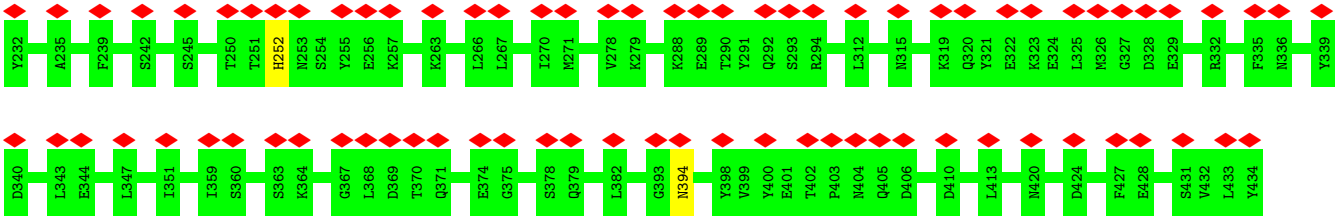


• Molecule 24: 26S proteasome regulatory subunit RPN6

Chain Q:

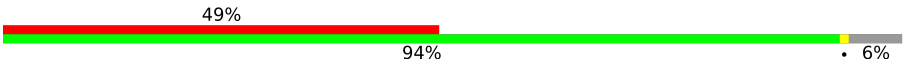


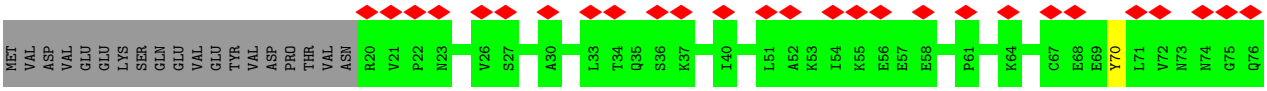




• Molecule 25: 26S proteasome regulatory subunit RPN7

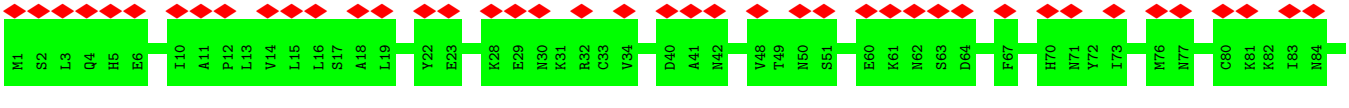
Chain R:

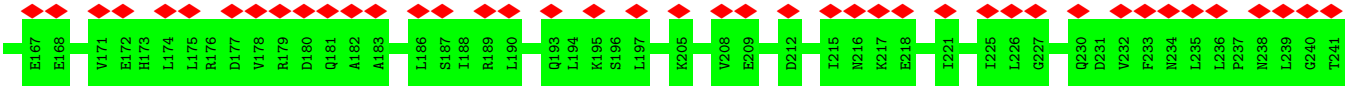


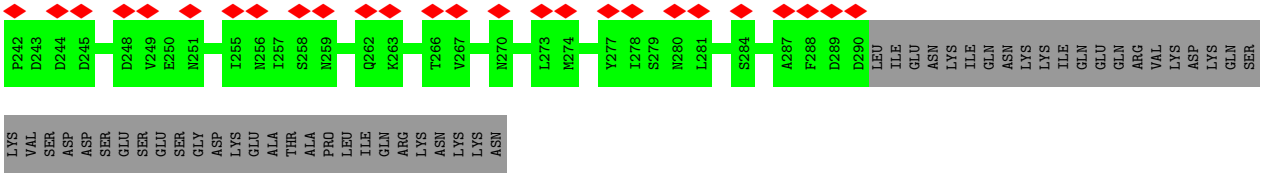


• Molecule 26: 26S proteasome regulatory subunit RPN8

Chain U:

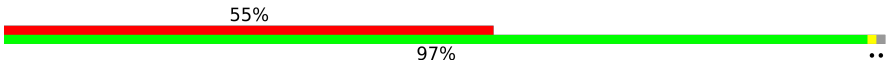


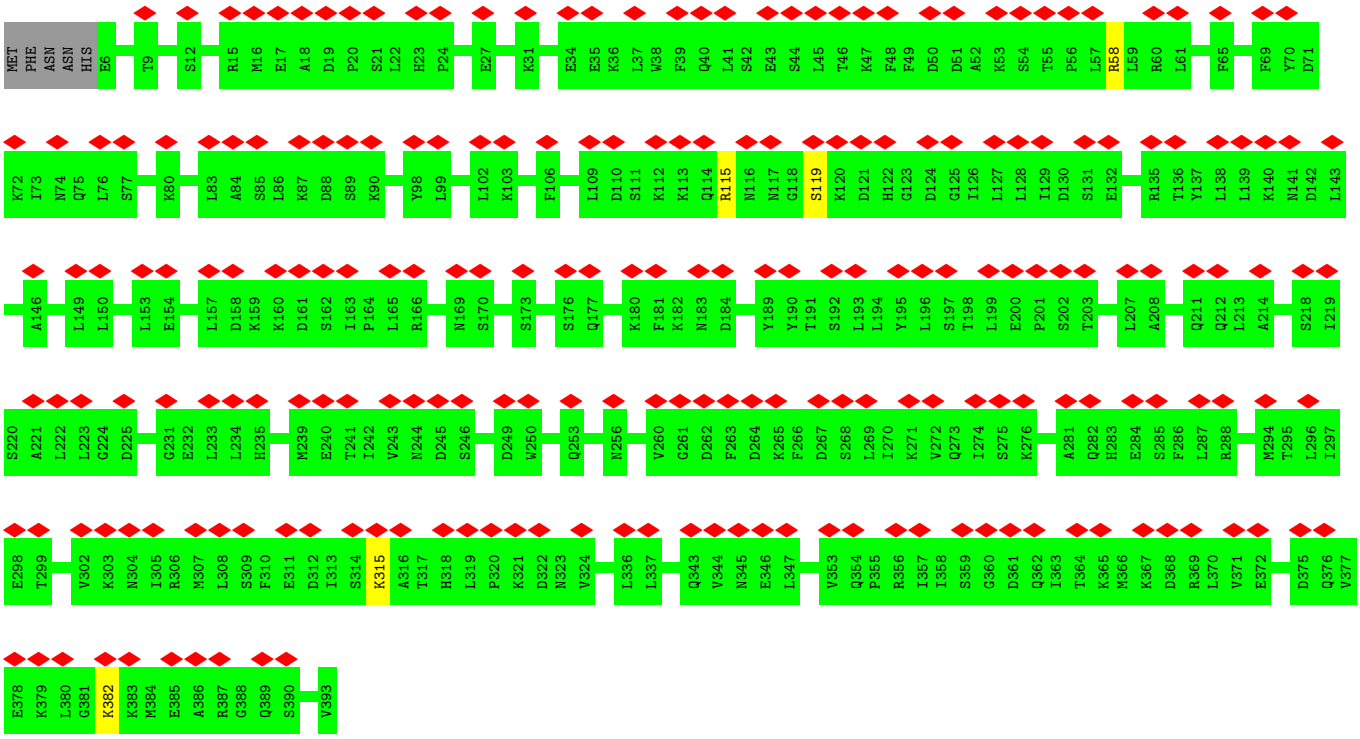




• Molecule 27: 26S proteasome regulatory subunit RPN9

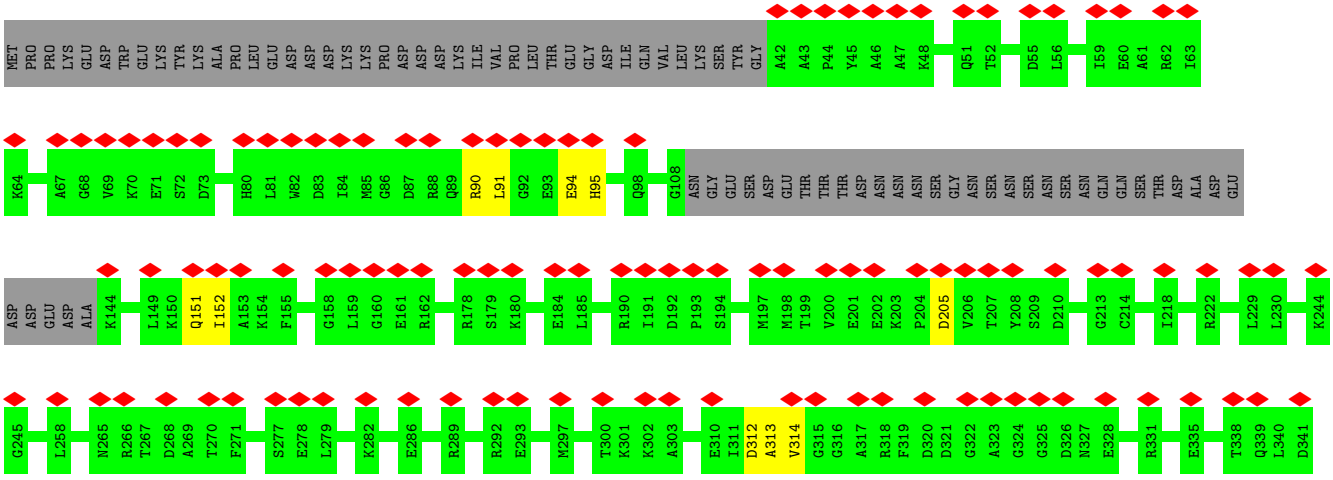
Chain O:

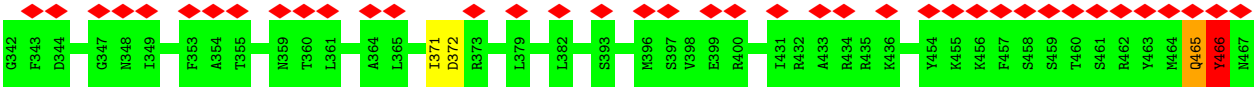




• Molecule 28: 26S proteasome regulatory subunit 7 homolog

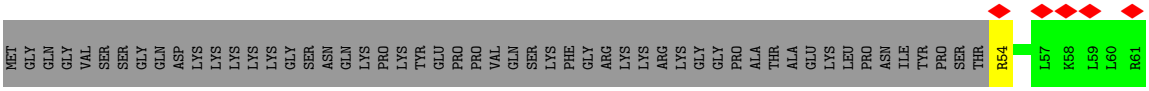
Chain H:

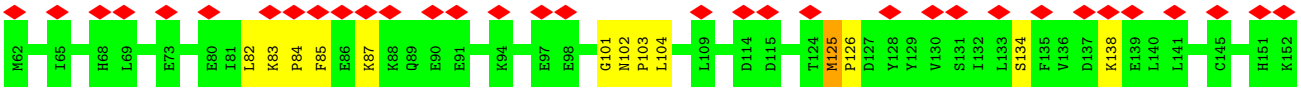


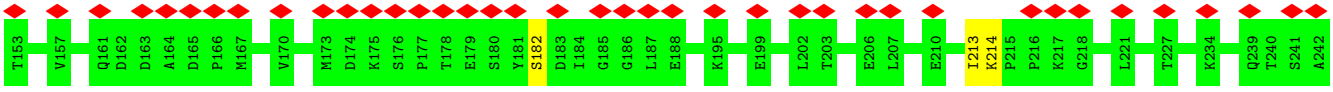


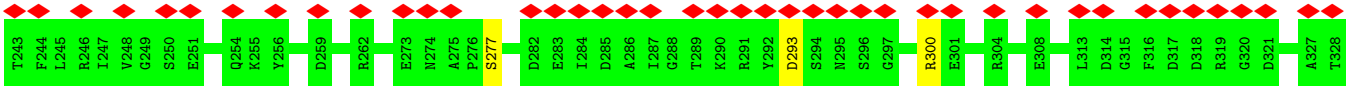
• Molecule 29: 26S proteasome regulatory subunit 4 homolog

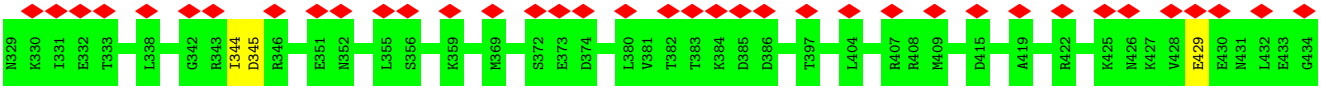
Chain I:





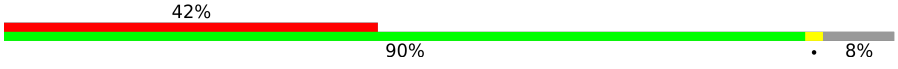


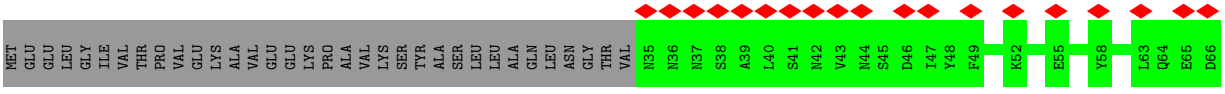


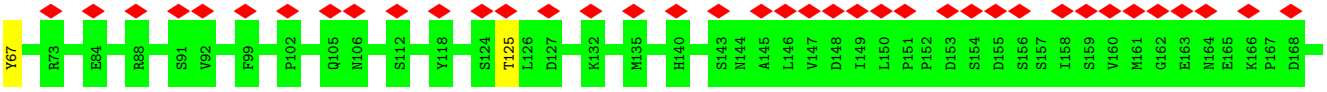


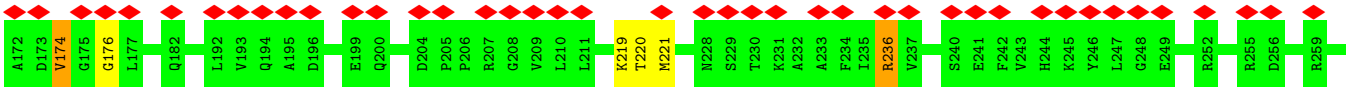
• Molecule 30: 26S proteasome regulatory subunit 6B homolog

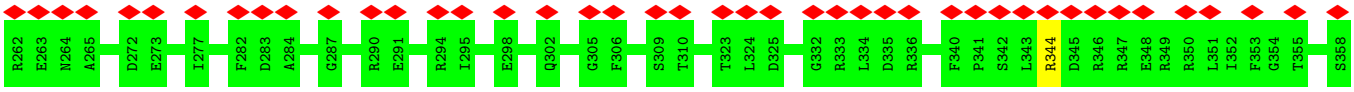
Chain K:

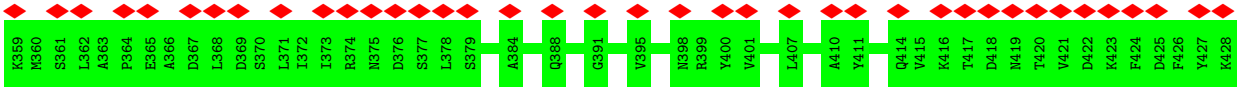






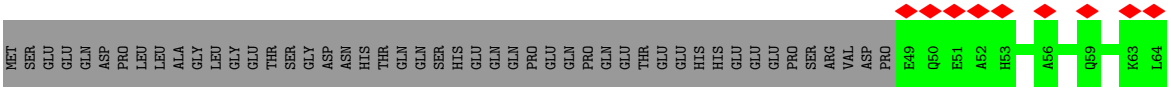


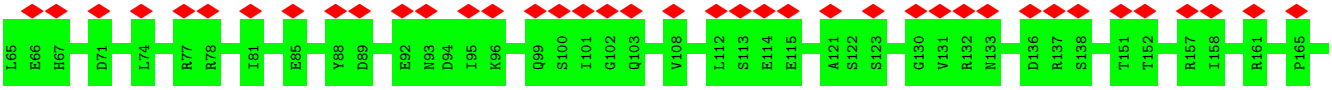


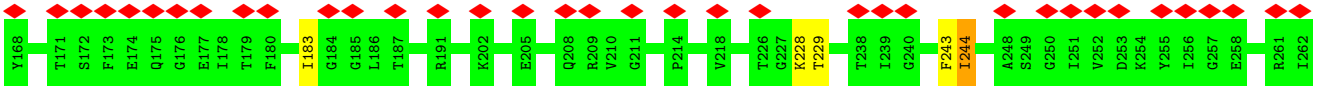


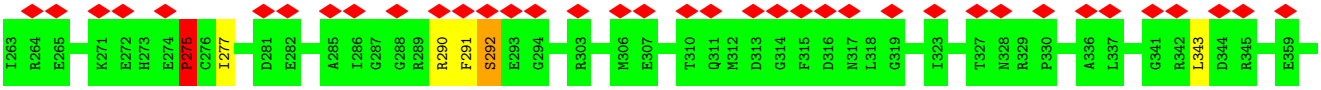
• Molecule 31: 26S proteasome subunit RPT4

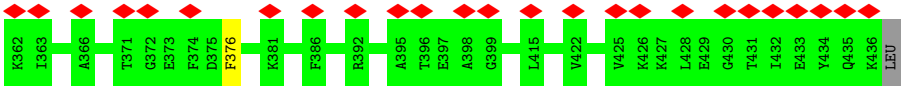
Chain L:





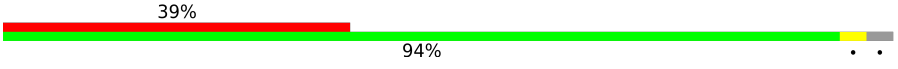


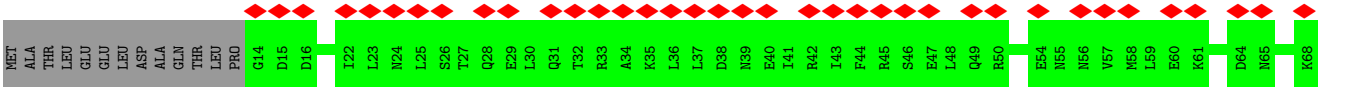


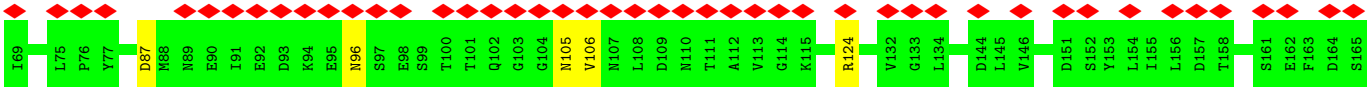


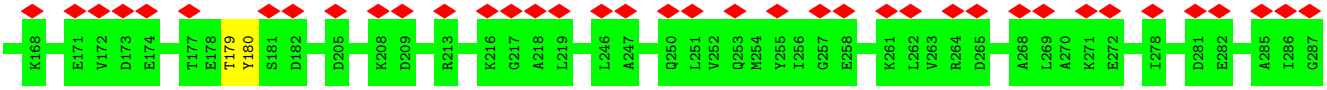
• Molecule 32: 26S proteasome regulatory subunit 6A

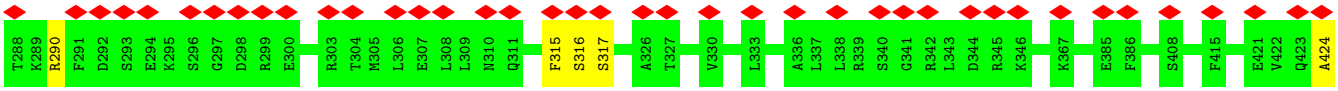
Chain M:

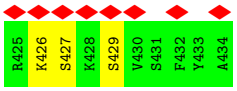






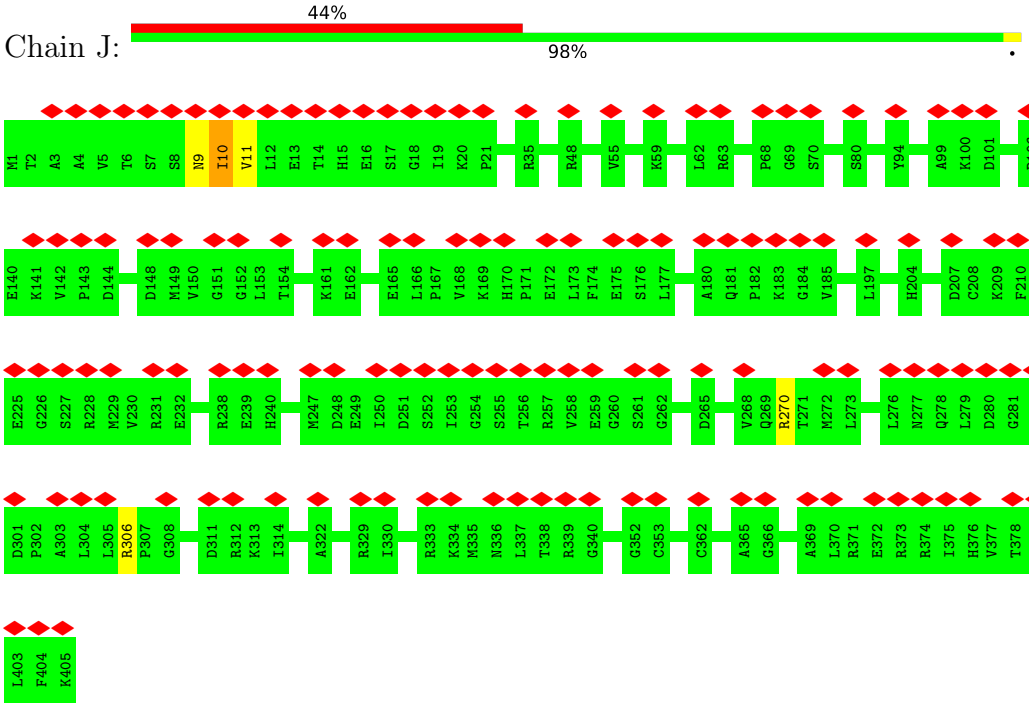






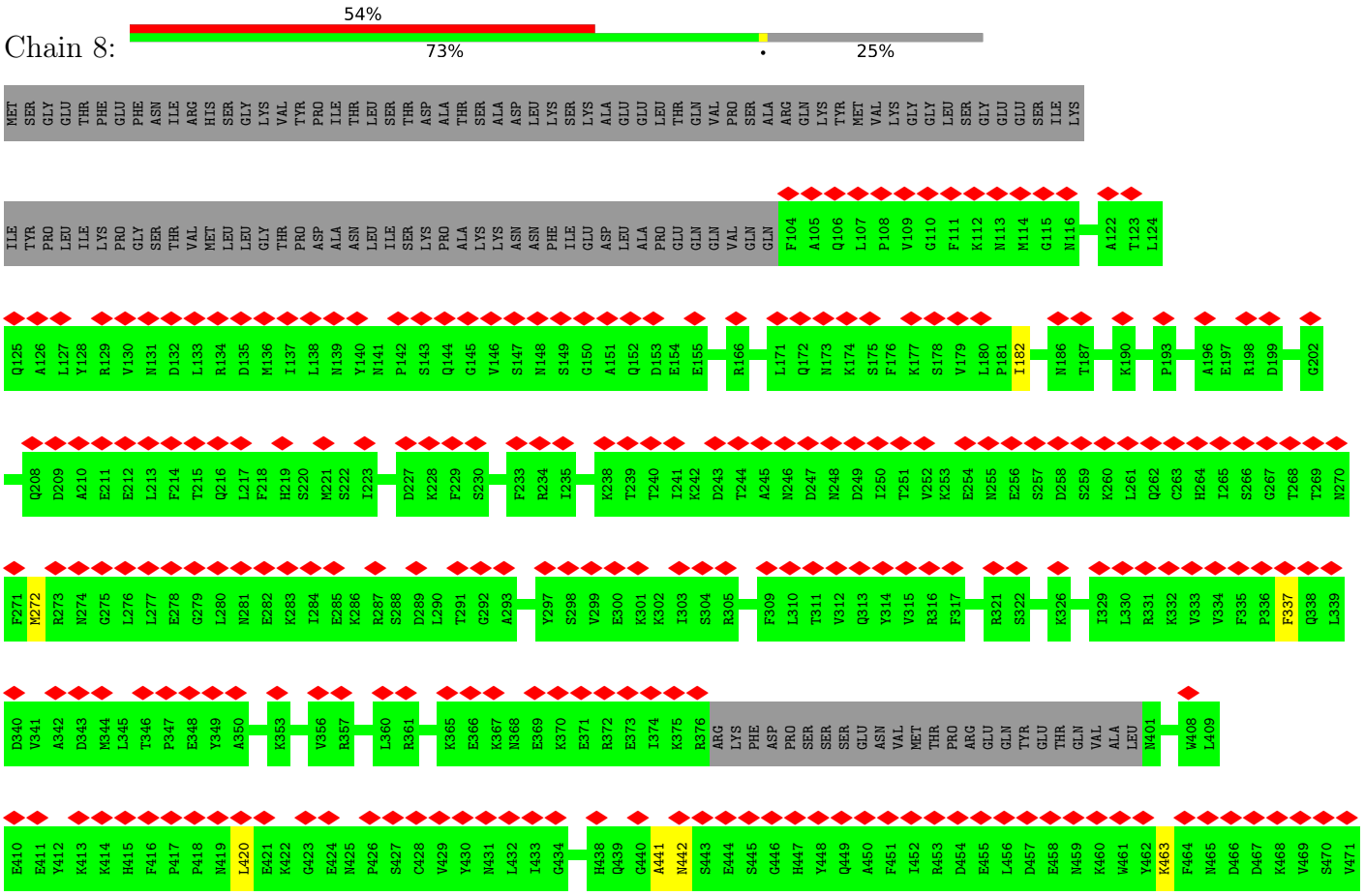
• Molecule 33: 26S proteasome regulatory subunit 8 homolog

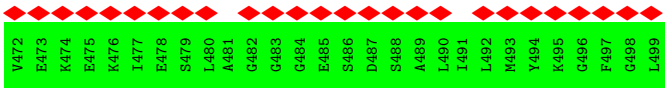
Chain J:



• Molecule 34: Ubiquitin carboxyl-terminal hydrolase

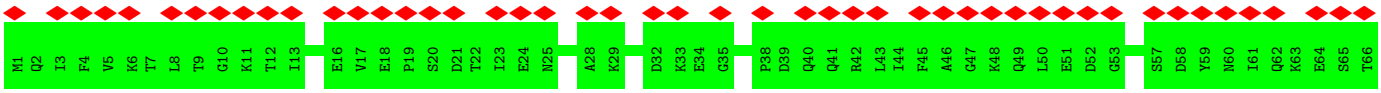
Chain 8:

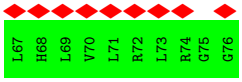




• Molecule 35: Polyubiquitin-B

Chain 9:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	74842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	26.593	Depositor
Minimum map value	-21.027	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.913	Depositor
Recommended contour level	5.2	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GLZ, ATP, 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	A	0.46	0/1950	0.96	16/2641 (0.6%)
1	a	0.46	0/1950	0.96	16/2641 (0.6%)
2	B	0.46	0/1944	0.73	3/2632 (0.1%)
2	b	0.46	0/1944	0.73	3/2632 (0.1%)
3	C	0.46	0/1934	1.12	14/2618 (0.5%)
3	c	0.46	0/1934	1.12	14/2618 (0.5%)
4	D	0.46	0/1879	0.62	0/2546
4	d	0.33	0/1879	0.60	0/2546
5	E	0.47	0/1952	0.85	7/2630 (0.3%)
5	e	0.47	0/1952	0.85	7/2630 (0.3%)
6	F	0.45	0/1800	0.82	6/2433 (0.2%)
6	f	0.45	0/1800	0.82	7/2433 (0.3%)
7	G	0.56	0/1925	0.98	16/2599 (0.6%)
7	g	0.56	0/1925	0.98	16/2599 (0.6%)
8	1	0.49	0/1541	0.92	9/2087 (0.4%)
8	h	0.58	0/1541	0.94	8/2087 (0.4%)
9	2	0.63	2/1750 (0.1%)	0.98	10/2373 (0.4%)
9	i	0.53	0/1750	0.95	11/2373 (0.5%)
10	3	0.52	0/1611	0.86	8/2174 (0.4%)
10	j	0.52	0/1611	0.86	8/2174 (0.4%)
11	4	0.54	0/1589	1.02	13/2142 (0.6%)
11	k	0.54	0/1589	1.02	13/2142 (0.6%)
12	5	0.54	0/1681	1.16	9/2274 (0.4%)
12	l	0.54	0/1681	1.16	9/2274 (0.4%)
13	6	0.49	0/1795	0.92	10/2420 (0.4%)
13	m	0.49	0/1795	0.92	10/2420 (0.4%)
14	7	0.44	0/1821	0.64	0/2470
14	n	0.35	0/1821	0.59	0/2470
15	W	0.52	2/1557 (0.1%)	0.72	5/2111 (0.2%)
16	V	0.42	0/2309	0.65	0/3115
17	T	0.31	0/2235	0.56	0/3017
18	X	0.29	0/1058	0.54	0/1432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	Y	0.31	0/741	0.64	1/1000 (0.1%)
20	Z	0.34	0/7122	0.61	3/9645 (0.0%)
21	N	0.36	0/6521	0.53	4/8824 (0.0%)
22	S	0.35	0/3966	0.57	0/5355
23	P	0.35	0/3663	0.53	0/4940
24	Q	0.34	0/3556	0.57	0/4787
25	R	0.37	0/3313	0.55	0/4469
26	U	0.45	0/2340	0.63	1/3168 (0.0%)
27	O	0.34	0/3247	0.54	0/4380
28	H	0.40	0/3113	0.62	2/4187 (0.0%)
29	I	0.50	0/3054	0.75	7/4111 (0.2%)
30	K	0.43	1/3156 (0.0%)	0.67	5/4261 (0.1%)
31	L	0.55	0/3128	0.76	5/4204 (0.1%)
32	M	0.40	0/3323	0.61	1/4478 (0.0%)
33	J	0.39	0/3212	0.63	1/4316 (0.0%)
34	8	0.41	0/3089	0.64	2/4144 (0.0%)
35	9	0.32	0/603	0.58	0/811
All	All	0.44	5/114650 (0.0%)	0.76	280/154833 (0.2%)

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
4	d	0	1
5	E	0	1
5	e	0	1
6	F	0	3
6	f	0	3
7	G	0	1
7	g	0	1
8	h	0	1
9	2	0	7
9	i	0	6
10	3	0	1
10	j	0	1
11	4	0	1
11	k	0	1
13	6	0	1
13	m	0	1
16	V	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
17	T	0	3
19	Y	0	1
20	Z	0	2
21	N	0	1
22	S	0	3
24	Q	0	2
25	R	0	1
27	O	0	1
28	H	0	8
29	I	0	6
30	K	0	2
31	L	0	6
32	M	0	4
33	J	0	4
34	8	0	2
All	All	0	78

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	117	PHE	CG-CD1	5.98	1.47	1.38
9	2	114	GLN	C-N	-5.54	1.21	1.34
30	K	67	TYR	CD1-CE1	-5.27	1.31	1.39
15	W	21	PHE	CG-CD1	5.10	1.46	1.38
15	W	25	ARG	CD-NE	5.02	1.54	1.46

