



Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 05:27 AM UTC

PDB ID : 6MSK / pdb_00006msk
EMDB ID : EMD-9222
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.20 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

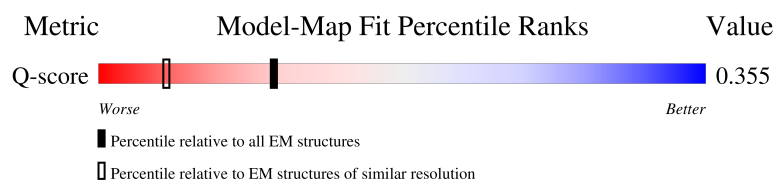
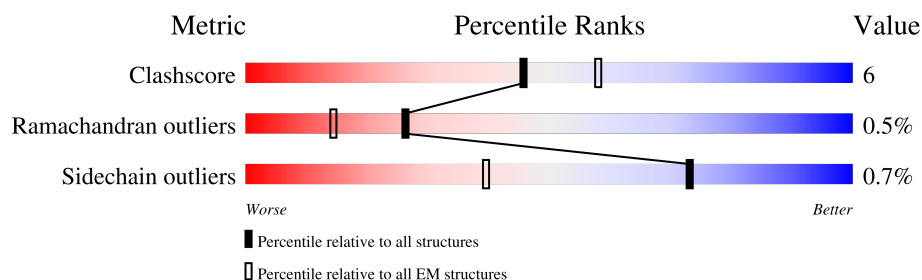
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	U	953	54% 73% 17% 8%
2	V	533	51% 68% 22% 10%
3	W	456	55% 77% 22% .
4	X	422	28% 79% 11% 10%

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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	309	
10	d	349	
11	e	70	
12	f	892	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	v	36	
20	G	245	
20	g	245	
21	H	233	
21	h	233	
22	I	260	
22	i	260	
23	J	247	
23	j	247	
24	K	240	
24	k	240	

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Mol	Chain	Length	Quality of chain
25	L	268	
25	l	268	
26	M	254	
26	m	254	
27	N	238	
27	n	238	
28	O	276	
28	o	276	
29	P	204	
29	p	204	
30	Q	201	
30	q	201	
31	R	262	
31	r	262	
32	S	240	
32	s	240	
33	T	263	
33	t	263	

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 105222 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	872	Total	C	N	O	S	0	0
			6828	4328	1157	1298	45		

- Molecule 2 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	456	Total	C	N	O	S	0	0
			3703	2339	635	704	25		

- Molecule 4 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	X	380	Total	C	N	O	S	0	0
			3009	1918	509	570	12		

- Molecule 5 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 6 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 7 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	d	257	Total	C	N	O	S	0	0
			2116	1371	346	390	9		

- Molecule 11 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	e	40	Total	C	N	O	S	0	0
			334	200	55	77	2		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	f	889	Total	C	N	O	S	0	0
			6866	4315	1174	1331	46		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

- Molecule 14 is a protein called Rpt2, NP_002793.2 (26SHA chain B).

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	411	Total	C	N	O	S	0	0
			3207	2022	548	622	15		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	396	Total	C	N	O	S	0	0
			3105	1954	558	576	17		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

- Molecule 18 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 19 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	v	36	Total	C	N	O	0	0
			180	108	36	36		

- Molecule 20 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	G	239	Total	C	N	O	S	0	0
			1820	1157	304	346	13		
20	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 21 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	H	230	Total	C	N	O	S	0	0
			1692	1073	285	329	5		
21	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
22	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 23 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	J	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		
23	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 24 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	K	228	Total	C	N	O	S	0	0
			1729	1086	284	349	10		
24	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 25 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		
25	l	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 26 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	m	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 27 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		
27	n	191	Total	C	N	O	S	0	0
			1430	893	245	280	12		

- Molecule 28 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	O	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		
28	o	220	Total	C	N	O	S	0	0
			1643	1033	280	318	12		

- Molecule 29 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		
29	p	204	Total	C	N	O	S	0	0
			1585	1010	262	294	19		

- Molecule 30 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
30	q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		

- Molecule 31 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		
31	r	201	Total	C	N	O	S	0	0
			1548	974	273	292	9		

- Molecule 32 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	S	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		
32	s	213	Total	C	N	O	S	0	0
			1641	1036	282	313	10		

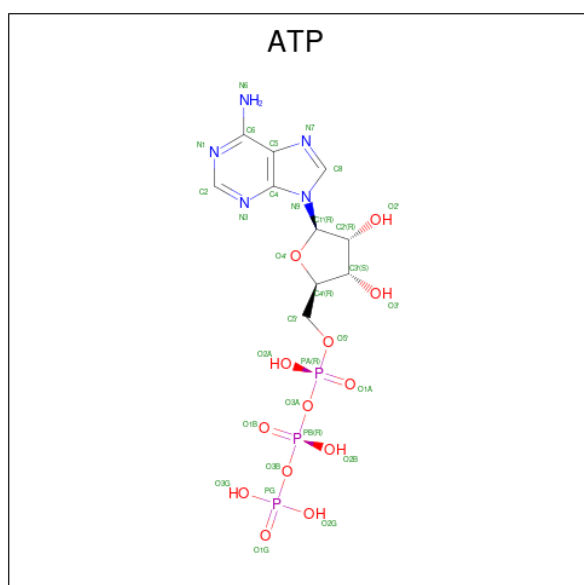
- Molecule 33 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
33	t	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	Zn	0
			1	1	

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



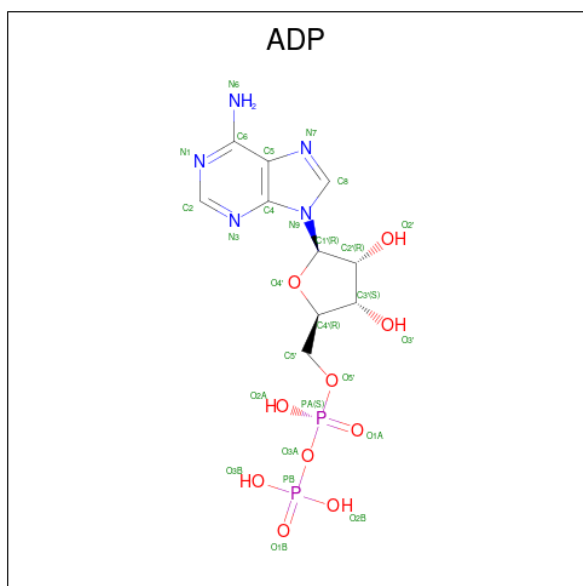
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Mol	Chain	Residues	Atoms					AltConf
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
36	A	1	Total	Mg	0
			1	1	
36	B	1	Total	Mg	0
			1	1	
36	C	1	Total	Mg	0
			1	1	
36	D	1	Total	Mg	0
			1	1	
36	F	1	Total	Mg	0
			1	1	

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

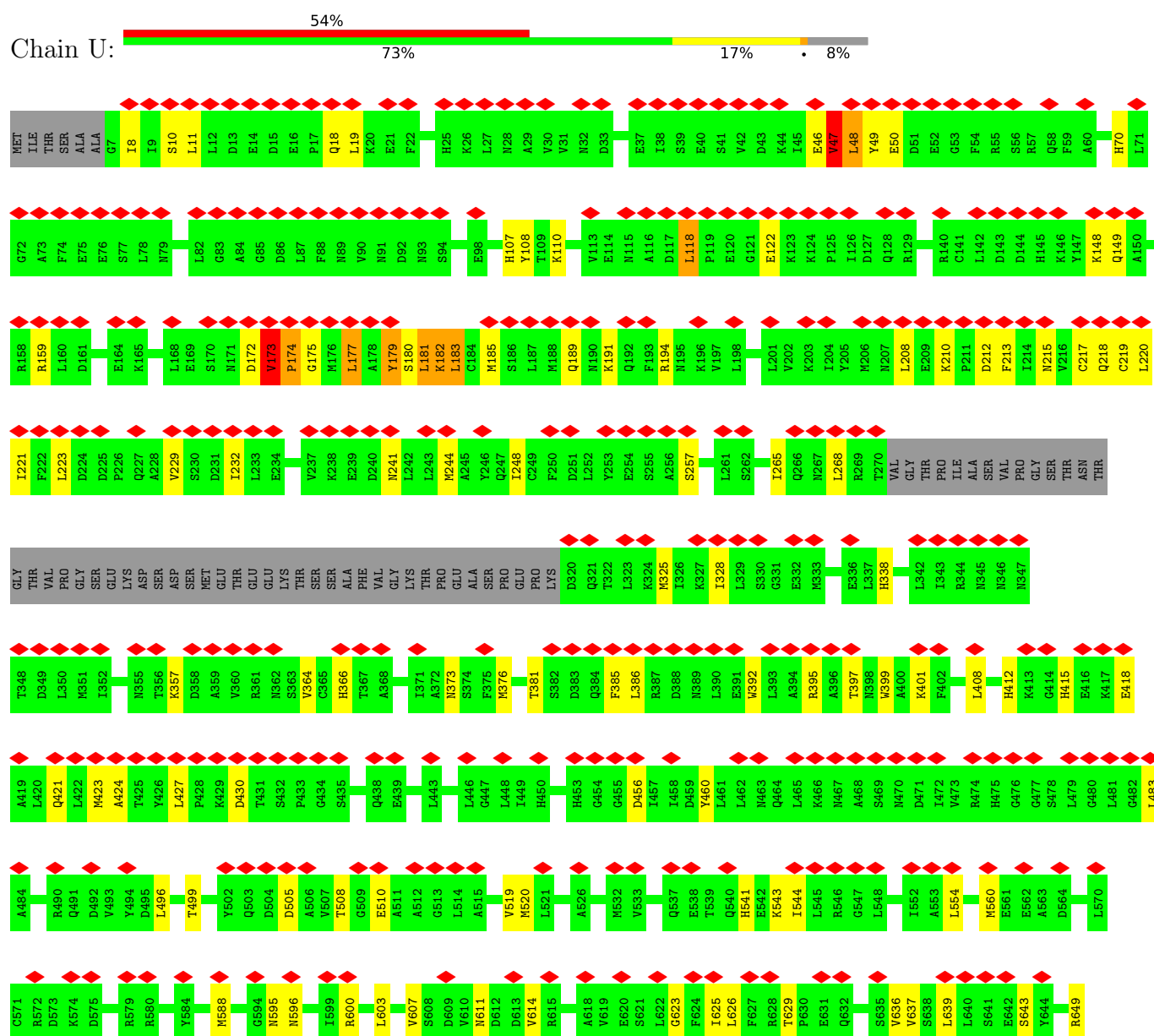


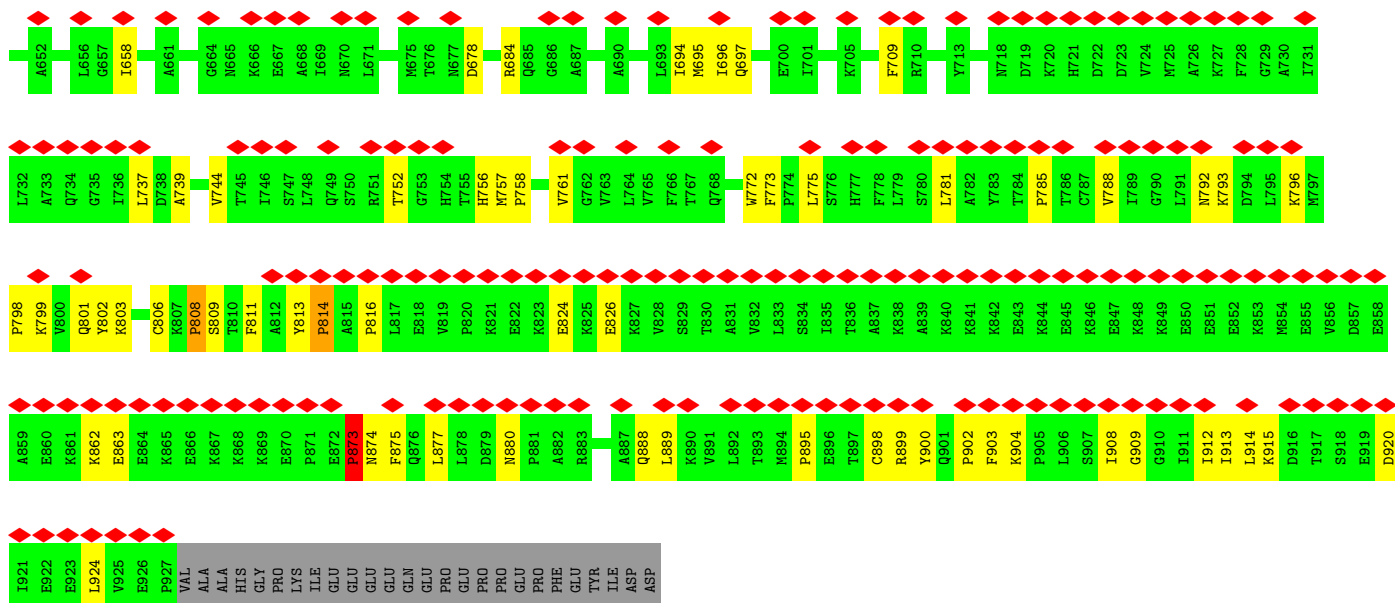
Mol	Chain	Residues	Atoms					AltConf
37	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

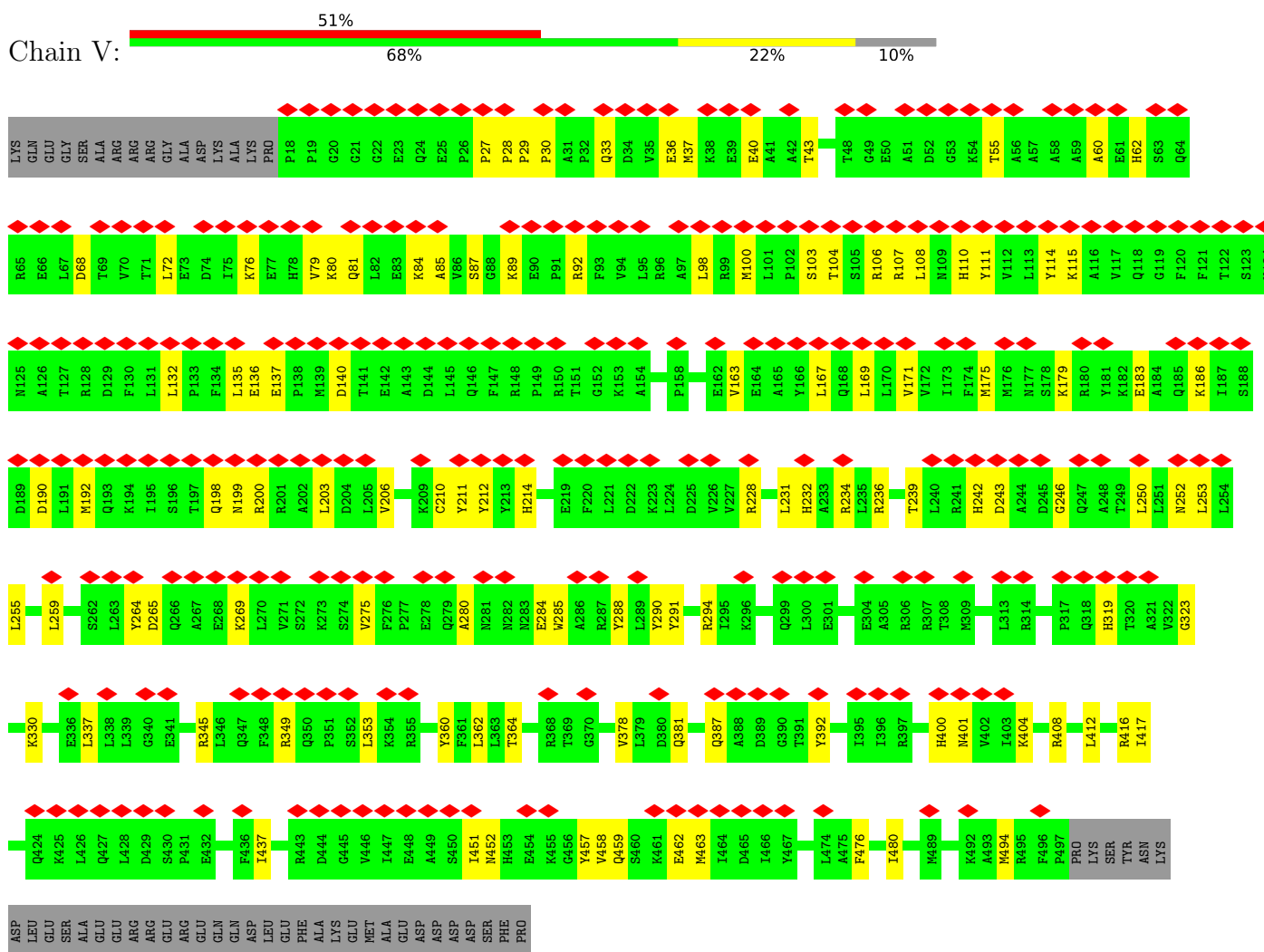
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S proteasome non-ATPase regulatory subunit 1

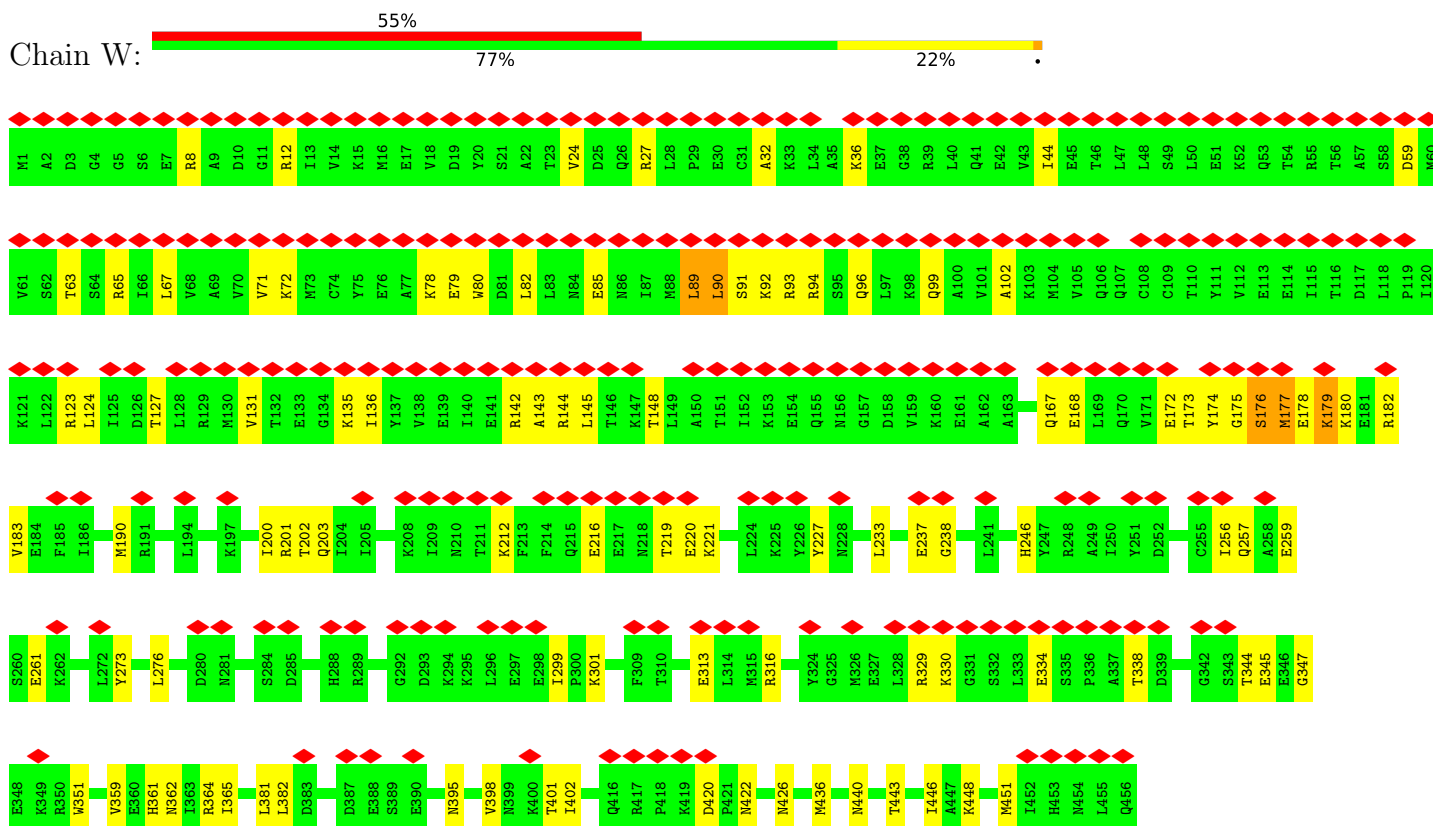




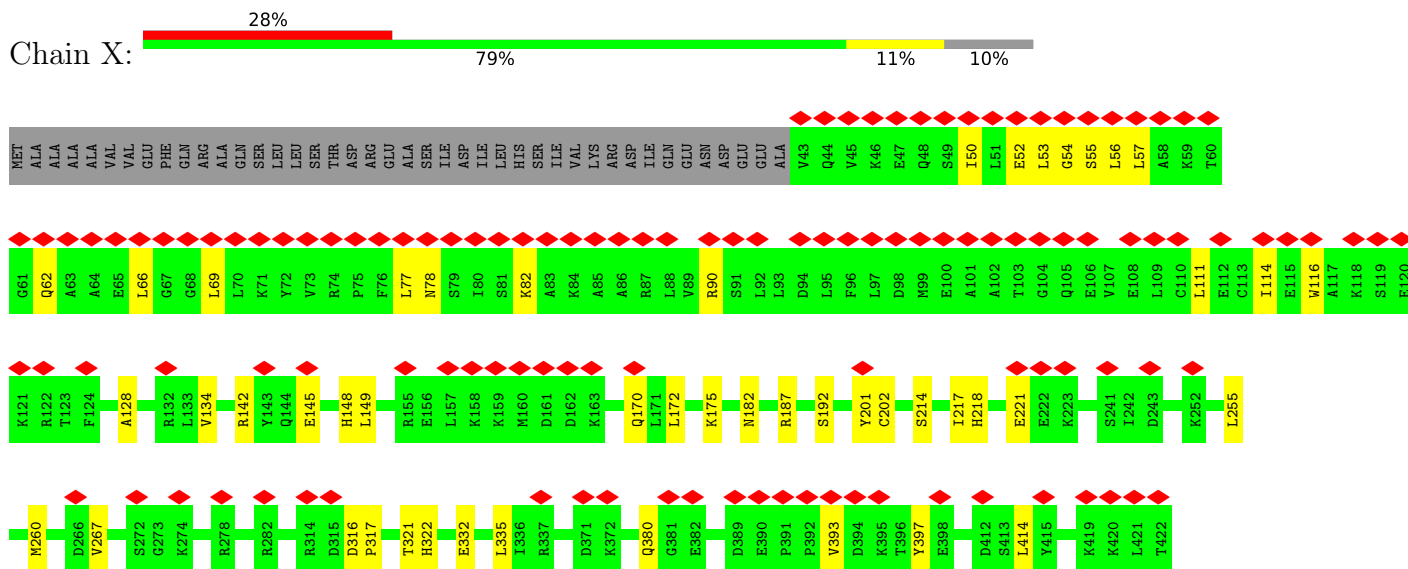
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3



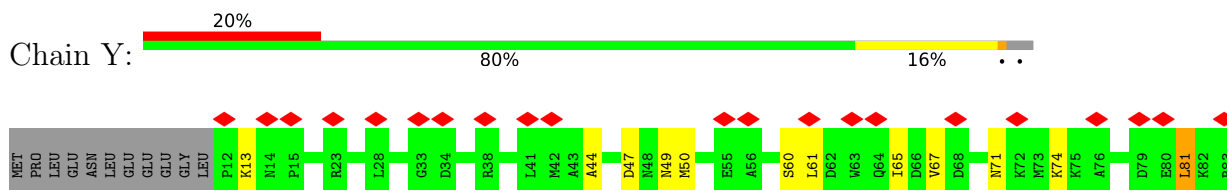
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

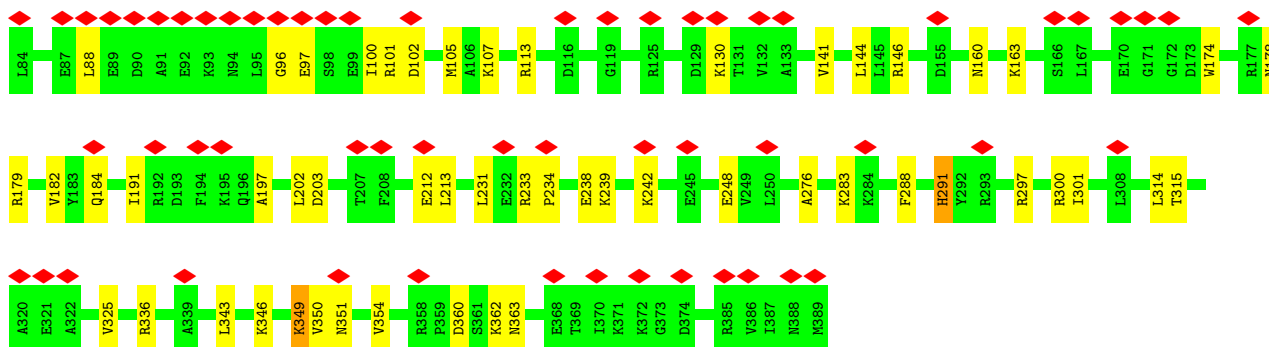


• Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

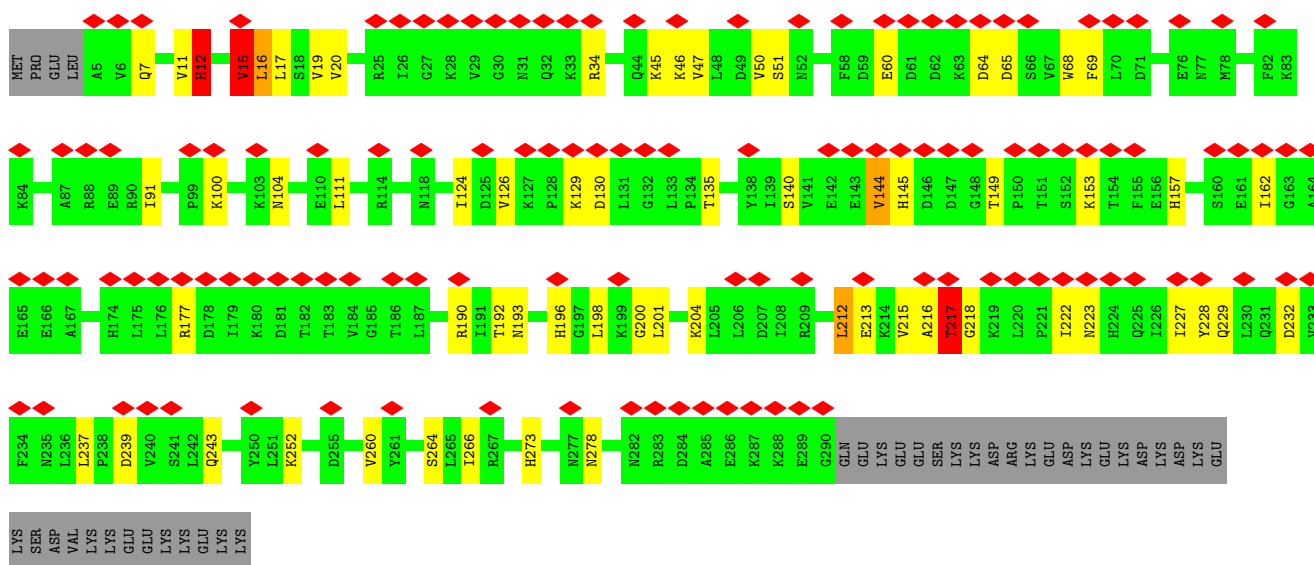


• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

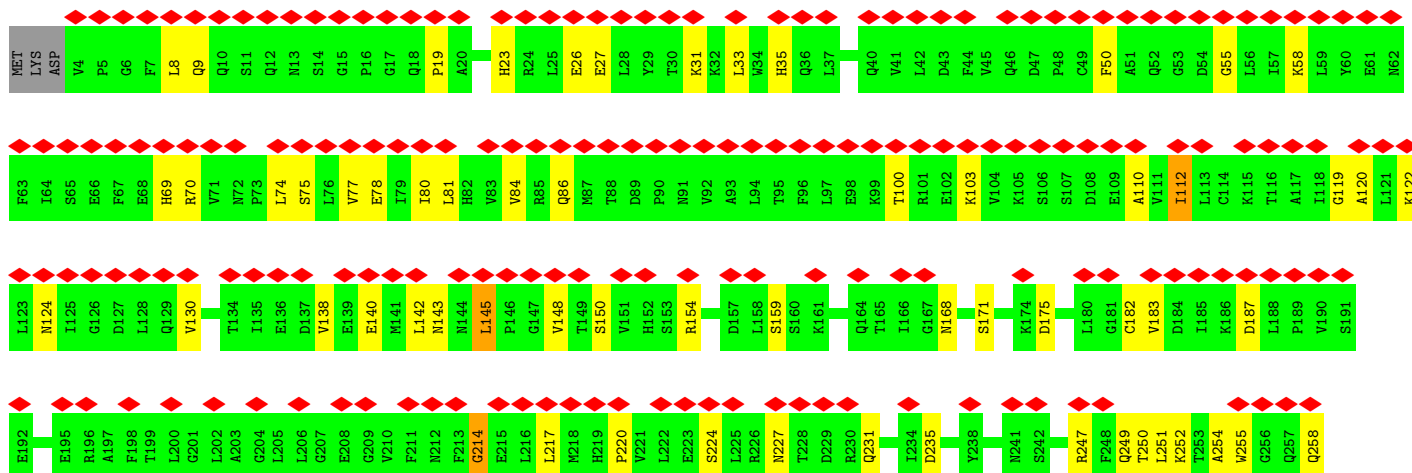
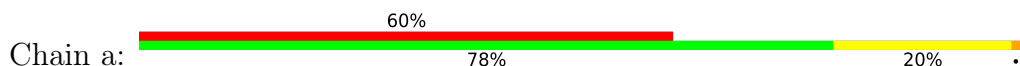


