Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 09:44 AM JST

PDB ID	:	5GJQ
EMDB ID	:	EMD-9511
Title	:	Structure of the human 26S proteasome bound to USP14-UbAl
Authors	:	Huang, X.L.; Luan, B.; Wu, J.P.; Shi, Y.G.
Deposited on	:	2016-07-01
Resolution	:	4.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

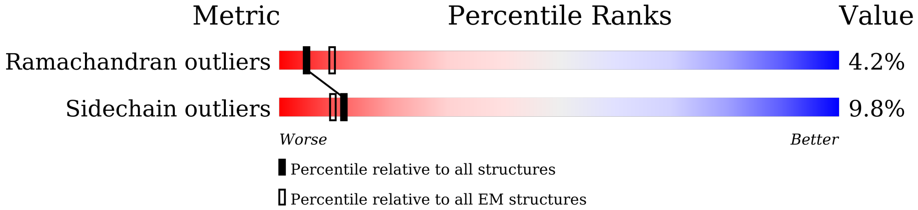
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance ⓘ

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

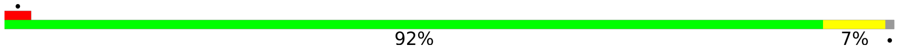
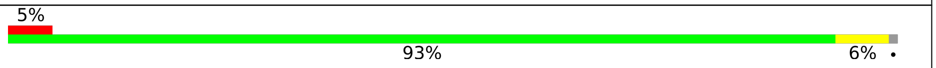
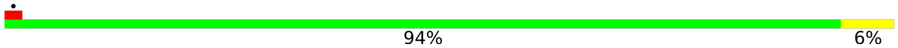
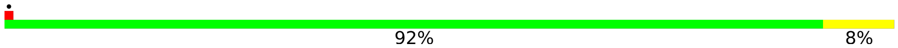
The reported resolution of this entry is 4.50 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	239	
1	o	239	
2	B	246	
2	h	246	
3	b	277	
3	p	277	
4	C	234	
4	i	234	
5	c	205	

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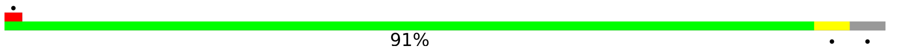
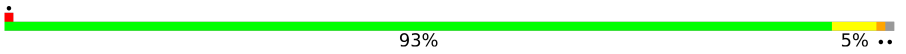
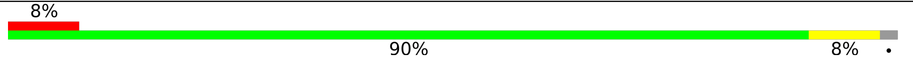
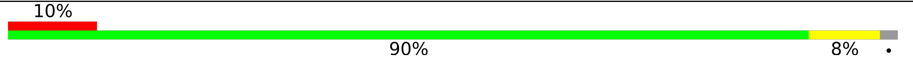
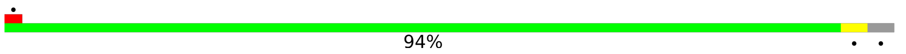
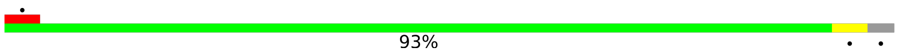
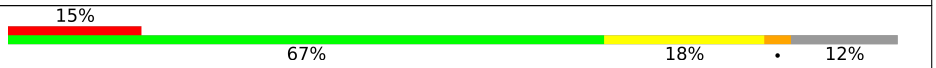
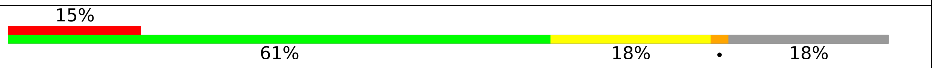
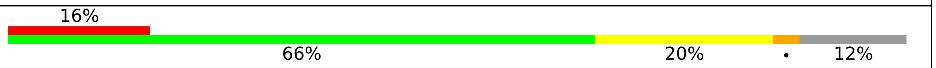
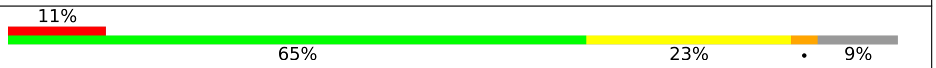
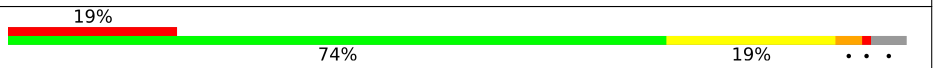
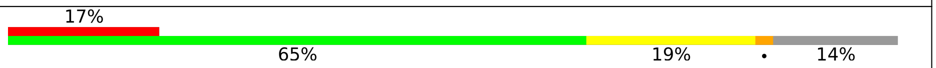
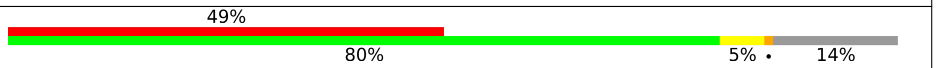
Mol	Chain	Length	Quality of chain
5	q	205	
6	D	261	
6	j	261	
7	d	201	
7	r	201	
8	E	248	
8	k	248	
9	e	263	
9	s	263	
10	F	241	
10	l	241	
11	f	241	
11	t	241	
12	G	263	
12	m	263	
13	g	264	
13	u	264	
14	H	433	
15	I	440	
16	J	406	
17	K	418	
18	L	389	
19	M	439	
20	N	953	
21	X	255	

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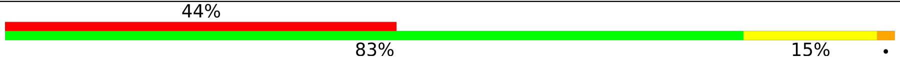
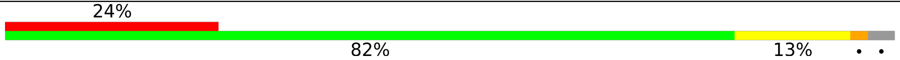
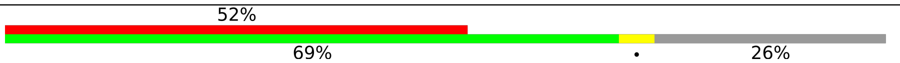
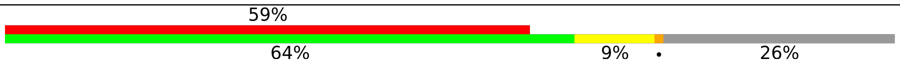
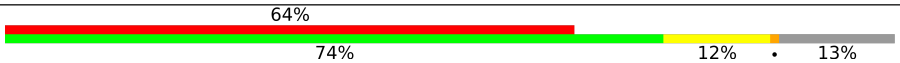
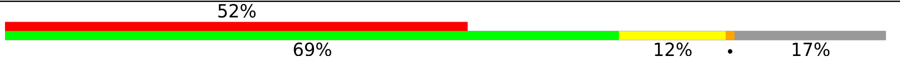
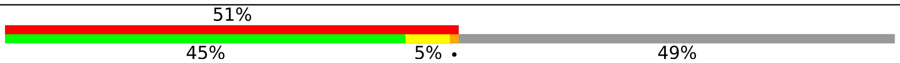
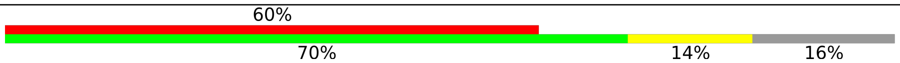
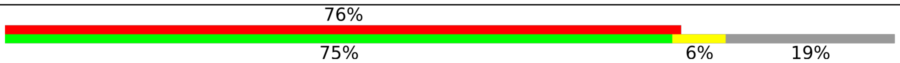
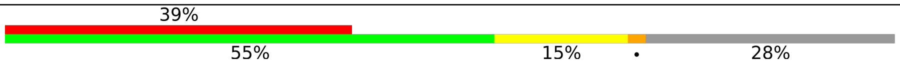
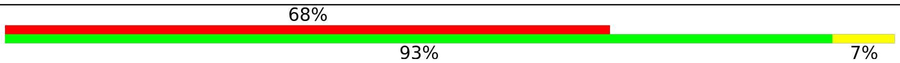
Mol	Chain	Length	Quality of chain
21	n	255	 89% 5% 5%
22	O	376	 73% 87% 11%
23	P	456	 57% 83% 7% 9%
24	Q	422	 44% 83% 15%
25	R	389	 24% 82% 13%
26	S	534	 52% 69% 26%
27	T	350	 59% 64% 9% 26%
28	U	324	 64% 74% 12% 13%
29	V	310	 52% 69% 12% 17%
30	W	377	 51% 45% 5% 49%
31	Y	70	 60% 70% 14% 16%
32	Z	908	 76% 75% 6% 19%
33	x	494	 39% 55% 15% 28%
34	y	76	 68% 93% 7%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 98461 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit beta type-6.

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

- Molecule 2 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 3 is a protein called Proteasome subunit beta type-7.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	233	Total	C	N	O	S	0	0
			1707	1081	287	334	5		
4	i	231	Total	C	N	O	S	0	0
			1744	1112	290	336	6		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	250	Total 1912	C 1204	N 329	O 371	S 8	0	0
6	j	250	Total 1913	C 1203	N 330	O 372	S 8	0	0

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

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

- Molecule 8 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 9 is a protein called Proteasome subunit beta type-5.

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

- Molecule 10 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	234	Total 1766	C 1108	N 290	O 357	S 11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	l	234	Total 1726	C 1107	N 291	O 317	S 11	0	0

- Molecule 11 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	f	213	Total 1641	C 1036	N 282	O 313	S 10	0	0
11	t	213	Total 1644	C 1039	N 282	O 313	S 10	0	0

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 13 is a protein called Proteasome subunit beta type-4.

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

- Molecule 14 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H	380	Total 2879	C 1809	N 513	O 539	S 18	0	0

- Molecule 15 is a protein called 26S protease regulatory subunit 4.

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

- Molecule 16 is a protein called 26S protease regulatory subunit 8.

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

- Molecule 17 is a protein called 26S protease regulatory subunit 6B.

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

- Molecule 18 is a protein called 26S protease regulatory subunit 10B.

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

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

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

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	823	Total	C	N	O	S	0	0
			5462	3499	933	1012	18		

- Molecule 21 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	372	Total	C	N	O	S	0	0
			2372	1518	405	438	11		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	413	2828	1819	489	514	6	0	0

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Q	421	2948	1864	509	567	8	0	0

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	R	376	2767	1794	461	503	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	S	395	2600	1662	463	472	3	0	0

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	T	258	1702	1102	280	315	5	0	0

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

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

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	V	257	2011	1276	341	377	17	0	0

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 31 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	Y	59	Total	C	N	O	0	0
			308	184	60	64		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

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

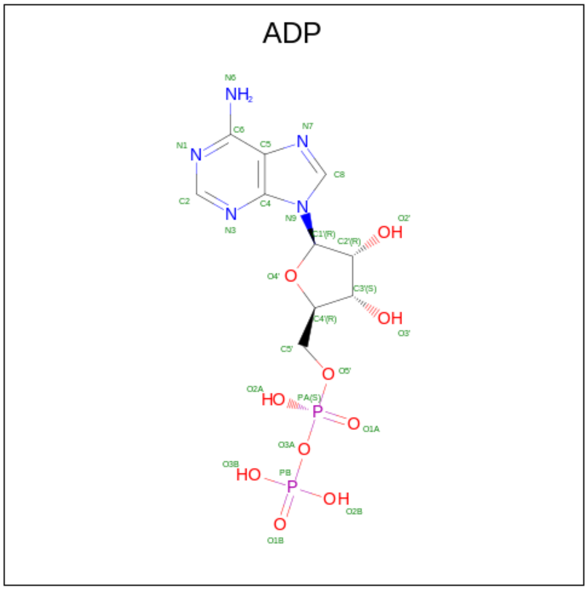
- Molecule 33 is a protein called Ubiquitin carboxyl-terminal hydrolase 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	x	355	Total	C	N	O	S	0	0
			2810	1782	470	538	20		

- Molecule 34 is a protein called Polyubiquitin-B.

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

- Molecule 35 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



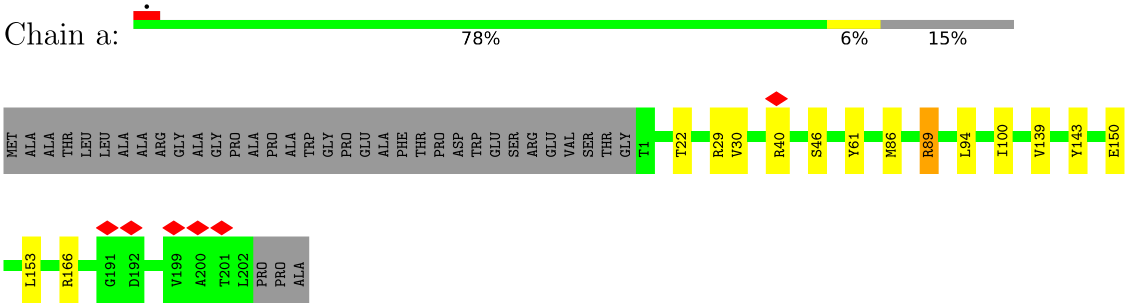
Mol	Chain	Residues	Atoms	AltConf
35	H	1	Total C N O P 27 10 5 10 2	0
35	I	1	Total C N O P 27 10 5 10 2	0
35	J	1	Total C N O P 27 10 5 10 2	0
35	K	1	Total C N O P 27 10 5 10 2	0
35	L	1	Total C N O P 27 10 5 10 2	0
35	M	1	Total C N O P 27 10 5 10 2	0

3 Residue-property plots ⓘ

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

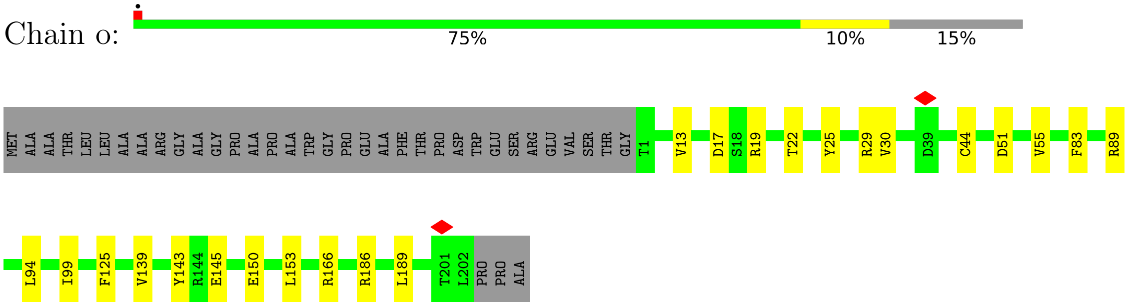
- Molecule 1: Proteasome subunit beta type-6

Chain a:



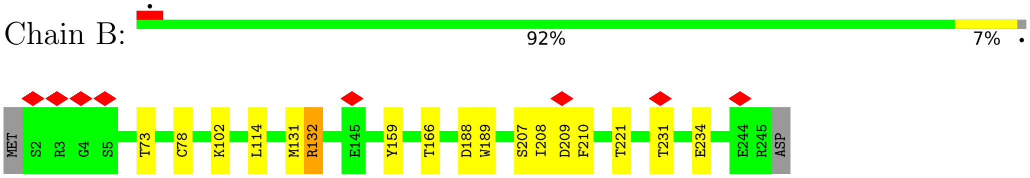
- Molecule 1: Proteasome subunit beta type-6

Chain o:



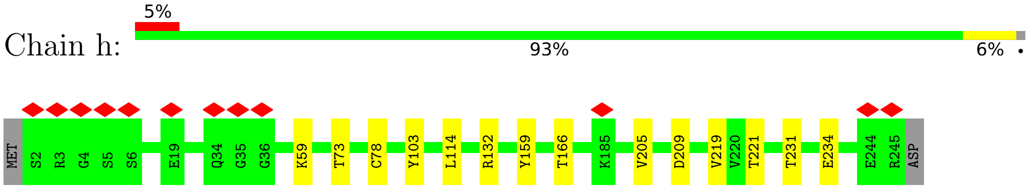
- Molecule 2: Proteasome subunit alpha type-6

Chain B:



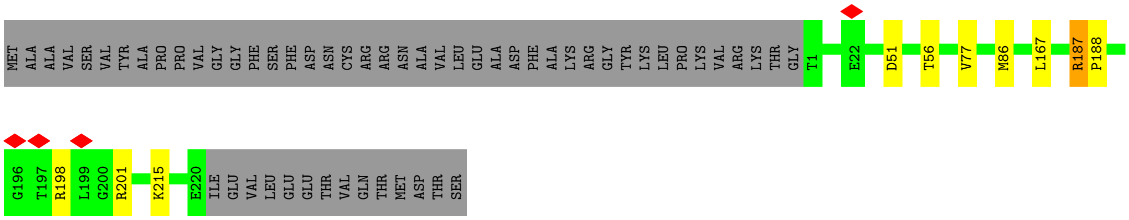
- Molecule 2: Proteasome subunit alpha type-6

Chain h:



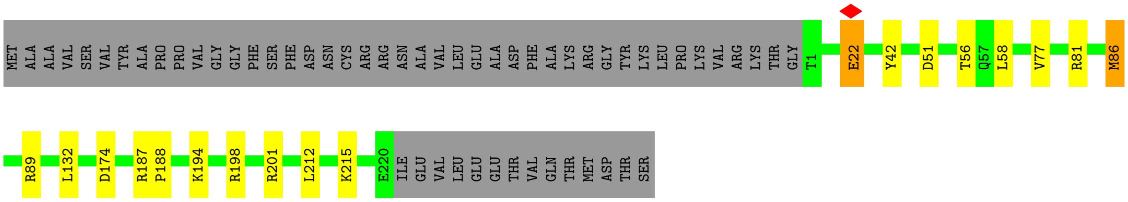
- Molecule 3: Proteasome subunit beta type-7

Chain b:



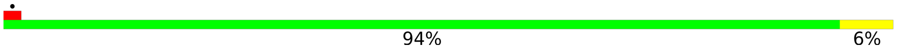
- Molecule 3: Proteasome subunit beta type-7

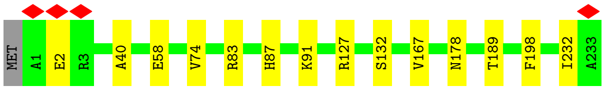
Chain p:



- Molecule 4: Proteasome subunit alpha type-2

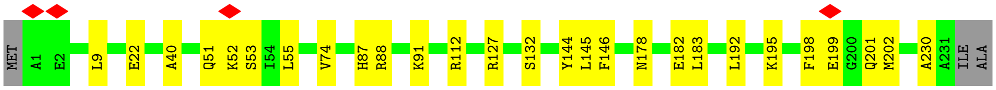
Chain C:





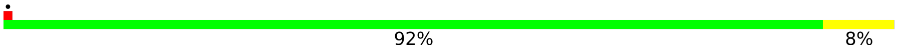
- Molecule 4: Proteasome subunit alpha type-2

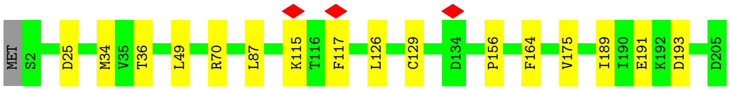
Chain i:



- Molecule 5: Proteasome subunit beta type-3

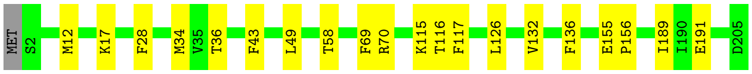
Chain c:





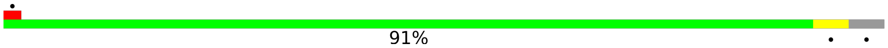
- Molecule 5: Proteasome subunit beta type-3

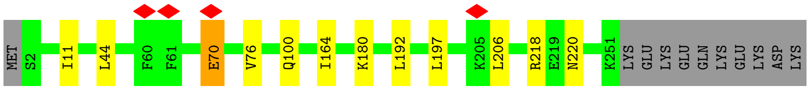
Chain q:



- Molecule 6: Proteasome subunit alpha type-4

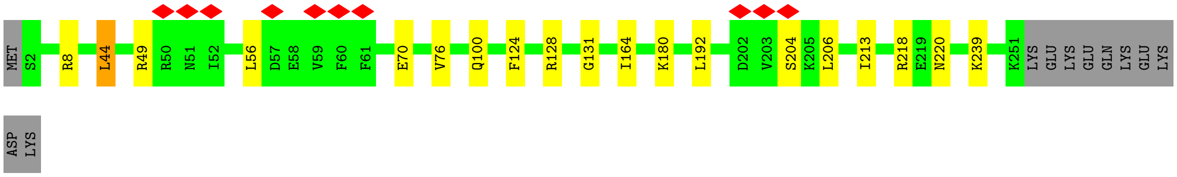
Chain D:





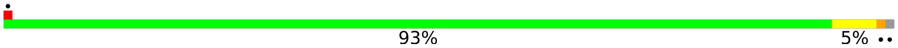
- Molecule 6: Proteasome subunit alpha type-4

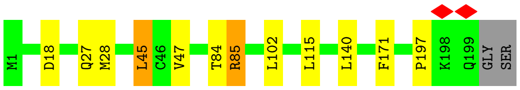
Chain j:



- Molecule 7: Proteasome subunit beta type-2

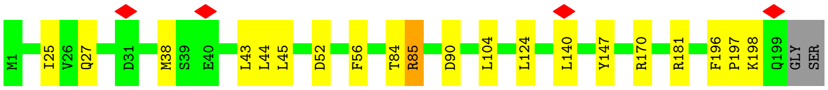
Chain d:





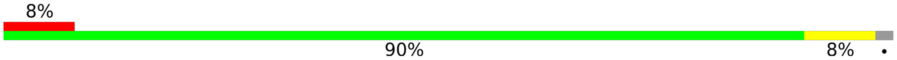
- Molecule 7: Proteasome subunit beta type-2

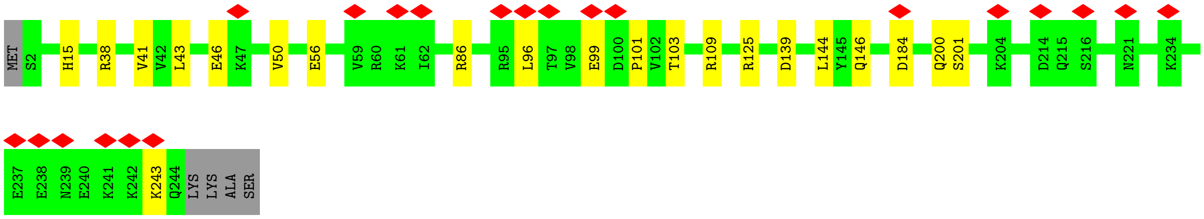
Chain r:



- Molecule 8: Proteasome subunit alpha type-7

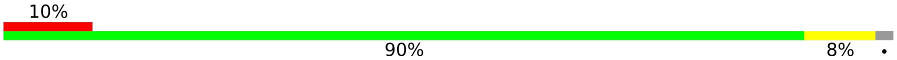
Chain E:

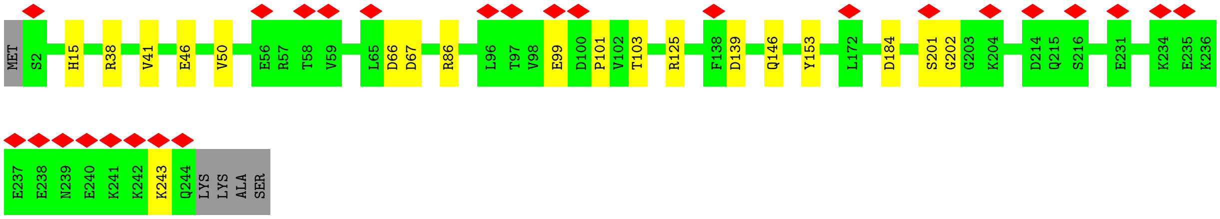




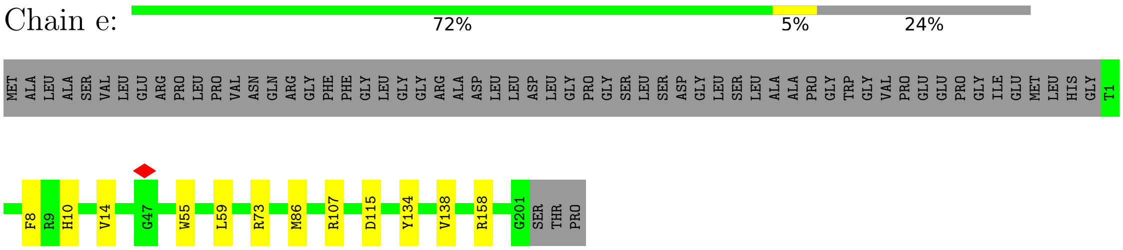
- Molecule 8: Proteasome subunit alpha type-7

Chain k:

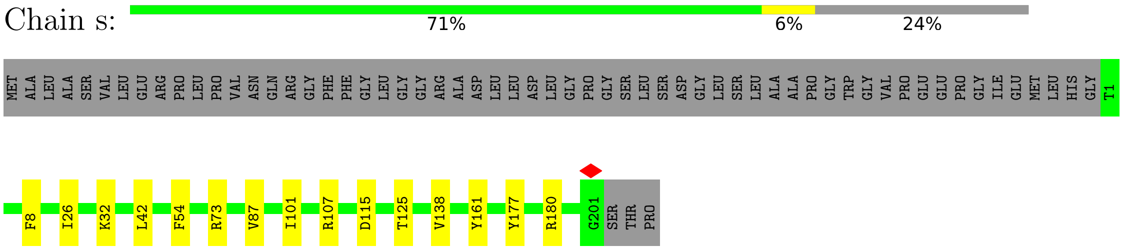




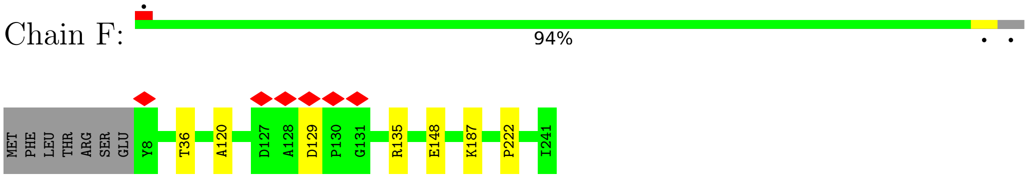
- Molecule 9: Proteasome subunit beta type-5



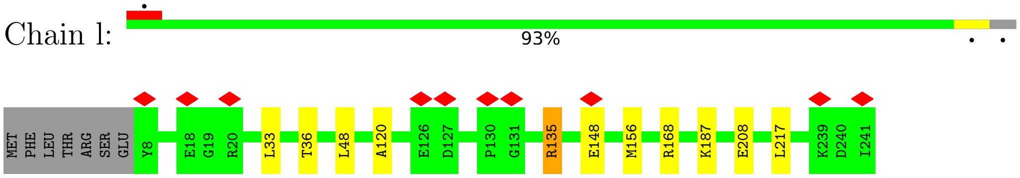
- Molecule 9: Proteasome subunit beta type-5



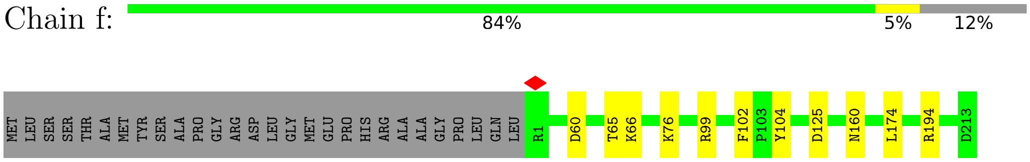
- Molecule 10: Proteasome subunit alpha type-5