All (280) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	19	LEU	CB-CG-CD1	33.56	168.05	111.00
3	C	19	LEU	CB-CG-CD1	33.56	168.05	111.00
12	l	161	LEU	CB-CG-CD1	26.10	155.36	111.00
12	5	161	LEU	CB-CG-CD1	26.09	155.36	111.00
12	5	161	LEU	CB-CG-CD2	-21.01	75.28	111.00
12	l	161	LEU	CB-CG-CD2	-21.01	75.29	111.00
11	k	163	LEU	CA-CB-CG	18.69	158.29	115.30
11	4	163	LEU	CA-CB-CG	18.68	158.26	115.30
12	5	144	ARG	CG-CD-NE	-17.93	74.14	111.80
12	l	144	ARG	CG-CD-NE	-17.93	74.16	111.80
3	C	19	LEU	CB-CG-CD2	-16.90	82.27	111.00
3	c	19	LEU	CB-CG-CD2	-16.90	82.27	111.00
7	g	115	ARG	NE-CZ-NH2	-15.58	112.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	115	ARG	NE-CZ-NH2	-15.55	112.53	120.30
5	E	33	LEU	CA-CB-CG	15.37	150.66	115.30
5	e	33	LEU	CA-CB-CG	15.37	150.65	115.30
6	F	102	LYS	CD-CE-NZ	12.78	141.09	111.70
6	f	102	LYS	CD-CE-NZ	12.77	141.06	111.70
5	e	3	LEU	CA-CB-CG	12.68	144.45	115.30
5	E	3	LEU	CA-CB-CG	12.65	144.39	115.30
7	g	57	LYS	CD-CE-NZ	-11.81	84.53	111.70
7	G	57	LYS	CD-CE-NZ	-11.80	84.55	111.70
13	m	109	ARG	NE-CZ-NH2	-11.74	114.43	120.30
13	6	109	ARG	NE-CZ-NH2	-11.64	114.48	120.30
8	1	152	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	A	210	MET	CB-CG-SD	10.97	145.30	112.40
1	a	210	MET	CB-CG-SD	10.96	145.27	112.40
8	h	124	LEU	CA-CB-CG	10.54	139.55	115.30
8	1	124	LEU	CA-CB-CG	10.53	139.52	115.30
13	m	109	ARG	NE-CZ-NH1	10.48	125.54	120.30
13	6	109	ARG	NE-CZ-NH1	10.47	125.53	120.30
9	i	94	LEU	CB-CG-CD1	10.37	128.62	111.00
9	2	94	LEU	CB-CG-CD1	10.36	128.61	111.00
9	2	243	LYS	CD-CE-NZ	10.21	135.18	111.70
9	i	243	LYS	CD-CE-NZ	10.20	135.16	111.70
8	h	54	ARG	NE-CZ-NH2	-10.00	115.30	120.30
8	1	54	ARG	NE-CZ-NH2	-9.98	115.31	120.30
8	1	173	LYS	CD-CE-NZ	9.89	134.46	111.70
8	h	173	LYS	CD-CE-NZ	9.89	134.45	111.70
7	g	167	LYS	CD-CE-NZ	9.82	134.28	111.70
7	G	167	LYS	CD-CE-NZ	9.80	134.24	111.70
1	A	187	LYS	CD-CE-NZ	9.65	133.90	111.70
1	a	187	LYS	CD-CE-NZ	9.63	133.84	111.70
7	G	81	LEU	CB-CG-CD2	-9.45	94.93	111.00
7	g	81	LEU	CB-CG-CD2	-9.45	94.94	111.00
1	A	98	LYS	CD-CE-NZ	9.25	132.97	111.70
1	a	98	LYS	CD-CE-NZ	9.24	132.95	111.70
3	c	19	LEU	CA-CB-CG	9.03	136.08	115.30
3	C	19	LEU	CA-CB-CG	9.03	136.06	115.30
13	6	141	ARG	NE-CZ-NH2	-8.98	115.81	120.30
13	m	141	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	A	24	ARG	CG-CD-NE	-8.86	93.19	111.80
1	A	232	LYS	CD-CE-NZ	8.86	132.07	111.70
1	a	232	LYS	CD-CE-NZ	8.85	132.06	111.70
1	a	24	ARG	CG-CD-NE	-8.84	93.23	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	232	LYS	CA-CB-CG	8.80	132.76	113.40
1	a	232	LYS	CA-CB-CG	8.79	132.73	113.40
11	k	163	LEU	CB-CG-CD2	8.71	125.81	111.00
11	4	163	LEU	CB-CG-CD2	8.71	125.80	111.00
1	a	62	LYS	CD-CE-NZ	8.70	131.72	111.70
1	A	62	LYS	CD-CE-NZ	8.70	131.72	111.70
2	b	116	LYS	CD-CE-NZ	8.64	131.57	111.70
2	B	116	LYS	CD-CE-NZ	8.64	131.57	111.70
11	k	170	LYS	CD-CE-NZ	8.63	131.54	111.70
11	4	170	LYS	CD-CE-NZ	8.60	131.48	111.70
13	m	72	LEU	CB-CG-CD2	8.59	125.61	111.00
13	6	72	LEU	CB-CG-CD2	8.59	125.59	111.00
10	3	42	LYS	CD-CE-NZ	8.52	131.29	111.70
10	j	42	LYS	CD-CE-NZ	8.51	131.27	111.70
31	L	229	THR	CA-CB-CG2	-8.48	100.52	112.40
12	l	161	LEU	CD1-CG-CD2	-8.47	85.09	110.50
12	5	161	LEU	CD1-CG-CD2	-8.47	85.10	110.50
3	c	18	ARG	NE-CZ-NH2	-8.39	116.10	120.30
7	g	93	ARG	NE-CZ-NH2	-8.38	116.11	120.30
7	G	86	ARG	CG-CD-NE	-8.37	94.23	111.80
3	C	18	ARG	NE-CZ-NH2	-8.36	116.12	120.30
7	g	86	ARG	CG-CD-NE	-8.35	94.26	111.80
7	G	93	ARG	NE-CZ-NH2	-8.29	116.16	120.30
9	i	118	LYS	CD-CE-NZ	8.28	130.74	111.70
5	E	3	LEU	CB-CG-CD2	-8.26	96.96	111.00
5	e	3	LEU	CB-CG-CD2	-8.24	97.00	111.00
3	c	19	LEU	CD1-CG-CD2	-8.23	85.81	110.50
3	C	19	LEU	CD1-CG-CD2	-8.23	85.81	110.50
3	C	92	ARG	NE-CZ-NH1	-8.16	116.22	120.30
3	c	92	ARG	NE-CZ-NH1	-8.07	116.26	120.30
8	h	45	ARG	NE-CZ-NH2	-8.06	116.27	120.30
8	1	45	ARG	NE-CZ-NH2	-8.01	116.29	120.30
9	i	118	LYS	CA-CB-CG	7.88	130.73	113.40
7	g	232	LYS	CD-CE-NZ	-7.82	93.71	111.70
7	G	232	LYS	CD-CE-NZ	-7.81	93.73	111.70
29	I	85	PHE	CB-CG-CD1	-7.80	115.34	120.80
29	I	54	ARG	NE-CZ-NH2	-7.78	116.41	120.30
31	L	275	PRO	CA-N-CD	-7.75	100.65	111.50
13	m	180	LEU	CB-CG-CD2	-7.69	97.92	111.00
7	G	81	LEU	CB-CG-CD1	7.68	124.06	111.00
29	I	125	MET	C-N-CD	-7.68	103.71	120.60
7	g	81	LEU	CB-CG-CD1	7.67	124.05	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	180	LEU	CB-CG-CD2	-7.66	97.97	111.00
11	4	163	LEU	CB-CG-CD1	-7.64	98.01	111.00
11	k	163	LEU	CB-CG-CD1	-7.62	98.04	111.00
5	e	33	LEU	CB-CG-CD2	7.61	123.93	111.00
5	E	33	LEU	CB-CG-CD2	7.61	123.93	111.00
11	4	96	ARG	NE-CZ-NH2	-7.53	116.53	120.30
10	3	98	ARG	NE-CZ-NH1	7.50	124.05	120.30
11	k	96	ARG	NE-CZ-NH2	-7.47	116.56	120.30
10	j	98	ARG	NE-CZ-NH1	7.47	124.03	120.30
29	I	54	ARG	NE-CZ-NH1	7.42	124.01	120.30
6	F	18	ARG	NE-CZ-NH1	-7.40	116.60	120.30
12	l	144	ARG	NE-CZ-NH2	-7.34	116.63	120.30
6	f	18	ARG	NE-CZ-NH1	-7.31	116.64	120.30
3	C	100	LYS	CG-CD-CE	7.31	133.83	111.90
7	G	185	GLU	CA-CB-CG	7.31	129.48	113.40
7	g	185	GLU	CA-CB-CG	7.31	129.48	113.40
2	B	236	ARG	NE-CZ-NH2	7.30	123.95	120.30
3	c	100	LYS	CG-CD-CE	7.30	133.79	111.90
5	e	3	LEU	CB-CG-CD1	7.30	123.40	111.00
5	E	3	LEU	CB-CG-CD1	7.29	123.39	111.00
2	b	236	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	a	190	LYS	CD-CE-NZ	7.23	128.32	111.70
9	i	220	LEU	CA-CB-CG	7.23	131.92	115.30
1	A	190	LYS	CD-CE-NZ	7.23	128.32	111.70
12	5	144	ARG	NE-CZ-NH2	-7.22	116.69	120.30
9	2	220	LEU	CA-CB-CG	7.21	131.89	115.30
30	K	219	LYS	O-C-N	-7.19	111.19	122.70
15	W	23	ARG	NE-CZ-NH1	7.15	123.88	120.30
7	G	178	LYS	CD-CE-NZ	7.11	128.04	111.70
7	g	178	LYS	CD-CE-NZ	7.10	128.03	111.70
11	k	70	ARG	NE-CZ-NH2	-7.00	116.80	120.30
11	4	70	ARG	NE-CZ-NH2	-6.97	116.82	120.30
5	E	86	ARG	NE-CZ-NH2	6.96	123.78	120.30
8	h	151	PHE	CB-CG-CD2	-6.94	115.94	120.80
5	e	86	ARG	NE-CZ-NH2	6.93	123.76	120.30
8	1	124	LEU	CB-CG-CD2	6.80	122.56	111.00
13	6	222	LYS	CD-CE-NZ	6.78	127.30	111.70
13	m	222	LYS	CD-CE-NZ	6.78	127.29	111.70
8	h	124	LEU	CB-CG-CD2	6.77	122.52	111.00
9	i	94	LEU	CB-CG-CD2	-6.73	99.56	111.00
9	2	94	LEU	CB-CG-CD2	-6.73	99.56	111.00
34	8	272	MET	CG-SD-CE	-6.67	89.53	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	144	ARG	CB-CG-CD	6.66	128.92	111.60
10	3	134	LYS	CD-CE-NZ	-6.66	96.38	111.70
12	l	144	ARG	CB-CG-CD	6.65	128.90	111.60
10	j	134	LYS	CD-CE-NZ	-6.65	96.41	111.70
3	C	228	LYS	CD-CE-NZ	6.64	126.98	111.70
3	c	228	LYS	CD-CE-NZ	6.63	126.96	111.70
9	2	65	ARG	NE-CZ-NH2	-6.57	117.01	120.30
9	i	65	ARG	NE-CZ-NH2	-6.56	117.02	120.30
12	5	271	LEU	CB-CG-CD1	6.54	122.12	111.00
12	l	271	LEU	CB-CG-CD1	6.54	122.11	111.00
21	N	597	ARG	CG-CD-NE	6.54	125.52	111.80
15	W	25	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	a	24	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	24	ARG	NE-CZ-NH1	6.36	123.48	120.30
7	g	81	LEU	CA-CB-CG	6.33	129.86	115.30
13	6	109	ARG	CB-CG-CD	6.32	128.04	111.60
7	G	81	LEU	CA-CB-CG	6.32	129.84	115.30
30	K	221	MET	C-N-CA	-6.32	105.90	121.70
13	m	109	ARG	CB-CG-CD	6.30	127.98	111.60
5	E	121	LEU	CB-CG-CD2	-6.28	100.32	111.00
5	e	121	LEU	CB-CG-CD2	-6.26	100.36	111.00
28	H	466	TYR	CB-CA-C	-6.25	97.90	110.40
6	f	202	ARG	NE-CZ-NH2	-6.24	117.18	120.30
6	f	181	LYS	CD-CE-NZ	-6.20	97.43	111.70
6	F	202	ARG	NE-CZ-NH2	-6.20	117.20	120.30
6	F	181	LYS	CD-CE-NZ	-6.19	97.46	111.70
11	k	93	ARG	NE-CZ-NH2	-6.17	117.22	120.30
30	K	220	THR	N-CA-CB	6.17	122.02	110.30
11	4	93	ARG	NE-CZ-NH2	-6.15	117.22	120.30
13	6	180	LEU	CB-CG-CD1	6.12	121.40	111.00
20	Z	173	ALA	C-N-CA	6.12	136.99	121.70
13	m	180	LEU	CB-CG-CD1	6.09	121.35	111.00
30	K	236	ARG	NE-CZ-NH2	-6.06	117.27	120.30
11	k	109	LYS	CD-CE-NZ	5.97	125.43	111.70
10	3	98	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	a	210	MET	CG-SD-CE	5.96	109.73	100.20
11	4	109	LYS	CD-CE-NZ	5.96	125.40	111.70
29	I	82	LEU	C-N-CA	5.95	136.57	121.70
2	b	91	LYS	CD-CE-NZ	5.95	125.38	111.70
1	A	210	MET	CG-SD-CE	5.93	109.69	100.20
11	k	19	LYS	CD-CE-NZ	5.93	125.33	111.70
10	j	98	ARG	NE-CZ-NH2	-5.92	117.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	91	LYS	CD-CE-NZ	5.92	125.31	111.70
11	4	19	LYS	CD-CE-NZ	5.91	125.28	111.70
12	5	161	LEU	CA-CB-CG	-5.91	101.72	115.30
12	l	161	LEU	CA-CB-CG	-5.90	101.74	115.30
31	L	244	ILE	CG1-CB-CG2	-5.89	98.45	111.40
1	A	96	ARG	CB-CG-CD	5.85	126.80	111.60
3	C	185	LYS	CB-CG-CD	5.84	126.80	111.60
3	c	185	LYS	CB-CG-CD	5.84	126.78	111.60
7	G	72	ARG	CG-CD-NE	-5.84	99.54	111.80
1	a	96	ARG	CB-CG-CD	5.83	126.75	111.60
11	4	86	GLN	CA-CB-CG	5.82	126.21	113.40
21	N	597	ARG	NE-CZ-NH2	-5.82	117.39	120.30
30	K	220	THR	C-N-CA	5.82	136.24	121.70
11	k	86	GLN	CA-CB-CG	5.81	126.18	113.40
7	g	72	ARG	CG-CD-NE	-5.80	99.61	111.80
31	L	277	ILE	N-CA-C	-5.79	95.37	111.00
10	j	65	GLU	CA-CB-CG	5.77	126.10	113.40
3	c	5	ARG	CA-CB-CG	5.76	126.06	113.40
1	A	58	LYS	CA-CB-CG	5.75	126.06	113.40
1	a	58	LYS	CA-CB-CG	5.75	126.06	113.40
3	C	5	ARG	CA-CB-CG	5.75	126.05	113.40
10	3	65	GLU	CA-CB-CG	5.75	126.05	113.40
3	c	92	ARG	NE-CZ-NH2	-5.71	117.45	120.30
12	5	94	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	a	190	LYS	CB-CG-CD	5.69	126.40	111.60
11	k	149	ARG	NE-CZ-NH2	-5.68	117.46	120.30
29	I	85	PHE	CB-CG-CD2	5.68	124.78	120.80
1	A	190	LYS	CB-CG-CD	5.68	126.38	111.60
1	A	137	LEU	CA-CB-CG	5.67	128.33	115.30
3	C	92	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	a	137	LEU	CA-CB-CG	5.66	128.32	115.30
12	l	94	ARG	NE-CZ-NH2	-5.66	117.47	120.30
11	4	149	ARG	NE-CZ-NH2	-5.66	117.47	120.30
10	j	18	LYS	CD-CE-NZ	-5.64	98.72	111.70
10	3	18	LYS	CD-CE-NZ	-5.64	98.73	111.70
1	a	58	LYS	CB-CG-CD	5.63	126.24	111.60
1	A	58	LYS	CB-CG-CD	5.63	126.23	111.60
13	m	108	LYS	CD-CE-NZ	-5.60	98.81	111.70
13	6	108	LYS	CD-CE-NZ	-5.60	98.83	111.70
11	4	143	LEU	CA-CB-CG	5.59	128.15	115.30
20	Z	174	GLU	N-CA-C	5.59	126.08	111.00
20	Z	174	GLU	N-CA-CB	-5.58	100.55	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	272	MET	O-C-N	5.58	131.62	122.70
11	k	143	LEU	CA-CB-CG	5.55	128.08	115.30
3	C	92	ARG	NH1-CZ-NH2	5.55	125.50	119.40
3	c	92	ARG	NH1-CZ-NH2	5.53	125.48	119.40
7	G	115	ARG	NH1-CZ-NH2	5.49	125.44	119.40
9	i	65	ARG	NE-CZ-NH1	-5.48	117.56	120.30
31	L	228	LYS	O-C-N	-5.47	113.94	122.70
8	h	151	PHE	CB-CG-CD1	5.47	124.63	120.80
9	2	227	GLU	CA-CB-CG	5.45	125.39	113.40
7	g	115	ARG	NH1-CZ-NH2	5.45	125.39	119.40
9	i	227	GLU	CA-CB-CG	5.44	125.36	113.40
9	2	65	ARG	NE-CZ-NH1	-5.43	117.58	120.30
15	W	20	ASP	CB-CG-OD1	5.43	123.19	118.30
8	h	54	ARG	NH1-CZ-NH2	5.40	125.34	119.40
10	j	134	LYS	CG-CD-CE	5.40	128.09	111.90
8	1	54	ARG	NH1-CZ-NH2	5.40	125.34	119.40
10	3	134	LYS	CG-CD-CE	5.40	128.09	111.90
9	i	104	ARG	NE-CZ-NH2	-5.37	117.61	120.30
11	k	182	LYS	CD-CE-NZ	-5.37	99.34	111.70
1	a	24	ARG	CD-NE-CZ	5.37	131.12	123.60
11	4	182	LYS	CD-CE-NZ	-5.36	99.37	111.70
1	A	24	ARG	CD-NE-CZ	5.35	131.09	123.60
9	i	65	ARG	NH1-CZ-NH2	5.35	125.28	119.40
9	2	65	ARG	NH1-CZ-NH2	5.34	125.27	119.40
3	c	5	ARG	CB-CG-CD	5.32	125.44	111.60
3	C	5	ARG	CB-CG-CD	5.32	125.43	111.60
7	G	23	GLN	CA-CB-CG	5.31	125.09	113.40
32	M	124	ARG	NE-CZ-NH2	-5.30	117.65	120.30
7	g	23	GLN	CA-CB-CG	5.29	125.03	113.40
6	f	82	ARG	CB-CG-CD	5.26	125.27	111.60
6	F	82	ARG	CB-CG-CD	5.26	125.28	111.60
28	H	466	TYR	N-CA-C	5.25	125.19	111.00
7	G	170	GLN	CA-CB-CG	5.25	124.94	113.40
9	2	104	ARG	NE-CZ-NH2	-5.25	117.68	120.30
7	g	170	GLN	CA-CB-CG	5.23	124.91	113.40
13	m	109	ARG	CG-CD-NE	-5.22	100.83	111.80
13	6	109	ARG	CG-CD-NE	-5.22	100.84	111.80
8	1	152	ARG	NE-CZ-NH1	5.21	122.90	120.30
15	W	21	PHE	N-CA-CB	5.20	119.96	110.60
3	c	113	ARG	NE-CZ-NH2	-5.17	117.71	120.30
10	j	18	LYS	CA-CB-CG	-5.17	102.03	113.40
7	G	57	LYS	CG-CD-CE	5.16	127.38	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	57	LYS	CG-CD-CE	5.15	127.35	111.90
21	N	269	LEU	CA-CB-CG	5.15	127.15	115.30
10	3	18	LYS	CA-CB-CG	-5.15	102.08	113.40
9	2	119	TYR	CB-CG-CD2	-5.13	117.92	121.00
33	J	270	ARG	NE-CZ-NH1	5.12	122.86	120.30
19	Y	32	ASP	N-CA-C	5.11	124.81	111.00
8	1	152	ARG	CD-NE-CZ	5.10	130.74	123.60
6	f	126	ARG	NE-CZ-NH2	-5.10	117.75	120.30
6	f	101	ARG	NE-CZ-NH2	-5.08	117.76	120.30
21	N	60	MET	CG-SD-CE	5.08	108.33	100.20
15	W	21	PHE	CB-CG-CD1	5.08	124.35	120.80
3	C	113	ARG	NE-CZ-NH2	-5.06	117.77	120.30
26	U	94	HIS	CA-CB-CG	5.03	122.16	113.60
6	F	101	ARG	NE-CZ-NH2	-5.02	117.79	120.30
29	I	277	SER	CB-CA-C	-5.01	100.58	110.10

There are no chirality outliers.