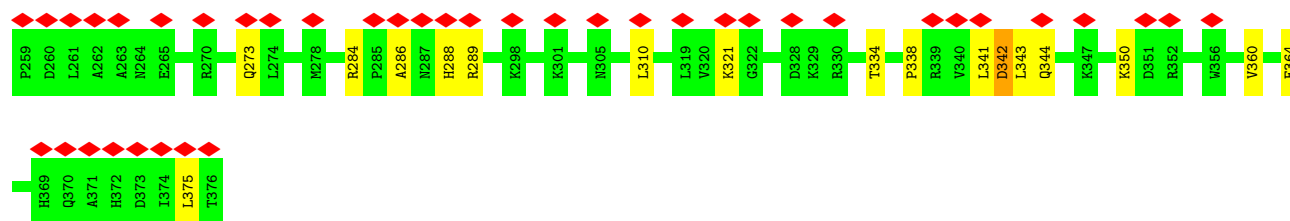


• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

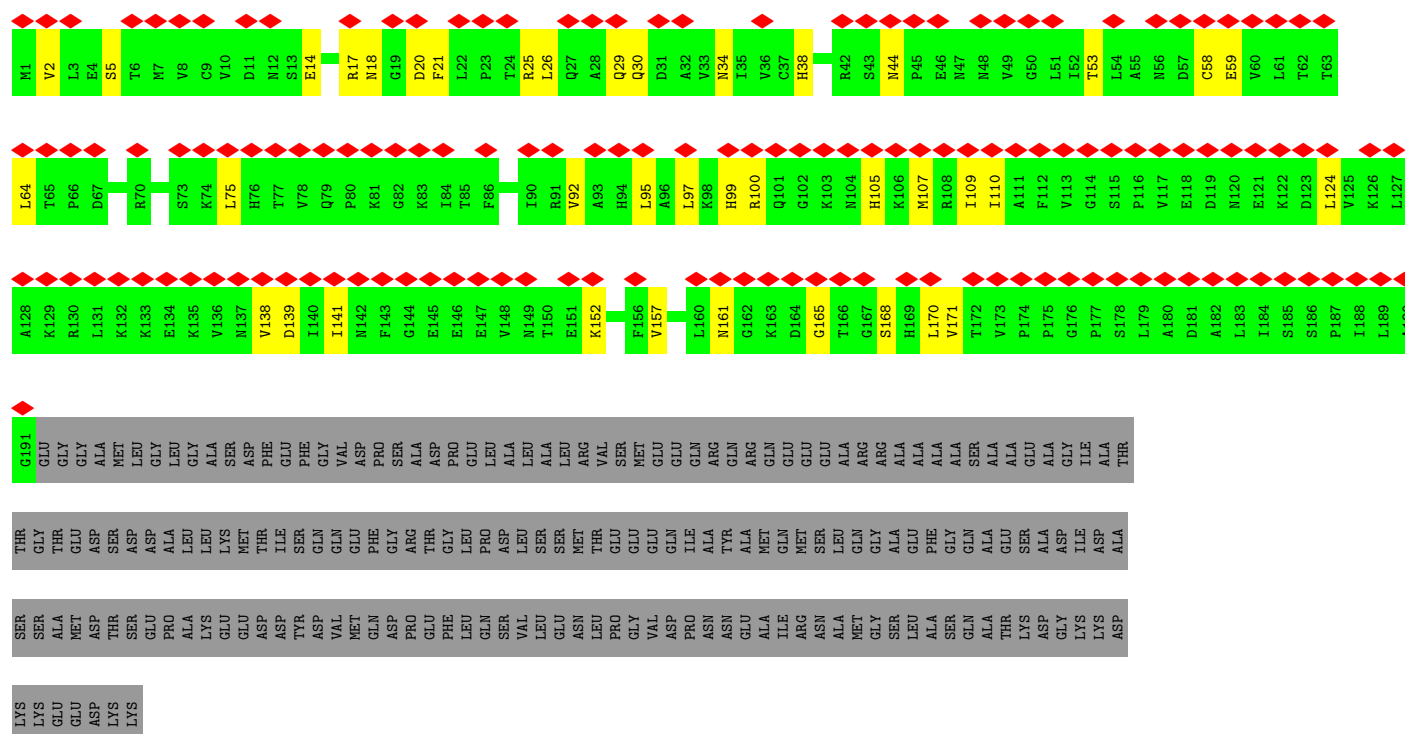
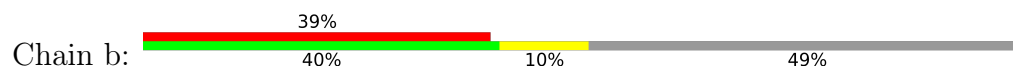


• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

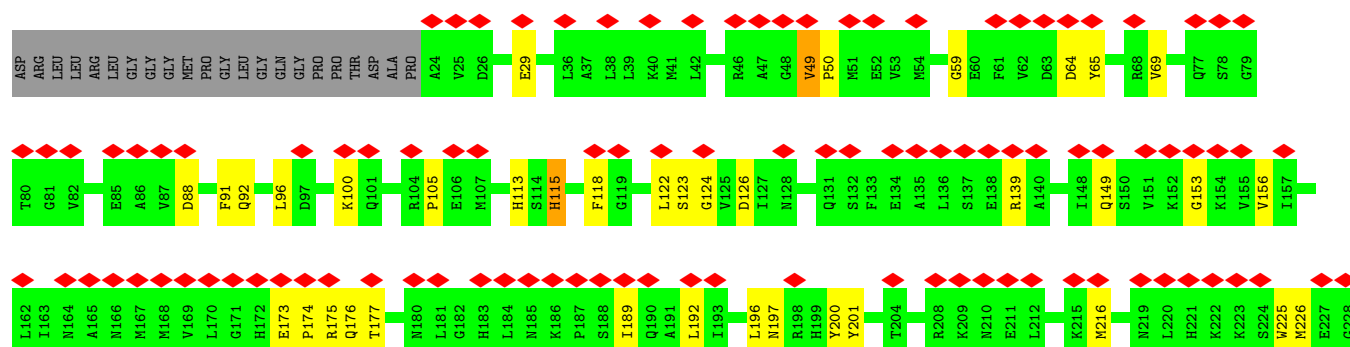


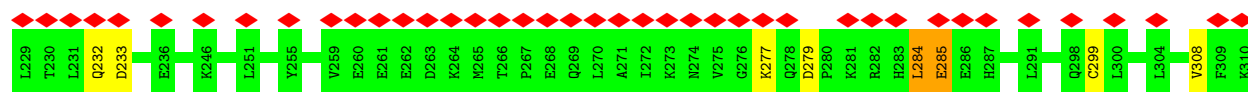


- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

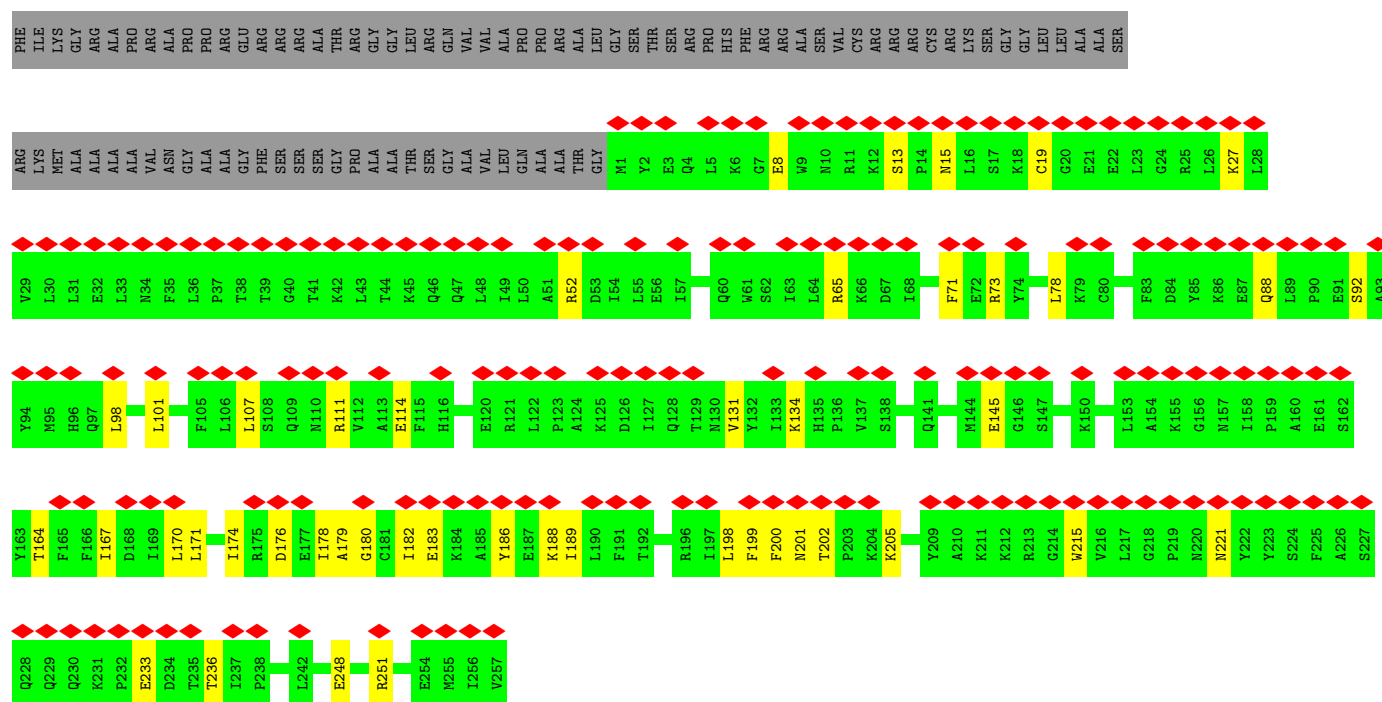


- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

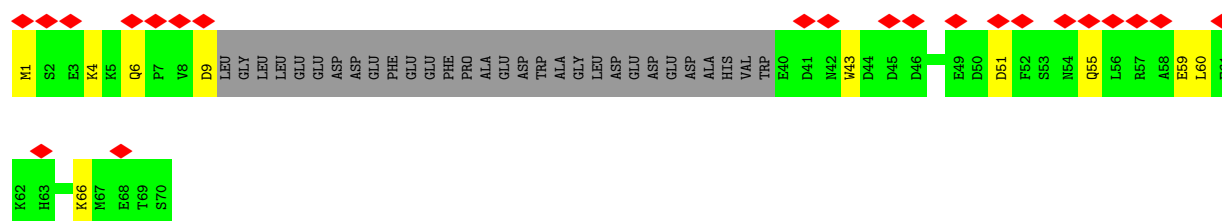
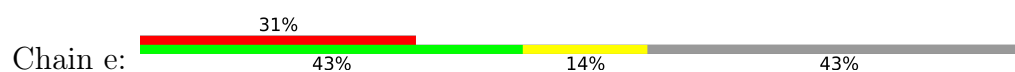




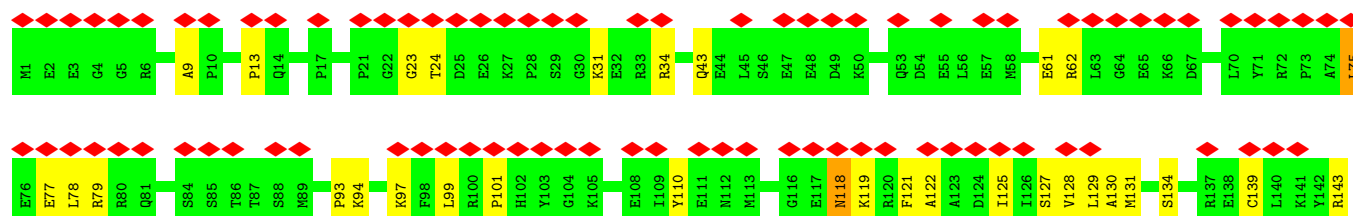
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

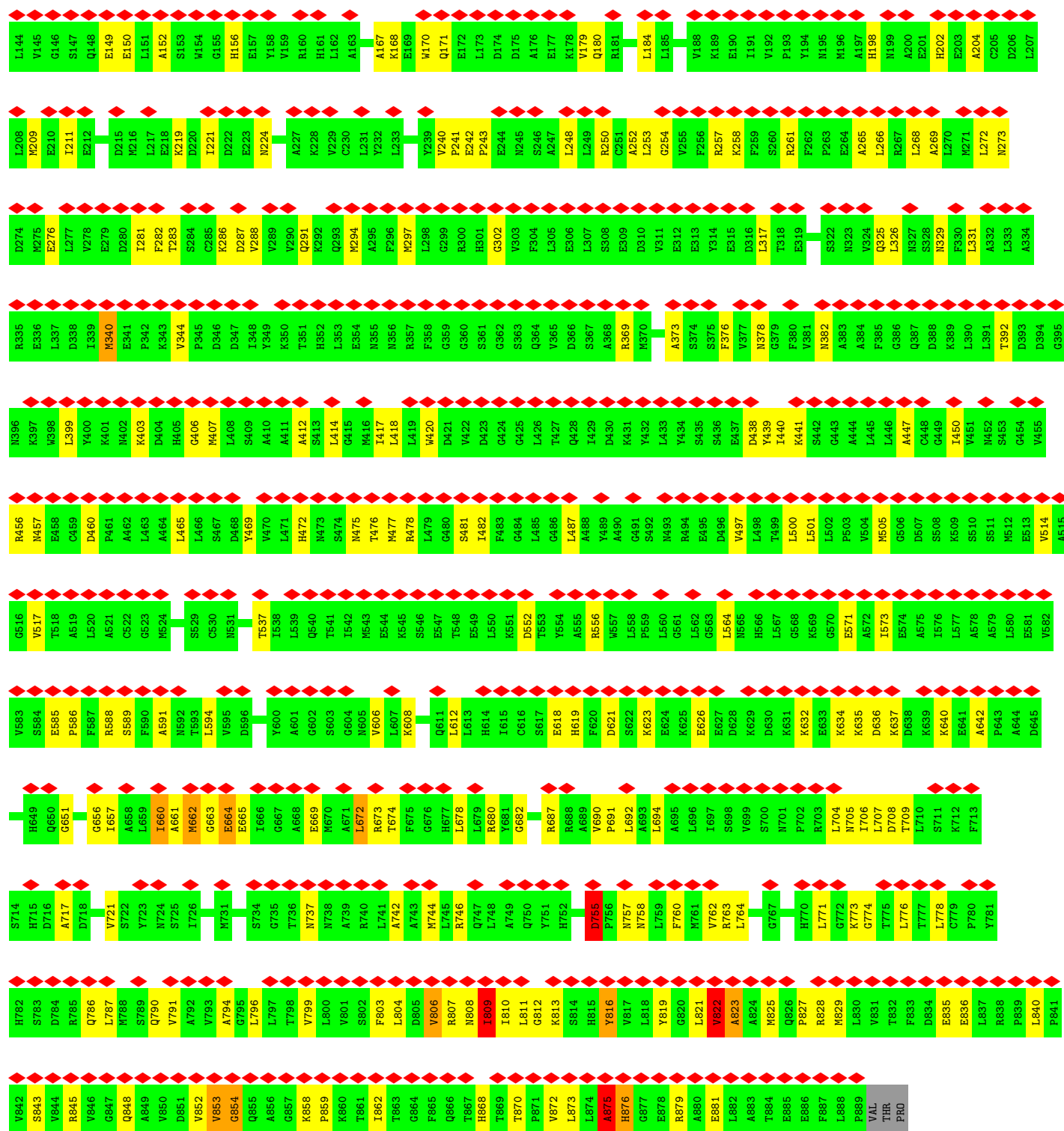


• Molecule 11: 26S proteasome complex subunit SEM1

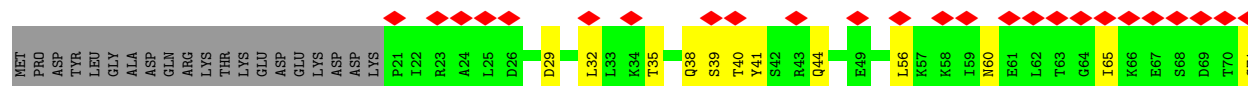
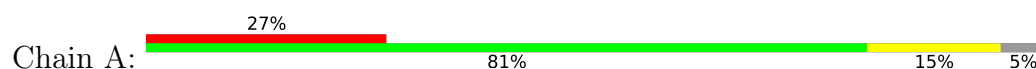


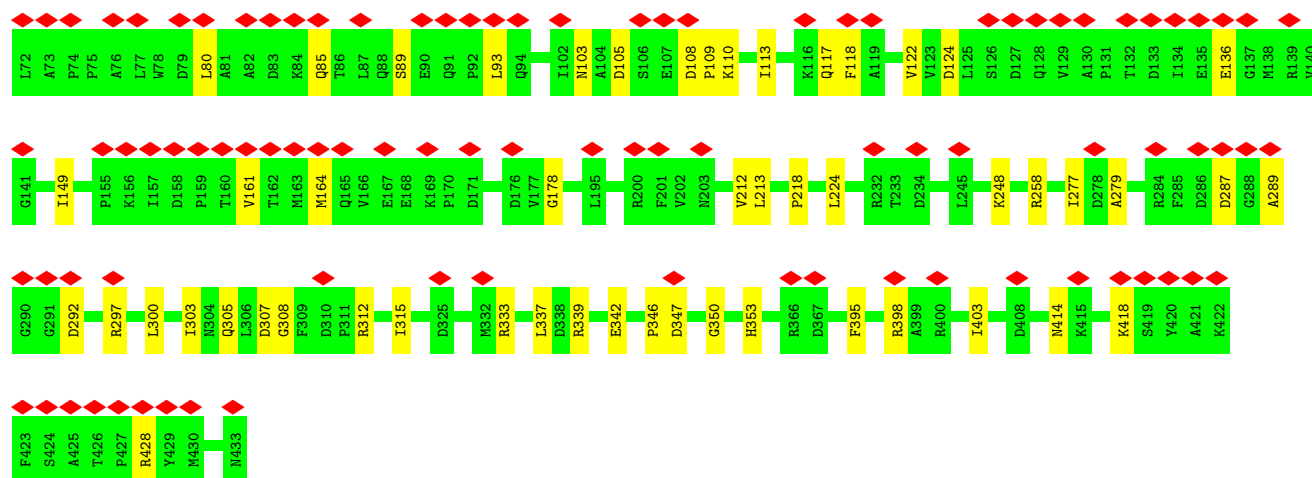
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2



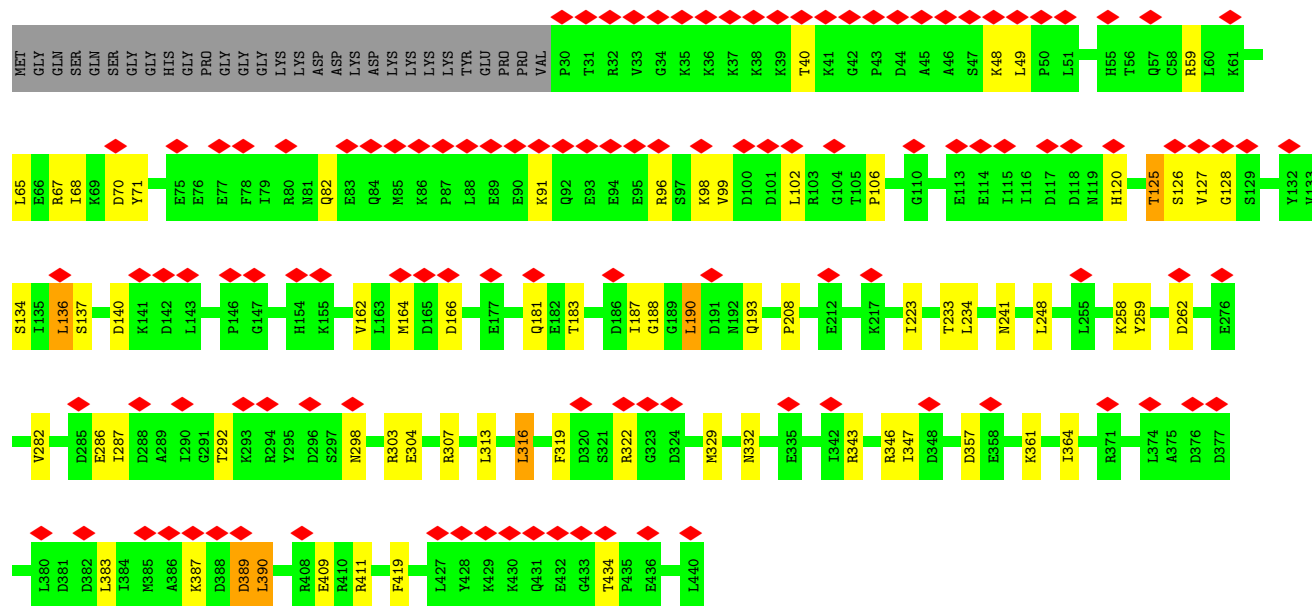
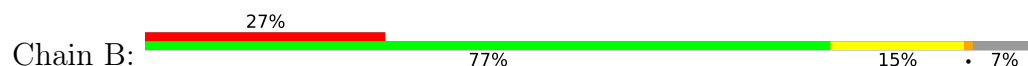


• Molecule 13: 26S proteasome regulatory subunit 7

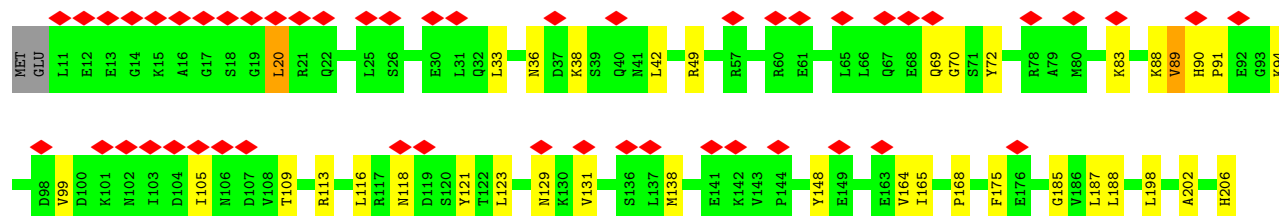
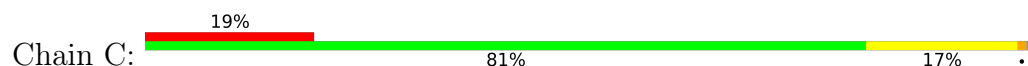


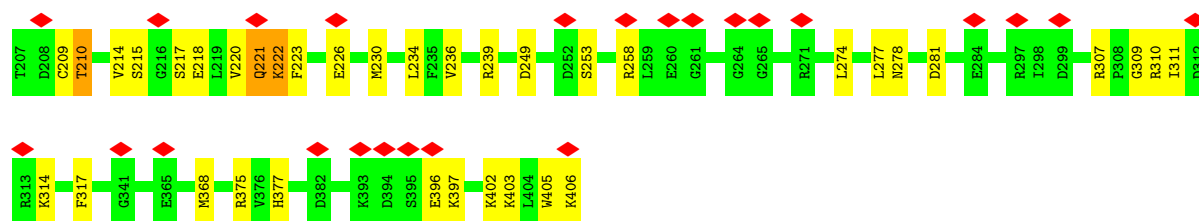


- Molecule 14: Rpt2, NP_002793.2 (26SHA chain B)

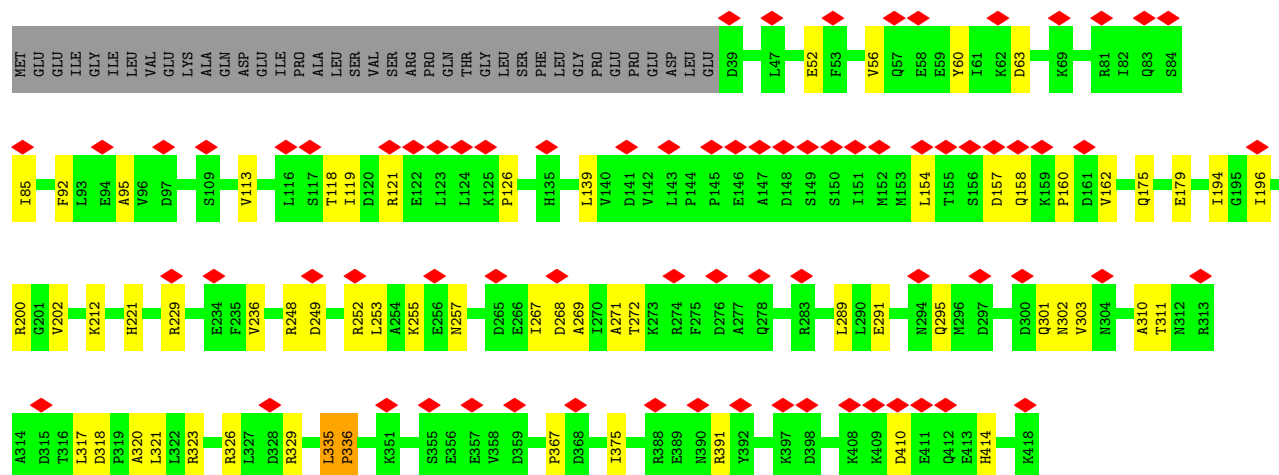
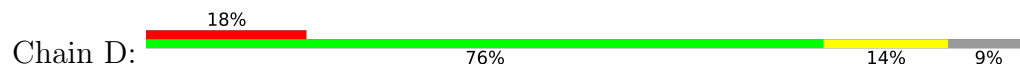