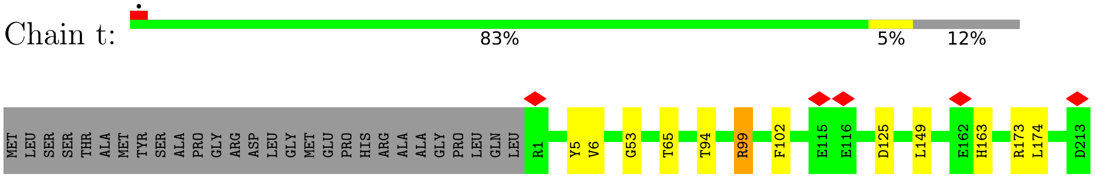
- Molecule 10: Proteasome subunit alpha type-5



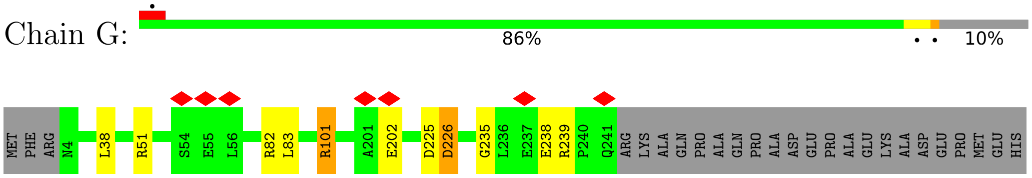
- Molecule 11: Proteasome subunit beta type-1



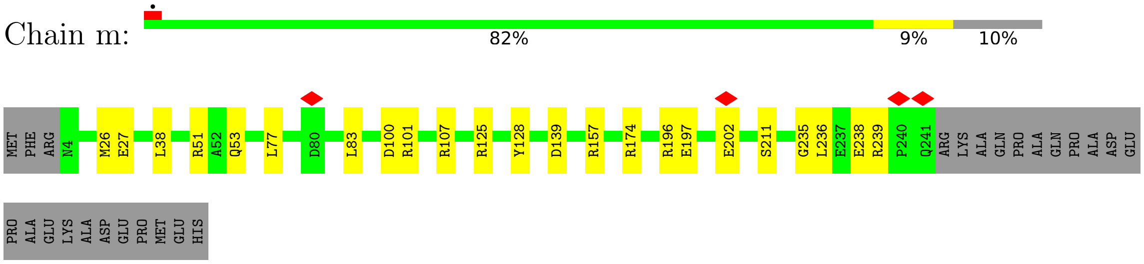
- Molecule 11: Proteasome subunit beta type-1



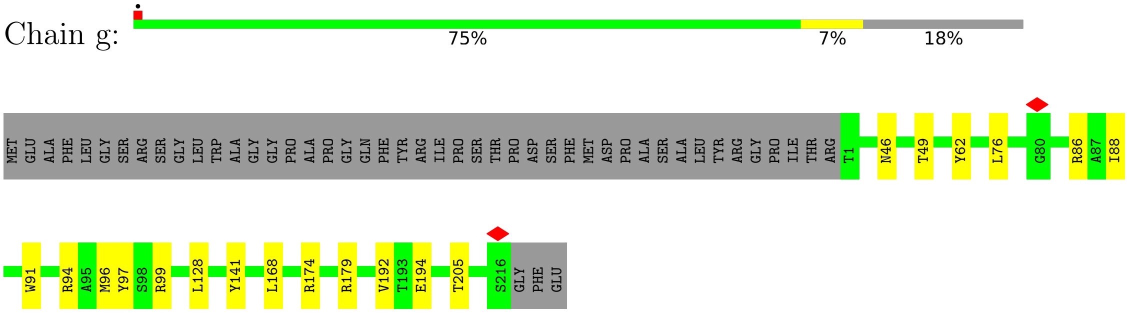
- Molecule 12: Proteasome subunit alpha type-1



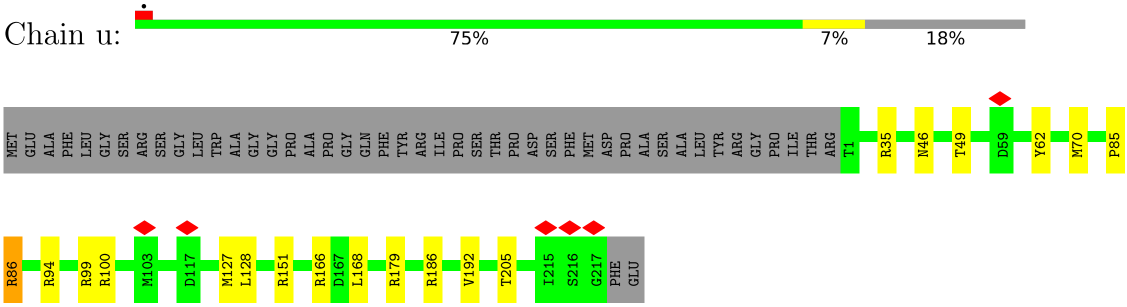
- Molecule 12: Proteasome subunit alpha type-1



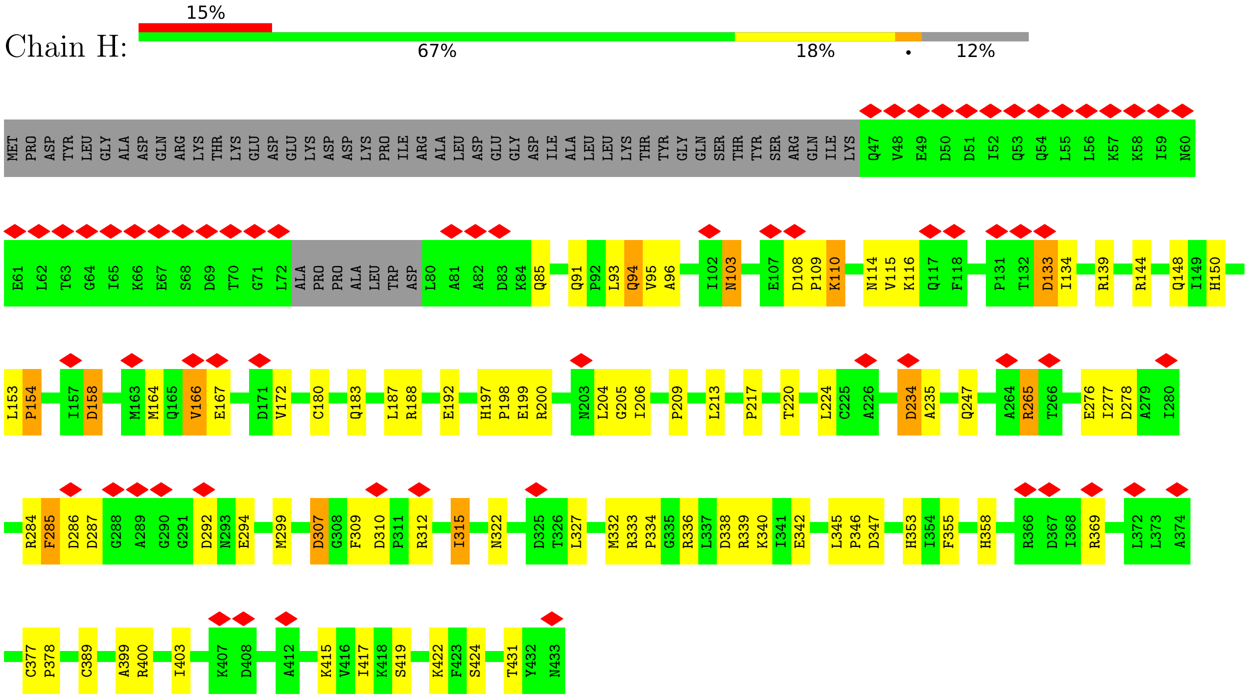
- Molecule 13: Proteasome subunit beta type-4



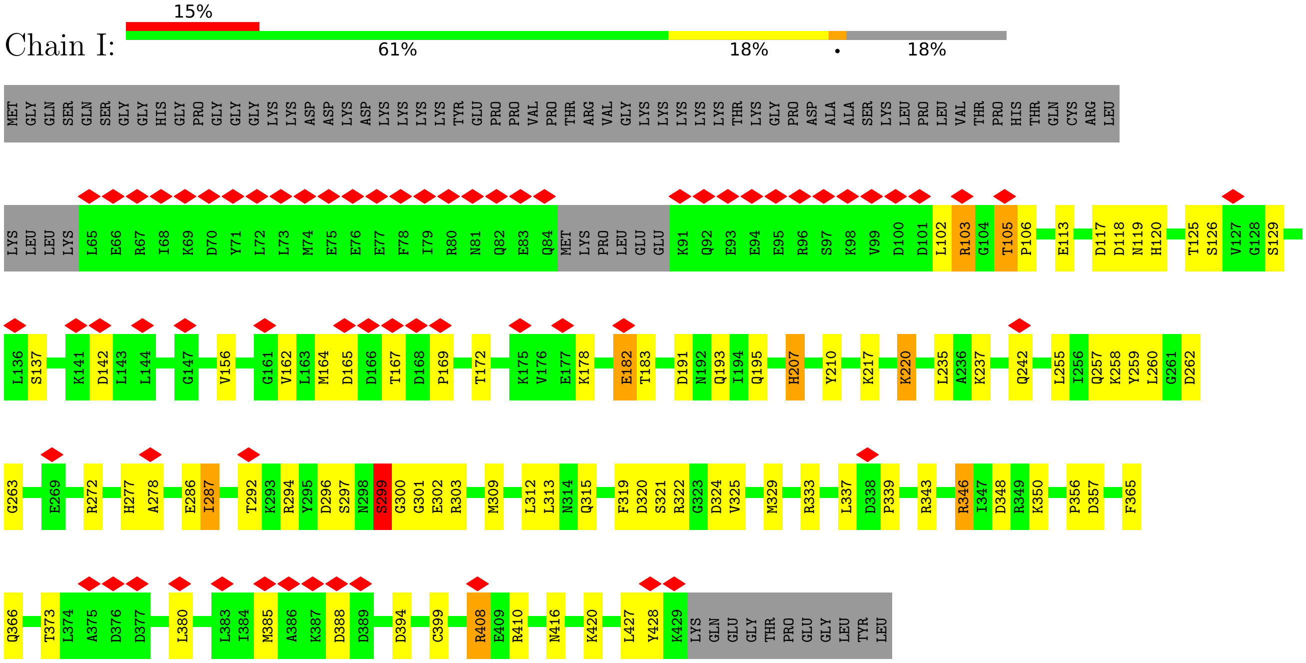
- Molecule 13: Proteasome subunit beta type-4



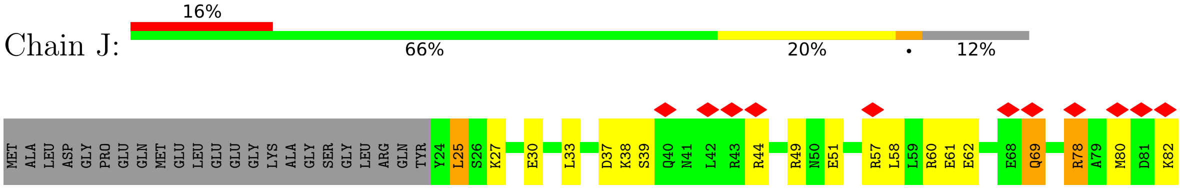
- Molecule 14: 26S protease regulatory subunit 7

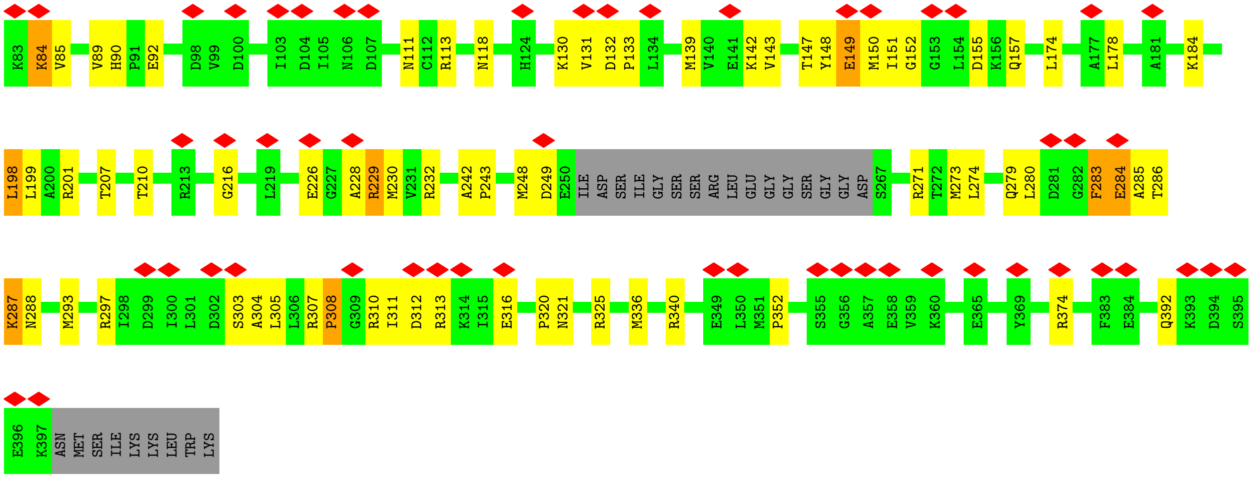


- Molecule 15: 26S protease regulatory subunit 4



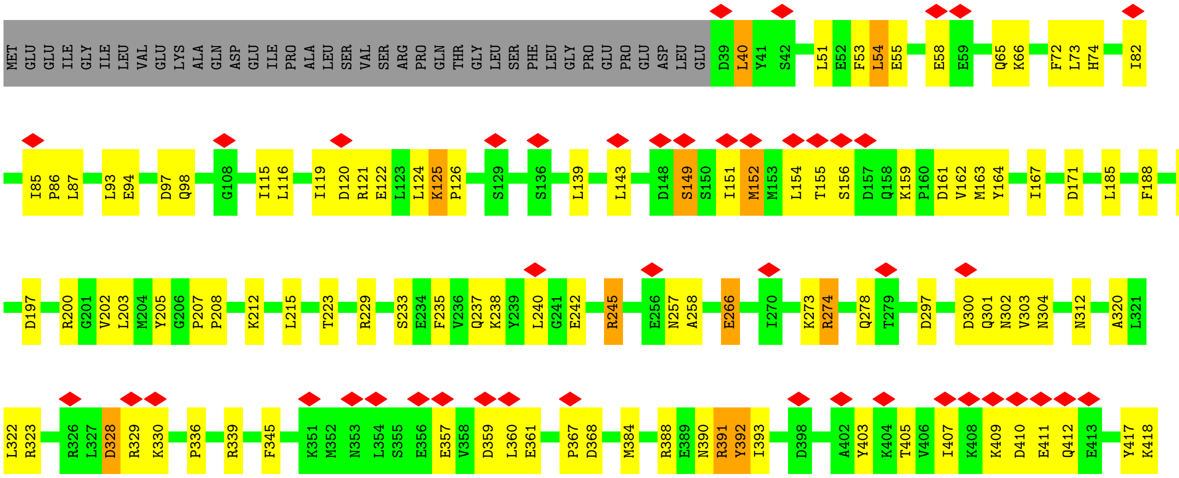
- Molecule 16: 26S protease regulatory subunit 8





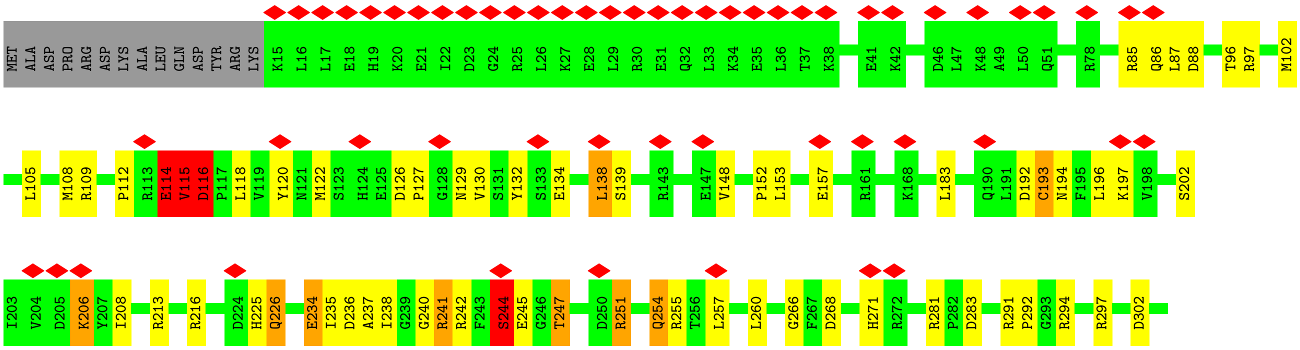
- Molecule 17: 26S protease regulatory subunit 6B

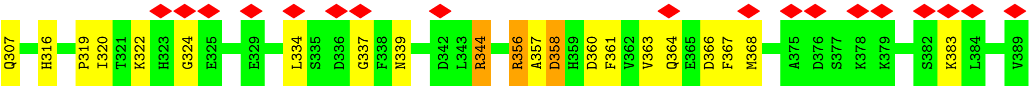
Chain K:



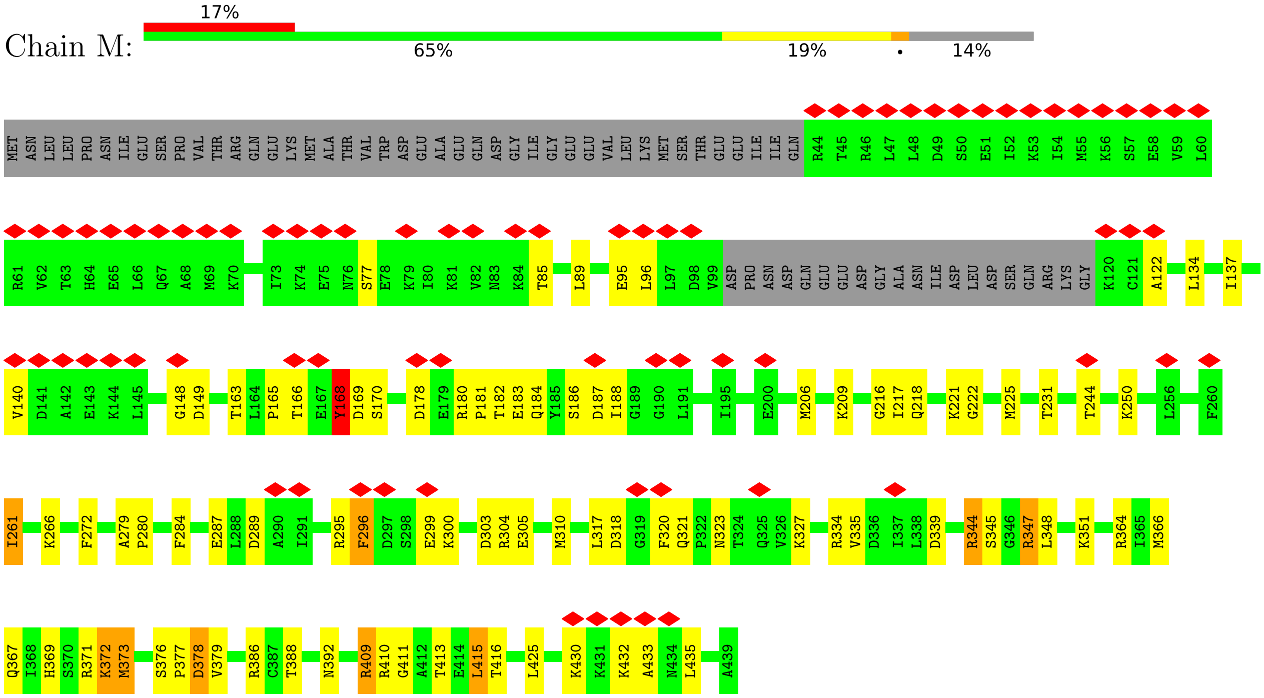
- Molecule 18: 26S protease regulatory subunit 10B

Chain L:

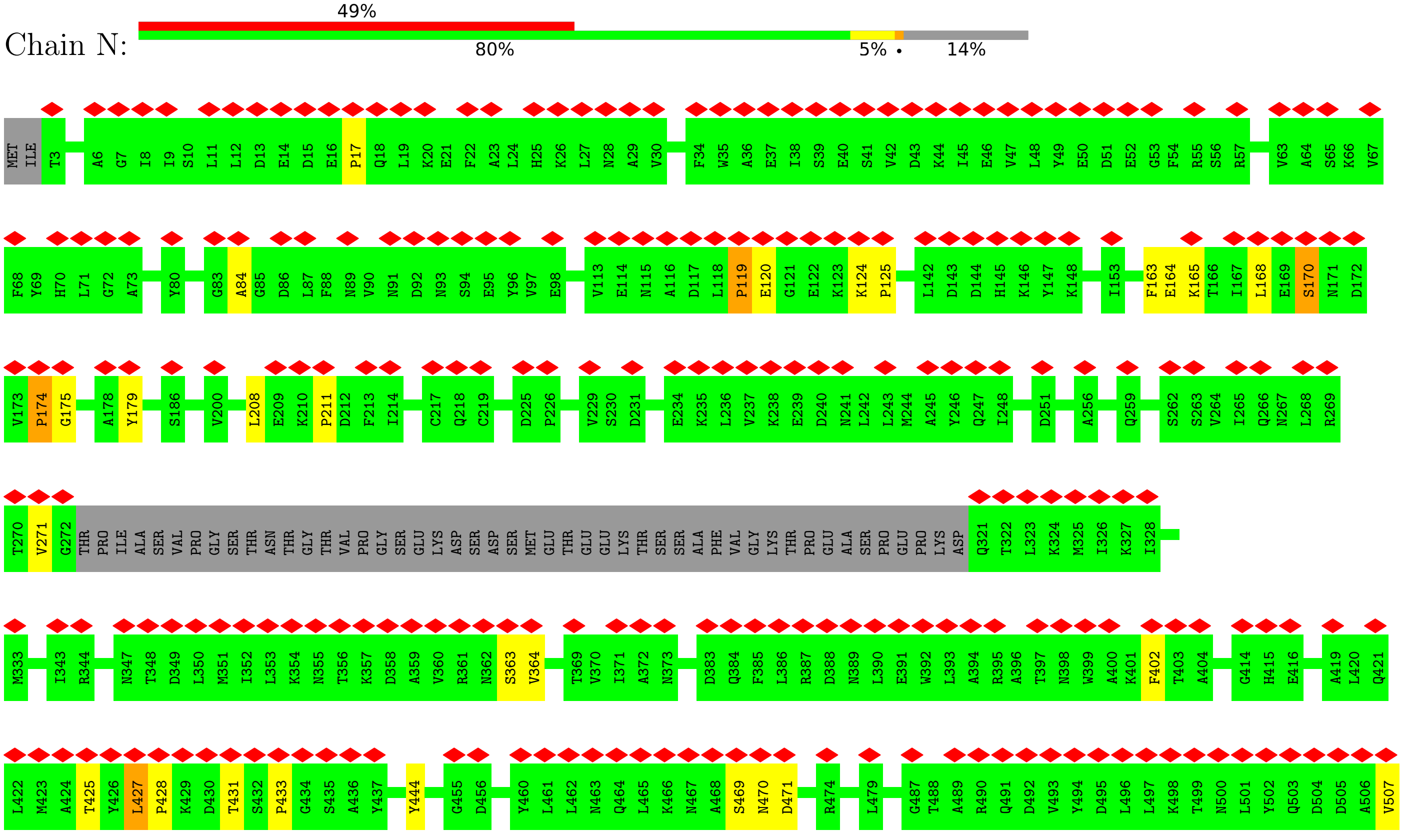


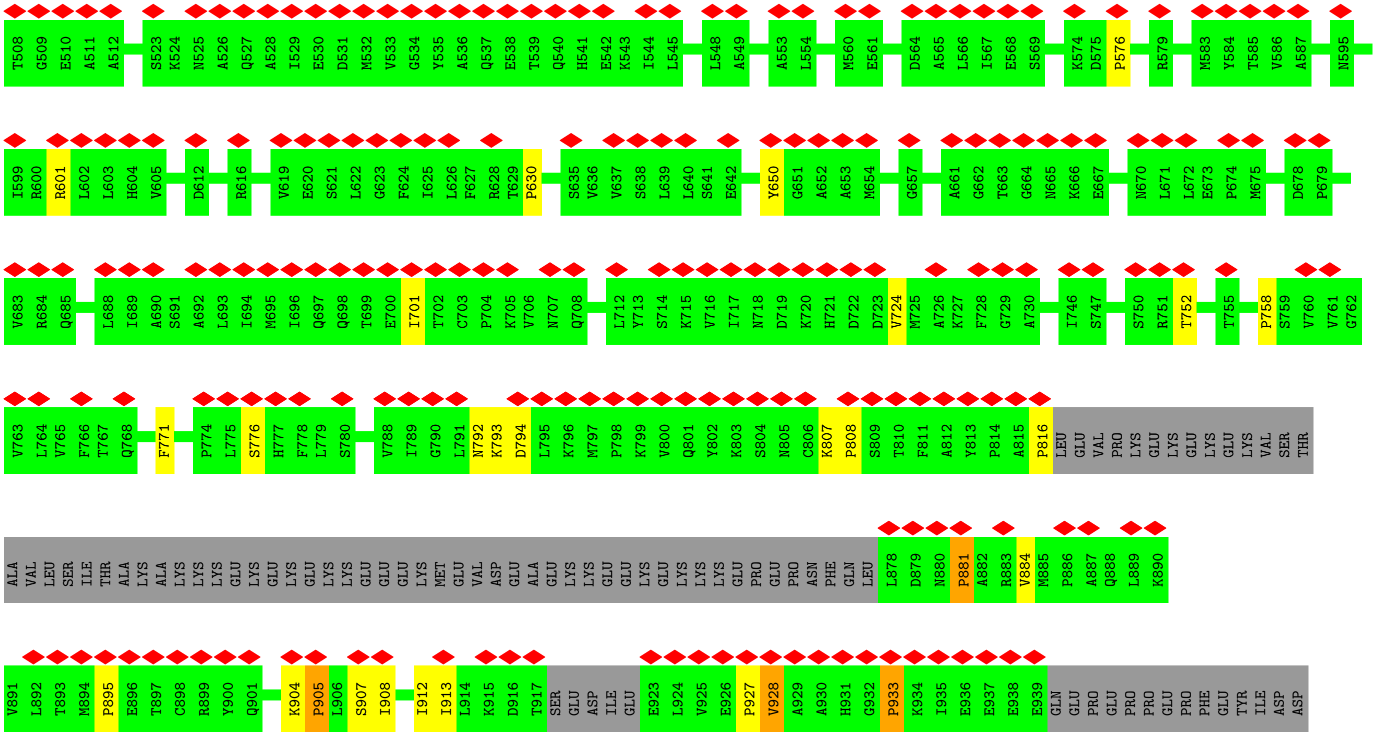


- Molecule 19: 26S protease regulatory subunit 6A

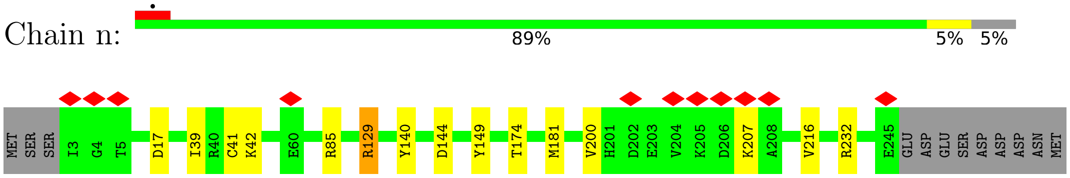


- Molecule 20: 26S proteasome non-ATPase regulatory subunit 1

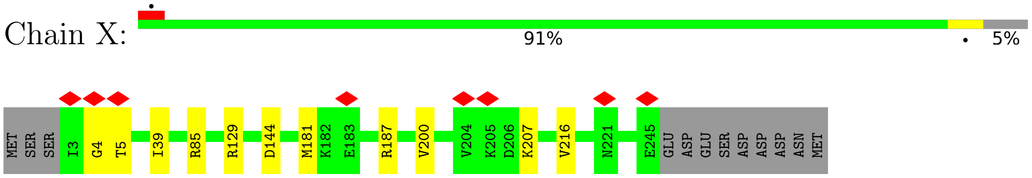




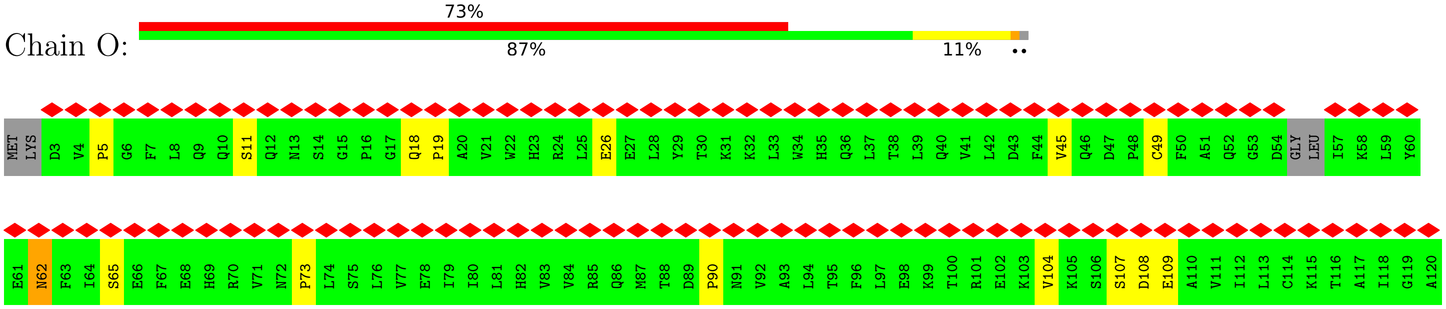
- Molecule 21: Proteasome subunit alpha type-3