All (78) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	2	119	TYR	Sidechain
9	2	152	TYR	Peptide
9	2	222	PRO	Peptide
9	2	252	ILE	Peptide
9	2	253	GLN	Peptide
9	2	254	GLU	Peptide
9	2	59	ASN	Peptide
10	3	31	SER	Peptide
11	4	1	MET	Peptide
13	6	39	THR	Peptide
34	8	337	PHE	Peptide
34	8	441	ALA	Peptide
5	E	15	PHE	Peptide
6	F	13	PHE	Peptide
6	F	18	ARG	Peptide
6	F	8	GLY	Peptide
7	G	70	VAL	Peptide
28	H	151	GLN	Peptide
28	H	205	ASP	Peptide
28	H	312	ASP	Peptide
28	H	313	ALA	Peptide
28	H	371	ILE	Peptide

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Mol	Chain	Res	Type	Group
28	H	465	GLN	Peptide
28	H	90	ARG	Peptide
28	H	94	GLU	Peptide
29	I	101	GLY	Peptide
29	I	104	LEU	Peptide
29	I	134	SER	Peptide
29	I	182	SER	Peptide
29	I	344	ILE	Peptide
29	I	429	GLU	Peptide
33	J	10	ILE	Peptide
33	J	286	LYS	Peptide
33	J	399	SER	Peptide
33	J	9	ASN	Peptide
30	K	125	THR	Peptide
30	K	174	VAL	Peptide
31	L	243	PHE	Peptide
31	L	244	ILE	Peptide
31	L	290	ARG	Peptide
31	L	292	SER	Peptide
31	L	343	LEU	Peptide
31	L	376	PHE	Peptide
32	M	105	ASN	Peptide
32	M	290	ARG	Peptide
32	M	315	PHE	Peptide
32	M	426	LYS	Peptide
21	N	528	ARG	Peptide
27	O	119	SER	Peptide
24	Q	161	LEU	Peptide
24	Q	67	THR	Peptide
25	R	70	TYR	Peptide
22	S	124	GLU	Peptide
22	S	127	THR	Peptide
22	S	448	LEU	Peptide
17	T	172	SER	Peptide
17	T	251	HIS	Peptide
17	T	91	SER	Peptide
16	V	270	TYR	Peptide
19	Y	31	GLU	Peptide
20	Z	173	ALA	Peptide
20	Z	84	ALA	Peptide
4	d	16	HIS	Peptide
5	e	15	PHE	Peptide

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Mol	Chain	Res	Type	Group
6	f	13	PHE	Peptide
6	f	18	ARG	Peptide
6	f	8	GLY	Peptide
7	g	70	VAL	Peptide
8	h	151	PHE	Sidechain
9	i	152	TYR	Peptide
9	i	222	PRO	Peptide
9	i	252	ILE	Peptide
9	i	253	GLN	Peptide
9	i	254	GLU	Peptide
9	i	59	ASN	Peptide
10	j	31	SER	Peptide
11	k	1	MET	Peptide
13	m	39	THR	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	A	240/252 (95%)	236 (98%)	4 (2%)	0	100	100
1	a	240/252 (95%)	236 (98%)	4 (2%)	0	100	100
2	B	247/250 (99%)	238 (96%)	7 (3%)	2 (1%)	19	60
2	b	247/250 (99%)	238 (96%)	7 (3%)	2 (1%)	19	60
3	C	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
3	c	242/258 (94%)	237 (98%)	5 (2%)	0	100	100
4	D	234/254 (92%)	224 (96%)	5 (2%)	5 (2%)	7	36
4	d	234/254 (92%)	224 (96%)	5 (2%)	5 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
5	E	247/260 (95%)	238 (96%)	6 (2%)	3 (1%)	13 50
5	e	247/260 (95%)	238 (96%)	6 (2%)	3 (1%)	13 50
6	F	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	34 72
6	f	229/234 (98%)	219 (96%)	9 (4%)	1 (0%)	34 72
7	G	240/288 (83%)	235 (98%)	4 (2%)	1 (0%)	34 72
7	g	240/288 (83%)	235 (98%)	4 (2%)	1 (0%)	34 72
8	1	194/215 (90%)	187 (96%)	6 (3%)	1 (0%)	29 69
8	h	194/215 (90%)	187 (96%)	5 (3%)	2 (1%)	15 54
9	2	224/261 (86%)	210 (94%)	10 (4%)	4 (2%)	8 40
9	i	224/261 (86%)	211 (94%)	10 (4%)	3 (1%)	12 48
10	3	202/205 (98%)	183 (91%)	18 (9%)	1 (0%)	29 69
10	j	202/205 (98%)	183 (91%)	18 (9%)	1 (0%)	29 69
11	4	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	29 69
11	k	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	29 69
12	5	210/287 (73%)	198 (94%)	12 (6%)	0	100 100
12	l	210/287 (73%)	198 (94%)	12 (6%)	0	100 100
13	6	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	29 69
13	m	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	29 69
14	7	227/266 (85%)	215 (95%)	10 (4%)	2 (1%)	17 56
14	n	227/266 (85%)	214 (94%)	11 (5%)	2 (1%)	17 56
15	W	195/268 (73%)	182 (93%)	12 (6%)	1 (0%)	29 69
16	V	287/306 (94%)	264 (92%)	19 (7%)	4 (1%)	11 46
17	T	264/274 (96%)	247 (94%)	13 (5%)	4 (2%)	10 45
18	X	125/156 (80%)	116 (93%)	8 (6%)	1 (1%)	19 60
19	Y	87/89 (98%)	73 (84%)	9 (10%)	5 (6%)	1 18
20	Z	902/993 (91%)	822 (91%)	65 (7%)	15 (2%)	9 42
21	N	828/945 (88%)	800 (97%)	26 (3%)	2 (0%)	47 81
22	S	473/523 (90%)	439 (93%)	27 (6%)	7 (2%)	10 45
23	P	438/445 (98%)	419 (96%)	17 (4%)	2 (0%)	29 69
24	Q	432/434 (100%)	404 (94%)	27 (6%)	1 (0%)	47 81
25	R	403/429 (94%)	384 (95%)	18 (4%)	1 (0%)	47 81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	U	288/338 (85%)	280 (97%)	8 (3%)	0	100	100
27	O	386/393 (98%)	373 (97%)	13 (3%)	0	100	100
28	H	387/467 (83%)	353 (91%)	27 (7%)	7 (2%)	8	40
29	I	382/437 (87%)	342 (90%)	29 (8%)	11 (3%)	4	29
30	K	392/428 (92%)	371 (95%)	18 (5%)	3 (1%)	19	60
31	L	386/437 (88%)	358 (93%)	25 (6%)	3 (1%)	19	60
32	M	419/434 (96%)	387 (92%)	22 (5%)	10 (2%)	6	33
33	J	403/405 (100%)	368 (91%)	31 (8%)	4 (1%)	15	54
34	8	368/499 (74%)	345 (94%)	20 (5%)	3 (1%)	19	60
35	9	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
All	All	14217/15714 (90%)	13424 (94%)	665 (5%)	128 (1%)	21	56

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	125	GLY
4	d	101	GLU
4	d	204	GLN
8	h	116	LYS
9	i	200	SER
14	n	110	ASP
2	B	125	GLY
4	D	204	GLN
8	1	116	LYS
9	2	200	SER
14	7	110	ASP
16	V	59	ASP
16	V	184	ASN
16	V	271	VAL
17	T	138	ASP
18	X	39	GLU
19	Y	4	ASP
19	Y	32	ASP
20	Z	5	SER
20	Z	142	ASP
20	Z	174	GLU
20	Z	309	GLN
20	Z	366	LYS

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Mol	Chain	Res	Type
20	Z	443	ASP
20	Z	444	GLU
20	Z	498	ALA
20	Z	926	ASN
21	N	150	LEU
22	S	69	LEU
22	S	98	SER
22	S	449	LEU
25	R	280	ILE
28	H	95	HIS
28	H	152	ILE
28	H	465	GLN
28	H	466	TYR
29	I	102	ASN
29	I	125	MET
29	I	213	ILE
30	K	344	ARG
31	L	275	PRO
31	L	292	SER
32	M	96	ASN
32	M	179	THR
32	M	316	SER
32	M	427	SER
32	M	429	SER
33	J	10	ILE
33	J	285	SER
34	8	182	ILE
4	d	205	THR
5	e	211	LYS
6	f	205	SER
7	g	71	ASP
4	D	102	ASP
4	D	103	PRO
4	D	205	THR
5	E	211	LYS
6	F	205	SER
7	G	71	ASP
17	T	92	ASN
19	Y	33	ASP
19	Y	45	ASN
20	Z	310	LEU
23	P	90	LYS

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Mol	Chain	Res	Type
23	P	131	PHE
28	H	314	VAL
29	I	126	PRO
29	I	293	ASP
30	K	174	VAL
32	M	87	ASP
32	M	106	VAL
33	J	400	VAL
34	8	442	ASN
4	d	102	ASP
4	d	103	PRO
5	e	128	SER
9	i	153	TYR
5	E	128	SER
9	2	120	GLN
9	2	153	TYR
19	Y	31	GLU
20	Z	85	VAL
20	Z	802	ASP
21	N	361	ASN
22	S	68	LEU
22	S	119	TYR
24	Q	51	ARG
29	I	84	PRO
29	I	103	PRO
29	I	138	LYS
31	L	291	PHE
32	M	180	TYR
32	M	317	SER
34	8	420	LEU
9	i	254	GLU
13	m	138	SER
4	D	101	GLU
9	2	254	GLU
13	6	138	SER
15	W	23	ARG
20	Z	173	ALA
20	Z	377	ALA
28	H	91	LEU
28	H	372	ASP
29	I	83	LYS
10	j	32	GLN

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Mol	Chain	Res	Type
11	k	10	GLN
14	n	111	ASN
10	3	32	GLN
11	4	10	GLN
16	V	258	GLU
17	T	139	ASP
17	T	258	ASN
22	S	153	GLU
29	I	345	ASP
5	e	129	GLY
8	h	154	ASN
5	E	129	GLY
32	M	424	ALA
33	J	11	VAL
29	I	214	LYS
30	K	176	GLY
14	7	111	ASN
20	Z	612	GLY
22	S	83	PRO
2	b	16	GLY
2	B	16	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	206/210 (98%)	171 (83%)	35 (17%)	2 12
1	a	206/210 (98%)	170 (82%)	36 (18%)	2 11
2	B	208/209 (100%)	162 (78%)	46 (22%)	1 6
2	b	208/209 (100%)	162 (78%)	46 (22%)	1 6
3	C	203/216 (94%)	162 (80%)	41 (20%)	1 7
3	c	203/216 (94%)	162 (80%)	41 (20%)	1 7
4	D	209/226 (92%)	209 (100%)	0	100 100
4	d	209/226 (92%)	207 (99%)	2 (1%)	76 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	E	205/215 (95%)	171 (83%)	34 (17%)	2 12
5	e	205/215 (95%)	171 (83%)	34 (17%)	2 12
6	F	190/193 (98%)	157 (83%)	33 (17%)	2 11
6	f	190/193 (98%)	157 (83%)	33 (17%)	2 11
7	G	200/239 (84%)	165 (82%)	35 (18%)	2 11
7	g	200/239 (84%)	165 (82%)	35 (18%)	2 11
8	1	162/178 (91%)	133 (82%)	29 (18%)	2 10
8	h	162/178 (91%)	135 (83%)	27 (17%)	2 12
9	2	185/214 (86%)	135 (73%)	50 (27%)	0 3
9	i	185/214 (86%)	134 (72%)	51 (28%)	0 3
10	3	172/173 (99%)	148 (86%)	24 (14%)	3 17
10	j	172/173 (99%)	148 (86%)	24 (14%)	3 17
11	4	173/175 (99%)	141 (82%)	32 (18%)	1 9
11	k	173/175 (99%)	141 (82%)	32 (18%)	1 9
12	5	169/235 (72%)	139 (82%)	30 (18%)	2 10
12	l	169/235 (72%)	139 (82%)	30 (18%)	2 10
13	6	185/201 (92%)	155 (84%)	30 (16%)	2 13
13	m	185/201 (92%)	155 (84%)	30 (16%)	2 13
14	7	195/224 (87%)	195 (100%)	0	100 100
14	n	195/224 (87%)	194 (100%)	1 (0%)	88 93
15	W	171/230 (74%)	170 (99%)	1 (1%)	86 92
16	V	253/268 (94%)	252 (100%)	1 (0%)	91 94
17	T	249/256 (97%)	249 (100%)	0	100 100
18	X	116/144 (81%)	116 (100%)	0	100 100
19	Y	81/81 (100%)	81 (100%)	0	100 100
20	Z	773/850 (91%)	772 (100%)	1 (0%)	93 97
21	N	698/797 (88%)	695 (100%)	3 (0%)	91 94
22	S	447/489 (91%)	446 (100%)	1 (0%)	93 96
23	P	412/415 (99%)	411 (100%)	1 (0%)	93 96
24	Q	391/391 (100%)	387 (99%)	4 (1%)	76 86
25	R	356/379 (94%)	355 (100%)	1 (0%)	92 95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	U	263/308 (85%)	263 (100%)	0	100 100
27	O	363/368 (99%)	359 (99%)	4 (1%)	73 84
28	H	330/399 (83%)	329 (100%)	1 (0%)	92 95
29	I	341/385 (89%)	339 (99%)	2 (1%)	86 92
30	K	346/374 (92%)	345 (100%)	1 (0%)	92 95
31	L	332/377 (88%)	330 (99%)	2 (1%)	86 92
32	M	364/375 (97%)	364 (100%)	0	100 100
33	J	352/352 (100%)	351 (100%)	1 (0%)	92 95
34	8	337/449 (75%)	336 (100%)	1 (0%)	92 95
35	9	68/68 (100%)	68 (100%)	0	100 100
All	All	12367/13571 (91%)	11501 (93%)	866 (7%)	19 40

All (866) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	13	ASP
1	a	14	ARG
1	a	20	SER
1	a	22	GLU
1	a	27	GLN
1	a	36	ASN
1	a	45	VAL
1	a	54	ILE
1	a	56	GLN
1	a	58	LYS
1	a	62	LYS
1	a	67	THR
1	a	74	CYS
1	a	84	ASN
1	a	96	ARG
1	a	103	GLU
1	a	129	THR
1	a	134	MET
1	a	137	LEU
1	a	148	GLU
1	a	153	SER
1	a	156	LYS
1	a	157	THR

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Mol	Chain	Res	Type
1	a	174	LYS
1	a	175	GLN
1	a	176	GLN
1	a	177	GLU
1	a	190	LYS
1	a	208	THR
1	a	210	MET
1	a	216	THR
1	a	217	GLU
1	a	219	SER
1	a	230	LYS
1	a	232	LYS
1	a	250	GLU
2	b	8	SER
2	b	15	SER
2	b	17	LYS
2	b	21	ILE
2	b	33	THR
2	b	51	SER
2	b	55	LEU
2	b	59	GLU
2	b	70	ASP
2	b	85	LEU
2	b	89	SER
2	b	92	VAL
2	b	96	SER
2	b	97	TYR
2	b	98	LYS
2	b	109	LEU
2	b	112	SER
2	b	114	VAL
2	b	124	SER
2	b	128	ARG
2	b	132	VAL
2	b	133	SER
2	b	141	GLU
2	b	146	SER
2	b	151	ASP
2	b	156	TYR
2	b	166	LYS
2	b	169	VAL
2	b	176	GLU

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Mol	Chain	Res	Type
2	b	178	ARG
2	b	181	ASP
2	b	186	GLU
2	b	198	GLU
2	b	199	SER
2	b	203	GLU
2	b	205	ASN
2	b	216	ASP
2	b	217	GLU
2	b	230	ASP
2	b	231	LYS
2	b	236	ARG
2	b	239	THR
2	b	241	GLN
2	b	242	GLU
2	b	245	ASP
2	b	248	GLU
3	c	3	SER
3	c	5	ARG
3	c	8	SER
3	c	11	THR
3	c	18	ARG
3	c	19	LEU
3	c	27	GLU
3	c	36	ILE
3	c	45	VAL
3	c	51	LYS
3	c	52	VAL
3	c	61	THR
3	c	64	GLU
3	c	80	LEU
3	c	81	THR
3	c	93	ILE
3	c	99	LEU
3	c	100	LYS
3	c	110	ILE
3	c	113	ARG
3	c	115	LEU
3	c	118	ILE
3	c	123	THR
3	c	134	SER
3	c	142	ASP

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Mol	Chain	Res	Type
3	c	152	ASN
3	c	154	SER
3	c	170	SER
3	c	177	GLN
3	c	178	MET
3	c	181	LYS
3	c	182	ASP
3	c	183	ASP
3	c	185	LYS
3	c	203	SER
3	c	204	SER
3	c	209	ASP
3	c	221	ASN
3	c	227	GLN
3	c	228	LYS
3	c	231	LYS
4	d	127	ARG
4	d	177	LYS
5	e	2	PHE
5	e	4	THR
5	e	7	GLU
5	e	9	ASP
5	e	10	ARG
5	e	16	SER
5	e	21	LEU
5	e	24	VAL
5	e	25	GLU
5	e	36	THR
5	e	47	VAL
5	e	48	LEU
5	e	61	SER
5	e	64	ILE
5	e	78	MET
5	e	82	THR
5	e	104	ASP
5	e	110	GLU
5	e	116	VAL
5	e	128	SER
5	e	130	GLU
5	e	131	GLU
5	e	136	ARG
5	e	174	SER

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Mol	Chain	Res	Type
5	e	177	GLU
5	e	186	GLU
5	e	190	SER
5	e	195	GLU
5	e	202	LYS
5	e	205	LYS
5	e	206	GLN
5	e	209	GLU
5	e	211	LYS
5	e	234	GLU
6	f	9	ASP
6	f	10	THR
6	f	14	SER
6	f	18	ARG
6	f	26	LEU
6	f	30	LYS
6	f	31	GLN
6	f	33	SER
6	f	36	VAL
6	f	51	ARG
6	f	55	GLU
6	f	61	LYS
6	f	82	ARG
6	f	91	GLN
6	f	94	TYR
6	f	97	LEU
6	f	105	VAL
6	f	107	ARG
6	f	111	LEU
6	f	114	ASP
6	f	119	ASN
6	f	122	SER
6	f	140	SER
6	f	148	GLN
6	f	174	ARG
6	f	177	ASP
6	f	181	LYS
6	f	199	GLN
6	f	200	SER
6	f	218	LYS
6	f	219	ASP
6	f	220	THR