- Molecule 15: 26S proteasome regulatory subunit 8

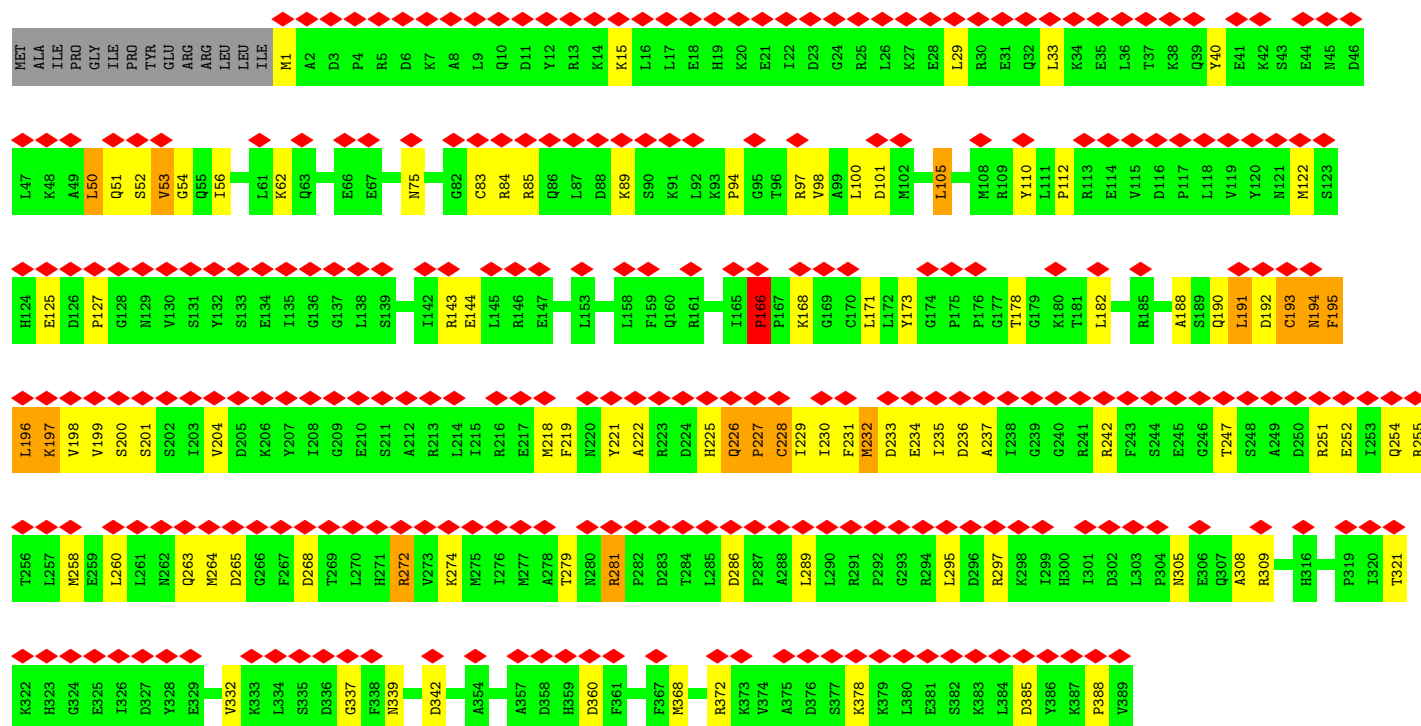
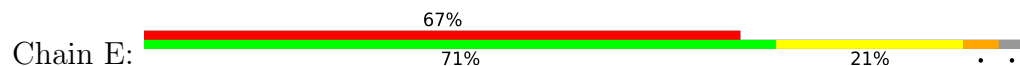




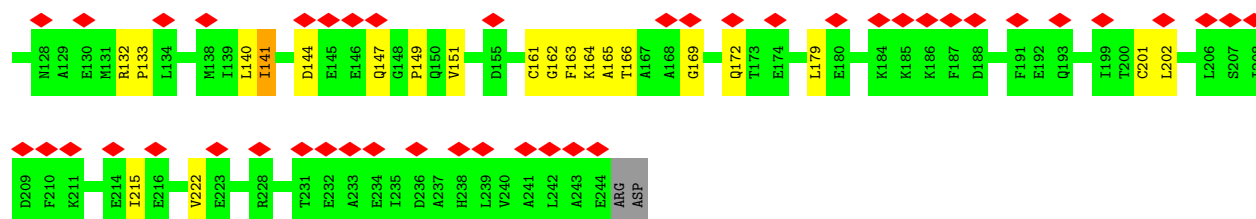
• Molecule 16: 26S proteasome regulatory subunit 6B



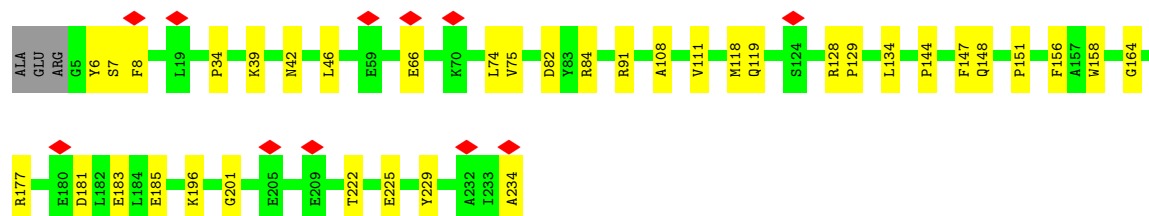
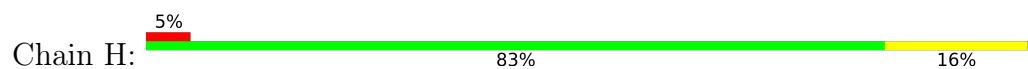
• Molecule 17: 26S proteasome regulatory subunit 10B



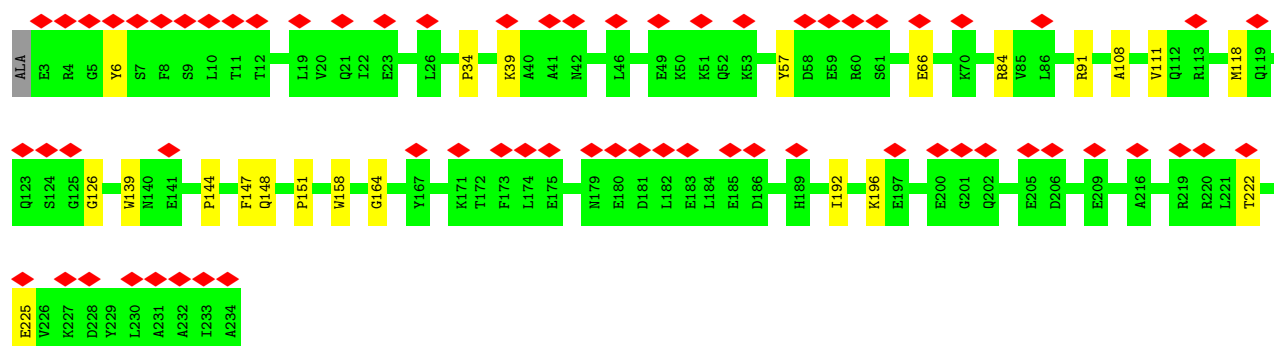
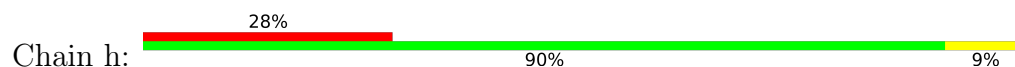
SER	ARG	GLY
S5		
S6		
A7		
G8		
F9		
D10		
R11		
H12		
I13		
T14		
I15		
E19		
G20		
R21		
L22		
Y23		
Q24		
I32		
N33		
Q34		
A41		
V42		
R43		
G44		
K45		
D46		
Q53		
K54		
K55		
V56		
P57		
D58		
K59		
L60		
L61		
D62		
L69		
E74		
G82		
M83		
D86		
S89		
E108		
L114		
D120		



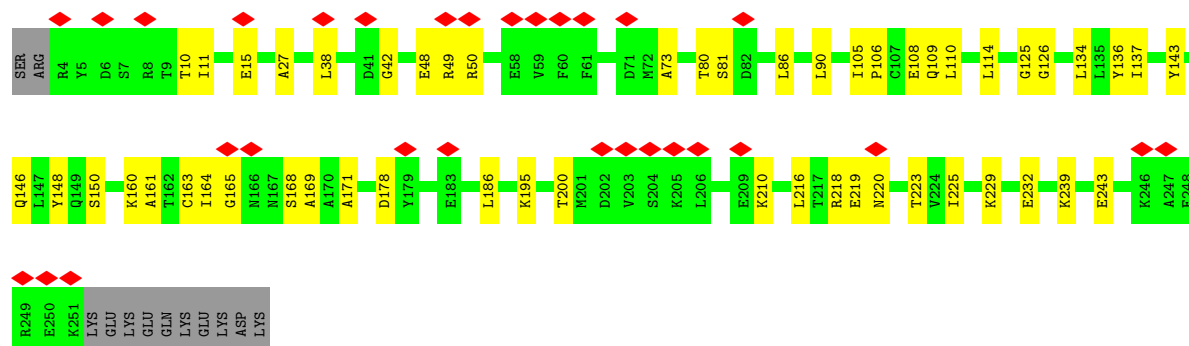
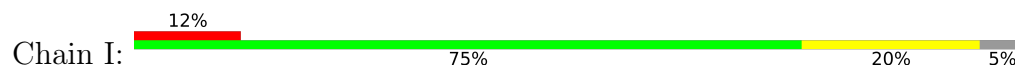
• Molecule 21: Proteasome subunit alpha type-2



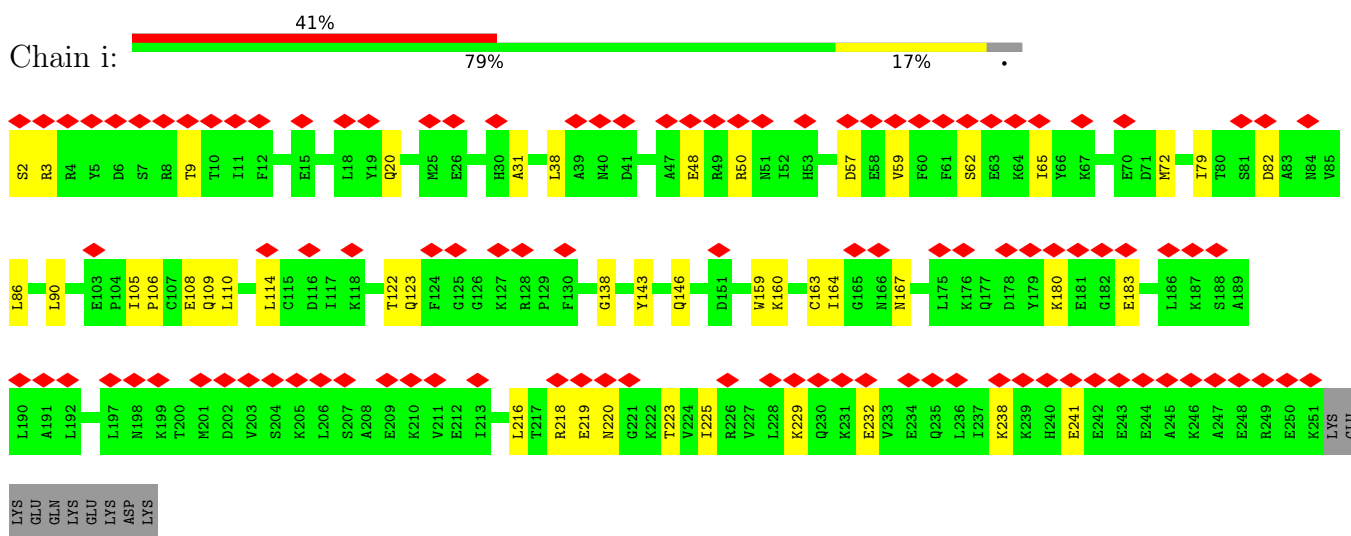
• Molecule 21: Proteasome subunit alpha type-2



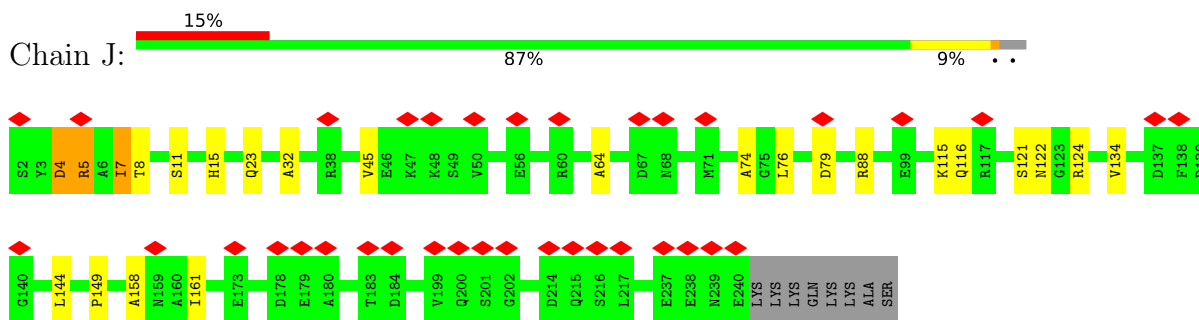
• Molecule 22: Proteasome subunit alpha type-4



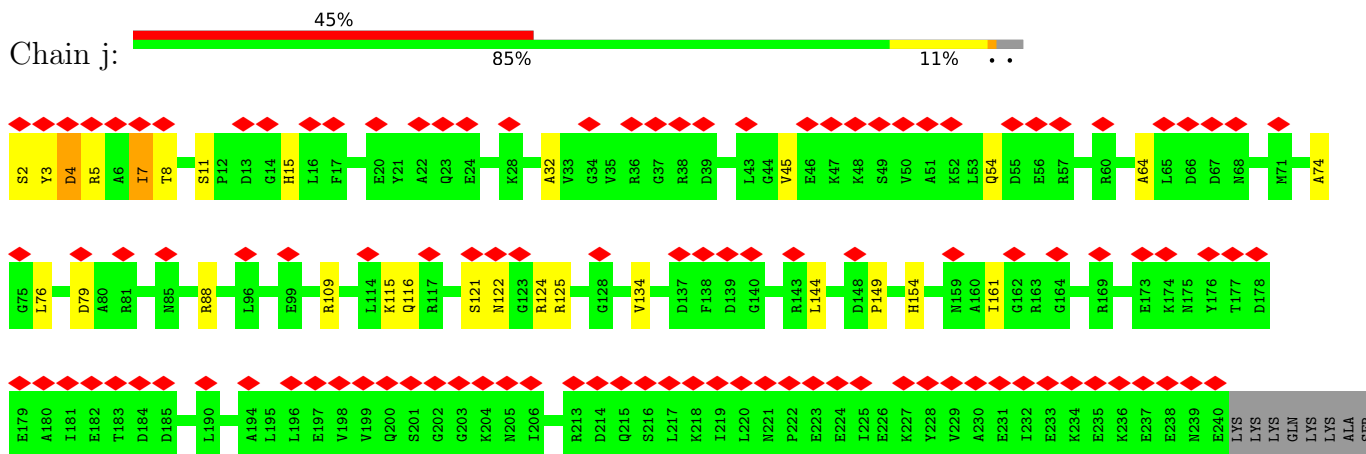
• Molecule 22: Proteasome subunit alpha type-4



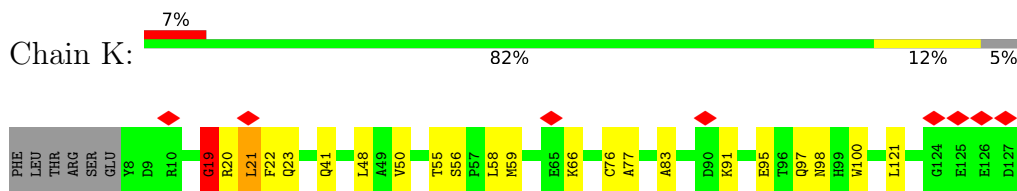
- Molecule 23: Proteasome subunit alpha type-7

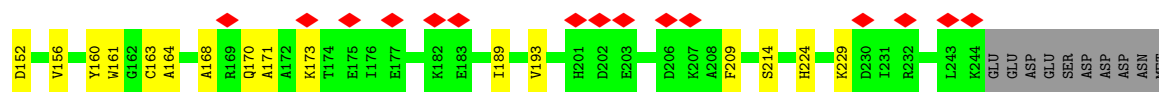


- Molecule 23: Proteasome subunit alpha type-7

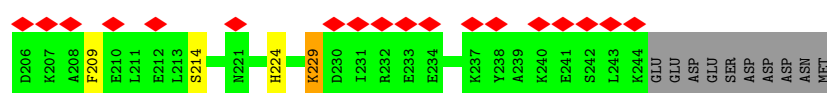
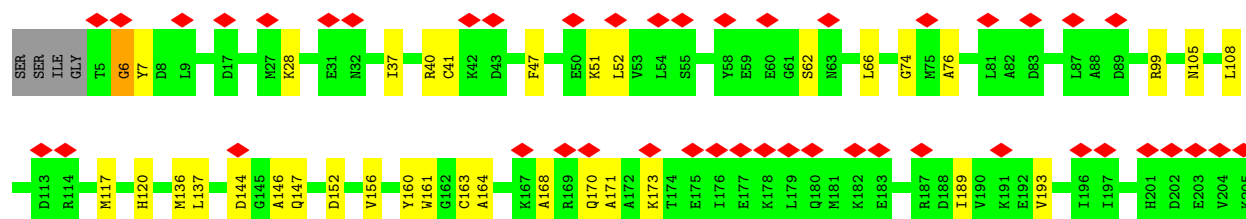
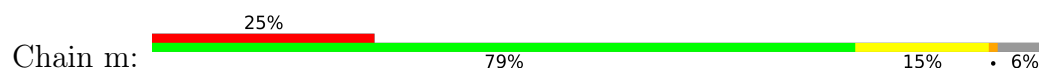


- Molecule 24: Proteasome subunit alpha type-5

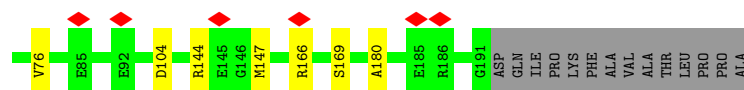
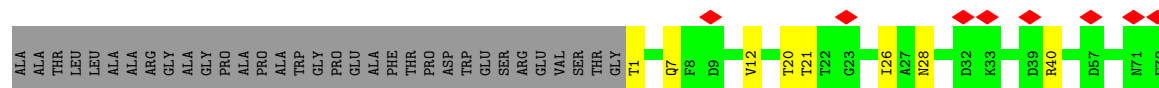
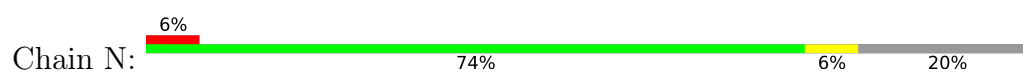




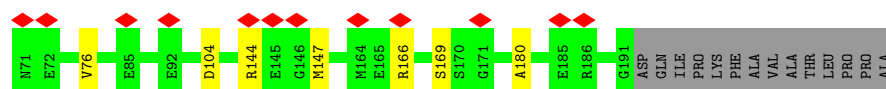
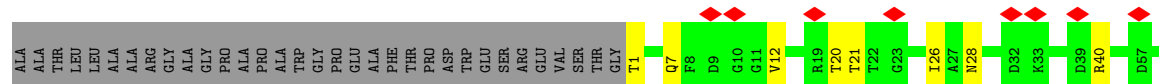
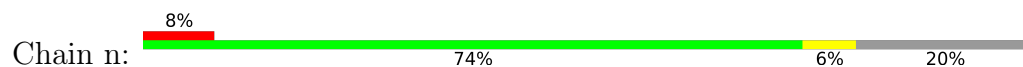
• Molecule 26: Proteasome subunit alpha type-3



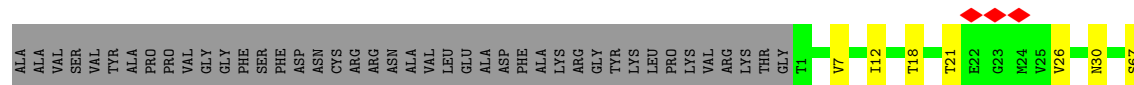
• Molecule 27: Proteasome subunit beta type-6

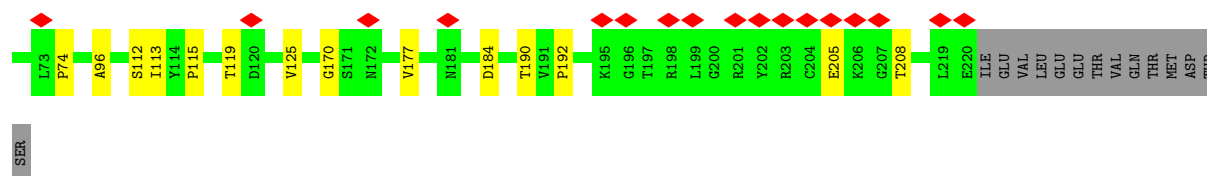


• Molecule 27: Proteasome subunit beta type-6

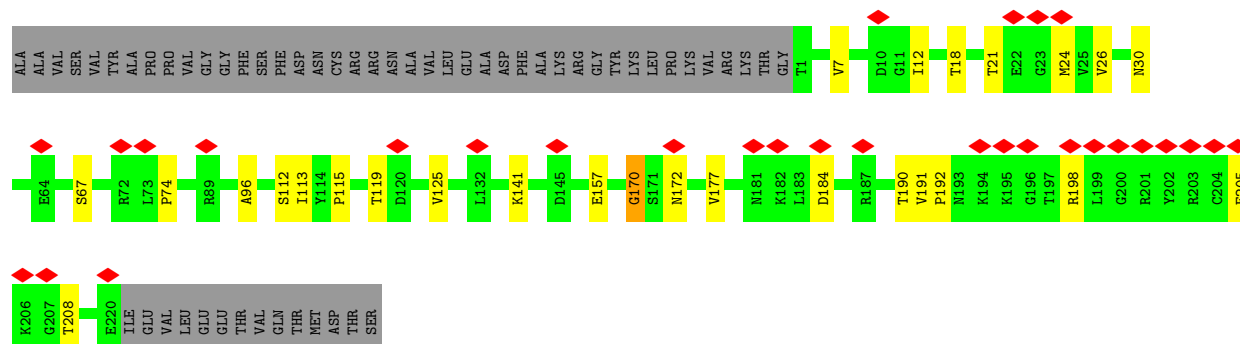


• Molecule 28: Proteasome subunit beta type-7





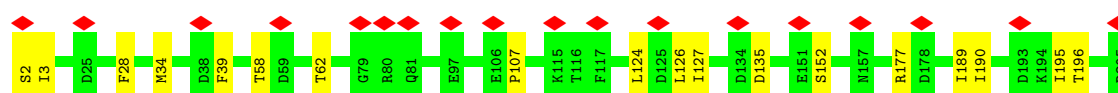
• Molecule 28: Proteasome subunit beta type-7



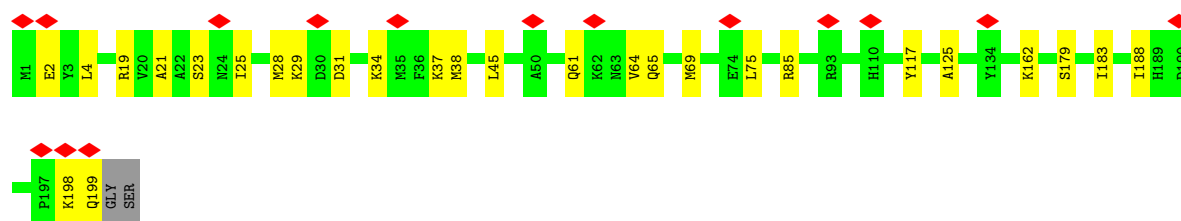
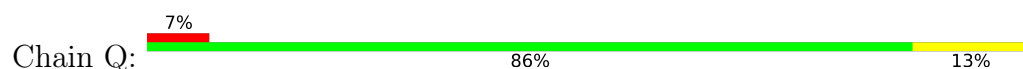
• Molecule 29: Proteasome subunit beta type-3



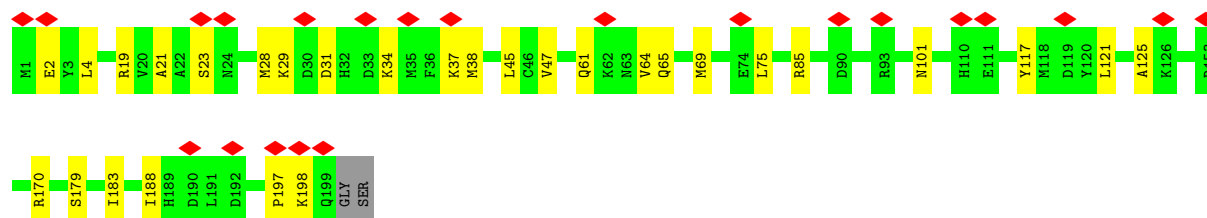
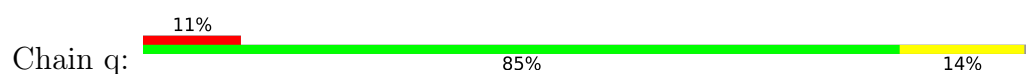
• Molecule 29: Proteasome subunit beta type-3



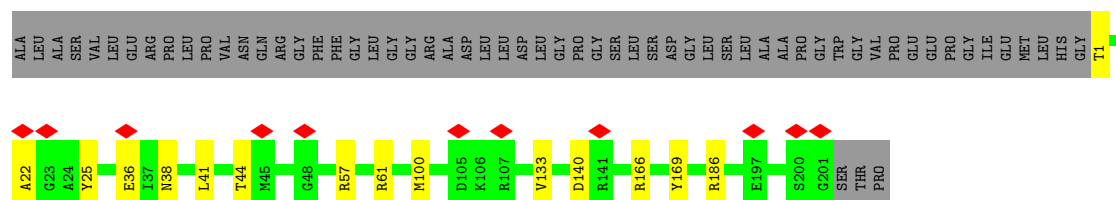
• Molecule 30: Proteasome subunit beta type-2



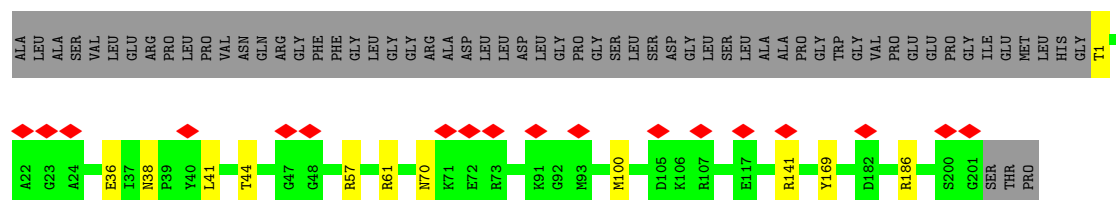
• Molecule 30: Proteasome subunit beta type-2



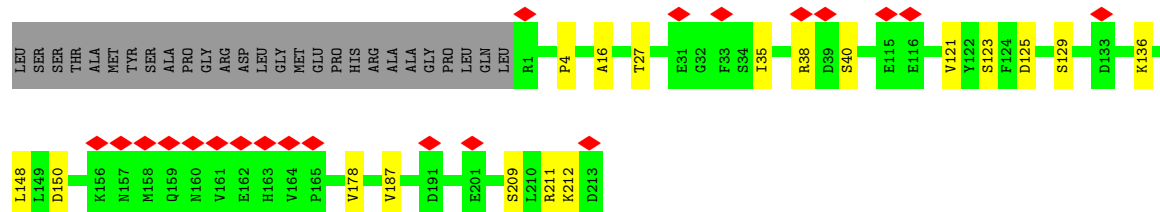
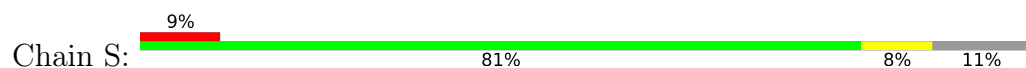
• Molecule 31: Proteasome subunit beta type-5



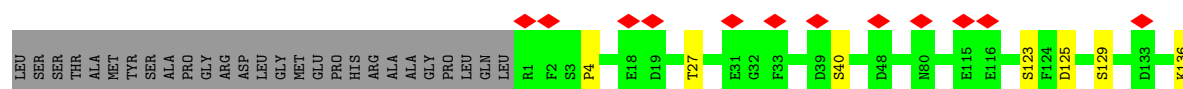
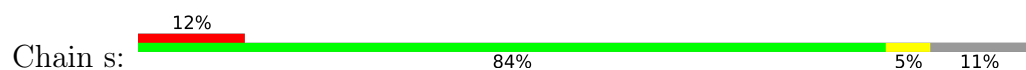
• Molecule 31: Proteasome subunit beta type-5