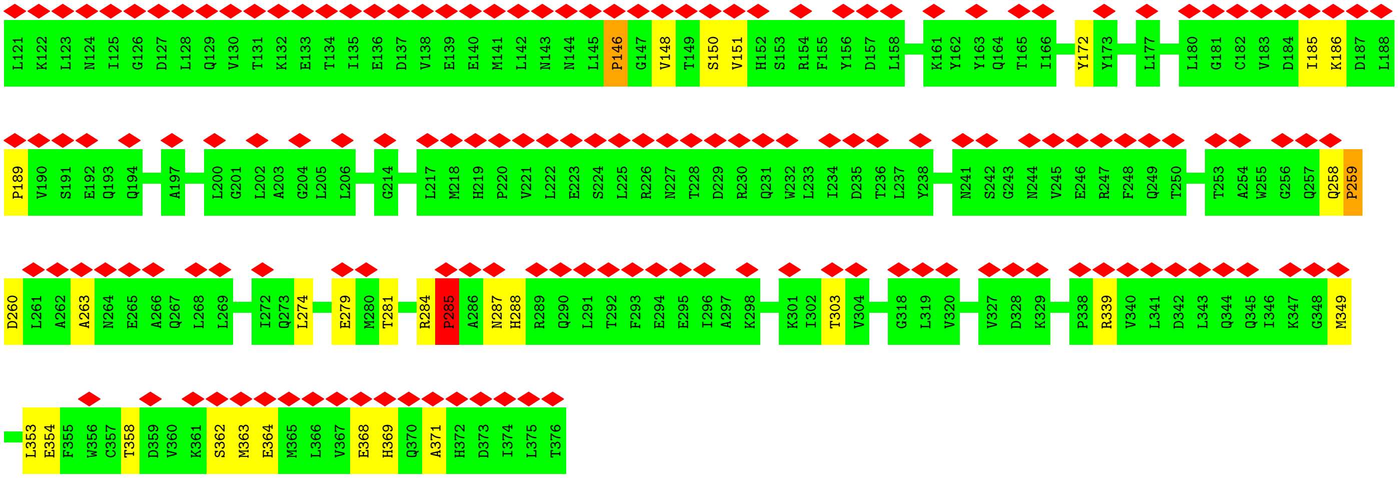


- Molecule 21: Proteasome subunit alpha type-3

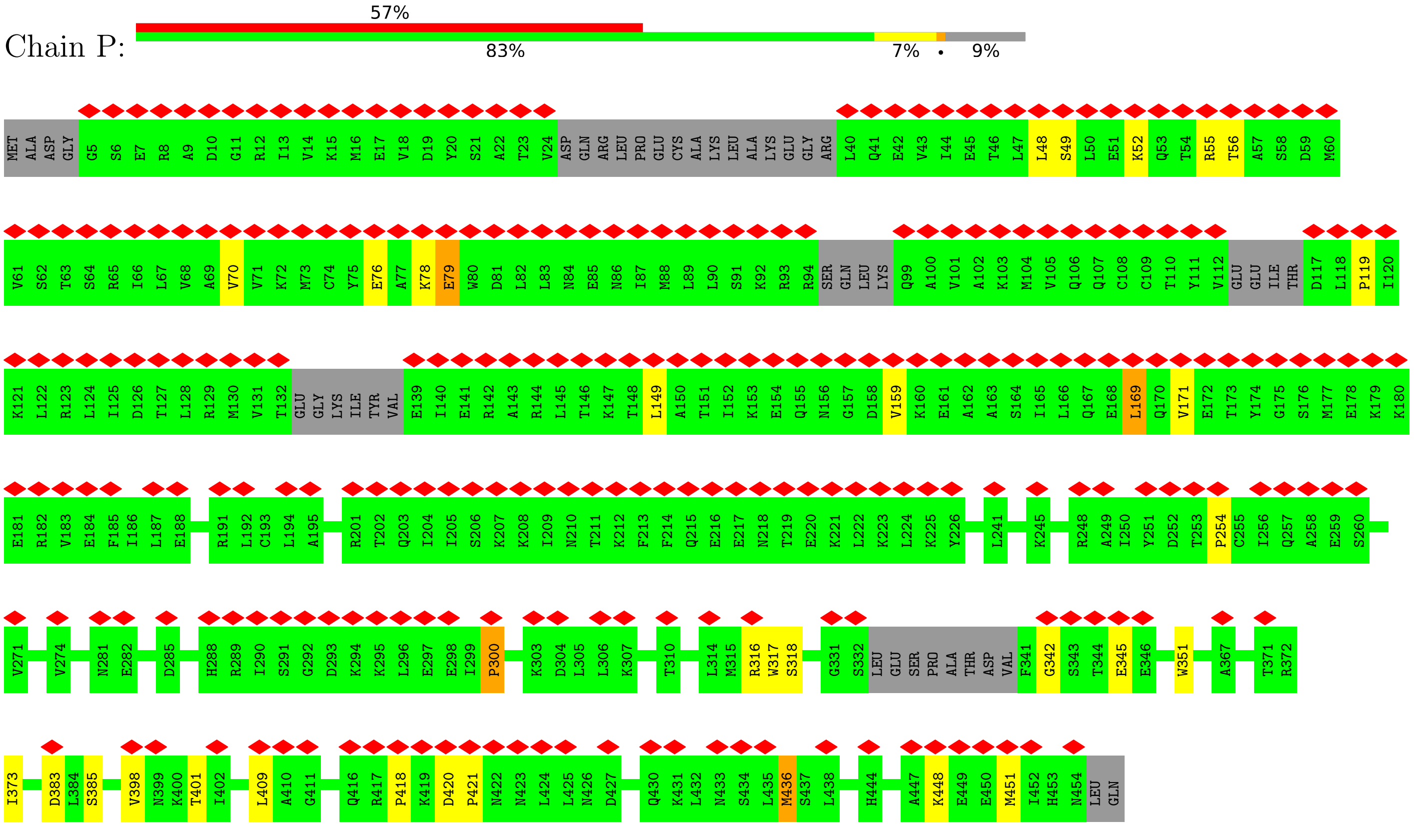


- Molecule 22: 26S proteasome non-ATPase regulatory subunit 13

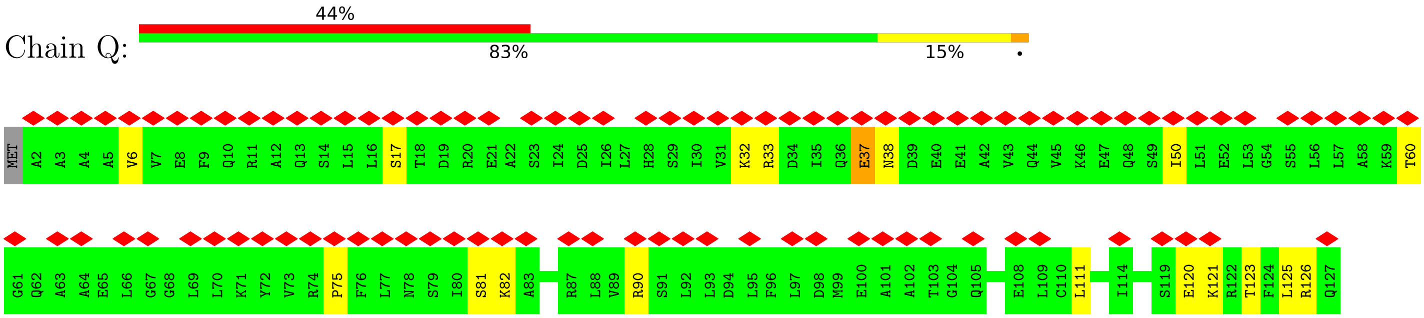


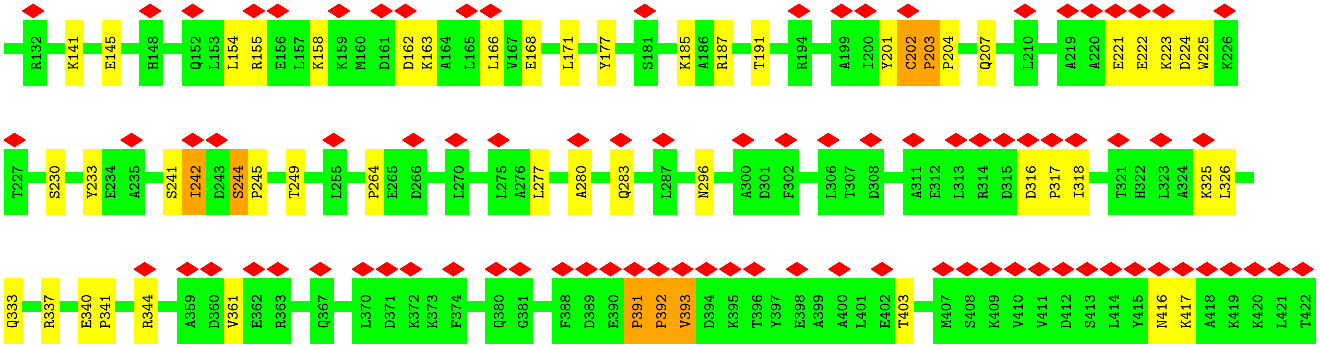


- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12



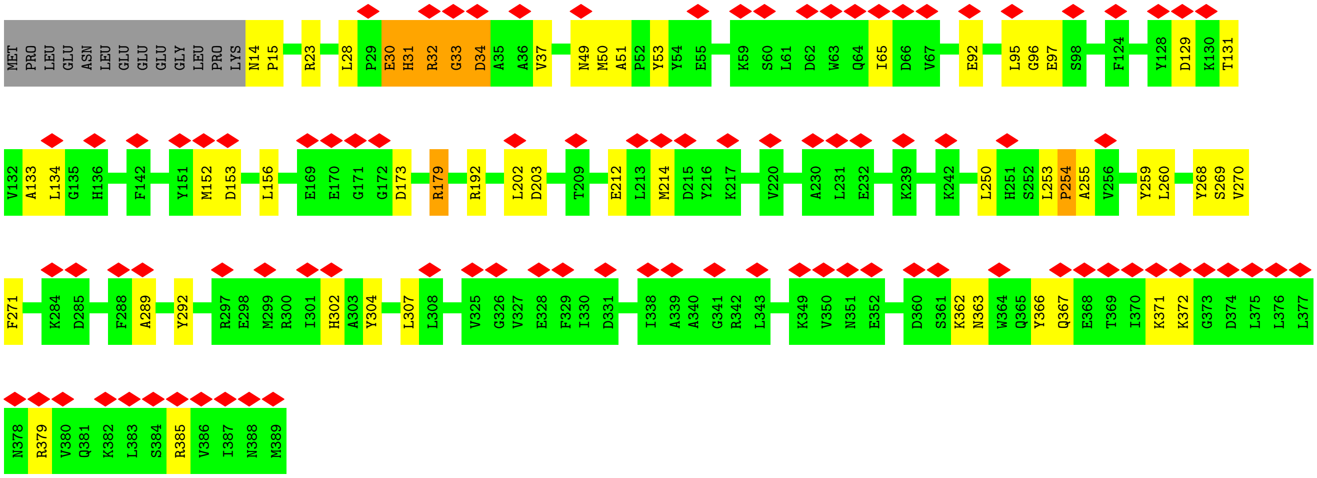
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11





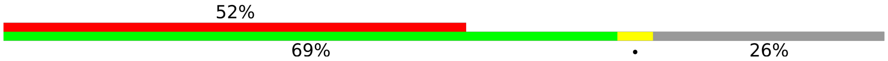
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

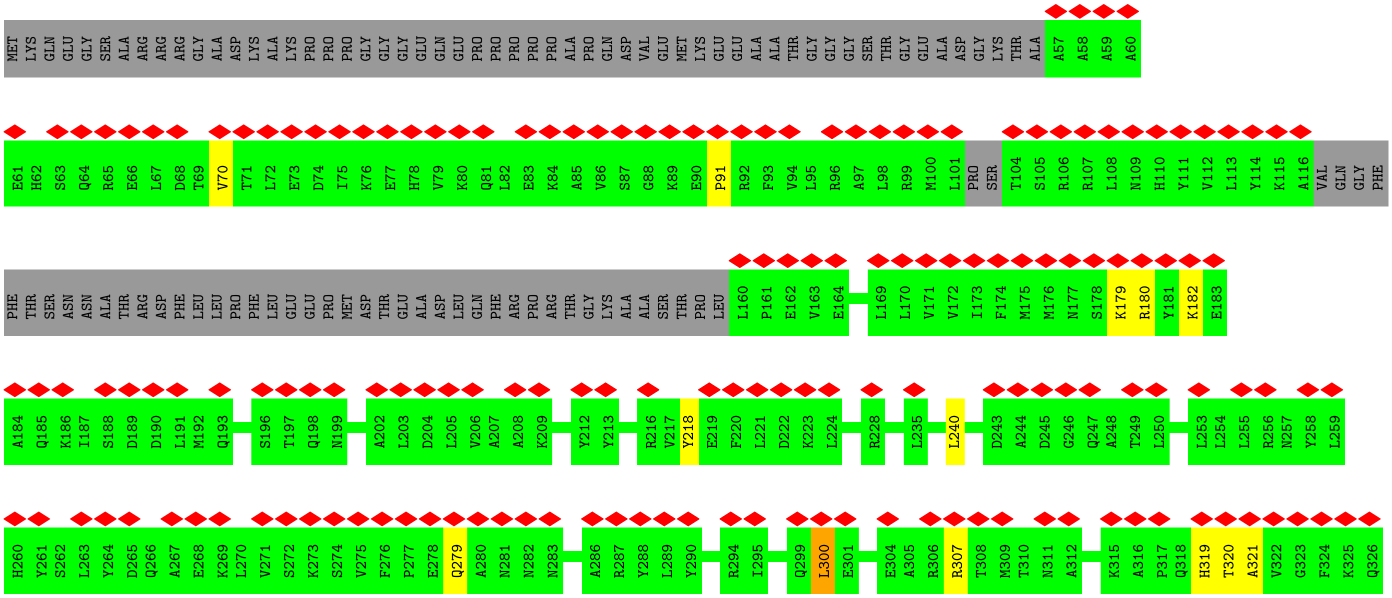
Chain R:



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

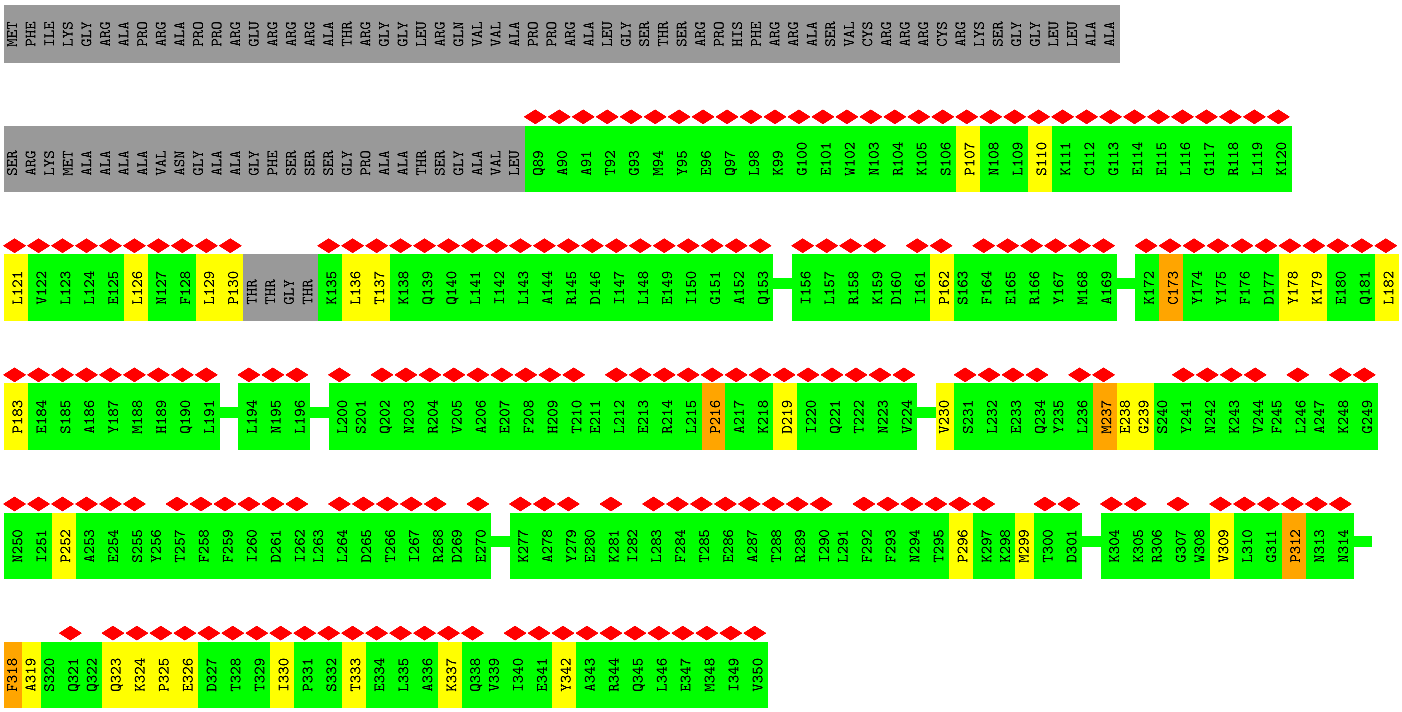
Chain S:





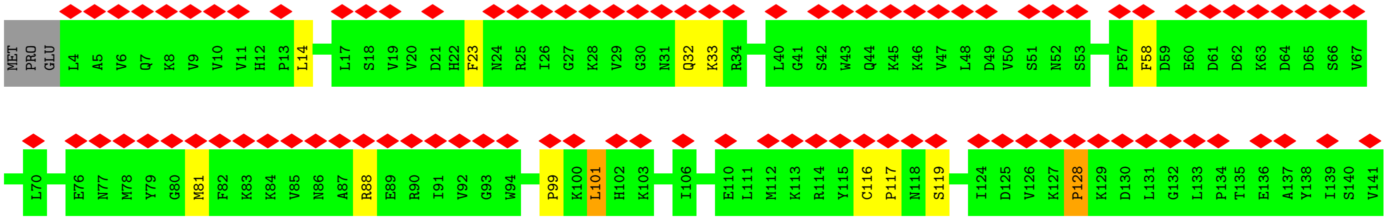
- Molecule 27: 26S proteasome non-ATPase regulatory subunit 8

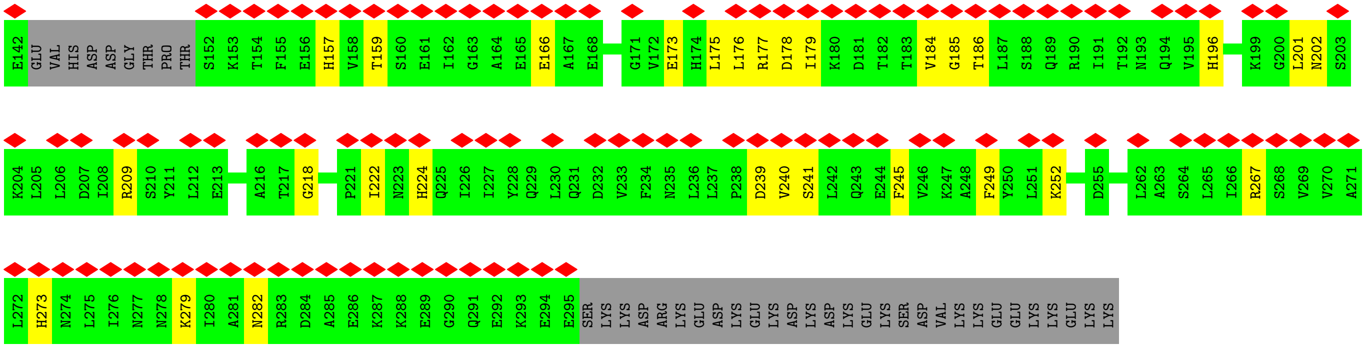
Chain T:



- Molecule 28: 26S proteasome non-ATPase regulatory subunit 7

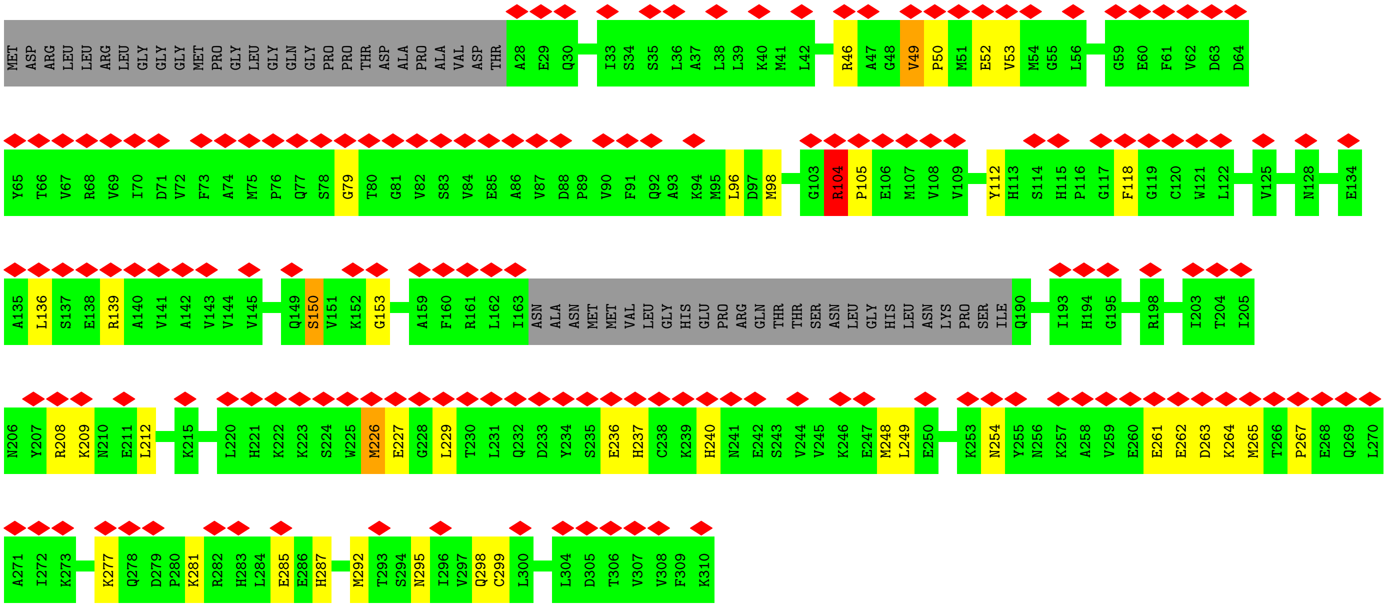
Chain U:





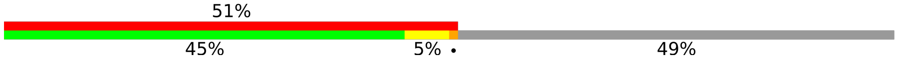
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

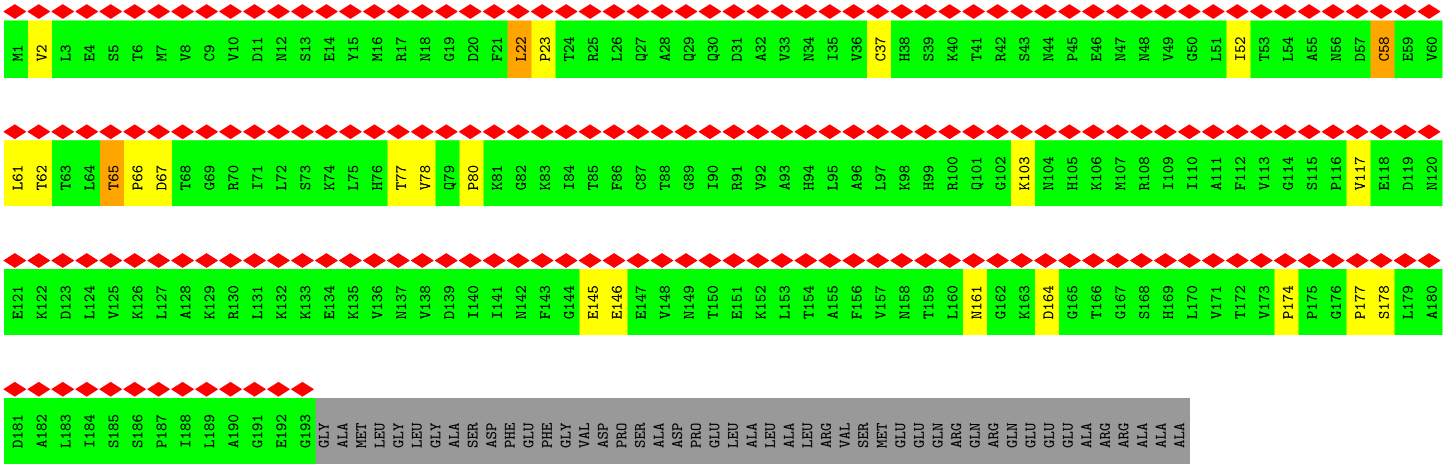
Chain V:

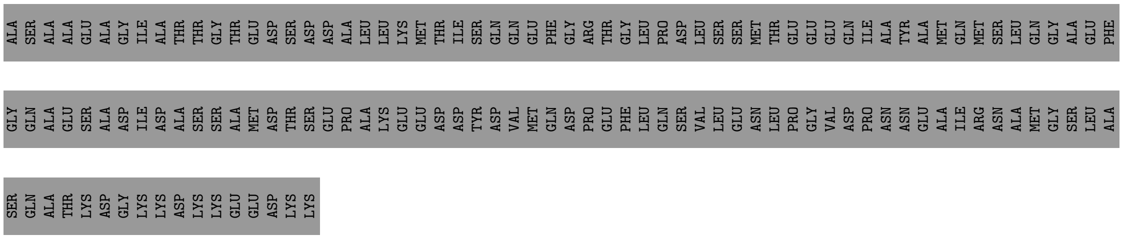


- Molecule 30: 26S proteasome non-ATPase regulatory subunit 4

Chain W:

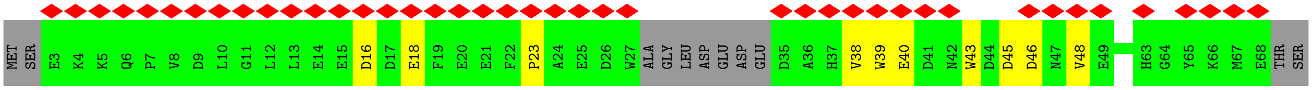






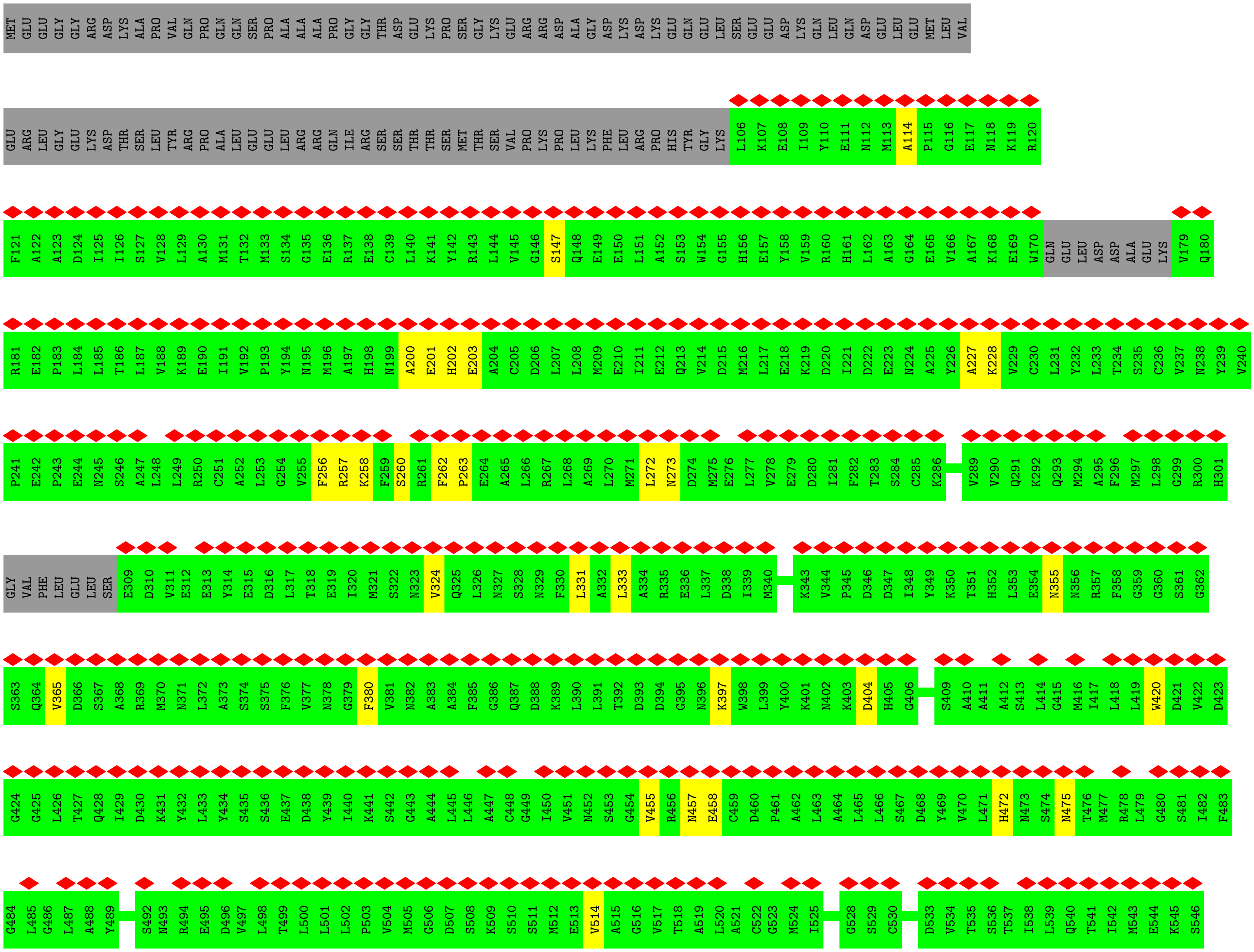
- Molecule 31: 26S proteasome complex subunit DSS1

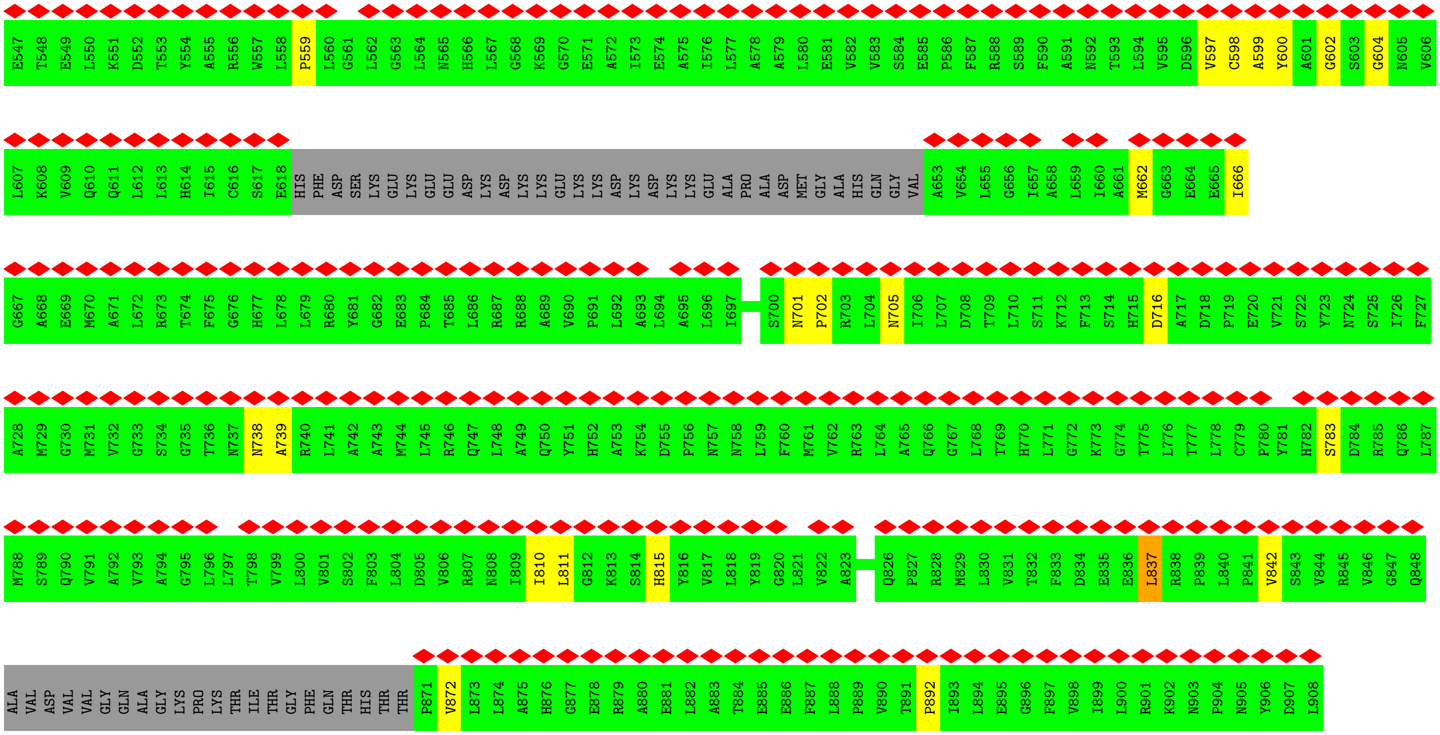
Chain Y:



- Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

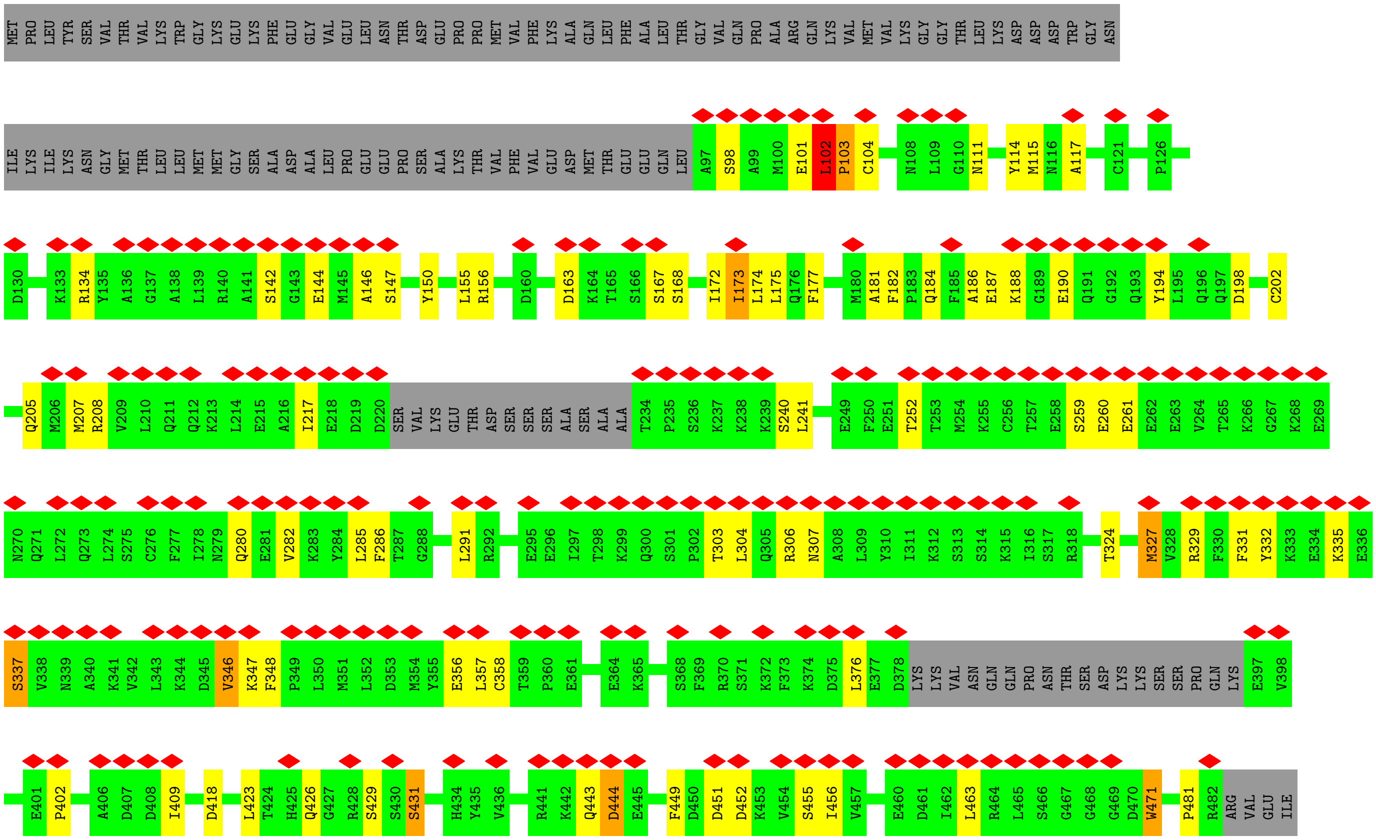
Chain Z:





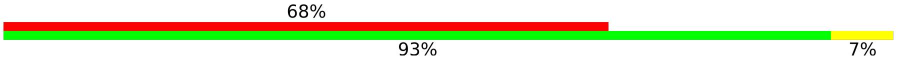
- Molecule 33: Ubiquitin carboxyl-terminal hydrolase 14

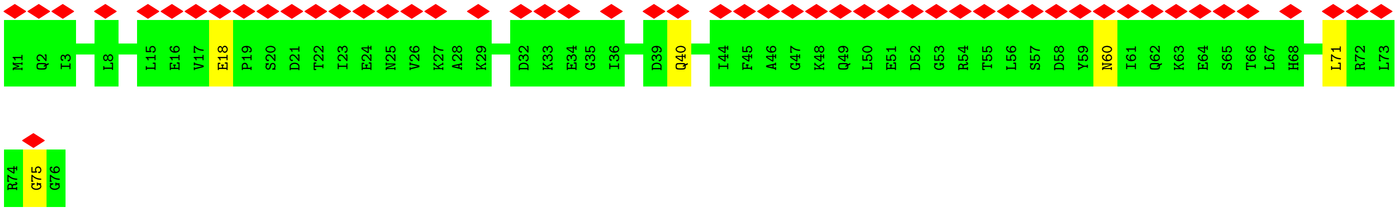
Chain x:



- Molecule 34: Polyubiquitin-B

Chain y:





4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	141293	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	37	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.171	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.033	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GLZ, 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	1.10	3/1535 (0.2%)	1.10	6/2078 (0.3%)
1	o	1.13	4/1535 (0.3%)	1.18	13/2078 (0.6%)
2	B	0.83	1/1878 (0.1%)	0.88	2/2549 (0.1%)
2	h	1.01	0/1886	1.00	2/2557 (0.1%)
3	b	0.98	0/1670	1.06	2/2265 (0.1%)
3	p	1.06	2/1670 (0.1%)	1.15	8/2265 (0.4%)
4	C	0.82	0/1742	0.89	4/2372 (0.2%)
4	i	1.11	5/1780 (0.3%)	1.10	7/2417 (0.3%)
5	c	1.08	2/1614 (0.1%)	1.11	6/2177 (0.3%)
5	q	1.21	5/1614 (0.3%)	1.19	4/2177 (0.2%)
6	D	0.81	2/1942 (0.1%)	0.89	1/2628 (0.0%)
6	j	0.99	1/1943 (0.1%)	1.04	7/2629 (0.3%)
7	d	0.99	0/1603	1.09	6/2174 (0.3%)
7	r	1.12	2/1603 (0.1%)	1.17	10/2174 (0.5%)
8	E	0.78	0/1748	0.88	5/2386 (0.2%)
8	k	0.95	2/1716 (0.1%)	1.04	5/2347 (0.2%)
9	e	1.08	2/1579 (0.1%)	1.11	7/2134 (0.3%)
9	s	1.13	4/1582 (0.3%)	1.10	6/2138 (0.3%)
10	F	0.76	0/1794	0.84	0/2430
10	l	0.95	1/1753 (0.1%)	1.01	4/2346 (0.2%)
11	f	1.03	1/1671 (0.1%)	1.05	2/2253 (0.1%)
11	t	1.08	2/1674 (0.1%)	1.14	4/2257 (0.2%)
12	G	0.77	0/1885	0.88	3/2552 (0.1%)
12	m	0.95	1/1885 (0.1%)	1.01	4/2552 (0.2%)
13	g	1.01	3/1705 (0.2%)	1.06	7/2312 (0.3%)
13	u	1.04	1/1711 (0.1%)	1.10	9/2319 (0.4%)
14	H	0.82	1/2925 (0.0%)	1.09	8/3952 (0.2%)
15	I	0.80	1/2756 (0.0%)	1.01	8/3727 (0.2%)
16	J	0.77	0/2857	0.95	4/3844 (0.1%)
17	K	0.81	1/3089 (0.0%)	0.99	7/4168 (0.2%)
18	L	0.79	4/2904 (0.1%)	1.09	12/3924 (0.3%)
19	M	0.75	0/2896	0.91	3/3912 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	N	0.41	1/5520 (0.0%)	0.60	1/7446 (0.0%)
21	X	0.83	0/1908	0.87	1/2575 (0.0%)
21	n	0.93	2/1908 (0.1%)	0.98	4/2575 (0.2%)
22	O	0.56	0/2387	0.74	3/3211 (0.1%)
23	P	0.54	0/2857	0.72	4/3855 (0.1%)
24	Q	0.62	1/2981 (0.0%)	0.76	4/4045 (0.1%)
25	R	0.65	1/2817 (0.0%)	0.80	6/3811 (0.2%)
26	S	0.57	0/2623	0.70	2/3545 (0.1%)
27	T	0.56	0/1716	0.68	3/2310 (0.1%)
28	U	0.58	0/2167	0.75	2/2936 (0.1%)
29	V	0.60	0/2047	0.83	4/2763 (0.1%)
30	W	0.52	0/1312	0.76	3/1769 (0.2%)
31	Y	0.58	0/307	0.84	1/424 (0.2%)
32	Z	0.32	0/3603	0.53	1/5005 (0.0%)
33	x	0.67	0/2860	0.90	2/3852 (0.1%)
34	y	0.60	0/603	0.75	0/811
All	All	0.83	56/99761 (0.1%)	0.94	217/135026 (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
3	b	0	2
4	i	0	1
6	j	0	1
7	r	0	1
14	H	0	1
15	I	0	4
16	J	0	1
17	K	0	1
18	L	0	4
19	M	0	2
20	N	0	3
22	O	0	2
23	P	0	2
24	Q	0	6
25	R	0	5
27	T	0	1
28	U	0	1
29	V	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
30	W	0	7
31	Y	0	2
32	Z	0	7
34	y	0	2
All	All	0	59

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	q	155	GLU	CD-OE2	13.15	1.40	1.25
18	L	116	ASP	N-CA	-10.28	1.25	1.46
4	i	22	GLU	CG-CD	8.89	1.65	1.51
3	p	81	ARG	CZ-NH2	8.66	1.44	1.33
5	c	164	PHE	CG-CD1	-8.04	1.26	1.38
6	D	70	GLU	CG-CD	7.97	1.64	1.51
1	a	61	TYR	CB-CG	7.67	1.63	1.51
14	H	133	ASP	CB-CG	7.06	1.66	1.51
13	u	62	TYR	CB-CG	-6.95	1.41	1.51
18	L	115	VAL	CA-CB	-6.94	1.40	1.54
6	j	70	GLU	CG-CD	6.86	1.62	1.51
24	Q	163	LYS	N-CA	-6.79	1.32	1.46
9	s	177	TYR	CE2-CZ	6.56	1.47	1.38
1	o	44	CYS	CB-SG	-6.38	1.71	1.82
15	I	142	ASP	CB-CG	6.30	1.65	1.51
11	f	104	TYR	CE1-CZ	-6.15	1.30	1.38
8	k	67	ASP	CB-CG	6.15	1.64	1.51
1	a	61	TYR	CG-CD1	6.05	1.47	1.39
4	i	127	ARG	CZ-NH1	5.98	1.40	1.33
13	g	62	TYR	CE1-CZ	5.96	1.46	1.38
5	q	155	GLU	CG-CD	5.88	1.60	1.51
6	D	70	GLU	CB-CG	5.83	1.63	1.52
1	a	143	TYR	CG-CD2	5.81	1.46	1.39
12	m	128	TYR	CG-CD2	-5.80	1.31	1.39
9	e	134	TYR	CG-CD2	-5.78	1.31	1.39
1	o	13	VAL	C-O	-5.77	1.12	1.23
5	c	129	CYS	CB-SG	5.75	1.92	1.82
1	o	143	TYR	CG-CD2	5.65	1.46	1.39
9	s	161	TYR	CE1-CZ	5.65	1.45	1.38
9	e	55	TRP	CB-CG	-5.63	1.40	1.50
10	l	217	LEU	N-CA	-5.63	1.35	1.46
7	r	147	TYR	CG-CD1	-5.61	1.31	1.39
8	k	153	TYR	CG-CD2	-5.59	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	t	53	GLY	CA-C	5.51	1.60	1.51
2	B	159	TYR	CE1-CZ	5.49	1.45	1.38
5	q	28	PHE	C-O	5.45	1.33	1.23
11	t	5	TYR	CG-CD1	-5.45	1.32	1.39
21	n	149	TYR	CE1-CZ	5.42	1.45	1.38
17	K	235	PHE	CG-CD1	5.39	1.46	1.38
5	q	136	PHE	CB-CG	-5.39	1.42	1.51
7	r	56	PHE	CB-CG	-5.38	1.42	1.51
1	o	83	PHE	CG-CD1	-5.33	1.30	1.38
21	n	140	TYR	CE1-CZ	5.24	1.45	1.38
4	i	144	TYR	CE2-CZ	5.23	1.45	1.38
9	s	125	THR	CB-CG2	5.22	1.69	1.52
9	s	177	TYR	CG-CD1	5.20	1.46	1.39
18	L	114	GLU	CD-OE2	-5.20	1.20	1.25
13	g	97	TYR	CE1-CZ	5.20	1.45	1.38
3	p	42	TYR	CE1-CZ	5.15	1.45	1.38
13	g	91	TRP	CB-CG	-5.14	1.41	1.50
5	q	43	PHE	CG-CD2	-5.12	1.31	1.38
4	i	144	TYR	CG-CD1	5.06	1.45	1.39
4	i	146	PHE	CG-CD1	5.03	1.46	1.38
18	L	115	VAL	N-CA	5.02	1.56	1.46
20	N	428	PRO	N-CD	5.01	1.54	1.47
25	R	33	GLY	C-O	5.01	1.31	1.23