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Mol	Chain	Res	Type
6	f	223	THR
7	g	13	SER
7	g	20	ARG
7	g	23	GLN
7	g	29	LYS
7	g	36	THR
7	g	55	THR
7	g	57	LYS
7	g	62	GLN
7	g	63	LYS
7	g	72	ARG
7	g	86	ARG
7	g	89	VAL
7	g	100	LYS
7	g	105	THR
7	g	112	PHE
7	g	116	LEU
7	g	135	SER
7	g	143	LYS
7	g	154	SER
7	g	161	LYS
7	g	169	ARG
7	g	170	GLN
7	g	175	GLU
7	g	178	LYS
7	g	181	ASP
7	g	185	GLU
7	g	198	LYS
7	g	205	GLU
7	g	209	GLU
7	g	210	LYS
7	g	215	GLU
7	g	220	SER
7	g	227	LEU
7	g	232	LYS
7	g	247	ILE
8	h	11	SER
8	h	19	ASP
8	h	27	SER
8	h	29	THR
8	h	31	THR
8	h	37	ASN

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Mol	Chain	Res	Type
8	h	45	ARG
8	h	52	CYS
8	h	54	ARG
8	h	55	SER
8	h	57	SER
8	h	81	THR
8	h	83	SER
8	h	85	GLU
8	h	91	PHE
8	h	95	CYS
8	h	99	LYS
8	h	124	LEU
8	h	127	SER
8	h	128	VAL
8	h	147	CYS
8	h	159	GLU
8	h	162	ASP
8	h	169	SER
8	h	177	SER
8	h	178	SER
8	h	200	ASP
9	i	36	LYS
9	i	37	PHE
9	i	49	SER
9	i	51	GLN
9	i	54	ILE
9	i	57	ASP
9	i	60	CYS
9	i	63	LEU
9	i	65	ARG
9	i	67	SER
9	i	82	GLU
9	i	85	THR
9	i	86	GLN
9	i	87	LEU
9	i	90	SER
9	i	92	ILE
9	i	94	LEU
9	i	99	THR
9	i	104	ARG
9	i	110	GLN
9	i	114	GLN

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Mol	Chain	Res	Type
9	i	118	LYS
9	i	127	LEU
9	i	128	ILE
9	i	141	SER
9	i	143	HIS
9	i	147	SER
9	i	149	ASP
9	i	156	LEU
9	i	170	HIS
9	i	172	LYS
9	i	177	LYS
9	i	178	GLU
9	i	181	ILE
9	i	186	ASP
9	i	189	GLN
9	i	204	VAL
9	i	211	LYS
9	i	212	ASP
9	i	214	GLU
9	i	216	LEU
9	i	217	ARG
9	i	220	LEU
9	i	227	GLU
9	i	230	LYS
9	i	231	SER
9	i	243	LYS
9	i	244	GLU
9	i	246	ILE
9	i	250	CYS
9	i	252	ILE
10	j	3	ASP
10	j	5	SER
10	j	6	SER
10	j	15	MET
10	j	18	LYS
10	j	31	SER
10	j	33	SER
10	j	61	THR
10	j	63	LEU
10	j	70	LYS
10	j	71	THR
10	j	73	LEU

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Mol	Chain	Res	Type
10	j	86	THR
10	j	93	SER
10	j	114	SER
10	j	118	LYS
10	j	134	LYS
10	j	136	PHE
10	j	139	SER
10	j	143	SER
10	j	147	PHE
10	j	157	ASN
10	j	161	GLU
10	j	177	ARG
11	k	7	ILE
11	k	12	SER
11	k	13	VAL
11	k	17	SER
11	k	25	ILE
11	k	29	LYS
11	k	30	ASP
11	k	31	SER
11	k	39	SER
11	k	44	MET
11	k	45	SER
11	k	54	VAL
11	k	65	GLN
11	k	69	ILE
11	k	71	GLU
11	k	78	GLN
11	k	86	GLN
11	k	90	LYS
11	k	91	SER
11	k	94	SER
11	k	96	ARG
11	k	109	LYS
11	k	110	LYS
11	k	125	LYS
11	k	135	TYR
11	k	140	THR
11	k	153	THR
11	k	155	GLU
11	k	169	GLU
11	k	175	ASP

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Mol	Chain	Res	Type
11	k	182	LYS
11	k	186	LYS
12	l	77	THR
12	l	84	GLN
12	l	96	THR
12	l	100	TRP
12	l	103	SER
12	l	105	THR
12	l	106	VAL
12	l	107	LYS
12	l	111	GLU
12	l	129	PHE
12	l	138	CYS
12	l	147	GLU
12	l	150	SER
12	l	159	SER
12	l	161	LEU
12	l	175	MET
12	l	181	ARG
12	l	182	LYS
12	l	192	SER
12	l	201	ILE
12	l	217	SER
12	l	224	SER
12	l	227	ASP
12	l	258	ASP
12	l	261	ILE
12	l	267	ASP
12	l	271	LEU
12	l	274	LYS
12	l	285	VAL
12	l	286	ILE
13	m	27	ASP
13	m	39	THR
13	m	40	ASP
13	m	42	SER
13	m	58	ILE
13	m	61	SER
13	m	72	LEU
13	m	73	VAL
13	m	74	LYS
13	m	75	ARG

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Mol	Chain	Res	Type
13	m	93	SER
13	m	96	SER
13	m	108	LYS
13	m	109	ARG
13	m	116	HIS
13	m	118	ILE
13	m	124	GLU
13	m	125	ASP
13	m	140	GLU
13	m	141	ARG
13	m	143	GLN
13	m	144	CYS
13	m	158	LEU
13	m	161	GLN
13	m	177	LYS
13	m	184	SER
13	m	186	GLU
13	m	187	GLU
13	m	198	SER
13	m	217	LYS
14	n	137	ARG
1	A	13	ASP
1	A	14	ARG
1	A	20	SER
1	A	22	GLU
1	A	27	GLN
1	A	45	VAL
1	A	54	ILE
1	A	56	GLN
1	A	58	LYS
1	A	62	LYS
1	A	67	THR
1	A	74	CYS
1	A	84	ASN
1	A	96	ARG
1	A	103	GLU
1	A	129	THR
1	A	134	MET
1	A	137	LEU
1	A	148	GLU
1	A	153	SER
1	A	156	LYS

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Mol	Chain	Res	Type
1	A	157	THR
1	A	174	LYS
1	A	175	GLN
1	A	176	GLN
1	A	177	GLU
1	A	190	LYS
1	A	208	THR
1	A	210	MET
1	A	216	THR
1	A	217	GLU
1	A	219	SER
1	A	230	LYS
1	A	232	LYS
1	A	250	GLU
2	B	8	SER
2	B	15	SER
2	B	17	LYS
2	B	21	ILE
2	B	33	THR
2	B	51	SER
2	B	55	LEU
2	B	59	GLU
2	B	70	ASP
2	B	85	LEU
2	B	89	SER
2	B	92	VAL
2	B	96	SER
2	B	97	TYR
2	B	98	LYS
2	B	109	LEU
2	B	112	SER
2	B	114	VAL
2	B	124	SER
2	B	128	ARG
2	B	132	VAL
2	B	133	SER
2	B	141	GLU
2	B	146	SER
2	B	151	ASP
2	B	156	TYR
2	B	166	LYS
2	B	169	VAL

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Mol	Chain	Res	Type
2	B	176	GLU
2	B	178	ARG
2	B	181	ASP
2	B	186	GLU
2	B	198	GLU
2	B	199	SER
2	B	203	GLU
2	B	205	ASN
2	B	216	ASP
2	B	217	GLU
2	B	230	ASP
2	B	231	LYS
2	B	236	ARG
2	B	239	THR
2	B	241	GLN
2	B	242	GLU
2	B	245	ASP
2	B	248	GLU
3	C	3	SER
3	C	5	ARG
3	C	8	SER
3	C	11	THR
3	C	18	ARG
3	C	19	LEU
3	C	27	GLU
3	C	36	ILE
3	C	45	VAL
3	C	51	LYS
3	C	52	VAL
3	C	61	THR
3	C	64	GLU
3	C	80	LEU
3	C	81	THR
3	C	93	ILE
3	C	99	LEU
3	C	100	LYS
3	C	110	ILE
3	C	113	ARG
3	C	115	LEU
3	C	118	ILE
3	C	123	THR
3	C	134	SER

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Mol	Chain	Res	Type
3	C	142	ASP
3	C	152	ASN
3	C	154	SER
3	C	170	SER
3	C	177	GLN
3	C	178	MET
3	C	181	LYS
3	C	182	ASP
3	C	183	ASP
3	C	185	LYS
3	C	203	SER
3	C	204	SER
3	C	209	ASP
3	C	221	ASN
3	C	227	GLN
3	C	228	LYS
3	C	231	LYS
5	E	2	PHE
5	E	4	THR
5	E	7	GLU
5	E	9	ASP
5	E	10	ARG
5	E	16	SER
5	E	21	LEU
5	E	24	VAL
5	E	25	GLU
5	E	36	THR
5	E	47	VAL
5	E	48	LEU
5	E	61	SER
5	E	64	ILE
5	E	78	MET
5	E	82	THR
5	E	104	ASP
5	E	110	GLU
5	E	116	VAL
5	E	128	SER
5	E	130	GLU
5	E	131	GLU
5	E	136	ARG
5	E	174	SER
5	E	177	GLU

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Mol	Chain	Res	Type
5	E	186	GLU
5	E	190	SER
5	E	195	GLU
5	E	202	LYS
5	E	205	LYS
5	E	206	GLN
5	E	209	GLU
5	E	211	LYS
5	E	234	GLU
6	F	9	ASP
6	F	10	THR
6	F	14	SER
6	F	18	ARG
6	F	26	LEU
6	F	30	LYS
6	F	31	GLN
6	F	33	SER
6	F	36	VAL
6	F	51	ARG
6	F	55	GLU
6	F	61	LYS
6	F	82	ARG
6	F	91	GLN
6	F	94	TYR
6	F	97	LEU
6	F	105	VAL
6	F	107	ARG
6	F	111	LEU
6	F	114	ASP
6	F	119	ASN
6	F	122	SER
6	F	140	SER
6	F	148	GLN
6	F	174	ARG
6	F	177	ASP
6	F	181	LYS
6	F	199	GLN
6	F	200	SER
6	F	218	LYS
6	F	219	ASP
6	F	220	THR
6	F	223	THR

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Mol	Chain	Res	Type
7	G	13	SER
7	G	20	ARG
7	G	23	GLN
7	G	29	LYS
7	G	36	THR
7	G	55	THR
7	G	57	LYS
7	G	62	GLN
7	G	63	LYS
7	G	72	ARG
7	G	86	ARG
7	G	89	VAL
7	G	100	LYS
7	G	105	THR
7	G	112	PHE
7	G	116	LEU
7	G	135	SER
7	G	143	LYS
7	G	154	SER
7	G	161	LYS
7	G	169	ARG
7	G	170	GLN
7	G	175	GLU
7	G	178	LYS
7	G	181	ASP
7	G	185	GLU
7	G	198	LYS
7	G	205	GLU
7	G	209	GLU
7	G	210	LYS
7	G	215	GLU
7	G	220	SER
7	G	227	LEU
7	G	232	LYS
7	G	247	ILE
8	1	11	SER
8	1	19	ASP
8	1	27	SER
8	1	29	THR
8	1	31	THR
8	1	37	ASN
8	1	45	ARG

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Mol	Chain	Res	Type
8	1	52	CYS
8	1	54	ARG
8	1	55	SER
8	1	57	SER
8	1	81	THR
8	1	83	SER
8	1	85	GLU
8	1	91	PHE
8	1	95	CYS
8	1	99	LYS
8	1	124	LEU
8	1	127	SER
8	1	128	VAL
8	1	147	CYS
8	1	152	ARG
8	1	153	GLU
8	1	159	GLU
8	1	162	ASP
8	1	169	SER
8	1	177	SER
8	1	178	SER
8	1	200	ASP
9	2	36	LYS
9	2	37	PHE
9	2	49	SER
9	2	51	GLN
9	2	54	ILE
9	2	57	ASP
9	2	60	CYS
9	2	63	LEU
9	2	65	ARG
9	2	67	SER
9	2	82	GLU
9	2	85	THR
9	2	86	GLN
9	2	87	LEU
9	2	90	SER
9	2	92	ILE
9	2	94	LEU
9	2	99	THR
9	2	104	ARG
9	2	110	GLN

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Mol	Chain	Res	Type
9	2	114	GLN
9	2	127	LEU
9	2	128	ILE
9	2	141	SER
9	2	143	HIS
9	2	147	SER
9	2	149	ASP
9	2	156	LEU
9	2	170	HIS
9	2	172	LYS
9	2	177	LYS
9	2	178	GLU
9	2	181	ILE
9	2	186	ASP
9	2	189	GLN
9	2	204	VAL
9	2	211	LYS
9	2	212	ASP
9	2	214	GLU
9	2	216	LEU
9	2	217	ARG
9	2	220	LEU
9	2	227	GLU
9	2	230	LYS
9	2	231	SER
9	2	243	LYS
9	2	244	GLU
9	2	246	ILE
9	2	250	CYS
9	2	252	ILE
10	3	3	ASP
10	3	5	SER
10	3	6	SER
10	3	15	MET
10	3	18	LYS
10	3	31	SER
10	3	33	SER
10	3	61	THR
10	3	63	LEU
10	3	70	LYS
10	3	71	THR
10	3	73	LEU

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Mol	Chain	Res	Type
10	3	86	THR
10	3	93	SER
10	3	114	SER
10	3	118	LYS
10	3	134	LYS
10	3	136	PHE
10	3	139	SER
10	3	143	SER
10	3	147	PHE
10	3	157	ASN
10	3	161	GLU
10	3	177	ARG
11	4	7	ILE
11	4	12	SER
11	4	13	VAL
11	4	17	SER
11	4	25	ILE
11	4	29	LYS
11	4	30	ASP
11	4	31	SER
11	4	39	SER
11	4	44	MET
11	4	45	SER
11	4	54	VAL
11	4	65	GLN
11	4	69	ILE
11	4	71	GLU
11	4	78	GLN
11	4	86	GLN
11	4	90	LYS
11	4	91	SER
11	4	94	SER
11	4	96	ARG
11	4	109	LYS
11	4	110	LYS
11	4	125	LYS
11	4	135	TYR
11	4	140	THR
11	4	153	THR
11	4	155	GLU
11	4	169	GLU
11	4	175	ASP

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Mol	Chain	Res	Type
11	4	182	LYS
11	4	186	LYS
12	5	77	THR
12	5	84	GLN
12	5	96	THR
12	5	100	TRP
12	5	103	SER
12	5	105	THR
12	5	106	VAL
12	5	107	LYS
12	5	111	GLU
12	5	129	PHE
12	5	138	CYS
12	5	147	GLU
12	5	150	SER
12	5	159	SER
12	5	161	LEU
12	5	175	MET
12	5	181	ARG
12	5	182	LYS
12	5	192	SER
12	5	201	ILE
12	5	217	SER
12	5	224	SER
12	5	227	ASP
12	5	258	ASP
12	5	261	ILE
12	5	267	ASP
12	5	271	LEU
12	5	274	LYS
12	5	285	VAL
12	5	286	ILE
13	6	27	ASP
13	6	39	THR
13	6	40	ASP
13	6	42	SER
13	6	58	ILE
13	6	61	SER
13	6	72	LEU
13	6	73	VAL
13	6	74	LYS
13	6	75	ARG

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Mol	Chain	Res	Type
13	6	93	SER
13	6	96	SER
13	6	108	LYS
13	6	109	ARG
13	6	116	HIS
13	6	118	ILE
13	6	124	GLU
13	6	125	ASP
13	6	140	GLU
13	6	141	ARG
13	6	143	GLN
13	6	144	CYS
13	6	158	LEU
13	6	161	GLN
13	6	177	LYS
13	6	184	SER
13	6	186	GLU
13	6	187	GLU
13	6	198	SER
13	6	217	LYS
15	W	134	LYS
16	V	20	ARG
20	Z	774	ARG
21	N	398	ARG
21	N	858	LYS
21	N	864	LYS
22	S	358	LYS
23	P	23	LYS
24	Q	93	THR
24	Q	111	LEU
24	Q	252	HIS
24	Q	394	ASN
25	R	351	LYS
27	O	58	ARG
27	O	115	ARG
27	O	315	LYS
27	O	382	LYS
28	H	466	TYR
29	I	87	LYS
29	I	300	ARG
30	K	236	ARG
31	L	183	ILE

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Mol	Chain	Res	Type
31	L	275	PRO
33	J	306	ARG
34	8	463	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	37	GLN
1	a	84	ASN
1	a	176	GLN
3	c	168	ASN
3	c	177	GLN
3	c	227	GLN
4	d	94	GLN
5	e	99	HIS
5	e	114	GLN
6	f	60	GLN
6	f	90	GLN
6	f	119	ASN
7	g	68	GLN
7	g	170	GLN
8	h	170	GLN
9	i	223	ASN
9	i	248	ASN
10	j	8	ASN
10	j	38	ASN
10	j	48	HIS
10	j	173	ASN
11	k	37	GLN
11	k	41	HIS
11	k	61	GLN
11	k	63	ASN
11	k	86	GLN
12	l	84	GLN
12	l	218	ASN
13	m	84	HIS
13	m	102	GLN
13	m	143	GLN
13	m	161	GLN
13	m	166	ASN
13	m	205	GLN
1	A	37	GLN