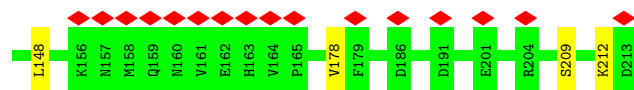


• Molecule 32: Proteasome subunit beta type-1

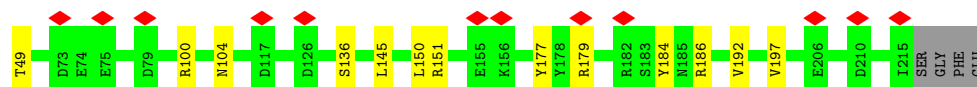
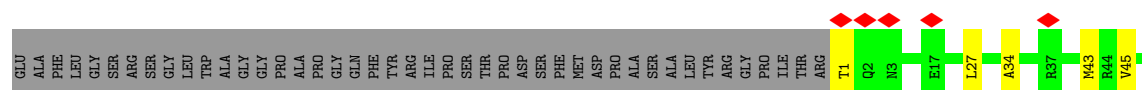
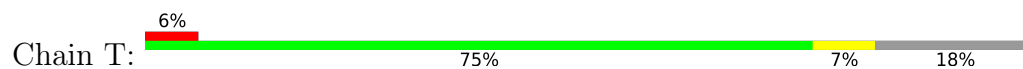


• Molecule 32: Proteasome subunit beta type-1

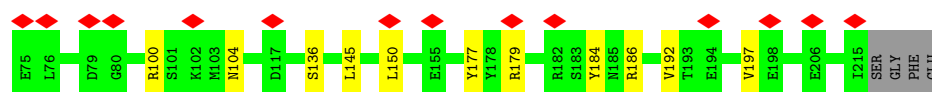
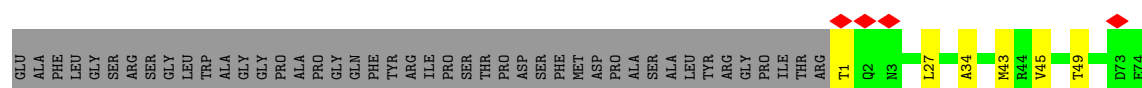
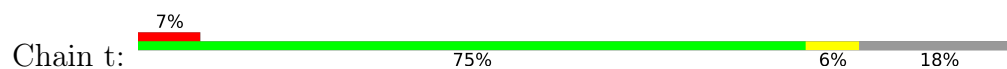




- Molecule 33: Proteasome subunit beta type-4



- Molecule 33: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	348646	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.006	Depositor
Map size ($\text{\AA}$)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.685, 0.685, 0.685	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	U	0.25	0/6945	0.68	12/9382 (0.1%)
2	V	0.26	0/3929	0.69	2/5309 (0.0%)
3	W	0.24	0/3751	0.63	2/5042 (0.0%)
4	X	0.20	0/3053	0.54	0/4115
5	Y	0.24	0/3173	0.64	0/4273
6	Z	0.24	0/2324	0.76	7/3150 (0.2%)
7	a	0.24	0/3053	0.67	2/4133 (0.0%)
8	b	0.22	0/1478	0.61	0/2001
9	c	0.25	0/2302	0.75	2/3110 (0.1%)
10	d	0.24	0/2162	0.65	4/2919 (0.1%)
11	e	0.24	0/338	0.71	0/450
12	f	0.29	0/6980	0.80	11/9433 (0.1%)
13	A	0.22	0/3283	0.59	0/4433
14	B	0.26	0/3254	0.72	4/4388 (0.1%)
15	C	0.24	0/3146	0.65	2/4226 (0.0%)
16	D	0.25	0/3090	0.65	1/4168 (0.0%)
17	E	0.26	0/3145	0.74	6/4233 (0.1%)
18	F	0.22	0/3137	0.62	2/4223 (0.0%)
20	G	0.22	0/1853	0.57	0/2515
20	g	0.19	0/1859	0.54	0/2523
21	H	0.21	0/1727	0.52	0/2350
21	h	0.18	0/1743	0.44	0/2372
22	I	0.23	0/1925	0.65	4/2606 (0.2%)
22	i	0.18	0/1942	0.53	0/2628
23	J	0.18	0/1728	0.52	2/2358 (0.1%)
23	j	0.19	0/1728	0.53	2/2358 (0.1%)
24	K	0.22	0/1755	0.60	4/2375 (0.2%)
24	k	0.18	0/1747	0.47	0/2364
25	L	0.27	0/1885	0.53	1/2552 (0.0%)
25	l	0.27	0/1885	0.53	1/2552 (0.0%)
26	M	0.19	0/1891	0.55	2/2552 (0.1%)
26	m	0.19	0/1891	0.55	2/2552 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
27	N	0.17	0/1454	0.49	0/1967
27	n	0.17	0/1454	0.49	0/1967
28	O	0.18	0/1670	0.42	0/2265
28	o	0.18	0/1670	0.42	0/2265
29	P	0.17	0/1614	0.40	0/2177
29	p	0.17	0/1614	0.40	0/2177
30	Q	0.18	0/1603	0.47	0/2174
30	q	0.18	0/1603	0.47	0/2174
31	R	0.16	0/1579	0.37	0/2134
31	r	0.16	0/1579	0.37	0/2134
32	S	0.17	0/1671	0.42	0/2253
32	s	0.17	0/1671	0.42	0/2253
33	T	0.18	0/1700	0.43	0/2305
33	t	0.18	0/1700	0.43	0/2305
All	All	0.23	0/106684	0.60	75/144195 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	U	0	5
2	V	0	2
3	W	0	3
4	X	0	2
5	Y	0	5
6	Z	0	3
7	a	0	1
8	b	0	1
9	c	0	2
10	d	0	3
11	e	0	1
12	f	0	12
14	B	0	4
15	C	0	2
16	D	0	4
17	E	0	3
18	F	0	1
20	G	0	2
20	g	0	1
21	H	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
22	I	0	1
24	K	0	2
24	k	0	1
26	M	0	2
26	m	0	2
28	O	0	1
28	o	0	1
All	All	0	68

There are no bond length outliers.

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	217	THR	N-CA-C	-13.12	97.04	111.07
1	U	173	VAL	CA-C-N	10.72	133.24	119.84
1	U	173	VAL	C-N-CA	10.72	133.24	119.84
24	K	21	LEU	CA-C-N	9.20	138.26	121.70
24	K	21	LEU	C-N-CA	9.20	138.26	121.70
6	Z	216	ALA	N-CA-C	-8.45	101.30	111.69
17	E	228	CYS	CA-C-N	-7.73	112.58	123.10
17	E	228	CYS	C-N-CA	-7.73	112.58	123.10
1	U	813	TYR	CA-CB-CG	7.43	127.28	113.90
15	C	397	LYS	CA-C-N	7.23	135.35	121.54
15	C	397	LYS	C-N-CA	7.23	135.35	121.54
22	I	15	GLU	CA-C-N	7.12	134.52	121.70
22	I	15	GLU	C-N-CA	7.12	134.52	121.70
22	I	15	GLU	N-CA-CB	-6.81	106.41	114.17
6	Z	15	VAL	N-CA-C	6.77	116.92	110.42
24	K	19	GLY	CA-C-N	6.66	133.69	121.70
24	K	19	GLY	C-N-CA	6.66	133.69	121.70
10	d	236	THR	CA-C-N	6.38	126.56	120.43
10	d	236	THR	C-N-CA	6.38	126.56	120.43
16	D	236	VAL	N-CA-C	-6.25	106.34	111.91
1	U	172	ASP	O-C-N	6.18	130.39	123.40
12	f	875	ALA	CA-C-N	6.03	133.06	121.54
12	f	875	ALA	C-N-CA	6.03	133.06	121.54
23	j	4	ASP	CA-C-N	5.99	132.99	121.54
23	j	4	ASP	C-N-CA	5.99	132.99	121.54
23	J	4	ASP	CA-C-N	5.98	132.95	121.54
23	J	4	ASP	C-N-CA	5.98	132.95	121.54
1	U	796	LYS	CA-C-N	-5.97	111.43	122.06
1	U	796	LYS	C-N-CA	-5.97	111.43	122.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	c	200	TYR	CA-C-N	5.97	132.93	121.54
9	c	200	TYR	C-N-CA	5.97	132.93	121.54
17	E	251	ARG	CA-C-O	-5.95	112.00	120.51
22	I	15	GLU	N-CA-C	5.88	122.51	113.28
7	a	214	GLY	CA-C-N	5.87	132.75	121.54
7	a	214	GLY	C-N-CA	5.87	132.75	121.54
1	U	873	PRO	CA-C-N	5.76	132.54	121.54
1	U	873	PRO	C-N-CA	5.76	132.54	121.54
12	f	868	HIS	CA-C-N	5.70	132.43	121.54
12	f	868	HIS	C-N-CA	5.70	132.43	121.54
18	F	72	LYS	CA-C-N	5.66	132.16	121.97
18	F	72	LYS	C-N-CA	5.66	132.16	121.97
6	Z	64	ASP	CA-C-N	5.58	132.20	121.54
6	Z	64	ASP	C-N-CA	5.58	132.20	121.54
25	l	118	ILE	CA-CB-CG1	5.56	119.85	110.40
25	L	118	ILE	CA-CB-CG1	5.56	119.84	110.40
1	U	809	SER	N-CA-C	5.53	116.66	108.86
17	E	225	HIS	CA-C-N	5.42	135.02	121.80
17	E	225	HIS	C-N-CA	5.42	135.02	121.80
6	Z	12	HIS	CA-C-N	-5.39	113.36	120.96
6	Z	12	HIS	C-N-CA	-5.39	113.36	120.96
1	U	223	LEU	CA-C-N	5.37	131.79	121.54
1	U	223	LEU	C-N-CA	5.37	131.79	121.54
12	f	822	VAL	CA-C-N	5.33	131.72	121.54
12	f	822	VAL	C-N-CA	5.33	131.72	121.54
2	V	27	PRO	N-CA-C	5.32	117.19	110.70
12	f	254	GLY	N-CA-C	5.20	118.53	112.50
14	B	164	MET	CA-C-N	5.20	131.47	121.54
14	B	164	MET	C-N-CA	5.20	131.47	121.54
12	f	619	HIS	CA-C-N	5.18	131.44	121.54
12	f	619	HIS	C-N-CA	5.18	131.44	121.54
10	d	198	LEU	CA-C-N	5.17	131.42	121.54
10	d	198	LEU	C-N-CA	5.17	131.42	121.54
12	f	858	LYS	CA-C-N	-5.14	113.41	119.84
12	f	858	LYS	C-N-CA	-5.14	113.41	119.84
2	V	28	PRO	N-CA-C	5.11	116.94	110.70
26	m	6	GLY	CA-C-N	5.10	131.29	121.54
26	m	6	GLY	C-N-CA	5.10	131.29	121.54
14	B	136	LEU	CA-C-N	5.08	131.25	121.54
14	B	136	LEU	C-N-CA	5.08	131.25	121.54
26	M	6	GLY	CA-C-N	5.08	131.24	121.54
26	M	6	GLY	C-N-CA	5.08	131.24	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	W	44	ILE	CA-C-N	5.04	131.17	121.54
3	W	44	ILE	C-N-CA	5.04	131.17	121.54
17	E	272	ARG	CA-CB-CG	5.03	124.17	114.10
1	U	182	LYS	N-CA-C	-5.02	105.50	110.97

There are no chirality outliers.

All (68) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	B	136	LEU	Peptide
14	B	319	PHE	Peptide
14	B	434	THR	Peptide
14	B	91	LYS	Peptide
15	C	220	VAL	Peptide
15	C	89	VAL	Peptide
16	D	268	ASP	Peptide
16	D	335	LEU	Peptide
16	D	336	PRO	Peptide
16	D	410	ASP	Peptide
17	E	1	MET	Peptide
17	E	166	PRO	Peptide
17	E	281	ARG	Peptide
18	F	343	LEU	Peptide
20	G	209	ASP	Peptide
20	G	222	VAL	Peptide
21	H	6	TYR	Peptide
22	I	10	THR	Peptide
24	K	19	GLY	Peptide
24	K	232	GLU	Peptide
26	M	229	LYS	Peptide
26	M	6	GLY	Peptide
28	O	170	GLY	Peptide
1	U	415	HIS	Peptide
1	U	423	MET	Peptide
1	U	808	PRO	Peptide
1	U	811	PHE	Peptide
1	U	873	PRO	Peptide
2	V	192	MET	Peptide
2	V	29	PRO	Peptide
3	W	172	GLU	Peptide
3	W	313	GLU	Peptide
3	W	90	LEU	Peptide