All (217) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	115	VAL	CA-C-N	-22.22	68.32	117.20
14	H	336	ARG	NE-CZ-NH1	-21.51	109.54	120.30
18	L	115	VAL	C-N-CA	-18.03	76.64	121.70
14	H	336	ARG	NE-CZ-NH2	16.39	128.50	120.30
17	K	200	ARG	NE-CZ-NH1	14.57	127.59	120.30
17	K	200	ARG	NE-CZ-NH2	-13.07	113.76	120.30
23	P	420	ASP	C-N-CD	-11.98	94.25	120.60
22	O	62	ASN	O-C-N	-11.76	103.88	122.70
29	V	139	ARG	NE-CZ-NH2	-11.62	114.49	120.30
18	L	115	VAL	O-C-N	10.84	140.04	122.70
21	n	129	ARG	NE-CZ-NH2	-10.64	114.98	120.30
19	M	168	TYR	CB-CA-C	-10.51	89.39	110.40
7	d	28	MET	CG-SD-CE	-9.65	84.76	100.20
29	V	139	ARG	NE-CZ-NH1	9.30	124.95	120.30
9	e	59	LEU	CB-CG-CD2	9.21	126.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	g	179	ARG	NE-CZ-NH1	9.04	124.82	120.30
5	q	70	ARG	NE-CZ-NH2	-9.01	115.80	120.30
4	i	127	ARG	NE-CZ-NH2	-8.89	115.86	120.30
6	j	128	ARG	NE-CZ-NH2	-8.88	115.86	120.30
15	I	142	ASP	CB-CG-OD1	8.57	126.02	118.30
5	c	70	ARG	NE-CZ-NH2	-8.56	116.02	120.30
8	k	125	ARG	NE-CZ-NH2	-8.17	116.21	120.30
12	m	100	ASP	CB-CG-OD1	-8.14	110.97	118.30
13	u	179	ARG	NE-CZ-NH1	8.01	124.30	120.30
13	u	86	ARG	NE-CZ-NH2	-7.99	116.30	120.30
10	l	135	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	o	166	ARG	NE-CZ-NH1	7.96	124.28	120.30
15	I	408	ARG	NE-CZ-NH1	7.95	124.27	120.30
9	s	42	LEU	CB-CG-CD2	7.84	124.34	111.00
2	B	132	ARG	NE-CZ-NH2	-7.84	116.38	120.30
14	H	315	ILE	N-CA-C	-7.78	90.00	111.00
30	W	52	ILE	CB-CA-C	-7.69	96.21	111.60
17	K	40	LEU	CB-CG-CD1	7.59	123.91	111.00
8	k	153	TYR	CB-CG-CD1	7.57	125.54	121.00
7	r	140	LEU	CB-CG-CD2	7.52	123.78	111.00
7	r	85	ARG	NE-CZ-NH2	-7.45	116.57	120.30
3	p	89	ARG	NE-CZ-NH1	7.43	124.01	120.30
14	H	339	ARG	NE-CZ-NH2	-7.41	116.59	120.30
7	r	44	LEU	CB-CG-CD1	-7.29	98.61	111.00
3	p	86	MET	CB-CG-SD	7.28	134.25	112.40
24	Q	391	PRO	N-CA-CB	7.08	111.80	103.30
24	Q	75	PRO	N-CA-CB	7.08	111.79	103.30
21	n	232	ARG	NE-CZ-NH1	7.06	123.83	120.30
25	R	33	GLY	N-CA-C	-7.02	95.56	113.10
1	o	189	LEU	CB-CG-CD1	-7.00	99.10	111.00
6	D	70	GLU	OE1-CD-OE2	-6.98	114.92	123.30
6	j	49	ARG	NE-CZ-NH1	-6.92	116.84	120.30
22	O	285	PRO	N-CA-CB	6.91	111.59	103.30
1	a	89	ARG	NE-CZ-NH1	6.91	123.75	120.30
25	R	129	ASP	CB-CG-OD1	6.88	124.49	118.30
1	a	94	LEU	CB-CG-CD2	6.87	122.69	111.00
3	p	51	ASP	CB-CG-OD1	6.85	124.47	118.30
7	r	104	LEU	CB-CG-CD1	-6.83	99.39	111.00
15	I	394	ASP	CB-CG-OD2	6.83	124.44	118.30
13	u	166	ARG	NE-CZ-NH2	-6.81	116.90	120.30
9	s	54	PHE	CB-CG-CD2	-6.80	116.04	120.80
15	I	325	VAL	N-CA-C	-6.72	92.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	U	14	LEU	CB-CG-CD2	6.72	122.43	111.00
3	p	81	ARG	NE-CZ-NH1	-6.72	116.94	120.30
18	L	251	ARG	NE-CZ-NH1	-6.71	116.94	120.30
14	H	265	ARG	NE-CZ-NH1	6.67	123.64	120.30
21	n	85	ARG	NE-CZ-NH2	-6.63	116.99	120.30
13	u	151	ARG	NE-CZ-NH2	-6.62	116.99	120.30
3	b	167	LEU	CB-CG-CD1	6.55	122.13	111.00
1	a	29	ARG	NE-CZ-NH2	-6.50	117.05	120.30
32	Z	201	GLU	N-CA-CB	-6.50	98.89	110.60
15	I	102	LEU	CB-CG-CD1	-6.50	99.95	111.00
15	I	165	ASP	CB-CG-OD1	6.34	124.01	118.30
18	L	148	VAL	CB-CA-C	6.33	123.42	111.40
19	M	169	ASP	N-CA-C	6.33	128.08	111.00
13	u	151	ARG	NE-CZ-NH1	6.33	123.46	120.30
27	T	121	LEU	CB-CG-CD2	-6.23	100.40	111.00
9	s	180	ARG	NE-CZ-NH2	6.23	123.41	120.30
4	i	112	ARG	NE-CZ-NH1	6.21	123.41	120.30
18	L	294	ARG	NE-CZ-NH1	6.21	123.40	120.30
5	c	70	ARG	NE-CZ-NH1	6.17	123.39	120.30
21	n	129	ARG	NE-CZ-NH1	6.15	123.38	120.30
11	t	173	ARG	NE-CZ-NH2	-6.13	117.24	120.30
7	d	140	LEU	CB-CG-CD2	6.12	121.41	111.00
8	k	86	ARG	NE-CZ-NH2	-6.11	117.24	120.30
9	s	107	ARG	NE-CZ-NH1	6.10	123.35	120.30
18	L	356	ARG	NE-CZ-NH1	6.08	123.34	120.30
4	i	55	LEU	CB-CG-CD2	-6.08	100.67	111.00
22	O	259	PRO	N-CA-CB	6.07	110.59	103.30
3	p	58	LEU	CB-CG-CD1	-6.05	100.71	111.00
14	H	91	GLN	C-N-CD	6.05	141.10	128.40
4	i	88	ARG	NE-CZ-NH1	6.03	123.32	120.30
8	k	66	ASP	CB-CG-OD2	6.03	123.73	118.30
4	C	127	ARG	NE-CZ-NH2	-6.02	117.29	120.30
20	N	427	LEU	C-N-CD	6.02	141.04	128.40
1	o	186	ARG	NE-CZ-NH2	-5.98	117.31	120.30
11	f	60	ASP	CB-CG-OD2	-5.97	112.92	118.30
15	I	263	GLY	C-N-CD	-5.97	107.46	120.60
15	I	346	ARG	NE-CZ-NH1	5.97	123.28	120.30
16	J	374	ARG	NE-CZ-NH1	5.97	123.28	120.30
25	R	179	ARG	NE-CZ-NH1	5.94	123.27	120.30
6	j	8	ARG	NE-CZ-NH2	-5.93	117.34	120.30
9	e	158	ARG	NE-CZ-NH2	-5.92	117.34	120.30
18	L	236	ASP	CB-CG-OD2	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	u	86	ARG	NE-CZ-NH1	5.89	123.24	120.30
7	d	85	ARG	NE-CZ-NH2	-5.88	117.36	120.30
7	r	52	ASP	CB-CG-OD2	-5.87	113.01	118.30
7	d	115	LEU	CB-CG-CD1	-5.85	101.05	111.00
8	k	153	TYR	CB-CG-CD2	-5.82	117.51	121.00
29	V	249	LEU	CB-CG-CD1	-5.82	101.11	111.00
7	r	104	LEU	CB-CG-CD2	5.81	120.87	111.00
1	o	29	ARG	NE-CZ-NH2	-5.80	117.40	120.30
8	E	144	LEU	CB-CG-CD2	5.79	120.84	111.00
3	b	51	ASP	CB-CG-OD1	5.78	123.50	118.30
1	a	40	ARG	NE-CZ-NH1	5.77	123.19	120.30
16	J	311	ILE	N-CA-C	-5.77	95.41	111.00
8	E	125	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	o	44	CYS	CA-CB-SG	-5.77	103.61	114.00
28	U	81	MET	CG-SD-CE	5.74	109.38	100.20
1	a	100	ILE	CG1-CB-CG2	-5.73	98.79	111.40
16	J	325	ARG	NE-CZ-NH2	-5.73	117.43	120.30
33	x	102	LEU	N-CA-C	5.71	126.43	111.00
4	i	9	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	o	25	TYR	CB-CG-CD1	-5.71	117.58	121.00
17	K	245	ARG	NE-CZ-NH2	-5.69	117.45	120.30
10	l	135	ARG	NE-CZ-NH2	-5.68	117.46	120.30
23	P	79	GLU	N-CA-CB	-5.67	100.39	110.60
9	s	101	ILE	CG1-CB-CG2	-5.67	98.92	111.40
5	c	164	PHE	CB-CG-CD2	5.66	124.76	120.80
1	o	55	VAL	CG1-CB-CG2	-5.63	101.89	110.90
8	E	86	ARG	NE-CZ-NH2	-5.63	117.49	120.30
5	c	25	ASP	CB-CG-OD2	-5.62	113.24	118.30
30	W	65	THR	N-CA-C	5.62	126.18	111.00
18	L	297	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	o	51	ASP	CB-CG-OD2	-5.61	113.25	118.30
9	e	158	ARG	NE-CZ-NH1	5.61	123.11	120.30
12	m	128	TYR	CB-CG-CD1	5.60	124.36	121.00
3	p	174	ASP	CB-CG-OD1	5.60	123.34	118.30
26	S	91	PRO	N-CA-CB	5.59	110.01	103.30
18	L	297	ARG	NE-CZ-NH1	5.58	123.09	120.30
6	j	8	ARG	NE-CZ-NH1	5.58	123.09	120.30
12	m	125	ARG	NE-CZ-NH1	5.57	123.08	120.30
7	r	181	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	a	166	ARG	NE-CZ-NH1	5.53	123.07	120.30
17	K	54	LEU	CB-CG-CD1	5.51	120.37	111.00
2	h	103	TYR	CB-CG-CD2	-5.51	117.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	91	LYS	CD-CE-NZ	5.50	124.34	111.70
13	g	174	ARG	NE-CZ-NH1	5.49	123.04	120.30
29	V	104	ARG	NE-CZ-NH1	5.48	123.04	120.30
9	e	14	VAL	CG1-CB-CG2	-5.47	102.15	110.90
3	p	22	GLU	CA-CB-CG	5.47	125.43	113.40
1	o	166	ARG	CD-NE-CZ	5.46	131.24	123.60
6	j	44	LEU	CA-CB-CG	5.45	127.84	115.30
10	l	48	LEU	CB-CG-CD1	-5.45	101.74	111.00
24	Q	33	ARG	N-CA-C	5.45	125.70	111.00
7	d	28	MET	CB-CG-SD	5.43	128.68	112.40
25	R	31	HIS	N-CA-C	-5.42	96.36	111.00
25	R	96	GLY	N-CA-C	-5.41	99.57	113.10
10	l	33	LEU	CB-CG-CD1	5.40	120.19	111.00
9	e	107	ARG	CG-CD-NE	5.39	123.13	111.80
13	g	174	ARG	NE-CZ-NH2	-5.39	117.61	120.30
2	B	159	TYR	CB-CA-C	-5.39	99.62	110.40
12	G	101	ARG	NE-CZ-NH1	5.38	122.99	120.30
9	e	86	MET	CG-SD-CE	5.37	108.78	100.20
1	o	94	LEU	CB-CG-CD2	5.37	120.12	111.00
27	T	252	PRO	N-CA-CB	5.36	109.74	103.30
1	o	99	ILE	CG1-CB-CG2	-5.36	99.61	111.40
4	C	83	ARG	NE-CZ-NH2	5.35	122.98	120.30
30	W	58	CYS	CA-CB-SG	-5.34	104.39	114.00
17	K	116	LEU	CB-CG-CD2	-5.34	101.93	111.00
13	u	127	MET	CG-SD-CE	-5.32	91.68	100.20
13	g	76	LEU	CB-CG-CD2	5.32	120.04	111.00
6	j	124	PHE	CB-CG-CD1	-5.32	117.08	120.80
4	i	22	GLU	OE1-CD-OE2	-5.32	116.92	123.30
11	f	194	ARG	NE-CZ-NH2	-5.31	117.64	120.30
13	g	128	LEU	CB-CG-CD1	5.31	120.02	111.00
33	x	103	PRO	N-CA-C	5.30	125.87	112.10
13	g	96	MET	CG-SD-CE	-5.29	91.73	100.20
7	d	45	LEU	CA-CB-CG	5.28	127.45	115.30
23	P	448	LYS	CD-CE-NZ	5.28	123.85	111.70
7	r	90	ASP	CB-CG-OD1	5.27	123.05	118.30
8	E	109	ARG	NE-CZ-NH1	5.27	122.93	120.30
2	h	219	VAL	CG1-CB-CG2	5.26	119.32	110.90
31	Y	23	PRO	N-CA-CB	5.25	109.60	103.30
11	t	99	ARG	NE-CZ-NH2	-5.25	117.68	120.30
8	E	96	LEU	CA-CB-CG	5.23	127.33	115.30
12	G	82	ARG	NE-CZ-NH2	-5.23	117.69	120.30
14	H	336	ARG	CG-CD-NE	5.19	122.70	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	J	198	LEU	CB-CG-CD2	5.19	119.83	111.00
27	T	173	CYS	CA-CB-SG	-5.19	104.67	114.00
19	M	347	ARG	NE-CZ-NH1	5.18	122.89	120.30
18	L	344	ARG	NE-CZ-NH1	5.17	122.89	120.30
5	q	69	PHE	CB-CG-CD2	-5.15	117.20	120.80
11	t	94	THR	CA-CB-CG2	-5.15	105.20	112.40
7	r	124	LEU	CB-CG-CD1	-5.14	102.26	111.00
5	q	12	MET	CB-CG-SD	-5.14	96.99	112.40
9	s	26	ILE	CG1-CB-CG2	-5.14	100.10	111.40
7	r	43	LEU	CB-CG-CD2	5.11	119.69	111.00
23	P	436	MET	CG-SD-CE	5.11	108.37	100.20
13	g	88	ILE	CG1-CB-CG2	-5.10	100.18	111.40
14	H	224	LEU	CB-CG-CD1	-5.10	102.33	111.00
18	L	291	ARG	NE-CZ-NH1	5.09	122.85	120.30
4	C	83	ARG	NE-CZ-NH1	-5.09	117.76	120.30
26	S	240	LEU	CB-CG-CD1	-5.09	102.35	111.00
4	i	145	LEU	CB-CG-CD2	5.08	119.64	111.00
21	X	85	ARG	NE-CZ-NH1	5.07	122.84	120.30
5	c	164	PHE	CB-CG-CD1	-5.07	117.25	120.80
6	j	128	ARG	NE-CZ-NH1	5.07	122.83	120.30
11	t	149	LEU	CB-CG-CD2	5.06	119.60	111.00
24	Q	203	PRO	CA-N-CD	-5.05	104.42	111.50
13	u	128	LEU	CB-CG-CD2	-5.05	102.41	111.00
13	u	35	ARG	NE-CZ-NH2	-5.05	117.78	120.30
3	p	212	LEU	CB-CG-CD1	-5.05	102.42	111.00
5	c	87	LEU	CB-CG-CD1	5.04	119.56	111.00
5	q	58	THR	CA-CB-CG2	-5.03	105.35	112.40
17	K	215	LEU	CB-CG-CD1	-5.03	102.45	111.00
9	e	73	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	o	125	PHE	CB-CG-CD2	-5.03	117.28	120.80
12	m	107	ARG	NE-CZ-NH2	-5.02	117.79	120.30
12	G	51	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	o	19	ARG	NE-CZ-NH2	-5.01	117.80	120.30
25	R	34	ASP	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	H	154	PRO	Peptide
15	I	105	THR	Peptide
15	I	137	SER	Peptide

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Mol	Chain	Res	Type	Group
15	I	299	SER	Peptide,Mainchain
16	J	242	ALA	Peptide
17	K	149	SER	Peptide
18	L	115	VAL	Mainchain
18	L	226	GLN	Peptide,Mainchain
18	L	244	SER	Peptide
19	M	279	ALA	Peptide,Mainchain
20	N	208	LEU	Peptide
20	N	724	VAL	Peptide
20	N	807	LYS	Peptide
22	O	285	PRO	Peptide
22	O	62	ASN	Mainchain
23	P	78	LYS	Peptide,Mainchain
24	Q	162	ASP	Peptide
24	Q	202	CYS	Peptide,Mainchain
24	Q	32	LYS	Peptide,Mainchain
24	Q	37	GLU	Peptide
25	R	14	ASN	Peptide
25	R	30	GLU	Peptide
25	R	32	ARG	Peptide
25	R	33	GLY	Peptide
25	R	95	LEU	Peptide
27	T	318	PHE	Peptide
28	U	239	ASP	Peptide
29	V	112	TYR	Peptide
29	V	49	VAL	Peptide,Mainchain
30	W	103	LYS	Peptide
30	W	145	GLU	Peptide
30	W	146	GLU	Peptide
30	W	161	ASN	Peptide
30	W	2	VAL	Peptide
30	W	22	LEU	Peptide,Mainchain
31	Y	16	ASP	Peptide
31	Y	43	TRP	Peptide
32	Z	147	SER	Peptide
32	Z	200	ALA	Peptide,Mainchain
32	Z	260	SER	Peptide,Mainchain
32	Z	355	ASN	Peptide
32	Z	837	LEU	Peptide
3	b	187	ARG	Peptide,Mainchain
4	i	230	ALA	Peptide
6	j	56	LEU	Peptide

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Mol	Chain	Res	Type	Group
7	r	196	PHE	Peptide
34	y	75	GLY	Peptide,Mainchain

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	29	68
1	o	200/239 (84%)	195 (98%)	4 (2%)	1 (0%)	29	68
2	B	242/246 (98%)	228 (94%)	9 (4%)	5 (2%)	7	39
2	h	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
3	b	218/277 (79%)	210 (96%)	7 (3%)	1 (0%)	29	68
3	p	218/277 (79%)	207 (95%)	9 (4%)	2 (1%)	17	56
4	C	231/234 (99%)	204 (88%)	24 (10%)	3 (1%)	12	48
4	i	229/234 (98%)	202 (88%)	24 (10%)	3 (1%)	12	48
5	c	202/205 (98%)	189 (94%)	11 (5%)	2 (1%)	15	54
5	q	202/205 (98%)	188 (93%)	11 (5%)	3 (2%)	10	46
6	D	248/261 (95%)	236 (95%)	11 (4%)	1 (0%)	34	72
6	j	248/261 (95%)	233 (94%)	12 (5%)	3 (1%)	13	50
7	d	197/201 (98%)	186 (94%)	10 (5%)	1 (0%)	29	68
7	r	197/201 (98%)	186 (94%)	9 (5%)	2 (1%)	15	54
8	E	241/248 (97%)	223 (92%)	12 (5%)	6 (2%)	5	35
8	k	241/248 (97%)	224 (93%)	11 (5%)	6 (2%)	5	35
9	e	199/263 (76%)	195 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	s	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
10	F	232/241 (96%)	216 (93%)	14 (6%)	2 (1%)	17	56
10	l	232/241 (96%)	215 (93%)	15 (6%)	2 (1%)	17	56
11	f	211/241 (88%)	205 (97%)	6 (3%)	0	100	100
11	t	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
12	G	236/263 (90%)	223 (94%)	10 (4%)	3 (1%)	12	48
12	m	236/263 (90%)	222 (94%)	10 (4%)	4 (2%)	9	43
13	g	214/264 (81%)	203 (95%)	10 (5%)	1 (0%)	29	68
13	u	215/264 (81%)	205 (95%)	9 (4%)	1 (0%)	29	68
14	H	376/433 (87%)	254 (68%)	81 (22%)	41 (11%)	0	8
15	I	355/440 (81%)	264 (74%)	63 (18%)	28 (8%)	1	14
16	J	354/406 (87%)	253 (72%)	68 (19%)	33 (9%)	0	12
17	K	378/418 (90%)	260 (69%)	73 (19%)	45 (12%)	0	6
18	L	373/389 (96%)	268 (72%)	69 (18%)	36 (10%)	0	11
19	M	372/439 (85%)	257 (69%)	72 (19%)	43 (12%)	0	6
20	N	815/953 (86%)	610 (75%)	176 (22%)	29 (4%)	3	28
21	X	241/255 (94%)	233 (97%)	5 (2%)	3 (1%)	13	50
21	n	241/255 (94%)	232 (96%)	7 (3%)	2 (1%)	19	60
22	O	368/376 (98%)	292 (79%)	55 (15%)	21 (6%)	1	20
23	P	401/456 (88%)	333 (83%)	55 (14%)	13 (3%)	4	30
24	Q	419/422 (99%)	324 (77%)	67 (16%)	28 (7%)	1	18
25	R	374/389 (96%)	292 (78%)	60 (16%)	22 (6%)	1	20
26	S	389/534 (73%)	332 (85%)	42 (11%)	15 (4%)	3	26
27	T	254/350 (73%)	191 (75%)	44 (17%)	19 (8%)	1	15
28	U	279/324 (86%)	224 (80%)	42 (15%)	13 (5%)	2	24
29	V	253/310 (82%)	210 (83%)	32 (13%)	11 (4%)	2	25
30	W	191/377 (51%)	143 (75%)	38 (20%)	10 (5%)	2	22
31	Y	55/70 (79%)	36 (66%)	12 (22%)	7 (13%)	0	5
32	Z	722/908 (80%)	560 (78%)	113 (16%)	49 (7%)	1	17
33	x	349/494 (71%)	245 (70%)	62 (18%)	42 (12%)	0	6
34	y	74/76 (97%)	71 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	13374/15440 (87%)	11297 (84%)	1514 (11%)	563 (4%)	5	25

All (563) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	120	ALA
12	G	238	GLU
14	H	95	VAL
14	H	108	ASP
14	H	109	PRO
14	H	115	VAL
14	H	116	LYS
14	H	133	ASP
14	H	154	PRO
14	H	167	GLU
14	H	234	ASP
14	H	285	PHE
14	H	307	ASP
14	H	346	PRO
14	H	424	SER
15	I	207	HIS
15	I	220	LYS
15	I	277	HIS
15	I	278	ALA
15	I	292	THR
15	I	300	GLY
15	I	321	SER
15	I	356	PRO
15	I	357	ASP
15	I	380	LEU
15	I	416	ASN
4	i	40	ALA
16	J	84	LYS
16	J	89	VAL
16	J	90	HIS
16	J	92	GLU
16	J	131	VAL
16	J	133	PRO
16	J	149	GLU
16	J	150	MET
16	J	151	ILE
16	J	152	GLY

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Mol	Chain	Res	Type
16	J	229	ARG
16	J	284	GLU
16	J	288	ASN
16	J	310	ARG
16	J	352	PRO
17	K	85	ILE
17	K	97	ASP
17	K	119	ILE
17	K	120	ASP
17	K	122	GLU
17	K	125	LYS
17	K	126	PRO
17	K	149	SER
17	K	152	MET
17	K	155	THR
17	K	162	VAL
17	K	223	THR
17	K	258	ALA
17	K	273	LYS
17	K	274	ARG
17	K	278	GLN
17	K	300	ASP
17	K	303	VAL
17	K	336	PRO
17	K	360	LEU
17	K	367	PRO
17	K	391	ARG
17	K	409	LYS
17	K	411	GLU
8	k	50	VAL
18	L	85	ARG
18	L	88	ASP
18	L	109	ARG
18	L	114	GLU
18	L	116	ASP
18	L	127	PRO
18	L	139	SER
18	L	206	LYS
18	L	237	ALA
18	L	247	THR
18	L	324	GLY
18	L	358	ASP

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Mol	Chain	Res	Type
19	M	137	ILE
19	M	140	VAL
19	M	184	GLN
19	M	218	GLN
19	M	244	THR
19	M	261	ILE
19	M	345	SER
19	M	378	ASP
19	M	379	VAL
19	M	413	THR
19	M	433	ALA
20	N	164	GLU
20	N	170	SER
20	N	701	ILE
20	N	752	THR
20	N	792	ASN
20	N	793	LYS
20	N	881	PRO
20	N	905	PRO
20	N	933	PRO
22	O	104	VAL
22	O	109	GLU
22	O	146	PRO
22	O	284	ARG
22	O	285	PRO
22	O	369	HIS
22	O	371	ALA
23	P	169	LEU
23	P	300	PRO
23	P	409	LEU
24	Q	121	LYS
24	Q	141	LYS
24	Q	201	TYR
24	Q	204	PRO
24	Q	277	LEU
24	Q	280	ALA
24	Q	391	PRO
24	Q	393	VAL
5	q	156	PRO
25	R	28	LEU
25	R	31	HIS
25	R	34	ASP

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Mol	Chain	Res	Type
25	R	37	VAL
25	R	131	THR
25	R	254	PRO
25	R	268	TYR
25	R	269	SER
25	R	289	ALA
26	S	180	ARG
26	S	218	TYR
26	S	279	GLN
26	S	321	ALA
26	S	346	LEU
26	S	351	PRO
26	S	464	ILE
26	S	466	ILE
27	T	129	LEU
27	T	216	PRO
27	T	312	PRO
27	T	319	ALA
27	T	323	GLN
27	T	325	PRO
28	U	117	PRO
28	U	128	PRO
28	U	186	THR
28	U	222	ILE
28	U	224	HIS
28	U	240	VAL
28	U	241	SER
29	V	52	GLU
29	V	226	MET
30	W	62	THR
30	W	65	THR
30	W	66	PRO
30	W	67	ASP
30	W	78	VAL
21	X	207	LYS
31	Y	38	VAL
31	Y	40	GLU
31	Y	45	ASP
31	Y	48	VAL
32	Z	203	GLU
32	Z	228	LYS
32	Z	256	PHE

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Mol	Chain	Res	Type
32	Z	257	ARG
32	Z	258	LYS
32	Z	272	LEU
32	Z	273	ASN
32	Z	324	VAL
32	Z	404	ASP
32	Z	457	ASN
32	Z	662	MET
32	Z	666	ILE
32	Z	701	ASN
32	Z	705	ASN
32	Z	810	ILE
32	Z	815	HIS
32	Z	837	LEU
32	Z	892	PRO
33	x	146	ALA
33	x	167	SER
33	x	168	SER
33	x	173	ILE
33	x	181	ALA
33	x	190	GLU
33	x	259	SER
33	x	260	GLU
33	x	261	GLU
33	x	291	LEU
33	x	337	SER
33	x	376	LEU
33	x	409	ILE
33	x	443	GLN
33	x	449	PHE
33	x	451	ASP
33	x	481	PRO
3	b	188	PRO
4	C	40	ALA
4	C	198	PHE
5	c	117	PHE
5	c	156	PRO
8	E	46	GLU
8	E	50	VAL
8	E	101	PRO
13	g	46	ASN
14	H	93	LEU

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Mol	Chain	Res	Type
14	H	110	LYS
14	H	134	ILE
14	H	197	HIS
14	H	205	GLY
14	H	206	ILE
14	H	292	ASP
14	H	378	PRO
14	H	399	ALA
14	H	417	ILE
15	I	103	ARG
15	I	106	PRO
15	I	119	ASN
15	I	191	ASP
15	I	296	ASP
15	I	297	SER
15	I	301	GLY
15	I	427	LEU
16	J	37	ASP
16	J	78	ARG
16	J	148	TYR
16	J	287	LYS
6	j	131	GLY
17	K	121	ARG
17	K	151	ILE
17	K	156	SER
17	K	304	ASN
17	K	320	ALA
17	K	393	ILE
17	K	410	ASP
17	K	412	GLN
8	k	101	PRO
18	L	192	ASP
18	L	193	CYS
18	L	208	ILE
18	L	241	ARG
18	L	244	SER
18	L	266	GLY
18	L	337	GLY
18	L	357	ALA
10	l	120	ALA
10	l	187	LYS
19	M	85	THR

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Mol	Chain	Res	Type
19	M	165	PRO
19	M	168	TYR
19	M	216	GLY
19	M	280	PRO
19	M	300	LYS
19	M	372	LYS
19	M	409	ARG
12	m	197	GLU
12	m	238	GLU
20	N	120	GLU
20	N	174	PRO
20	N	175	GLY
20	N	427	LEU
20	N	776	SER
20	N	908	ILE
21	n	207	LYS
22	O	107	SER
22	O	148	VAL
22	O	150	SER
22	O	258	GLN
22	O	260	ASP
22	O	287	ASN
23	P	79	GLU
23	P	316	ARG
23	P	342	GLY
24	Q	6	VAL
24	Q	37	GLU
24	Q	38	ASN
24	Q	123	THR
24	Q	203	PRO
24	Q	221	GLU
24	Q	242	ILE
24	Q	392	PRO
5	q	117	PHE
25	R	32	ARG
25	R	133	ALA
26	S	179	LYS
26	S	182	LYS
26	S	319	HIS
27	T	179	LYS
27	T	318	PHE
27	T	324	LYS

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Mol	Chain	Res	Type
28	U	99	PRO
28	U	101	LEU
28	U	218	GLY
29	V	49	VAL
29	V	53	VAL
29	V	104	ARG
29	V	153	GLY
29	V	263	ASP
21	X	4	GLY
31	Y	46	ASP
32	Z	333	LEU
32	Z	365	VAL
32	Z	455	VAL
32	Z	514	VAL
32	Z	599	ALA
32	Z	600	TYR
33	x	102	LEU
33	x	142	SER
33	x	184	GLN
33	x	186	ALA
33	x	304	LEU
33	x	327	MET
33	x	335	LYS
33	x	356	GLU
33	x	402	PRO
33	x	429	SER
33	x	431	SER
33	x	444	ASP
2	B	210	PHE
8	E	201	SER
8	E	243	LYS
10	F	187	LYS
12	G	226	ASP
12	G	235	GLY
14	H	94	GLN
14	H	103	ASN
14	H	209	PRO
14	H	235	ALA
14	H	309	PHE
14	H	310	ASP
14	H	347	ASP
15	I	167	THR

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Mol	Chain	Res	Type
15	I	172	THR
15	I	182	GLU
16	J	27	LYS
16	J	283	PHE
16	J	304	ALA
16	J	308	PRO
17	K	207	PRO
17	K	390	ASN
17	K	392	TYR
8	k	46	GLU
8	k	201	SER
8	k	202	GLY
18	L	138	LEU
18	L	157	GLU
18	L	194	ASN
18	L	254	GLN
18	L	339	ASN
18	L	366	ASP
19	M	122	ALA
19	M	180	ARG
19	M	217	ILE
19	M	222	GLY
19	M	287	GLU
19	M	344	ARG
19	M	371	ARG
19	M	377	PRO
19	M	410	ARG
19	M	411	GLY
19	M	415	LEU
19	M	432	LYS
12	m	235	GLY
20	N	119	PRO
20	N	163	PHE
20	N	771	PHE
20	N	884	VAL
20	N	907	SER
22	O	259	PRO
23	P	56	THR
23	P	76	GLU
23	P	345	GLU
24	Q	17	SER
24	Q	81	SER

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Mol	Chain	Res	Type
24	Q	202	CYS
24	Q	245	PRO
25	R	30	GLU
25	R	49	ASN
25	R	51	ALA
25	R	65	ILE
25	R	156	LEU
26	S	354	LYS
27	T	237	MET
27	T	238	GLU
27	T	326	GLU
28	U	185	GLY
29	V	150	SER
30	W	77	THR
31	Y	18	GLU
31	Y	39	TRP
32	Z	227	ALA
32	Z	397	LYS
32	Z	420	TRP
32	Z	458	GLU
32	Z	472	HIS
32	Z	598	CYS
32	Z	738	ASN
32	Z	739	ALA
32	Z	811	LEU
33	x	144	GLU
33	x	187	GLU
33	x	240	SER
33	x	280	GLN
33	x	463	LEU
2	B	207	SER
4	C	232	ILE
6	D	206	LEU
14	H	85	GLN
14	H	139	ARG
14	H	286	ASP
15	I	217	LYS
15	I	299	SER
15	I	320	ASP
15	I	428	TYR
4	i	202	MET
16	J	25	LEU

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Mol	Chain	Res	Type
16	J	69	GLN
16	J	132	ASP
16	J	228	ALA
16	J	297	ARG
6	j	204	SER
17	K	161	ASP
17	K	208	PRO
17	K	266	GLU
17	K	328	ASP
17	K	368	ASP
17	K	417	TYR
18	L	360	ASP
19	M	77	SER
19	M	321	GLN
19	M	347	ARG
19	M	373	MET
19	M	392	ASN
20	N	470	ASN
20	N	912	ILE
20	N	927	PRO
22	O	108	ASP
22	O	288	HIS
23	P	385	SER
23	P	418	PRO
3	p	187	ARG
24	Q	60	THR
24	Q	225	TRP
24	Q	344	ARG
25	R	53	TYR
25	R	152	MET
25	R	153	ASP
26	S	300	LEU
26	S	350	GLN
27	T	136	LEU
27	T	178	TYR
27	T	239	GLY
28	U	179	ILE
13	u	46	ASN
29	V	292	MET
30	W	22	LEU
30	W	164	ASP
32	Z	202	HIS

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Mol	Chain	Res	Type
32	Z	262	PHE
32	Z	331	LEU
32	Z	475	ASN
32	Z	597	VAL
32	Z	716	ASP
32	Z	783	SER
32	Z	842	VAL
33	x	285	LEU
33	x	303	THR
33	x	306	ARG
2	B	189	TRP
7	d	197	PRO
8	E	200	GLN
14	H	96	ALA
14	H	144	ARG
14	H	158	ASP
14	H	192	GLU
15	I	169	PRO
4	i	53	SER
16	J	243	PRO
16	J	285	ALA
16	J	312	ASP
6	j	206	LEU
17	K	257	ASN
8	k	243	LYS
18	L	112	PRO
18	L	152	PRO
18	L	234	GLU
18	L	319	PRO
19	M	186	SER
19	M	376	SER
20	N	904	LYS
20	N	928	VAL
21	n	216	VAL
22	O	186	LYS
23	P	421	PRO
24	Q	244	SER
25	R	255	ALA
7	r	198	LYS
27	T	219	ASP
27	T	299	MET
28	U	119	SER