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Mol	Chain	Res	Type
1	A	84	ASN
3	C	168	ASN
3	C	227	GLN
4	D	79	ASN
5	E	99	HIS
6	F	60	GLN
6	F	90	GLN
6	F	119	ASN
7	G	68	GLN
7	G	170	GLN
9	2	223	ASN
9	2	248	ASN
10	3	8	ASN
10	3	48	HIS
10	3	173	ASN
11	4	37	GLN
11	4	41	HIS
11	4	61	GLN
11	4	63	ASN
11	4	86	GLN
12	5	84	GLN
12	5	218	ASN
13	6	84	HIS
13	6	102	GLN
13	6	161	GLN
13	6	166	ASN
13	6	205	GLN
14	7	158	GLN
15	W	149	GLN
15	W	170	HIS
16	V	102	GLN
16	V	184	ASN
16	V	186	GLN
16	V	190	HIS
16	V	200	ASN
16	V	279	HIS
16	V	290	ASN
17	T	71	GLN
17	T	230	ASN
19	Y	52	ASN
20	Z	110	ASN
20	Z	214	HIS

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Mol	Chain	Res	Type
20	Z	243	GLN
20	Z	276	ASN
20	Z	327	GLN
20	Z	387	ASN
20	Z	577	GLN
20	Z	628	ASN
20	Z	823	ASN
20	Z	868	ASN
20	Z	874	ASN
20	Z	897	HIS
20	Z	905	ASN
20	Z	926	ASN
20	Z	931	GLN
21	N	233	ASN
21	N	336	ASN
21	N	340	HIS
21	N	346	ASN
21	N	375	HIS
21	N	506	GLN
21	N	654	GLN
21	N	747	HIS
21	N	877	GLN
22	S	154	GLN
22	S	177	ASN
22	S	312	GLN
22	S	412	ASN
23	P	33	ASN
23	P	94	GLN
23	P	222	ASN
23	P	275	ASN
23	P	394	ASN
23	P	413	ASN
23	P	440	HIS
24	Q	19	GLN
24	Q	80	HIS
25	R	314	ASN
25	R	385	ASN
25	R	397	ASN
25	R	401	HIS
26	U	21	HIS
26	U	193	GLN
26	U	238	ASN

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Mol	Chain	Res	Type
26	U	260	ASN
27	O	177	GLN
27	O	354	GLN
28	H	98	GLN
28	H	151	GLN
28	H	339	GLN
29	I	102	ASN
29	I	150	HIS
29	I	151	HIS
29	I	204	HIS
29	I	238	ASN
29	I	295	ASN
29	I	426	ASN
30	K	36	ASN
30	K	83	GLN
30	K	264	ASN
31	L	50	GLN
31	L	175	GLN
31	L	317	ASN
32	M	53	HIS
32	M	71	ASN
32	M	328	ASN
33	J	123	HIS
33	J	170	HIS
34	8	106	GLN
34	8	264	HIS
34	8	338	GLN
34	8	415	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
35	GLZ	9	76	35	3,3,3	0.58	0	0,2,2	-	-

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
35	GLZ	9	76	35	-	0/0/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	ATP	K	501	37	26,33,33	1.07	2 (7%)	31,52,52	2.06	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	ADP	J	501	37	24,29,29	1.21	3 (12%)	29,45,45	2.29	9 (31%)
36	ATP	L	501	37	26,33,33	1.50	6 (23%)	31,52,52	1.42	3 (9%)
36	ATP	I	501	33,37	26,33,33	1.13	3 (11%)	31,52,52	2.05	10 (32%)
36	ATP	M	501	32,37	26,33,33	0.77	0	31,52,52	1.63	5 (16%)
36	ATP	H	501	37,28	26,33,33	0.90	0	31,52,52	1.87	10 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	K	501	37	-	5/18/38/38	0/3/3/3
38	ADP	J	501	37	-	4/12/32/32	0/3/3/3
36	ATP	L	501	37	-	4/18/38/38	0/3/3/3
36	ATP	I	501	33,37	-	4/18/38/38	0/3/3/3
36	ATP	M	501	32,37	-	4/18/38/38	0/3/3/3
36	ATP	H	501	37,28	-	6/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	J	501	ADP	O4'-C1'	3.40	1.45	1.41
36	L	501	ATP	C4-N3	-3.20	1.31	1.35
36	L	501	ATP	C5-N7	-2.70	1.29	1.39
36	K	501	ATP	C6-C5	2.60	1.53	1.43
38	J	501	ADP	C5'-C4'	-2.56	1.43	1.51
36	L	501	ATP	C2-N1	2.53	1.38	1.33
36	L	501	ATP	PB-O2B	-2.52	1.43	1.55
36	L	501	ATP	C2-N3	2.41	1.36	1.32
36	K	501	ATP	C2-N3	2.31	1.35	1.32
36	I	501	ATP	C5-C4	2.29	1.47	1.40
36	L	501	ATP	C2'-C1'	-2.16	1.50	1.53
36	I	501	ATP	C2-N3	2.13	1.35	1.32
38	J	501	ADP	O4'-C4'	2.04	1.49	1.45
36	I	501	ATP	O5'-C5'	-2.01	1.37	1.44

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	J	501	ADP	N3-C2-N1	-5.69	119.79	128.68
36	K	501	ATP	C5-C6-N6	-5.62	111.81	120.35
38	J	501	ADP	C5'-C4'-C3'	5.32	135.12	115.18
38	J	501	ADP	C3'-C2'-C1'	5.20	108.80	100.98
36	M	501	ATP	N3-C2-N1	-4.90	121.02	128.68
36	H	501	ATP	N3-C2-N1	-4.90	121.03	128.68
36	I	501	ATP	O5'-C5'-C4'	-4.82	92.40	108.99
36	L	501	ATP	PA-O3A-PB	4.74	149.09	132.83
36	K	501	ATP	C2-N1-C6	-4.72	110.68	118.75
36	I	501	ATP	O4'-C4'-C3'	4.21	113.44	105.11
38	J	501	ADP	C5-C6-N6	-4.14	114.07	120.35
36	I	501	ATP	N3-C2-N1	-3.91	122.57	128.68
36	I	501	ATP	C3'-C2'-C1'	3.61	106.41	100.98
36	K	501	ATP	C4-C5-N7	-3.56	105.68	109.40
36	M	501	ATP	C1'-N9-C4	-3.52	120.45	126.64
36	K	501	ATP	N6-C6-N1	3.42	125.68	118.57
36	M	501	ATP	O4'-C1'-C2'	3.37	111.85	106.93
36	I	501	ATP	O4'-C4'-C5'	3.26	120.11	109.37
36	H	501	ATP	C5-C6-N6	-3.19	115.50	120.35
36	K	501	ATP	O5'-PA-O1A	-3.08	97.05	109.07
36	K	501	ATP	O5'-C5'-C4'	3.00	119.31	108.99
36	H	501	ATP	C3'-C2'-C1'	2.96	105.43	100.98
36	K	501	ATP	PA-O3A-PB	2.94	142.93	132.83
36	M	501	ATP	C5-C6-N6	-2.81	116.08	120.35
36	H	501	ATP	C1'-N9-C4	-2.80	121.71	126.64
36	H	501	ATP	O5'-C5'-C4'	2.78	118.57	108.99
36	I	501	ATP	O3'-C3'-C2'	2.69	120.54	111.82
36	L	501	ATP	O4'-C1'-C2'	2.66	110.82	106.93
38	J	501	ADP	O4'-C1'-C2'	-2.65	103.05	106.93
36	H	501	ATP	O4'-C1'-C2'	-2.61	103.11	106.93
36	M	501	ATP	PB-O3B-PG	-2.52	124.18	132.83
36	L	501	ATP	O3G-PG-O2G	2.41	116.83	107.64
38	J	501	ADP	O5'-PA-O1A	-2.33	99.97	109.07
36	H	501	ATP	O5'-PA-O1A	-2.33	99.98	109.07
38	J	501	ADP	C1'-N9-C4	-2.32	122.56	126.64
36	I	501	ATP	C4-C5-N7	-2.32	106.98	109.40
36	I	501	ATP	O2'-C2'-C3'	2.24	119.06	111.82
36	H	501	ATP	O2A-PA-O1A	2.20	123.10	112.24
38	J	501	ADP	N6-C6-N1	2.20	123.13	118.57
36	K	501	ATP	O3G-PG-O2G	2.16	115.88	107.64
36	H	501	ATP	O2G-PG-O1G	2.14	119.07	110.68
38	J	501	ADP	O4'-C4'-C5'	-2.08	102.53	109.37
36	H	501	ATP	PA-O3A-PB	-2.07	125.71	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	I	501	ATP	N6-C6-N1	2.06	122.85	118.57
36	I	501	ATP	O3G-PG-O2G	2.04	115.43	107.64

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	H	501	ATP	PB-O3B-PG-O3G
36	H	501	ATP	C5'-O5'-PA-O2A
36	H	501	ATP	C5'-O5'-PA-O3A
36	I	501	ATP	C5'-O5'-PA-O1A
36	I	501	ATP	C5'-O5'-PA-O2A
36	K	501	ATP	PB-O3B-PG-O2G
36	K	501	ATP	PB-O3B-PG-O3G
36	L	501	ATP	C5'-O5'-PA-O3A
36	M	501	ATP	PB-O3B-PG-O2G
36	M	501	ATP	C5'-O5'-PA-O2A
36	M	501	ATP	C5'-O5'-PA-O3A
36	I	501	ATP	O4'-C4'-C5'-O5'
38	J	501	ADP	O4'-C4'-C5'-O5'
36	H	501	ATP	PB-O3B-PG-O2G
36	H	501	ATP	PG-O3B-PB-O2B
36	L	501	ATP	C5'-O5'-PA-O2A
36	K	501	ATP	PG-O3B-PB-O2B
36	L	501	ATP	O4'-C4'-C5'-O5'
36	L	501	ATP	C3'-C4'-C5'-O5'
36	M	501	ATP	PB-O3B-PG-O3G
38	J	501	ADP	PA-O3A-PB-O2B
38	J	501	ADP	PA-O3A-PB-O3B
36	I	501	ATP	C5'-O5'-PA-O3A
38	J	501	ADP	C5'-O5'-PA-O3A
36	H	501	ATP	PG-O3B-PB-O1B
36	K	501	ATP	PG-O3B-PB-O1B
36	K	501	ATP	PB-O3B-PG-O1G

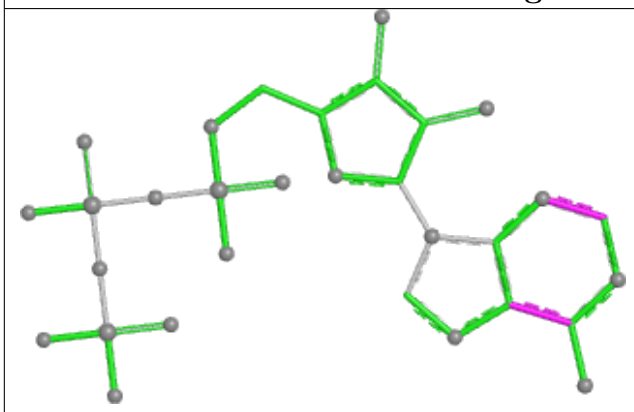
There are no ring outliers.

No monomer is involved in short contacts.

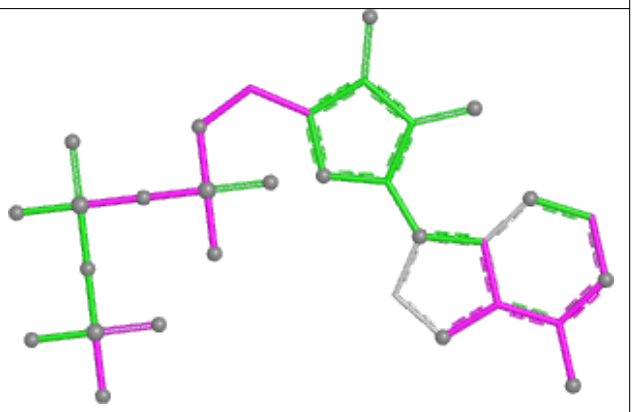
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

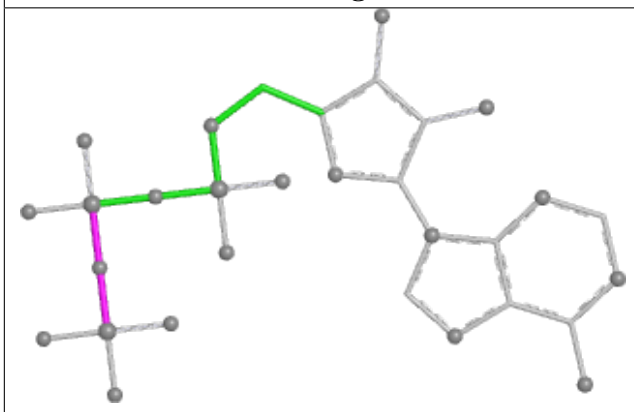
Ligand ATP K 501



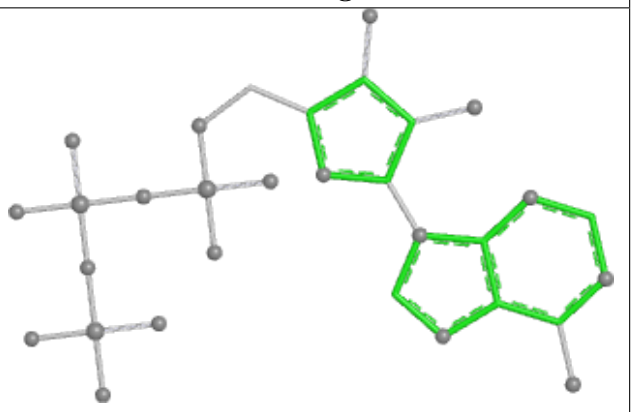
Bond lengths



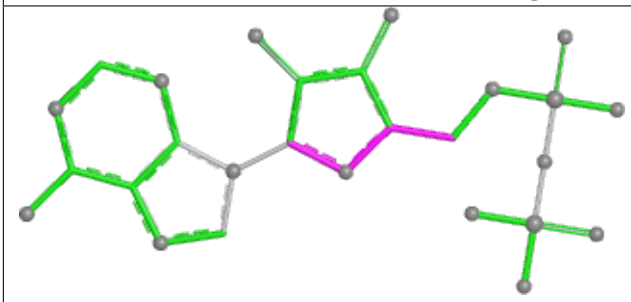
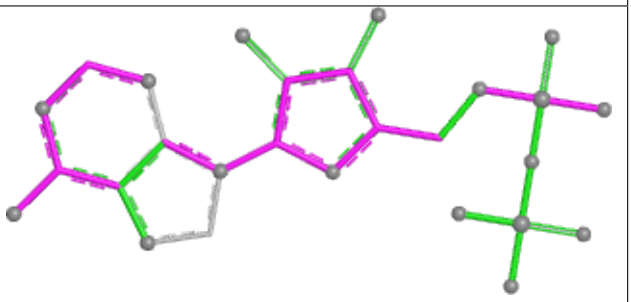
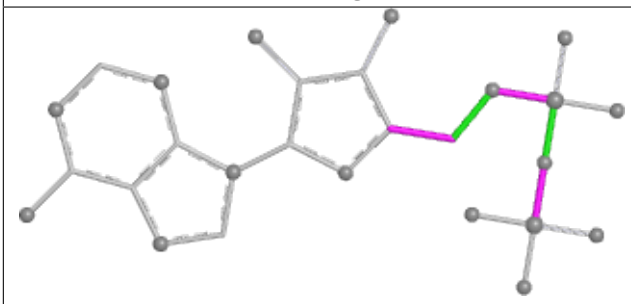
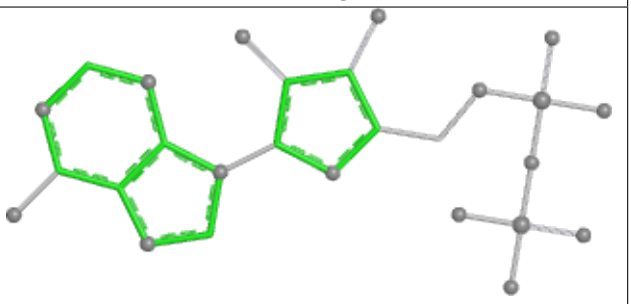
Bond angles