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Mol	Chain	Res	Type	Group
4	X	142	ARG	Peptide
4	X	202	CYS	Peptide
5	Y	174	TRP	Peptide
5	Y	233	ARG	Peptide
5	Y	291	HIS	Peptide
5	Y	349	LYS	Peptide
5	Y	65	ILE	Peptide
6	Z	144	VAL	Peptide
6	Z	237	LEU	Peptide
6	Z	69	PHE	Peptide
7	a	341	LEU	Peptide
8	b	21	PHE	Peptide
9	c	232	GLN	Peptide
9	c	279	ASP	Peptide
10	d	201	ASN	Peptide
10	d	202	THR	Peptide
10	d	88	GLN	Peptide
11	e	6	GLN	Peptide
12	f	340	MET	Peptide
12	f	642	ALA	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	809	ILE	Peptide
12	f	816	TYR	Peptide
12	f	822	VAL	Peptide
12	f	823	ALA	Peptide
12	f	854	GLY	Peptide
12	f	870	THR	Peptide
12	f	875	ALA	Peptide
20	g	222	VAL	Peptide
24	k	9	ASP	Peptide
26	m	229	LYS	Peptide
26	m	6	GLY	Peptide
28	o	170	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6828	0	6884	110	0
2	V	3852	0	3893	73	0
3	W	3703	0	3822	73	0
4	X	3009	0	3113	26	0
5	Y	3115	0	3120	40	0
6	Z	2281	0	2312	54	0
7	a	2995	0	3012	47	0
8	b	1458	0	1505	24	0
9	c	2260	0	2276	37	0
10	d	2116	0	2146	25	0
11	e	334	0	294	9	0
12	f	6866	0	6866	154	0
13	A	3229	0	3260	46	0
14	B	3207	0	3278	51	0
15	C	3105	0	3218	51	0
16	D	3040	0	3075	32	0
17	E	3097	0	3174	111	0
18	F	3098	0	3186	39	0
19	v	180	0	42	19	0
20	G	1820	0	1791	30	0
20	g	1826	0	1796	19	0
21	H	1692	0	1586	24	0
21	h	1708	0	1594	13	0
22	I	1895	0	1833	31	0
22	i	1912	0	1851	26	0
23	J	1704	0	1517	17	0
23	j	1704	0	1517	21	0
24	K	1729	0	1680	20	0
24	k	1722	0	1673	21	0
25	L	1850	0	1822	13	0
25	l	1850	0	1822	15	0
26	M	1856	0	1814	22	0
26	m	1856	0	1814	24	0
27	N	1430	0	1398	8	0
27	n	1430	0	1398	8	0
28	O	1643	0	1644	10	0
28	o	1643	0	1644	15	0
29	P	1585	0	1598	10	0
29	p	1585	0	1598	12	0
30	Q	1570	0	1547	18	0
30	q	1570	0	1547	18	0
31	R	1548	0	1499	11	0
31	r	1548	0	1499	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	S	1641	0	1618	13	0
32	s	1641	0	1618	6	0
33	T	1667	0	1628	14	0
33	t	1667	0	1628	11	0
34	c	1	0	0	0	0
35	A	31	0	12	1	0
35	B	31	0	12	2	0
35	C	31	0	12	2	0
35	F	31	0	12	1	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	C	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	D	27	0	12	0	0
All	All	105222	0	104510	1298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:196:LEU:O	17:E:197:LYS:HG3	1.19	1.29
12:f:657:ILE:O	12:f:661:ALA:HB3	1.44	1.16
17:E:235:ILE:CG2	17:E:279:THR:HB	1.78	1.11
17:E:196:LEU:O	17:E:197:LYS:CG	2.00	1.09
17:E:235:ILE:HG22	17:E:279:THR:HB	1.05	1.03
1:U:47:VAL:HG12	1:U:48:LEU:N	1.75	1.01
9:c:115:HIS:HD2	9:c:118:PHE:HZ	1.09	1.01
9:c:115:HIS:HD2	9:c:118:PHE:CZ	1.81	0.99
1:U:174:PRO:HB3	1:U:208:LEU:HD11	1.44	0.99
1:U:148:LYS:HE3	1:U:179:TYR:CE2	1.96	0.99
14:B:127:VAL:HG11	19:v:27:UNK:CB	1.92	0.97
17:E:235:ILE:HG22	17:E:279:THR:CB	1.95	0.97
9:c:50:PRO:HG2	17:E:53:VAL:CG1	1.95	0.95
17:E:198:VAL:HG11	17:E:232:MET:SD	2.05	0.95
17:E:127:PRO:HB3	17:E:193:CYS:SG	2.11	0.89
17:E:235:ILE:CG2	17:E:279:THR:CB	2.49	0.88
3:W:142:ARG:HH22	3:W:178:GLU:HB2	1.37	0.88
9:c:115:HIS:CD2	9:c:118:PHE:CZ	2.61	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:115:HIS:CD2	9:c:118:PHE:HZ	1.93	0.87
17:E:235:ILE:CG2	17:E:279:THR:CG2	2.54	0.85
1:U:173:VAL:HG12	1:U:175:GLY:H	1.42	0.85
9:c:50:PRO:HG2	17:E:53:VAL:HG11	1.58	0.84
17:E:188:ALA:HA	17:E:192:ASP:CB	2.07	0.84
3:W:178:GLU:H	3:W:182:ARG:HB2	1.42	0.84
17:E:198:VAL:HB	17:E:232:MET:HA	1.59	0.84
19:v:22:UNK:O	19:v:23:UNK:O	1.98	0.82
6:Z:11:VAL:HB	6:Z:162:ILE:HD13	1.61	0.81
1:U:47:VAL:HG12	1:U:48:LEU:H	1.45	0.81
12:f:662:MET:SD	13:A:65:ILE:HG21	2.21	0.80
3:W:142:ARG:NH2	3:W:178:GLU:HB2	1.95	0.80
6:Z:16:LEU:HD23	6:Z:17:LEU:H	1.47	0.80
12:f:657:ILE:O	12:f:661:ALA:CB	2.29	0.79
1:U:180:SER:O	1:U:183:LEU:HB2	1.81	0.79
18:F:300:LYS:HE3	18:F:300:LYS:O	1.84	0.78
3:W:178:GLU:H	3:W:182:ARG:CB	1.97	0.77
3:W:142:ARG:HH22	3:W:178:GLU:CB	1.98	0.75
17:E:194:ASN:CB	17:E:229:ILE:H	1.98	0.75
17:E:222:ALA:HB1	17:E:228:CYS:SG	2.25	0.75
6:Z:16:LEU:CD2	6:Z:17:LEU:H	1.99	0.75
17:E:198:VAL:HG11	17:E:232:MET:CE	2.16	0.74
17:E:235:ILE:HG23	17:E:236:ASP:H	1.52	0.74
14:B:127:VAL:CG1	19:v:27:UNK:CB	2.67	0.72
1:U:903:PHE:HB2	1:U:915:LYS:HB2	1.71	0.72
17:E:194:ASN:CG	17:E:229:ILE:H	1.96	0.72
12:f:828:ARG:CZ	12:f:843:SER:OG	2.37	0.71
13:A:29:ASP:HA	13:A:32:LEU:HD23	1.70	0.71
14:B:304:GLU:OE2	19:v:18:UNK:CB	2.37	0.71
3:W:178:GLU:O	3:W:180:LYS:N	2.23	0.71
17:E:235:ILE:HG23	17:E:279:THR:CG2	2.20	0.71
1:U:47:VAL:O	1:U:49:TYR:N	2.24	0.71
17:E:235:ILE:HG23	17:E:279:THR:HG21	1.72	0.70
3:W:8:ARG:HB3	3:W:27:ARG:HD3	1.74	0.70
3:W:142:ARG:HH22	3:W:178:GLU:CG	2.04	0.70
17:E:198:VAL:CG1	17:E:232:MET:SD	2.79	0.70
17:E:235:ILE:HG23	17:E:236:ASP:N	2.05	0.70
3:W:175:GLY:O	3:W:176:SER:OG	2.09	0.69
4:X:260:MET:HE1	4:X:322:HIS:HB3	1.74	0.69
12:f:828:ARG:NE	12:f:843:SER:OG	2.26	0.69
15:C:277:LEU:HG	15:C:310:ARG:HH12	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:10:SER:HB2	10:d:73:ARG:HG3	1.75	0.69
15:C:222:LYS:HG2	15:C:222:LYS:O	1.92	0.68
17:E:52:SER:C	17:E:54:GLY:H	2.01	0.68
17:E:52:SER:O	17:E:54:GLY:N	2.25	0.68
17:E:194:ASN:ND2	17:E:228:CYS:HA	2.09	0.68
15:C:368:MET:HG2	16:D:329:ARG:HH22	1.59	0.68
5:Y:288:PHE:HA	5:Y:291:HIS:HD2	1.60	0.67
1:U:47:VAL:CG1	1:U:48:LEU:N	2.48	0.66
17:E:188:ALA:HA	17:E:192:ASP:CG	2.20	0.66
3:W:177:MET:HA	3:W:182:ARG:HG2	1.78	0.66
12:f:660:ILE:HG13	12:f:660:ILE:O	1.95	0.66
6:Z:12:HIS:HB2	6:Z:50:VAL:O	1.94	0.66
17:E:188:ALA:HA	17:E:192:ASP:HB3	1.78	0.65
17:E:195:PHE:O	17:E:231:PHE:HB3	1.97	0.65
12:f:61:GLU:OE2	12:f:62:ARG:NH1	2.30	0.65
14:B:389:ASP:O	14:B:390:LEU:HB3	1.97	0.65
1:U:639:LEU:HD21	15:C:49:ARG:HD2	1.79	0.65
6:Z:15:VAL:O	6:Z:19:VAL:HG23	1.97	0.65
13:A:122:VAL:HB	18:F:88:TYR:HB2	1.77	0.65
3:W:201:ARG:HH22	16:D:391:ARG:HA	1.60	0.65
1:U:182:LYS:O	1:U:185:MET:N	2.25	0.64
1:U:148:LYS:HE3	1:U:179:TYR:CZ	2.33	0.64
1:U:148:LYS:HE3	1:U:179:TYR:HE2	1.59	0.64
2:V:280:ALA:HB1	2:V:284:GLU:HB3	1.78	0.64
3:W:329:ARG:HG3	3:W:330:LYS:HG2	1.80	0.64
6:Z:16:LEU:CG	6:Z:17:LEU:H	2.11	0.64
22:I:218:ARG:NH1	22:I:223:THR:OG1	2.31	0.64
17:E:195:PHE:CD1	17:E:231:PHE:HB2	2.33	0.64
12:f:125:ILE:HD13	12:f:129:LEU:HB2	1.80	0.64
3:W:299:ILE:HG22	3:W:301:LYS:H	1.64	0.63
27:N:21:THR:HG22	27:N:26:ILE:HG13	1.81	0.63
32:S:27:THR:HB	32:S:40:SER:H	1.63	0.63
27:n:21:THR:HG22	27:n:26:ILE:HG13	1.81	0.63
4:X:255:LEU:HD22	4:X:267:VAL:HG13	1.80	0.63
9:c:113:HIS:CD2	9:c:115:HIS:CE1	2.87	0.63
32:s:27:THR:HB	32:s:40:SER:H	1.63	0.63
12:f:721:VAL:HG11	14:B:208:PRO:HD2	1.80	0.63
2:V:37:MET:SD	2:V:92:ARG:NH1	2.71	0.62
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.81	0.62
3:W:178:GLU:O	3:W:179:LYS:C	2.41	0.62
5:Y:360:ASP:H	5:Y:363:ASN:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:125:ILE:HD11	12:f:128:VAL:HB	1.82	0.62
3:W:142:ARG:HG2	3:W:145:LEU:HD12	1.82	0.62
17:E:127:PRO:CB	17:E:193:CYS:SG	2.87	0.62
17:E:196:LEU:CD1	17:E:230:ILE:HD13	2.30	0.62
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.32	0.62
12:f:673:ARG:HH22	12:f:709:THR:HA	1.63	0.62
17:E:222:ALA:CB	17:E:228:CYS:SG	2.88	0.62
26:m:214:SER:OG	26:m:224:HIS:NE2	2.32	0.62
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.82	0.62
15:C:198:LEU:HD11	35:C:501:ATP:H2'	1.82	0.61
15:C:69:GLN:HB3	15:C:118:ASN:HD21	1.63	0.61
22:I:143:TYR:HB2	22:I:146:GLN:HE21	1.64	0.61
3:W:175:GLY:O	3:W:176:SER:CB	2.47	0.61
26:M:214:SER:OG	26:M:224:HIS:NE2	2.32	0.61
10:d:188:LYS:HD2	10:d:221:ASN:HD21	1.65	0.61
2:V:476:PHE:HB3	6:Z:260:VAL:HG21	1.81	0.61
3:W:362:ASN:HD22	3:W:365:ILE:HD11	1.66	0.61
4:X:182:ASN:ND2	5:Y:248:GLU:OE2	2.33	0.61
17:E:196:LEU:HD13	17:E:230:ILE:HD13	1.82	0.61
2:V:198:GLN:HE22	15:C:33:LEU:HD11	1.66	0.61
1:U:505:ASP:HB3	1:U:508:THR:HG22	1.83	0.61
17:E:286:ASP:HB3	17:E:289:LEU:HB2	1.81	0.61
13:A:118:PHE:HE1	19:v:28:UNK:CB	2.12	0.60
12:f:618:GLU:HG2	14:B:82:GLN:OE1	2.01	0.60
6:Z:11:VAL:CB	6:Z:162:ILE:HD13	2.31	0.60
14:B:313:LEU:O	14:B:346:ARG:NH1	2.35	0.60
12:f:127:SER:HA	12:f:131:MET:HB2	1.82	0.60
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.83	0.60
3:W:142:ARG:HH12	3:W:178:GLU:HG3	1.66	0.60
12:f:586:PRO:HA	12:f:589:SER:HB2	1.83	0.60
7:a:286:ALA:HA	7:a:289:ARG:HB3	1.83	0.60
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.83	0.60
21:H:39:LYS:HE2	21:H:144:PRO:HG2	1.83	0.60
9:c:192:LEU:HA	9:c:196:LEU:HB2	1.84	0.60
20:G:127:GLN:NE2	21:H:128:ARG:O	2.35	0.60
2:V:55:THR:OG1	15:C:36:ASN:ND2	2.35	0.60
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.84	0.59
17:E:234:GLU:HB2	17:E:237:ALA:HB3	1.84	0.59
3:W:273:TYR:HB2	3:W:276:LEU:HB2	1.83	0.59
1:U:366:HIS:HE1	1:U:395:ARG:HD2	1.65	0.59
12:f:704:LEU:HA	12:f:707:LEU:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:198:HIS:O	12:f:202:HIS:N	2.36	0.59
18:F:206:MET:HE3	18:F:246:ALA:HB2	1.85	0.59
22:I:219:GLU:OE2	22:I:220:ASN:ND2	2.36	0.59
31:R:166:ARG:NH2	29:p:34:MET:O	2.35	0.59
1:U:194:ARG:HH11	1:U:218:GLN:HE21	1.50	0.59
2:V:100:MET:H	2:V:103:SER:HB2	1.67	0.59
9:c:174:PRO:O	9:c:176:GLN:NE2	2.35	0.59
12:f:811:LEU:HD11	12:f:862:ILE:HB	1.84	0.59
20:G:123:GLN:NE2	21:H:82:ASP:OD1	2.35	0.59
3:W:436:MET:HE3	9:c:226:MET:HB2	1.83	0.59
17:E:29:LEU:HB3	18:F:62:VAL:HG11	1.85	0.59
1:U:798:PRO:O	1:U:880:ASN:ND2	2.34	0.58
6:Z:212:LEU:HA	6:Z:215:VAL:HG12	1.85	0.58
7:a:35:HIS:NE2	8:b:14:GLU:O	2.36	0.58
20:G:67:THR:HG23	20:G:216:GLU:HG2	1.85	0.58
26:m:51:LYS:NZ	26:m:62:SER:O	2.36	0.58
2:V:79:VAL:HG13	2:V:81:GLN:H	1.68	0.58
12:f:672:LEU:HD21	12:f:690:VAL:HG22	1.83	0.58
16:D:212:LYS:NZ	16:D:311:THR:O	2.36	0.58
8:b:110:ILE:HG22	8:b:139:ASP:HB2	1.85	0.58
9:c:189:ILE:HA	9:c:192:LEU:HG	1.86	0.58
12:f:872:VAL:HG21	12:f:881:GLU:H	1.67	0.58
26:M:52:LEU:HA	26:M:209:PHE:HA	1.85	0.58
13:A:103:ASN:ND2	18:F:167:GLU:OE1	2.36	0.58
30:q:117:TYR:HB3	30:q:125:ALA:HB3	1.86	0.58
1:U:600:ARG:HE	16:D:56:VAL:HG22	1.68	0.58
8:b:161:ASN:HD21	8:b:168:SER:H	1.51	0.58
30:Q:117:TYR:HB3	30:Q:125:ALA:HB3	1.86	0.58
2:V:452:ASN:HB3	2:V:457:TYR:HB2	1.84	0.58
15:C:113:ARG:NH2	15:C:129:ASN:O	2.36	0.58
9:c:123:SER:OG	19:v:33:UNK:CB	2.52	0.58
17:E:260:LEU:HD22	17:E:264:MET:HE3	1.84	0.58
22:I:163:CYS:SG	22:I:164:ILE:N	2.75	0.58
21:h:39:LYS:HE2	21:h:144:PRO:HG2	1.85	0.58
27:n:1:THR:N	27:n:169:SER:O	2.37	0.58
6:Z:16:LEU:HD23	6:Z:17:LEU:N	2.18	0.58
9:c:29:GLU:HG3	9:c:65:TYR:HB2	1.85	0.58
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.84	0.58
1:U:596:ASN:ND2	16:D:52:GLU:OE1	2.37	0.58
26:M:51:LYS:NZ	26:M:62:SER:O	2.36	0.58
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:T:145:LEU:HD22	33:T:179:ARG:HH11	1.69	0.58
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.37	0.57
3:W:190:MET:HB2	3:W:202:THR:HG23	1.86	0.57
15:C:164:VAL:HG13	15:C:165:ILE:HG13	1.85	0.57
2:V:163:VAL:HA	2:V:175:MET:HE2	1.86	0.57
13:A:428:ARG:NH2	23:J:23:GLN:O	2.37	0.57
26:m:52:LEU:HA	26:m:209:PHE:HA	1.85	0.57
2:V:416:ARG:NH1	5:Y:351:ASN:OD1	2.37	0.57
9:c:64:ASP:O	9:c:139:ARG:NH2	2.35	0.57
2:V:137:GLU:HA	2:V:140:ASP:HB2	1.85	0.57
12:f:150:GLU:O	12:f:156:HIS:ND1	2.37	0.57
12:f:469:TYR:O	12:f:472:HIS:ND1	2.32	0.57
12:f:556:ARG:HD3	12:f:786:GLN:HB2	1.86	0.57
14:B:258:LYS:HD3	15:C:226:GLU:HG2	1.87	0.57
27:N:1:THR:N	27:N:169:SER:O	2.37	0.57
6:Z:7:GLN:HB2	6:Z:46:LYS:HG2	1.87	0.57
17:E:337:GLY:O	17:E:378:LYS:NZ	2.35	0.57
19:v:22:UNK:C	19:v:23:UNK:O	2.53	0.57
3:W:448:LYS:HE2	6:Z:157:HIS:HB2	1.86	0.57
10:d:78:LEU:HD13	10:d:98:LEU:HD21	1.86	0.57
3:W:80:TRP:NE1	20:G:244:GLU:OE1	2.37	0.57
4:X:170:GLN:NE2	4:X:192:SER:OG	2.38	0.57
8:b:97:LEU:HD23	8:b:107:MET:HB3	1.87	0.57
15:C:215:SER:HA	15:C:249:ASP:HB2	1.85	0.57
3:W:91:SER:HB3	3:W:96:GLN:HE22	1.69	0.57
7:a:182:CYS:SG	7:a:183:VAL:N	2.77	0.57
16:D:272:THR:HB	16:D:317:LEU:HA	1.85	0.57
30:Q:198:LYS:H	30:q:198:LYS:H	1.52	0.57
33:t:145:LEU:HD22	33:t:179:ARG:HH11	1.69	0.57
3:W:92:LYS:HB3	3:W:94:ARG:HB3	1.87	0.57
6:Z:16:LEU:CG	6:Z:17:LEU:N	2.68	0.57
6:Z:212:LEU:HD13	7:a:350:LYS:HG2	1.87	0.57
13:A:80:LEU:O	13:A:85:GLN:NE2	2.38	0.57
18:F:300:LYS:HE3	18:F:300:LYS:C	2.29	0.57
1:U:788:VAL:HG12	1:U:909:GLY:HA2	1.87	0.57
12:f:378:ASN:HD21	12:f:392:THR:HG22	1.70	0.56
24:K:221:GLN:HB2	24:K:224:GLN:HB3	1.85	0.56
6:Z:16:LEU:HD23	6:Z:16:LEU:N	2.20	0.56
6:Z:16:LEU:HG	6:Z:17:LEU:N	2.20	0.56
9:c:50:PRO:CG	17:E:53:VAL:HG11	2.31	0.56
12:f:875:ALA:O	12:f:876:HIS:ND1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:345:ARG:HH12	2:V:353:LEU:HD11	1.70	0.56
5:Y:202:LEU:HD21	5:Y:239:LYS:HB3	1.86	0.56
7:a:273:GLN:HB3	7:a:310:LEU:HD11	1.88	0.56
13:A:212:VAL:HG22	13:A:339:ARG:HB3	1.87	0.56
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.37	0.56
26:M:163:CYS:SG	26:M:164:ALA:N	2.78	0.56
2:V:85:ALA:O	2:V:89:LYS:NZ	2.39	0.56
15:C:375:ARG:HG2	15:C:377:HIS:H	1.69	0.56
7:a:74:LEU:HD23	7:a:110:ALA:HB2	1.87	0.56
10:d:52:ARG:HH22	10:d:92:SER:HB3	1.71	0.56
21:H:42:ASN:ND2	21:H:183:GLU:OE1	2.39	0.56
24:k:76:CYS:SG	24:k:77:ALA:N	2.79	0.56
1:U:47:VAL:C	1:U:49:TYR:N	2.64	0.56
2:V:68:ASP:O	2:V:72:LEU:N	2.38	0.56
12:f:77:GLU:OE1	12:f:79:ARG:NH1	2.38	0.56
26:M:47:PHE:HB2	26:M:214:SER:HB3	1.88	0.56
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.87	0.56
20:G:43:ARG:NH1	20:G:149:PRO:O	2.39	0.56
1:U:814:PRO:HB2	1:U:816:PRO:HD3	1.88	0.56
22:I:90:LEU:HD12	22:I:114:LEU:HD22	1.88	0.56
5:Y:88:LEU:HG	5:Y:100:ILE:HG13	1.88	0.55
12:f:828:ARG:CD	12:f:843:SER:OG	2.54	0.55
15:C:88:LYS:HB2	15:C:94:LYS:HG2	1.86	0.55
17:E:75:ASN:ND2	18:F:129:ARG:O	2.39	0.55
1:U:257:SER:HB2	1:U:757:MET:HE3	1.87	0.55
3:W:316:ARG:HH12	3:W:381:LEU:HA	1.71	0.55
23:j:74:ALA:HB2	23:j:161:ILE:HD13	1.88	0.55
26:m:163:CYS:SG	26:m:164:ALA:N	2.78	0.55
14:B:106:PRO:HB3	15:C:121:TYR:HB2	1.87	0.55
1:U:217:CYS:HG	1:U:752:THR:HG1	1.55	0.55
8:b:141:ILE:HA	8:b:171:VAL:HB	1.88	0.55
12:f:594:LEU:O	12:f:635:LYS:NZ	2.40	0.55
12:f:663:GLY:O	12:f:664:GLU:HG3	2.06	0.55
15:C:99:VAL:HG12	15:C:123:LEU:HD12	1.89	0.55
17:E:263:GLN:HA	17:E:268:ASP:HB3	1.88	0.55
20:g:165:ALA:HB1	20:g:179:LEU:HD13	1.89	0.55
25:l:189:LYS:HA	25:l:192:LEU:HG	1.89	0.55
12:f:378:ASN:OD1	12:f:382:ASN:ND2	2.40	0.55
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.87	0.55
32:S:150:ASP:OD2	29:p:177:ARG:NH2	2.38	0.55
24:k:209:LYS:O	24:k:214:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:441:LYS:HB2	12:f:477:MET:HE1	1.88	0.55
12:f:680:ARG:HB2	12:f:763:ARG:HE	1.72	0.55
12:f:758:ASN:HB2	12:f:809:ILE:HG21	1.88	0.55
23:J:74:ALA:HB2	23:J:161:ILE:HD13	1.88	0.55
22:i:38:LEU:HD13	22:i:160:LYS:HA	1.88	0.55
26:m:47:PHE:HB2	26:m:214:SER:HB3	1.88	0.55
2:V:252:ASN:HD21	2:V:288:TYR:HB2	1.71	0.55
4:X:332:GLU:HA	4:X:335:LEU:HB2	1.89	0.55
17:E:200:SER:CB	17:E:234:GLU:O	2.55	0.55
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.87	0.55
14:B:125:THR:OG1	14:B:126:SER:N	2.38	0.55
1:U:189:GLN:NE2	1:U:595:ASN:OD1	2.39	0.55
1:U:376:MET:HA	1:U:739:ALA:HA	1.89	0.55
2:V:416:ARG:HA	2:V:459:GLN:HA	1.89	0.55
7:a:284:ARG:HD3	7:a:288:HIS:H	1.71	0.55
22:i:219:GLU:OE2	22:i:220:ASN:ND2	2.40	0.55
1:U:219:CYS:SG	1:U:220:LEU:N	2.79	0.55
12:f:552:ASP:HB3	12:f:556:ARG:HG3	1.88	0.55
1:U:623:GLY:HA3	1:U:658:ILE:HG13	1.90	0.54
2:V:451:ILE:HG23	2:V:458:VAL:HG22	1.88	0.54
5:Y:314:LEU:O	5:Y:354:VAL:N	2.40	0.54
12:f:209:MET:HG3	12:f:211:ILE:H	1.72	0.54
22:i:79:ILE:HG22	22:i:82:ASP:H	1.72	0.54
12:f:465:LEU:O	12:f:481:SER:OG	2.25	0.54
28:O:113:ILE:HG12	28:O:119:THR:HG22	1.89	0.54
22:i:31:ALA:O	22:i:167:ASN:ND2	2.40	0.54
22:i:218:ARG:NH1	22:i:223:THR:OG1	2.37	0.54
1:U:174:PRO:CB	1:U:208:LEU:HD11	2.30	0.54
2:V:265:ASP:O	2:V:269:LYS:NZ	2.40	0.54
14:B:234:LEU:HD11	35:B:501:ATP:H2'	1.90	0.54
12:f:873:LEU:HG	12:f:875:ALA:H	1.73	0.54
17:E:50:LEU:O	17:E:51:GLN:HG3	2.07	0.54
20:G:165:ALA:HB1	20:G:179:LEU:HD13	1.88	0.54
6:Z:129:LYS:HE2	9:c:216:MET:HB3	1.90	0.54
12:f:378:ASN:O	12:f:382:ASN:ND2	2.39	0.54
4:X:90:ARG:HH21	4:X:128:ALA:HB1	1.72	0.54
12:f:139:CYS:O	12:f:143:ARG:NH1	2.41	0.54
12:f:673:ARG:NH1	12:f:708:ASP:OD2	2.41	0.54
24:k:117:SER:HB3	25:l:82:ARG:HH22	1.73	0.54
25:l:186:GLU:HA	25:l:189:LYS:HG2	1.90	0.54
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:217:THR:HG22	6:Z:218:GLY:N	2.22	0.54
13:A:342:GLU:OE2	18:F:431:LYS:NZ	2.41	0.54
16:D:119:ILE:O	16:D:121:ARG:NH1	2.41	0.54
16:D:271:ALA:HA	16:D:289:LEU:HD21	1.90	0.54
18:F:184:GLN:OE1	18:F:243:GLN:NE2	2.41	0.54
25:L:134:ILE:HB	25:L:145:PHE:HB2	1.89	0.54
28:o:190:THR:HG22	28:o:192:PRO:HD3	1.89	0.54
1:U:179:TYR:CD1	1:U:179:TYR:C	2.86	0.54
7:a:8:LEU:HD11	7:a:26:GLU:HB3	1.90	0.54
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.90	0.54
17:E:52:SER:C	17:E:54:GLY:N	2.65	0.54
2:V:80:LYS:O	2:V:87:SER:N	2.41	0.54
15:C:185:GLY:HA3	15:C:311:ILE:HA	1.90	0.54
3:W:220:GLU:HG3	3:W:221:LYS:HG2	1.89	0.54
5:Y:325:VAL:O	11:e:66:LYS:NZ	2.39	0.54
15:C:396:GLU:O	15:C:402:LYS:NZ	2.41	0.54
25:l:134:ILE:HB	25:l:145:PHE:HB2	1.89	0.54
27:n:40:ARG:NH1	27:n:180:ALA:O	2.41	0.54
28:o:113:ILE:HG12	28:o:119:THR:HG22	1.89	0.54
14:B:304:GLU:CD	19:v:18:UNK:CB	2.81	0.53
15:C:218:GLU:O	15:C:221:GLN:NE2	2.41	0.53
20:G:53:GLN:HA	20:G:215:ILE:HA	1.89	0.53
25:L:189:LYS:HA	25:L:192:LEU:HG	1.89	0.53
33:t:27:LEU:HD22	33:t:184:TYR:HB2	1.90	0.53
10:d:19:CYS:SG	10:d:65:ARG:NH1	2.79	0.53
12:f:202:HIS:ND1	12:f:242:GLU:OE2	2.41	0.53
13:A:224:LEU:HD11	35:A:501:ATP:H2'	1.90	0.53
12:f:809:ILE:HG23	12:f:810:ILE:HG12	1.91	0.53
12:f:828:ARG:HD2	12:f:843:SER:OG	2.07	0.53
17:E:199:VAL:O	17:E:234:GLU:HG3	2.08	0.53
33:T:27:LEU:HD22	33:T:184:TYR:HB2	1.91	0.53
2:V:400:HIS:HA	10:d:145:GLU:HG3	1.91	0.53
3:W:145:LEU:HA	3:W:148:THR:HG22	1.90	0.53
6:Z:68:TRP:CG	6:Z:104:ASN:HD21	2.26	0.53
6:Z:200:GLY:HA3	9:c:225:TRP:HE1	1.73	0.53
14:B:258:LYS:O	19:v:19:UNK:N	2.42	0.53
1:U:373:ASN:HD22	1:U:385:PHE:HD2	1.55	0.53
2:V:200:ARG:NH1	2:V:242:HIS:O	2.42	0.53
2:V:228:ARG:O	2:V:232:HIS:ND1	2.38	0.53
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.90	0.53
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:97:ARG:NH2	17:E:112:PRO:O	2.42	0.53
17:E:272:ARG:O	17:E:274:LYS:NZ	2.42	0.53
33:t:27:LEU:HD11	33:t:34:ALA:HB1	1.91	0.53
15:C:215:SER:OG	15:C:218:GLU:OE1	2.27	0.53
25:L:186:GLU:HA	25:L:189:LYS:HG2	1.90	0.53
25:L:196:ARG:HH21	25:L:239:ARG:HG3	1.73	0.53
27:N:40:ARG:NH1	27:N:180:ALA:O	2.41	0.53
33:T:27:LEU:HD11	33:T:34:ALA:HB1	1.91	0.53
29:p:62:THR:OG1	30:q:85:ARG:NH2	2.41	0.53
3:W:173:THR:HG23	3:W:182:ARG:HH11	1.74	0.53
3:W:177:MET:HB3	3:W:182:ARG:HG2	1.90	0.53
8:b:30:GLN:HG3	8:b:75:LEU:HD13	1.91	0.53
10:d:131:VAL:HA	10:d:134:LYS:HB3	1.91	0.53
20:G:67:THR:HG22	20:G:69:LEU:H	1.74	0.53
1:U:483:LEU:HD11	1:U:781:LEU:HD11	1.91	0.53
2:V:106:ARG:O	2:V:110:HIS:ND1	2.42	0.53
14:B:332:ASN:HB2	15:C:258:ARG:HH22	1.72	0.53
28:O:190:THR:HG22	28:O:192:PRO:HD3	1.89	0.53
25:l:196:ARG:HH21	25:l:239:ARG:HG3	1.73	0.53
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.90	0.53
35:C:501:ATP:O2B	16:D:323:ARG:NH1	2.41	0.53
17:E:33:LEU:HD11	18:F:62:VAL:HG13	1.90	0.53
1:U:889:LEU:HD13	1:U:908:ILE:HG13	1.90	0.52
2:V:349:ARG:HA	2:V:353:LEU:HD23	1.90	0.52
3:W:12:ARG:HD2	3:W:24:VAL:HG22	1.91	0.52
6:Z:16:LEU:HG	6:Z:17:LEU:H	1.74	0.52
12:f:240:VAL:HG13	12:f:257:ARG:HE	1.74	0.52
17:E:235:ILE:CG2	17:E:236:ASP:H	2.21	0.52
20:G:169:GLY:O	20:G:172:GLN:NE2	2.41	0.52
32:s:125:ASP:OD1	32:s:129:SER:N	2.42	0.52
1:U:697:GLN:NE2	1:U:744:VAL:O	2.43	0.52
6:Z:252:LYS:HE2	9:c:299:CYS:HB2	1.91	0.52
9:c:113:HIS:CD2	9:c:115:HIS:ND1	2.77	0.52
10:d:111:ARG:HB3	10:d:114:GLU:HB2	1.90	0.52
10:d:183:GLU:OE2	10:d:215:TRP:NE1	2.43	0.52
13:A:308:GLY:HA2	18:F:234:THR:HG21	1.90	0.52
15:C:72:TYR:HB2	15:C:116:LEU:HB3	1.91	0.52
25:L:148:CYS:SG	25:L:150:SER:OG	2.67	0.52
2:V:264:TYR:OH	10:d:114:GLU:OE1	2.27	0.52
19:v:11:UNK:O	19:v:12:UNK:CB	2.56	0.52
21:H:111:VAL:HG21	21:H:147:PHE:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:M:99:ARG:NH2	26:M:105:ASN:OD1	2.42	0.52
1:U:397:THR:OG1	1:U:401:LYS:NZ	2.42	0.52
13:A:300:LEU:HD23	13:A:303:ILE:HD12	1.92	0.52
25:l:155:ASP:HB3	26:m:62:SER:HB2	1.90	0.52
3:W:220:GLU:O	3:W:257:GLN:NE2	2.42	0.52
12:f:291:GLN:HE21	12:f:879:ARG:HH21	1.56	0.52
17:E:52:SER:OG	18:F:159:LEU:HD12	2.08	0.52
26:m:99:ARG:NH2	26:m:105:ASN:OD1	2.42	0.52
13:A:213:LEU:HD12	13:A:337:LEU:HD13	1.91	0.52
14:B:383:LEU:HD11	14:B:419:PHE:HB3	1.91	0.52
14:B:389:ASP:O	14:B:390:LEU:CB	2.56	0.52
17:E:196:LEU:C	17:E:197:LYS:HG3	2.21	0.52
33:t:192:VAL:HG12	33:t:197:VAL:HG22	1.92	0.52
2:V:412:LEU:O	5:Y:346:LYS:NZ	2.42	0.52
27:N:166:ARG:HH22	33:t:177:TYR:HE1	1.58	0.52
5:Y:191:ILE:H	11:e:43:TRP:HZ3	1.58	0.52
6:Z:145:HIS:HD1	6:Z:149:THR:HG1	1.51	0.52
6:Z:198:LEU:HG	6:Z:201:LEU:HD12	1.91	0.52
7:a:23:HIS:HA	7:a:26:GLU:HG2	1.91	0.52
12:f:571:GLU:HG3	12:f:573:ILE:H	1.73	0.52
12:f:836:GLU:H	12:f:840:LEU:HD21	1.74	0.52
17:E:171:LEU:HB2	17:E:295:LEU:HD22	1.92	0.52
32:S:125:ASP:OD1	32:S:129:SER:N	2.42	0.52
3:W:183:VAL:HG21	3:W:212:LYS:HG2	1.90	0.52
3:W:440:ASN:OD1	6:Z:204:LYS:NZ	2.42	0.52
17:E:201:SER:O	17:E:204:VAL:HG22	2.10	0.52
17:E:235:ILE:CG2	17:E:236:ASP:N	2.73	0.52
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.42	0.52
3:W:347:GLY:O	3:W:351:TRP:N	2.43	0.52
6:Z:16:LEU:CD2	6:Z:16:LEU:N	2.73	0.52
16:D:253:LEU:O	16:D:257:ASN:ND2	2.43	0.52
22:I:106:PRO:HD2	22:I:109:GLN:HE21	1.75	0.52
20:g:43:ARG:NH1	20:g:149:PRO:O	2.43	0.52
24:k:48:LEU:HD21	24:k:77:ALA:HB2	1.92	0.52
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.92	0.51
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.91	0.51
12:f:812:GLY:HA3	12:f:853:VAL:HA	1.92	0.51
12:f:816:TYR:HB3	12:f:821:LEU:HD13	1.92	0.51
17:E:309:ARG:NH1	17:E:332:VAL:O	2.43	0.51
20:G:201:CYS:SG	20:G:202:LEU:N	2.83	0.51
22:I:38:LEU:HG	22:I:160:LYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:g:201:CYS:SG	20:g:202:LEU:N	2.83	0.51
1:U:799:LYS:NZ	1:U:924:LEU:O	2.42	0.51
2:V:212:TYR:HB3	11:e:4:LYS:HE2	1.91	0.51
3:W:359:VAL:HG23	3:W:382:LEU:HD22	1.93	0.51
6:Z:223:ASN:HB3	6:Z:227:ILE:HB	1.92	0.51
13:A:297:ARG:HH12	18:F:306:VAL:HG21	1.75	0.51
14:B:98:LYS:O	14:B:102:LEU:N	2.43	0.51
15:C:281:ASP:OD2	15:C:307:ARG:NH2	2.44	0.51
17:E:98:VAL:HA	17:E:110:TYR:HA	1.92	0.51
26:m:40:ARG:NH1	26:m:146:ALA:O	2.43	0.51
1:U:862:LYS:HD2	1:U:863:GLU:HB3	1.92	0.51
8:b:2:VAL:O	8:b:44:ASN:ND2	2.43	0.51
13:A:118:PHE:CE1	19:v:28:UNK:CB	2.93	0.51
14:B:181:GLN:O	14:B:241:ASN:ND2	2.43	0.51
17:E:83:CYS:HB2	17:E:89:LYS:HE2	1.91	0.51
18:F:31:GLU:OE1	18:F:35:LYS:NZ	2.43	0.51
30:Q:4:LEU:HD22	30:Q:45:LEU:HD13	1.92	0.51
33:T:192:VAL:HG12	33:T:197:VAL:HG22	1.92	0.51
28:o:7:VAL:HG22	28:o:12:ILE:HG12	1.91	0.51
30:q:21:ALA:HB3	30:q:29:LYS:HB3	1.92	0.51
1:U:11:LEU:HD22	1:U:19:LEU:HD11	1.92	0.51
12:f:682:GLY:HA3	12:f:687:ARG:HH11	1.76	0.51
12:f:705:ASN:HB3	12:f:787:LEU:HD21	1.92	0.51
26:M:40:ARG:NH1	26:M:146:ALA:O	2.43	0.51
30:Q:21:ALA:HB3	30:Q:29:LYS:HB3	1.92	0.51
21:h:34:PRO:HA	21:h:164:GLY:HA3	1.92	0.51
22:i:57:ASP:HB3	22:i:59:VAL:HG13	1.92	0.51
30:q:4:LEU:HD22	30:q:45:LEU:HD13	1.92	0.51
1:U:399:TRP:HD1	9:c:176:GLN:HG2	1.75	0.51
24:K:48:LEU:HD21	24:K:77:ALA:HB2	1.91	0.51
24:K:97:GLN:HG3	31:R:61:ARG:HG2	1.92	0.51
26:M:170:GLN:HA	26:M:173:LYS:HE2	1.93	0.51
28:O:7:VAL:HG22	28:O:12:ILE:HG12	1.91	0.51
31:R:1:THR:N	31:R:169:TYR:O	2.44	0.51
26:m:170:GLN:HA	26:m:173:LYS:HE2	1.93	0.51
32:s:209:SER:OG	32:s:212:LYS:NZ	2.44	0.51
5:Y:336:ARG:NH1	11:e:55:GLN:OE1	2.44	0.51
12:f:606:VAL:HG11	14:B:70:ASP:HB3	1.93	0.51
17:E:242:ARG:O	17:E:281:ARG:NH2	2.44	0.51
20:G:41:ALA:HB3	20:G:166:THR:HB	1.92	0.51
20:g:169:GLY:O	20:g:172:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:265:ILE:HA	1:U:268:LEU:HD13	1.93	0.51
5:Y:13:LYS:HE3	5:Y:146:ARG:HD2	1.92	0.51
6:Z:11:VAL:HB	6:Z:162:ILE:CD1	2.36	0.51
24:k:41:GLN:NE2	24:k:151:PRO:O	2.44	0.51
24:k:97:GLN:HG3	31:r:61:ARG:HG2	1.93	0.51
31:r:1:THR:N	31:r:169:TYR:O	2.44	0.51
3:W:259:GLU:HG3	3:W:261:GLU:H	1.75	0.51
10:d:8:GLU:O	10:d:13:SER:OG	2.27	0.51
32:S:209:SER:OG	32:S:212:LYS:NZ	2.44	0.51
23:j:4:ASP:OD1	23:j:4:ASP:N	2.44	0.51
12:f:149:GLU:HG3	12:f:152:ALA:HB2	1.93	0.51
17:E:368:MET:HB3	17:E:372:ARG:HH12	1.76	0.51
22:i:216:LEU:HD12	22:i:225:ILE:HG12	1.91	0.51
33:t:1:THR:N	33:t:104:ASN:OD1	2.43	0.51
15:C:187:LEU:HD23	15:C:314:LYS:HE3	1.92	0.51
20:G:158:GLY:O	21:H:84:ARG:NH2	2.44	0.51
25:l:42:THR:O	25:l:137:TYR:OH	2.29	0.51
30:q:183:ILE:HG12	30:q:188:ILE:HG13	1.92	0.51
9:c:149:GLN:HB3	9:c:156:VAL:HG21	1.93	0.50
12:f:110:TYR:OH	12:f:118:ASN:ND2	2.43	0.50
17:E:166:PRO:HA	17:E:168:LYS:HE3	1.92	0.50
17:E:194:ASN:HD21	17:E:228:CYS:HA	1.74	0.50
1:U:900:TYR:HB3	1:U:914:LEU:HD21	1.91	0.50
2:V:179:LYS:HE3	2:V:214:HIS:HB2	1.92	0.50
7:a:140:GLU:O	7:a:143:ASN:ND2	2.44	0.50
10:d:179:ALA:HA	10:d:182:ILE:HG22	1.91	0.50
12:f:269:ALA:O	12:f:273:ASN:N	2.41	0.50
14:B:223:ILE:HG13	14:B:347:ILE:HG21	1.93	0.50
16:D:249:ASP:OD1	16:D:252:ARG:NH2	2.44	0.50
33:T:1:THR:N	33:T:104:ASN:OD1	2.43	0.50
24:k:37:ALA:HB2	24:k:50:VAL:HG23	1.93	0.50
1:U:47:VAL:O	1:U:48:LEU:C	2.54	0.50
1:U:418:GLU:HG3	1:U:421:GLN:HE21	1.75	0.50
3:W:72:LYS:HD3	3:W:123:ARG:HA	1.93	0.50
16:D:154:LEU:HD11	16:D:229:ARG:HE	1.76	0.50
25:l:157:ARG:HD2	25:l:176:MET:HE3	1.93	0.50
29:p:189:ILE:HG23	29:p:196:THR:HB	1.94	0.50
15:C:307:ARG:HD2	15:C:309:GLY:H	1.76	0.50
25:L:157:ARG:HD2	25:L:176:MET:HE3	1.93	0.50
21:h:139:TRP:HA	21:h:144:PRO:HA	1.94	0.50
24:k:221:GLN:HB2	24:k:224:GLN:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:401:ASN:HA	2:V:404:LYS:HB2	1.94	0.50
5:Y:300:ARG:NH2	11:e:59:GLU:OE1	2.44	0.50
7:a:120:ALA:O	7:a:124:ASN:ND2	2.45	0.50
15:C:217:SER:OG	16:D:291:GLU:OE1	2.29	0.50
17:E:195:PHE:HD1	17:E:231:PHE:HB2	1.75	0.50
20:g:120:ASP:OD1	21:h:84:ARG:NH1	2.44	0.50
31:r:38:ASN:HD22	31:r:41:LEU:HD12	1.77	0.50
7:a:70:ARG:HH21	8:b:17:ARG:HA	1.77	0.50
10:d:8:GLU:HG3	10:d:15:ASN:HD21	1.76	0.50
12:f:252:ALA:O	12:f:257:ARG:NH1	2.45	0.50
17:E:178:THR:HB	17:E:182:LEU:HD13	1.93	0.50
17:E:200:SER:HB2	17:E:234:GLU:O	2.11	0.50
20:G:114:LEU:HD22	20:G:140:LEU:HD21	1.93	0.50
32:S:148:LEU:HD23	32:S:178:VAL:HG12	1.93	0.50
22:i:48:GLU:OE2	22:i:50:ARG:NH2	2.45	0.50
1:U:421:GLN:HA	1:U:424:ALA:HB3	1.94	0.50
5:Y:47:ASP:OD1	5:Y:113:ARG:NE	2.38	0.50
5:Y:231:LEU:HB2	5:Y:234:PRO:HG2	1.94	0.50
7:a:70:ARG:O	8:b:17:ARG:NH1	2.40	0.50
12:f:612:LEU:HD21	12:f:636:ASP:HA	1.94	0.50
30:Q:183:ILE:HG12	30:Q:188:ILE:HG13	1.92	0.50
29:p:126:LEU:HD12	29:p:127:ILE:HG23	1.94	0.50
2:V:163:VAL:HG22	2:V:175:MET:HG2	1.94	0.50
7:a:33:LEU:HA	8:b:18:ASN:HB2	1.93	0.50
9:c:124:GLY:HA3	19:v:35:UNK:CB	2.42	0.50
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.93	0.50
32:S:35:ILE:O	33:T:151:ARG:NH2	2.38	0.50
2:V:167:LEU:HD12	2:V:169:LEU:H	1.76	0.50
3:W:203:GLN:HB3	3:W:233:LEU:HD21	1.94	0.50
20:G:56:VAL:HG13	20:G:61:LEU:HD22	1.93	0.50
30:Q:64:VAL:HG13	30:Q:75:LEU:HD12	1.94	0.50
21:h:66:GLU:OE2	21:h:91:ARG:NH2	2.44	0.50
17:E:101:ASP:HB3	17:E:105:LEU:H	1.77	0.49
17:E:198:VAL:HB	17:E:232:MET:CA	2.38	0.49
24:K:21:LEU:HB3	24:K:23:GLN:H	1.75	0.49
27:N:76:VAL:HG23	27:N:104:ASP:HB2	1.94	0.49
29:P:126:LEU:HD12	29:P:127:ILE:HG23	1.93	0.49
2:V:239:THR:HG23	2:V:243:ASP:HB2	1.93	0.49
12:f:373:ALA:HB2	12:f:744:MET:HA	1.94	0.49
12:f:742:ALA:O	12:f:746:ARG:NE	2.40	0.49
19:v:22:UNK:O	19:v:23:UNK:C	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:193:CYS:SG	17:E:194:ASN:N	2.85	0.49
17:E:232:MET:HG3	17:E:232:MET:O	2.07	0.49
21:H:66:GLU:OE2	21:H:91:ARG:NH2	2.45	0.49
7:a:227:ASN:O	7:a:231:GLN:NE2	2.44	0.49
8:b:161:ASN:HB2	8:b:165:GLY:HA3	1.94	0.49
10:d:248:GLU:HA	10:d:251:ARG:HB3	1.95	0.49
16:D:200:ARG:NH2	16:D:302:ASN:OD1	2.35	0.49
29:p:58:THR:OG1	30:q:121:LEU:O	2.23	0.49
1:U:554:LEU:HG	1:U:588:MET:HE1	1.94	0.49
1:U:696:ILE:HG22	1:U:737:LEU:HA	1.93	0.49
5:Y:141:VAL:HG13	5:Y:160:ASN:HB2	1.95	0.49
6:Z:192:THR:HG22	7:a:375:LEU:HG	1.94	0.49
9:c:122:LEU:HD12	9:c:126:ASP:HB3	1.94	0.49
12:f:171:GLN:HG3	12:f:179:VAL:HG22	1.95	0.49
12:f:257:ARG:HG2	12:f:272:LEU:HD13	1.94	0.49
12:f:618:GLU:HG2	14:B:82:GLN:CD	2.38	0.49
18:F:376:SER:HB3	18:F:414:GLU:HG3	1.94	0.49
31:R:38:ASN:HD22	31:R:41:LEU:HD12	1.77	0.49
32:s:148:LEU:HD23	32:s:178:VAL:HG12	1.93	0.49
1:U:510:GLU:HG3	1:U:543:LYS:HB3	1.95	0.49
13:A:41:TYR:HA	13:A:44:GLN:HB3	1.94	0.49
13:A:71:GLY:HA2	14:B:162:VAL:HG12	1.93	0.49
17:E:196:LEU:HD13	17:E:230:ILE:CD1	2.43	0.49
18:F:50:SER:O	18:F:54:ILE:N	2.38	0.49
20:g:89:SER:OG	26:m:117:MET:SD	2.70	0.49
3:W:123:ARG:HH12	3:W:127:THR:HB	1.77	0.49
5:Y:96:GLY:O	5:Y:130:LYS:NZ	2.44	0.49
8:b:100:ARG:NH1	8:b:105:HIS:O	2.46	0.49
12:f:482:ILE:HG22	12:f:501:LEU:HD22	1.94	0.49
20:g:11:ARG:O	20:g:24:GLN:NE2	2.46	0.49
30:q:64:VAL:HG13	30:q:75:LEU:HD12	1.94	0.49
12:f:369:ARG:NH2	12:f:791:VAL:O	2.45	0.49
13:A:178:GLY:HA3	13:A:353:HIS:HD2	1.78	0.49
14:B:188:GLY:HA3	14:B:364:ILE:HD13	1.94	0.49
16:D:248:ARG:HG2	16:D:295:GLN:HE22	1.78	0.49
17:E:127:PRO:CA	17:E:193:CYS:SG	3.01	0.49
20:G:43:ARG:HH21	20:G:164:LYS:HG2	1.76	0.49
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.94	0.49
5:Y:102:ASP:HA	5:Y:105:MET:HG2	1.94	0.49
29:P:189:ILE:HG23	29:P:196:THR:HB	1.94	0.49
24:k:121:LEU:HD13	25:l:79:ALA:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:s:123:SER:HB3	32:s:136:LYS:HG3	1.95	0.49
7:a:342:ASP:O	7:a:344:GLN:N	2.46	0.49
12:f:240:VAL:O	12:f:257:ARG:NH2	2.36	0.49
12:f:288:VAL:HA	12:f:291:GLN:HG2	1.94	0.49
13:A:35:THR:O	13:A:39:SER:OG	2.31	0.49
17:E:125:GLU:OE1	17:E:221:TYR:OH	2.31	0.49
24:K:41:GLN:NE2	24:K:151:PRO:O	2.45	0.49
24:K:77:ALA:HB3	24:K:142:LEU:HB2	1.95	0.49
1:U:678:ASP:O	1:U:684:ARG:NH1	2.40	0.48
1:U:898:CYS:SG	1:U:899:ARG:N	2.86	0.48
2:V:33:GLN:NE2	2:V:84:LYS:O	2.46	0.48
3:W:59:ASP:HB3	3:W:71:VAL:HG23	1.95	0.48
7:a:360:VAL:HG22	9:c:308:VAL:HG13	1.95	0.48
9:c:124:GLY:CA	19:v:35:UNK:CB	2.91	0.48
22:i:143:TYR:HB2	22:i:146:GLN:HE21	1.77	0.48
28:o:198:ARG:NH1	29:p:152:SER:O	2.45	0.48
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.94	0.48
3:W:99:GLN:HA	3:W:102:ALA:HB3	1.94	0.48
3:W:344:THR:OG1	3:W:345:GLU:OE1	2.30	0.48
10:d:182:ILE:HD12	10:d:186:TYR:HD2	1.78	0.48
12:f:253:LEU:HD11	12:f:272:LEU:HB3	1.95	0.48
17:E:168:LYS:NZ	17:E:265:ASP:OD2	2.37	0.48
21:H:196:LYS:NZ	21:H:234:ALA:O	2.41	0.48
30:q:38:MET:O	30:q:65:GLN:NE2	2.45	0.48
1:U:47:VAL:C	1:U:49:TYR:H	2.22	0.48
3:W:65:ARG:HG3	3:W:67:LEU:H	1.78	0.48
5:Y:179:ARG:HH11	5:Y:182:VAL:HG11	1.77	0.48
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.95	0.48
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.95	0.48
16:D:367:PRO:HG2	21:H:201:GLY:HA2	1.95	0.48
17:E:84:ARG:O	17:E:85:ARG:NE	2.43	0.48