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Mol	Chain	Res	Type
32	Z	114	ALA
32	Z	602	GLY
33	x	103	PRO
33	x	117	ALA
2	B	188	ASP
14	H	166	VAL
15	I	287	ILE
16	J	216	GLY
17	K	86	PRO
17	K	197	ASP
17	K	407	ILE
18	L	115	VAL
18	L	126	ASP
18	L	292	PRO
19	M	188	ILE
19	M	296	PHE
12	m	53	GLN
20	N	84	ALA
22	O	26	GLU
22	O	263	ALA
23	P	171	VAL
3	p	188	PRO
24	Q	340	GLU
5	q	17	LYS
25	R	192	ARG
25	R	253	LEU
7	r	197	PRO
30	W	177	PRO
32	Z	263	PRO
32	Z	380	PHE
32	Z	559	PRO
33	x	194	TYR
33	x	471	TRP
14	H	172	VAL
14	H	198	PRO
14	H	333	ARG
19	M	148	GLY
19	M	335	VAL
26	S	70	VAL
27	T	330	ILE
29	V	79	GLY
32	Z	604	GLY

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Mol	Chain	Res	Type
18	L	130	VAL
24	Q	341	PRO
24	Q	361	VAL
27	T	230	VAL
30	W	117	VAL
2	B	208	ILE
19	M	181	PRO
20	N	913	ILE
22	O	185	ILE
1	o	30	VAL
16	J	320	PRO
18	L	240	GLY
20	N	507	VAL
22	O	18	GLN
24	Q	50	ILE
21	X	216	VAL
32	Z	702	PRO
32	Z	872	VAL
33	x	346	VAL
1	a	30	VAL
20	N	124	LYS
29	V	267	PRO

5.3.2 Protein sidechains ⓘ

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	155/181 (86%)	148 (96%)	7 (4%)	27	54
1	o	155/181 (86%)	148 (96%)	7 (4%)	27	54
2	B	193/210 (92%)	182 (94%)	11 (6%)	20	48
2	h	195/210 (93%)	183 (94%)	12 (6%)	18	45
3	b	177/228 (78%)	170 (96%)	7 (4%)	31	56
3	p	177/228 (78%)	168 (95%)	9 (5%)	24	50
4	C	163/191 (85%)	155 (95%)	8 (5%)	25	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	i	177/191 (93%)	163 (92%)	14 (8%)	12	38
5	c	172/174 (99%)	163 (95%)	9 (5%)	23	50
5	q	172/174 (99%)	163 (95%)	9 (5%)	23	50
6	D	193/221 (87%)	182 (94%)	11 (6%)	20	48
6	j	193/221 (87%)	183 (95%)	10 (5%)	23	50
7	d	164/171 (96%)	156 (95%)	8 (5%)	25	51
7	r	164/171 (96%)	157 (96%)	7 (4%)	29	55
8	E	152/211 (72%)	142 (93%)	10 (7%)	16	43
8	k	142/211 (67%)	134 (94%)	8 (6%)	21	48
9	e	153/202 (76%)	149 (97%)	4 (3%)	46	67
9	s	154/202 (76%)	148 (96%)	6 (4%)	32	57
10	F	190/203 (94%)	185 (97%)	5 (3%)	46	67
10	l	191/203 (94%)	185 (97%)	6 (3%)	40	63
11	f	174/199 (87%)	166 (95%)	8 (5%)	27	53
11	t	175/199 (88%)	168 (96%)	7 (4%)	31	56
12	G	198/224 (88%)	191 (96%)	7 (4%)	36	60
12	m	198/224 (88%)	183 (92%)	15 (8%)	13	40
13	g	175/215 (81%)	166 (95%)	9 (5%)	24	50
13	u	175/215 (81%)	164 (94%)	11 (6%)	18	44
14	H	292/372 (78%)	238 (82%)	54 (18%)	1	10
15	I	291/385 (76%)	231 (79%)	60 (21%)	1	7
16	J	310/352 (88%)	246 (79%)	64 (21%)	1	7
17	K	333/366 (91%)	268 (80%)	65 (20%)	1	9
18	L	298/341 (87%)	239 (80%)	59 (20%)	1	9
19	M	296/379 (78%)	240 (81%)	56 (19%)	1	9
20	N	377/816 (46%)	345 (92%)	32 (8%)	10	36
21	X	193/212 (91%)	186 (96%)	7 (4%)	35	60
21	n	193/212 (91%)	184 (95%)	9 (5%)	26	52
22	O	144/336 (43%)	119 (83%)	25 (17%)	2	12
23	P	202/416 (49%)	182 (90%)	20 (10%)	8	28
24	Q	249/362 (69%)	207 (83%)	42 (17%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	R	226/344 (66%)	196 (87%)	30 (13%)	4	20
26	S	163/460 (35%)	153 (94%)	10 (6%)	18	46
27	T	109/294 (37%)	92 (84%)	17 (16%)	2	16
28	U	212/295 (72%)	184 (87%)	28 (13%)	4	20
29	V	219/268 (82%)	188 (86%)	31 (14%)	3	18
30	W	109/312 (35%)	102 (94%)	7 (6%)	17	44
31	Y	4/63 (6%)	4 (100%)	0	100	100
33	x	305/439 (70%)	254 (83%)	51 (17%)	2	14
34	y	68/68 (100%)	64 (94%)	4 (6%)	19	47
All	All	9120/12352 (74%)	8224 (90%)	896 (10%)	11	28

All (896) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	22	THR
1	a	46	SER
1	a	86	MET
1	a	89	ARG
1	a	139	VAL
1	a	150	GLU
1	a	153	LEU
2	B	73	THR
2	B	78	CYS
2	B	102	LYS
2	B	114	LEU
2	B	131	MET
2	B	132	ARG
2	B	166	THR
2	B	209	ASP
2	B	221	THR
2	B	231	THR
2	B	234	GLU
3	b	56	THR
3	b	77	VAL
3	b	86	MET
3	b	187	ARG
3	b	198	ARG
3	b	201	ARG
3	b	215	LYS

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Mol	Chain	Res	Type
4	C	2	GLU
4	C	58	GLU
4	C	74	VAL
4	C	87	HIS
4	C	132	SER
4	C	167	VAL
4	C	178	ASN
4	C	189	THR
5	c	34	MET
5	c	36	THR
5	c	49	LEU
5	c	115	LYS
5	c	126	LEU
5	c	175	VAL
5	c	189	ILE
5	c	191	GLU
5	c	193	ASP
6	D	11	ILE
6	D	44	LEU
6	D	70	GLU
6	D	76	VAL
6	D	100	GLN
6	D	164	ILE
6	D	180	LYS
6	D	192	LEU
6	D	197	LEU
6	D	218	ARG
6	D	220	ASN
7	d	18	ASP
7	d	27	GLN
7	d	45	LEU
7	d	47	VAL
7	d	84	THR
7	d	85	ARG
7	d	102	LEU
7	d	171	PHE
8	E	15	HIS
8	E	38	ARG
8	E	41	VAL
8	E	43	LEU
8	E	56	GLU
8	E	99	GLU

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Mol	Chain	Res	Type
8	E	103	THR
8	E	139	ASP
8	E	146	GLN
8	E	184	ASP
9	e	8	PHE
9	e	10	HIS
9	e	115	ASP
9	e	138	VAL
10	F	36	THR
10	F	129	ASP
10	F	135	ARG
10	F	148	GLU
10	F	222	PRO
11	f	65	THR
11	f	66	LYS
11	f	76	LYS
11	f	99	ARG
11	f	102	PHE
11	f	125	ASP
11	f	160	ASN
11	f	174	LEU
12	G	38	LEU
12	G	83	LEU
12	G	101	ARG
12	G	202	GLU
12	G	225	ASP
12	G	226	ASP
12	G	239	ARG
13	g	49	THR
13	g	86	ARG
13	g	94	ARG
13	g	99	ARG
13	g	141	TYR
13	g	168	LEU
13	g	192	VAL
13	g	194	GLU
13	g	205	THR
14	H	94	GLN
14	H	103	ASN
14	H	110	LYS
14	H	114	ASN
14	H	148	GLN

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Mol	Chain	Res	Type
14	H	150	HIS
14	H	153	LEU
14	H	158	ASP
14	H	164	MET
14	H	166	VAL
14	H	180	CYS
14	H	183	GLN
14	H	187	LEU
14	H	188	ARG
14	H	199	GLU
14	H	200	ARG
14	H	204	LEU
14	H	213	LEU
14	H	217	PRO
14	H	220	THR
14	H	234	ASP
14	H	247	GLN
14	H	265	ARG
14	H	276	GLU
14	H	277	ILE
14	H	278	ASP
14	H	284	ARG
14	H	285	PHE
14	H	287	ASP
14	H	294	GLU
14	H	299	MET
14	H	307	ASP
14	H	312	ARG
14	H	315	ILE
14	H	322	ASN
14	H	327	LEU
14	H	332	MET
14	H	334	PRO
14	H	338	ASP
14	H	340	LYS
14	H	342	GLU
14	H	345	LEU
14	H	353	HIS
14	H	355	PHE
14	H	358	HIS
14	H	369	ARG
14	H	377	CYS

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Mol	Chain	Res	Type
14	H	389	CYS
14	H	400	ARG
14	H	403	ILE
14	H	415	LYS
14	H	419	SER
14	H	422	LYS
14	H	431	THR
2	h	59	LYS
2	h	73	THR
2	h	78	CYS
2	h	114	LEU
2	h	132	ARG
2	h	159	TYR
2	h	166	THR
2	h	205	VAL
2	h	209	ASP
2	h	221	THR
2	h	231	THR
2	h	234	GLU
15	I	103	ARG
15	I	105	THR
15	I	113	GLU
15	I	117	ASP
15	I	118	ASP
15	I	120	HIS
15	I	125	THR
15	I	126	SER
15	I	129	SER
15	I	156	VAL
15	I	162	VAL
15	I	164	MET
15	I	178	LYS
15	I	182	GLU
15	I	183	THR
15	I	193	GLN
15	I	195	GLN
15	I	207	HIS
15	I	210	TYR
15	I	220	LYS
15	I	235	LEU
15	I	237	LYS
15	I	242	GLN

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Mol	Chain	Res	Type
15	I	255	LEU
15	I	257	GLN
15	I	258	LYS
15	I	259	TYR
15	I	260	LEU
15	I	262	ASP
15	I	272	ARG
15	I	286	GLU
15	I	287	ILE
15	I	294	ARG
15	I	299	SER
15	I	302	GLU
15	I	303	ARG
15	I	309	MET
15	I	312	LEU
15	I	313	LEU
15	I	315	GLN
15	I	319	PHE
15	I	322	ARG
15	I	324	ASP
15	I	329	MET
15	I	333	ARG
15	I	337	LEU
15	I	339	PRO
15	I	343	ARG
15	I	346	ARG
15	I	348	ASP
15	I	350	LYS
15	I	365	PHE
15	I	366	GLN
15	I	373	THR
15	I	385	MET
15	I	388	ASP
15	I	399	CYS
15	I	408	ARG
15	I	410	ARG
15	I	420	LYS
4	i	51	GLN
4	i	52	LYS
4	i	74	VAL
4	i	87	HIS
4	i	91	LYS

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Mol	Chain	Res	Type
4	i	132	SER
4	i	178	ASN
4	i	182	GLU
4	i	183	LEU
4	i	192	LEU
4	i	195	LYS
4	i	198	PHE
4	i	199	GLU
4	i	201	GLN
16	J	25	LEU
16	J	30	GLU
16	J	33	LEU
16	J	38	LYS
16	J	39	SER
16	J	44	ARG
16	J	49	ARG
16	J	51	GLU
16	J	57	ARG
16	J	58	LEU
16	J	60	ARG
16	J	61	GLU
16	J	62	GLU
16	J	69	GLN
16	J	78	ARG
16	J	80	MET
16	J	82	LYS
16	J	84	LYS
16	J	85	VAL
16	J	111	ASN
16	J	113	ARG
16	J	118	ASN
16	J	130	LYS
16	J	139	MET
16	J	142	LYS
16	J	143	VAL
16	J	147	THR
16	J	149	GLU
16	J	155	ASP
16	J	157	GLN
16	J	174	LEU
16	J	178	LEU
16	J	184	LYS

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Mol	Chain	Res	Type
16	J	198	LEU
16	J	199	LEU
16	J	201	ARG
16	J	207	THR
16	J	210	THR
16	J	226	GLU
16	J	229	ARG
16	J	230	MET
16	J	232	ARG
16	J	248	MET
16	J	249	ASP
16	J	271	ARG
16	J	273	MET
16	J	274	LEU
16	J	279	GLN
16	J	280	LEU
16	J	283	PHE
16	J	284	GLU
16	J	286	THR
16	J	287	LYS
16	J	293	MET
16	J	303	SER
16	J	305	LEU
16	J	307	ARG
16	J	308	PRO
16	J	313	ARG
16	J	316	GLU
16	J	321	ASN
16	J	336	MET
16	J	340	ARG
16	J	392	GLN
6	j	44	LEU
6	j	76	VAL
6	j	100	GLN
6	j	164	ILE
6	j	180	LYS
6	j	192	LEU
6	j	213	ILE
6	j	218	ARG
6	j	220	ASN
6	j	239	LYS
17	K	40	LEU

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Mol	Chain	Res	Type
17	K	51	LEU
17	K	53	PHE
17	K	54	LEU
17	K	55	GLU
17	K	58	GLU
17	K	65	GLN
17	K	66	LYS
17	K	72	PHE
17	K	73	LEU
17	K	74	HIS
17	K	82	ILE
17	K	87	LEU
17	K	93	LEU
17	K	94	GLU
17	K	98	GLN
17	K	115	ILE
17	K	124	LEU
17	K	125	LYS
17	K	139	LEU
17	K	143	LEU
17	K	152	MET
17	K	154	LEU
17	K	159	LYS
17	K	163	MET
17	K	164	TYR
17	K	167	ILE
17	K	171	ASP
17	K	185	LEU
17	K	188	PHE
17	K	193	GLN
17	K	202	VAL
17	K	203	LEU
17	K	205	TYR
17	K	212	LYS
17	K	229	ARG
17	K	233	SER
17	K	237	GLN
17	K	238	LYS
17	K	240	LEU
17	K	242	GLU
17	K	245	ARG
17	K	266	GLU

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Mol	Chain	Res	Type
17	K	274	ARG
17	K	297	ASP
17	K	301	GLN
17	K	302	ASN
17	K	312	ASN
17	K	322	LEU
17	K	323	ARG
17	K	328	ASP
17	K	329	ARG
17	K	330	LYS
17	K	339	ARG
17	K	345	PHE
17	K	357	GLU
17	K	359	ASP
17	K	361	GLU
17	K	384	MET
17	K	388	ARG
17	K	391	ARG
17	K	392	TYR
17	K	403	TYR
17	K	405	THR
17	K	418	LYS
8	k	15	HIS
8	k	38	ARG
8	k	41	VAL
8	k	99	GLU
8	k	103	THR
8	k	139	ASP
8	k	146	GLN
8	k	184	ASP
18	L	86	GLN
18	L	87	LEU
18	L	96	THR
18	L	97	ARG
18	L	102	MET
18	L	105	LEU
18	L	108	MET
18	L	114	GLU
18	L	116	ASP
18	L	118	LEU
18	L	120	TYR
18	L	122	MET

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Mol	Chain	Res	Type
18	L	129	ASN
18	L	132	TYR
18	L	134	GLU
18	L	138	LEU
18	L	153	LEU
18	L	183	LEU
18	L	193	CYS
18	L	196	LEU
18	L	197	LYS
18	L	202	SER
18	L	206	LYS
18	L	213	ARG
18	L	216	ARG
18	L	225	HIS
18	L	226	GLN
18	L	234	GLU
18	L	235	ILE
18	L	238	ILE
18	L	241	ARG
18	L	242	ARG
18	L	244	SER
18	L	245	GLU
18	L	247	THR
18	L	251	ARG
18	L	254	GLN
18	L	255	ARG
18	L	257	LEU
18	L	260	LEU
18	L	268	ASP
18	L	271	HIS
18	L	281	ARG
18	L	283	ASP
18	L	302	ASP
18	L	307	GLN
18	L	316	HIS
18	L	320	ILE
18	L	322	LYS
18	L	334	LEU
18	L	344	ARG
18	L	356	ARG
18	L	358	ASP
18	L	361	PHE

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Mol	Chain	Res	Type
18	L	363	VAL
18	L	364	GLN
18	L	367	PHE
18	L	368	MET
18	L	383	LYS
10	l	36	THR
10	l	135	ARG
10	l	148	GLU
10	l	156	MET
10	l	168	ARG
10	l	208	GLU
19	M	89	LEU
19	M	95	GLU
19	M	96	LEU
19	M	134	LEU
19	M	149	ASP
19	M	163	THR
19	M	166	THR
19	M	168	TYR
19	M	170	SER
19	M	178	ASP
19	M	182	THR
19	M	183	GLU
19	M	187	ASP
19	M	206	MET
19	M	209	LYS
19	M	221	LYS
19	M	225	MET
19	M	231	THR
19	M	250	LYS
19	M	261	ILE
19	M	266	LYS
19	M	272	PHE
19	M	284	PHE
19	M	289	ASP
19	M	295	ARG
19	M	296	PHE
19	M	299	GLU
19	M	303	ASP
19	M	304	ARG
19	M	305	GLU
19	M	310	MET

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Mol	Chain	Res	Type
19	M	317	LEU
19	M	318	ASP
19	M	320	PHE
19	M	323	ASN
19	M	327	LYS
19	M	334	ARG
19	M	339	ASP
19	M	344	ARG
19	M	348	LEU
19	M	351	LYS
19	M	364	ARG
19	M	366	MET
19	M	367	GLN
19	M	369	HIS
19	M	372	LYS
19	M	373	MET
19	M	378	ASP
19	M	386	ARG
19	M	388	THR
19	M	409	ARG
19	M	415	LEU
19	M	416	THR
19	M	425	LEU
19	M	430	LYS
19	M	435	LEU
12	m	26	MET
12	m	27	GLU
12	m	38	LEU
12	m	51	ARG
12	m	77	LEU
12	m	83	LEU
12	m	101	ARG
12	m	139	ASP
12	m	157	ARG
12	m	174	ARG
12	m	196	ARG
12	m	202	GLU
12	m	211	SER
12	m	236	LEU
12	m	239	ARG
20	N	17	PRO
20	N	119	PRO

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Mol	Chain	Res	Type
20	N	125	PRO
20	N	165	LYS
20	N	168	LEU
20	N	170	SER
20	N	174	PRO
20	N	179	TYR
20	N	211	PRO
20	N	271	VAL
20	N	363	SER
20	N	364	VAL
20	N	402	PHE
20	N	425	THR
20	N	431	THR
20	N	433	PRO
20	N	444	TYR
20	N	469	SER
20	N	471	ASP
20	N	576	PRO
20	N	601	ARG
20	N	630	PRO
20	N	650	TYR
20	N	758	PRO
20	N	794	ASP
20	N	808	PRO
20	N	816	PRO
20	N	881	PRO
20	N	895	PRO
20	N	905	PRO
20	N	928	VAL
20	N	933	PRO
21	n	17	ASP
21	n	39	ILE
21	n	41	CYS
21	n	42	LYS
21	n	129	ARG
21	n	144	ASP
21	n	174	THR
21	n	181	MET
21	n	200	VAL
22	O	5	PRO
22	O	11	SER
22	O	19	PRO

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Mol	Chain	Res	Type
22	O	45	VAL
22	O	49	CYS
22	O	65	SER
22	O	73	PRO
22	O	90	PRO
22	O	146	PRO
22	O	151	VAL
22	O	172	TYR
22	O	189	PRO
22	O	274	LEU
22	O	279	GLU
22	O	281	THR
22	O	303	THR
22	O	339	ARG
22	O	349	MET
22	O	353	LEU
22	O	354	GLU
22	O	358	THR
22	O	362	SER
22	O	363	MET
22	O	364	GLU
22	O	368	GLU
1	o	17	ASP
1	o	22	THR
1	o	89	ARG
1	o	139	VAL
1	o	145	GLU
1	o	150	GLU
1	o	153	LEU
23	P	48	LEU
23	P	49	SER
23	P	52	LYS
23	P	55	ARG
23	P	70	VAL
23	P	119	PRO
23	P	149	LEU
23	P	159	VAL
23	P	169	LEU
23	P	254	PRO
23	P	300	PRO
23	P	317	TRP
23	P	318	SER

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Mol	Chain	Res	Type
23	P	351	TRP
23	P	373	ILE
23	P	383	ASP
23	P	398	VAL
23	P	401	THR
23	P	436	MET
23	P	451	MET
3	p	22	GLU
3	p	56	THR
3	p	77	VAL
3	p	86	MET
3	p	132	LEU
3	p	194	LYS
3	p	198	ARG
3	p	201	ARG
3	p	215	LYS
24	Q	82	LYS
24	Q	90	ARG
24	Q	111	LEU
24	Q	120	GLU
24	Q	125	LEU
24	Q	126	ARG
24	Q	145	GLU
24	Q	154	LEU
24	Q	155	ARG
24	Q	158	LYS
24	Q	166	LEU
24	Q	168	GLU
24	Q	171	LEU
24	Q	177	TYR
24	Q	185	LYS
24	Q	187	ARG
24	Q	191	THR
24	Q	207	GLN
24	Q	222	GLU
24	Q	223	LYS
24	Q	224	ASP
24	Q	230	SER
24	Q	233	TYR
24	Q	241	SER
24	Q	242	ILE
24	Q	244	SER

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Mol	Chain	Res	Type
24	Q	249	THR
24	Q	264	PRO
24	Q	283	GLN
24	Q	296	ASN
24	Q	316	ASP
24	Q	317	PRO
24	Q	318	ILE
24	Q	325	LYS
24	Q	326	LEU
24	Q	333	GLN
24	Q	337	ARG
24	Q	392	PRO
24	Q	393	VAL
24	Q	403	THR
24	Q	416	ASN
24	Q	417	LYS
5	q	34	MET
5	q	36	THR
5	q	49	LEU
5	q	115	LYS
5	q	116	THR
5	q	126	LEU
5	q	132	VAL
5	q	189	ILE
5	q	191	GLU
25	R	15	PRO
25	R	23	ARG
25	R	50	MET
25	R	92	GLU
25	R	97	GLU
25	R	134	LEU
25	R	173	ASP
25	R	179	ARG
25	R	202	LEU
25	R	203	ASP
25	R	212	GLU
25	R	214	MET
25	R	250	LEU
25	R	254	PRO
25	R	259	TYR
25	R	260	LEU
25	R	270	VAL

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Mol	Chain	Res	Type
25	R	271	PHE
25	R	292	TYR
25	R	302	HIS
25	R	304	TYR
25	R	307	LEU
25	R	362	LYS
25	R	363	ASN
25	R	366	TYR
25	R	367	GLN
25	R	371	LYS
25	R	372	LYS
25	R	379	ARG
25	R	385	ARG
7	r	25	ILE
7	r	27	GLN
7	r	38	MET
7	r	45	LEU
7	r	84	THR
7	r	85	ARG
7	r	170	ARG
26	S	300	LEU
26	S	307	ARG
26	S	320	THR
26	S	351	PRO
26	S	431	PRO
26	S	467	TYR
26	S	469	THR
26	S	477	HIS
26	S	479	ARG
26	S	482	PHE
9	s	8	PHE
9	s	32	LYS
9	s	73	ARG
9	s	87	VAL
9	s	115	ASP
9	s	138	VAL
27	T	107	PRO
27	T	110	SER
27	T	126	LEU
27	T	130	PRO
27	T	137	THR
27	T	162	PRO

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Mol	Chain	Res	Type
27	T	173	CYS
27	T	182	LEU
27	T	183	PRO
27	T	216	PRO
27	T	237	MET
27	T	296	PRO
27	T	309	VAL
27	T	312	PRO
27	T	333	THR
27	T	337	LYS
27	T	342	TYR
11	t	6	VAL
11	t	65	THR
11	t	99	ARG
11	t	102	PHE
11	t	125	ASP
11	t	163	HIS
11	t	174	LEU
28	U	23	PHE
28	U	32	GLN
28	U	33	LYS
28	U	58	PHE
28	U	88	ARG
28	U	101	LEU
28	U	116	CYS
28	U	128	PRO
28	U	157	HIS
28	U	159	THR
28	U	166	GLU
28	U	173	GLU
28	U	175	LEU
28	U	176	LEU
28	U	177	ARG
28	U	178	ASP
28	U	184	VAL
28	U	196	HIS
28	U	201	LEU
28	U	202	ASN
28	U	209	ARG
28	U	245	PHE
28	U	249	PHE
28	U	252	LYS

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Mol	Chain	Res	Type
28	U	267	ARG
28	U	273	HIS
28	U	279	LYS
28	U	282	ASN
13	u	49	THR
13	u	70	MET
13	u	85	PRO
13	u	86	ARG
13	u	94	ARG
13	u	99	ARG
13	u	100	ARG
13	u	168	LEU
13	u	186	ARG
13	u	192	VAL
13	u	205	THR
29	V	46	ARG
29	V	50	PRO
29	V	96	LEU
29	V	98	MET
29	V	104	ARG
29	V	105	PRO
29	V	118	PHE
29	V	136	LEU
29	V	150	SER
29	V	208	ARG
29	V	209	LYS
29	V	212	LEU
29	V	226	MET
29	V	227	GLU
29	V	229	LEU
29	V	236	GLU
29	V	237	HIS
29	V	240	HIS
29	V	248	MET
29	V	254	ASN
29	V	261	GLU
29	V	262	GLU
29	V	264	LYS
29	V	265	MET
29	V	277	LYS
29	V	281	LYS
29	V	285	GLU

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Mol	Chain	Res	Type
29	V	287	HIS
29	V	295	ASN
29	V	298	GLN
29	V	299	CYS
30	W	23	PRO
30	W	37	CYS
30	W	58	CYS
30	W	61	LEU
30	W	80	PRO
30	W	174	PRO
30	W	178	SER
21	X	5	THR
21	X	39	ILE
21	X	129	ARG
21	X	144	ASP
21	X	181	MET
21	X	187	ARG
21	X	200	VAL
33	x	98	SER
33	x	101	GLU
33	x	102	LEU
33	x	104	CYS
33	x	111	ASN
33	x	114	TYR
33	x	115	MET
33	x	134	ARG
33	x	147	SER
33	x	150	TYR
33	x	155	LEU
33	x	156	ARG
33	x	163	ASP
33	x	172	ILE
33	x	173	ILE
33	x	174	LEU
33	x	175	LEU
33	x	177	PHE
33	x	182	PHE
33	x	188	LYS
33	x	198	ASP
33	x	202	CYS
33	x	205	GLN
33	x	207	MET

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Mol	Chain	Res	Type
33	x	208	ARG
33	x	217	ILE
33	x	241	LEU
33	x	252	THR
33	x	282	VAL
33	x	286	PHE
33	x	307	ASN
33	x	324	THR
33	x	327	MET
33	x	329	ARG
33	x	331	PHE
33	x	332	TYR
33	x	337	SER
33	x	346	VAL
33	x	347	LYS
33	x	348	PHE
33	x	357	LEU
33	x	358	CYS
33	x	418	ASP
33	x	423	LEU
33	x	426	GLN
33	x	431	SER
33	x	444	ASP
33	x	452	ASP
33	x	455	SER
33	x	456	ILE
33	x	471	TRP
34	y	18	GLU
34	y	40	GLN
34	y	60	ASN
34	y	71	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	100	ASN
6	D	100	GLN
6	D	155	ASN
8	E	54	GLN
8	E	92	GLN
9	e	38	ASN
10	F	182	GLN

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Mol	Chain	Res	Type
11	f	146	GLN
11	f	157	ASN
12	G	5	GLN
13	g	81	HIS
14	H	114	ASN
14	H	117	GLN
14	H	148	GLN
14	H	203	ASN
14	H	247	GLN
14	H	293	ASN
14	H	305	GLN
14	H	322	ASN
14	H	433	ASN
2	h	53	GLN
15	I	120	HIS
15	I	181	GLN
15	I	193	GLN
15	I	207	HIS
15	I	241	ASN
15	I	298	ASN
15	I	315	GLN
15	I	332	ASN
4	i	94	GLN
16	J	36	ASN
16	J	69	GLN
16	J	118	ASN
16	J	206	HIS
16	J	337	ASN
16	J	380	GLN
6	j	142	HIS
17	K	67	ASN
17	K	74	HIS
17	K	99	ASN
17	K	110	ASN
17	K	173	GLN
17	K	175	GLN
17	K	221	HIS
17	K	222	HIS
17	K	237	GLN
17	K	257	ASN
17	K	286	GLN
17	K	302	ASN