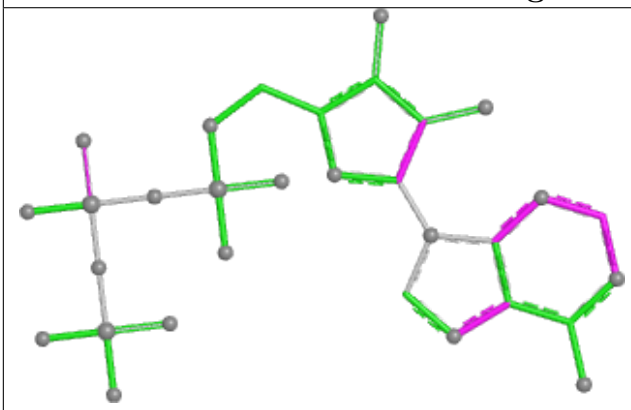
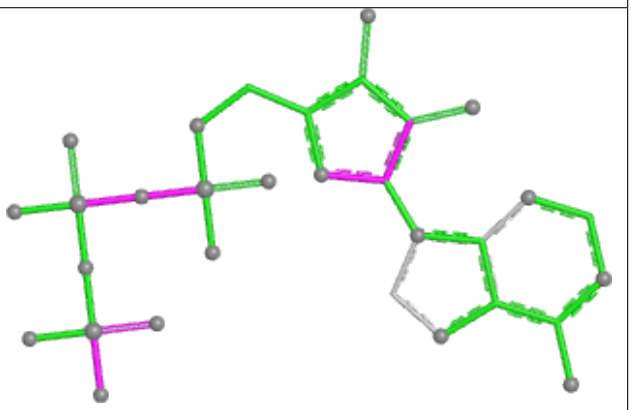
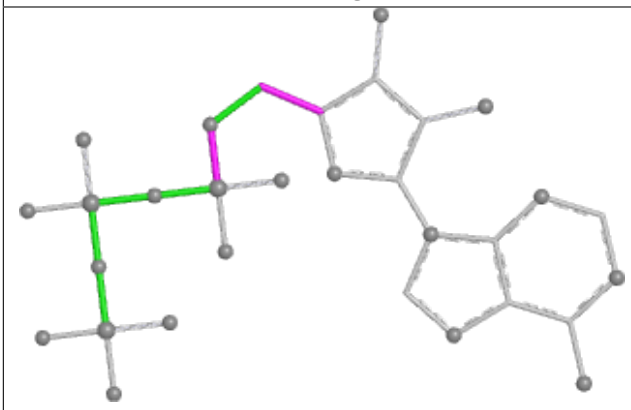
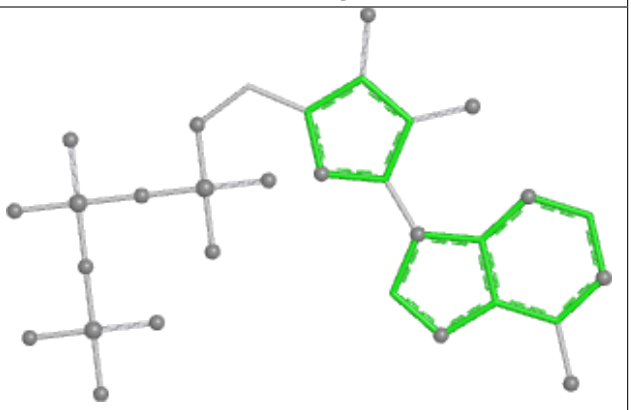


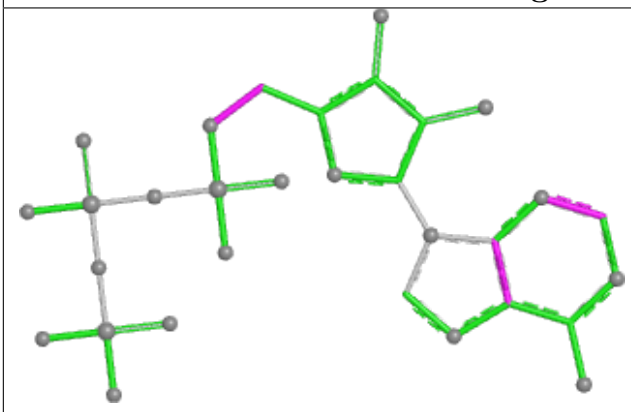
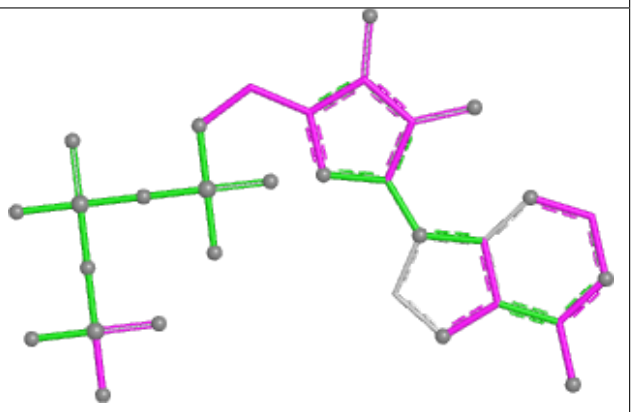
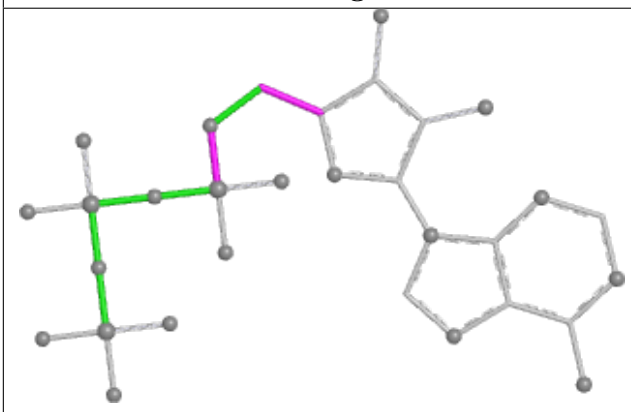
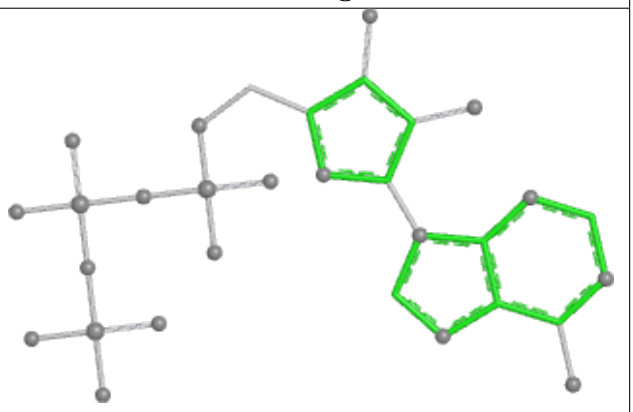
Torsions

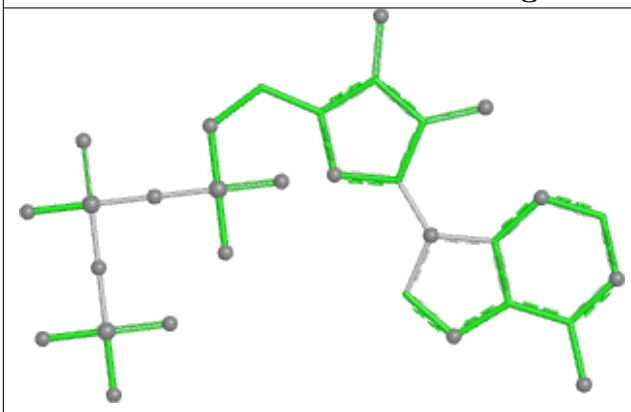
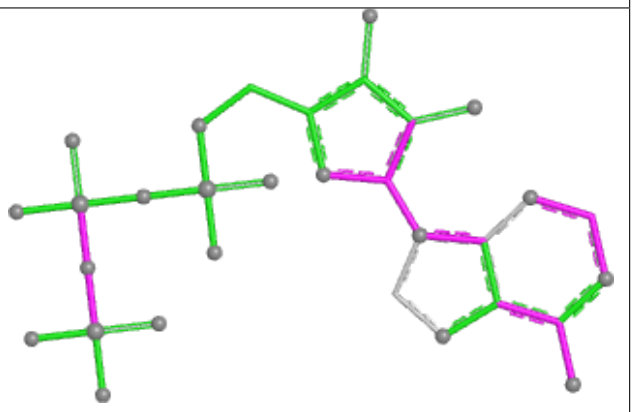
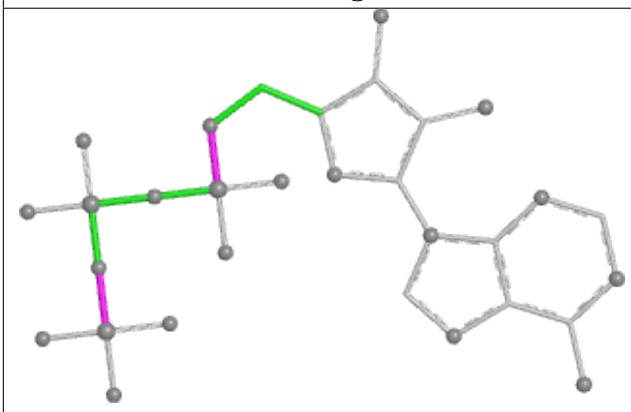
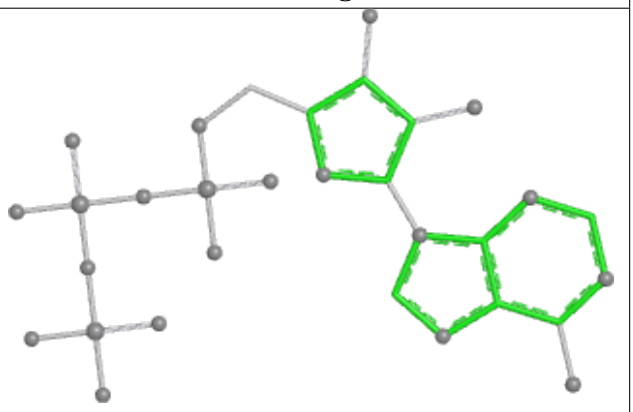


Rings

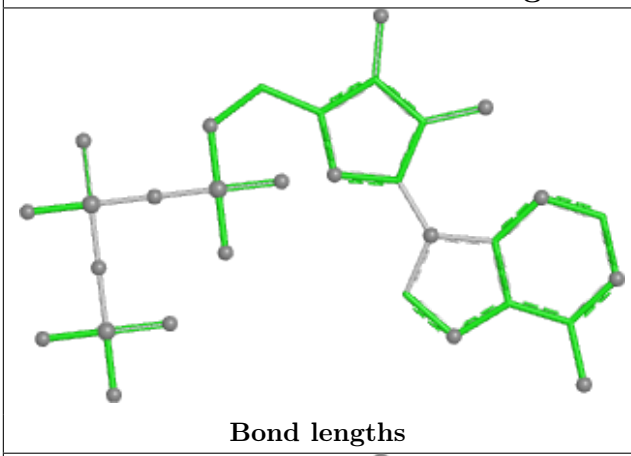
Ligand ADP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

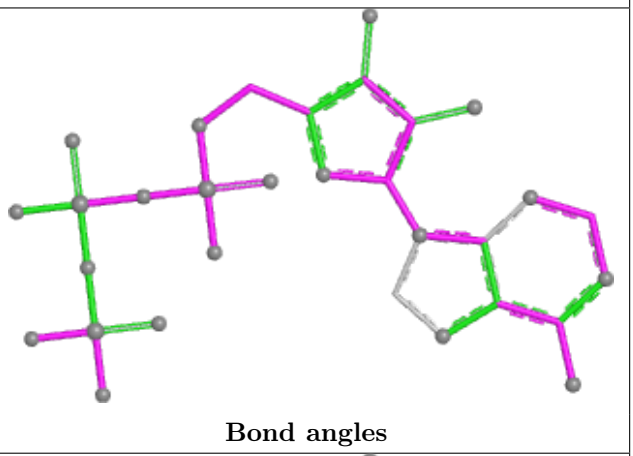
Ligand ATP I 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ATP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

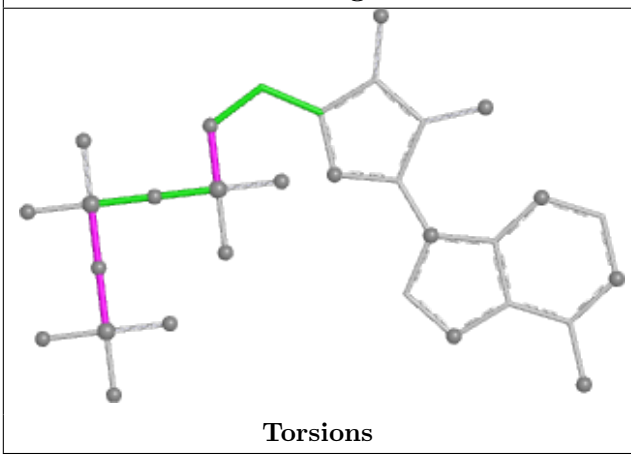
Ligand ATP H 501



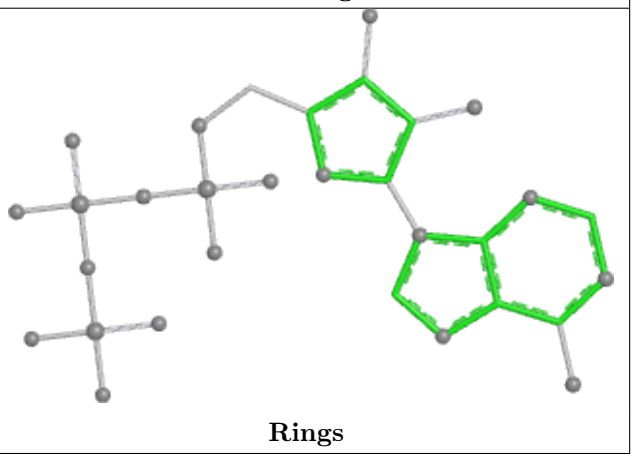
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

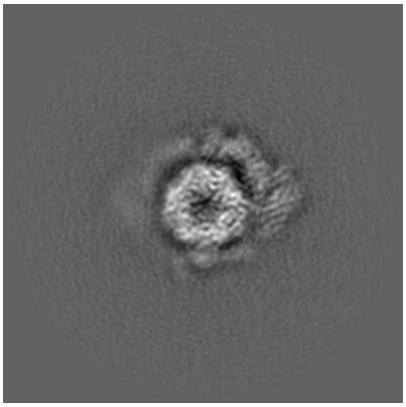
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-14085. These allow visual inspection of the internal detail of the map and identification of artifacts.

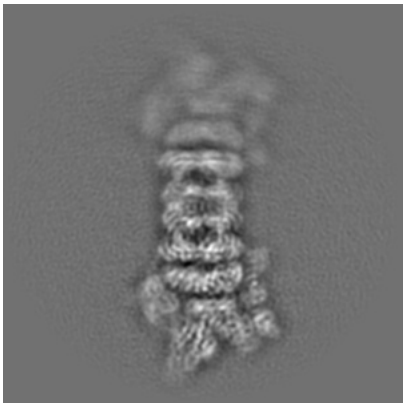
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

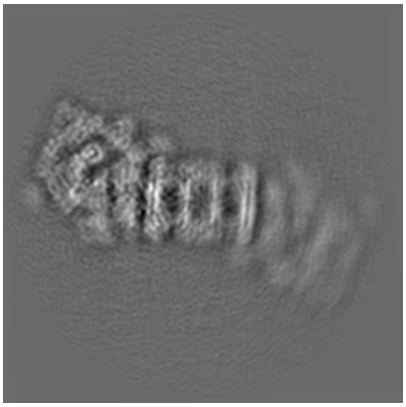
6.1.1 Primary map



X



Y

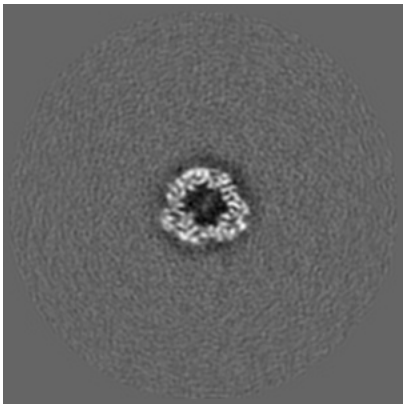


Z

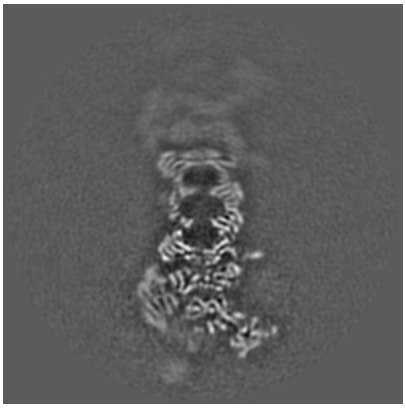
The images above show the map projected in three orthogonal directions.