17:E:194:ASN:CG	17:E:228:CYS:HA	2.37	0.48
22:i:159:TRP:HA	23:j:54:GLN:HA	1.95	0.48
25:l:41:LYS:NZ	25:l:180:MET:O	2.42	0.48
25:l:189:LYS:O	25:l:193:ARG:NH1	2.46	0.48
27:n:76:VAL:HG23	27:n:104:ASP:HB2	1.93	0.48
1:U:208:LEU:HD23	1:U:210:LYS:H	1.78	0.48
3:W:63:THR:HG21	3:W:71:VAL:H	1.78	0.48
25:L:186:GLU:O	25:L:190:HIS:N	2.45	0.48
25:L:189:LYS:O	25:L:193:ARG:NH1	2.46	0.48
25:l:186:GLU:O	25:l:190:HIS:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:78:ASN:HA	4:X:82:LYS:HE3	1.95	0.48
8:b:5:SER:HB3	8:b:64:LEU:HD21	1.95	0.48
12:f:23:GLY:HA3	12:f:34:ARG:HH22	1.78	0.48
20:G:120:ASP:OD1	21:H:84:ARG:NH1	2.46	0.48
22:i:163:CYS:SG	22:i:164:ILE:N	2.75	0.48
1:U:229:VAL:HA	1:U:232:ILE:HG12	1.96	0.48
1:U:325:MET:HA	1:U:328:ILE:HG12	1.95	0.48
2:V:228:ARG:NH2	2:V:253:LEU:O	2.46	0.48
9:c:100:LYS:HG2	9:c:105:PRO:HB3	1.94	0.48
12:f:828:ARG:CZ	12:f:843:SER:HG	2.26	0.48
22:I:239:LYS:NZ	22:I:243:GLU:OE2	2.46	0.48
20:g:43:ARG:HH21	20:g:164:LYS:HG2	1.79	0.48
1:U:643:SER:O	1:U:649:ARG:NH1	2.46	0.48
17:E:192:ASP:O	17:E:193:CYS:HB3	2.14	0.48
22:I:42:GLY:HA3	22:I:186:LEU:HD21	1.96	0.48
23:J:4:ASP:OD1	23:J:4:ASP:N	2.44	0.48
32:S:123:SER:HB3	32:S:136:LYS:HG3	1.95	0.48
32:s:4:PRO:O	33:t:100:ARG:NH2	2.46	0.48
1:U:824:GLU:HB3	1:U:826:GLU:HB2	1.94	0.48
2:V:203:LEU:HA	2:V:206:VAL:HB	1.96	0.48
3:W:443:THR:HA	3:W:446:ILE:HG12	1.95	0.48
8:b:109:ILE:HB	8:b:138:VAL:HG22	1.96	0.48
9:c:173:GLU:HG3	9:c:175:ARG:HD2	1.95	0.48
22:I:105:ILE:HD11	22:I:109:GLN:HG3	1.96	0.48
24:K:76:CYS:SG	24:K:77:ALA:N	2.87	0.48
22:i:105:ILE:HD11	22:i:109:GLN:HG3	1.95	0.48
1:U:643:SER:HA	15:C:49:ARG:HH22	1.78	0.48
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.94	0.48
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.47	0.48
23:J:158:ALA:HB3	24:K:58:LEU:HD13	1.95	0.48
28:O:177:VAL:HB	28:O:184:ASP:HB2	1.95	0.48
32:S:187:VAL:HG21	28:o:24:MET:HE3	1.96	0.48
2:V:179:LYS:HD2	2:V:210:CYS:HB2	1.96	0.48
4:X:316:ASP:OD2	4:X:321:THR:OG1	2.31	0.48
5:Y:297:ARG:HH12	11:e:51:ASP:HB3	1.79	0.48
8:b:58:CYS:HB3	8:b:92:VAL:HG11	1.95	0.48
18:F:339:ASP:HB3	18:F:342:LEU:HD13	1.96	0.48
32:S:211:ARG:HH22	28:o:170:GLY:HA2	1.78	0.48
22:i:2:SER:OG	22:i:3:ARG:N	2.46	0.48
1:U:381:THR:HG22	1:U:412:HIS:HA	1.96	0.47
15:C:83:LYS:H	15:C:105:ILE:HD11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:127:PRO:HA	17:E:193:CYS:SG	2.54	0.47
18:F:228:PRO:O	18:F:233:LYS:NZ	2.47	0.47
21:H:222:THR:OG1	21:H:225:GLU:OE1	2.26	0.47
22:I:105:ILE:HG12	22:I:110:LEU:HB2	1.96	0.47
28:o:177:VAL:HB	28:o:184:ASP:HB2	1.95	0.47
6:Z:45:LYS:HB3	6:Z:47:VAL:HG12	1.95	0.47
8:b:34:ASN:O	8:b:38:HIS:ND1	2.38	0.47
13:A:279:ALA:HB1	14:B:307:ARG:HG3	1.95	0.47
17:E:235:ILE:HG23	17:E:279:THR:CB	2.38	0.47
24:K:91:LYS:HG2	24:K:95:GLU:HG2	1.96	0.47
26:m:66:LEU:HD13	26:m:214:SER:HB2	1.96	0.47
3:W:82:LEU:HA	3:W:85:GLU:HB2	1.95	0.47
5:Y:238:GLU:HA	5:Y:242:LYS:HB2	1.96	0.47
5:Y:212:GLU:HG3	5:Y:213:LEU:HG	1.95	0.47
7:a:27:GLU:OE1	7:a:31:LYS:NZ	2.47	0.47
21:H:119:GLN:NE2	22:I:81:SER:O	2.47	0.47
24:K:100:TRP:O	31:R:57:ARG:NH2	2.47	0.47
23:j:116:GLN:HE22	24:k:83:ALA:HB1	1.79	0.47
8:b:95:LEU:O	8:b:99:HIS:ND1	2.47	0.47
9:c:50:PRO:HG2	17:E:53:VAL:HG13	1.89	0.47
13:A:113:ILE:HD11	13:A:149:ILE:HD11	1.95	0.47
17:E:193:CYS:O	17:E:194:ASN:C	2.57	0.47
18:F:222:GLY:HA3	18:F:348:LEU:HA	1.96	0.47
20:G:144:ASP:HB3	20:G:147:GLN:HB2	1.96	0.47
24:K:236:GLU:HA	24:K:239:LYS:HE3	1.95	0.47
22:i:62:SER:OG	22:i:65:ILE:O	2.32	0.47
24:k:100:TRP:O	31:r:57:ARG:NH2	2.47	0.47
24:k:169:ALA:O	24:k:174:SER:OG	2.32	0.47
3:W:216:GLU:HA	3:W:219:THR:HB	1.96	0.47
5:Y:44:ALA:HA	5:Y:49:ASN:HD22	1.79	0.47
22:I:86:LEU:HD22	22:I:114:LEU:HD11	1.94	0.47
26:M:66:LEU:HD13	26:M:214:SER:HB2	1.96	0.47
30:Q:199:GLN:H	30:q:197:PRO:HA	1.80	0.47
29:p:135:ASP:OD1	29:p:135:ASP:N	2.48	0.47
1:U:895:PRO:HG2	1:U:902:PRO:HD3	1.96	0.47
2:V:107:ARG:HA	2:V:110:HIS:HD1	1.78	0.47
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.96	0.47
7:a:112:ILE:H	7:a:112:ILE:HG13	1.58	0.47
12:f:168:LYS:HD3	12:f:204:ALA:HB1	1.97	0.47
12:f:637:LYS:HE2	12:f:673:ARG:HB2	1.96	0.47
13:A:103:ASN:HA	13:A:136:GLU:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:252:GLU:HA	17:E:255:ARG:HE	1.80	0.47
20:G:32:ILE:HA	20:G:82:GLY:HA2	1.97	0.47
22:I:11:ILE:HD13	23:J:5:ARG:HA	1.97	0.47
32:S:4:PRO:O	33:T:100:ARG:NH2	2.47	0.47
22:i:9:THR:HA	22:i:20:GLN:HG3	1.97	0.47
29:p:2:SER:OG	29:p:3:ILE:N	2.47	0.47
5:Y:179:ARG:HA	5:Y:179:ARG:HD3	1.69	0.47
7:a:214:GLY:HA2	7:a:217:LEU:HD13	1.97	0.47
9:c:49:VAL:HG23	9:c:50:PRO:HD3	1.96	0.47
12:f:202:HIS:CE1	12:f:241:PRO:HB2	2.50	0.47
12:f:640:LYS:HD3	12:f:651:GLY:HA3	1.96	0.47
15:C:113:ARG:HD2	15:C:131:VAL:HG13	1.95	0.47
15:C:403:LYS:HG3	21:H:156:PHE:HE1	1.80	0.47
5:Y:60:SER:OG	5:Y:61:LEU:N	2.47	0.47
13:A:218:PRO:HB2	14:B:343:ARG:HD3	1.95	0.47
19:v:15:UNK:O	19:v:16:UNK:C	2.63	0.47
23:J:7:ILE:HD12	23:J:8:THR:HG23	1.97	0.47
28:O:205:GLU:HB2	28:O:208:THR:HB	1.97	0.47
20:g:41:ALA:HB3	20:g:166:THR:HB	1.96	0.47
28:o:205:GLU:HB2	28:o:208:THR:HB	1.97	0.47
6:Z:192:THR:O	6:Z:196:HIS:ND1	2.47	0.47
29:P:190:ILE:HG22	29:P:195:ILE:HG23	1.97	0.47
30:Q:38:MET:O	30:Q:65:GLN:NE2	2.45	0.47
23:j:109:ARG:NH2	31:r:70:ASN:OD1	2.48	0.47
26:m:152:ASP:OD1	26:m:156:VAL:N	2.48	0.47
30:q:19:ARG:HH21	30:q:31:ASP:HB2	1.79	0.47
1:U:801:GLN:HB3	1:U:877:LEU:HD22	1.97	0.46
13:A:56:LEU:HD11	14:B:48:LYS:HD3	1.97	0.46
14:B:287:ILE:HG12	14:B:329:MET:HB3	1.97	0.46
22:i:105:ILE:HG12	22:i:110:LEU:HB2	1.96	0.46
1:U:181:LEU:C	1:U:181:LEU:HD23	2.40	0.46
2:V:417:ILE:HD12	5:Y:349:LYS:HB2	1.98	0.46
7:a:150:SER:OG	7:a:154:ARG:NH1	2.48	0.46
7:a:247:ARG:HH21	7:a:250:THR:HG23	1.80	0.46
12:f:505:MET:HE3	12:f:537:THR:HG22	1.98	0.46
12:f:827:PRO:HG2	12:f:848:GLN:HB3	1.96	0.46
13:A:248:LYS:HG2	19:v:21:UNK:CB	2.44	0.46
1:U:519:VAL:HG23	1:U:520:MET:HG2	1.97	0.46
1:U:607:VAL:HG11	16:D:63:ASP:HB3	1.97	0.46
7:a:321:LYS:O	7:a:334:THR:OG1	2.34	0.46
13:A:339:ARG:NH1	18:F:426:GLU:OE2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:C:406:LYS:HE2	22:I:80:THR:HG22	1.97	0.46
29:p:190:ILE:HG22	29:p:195:ILE:HG23	1.97	0.46
4:X:145:GLU:HA	4:X:148:HIS:HB2	1.95	0.46
12:f:717:ALA:HB1	12:f:760:PHE:HB2	1.97	0.46
13:A:307:ASP:OD2	13:A:333:ARG:NH2	2.49	0.46
18:F:206:MET:HA	18:F:325:GLN:HE21	1.80	0.46
33:T:177:TYR:HE1	27:n:166:ARG:HH22	1.62	0.46
20:g:163:PHE:HB3	21:h:57:TYR:HA	1.98	0.46
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.81	0.46
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.96	0.46
12:f:612:LEU:HA	12:f:632:LYS:HD2	1.96	0.46
13:A:117:GLN:HE22	14:B:128:GLY:HA3	1.80	0.46
29:P:2:SER:OG	29:P:3:ILE:N	2.47	0.46
2:V:183:GLU:HA	2:V:186:LYS:HB3	1.98	0.46
12:f:243:PRO:HD2	12:f:257:ARG:HH22	1.79	0.46
13:A:89:SER:HA	13:A:93:LEU:HD23	1.98	0.46
13:A:395:PHE:HA	13:A:398:ARG:HD2	1.98	0.46
17:E:122:MET:HB2	17:E:218:MET:HG2	1.97	0.46
18:F:72:LYS:O	18:F:74:LYS:N	2.48	0.46
18:F:249:LEU:HD23	18:F:283:ILE:HG12	1.97	0.46
23:J:134:VAL:HG22	23:J:144:LEU:HB2	1.98	0.46
26:M:152:ASP:OD1	26:M:156:VAL:N	2.48	0.46
2:V:110:HIS:HD2	2:V:114:TYR:HE2	1.63	0.46
2:V:480:ILE:HD11	6:Z:260:VAL:HA	1.98	0.46
3:W:422:ASN:O	3:W:426:ASN:N	2.48	0.46
7:a:75:SER:HA	7:a:78:GLU:HB2	1.97	0.46
7:a:119:GLY:HA2	7:a:122:LYS:HB3	1.98	0.46
9:c:196:LEU:HA	9:c:197:ASN:HA	1.70	0.46
16:D:202:VAL:HA	16:D:329:ARG:HB2	1.98	0.46
17:E:339:ASN:HB3	17:E:342:ASP:HB2	1.98	0.46
27:N:20:THR:HB	27:N:28:ASN:HB3	1.97	0.46
27:N:144:ARG:H	27:N:147:MET:HE3	1.80	0.46
33:T:136:SER:HB2	33:T:150:LEU:HD13	1.98	0.46
1:U:773:PHE:H	9:c:177:THR:HB	1.79	0.46
3:W:227:TYR:HB3	3:W:246:HIS:NE2	2.30	0.46
5:Y:50:MET:HE1	5:Y:67:VAL:HG13	1.97	0.46
15:C:138:MET:HE3	15:C:234:LEU:HD13	1.97	0.46
17:E:62:LYS:HA	17:E:94:PRO:HB3	1.98	0.46
20:g:144:ASP:HB3	20:g:147:GLN:HB2	1.97	0.46
4:X:134:VAL:HB	4:X:149:LEU:HD23	1.97	0.46
7:a:168:ASN:OD1	7:a:171:SER:OG	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:626:GLU:OE1	12:f:665:GLU:HB3	2.16	0.46
15:C:236:VAL:HA	15:C:239:ARG:HD3	1.96	0.46
15:C:307:ARG:HH21	15:C:310:ARG:HE	1.63	0.46
16:D:320:ALA:O	16:D:326:ARG:NH2	2.49	0.46
17:E:305:ASN:HB3	17:E:308:ALA:H	1.80	0.46
19:v:7:UNK:C	19:v:9:UNK:N	2.77	0.46
32:S:35:ILE:HB	33:T:151:ARG:HH12	1.81	0.46
1:U:118:LEU:HD13	1:U:122:GLU:HG3	1.98	0.46
4:X:380:GLN:HB3	5:Y:315:THR:HG22	1.98	0.46
4:X:397:TYR:OH	5:Y:362:LYS:NZ	2.47	0.46
6:Z:20:VAL:HG22	6:Z:126:VAL:HG23	1.96	0.46
12:f:24:THR:HG23	12:f:31:LYS:HG3	1.97	0.46
12:f:75:LEU:HD12	12:f:78:LEU:HD13	1.98	0.46
12:f:813:LYS:NZ	12:f:819:TYR:OH	2.34	0.46
14:B:259:TYR:HA	19:v:19:UNK:O	2.16	0.46
20:G:199:ILE:HD12	20:G:210:PHE:HZ	1.80	0.46
30:Q:19:ARG:HH21	30:Q:31:ASP:HB2	1.79	0.46
4:X:54:GLY:HA2	4:X:57:LEU:HD12	1.98	0.45
4:X:214:SER:O	4:X:218:HIS:ND1	2.39	0.45
6:Z:239:ASP:OD1	6:Z:239:ASP:N	2.49	0.45
22:i:86:LEU:HD22	22:i:114:LEU:HD11	1.97	0.45
23:j:32:ALA:HB2	23:j:45:VAL:HG23	1.98	0.45
23:j:134:VAL:HG22	23:j:144:LEU:HB2	1.98	0.45
33:t:136:SER:HB2	33:t:150:LEU:HD13	1.98	0.45
6:Z:124:ILE:HG22	6:Z:135:THR:HG22	1.98	0.45
8:b:18:ASN:OD1	8:b:18:ASN:N	2.49	0.45
17:E:254:GLN:HB3	17:E:258:MET:HE2	1.97	0.45
30:Q:25:ILE:HD11	31:R:133:VAL:HG11	1.96	0.45
27:n:144:ARG:H	27:n:147:MET:HE3	1.80	0.45
1:U:173:VAL:HA	1:U:174:PRO:HD3	1.55	0.45
2:V:323:GLY:HA2	11:e:9:ASP:HB2	1.98	0.45
4:X:260:MET:HE3	4:X:260:MET:HB2	1.76	0.45
5:Y:184:GLN:HB3	5:Y:197:ALA:HA	1.99	0.45
12:f:281:ILE:HA	12:f:282:PHE:HA	1.54	0.45
14:B:120:HIS:HA	14:B:134:SER:HA	1.98	0.45
17:E:56:ILE:HB	17:E:100:LEU:HB2	1.98	0.45
20:G:141:ILE:HG22	20:G:151:VAL:HG22	1.99	0.45
30:Q:2:GLU:HG3	30:Q:34:LYS:HE2	1.99	0.45
26:m:76:ALA:HB3	26:m:136:MET:HB2	1.99	0.45
27:n:20:THR:HB	27:n:28:ASN:HB3	1.97	0.45
10:d:71:PHE:HZ	10:d:101:LEU:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:P:28:PHE:HB2	29:P:39:PHE:HB2	1.99	0.45
23:j:7:ILE:HD12	23:j:8:THR:HG23	1.97	0.45
26:m:41:CYS:HB3	26:m:189:ILE:HG13	1.99	0.45
1:U:772:TRP:HD1	1:U:775:LEU:HG	1.82	0.45
6:Z:177:ARG:NH2	9:c:153:GLY:O	2.49	0.45
12:f:130:ALA:O	12:f:134:SER:N	2.49	0.45
12:f:778:LEU:HA	12:f:803:PHE:HB3	1.99	0.45
14:B:409:GLU:OE2	14:B:411:ARG:NH2	2.35	0.45
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.99	0.45
3:W:89:LEU:HD22	3:W:90:LEU:HD13	1.99	0.45
12:f:184:LEU:HG	14:B:59:ARG:HB2	1.98	0.45
12:f:417:ILE:HG22	12:f:418:LEU:HD12	1.98	0.45
20:g:141:ILE:HG22	20:g:151:VAL:HG22	1.98	0.45
1:U:603:LEU:HD21	16:D:60:TYR:HB2	1.99	0.45
4:X:57:LEU:HD13	4:X:66:LEU:HA	1.99	0.45
14:B:67:ARG:NH2	14:B:71:TYR:OH	2.49	0.45
22:I:48:GLU:OE2	22:I:50:ARG:NH2	2.50	0.45
22:I:165:GLY:O	22:I:168:SER:N	2.47	0.45
22:I:216:LEU:HD12	22:I:225:ILE:HG12	1.98	0.45
26:M:168:ALA:HB1	26:M:171:ALA:HB3	1.99	0.45
23:j:32:ALA:HB3	23:j:161:ILE:HD11	1.98	0.45
12:f:564:LEU:HD22	12:f:776:LEU:HG	1.99	0.45
21:H:34:PRO:HA	21:H:164:GLY:HA3	1.99	0.45
24:K:98:ASN:OD1	31:R:61:ARG:NH2	2.41	0.45
28:O:112:SER:HB3	28:O:125:VAL:HG11	1.98	0.45
26:m:168:ALA:HB1	26:m:171:ALA:HB3	1.99	0.45
30:q:37:LYS:O	30:q:61:GLN:NE2	2.46	0.45
6:Z:198:LEU:HD22	7:a:364:GLU:HB2	1.99	0.45
7:a:50:PHE:O	7:a:86:GLN:NE2	2.49	0.45
13:A:105:ASP:HB2	13:A:110:LYS:HB2	1.98	0.45
22:i:90:LEU:HD12	22:i:114:LEU:HD22	1.99	0.45
28:o:112:SER:HB3	28:o:125:VAL:HG11	1.98	0.45
1:U:177:LEU:HD13	1:U:177:LEU:N	2.32	0.45
3:W:446:ILE:HA	6:Z:227:ILE:HD11	1.99	0.45
5:Y:81:LEU:HD22	5:Y:107:LYS:HG2	1.98	0.45
6:Z:12:HIS:ND1	6:Z:51:SER:HA	2.32	0.45
12:f:403:LYS:HG3	12:f:406:GLY:H	1.82	0.45
14:B:248:LEU:HD12	14:B:282:VAL:HG22	1.98	0.45
25:L:42:THR:O	25:L:137:TYR:OH	2.29	0.45
31:R:36:GLU:OE2	31:R:186:ARG:NH2	2.50	0.45
1:U:180:SER:HA	1:U:183:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:57:LEU:HD23	4:X:62:GLN:HE21	1.82	0.44
6:Z:243:GLN:NE2	10:d:233:GLU:OE2	2.50	0.44
9:c:88:ASP:HB3	9:c:91:PHE:HB3	1.99	0.44
17:E:53:VAL:HG12	17:E:53:VAL:O	2.17	0.44
22:I:49:ARG:HB2	22:I:210:LYS:HA	1.98	0.44
23:J:32:ALA:HB2	23:J:45:VAL:HG23	1.98	0.44
26:M:41:CYS:HB3	26:M:189:ILE:HG13	1.99	0.44
20:g:53:GLN:HA	20:g:215:ILE:HA	1.99	0.44
20:g:132:ARG:HA	20:g:133:PRO:HD3	1.76	0.44
1:U:357:LYS:HE3	1:U:392:TRP:CD2	2.52	0.44
4:X:201:TYR:HD1	21:H:177:ARG:HA	1.82	0.44
12:f:773:LYS:HA	12:f:774:GLY:HA3	1.79	0.44
15:C:222:LYS:HD3	15:C:223:PHE:CE1	2.51	0.44
1:U:756:HIS:HB3	1:U:758:PRO:HD2	1.99	0.44
6:Z:140:SER:HB2	6:Z:153:LYS:HZ3	1.81	0.44
10:d:176:ASP:O	10:d:180:GLY:N	2.48	0.44
14:B:304:GLU:OE1	19:v:18:UNK:CB	2.66	0.44
15:C:198:LEU:O	15:C:202:ALA:N	2.44	0.44
22:I:229:LYS:N	22:I:232:GLU:OE2	2.47	0.44
23:J:32:ALA:HB3	23:J:161:ILE:HD11	1.98	0.44
26:m:37:ILE:HD11	26:m:193:VAL:HG13	1.99	0.44
2:V:190:ASP:OD2	2:V:234:ARG:NH1	2.35	0.44
4:X:414:LEU:HD11	6:Z:273:HIS:CE1	2.53	0.44
12:f:283:THR:O	12:f:287:ASP:N	2.46	0.44
28:o:96:ALA:H	28:o:115:PRO:HB3	1.82	0.44
2:V:132:LEU:HD23	2:V:135:LEU:HD12	2.00	0.44
7:a:122:LYS:HD3	7:a:130:VAL:HG13	1.99	0.44
12:f:755:ASP:OD1	12:f:755:ASP:N	2.50	0.44
21:h:192:ILE:O	21:h:196:LYS:N	2.46	0.44
1:U:802:TYR:HB3	1:U:895:PRO:HB3	1.98	0.44
17:E:235:ILE:HG21	17:E:279:THR:HG22	1.98	0.44
18:F:235:LEU:HG	35:F:501:ATP:H2'	2.00	0.44
24:K:121:LEU:HD13	25:L:79:ALA:HA	1.99	0.44
26:M:76:ALA:HB3	26:M:136:MET:HB2	1.99	0.44
1:U:803:LYS:HB2	1:U:875:PHE:HA	2.00	0.44
3:W:173:THR:HG23	3:W:182:ARG:HE	1.82	0.44
3:W:174:TYR:HA	17:E:143:ARG:HD2	1.99	0.44
3:W:237:GLU:HG2	3:W:238:GLY:H	1.83	0.44
7:a:19:PRO:HA	7:a:23:HIS:HD2	1.81	0.44
12:f:43:GLN:HG3	12:f:121:PHE:HB2	2.00	0.44
17:E:198:VAL:HG21	17:E:232:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:O:18:THR:HB	28:O:30:ASN:HA	2.00	0.44
30:q:2:GLU:HG3	30:q:34:LYS:HE2	1.99	0.44
12:f:438:ASP:HA	12:f:477:MET:HE2	2.00	0.44
17:E:194:ASN:HD22	17:E:229:ILE:HG12	1.82	0.44
22:I:178:ASP:OD2	22:I:195:LYS:NZ	2.37	0.44
23:J:11:SER:OG	23:J:15:HIS:N	2.51	0.44
20:g:114:LEU:HD22	20:g:140:LEU:HD21	2.00	0.44
28:o:67:SER:HB3	28:o:74:PRO:HG3	2.00	0.44
1:U:554:LEU:HD11	1:U:761:VAL:HG13	2.00	0.44
2:V:337:LEU:HD11	2:V:364:THR:HB	2.00	0.44
7:a:252:LYS:HA	7:a:255:TRP:HD1	1.82	0.44
15:C:148:TYR:HB2	15:C:206:HIS:CD2	2.53	0.44
15:C:405:TRP:HH2	22:I:27:ALA:HB1	1.83	0.44
17:E:190:GLN:O	17:E:191:LEU:C	2.60	0.44
21:h:222:THR:OG1	21:h:225:GLU:OE1	2.29	0.44
1:U:70:HIS:HA	2:V:236:ARG:HH22	1.83	0.43
1:U:212:ASP:H	1:U:215:ASN:HD21	1.65	0.43
2:V:199:ASN:O	2:V:203:LEU:N	2.42	0.43
2:V:243:ASP:OD1	2:V:246:GLY:N	2.50	0.43
4:X:53:LEU:HD23	4:X:56:LEU:HD12	2.00	0.43
6:Z:190:ARG:HA	6:Z:193:ASN:HD22	1.82	0.43
6:Z:229:GLN:HG3	7:a:338:PRO:HB2	1.99	0.43
12:f:852:VAL:O	12:f:854:GLY:N	2.43	0.43
22:I:108:GLU:OE2	22:I:146:GLN:NE2	2.51	0.43
26:M:37:ILE:HD11	26:M:193:VAL:HG13	1.99	0.43
21:h:108:ALA:HA	21:h:147:PHE:HE2	1.83	0.43
28:o:18:THR:HB	28:o:30:ASN:HA	2.00	0.43
1:U:900:TYR:OH	1:U:920:ASP:O	2.36	0.43
2:V:494:MET:HG2	6:Z:278:ASN:HD22	1.83	0.43
3:W:361:HIS:HA	3:W:364:ARG:HH11	1.84	0.43
7:a:145:LEU:HD12	7:a:148:VAL:HG23	1.99	0.43
12:f:656:GLY:O	12:f:660:ILE:CG2	2.66	0.43
28:O:67:SER:HB3	28:O:74:PRO:HG3	2.00	0.43
24:k:155:HIS:CE1	24:k:170:ILE:HG21	2.53	0.43
31:r:36:GLU:OE2	31:r:186:ARG:NH2	2.50	0.43
3:W:136:ILE:HG22	3:W:143:ALA:HB3	1.99	0.43
4:X:50:ILE:HG23	4:X:69:LEU:HD11	2.00	0.43
9:c:277:LYS:NZ	16:D:118:THR:O	2.51	0.43
14:B:303:ARG:O	14:B:307:ARG:N	2.49	0.43
28:O:96:ALA:H	28:O:115:PRO:HB3	1.82	0.43
23:j:7:ILE:HD11	23:j:122:ASN:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:p:28:PHE:HB2	29:p:39:PHE:HB2	1.99	0.43
1:U:456:ASP:O	1:U:460:TYR:N	2.46	0.43
12:f:167:ALA:HA	12:f:170:TRP:HD1	1.82	0.43
12:f:399:LEU:HD11	12:f:440:ILE:HG12	2.00	0.43
22:I:171:ALA:HB2	22:I:200:THR:HG21	2.00	0.43
33:T:43:MET:HE3	33:T:45:VAL:HG22	2.00	0.43
23:j:11:SER:OG	23:j:15:HIS:N	2.51	0.43
24:k:91:LYS:HE3	24:k:119:LEU:HD22	2.00	0.43
1:U:46:GLU:O	1:U:50:GLU:HG2	2.18	0.43
6:Z:130:ASP:OD1	6:Z:130:ASP:N	2.45	0.43
12:f:171:GLN:HE21	12:f:179:VAL:HA	1.83	0.43
17:E:235:ILE:CG2	17:E:279:THR:HG22	2.42	0.43
23:j:115:LYS:HD3	23:j:149:PRO:HA	1.99	0.43
1:U:149:GLN:NE2	15:C:20:LEU:O	2.50	0.43
13:A:346:PRO:HB3	13:A:350:GLY:HA3	1.99	0.43
16:D:194:ILE:HD12	16:D:196:ILE:HD11	2.00	0.43
17:E:194:ASN:ND2	17:E:229:ILE:N	2.66	0.43
23:J:115:LYS:HD3	23:J:149:PRO:HA	2.00	0.43
24:K:21:LEU:HA	24:K:22:PHE:HB2	2.00	0.43
25:L:46:LEU:HD13	25:L:73:SER:HB2	2.01	0.43
29:P:62:THR:OG1	30:Q:85:ARG:NH2	2.48	0.43
22:i:123:GLN:NE2	23:j:79:ASP:OD1	2.52	0.43
24:k:210:LEU:HD11	24:k:215:ILE:HG12	2.01	0.43
33:t:45:VAL:HB	33:t:49:THR:HG23	2.00	0.43
7:a:159:SER:OG	7:a:175:ASP:OD2	2.37	0.43
10:d:171:LEU:HD23	10:d:174:ILE:HD12	2.01	0.43
18:F:307:GLN:HA	18:F:310:MET:HB3	2.01	0.43
23:J:7:ILE:HD11	23:J:122:ASN:HA	2.01	0.43
29:P:58:THR:O	30:Q:85:ARG:NH2	2.52	0.43
33:T:184:TYR:CE2	33:T:186:ARG:HB3	2.54	0.43
22:i:238:LYS:HA	22:i:241:GLU:HB2	2.00	0.43
33:t:43:MET:HE3	33:t:45:VAL:HG22	2.00	0.43
12:f:665:GLU:HG2	12:f:669:GLU:HG3	2.01	0.43
12:f:762:VAL:HG13	12:f:806:VAL:HG13	2.01	0.43
25:L:41:LYS:NZ	25:L:180:MET:O	2.42	0.43
30:Q:37:LYS:O	30:Q:61:GLN:NE2	2.46	0.43
31:R:140:ASP:OD2	30:q:170:ARG:NE	2.40	0.43
32:S:38:ARG:HH12	33:T:151:ARG:HD3	1.84	0.43
23:j:121:SER:HB3	23:j:124:ARG:HD3	2.01	0.43
24:k:152:GLN:OE1	24:k:164:GLN:NE2	2.52	0.43
1:U:213:PHE:HE1	1:U:244:MET:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:496:LEU:HA	1:U:499:THR:HG22	2.00	0.43
1:U:792:ASN:HB3	1:U:914:LEU:HB3	2.01	0.43
2:V:37:MET:HE2	2:V:115:LYS:HE2	2.00	0.43
2:V:171:VAL:O	2:V:175:MET:N	2.42	0.43
2:V:378:VAL:HA	2:V:381:GLN:HB3	2.01	0.43
5:Y:144:LEU:HB3	5:Y:160:ASN:HD22	1.83	0.43
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.01	0.43
12:f:253:LEU:HA	12:f:257:ARG:HD3	2.01	0.43
12:f:705:ASN:OD1	12:f:706:ILE:N	2.48	0.43
17:E:194:ASN:CG	17:E:229:ILE:N	2.69	0.43
21:H:46:LEU:HD13	21:H:75:VAL:HG13	2.01	0.43
24:k:182:GLN:NE2	25:l:55:GLU:OE1	2.44	0.43
26:m:108:LEU:HD11	26:m:137:LEU:HB3	2.01	0.43
30:q:23:SER:HB2	30:q:28:MET:HE2	2.00	0.43
3:W:178:GLU:C	3:W:180:LYS:N	2.76	0.43
9:c:59:GLY:HA3	9:c:69:VAL:HA	2.00	0.43
13:A:258:ARG:HG2	13:A:305:GLN:HE22	1.82	0.43
17:E:40:TYR:HA	18:F:73:ILE:HD12	2.00	0.43
18:F:35:LYS:HE2	18:F:39:GLU:HG2	2.01	0.43
18:F:407:ALA:HB1	18:F:412:ALA:HB3	2.01	0.43
22:I:136:TYR:HB2	22:I:148:TYR:HB2	2.00	0.43
24:K:56:SER:HB3	24:K:59:MET:HB2	2.01	0.43
22:i:72:MET:HG2	22:i:138:GLY:HA3	2.01	0.43
6:Z:228:TYR:O	6:Z:232:ASP:N	2.50	0.42
10:d:107:LEU:HD22	10:d:170:LEU:HD11	2.01	0.42
12:f:276:GLU:O	12:f:286:LYS:NZ	2.39	0.42
13:A:161:VAL:HA	13:A:164:MET:HG2	2.00	0.42
17:E:190:GLN:O	17:E:192:ASP:N	2.52	0.42
17:E:385:ASP:OD1	17:E:385:ASP:N	2.50	0.42
21:H:225:GLU:O	21:H:229:TYR:N	2.49	0.42
29:P:36:THR:OG1	29:P:38:ASP:OD1	2.33	0.42
30:Q:23:SER:HB2	30:Q:28:MET:HE2	2.00	0.42
4:X:77:LEU:HD22	4:X:116:TRP:HH2	1.84	0.42
7:a:247:ARG:HH12	7:a:251:LEU:HD13	1.85	0.42
13:A:347:ASP:N	13:A:347:ASP:OD1	2.51	0.42
14:B:190:LEU:HD13	14:B:193:GLN:HB2	1.99	0.42
14:B:233:THR:OG1	35:B:501:ATP:O2B	2.32	0.42
15:C:168:PRO:HG3	15:C:175:PHE:HE2	1.84	0.42
22:I:165:GLY:O	22:I:169:ALA:N	2.53	0.42
23:J:121:SER:HB3	23:J:124:ARG:HD3	2.01	0.42
26:M:144:ASP:O	26:M:147:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Q:162:LYS:O	31:r:141:ARG:NH2	2.52	0.42
22:i:180:LYS:HE2	22:i:183:GLU:HG2	2.01	0.42
26:m:144:ASP:O	26:m:147:GLN:NE2	2.52	0.42
3:W:334:GLU:OE2	3:W:338:THR:OG1	2.36	0.42
4:X:187:ARG:NH2	4:X:221:GLU:OE2	2.52	0.42
12:f:412:ALA:HA	12:f:447:ALA:HB2	2.01	0.42
14:B:357:ASP:O	14:B:361:LYS:NZ	2.44	0.42
15:C:38:LYS:O	15:C:42:LEU:N	2.52	0.42
15:C:209:CYS:SG	15:C:210:THR:N	2.92	0.42
21:H:185:GLU:O	21:H:229:TYR:OH	2.37	0.42
29:P:135:ASP:OD1	29:P:135:ASP:N	2.48	0.42
22:i:108:GLU:OE2	22:i:146:GLN:NE2	2.49	0.42
30:q:47:VAL:O	30:q:101:ASN:N	2.42	0.42
7:a:9:GLN:HE22	7:a:23:HIS:CE1	2.37	0.42
8:b:20:ASP:CG	8:b:25:ARG:HH21	2.28	0.42
12:f:93:PRO:HB2	12:f:97:LYS:HE3	2.00	0.42
13:A:287:ASP:OD2	14:B:298:ASN:ND2	2.39	0.42
13:A:414:ASN:HA	13:A:418:LYS:HB2	2.01	0.42
21:H:148:GLN:OE1	21:H:158:TRP:NE1	2.52	0.42
24:K:50:VAL:HG21	24:K:66:LYS:HB3	2.02	0.42
20:g:56:VAL:HG13	20:g:61:LEU:HD22	2.00	0.42
23:j:64:ALA:O	23:j:88:ARG:NH1	2.53	0.42
1:U:19:LEU:HB2	10:d:27:LYS:HZ3	1.85	0.42
1:U:806:CYS:SG	1:U:888:GLN:NE2	2.92	0.42
2:V:108:LEU:HA	2:V:111:TYR:HD2	1.84	0.42
2:V:319:HIS:HE1	11:e:1:MET:HB3	1.83	0.42
5:Y:203:ASP:OD1	5:Y:203:ASP:N	2.43	0.42
7:a:55:GLY:HA2	7:a:58:LYS:HG2	2.00	0.42
9:c:284:LEU:HB3	9:c:285:GLU:H	1.49	0.42
12:f:478:ARG:HG3	12:f:514:VAL:HG11	2.00	0.42
12:f:674:THR:O	12:f:678:LEU:N	2.51	0.42
16:D:414:HIS:CE1	20:G:26:GLU:HB2	2.55	0.42
17:E:144:GLU:O	17:E:297:ARG:NH2	2.51	0.42
21:H:74:LEU:HD21	21:H:134:LEU:HD22	2.00	0.42
21:H:118:MET:HE2	21:H:151:PRO:HA	2.02	0.42
26:M:108:LEU:HD11	26:M:137:LEU:HB3	2.01	0.42
20:g:86:ASP:OD1	26:m:120:HIS:NE2	2.52	0.42
22:i:122:THR:HB	23:j:125:ARG:HH12	1.83	0.42
24:k:31:ILE:HD13	24:k:140:ALA:HB2	2.02	0.42
1:U:221:ILE:H	1:U:221:ILE:HG13	1.72	0.42
6:Z:34:ARG:NH1	6:Z:60:GLU:OE1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:692:LEU:HD22	14:B:40:THR:HB	2.00	0.42
12:f:764:LEU:HD12	12:f:771:LEU:HG	2.02	0.42
12:f:828:ARG:HG2	12:f:845:ARG:C	2.44	0.42
13:A:56:LEU:O	13:A:60:ASN:ND2	2.53	0.42
13:A:108:ASP:OD2	13:A:110:LYS:NZ	2.53	0.42
15:C:230:MET:O	15:C:234:LEU:N	2.52	0.42
20:G:58:ASP:HB3	20:G:61:LEU:HB2	2.02	0.42
22:I:73:ALA:HB3	22:I:137:ILE:HD11	2.02	0.42
23:J:64:ALA:O	23:J:88:ARG:NH1	2.53	0.42
33:T:45:VAL:HB	33:T:49:THR:HG23	2.00	0.42
29:p:107:PRO:HG2	29:p:124:LEU:HB2	2.01	0.42
2:V:401:ASN:HD21	2:V:408:ARG:HH12	1.68	0.42
3:W:89:LEU:H	20:G:209:ASP:HB2	1.85	0.42
17:E:173:TYR:HB2	17:E:388:PRO:HB2	2.02	0.42
17:E:232:MET:HE2	17:E:232:MET:HB2	1.76	0.42
18:F:275:ALA:O	18:F:281:SER:OG	2.38	0.42
20:G:86:ASP:OD1	26:M:120:HIS:NE2	2.45	0.42
24:K:210:LEU:HD11	24:K:215:ILE:HG12	2.01	0.42
26:M:40:ARG:HE	26:M:161:TRP:HD1	1.68	0.42
21:h:6:TYR:HE2	21:h:126:GLY:HA3	1.85	0.42
23:j:76:LEU:HD12	23:j:79:ASP:H	1.85	0.42
24:k:77:ALA:HB3	24:k:142:LEU:HB2	2.02	0.42
33:t:184:TYR:CE2	33:t:186:ARG:HB3	2.54	0.42
3:W:93:ARG:HE	3:W:135:LYS:H	1.68	0.42
3:W:178:GLU:H	3:W:182:ARG:HB3	1.81	0.42
6:Z:213:GLU:O	6:Z:217:THR:HB	2.19	0.42
7:a:100:THR:HA	7:a:103:LYS:HE2	2.02	0.42
12:f:594:LEU:HD13	12:f:594:LEU:HA	1.93	0.42
13:A:38:GLN:NE2	13:A:40:THR:OG1	2.53	0.42
13:A:258:ARG:NH2	18:F:255:GLN:HA	2.35	0.42
15:C:214:VAL:HG21	15:C:234:LEU:HD21	2.02	0.42
15:C:274:LEU:O	15:C:278:ASN:ND2	2.53	0.42
18:F:304:ARG:O	18:F:308:ARG:NH1	2.52	0.42
25:l:15:PRO:O	26:m:28:LYS:NZ	2.42	0.42
25:l:46:LEU:HD13	25:l:73:SER:HB2	2.01	0.42
1:U:179:TYR:CD1	1:U:179:TYR:O	2.73	0.42
1:U:191:LYS:HE3	1:U:560:MET:HG3	2.02	0.42
2:V:136:GLU:O	2:V:140:ASP:N	2.45	0.42
5:Y:276:ALA:HB1	11:e:60:LEU:HD13	2.01	0.42
17:E:198:VAL:O	17:E:233:ASP:O	2.37	0.42
28:o:141:LYS:NZ	28:o:157:GLU:OE2	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:8:ILE:H	1:U:8:ILE:HG13	1.74	0.42
1:U:386:LEU:HD22	1:U:408:LEU:HD13	2.02	0.42
1:U:792:ASN:OD1	1:U:793:LYS:N	2.50	0.42
2:V:60:ALA:HB3	2:V:62:HIS:CD2	2.54	0.42
5:Y:178:ASN:ND2	5:Y:212:GLU:OE1	2.53	0.42
13:A:289:ALA:HB1	18:F:296:PHE:HB3	2.01	0.42
14:B:187:ILE:HG22	14:B:234:LEU:HD13	2.00	0.42
15:C:83:LYS:HB3	15:C:99:VAL:HG22	2.01	0.42
20:G:175:SER:HA	20:G:205:VAL:HG21	2.01	0.42
3:W:32:ALA:O	3:W:36:LYS:N	2.52	0.41
7:a:254:ALA:O	7:a:258:GLN:NE2	2.53	0.41
12:f:460:ASP:N	12:f:460:ASP:OD1	2.52	0.41
14:B:316:LEU:HD22	14:B:322:ARG:HH12	1.85	0.41
18:F:421:MET:HA	18:F:424:ILE:HD12	2.02	0.41
20:G:132:ARG:HA	20:G:133:PRO:HD3	1.79	0.41
21:h:118:MET:HE2	21:h:151:PRO:HA	2.02	0.41
26:m:40:ARG:HE	26:m:161:TRP:HD1	1.68	0.41
26:m:160:TYR:HD2	26:m:163:CYS:HB2	1.85	0.41
1:U:889:LEU:HB3	1:U:908:ILE:HA	2.01	0.41
2:V:280:ALA:HB3	2:V:285:TRP:HB2	2.01	0.41
3:W:124:LEU:HA	3:W:127:THR:HG22	2.01	0.41
3:W:395:ASN:HA	3:W:398:VAL:HG22	2.02	0.41
7:a:138:VAL:O	7:a:142:LEU:N	2.52	0.41
12:f:180:GLN:HE22	12:f:835:GLU:HB3	1.85	0.41
12:f:248:LEU:HD12	12:f:250:ARG:HD3	2.02	0.41
12:f:608:LYS:HE3	12:f:608:LYS:HB3	1.85	0.41
12:f:618:GLU:HG2	14:B:82:GLN:NE2	2.35	0.41
13:A:124:ASP:HB2	18:F:86:LEU:HD21	2.02	0.41
18:F:221:LYS:HD3	18:F:322:PRO:HA	2.01	0.41
22:I:105:ILE:HA	22:I:106:PRO:HD3	1.83	0.41
23:J:116:GLN:HE22	24:K:83:ALA:HB1	1.85	0.41
29:P:107:PRO:HG2	29:P:124:LEU:HB2	2.01	0.41
31:R:44:THR:HG21	31:R:100:MET:HE3	2.02	0.41
21:h:111:VAL:HG21	21:h:147:PHE:HD2	1.84	0.41
1:U:611:ASN:HB3	1:U:614:VAL:HG12	2.01	0.41
2:V:36:GLU:HG3	2:V:76:LYS:HG2	2.02	0.41
6:Z:145:HIS:ND1	6:Z:149:THR:OG1	2.41	0.41
7:a:148:VAL:HG12	7:a:150:SER:H	1.86	0.41
17:E:194:ASN:HB2	17:E:229:ILE:H	1.79	0.41
27:N:7:GLN:HA	27:N:12:VAL:HA	2.03	0.41
31:R:22:ALA:N	31:R:25:TYR:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:182:LYS:O	1:U:183:LEU:C	2.63	0.41
5:Y:71:ASN:HA	5:Y:74:LYS:HG2	2.01	0.41
12:f:294:MET:HE1	12:f:456:ARG:HG2	2.02	0.41
18:F:311:LEU:O	18:F:315:ASN:N	2.46	0.41
21:H:108:ALA:HA	21:H:147:PHE:HE2	1.85	0.41
23:J:76:LEU:HD12	23:J:79:ASP:H	1.85	0.41
22:i:229:LYS:N	22:i:232:GLU:OE2	2.53	0.41
23:j:154:HIS:HE1	24:k:64:ILE:HG13	1.86	0.41
28:o:172:ASN:HD22	28:o:191:VAL:HG22	1.86	0.41
31:r:44:THR:HG21	31:r:100:MET:HE3	2.02	0.41
1:U:541:HIS:HB2	1:U:544:ILE:HG22	2.02	0.41
2:V:211:TYR:HA	2:V:214:HIS:HB3	2.02	0.41
6:Z:215:VAL:HG22	6:Z:222:ILE:HG13	2.03	0.41
10:d:164:THR:HA	10:d:167:ILE:HG12	2.03	0.41
12:f:31:LYS:HE2	12:f:31:LYS:HB3	1.92	0.41
12:f:265:ALA:HB3	12:f:268:LEU:HB2	2.02	0.41
12:f:407:MET:HE3	12:f:439:TYR:HB2	2.03	0.41
23:j:7:ILE:H	23:j:7:ILE:HG13	1.58	0.41
1:U:217:CYS:SG	1:U:752:THR:OG1	2.70	0.41
2:V:40:GLU:HA	2:V:43:THR:HB	2.02	0.41
12:f:414:LEU:HD23	12:f:417:ILE:HD12	2.03	0.41
12:f:621:ASP:O	12:f:623:LYS:N	2.51	0.41
15:C:70:GLY:HA3	16:D:113:VAL:HG12	2.03	0.41
17:E:194:ASN:ND2	17:E:229:ILE:H	2.18	0.41
17:E:321:THR:OG1	17:E:360:ASP:O	2.37	0.41
21:H:181:ASP:OD1	21:H:181:ASP:N	2.47	0.41
22:i:105:ILE:HA	22:i:106:PRO:HD3	1.84	0.41
1:U:427:LEU:HB2	1:U:430:ASP:HB2	2.03	0.41
2:V:231:LEU:HD11	2:V:250:LEU:HD22	2.02	0.41
12:f:663:GLY:C	12:f:664:GLU:HG3	2.45	0.41
13:A:312:ARG:HB2	13:A:315:ILE:HD13	2.01	0.41
15:C:99:VAL:HA	15:C:123:LEU:HB2	2.03	0.41
15:C:187:LEU:HB2	15:C:311:ILE:HG21	2.02	0.41
16:D:318:ASP:HB3	16:D:321:LEU:HD23	2.02	0.41
20:G:131:MET:HE3	26:M:124:LEU:HD13	2.02	0.41
30:Q:19:ARG:HH11	30:Q:179:SER:HB3	1.86	0.41
20:g:32:ILE:HA	20:g:82:GLY:HA2	2.03	0.41
26:m:229:LYS:HD3	26:m:229:LYS:HA	1.93	0.41
30:q:19:ARG:HH11	30:q:179:SER:HB3	1.86	0.41
1:U:904:LYS:HD3	1:U:912:ILE:HG22	2.03	0.41
2:V:462:GLU:HG2	2:V:463:MET:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:480:ILE:HD13	6:Z:264:SER:HB3	2.02	0.41
3:W:131:VAL:HG12	3:W:144:ARG:HE	1.86	0.41
5:Y:283:LYS:HD3	5:Y:288:PHE:HZ	1.84	0.41
8:b:124:LEU:HD21	8:b:152:LYS:HB3	2.02	0.41
12:f:662:MET:HE3	12:f:662:MET:HB3	1.92	0.41
12:f:721:VAL:HG21	14:B:208:PRO:HG2	2.02	0.41
20:G:89:SER:OG	26:M:117:MET:SD	2.79	0.41
28:O:21:THR:HG22	28:O:26:VAL:HA	2.03	0.41
26:m:74:GLY:HA3	26:m:224:HIS:CE1	2.56	0.41
27:n:7:GLN:HA	27:n:12:VAL:HA	2.02	0.41
2:V:255:LEU:HD22	2:V:291:TYR:HB3	2.03	0.41
2:V:259:LEU:HD21	2:V:294:ARG:HH11	1.86	0.41
3:W:200:ILE:HD12	3:W:203:GLN:HE21	1.86	0.41
4:X:111:LEU:HD23	4:X:114:ILE:HD12	2.03	0.41
6:Z:68:TRP:HH2	6:Z:111:LEU:HD13	1.86	0.41
7:a:81:LEU:HA	7:a:84:VAL:HG12	2.02	0.41
7:a:235:ASP:OD2	7:a:249:GLN:NE2	2.54	0.41
8:b:30:GLN:NE2	18:F:57:SER:OG	2.54	0.41
8:b:53:THR:HG22	8:b:59:GLU:H	1.86	0.41
10:d:200:PHE:HB2	10:d:205:LYS:HZ3	1.86	0.41
12:f:373:ALA:HA	12:f:376:PHE:HD2	1.86	0.41
20:G:132:ARG:HH21	26:M:20:VAL:HG21	1.86	0.41
22:I:38:LEU:HD12	22:I:161:ALA:HB2	2.03	0.41
24:K:19:GLY:HA3	24:K:20:ARG:HB3	2.02	0.41
1:U:18:GLN:HE21	10:d:27:LYS:HD2	1.86	0.41
1:U:248:ILE:HD12	1:U:248:ILE:HA	1.93	0.41
2:V:330:LYS:HG3	2:V:360:TYR:CE2	2.56	0.41
7:a:220:PRO:O	7:a:224:SER:OG	2.34	0.41
12:f:829:MET:H	12:f:845:ARG:HB3	1.86	0.41
14:B:65:LEU:HD23	14:B:68:ILE:HD12	2.02	0.41
17:E:191:LEU:HB3	17:E:192:ASP:H	1.62	0.41
24:k:109:VAL:HG23	24:k:147:ASP:HB3	2.02	0.41
28:o:21:THR:HG22	28:o:26:VAL:HA	2.03	0.41
1:U:338:HIS:HE1	1:U:785:PRO:HB3	1.85	0.40
2:V:98:LEU:HD23	2:V:104:THR:HA	2.02	0.40
4:X:52:GLU:O	4:X:55:SER:OG	2.34	0.40
8:b:26:LEU:HA	8:b:29:GLN:HG2	2.03	0.40
12:f:261:ARG:HG2	12:f:266:LEU:HD13	2.02	0.40
12:f:340:MET:SD	12:f:757:ASN:ND2	2.94	0.40
14:B:286:GLU:HG2	15:C:274:LEU:HD12	2.03	0.40
16:D:139:LEU:HA	16:D:139:LEU:HD23	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:212:LYS:HE2	16:D:310:ALA:HB1	2.03	0.40
20:G:16:PHE:HE2	21:H:129:PRO:HD2	1.85	0.40
26:M:160:TYR:HD2	26:M:163:CYS:HB2	1.85	0.40
12:f:9:ALA:HA	12:f:13:PRO:HD2	2.04	0.40
12:f:258:LYS:HG2	12:f:297:MET:HG3	2.04	0.40
13:A:277:ILE:H	13:A:277:ILE:HG13	1.68	0.40
14:B:140:ASP:OD1	14:B:140:ASP:N	2.54	0.40
16:D:157:ASP:HA	16:D:158:GLN:HA	1.73	0.40
3:W:78:LYS:HG3	3:W:79:GLU:HG3	2.02	0.40
3:W:420:ASP:OD1	3:W:420:ASP:N	2.54	0.40
12:f:180:GLN:HB3	12:f:219:LYS:NZ	2.36	0.40
12:f:331:LEU:HD12	12:f:813:LYS:HE2	2.03	0.40
12:f:812:GLY:HA2	12:f:825:MET:HE1	2.04	0.40
13:A:292:ASP:OD1	13:A:292:ASP:N	2.50	0.40
14:B:49:LEU:HD12	14:B:68:ILE:HD11	2.04	0.40
14:B:259:TYR:HB2	14:B:262:ASP:HB2	2.04	0.40
15:C:188:LEU:HB3	15:C:317:PHE:HE2	1.85	0.40
17:E:15:LYS:HA	18:F:47:LEU:HD22	2.03	0.40
22:I:125:GLY:HA2	22:I:126:GLY:HA2	1.72	0.40
22:I:134:LEU:N	22:I:150:SER:OG	2.49	0.40
23:J:88:ARG:NH1	30:Q:69:MET:O	2.54	0.40
23:j:2:SER:OG	23:j:3:TYR:N	2.55	0.40
23:j:88:ARG:NH1	30:q:69:MET:O	2.54	0.40
1:U:636:VAL:HG23	1:U:637:VAL:HG23	2.04	0.40
2:V:210:CYS:SG	2:V:211:TYR:N	2.95	0.40
2:V:387:GLN:HG2	2:V:392:TYR:CE1	2.57	0.40
10:d:176:ASP:HA	10:d:179:ALA:HB3	2.03	0.40
12:f:326:LEU:HD22	12:f:329:ASN:HB2	2.02	0.40
12:f:764:LEU:HD11	12:f:774:GLY:HA3	2.04	0.40
16:D:162:VAL:O	16:D:221:HIS:ND1	2.54	0.40
17:E:75:ASN:HD21	18:F:130:GLN:HG2	1.86	0.40
17:E:219:PHE:HA	17:E:222:ALA:HB3	2.03	0.40
17:E:226:GLN:O	17:E:227:PRO:C	2.62	0.40
20:g:161:CYS:SG	20:g:162:GLY:N	2.94	0.40
21:h:148:GLN:OE1	21:h:158:TRP:NE1	2.54	0.40
1:U:241:ASN:HD21	1:U:244:MET:HE3	1.86	0.40
1:U:772:TRP:CD1	1:U:775:LEU:HG	2.56	0.40
3:W:177:MET:CA	3:W:182:ARG:HG2	2.47	0.40
3:W:451:MET:HE2	6:Z:100:LYS:HA	2.04	0.40
5:Y:97:GLU:HA	5:Y:101:ARG:HG2	2.04	0.40
7:a:145:LEU:HD22	7:a:145:LEU:HA	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:92:GLN:HE21	9:c:96:LEU:HD11	1.87	0.40
12:f:325:GLN:HE21	12:f:420:TRP:HE3	1.68	0.40
14:B:96:ARG:HA	14:B:99:VAL:HB	2.03	0.40
16:D:92:PHE:HZ	16:D:95:ALA:HB2	1.86	0.40
16:D:255:LYS:HE2	16:D:301:GLN:HB3	2.04	0.40
17:E:226:GLN:HB2	17:E:227:PRO:CD	2.52	0.40
24:K:55:THR:OG1	24:K:59:MET:SD	2.71	0.40
25:L:207:THR:HG22	25:L:233:LEU:HD12	2.04	0.40
32:S:16:ALA:HB2	32:S:121:VAL:HG23	2.04	0.40