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Mol	Chain	Res	Type
17	K	304	ASN
17	K	312	ASN
18	L	51	GLN
18	L	75	ASN
18	L	226	GLN
18	L	339	ASN
10	l	182	GLN
19	M	321	GLN
19	M	333	ASN
20	N	259	GLN
20	N	345	ASN
20	N	347	ASN
20	N	596	ASN
20	N	645	ASN
20	N	697	GLN
20	N	880	ASN
22	O	273	GLN
22	O	287	ASN
22	O	369	HIS
1	o	71	ASN
23	P	288	HIS
23	P	361	HIS
23	P	423	ASN
23	P	444	HIS
23	P	454	ASN
24	Q	105	GLN
24	Q	127	GLN
24	Q	148	HIS
24	Q	152	GLN
24	Q	170	GLN
24	Q	207	GLN
24	Q	218	HIS
24	Q	334	ASN
5	q	93	ASN
25	R	136	HIS
25	R	178	ASN
25	R	280	GLN
25	R	291	HIS
25	R	344	HIS
25	R	381	GLN
26	S	242	HIS
26	S	299	GLN

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Mol	Chain	Res	Type
26	S	326	GLN
26	S	477	HIS
27	T	170	GLN
11	t	146	GLN
28	U	12	HIS
28	U	22	HIS
28	U	72	HIS
28	U	96	HIS
28	U	102	HIS
28	U	189	GLN
28	U	194	GLN
28	U	256	GLN
28	U	273	HIS
13	u	81	HIS
29	V	77	GLN
29	V	101	GLN
29	V	149	GLN
29	V	221	HIS
29	V	241	ASN
29	V	295	ASN
29	V	298	GLN
30	W	44	ASN
30	W	101	GLN
30	W	142	ASN
30	W	169	HIS
33	x	111	ASN
33	x	116	ASN
33	x	149	GLN
33	x	197	GLN
33	x	205	GLN
33	x	211	GLN
33	x	280	GLN
33	x	307	ASN
33	x	326	GLN
33	x	339	ASN
33	x	363	GLN
33	x	412	ASN
33	x	426	GLN
33	x	443	GLN
34	y	25	ASN
34	y	40	GLN
34	y	60	ASN

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Mol	Chain	Res	Type
34	y	68	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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	$\#\|Z\| > 2$
34	GLZ	y	76	34	3,3,3	0.74	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
34	GLZ	y	76	34	-	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	ADP	H	501	-	24,29,29	1.58	4 (16%)	29,45,45	2.76	10 (34%)
35	ADP	L	401	-	24,29,29	1.02	1 (4%)	29,45,45	1.74	8 (27%)
35	ADP	I	501	-	24,29,29	1.47	3 (12%)	29,45,45	1.90	6 (20%)
35	ADP	K	501	-	24,29,29	1.34	3 (12%)	29,45,45	1.92	11 (37%)
35	ADP	J	501	-	24,29,29	1.35	4 (16%)	29,45,45	2.15	9 (31%)
35	ADP	M	501	-	24,29,29	1.16	3 (12%)	29,45,45	1.81	10 (34%)

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	ADP	H	501	-	-	2/12/32/32	0/3/3/3
35	ADP	L	401	-	-	2/12/32/32	0/3/3/3
35	ADP	I	501	-	-	3/12/32/32	0/3/3/3
35	ADP	K	501	-	-	5/12/32/32	0/3/3/3
35	ADP	J	501	-	-	5/12/32/32	0/3/3/3
35	ADP	M	501	-	-	3/12/32/32	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	H	501	ADP	O4'-C1'	4.76	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	I	501	ADP	C5-C4	4.40	1.52	1.40
35	J	501	ADP	C2'-C1'	-2.91	1.49	1.53
35	H	501	ADP	C6-C5	2.90	1.54	1.43
35	K	501	ADP	O4'-C1'	2.80	1.45	1.41
35	I	501	ADP	C2-N3	2.76	1.36	1.32
35	J	501	ADP	C2-N3	2.74	1.36	1.32
35	L	401	ADP	C5-C4	2.73	1.48	1.40
35	M	501	ADP	C5-C4	2.65	1.47	1.40
35	J	501	ADP	O4'-C1'	2.56	1.44	1.41
35	K	501	ADP	C5-C4	2.53	1.47	1.40
35	J	501	ADP	O4'-C4'	-2.39	1.39	1.45
35	K	501	ADP	C2-N3	2.34	1.35	1.32
35	I	501	ADP	C8-N7	2.30	1.38	1.34
35	H	501	ADP	C2-N1	2.22	1.38	1.33
35	H	501	ADP	C5-C4	2.12	1.46	1.40
35	M	501	ADP	C2'-C1'	-2.06	1.50	1.53
35	M	501	ADP	C2-N3	2.04	1.35	1.32

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	H	501	ADP	C3'-C2'-C1'	7.83	112.77	100.98
35	H	501	ADP	O4'-C1'-C2'	-5.76	98.51	106.93
35	I	501	ADP	C3'-C2'-C1'	5.66	109.49	100.98
35	H	501	ADP	C4-C5-N7	-5.00	104.19	109.40
35	J	501	ADP	N3-C2-N1	-4.59	121.50	128.68
35	L	401	ADP	N3-C2-N1	-4.52	121.62	128.68
35	J	501	ADP	O4'-C1'-C2'	4.46	113.45	106.93
35	J	501	ADP	C4-C5-N7	-4.27	104.94	109.40
35	K	501	ADP	C4-C5-N7	-4.19	105.03	109.40
35	H	501	ADP	C5-C6-N6	3.97	126.38	120.35
35	K	501	ADP	O3B-PB-O1B	3.68	125.08	110.68
35	L	401	ADP	C1'-N9-C4	-3.59	120.34	126.64
35	J	501	ADP	C2'-C3'-C4'	3.54	109.53	102.64
35	H	501	ADP	N3-C2-N1	-3.51	123.19	128.68
35	M	501	ADP	PA-O3A-PB	-3.48	120.90	132.83
35	H	501	ADP	C1'-N9-C4	3.40	132.62	126.64
35	J	501	ADP	PA-O3A-PB	-3.36	121.29	132.83
35	M	501	ADP	N3-C2-N1	-3.36	123.43	128.68
35	M	501	ADP	O2B-PB-O3A	3.32	115.76	104.64
35	I	501	ADP	N3-C2-N1	-3.32	123.50	128.68
35	K	501	ADP	C3'-C2'-C1'	3.27	105.89	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	M	501	ADP	O4'-C1'-C2'	3.17	111.55	106.93
35	I	501	ADP	PA-O3A-PB	-3.08	122.25	132.83
35	H	501	ADP	O3B-PB-O2B	3.08	119.42	107.64
35	J	501	ADP	O3B-PB-O2B	3.07	119.38	107.64
35	H	501	ADP	O3B-PB-O1B	3.02	122.50	110.68
35	K	501	ADP	N3-C2-N1	-2.96	124.05	128.68
35	L	401	ADP	PA-O3A-PB	-2.91	122.83	132.83
35	M	501	ADP	C2'-C3'-C4'	2.89	108.25	102.64
35	H	501	ADP	O3B-PB-O3A	-2.88	94.99	104.64
35	J	501	ADP	O5'-C5'-C4'	2.77	118.54	108.99
35	J	501	ADP	O2'-C2'-C3'	-2.73	102.99	111.82
35	M	501	ADP	O2A-PA-O1A	2.73	125.72	112.24
35	K	501	ADP	O5'-C5'-C4'	2.61	117.96	108.99
35	I	501	ADP	C2-N1-C6	2.58	123.16	118.75
35	I	501	ADP	O5'-C5'-C4'	2.58	117.86	108.99
35	K	501	ADP	N6-C6-N1	2.55	123.87	118.57
35	L	401	ADP	O3A-PB-O1B	-2.47	97.51	111.19
35	M	501	ADP	N6-C6-N1	2.46	123.68	118.57
35	L	401	ADP	C2-N1-C6	2.43	122.91	118.75
35	K	501	ADP	O2A-PA-O1A	2.41	124.16	112.24
35	H	501	ADP	O5'-C5'-C4'	2.40	117.24	108.99
35	L	401	ADP	C4-C5-N7	-2.33	106.97	109.40
35	M	501	ADP	O3B-PB-O3A	-2.32	96.84	104.64
35	M	501	ADP	O3B-PB-O1B	2.28	119.63	110.68
35	K	501	ADP	O4'-C1'-C2'	-2.24	103.65	106.93
35	K	501	ADP	O3B-PB-O2B	2.22	116.14	107.64
35	K	501	ADP	O3A-PB-O1B	-2.20	99.00	111.19
35	M	501	ADP	O3A-PB-O1B	-2.17	99.16	111.19
35	L	401	ADP	C2'-C3'-C4'	2.16	106.84	102.64
35	L	401	ADP	N6-C6-N1	2.12	122.98	118.57
35	K	501	ADP	PA-O3A-PB	-2.09	125.66	132.83
35	J	501	ADP	C2-N1-C6	2.03	122.23	118.75
35	I	501	ADP	O3'-C3'-C2'	-2.01	105.33	111.82

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	H	501	ADP	O4'-C4'-C5'-O5'
35	I	501	ADP	O4'-C4'-C5'-O5'
35	J	501	ADP	C5'-O5'-PA-O1A
35	J	501	ADP	C5'-O5'-PA-O2A

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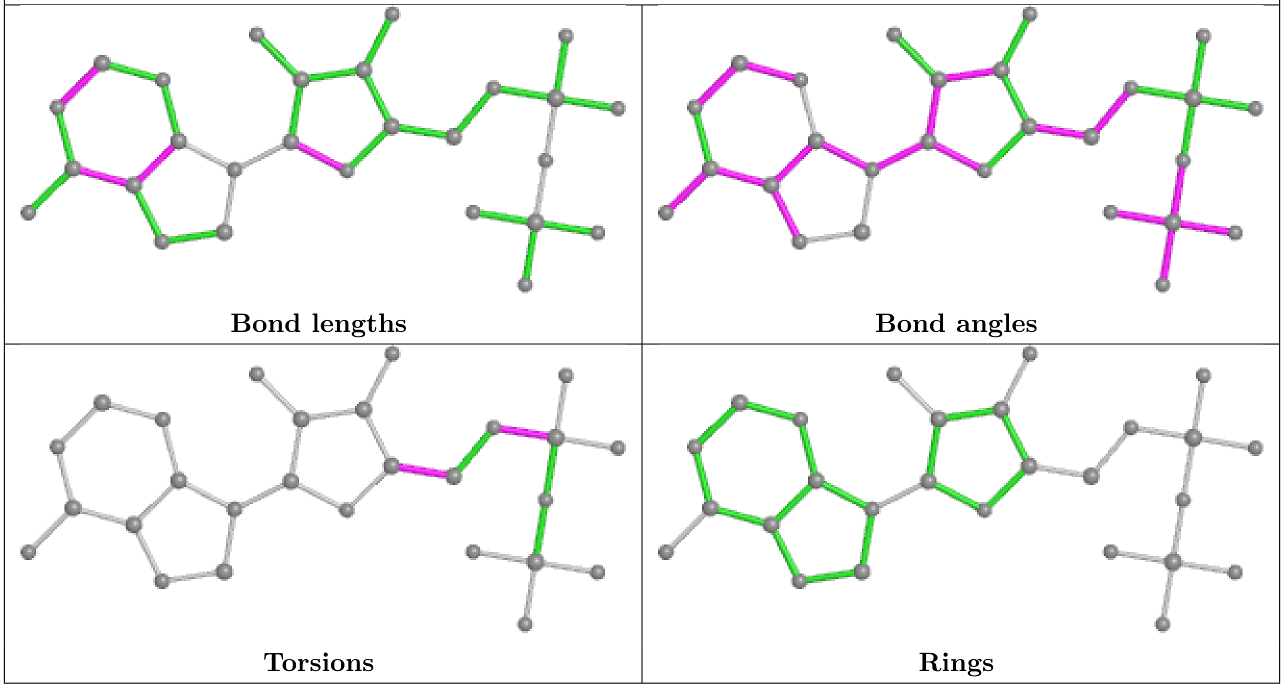
Mol	Chain	Res	Type	Atoms
35	J	501	ADP	C5'-O5'-PA-O3A
35	J	501	ADP	O4'-C4'-C5'-O5'
35	J	501	ADP	C3'-C4'-C5'-O5'
35	K	501	ADP	C5'-O5'-PA-O1A
35	L	401	ADP	C5'-O5'-PA-O3A
35	M	501	ADP	C5'-O5'-PA-O1A
35	M	501	ADP	C5'-O5'-PA-O2A
35	I	501	ADP	PB-O3A-PA-O2A
35	K	501	ADP	C5'-O5'-PA-O2A
35	L	401	ADP	C5'-O5'-PA-O2A
35	K	501	ADP	O4'-C4'-C5'-O5'
35	H	501	ADP	C5'-O5'-PA-O3A
35	K	501	ADP	C5'-O5'-PA-O3A
35	M	501	ADP	C5'-O5'-PA-O3A
35	I	501	ADP	PB-O3A-PA-O1A
35	K	501	ADP	C3'-C4'-C5'-O5'

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 ADP H 501



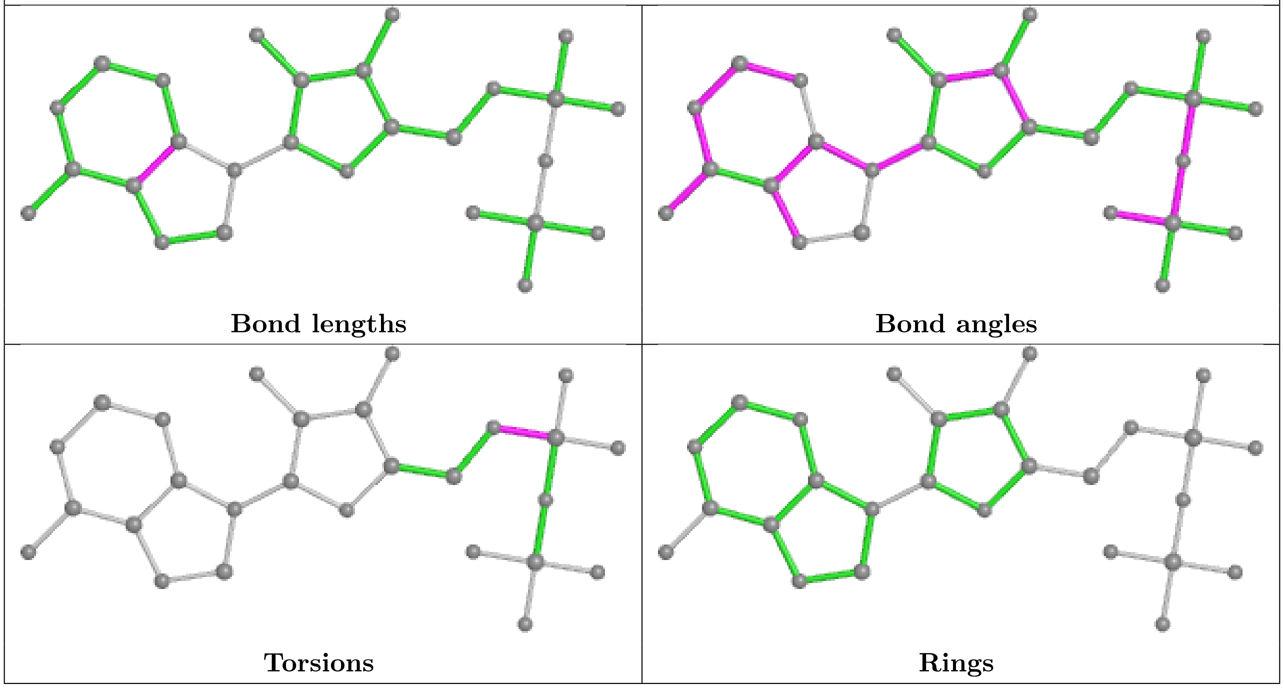
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP L 401



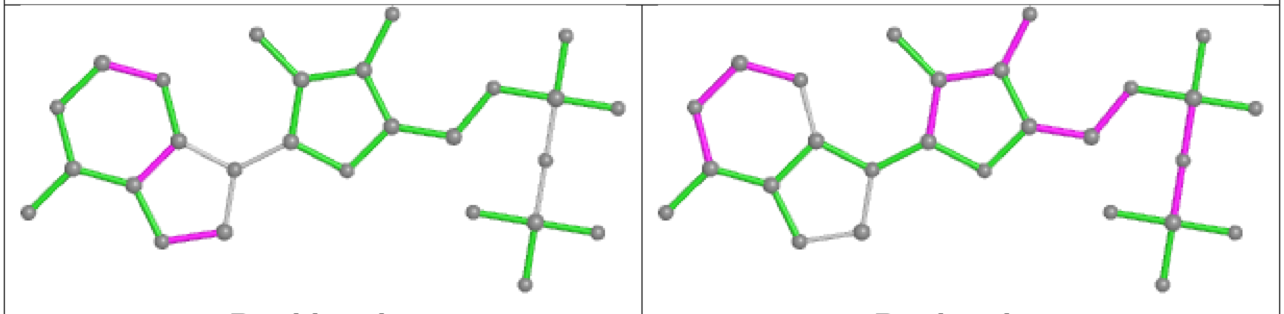
Bond lengths

Bond angles

Torsions

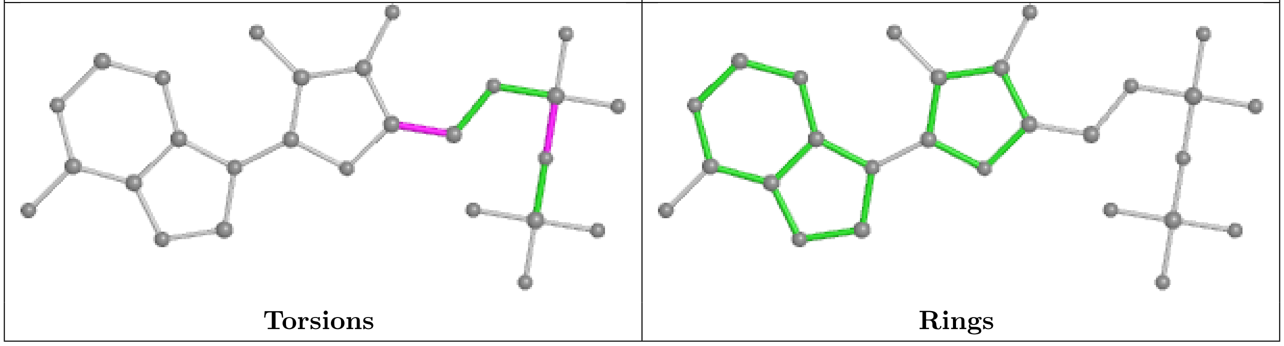
Rings

Ligand ADP I 501



Bond lengths

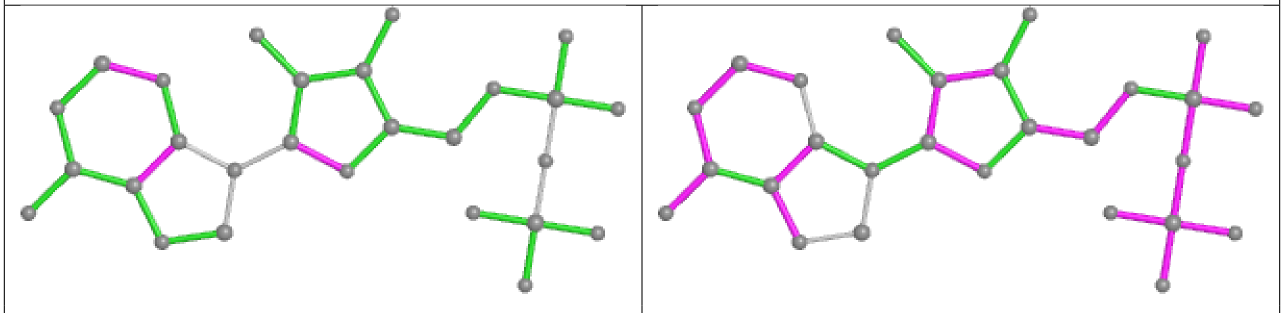
Bond angles



Torsions

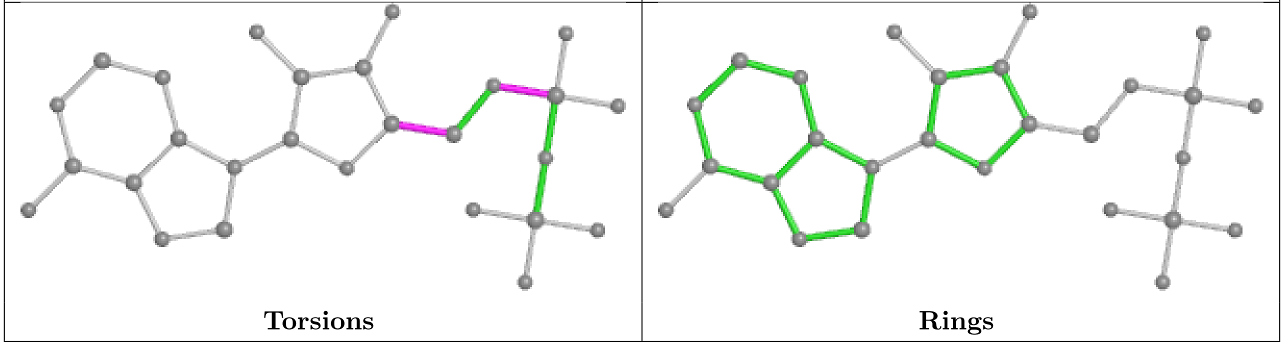
Rings

Ligand ADP K 501



Bond lengths

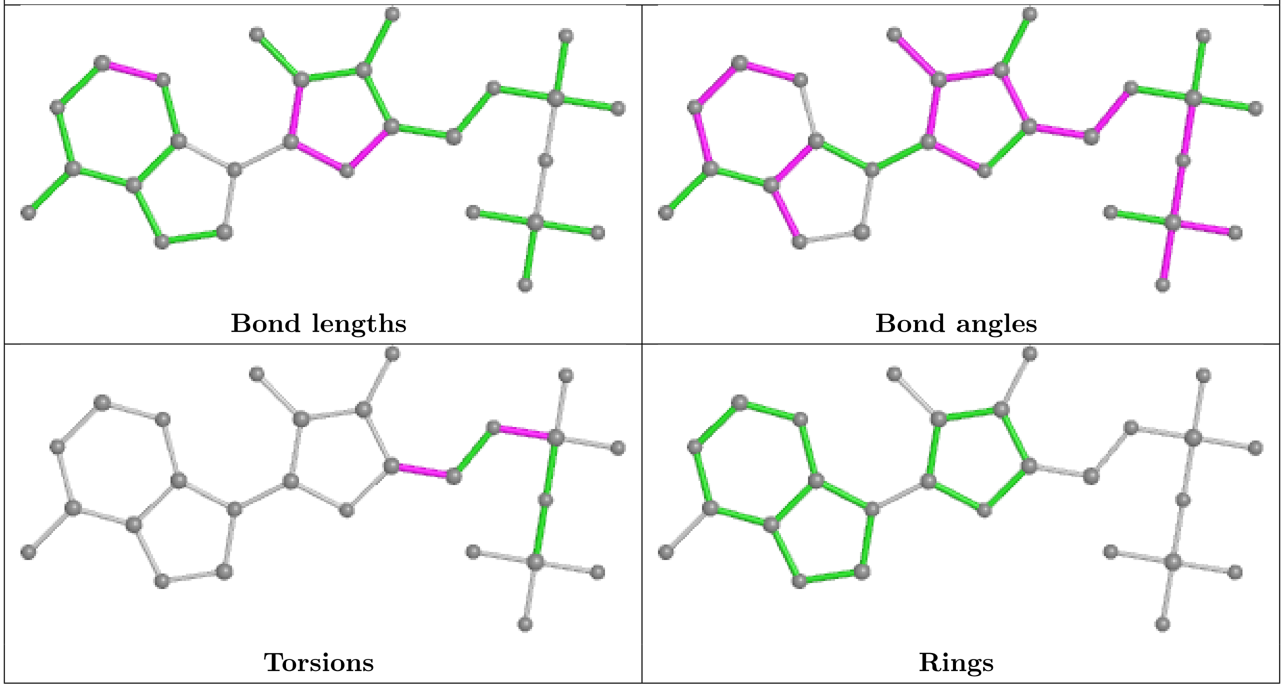
Bond angles



Torsions

Rings

Ligand ADP J 501



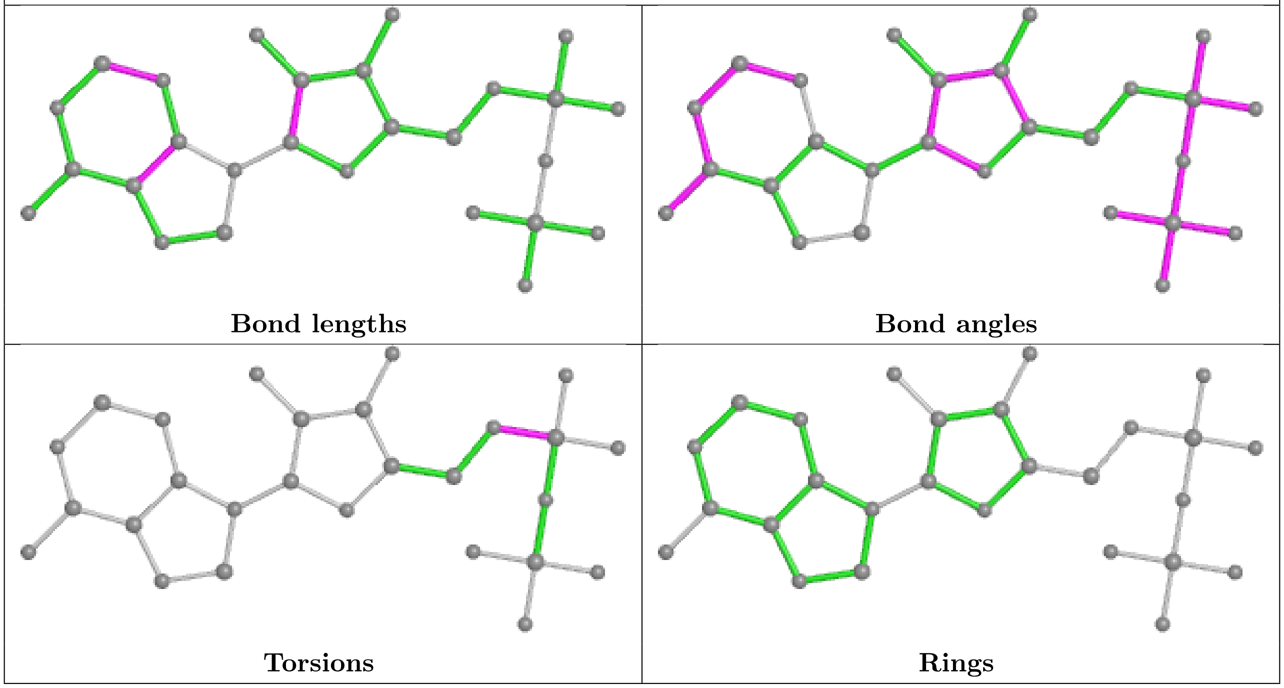
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP M 501