6.2 Central slices

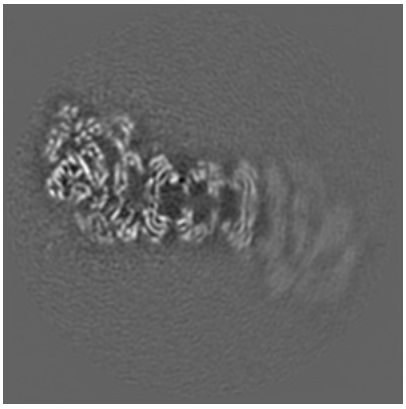
6.2.1 Primary map



X Index: 192



Y Index: 192

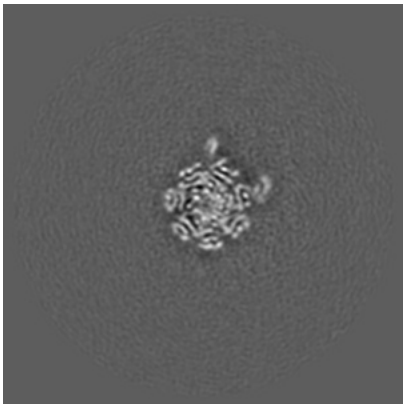


Z Index: 192

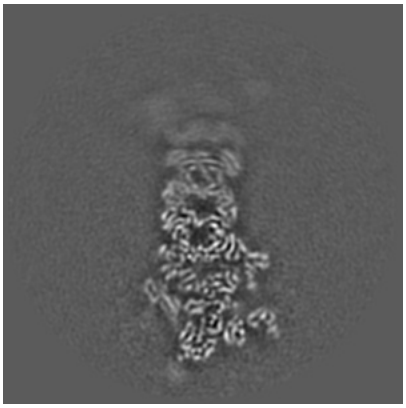
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

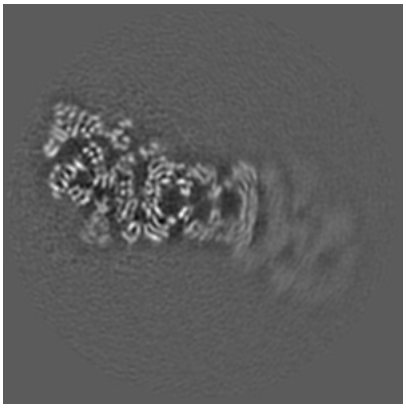
6.3.1 Primary map



X Index: 148



Y Index: 208

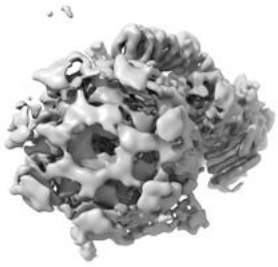


Z Index: 197

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

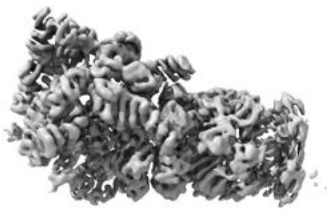
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

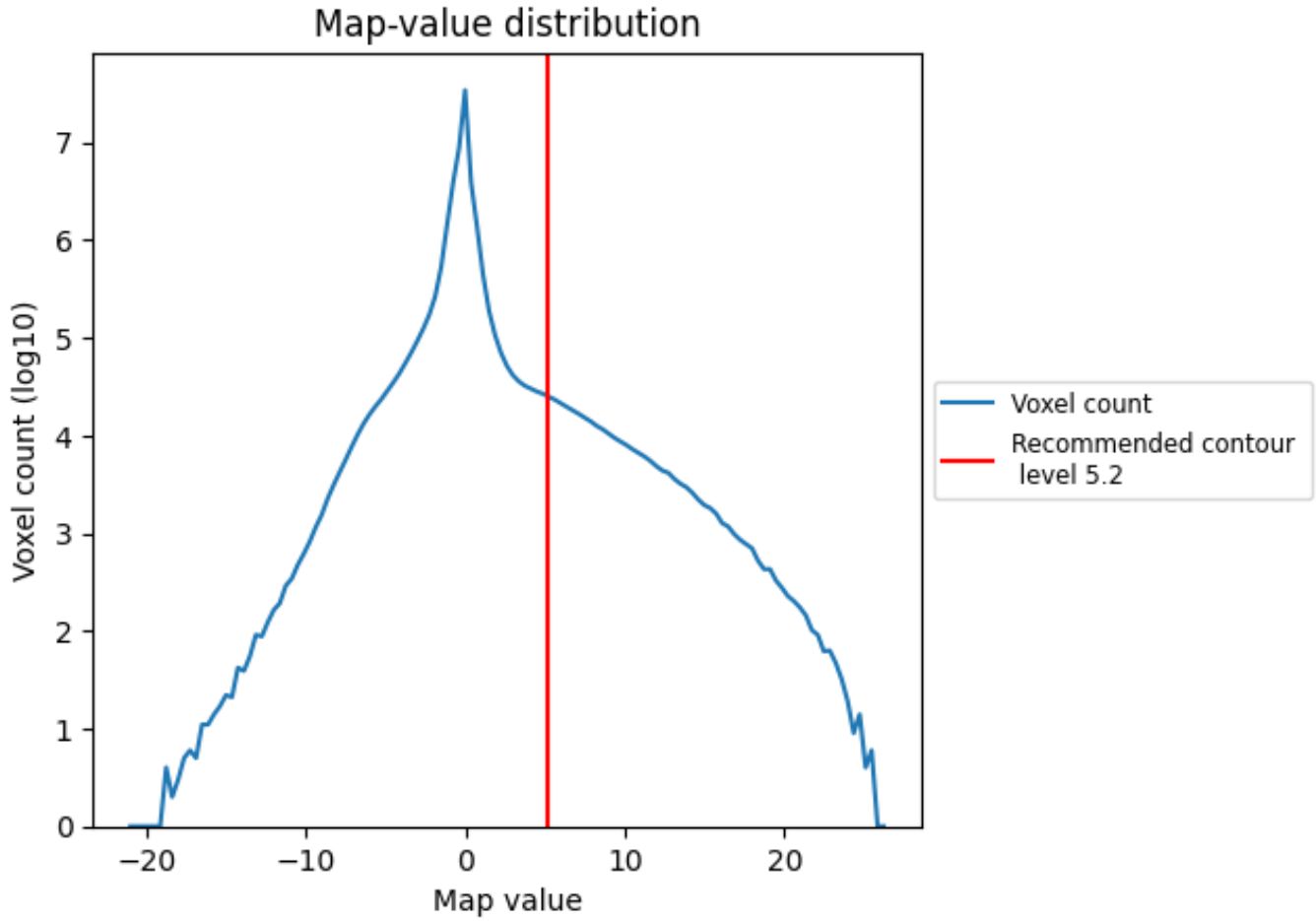
6.5 Mask visualisation (i)

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

7 Map analysis

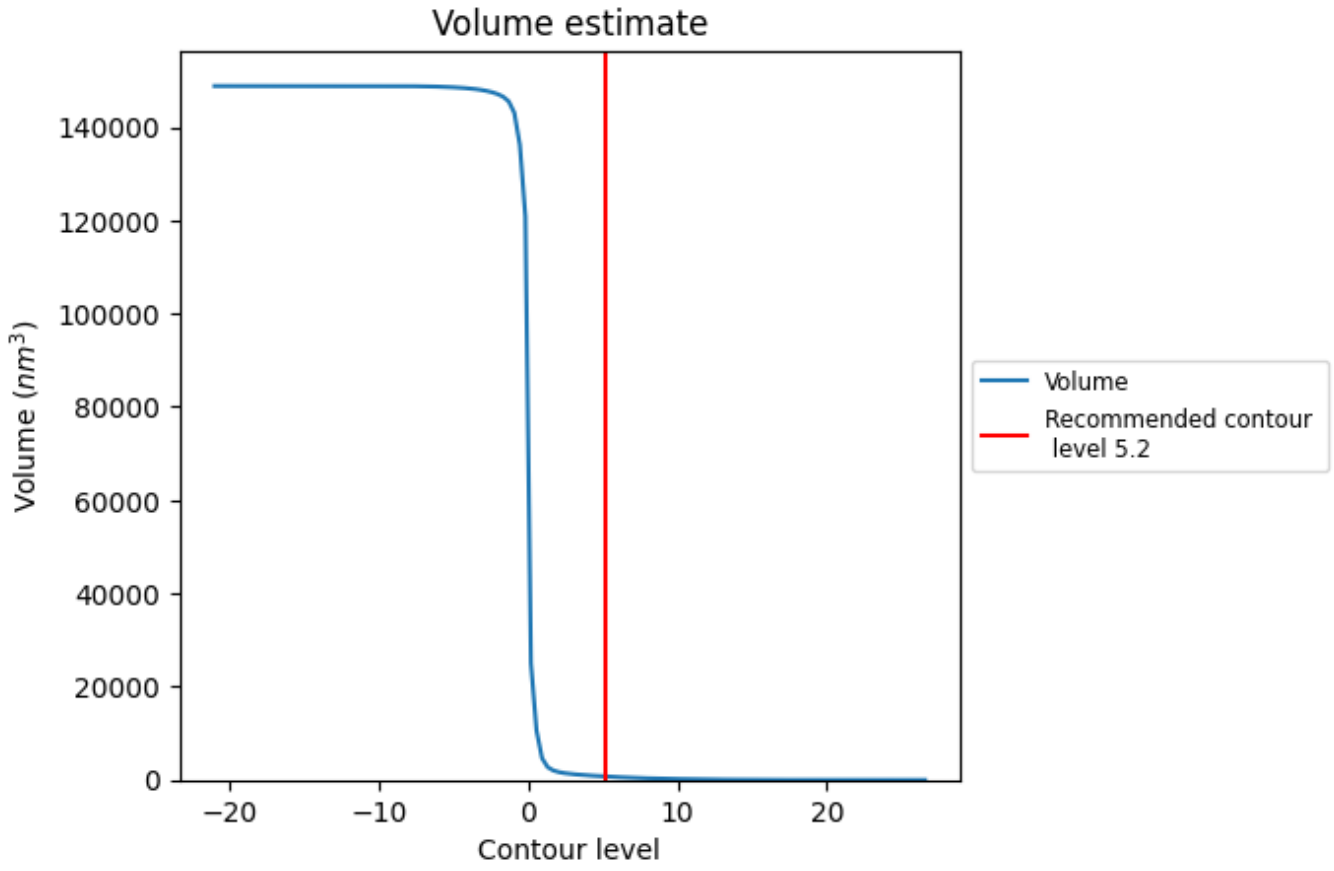
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

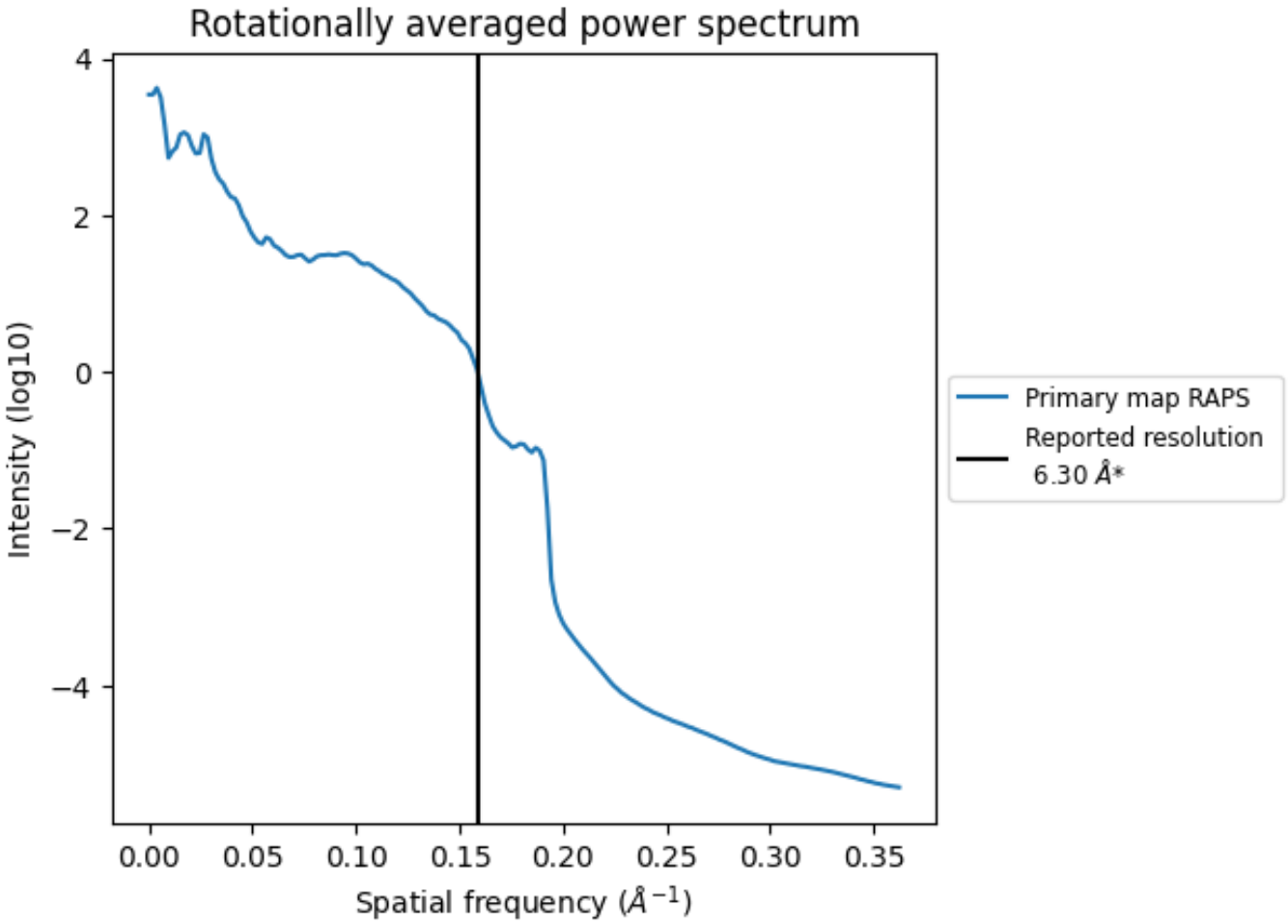
7.2 Volume estimate



The volume at the recommended contour level is 745 nm^3; this corresponds to an approximate mass of 673 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 0.159 $Å^{-1}$

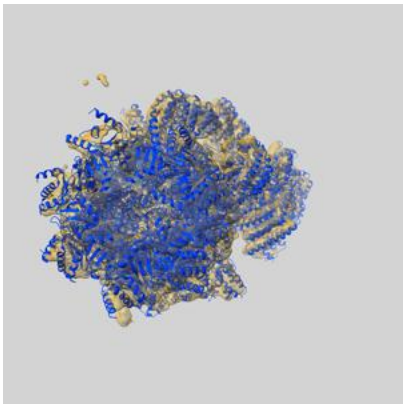
8 Fourier-Shell correlation (i)

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

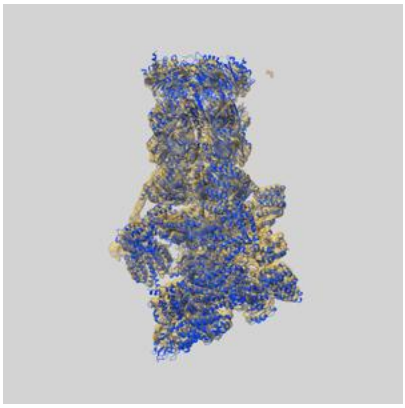
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-14085 and PDB model 7QO6. Per-residue inclusion information can be found in section 3 on page 13.

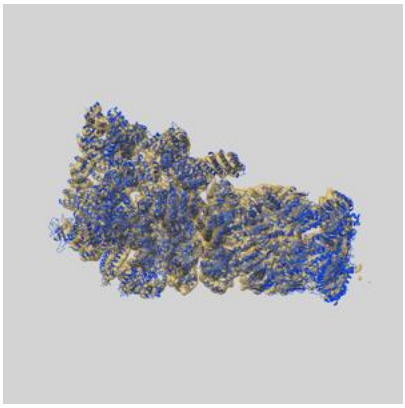
9.1 Map-model overlay



X



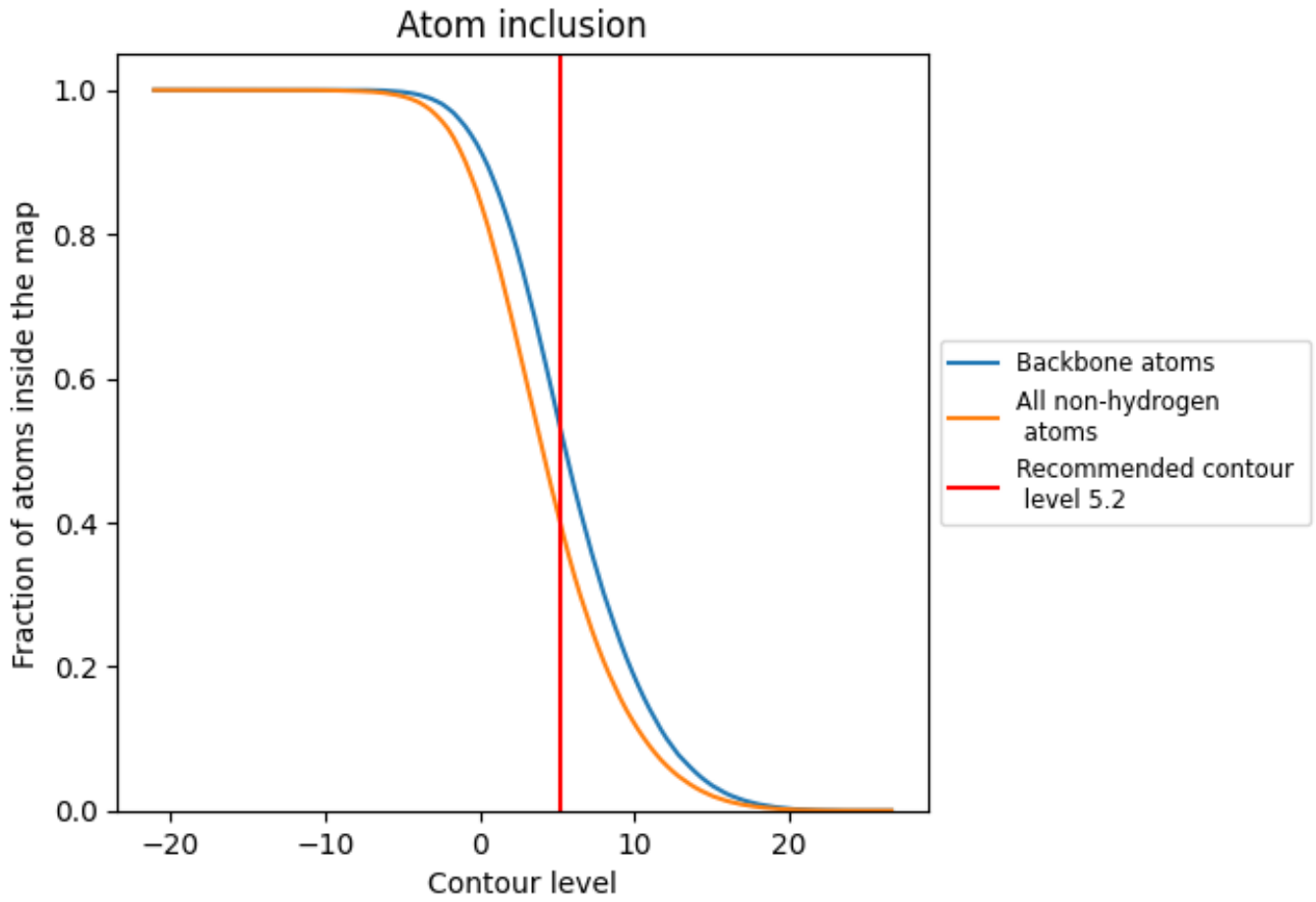
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 5.2 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 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 40% of all non-hydrogen atoms, are inside the map.