There are no symmetry-related clashes.

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	U	868/953 (91%)	781 (90%)	78 (9%)	9 (1%)	12	45
2	V	478/533 (90%)	414 (87%)	64 (13%)	0	100	100
3	W	454/456 (100%)	409 (90%)	43 (10%)	2 (0%)	30	62
4	X	378/422 (90%)	355 (94%)	22 (6%)	1 (0%)	36	68
5	Y	376/389 (97%)	336 (89%)	39 (10%)	1 (0%)	36	68
6	Z	284/324 (88%)	242 (85%)	40 (14%)	2 (1%)	18	52
7	a	371/376 (99%)	333 (90%)	34 (9%)	4 (1%)	11	43
8	b	189/377 (50%)	165 (87%)	24 (13%)	0	100	100
9	c	285/309 (92%)	248 (87%)	33 (12%)	4 (1%)	9	39
10	d	255/349 (73%)	212 (83%)	42 (16%)	1 (0%)	30	62
11	e	36/70 (51%)	29 (81%)	7 (19%)	0	100	100
12	f	887/892 (99%)	710 (80%)	166 (19%)	11 (1%)	10	42
13	A	411/433 (95%)	364 (89%)	46 (11%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	B	409/440 (93%)	355 (87%)	51 (12%)	3 (1%)	18	52
15	C	394/398 (99%)	353 (90%)	36 (9%)	5 (1%)	9	40
16	D	378/418 (90%)	317 (84%)	56 (15%)	5 (1%)	9	40
17	E	387/403 (96%)	323 (84%)	56 (14%)	8 (2%)	5	31
18	F	391/439 (89%)	339 (87%)	49 (12%)	3 (1%)	16	50
20	G	237/245 (97%)	207 (87%)	30 (13%)	0	100	100
20	g	238/245 (97%)	220 (92%)	18 (8%)	0	100	100
21	H	228/233 (98%)	218 (96%)	8 (4%)	2 (1%)	14	47
21	h	230/233 (99%)	222 (96%)	8 (4%)	0	100	100
22	I	246/260 (95%)	221 (90%)	25 (10%)	0	100	100
22	i	248/260 (95%)	223 (90%)	25 (10%)	0	100	100
23	J	237/247 (96%)	216 (91%)	20 (8%)	1 (0%)	30	62
23	j	237/247 (96%)	216 (91%)	20 (8%)	1 (0%)	30	62
24	K	224/240 (93%)	207 (92%)	17 (8%)	0	100	100
24	k	224/240 (93%)	210 (94%)	14 (6%)	0	100	100
25	L	236/268 (88%)	226 (96%)	10 (4%)	0	100	100
25	l	236/268 (88%)	226 (96%)	10 (4%)	0	100	100
26	M	238/254 (94%)	219 (92%)	18 (8%)	1 (0%)	30	62
26	m	238/254 (94%)	219 (92%)	18 (8%)	1 (0%)	30	62
27	N	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
27	n	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
28	O	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
28	o	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
29	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
29	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
30	Q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
30	q	197/201 (98%)	186 (94%)	11 (6%)	0	100	100
31	R	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
31	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
32	S	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
32	s	211/240 (88%)	205 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	T	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
33	t	213/263 (81%)	202 (95%)	11 (5%)	0	100	100
All	All	13386/14843 (90%)	12069 (90%)	1251 (9%)	66 (0%)	26	59