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

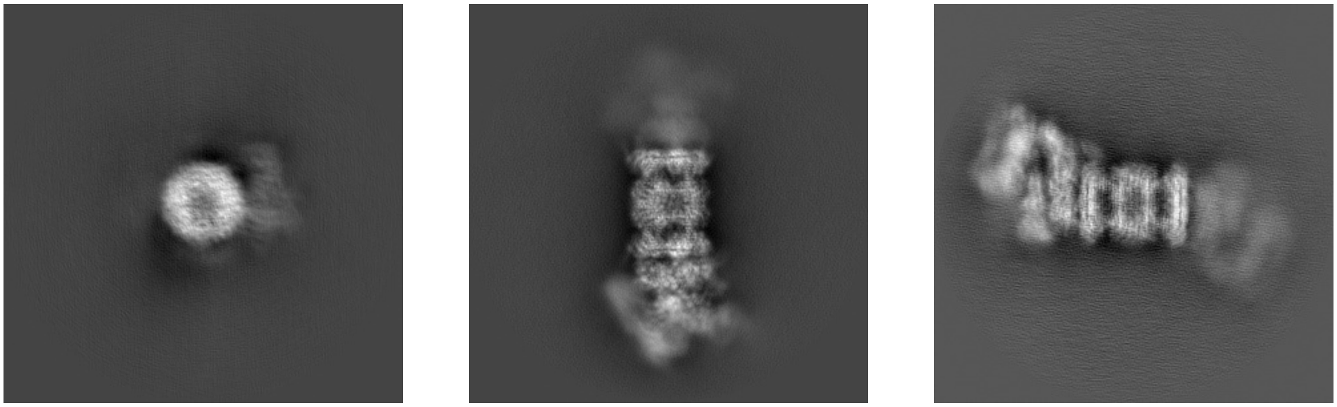
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-9511. 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

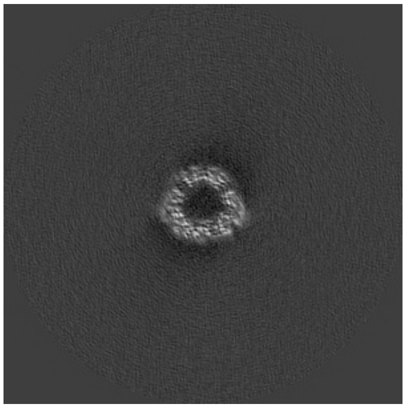


X Y Z

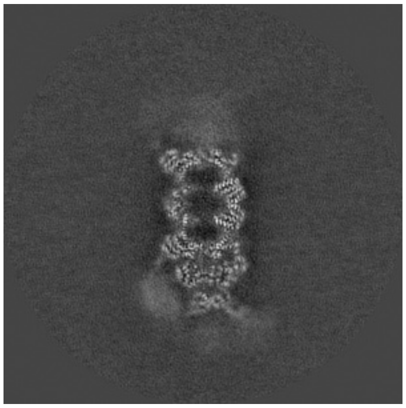
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

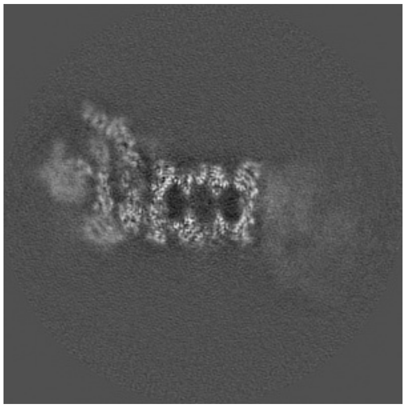
6.2.1 Primary map



X Index: 256



Y Index: 256

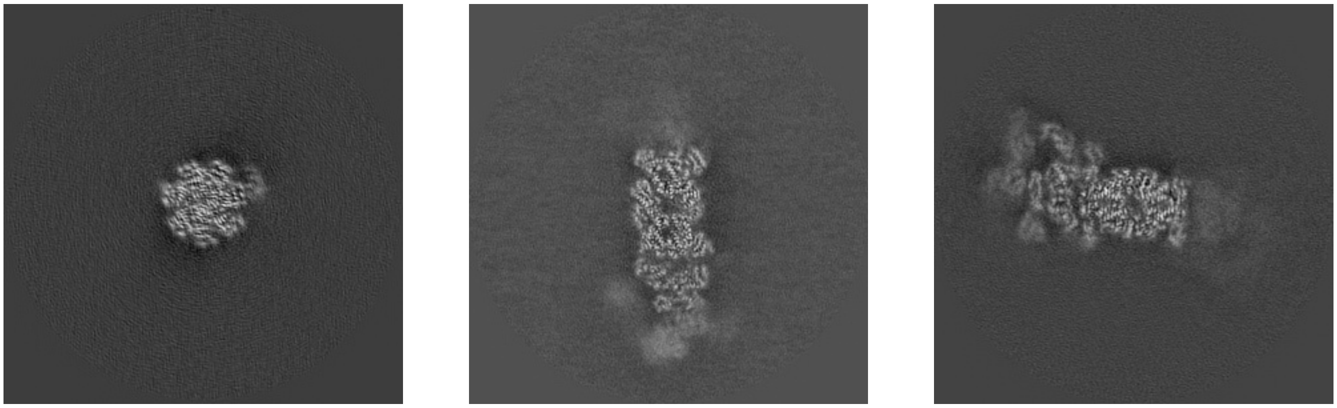


Z Index: 256

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

6.3 Largest variance slices

6.3.1 Primary map

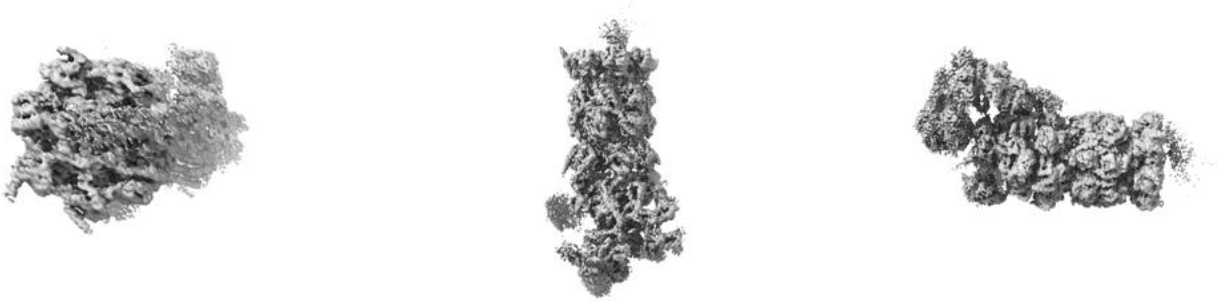


X Index: 202 Y Index: 278 Z Index: 280

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

6.4 Orthogonal surface views

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.033. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

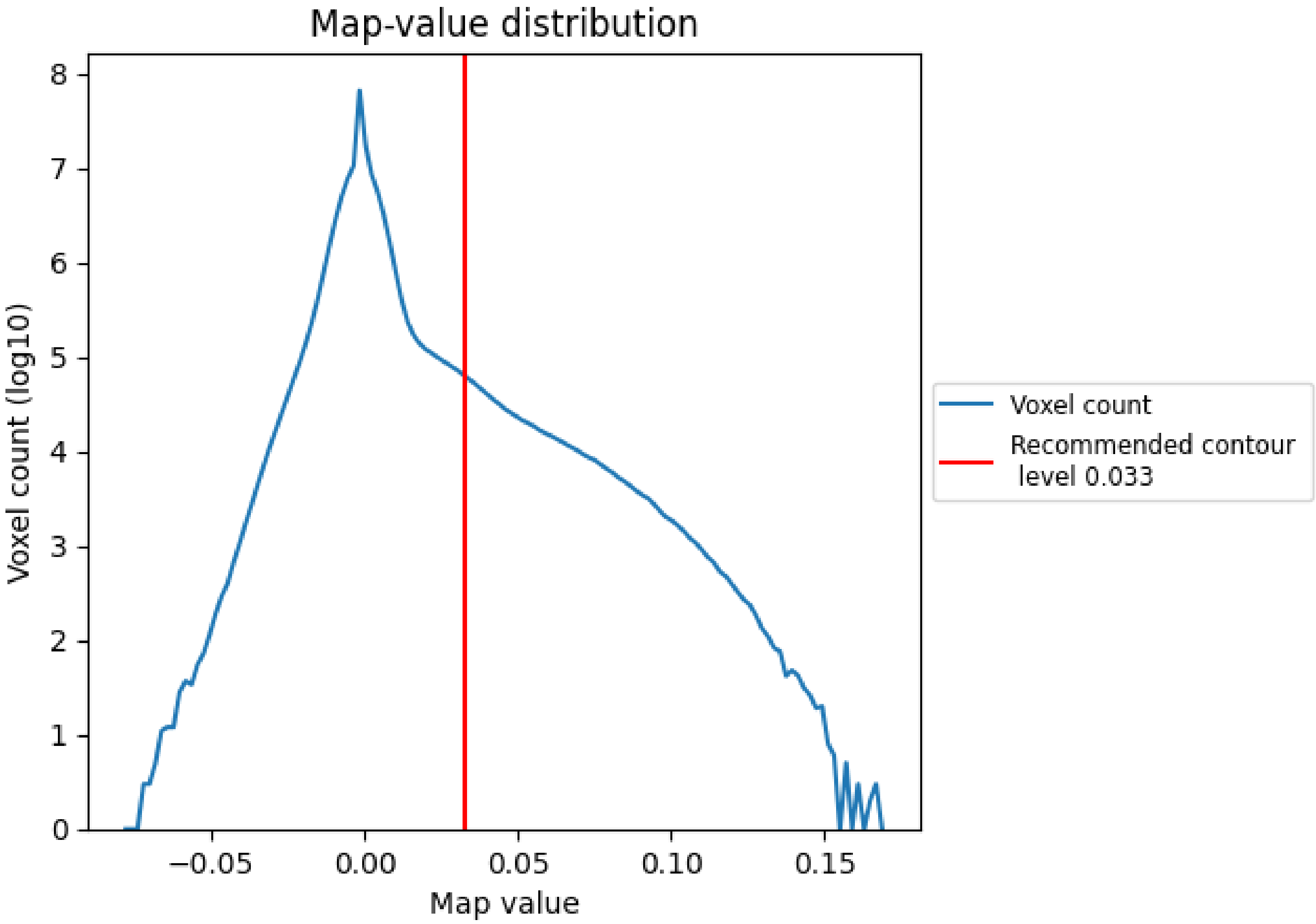
6.5 Mask visualisation ⓘ

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

7 Map analysis ⓘ

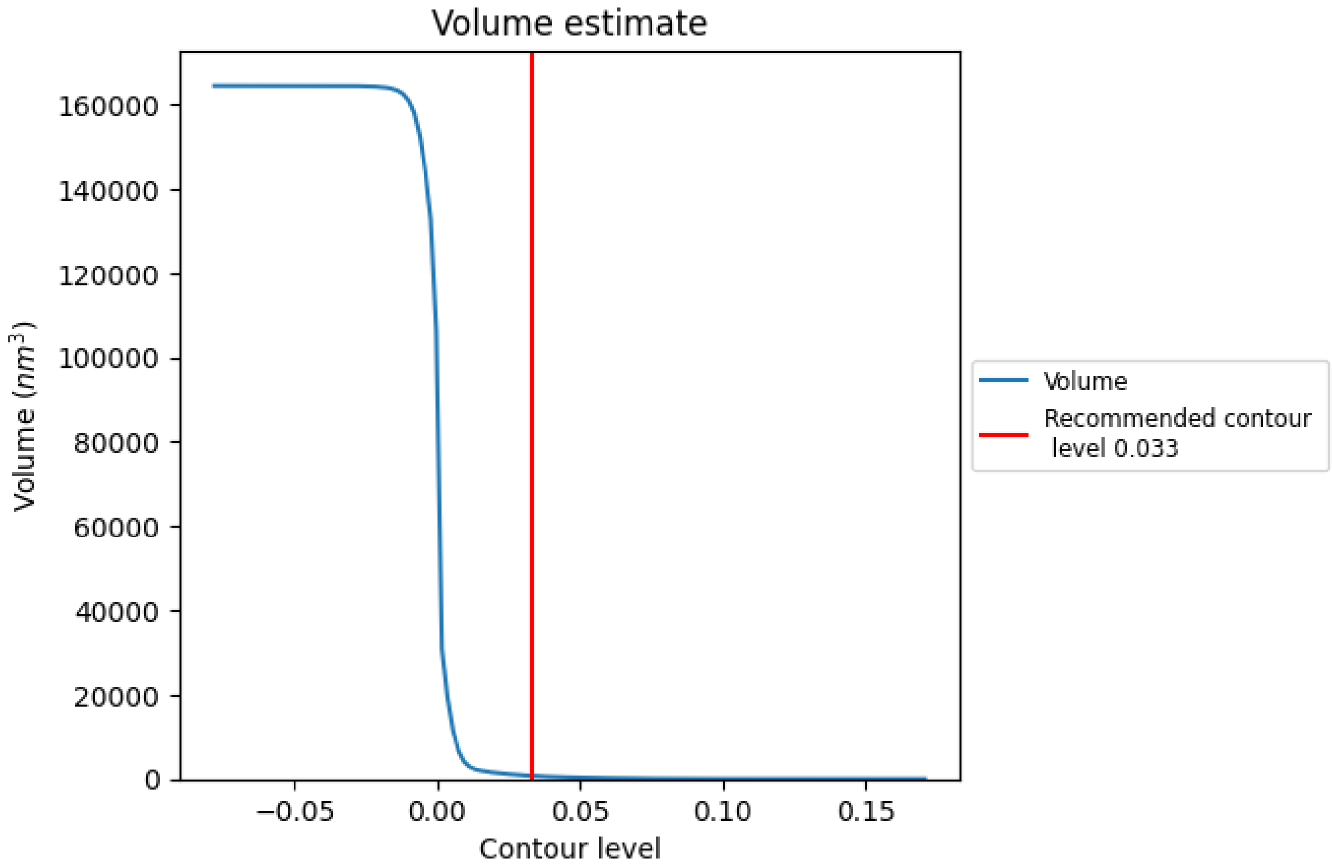
This section contains the results of statistical analysis of the map.

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.

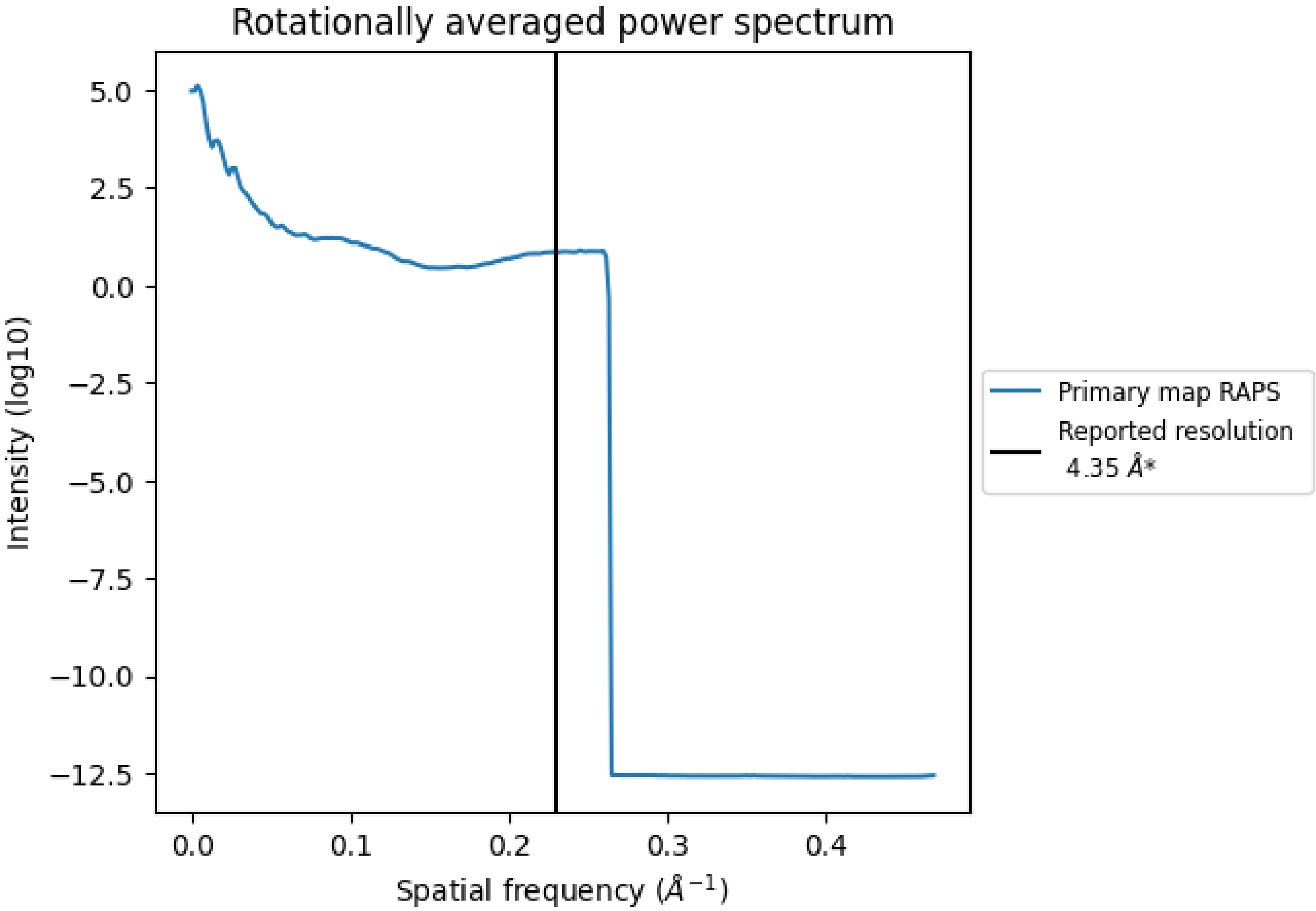
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 752 nm^3; this corresponds to an approximate mass of 679 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 0.230 Å^{-1}

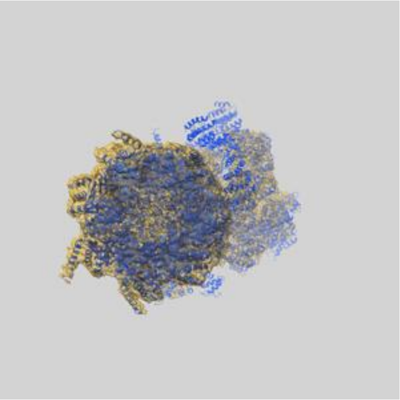
8 Fourier-Shell correlation ⓘ

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

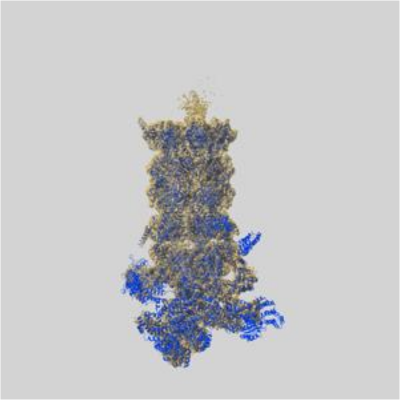
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-9511 and PDB model 5GJQ. Per-residue inclusion information can be found in section 3 on page 12.

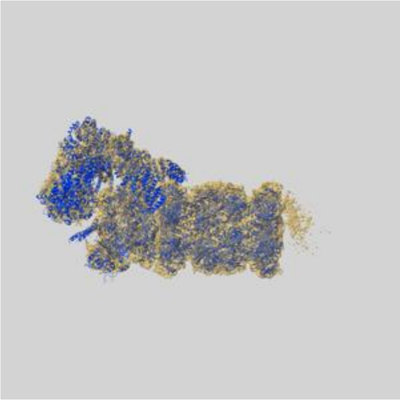
9.1 Map-model overlay ⓘ



X



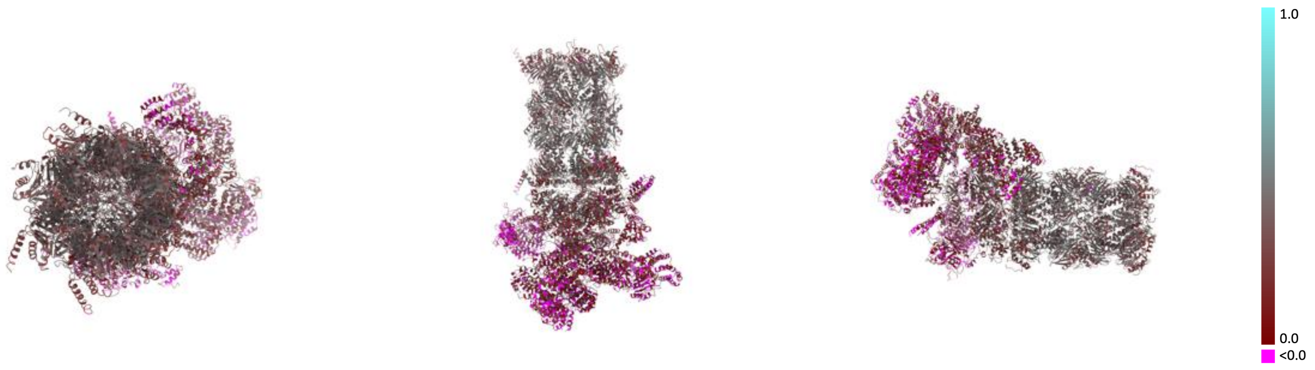
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.033 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

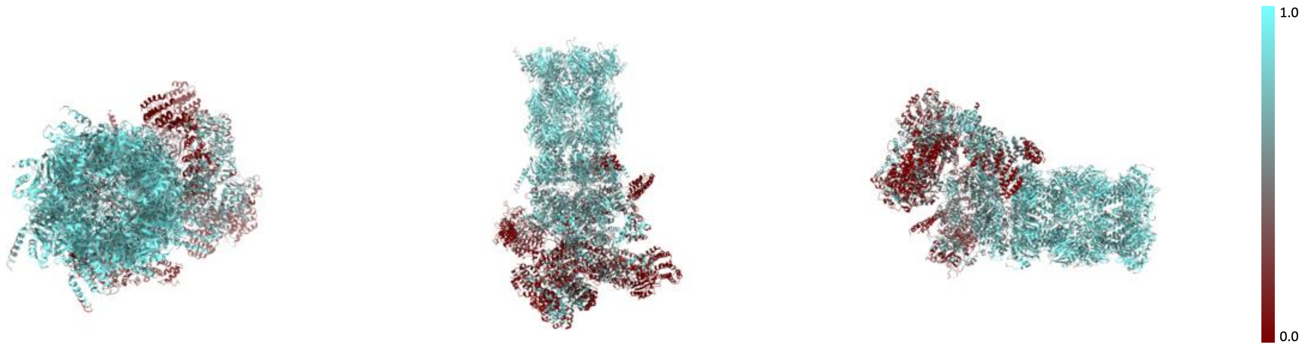
9.2 Q-score mapped to coordinate model



X Y Z

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

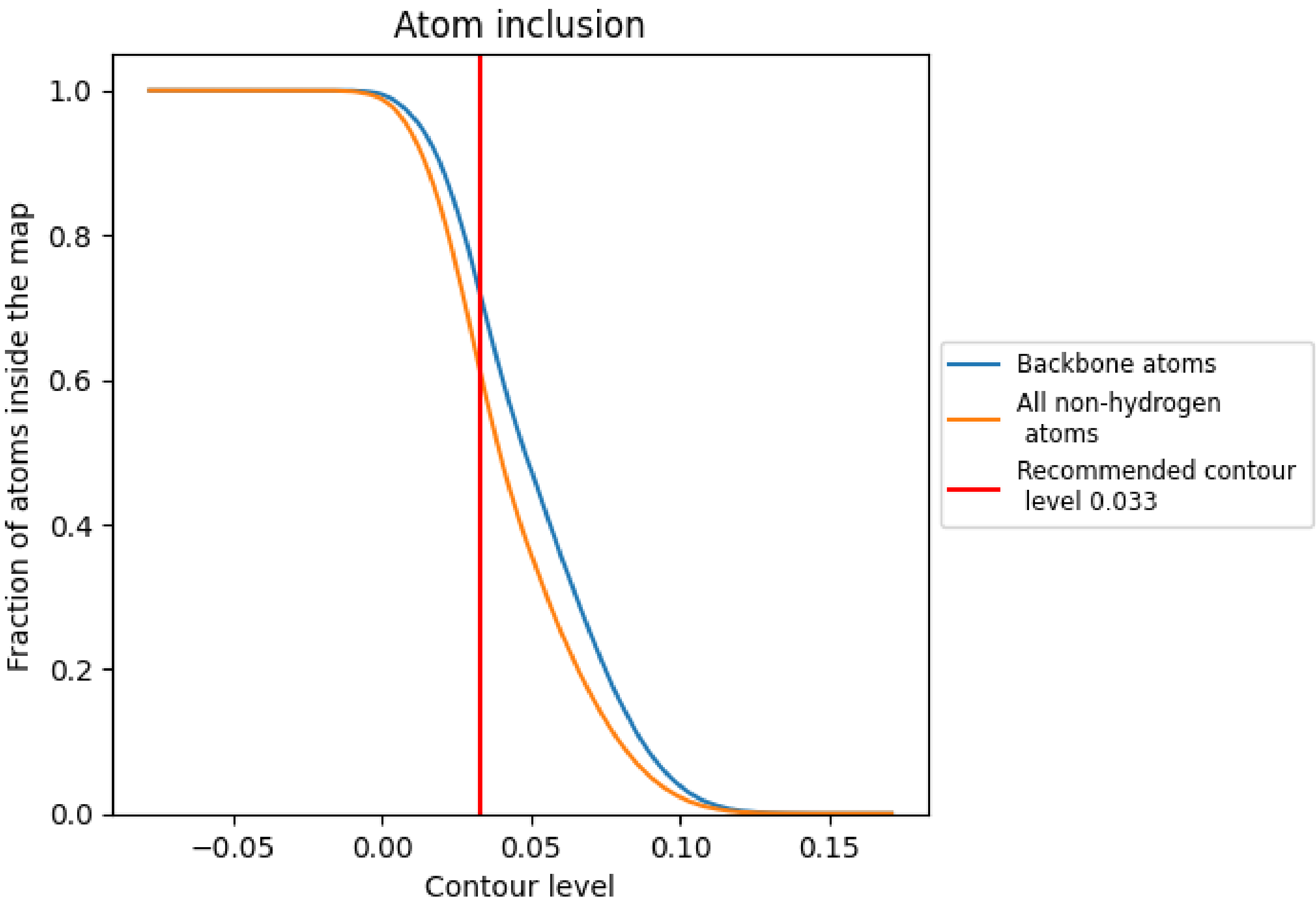
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.033).

9.4 Atom inclusion ⓘ



At the recommended contour level, 72% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.033) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6086	0.2740
B	0.7939	0.3520
C	0.8172	0.3590
D	0.8031	0.3480
E	0.7651	0.3130
F	0.7885	0.3570
G	0.8008	0.3490
H	0.6429	0.3090
I	0.6237	0.3070
J	0.6241	0.2940
K	0.6551	0.2840
L	0.6175	0.2840
M	0.6228	0.2930
N	0.3863	0.0710
O	0.2563	0.1060
P	0.3282	0.1410
Q	0.4816	0.2210
R	0.5944	0.2160
S	0.2863	0.1500
T	0.1912	0.1140
U	0.2700	0.1230
V	0.3095	0.1700
W	0.0054	0.0270
X	0.8119	0.3640
Y	0.2760	0.2040
Z	0.0793	0.0230
a	0.8084	0.3870
b	0.8042	0.3810
c	0.8055	0.3870
d	0.8300	0.3760
e	0.8264	0.3890
f	0.8467	0.3860
g	0.8618	0.4020
h	0.7822	0.3800
i	0.7943	0.3970

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Chain	Atom inclusion	Q-score
j	🟦 0.7643	🟫 0.3570
k	🟦 0.7647	🟫 0.3420
l	🟦 0.7860	🟫 0.3670
m	🟦 0.8124	🟫 0.3770
n	🟦 0.7874	🟫 0.3670
o	🟦 0.8395	🟫 0.3930
p	🟦 0.8346	🟫 0.3940
q	🟦 0.8350	🟫 0.4030
r	🟦 0.8143	🟫 0.3910
s	🟦 0.8594	🟫 0.3920
t	🟦 0.7998	🟫 0.3950
u	🟦 0.8162	🟫 0.3960
x	🟫 0.3774	🟥 0.1260
y	🟫 0.2703	🟥 0.0860