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	48	LEU
3	W	176	SER
3	W	179	LYS
7	a	343	LEU
9	c	285	GLU
12	f	808	ASN
12	f	853	VAL
16	D	335	LEU
17	E	53	VAL
17	E	194	ASN
18	F	73	ILE
23	J	5	ARG
23	j	5	ARG
1	U	47	VAL
1	U	183	LEU
1	U	874	ASN
7	a	69	HIS
7	a	187	ASP
9	c	233	ASP
12	f	876	HIS
14	B	390	LEU
26	M	7	TYR
26	m	7	TYR
5	Y	350	VAL
7	a	342	ASP
10	d	199	PHE
12	f	118	ASN
12	f	476	THR
12	f	664	GLU
12	f	823	ALA
12	f	859	PRO
14	B	166	ASP
16	D	160	PRO
17	E	191	LEU

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Mol	Chain	Res	Type
17	E	197	LYS
18	F	72	LYS
21	H	7	SER
4	X	317	PRO
6	Z	65	ASP
9	c	201	TYR
12	f	809	ILE
14	B	137	SER
15	C	89	VAL
15	C	90	HIS
15	C	221	GLN
16	D	269	ALA
17	E	193	CYS
18	F	301	ALA
21	H	8	PHE
1	U	173	VAL
1	U	808	PRO
1	U	873	PRO
9	c	284	LEU
12	f	475	ASN
16	D	336	PRO
12	f	755	ASP
13	A	109	PRO
15	C	253	SER
17	E	227	PRO
1	U	174	PRO
1	U	814	PRO
6	Z	144	VAL
16	D	126	PRO
17	E	166	PRO
15	C	91	PRO
17	E	226	GLN

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	U	748/816 (92%)	739 (99%)	9 (1%)	63	79
2	V	414/459 (90%)	411 (99%)	3 (1%)	76	83
3	W	416/416 (100%)	413 (99%)	3 (1%)	76	83
4	X	327/362 (90%)	325 (99%)	2 (1%)	78	84
5	Y	334/344 (97%)	333 (100%)	1 (0%)	86	88
6	Z	257/295 (87%)	250 (97%)	7 (3%)	39	68
7	a	333/336 (99%)	331 (99%)	2 (1%)	78	84
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	250 (99%)	2 (1%)	73	82
10	d	231/293 (79%)	229 (99%)	2 (1%)	70	81
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	745/748 (100%)	737 (99%)	8 (1%)	65	79
13	A	348/372 (94%)	347 (100%)	1 (0%)	86	88
14	B	357/385 (93%)	350 (98%)	7 (2%)	48	72
15	C	340/346 (98%)	336 (99%)	4 (1%)	63	79
16	D	333/366 (91%)	329 (99%)	4 (1%)	63	79
17	E	341/353 (97%)	335 (98%)	6 (2%)	51	74
18	F	340/379 (90%)	334 (98%)	6 (2%)	51	74
20	G	192/209 (92%)	192 (100%)	0	100	100
20	g	193/209 (92%)	192 (100%)	1 (0%)	81	85
21	H	163/190 (86%)	163 (100%)	0	100	100
21	h	164/190 (86%)	164 (100%)	0	100	100
22	I	191/220 (87%)	191 (100%)	0	100	100
22	i	193/220 (88%)	193 (100%)	0	100	100
23	J	152/210 (72%)	151 (99%)	1 (1%)	76	83
23	j	152/210 (72%)	151 (99%)	1 (1%)	76	83
24	K	187/202 (93%)	186 (100%)	1 (0%)	81	85
24	k	186/202 (92%)	183 (98%)	3 (2%)	55	75
25	L	198/229 (86%)	197 (100%)	1 (0%)	81	85
25	l	198/229 (86%)	197 (100%)	1 (0%)	81	85
26	M	192/211 (91%)	192 (100%)	0	100	100
26	m	192/211 (91%)	192 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	N	148/180 (82%)	148 (100%)	0	100	100
27	n	148/180 (82%)	148 (100%)	0	100	100
28	O	177/227 (78%)	177 (100%)	0	100	100
28	o	177/227 (78%)	177 (100%)	0	100	100
29	P	172/173 (99%)	172 (100%)	0	100	100
29	p	172/173 (99%)	172 (100%)	0	100	100
30	Q	164/171 (96%)	164 (100%)	0	100	100
30	q	164/171 (96%)	164 (100%)	0	100	100
31	R	153/201 (76%)	153 (100%)	0	100	100
31	r	153/201 (76%)	153 (100%)	0	100	100
32	S	174/198 (88%)	174 (100%)	0	100	100
32	s	174/198 (88%)	174 (100%)	0	100	100
33	T	175/214 (82%)	175 (100%)	0	100	100
33	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11200/12582 (89%)	11124 (99%)	76 (1%)	73	83

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	47	VAL
1	U	118	LEU
1	U	173	VAL
1	U	177	LEU
1	U	179	TYR
1	U	181	LEU
1	U	364	VAL
1	U	629	THR
1	U	913	ILE
2	V	275	VAL
2	V	362	LEU
2	V	437	ILE
3	W	89	LEU
3	W	177	MET
3	W	256	ILE
4	X	217	ILE
4	X	393	VAL
5	Y	81	LEU

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Mol	Chain	Res	Type
6	Z	12	HIS
6	Z	15	VAL
6	Z	16	LEU
6	Z	91	ILE
6	Z	212	LEU
6	Z	217	THR
6	Z	266	ILE
7	a	112	ILE
7	a	145	LEU
9	c	49	VAL
9	c	115	HIS
10	d	178	ILE
10	d	189	ILE
12	f	75	LEU
12	f	344	VAL
12	f	457	ASN
12	f	660	ILE
12	f	662	MET
12	f	672	LEU
12	f	806	VAL
12	f	822	VAL
13	A	403	ILE
14	B	125	THR
14	B	183	THR
14	B	190	LEU
14	B	292	THR
14	B	316	LEU
14	B	387	LYS
14	B	389	ASP
15	C	20	LEU
15	C	109	THR
15	C	210	THR
15	C	222	LYS
16	D	85	ILE
16	D	267	ILE
16	D	303	VAL
16	D	375	ILE
17	E	50	LEU
17	E	105	LEU
17	E	195	PHE
17	E	196	LEU
17	E	232	MET

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Mol	Chain	Res	Type
17	E	247	THR
18	F	54	ILE
18	F	59	VAL
18	F	298	SER
18	F	299	GLU
18	F	300	LYS
18	F	416	THR
23	J	7	ILE
24	K	139	VAL
25	L	118	ILE
20	g	141	ILE
23	j	7	ILE
24	k	113	THR
24	k	119	LEU
24	k	139	VAL
25	l	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (189) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	18	GLN
1	U	70	HIS
1	U	89	ASN
1	U	111	GLN
1	U	218	GLN
1	U	241	ASN
1	U	267	ASN
1	U	338	HIS
1	U	377	HIS
1	U	421	GLN
1	U	596	ASN
1	U	685	GLN
1	U	768	GLN
1	U	888	GLN
2	V	62	HIS
2	V	168	GLN
2	V	198	GLN
2	V	252	ASN
2	V	260	HIS
2	V	319	HIS
2	V	401	ASN
2	V	473	GLN

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Mol	Chain	Res	Type
2	V	487	HIS
3	W	106	GLN
3	W	107	GLN
3	W	203	GLN
3	W	362	ASN
3	W	454	ASN
4	X	170	GLN
4	X	198	ASN
4	X	213	GLN
4	X	349	HIS
4	X	416	ASN
5	Y	31	HIS
5	Y	48	ASN
5	Y	49	ASN
5	Y	77	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	273	GLN
5	Y	291	HIS
5	Y	365	GLN
5	Y	367	GLN
6	Z	32	GLN
6	Z	77	ASN
6	Z	109	ASN
6	Z	189	GLN
6	Z	193	ASN
6	Z	243	GLN
6	Z	256	GLN
7	a	9	GLN
7	a	86	GLN
7	a	124	ASN
7	a	227	ASN
7	a	249	GLN
7	a	257	GLN
7	a	273	GLN
7	a	288	HIS
8	b	30	GLN
8	b	161	ASN
9	c	92	GLN
9	c	115	HIS
9	c	130	GLN
9	c	149	GLN

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Mol	Chain	Res	Type
9	c	185	ASN
9	c	197	ASN
9	c	214	GLN
9	c	237	HIS
9	c	254	ASN
9	c	274	ASN
9	c	283	HIS
10	d	15	ASN
10	d	46	GLN
10	d	96	HIS
10	d	221	ASN
12	f	14	GLN
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	291	GLN
12	f	327	ASN
12	f	378	ASN
12	f	382	ASN
12	f	396	ASN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	619	HIS
12	f	737	ASN
12	f	747	GLN
12	f	752	HIS
12	f	766	GLN
12	f	786	GLN
12	f	815	HIS
13	A	54	GLN
13	A	60	ASN
13	A	94	GLN
13	A	203	ASN
13	A	247	GLN
13	A	304	ASN
13	A	353	HIS
14	B	154	HIS
14	B	181	GLN
14	B	195	GLN
14	B	368	HIS
15	C	32	GLN

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Mol	Chain	Res	Type
15	C	36	ASN
15	C	50	ASN
15	C	69	GLN
15	C	118	ASN
15	C	205	HIS
15	C	279	GLN
15	C	288	ASN
16	D	98	GLN
16	D	127	ASN
16	D	135	HIS
16	D	222	HIS
16	D	257	ASN
16	D	414	HIS
17	E	121	ASN
17	E	194	ASN
17	E	339	ASN
17	E	364	GLN
18	F	64	HIS
18	F	83	ASN
18	F	325	GLN
20	G	12	HIS
20	G	75	ASN
21	H	71	HIS
21	H	102	GLN
21	H	169	ASN
21	H	189	HIS
22	I	123	GLN
22	I	146	GLN
22	I	167	ASN
23	J	68	ASN
23	J	92	GLN
23	J	116	GLN
23	J	122	ASN
24	K	23	GLN
24	K	114	GLN
24	K	155	HIS
24	K	164	GLN
24	K	214	ASN
25	L	20	HIS
25	L	117	GLN
25	L	166	GLN
26	M	180	GLN

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Mol	Chain	Res	Type
28	O	62	ASN
28	O	172	ASN
29	P	18	ASN
30	Q	71	ASN
31	R	38	ASN
32	S	146	GLN
32	S	159	GLN
33	T	69	GLN
33	T	89	HIS
20	g	12	HIS
20	g	123	GLN
20	g	127	GLN
21	h	21	GLN
21	h	102	GLN
21	h	169	ASN
22	i	119	GLN
22	i	146	GLN
22	i	149	GLN
22	i	167	ASN
23	j	68	ASN
23	j	92	GLN
23	j	116	GLN
23	j	122	ASN
24	k	23	GLN
24	k	99	HIS
24	k	164	GLN
24	k	214	ASN
25	l	117	GLN
25	l	166	GLN
26	m	180	GLN
28	o	62	ASN
28	o	172	ASN
29	p	18	ASN
30	q	71	ASN
31	r	38	ASN
31	r	85	ASN
32	s	58	HIS
32	s	146	GLN
32	s	159	GLN
33	t	69	GLN
33	t	89	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
37	ADP	D	501	36	28,29,29	1.37	4 (14%)	43,45,45	1.88	9 (20%)
35	ATP	C	501	36	32,33,33	1.31	4 (12%)	48,52,52	1.81	7 (14%)
35	ATP	A	501	36	32,33,33	1.32	4 (12%)	48,52,52	1.79	10 (20%)
35	ATP	F	501	36	32,33,33	1.34	5 (15%)	48,52,52	1.81	8 (16%)
35	ATP	B	501	36	32,33,33	1.32	4 (12%)	48,52,52	1.90	9 (18%)

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
37	ADP	D	501	36	-	1/16/32/32	0/3/3/3
35	ATP	C	501	36	-	5/22/38/38	0/3/3/3
35	ATP	A	501	36	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	F	501	36	-	4/22/38/38	0/3/3/3
35	ATP	B	501	36	-	3/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	B	501	ATP	C5-C4	4.66	1.47	1.39
35	C	501	ATP	C5-C4	4.65	1.47	1.39
35	F	501	ATP	C5-C4	4.61	1.47	1.39
37	D	501	ADP	C5-C4	4.52	1.47	1.39
35	A	501	ATP	C5-C4	4.52	1.47	1.39
35	A	501	ATP	C5-C6	2.59	1.48	1.41
35	B	501	ATP	C5-N7	-2.59	1.34	1.39
35	C	501	ATP	C5-N7	-2.57	1.34	1.39
37	D	501	ADP	C5-C6	2.57	1.48	1.41
35	C	501	ATP	C5-C6	2.56	1.48	1.41
35	F	501	ATP	C5-C6	2.56	1.48	1.41
35	B	501	ATP	C5-C6	2.49	1.47	1.41
35	A	501	ATP	C5-N7	-2.44	1.34	1.39
35	F	501	ATP	C5-N7	-2.42	1.34	1.39
37	D	501	ADP	C5-N7	-2.39	1.34	1.39
35	A	501	ATP	C8-N7	2.18	1.35	1.31
37	D	501	ADP	C8-N7	2.16	1.35	1.31
35	C	501	ATP	C8-N7	2.13	1.35	1.31
35	F	501	ATP	C8-N7	2.10	1.35	1.31
35	B	501	ATP	C8-N7	2.06	1.35	1.31
35	F	501	ATP	C4-N9	-2.04	1.33	1.37

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	501	ATP	C5-C4-N3	-6.56	117.69	126.72
35	C	501	ATP	C5-C4-N3	-6.35	117.97	126.72
35	A	501	ATP	C5-C4-N3	-5.94	118.54	126.72
35	F	501	ATP	C5-C4-N3	-5.76	118.78	126.72
37	D	501	ADP	C5-C4-N3	-5.76	118.79	126.72
35	B	501	ATP	N3-C4-N9	5.41	136.38	127.17
35	C	501	ATP	N3-C4-N9	5.15	135.92	127.17
35	F	501	ATP	N3-C4-N9	4.79	135.31	127.17
35	A	501	ATP	N3-C4-N9	4.73	135.21	127.17
37	D	501	ADP	N3-C4-N9	4.68	135.13	127.17
35	B	501	ATP	C2-N3-C4	4.01	121.62	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	C	501	ATP	C2-N3-C4	3.95	121.47	111.83
35	A	501	ATP	C2-N3-C4	3.79	121.08	111.83
37	D	501	ADP	C2-N3-C4	3.69	120.83	111.83
35	F	501	ATP	C2-N3-C4	3.66	120.77	111.83
35	A	501	ATP	C4-C5-N7	-3.51	106.57	110.58
35	C	501	ATP	N3-C2-N1	-3.45	123.36	128.58
35	B	501	ATP	N3-C2-N1	-3.34	123.52	128.58
37	D	501	ADP	C4-C5-N7	-3.30	106.81	110.58
37	D	501	ADP	N3-C2-N1	-3.29	123.61	128.58
35	A	501	ATP	N3-C2-N1	-3.27	123.64	128.58
35	C	501	ATP	C4-C5-N7	-3.24	106.87	110.58
35	F	501	ATP	N3-C2-N1	-3.21	123.72	128.58
35	F	501	ATP	C4-C5-N7	-3.21	106.91	110.58
35	B	501	ATP	C4-C5-N7	-3.08	107.06	110.58
35	F	501	ATP	C4-N9-C8	2.90	108.78	105.74
35	B	501	ATP	C3'-C2'-C1'	2.88	106.92	101.46
37	D	501	ADP	C3'-C2'-C1'	2.84	106.83	101.46
37	D	501	ADP	C4-N9-C8	2.80	108.67	105.74
35	A	501	ATP	C4-N9-C8	2.72	108.59	105.74
35	F	501	ATP	C3'-C2'-C1'	2.66	106.50	101.46
35	A	501	ATP	C5-N7-C8	2.61	107.55	103.45
35	A	501	ATP	C3'-C2'-C1'	2.46	106.12	101.46
35	C	501	ATP	C5-N7-C8	2.45	107.30	103.45
37	D	501	ADP	C5-N7-C8	2.44	107.28	103.45
35	F	501	ATP	C5-N7-C8	2.40	107.22	103.45
35	B	501	ATP	C5-N7-C8	2.38	107.18	103.45
35	C	501	ATP	C4-N9-C8	2.32	108.18	105.74
35	B	501	ATP	C4-N9-C8	2.26	108.12	105.74
35	B	501	ATP	C1'-N9-C8	-2.13	122.36	127.09
35	A	501	ATP	C6-C5-N7	2.10	136.14	132.09
35	A	501	ATP	N9-C8-N7	-2.04	111.05	113.94
37	D	501	ADP	C6-C5-N7	2.02	135.99	132.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	C5'-O5'-PA-O1A
35	A	501	ATP	C5'-O5'-PA-O2A
35	A	501	ATP	C5'-O5'-PA-O3A
35	B	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	C5'-O5'-PA-O3A

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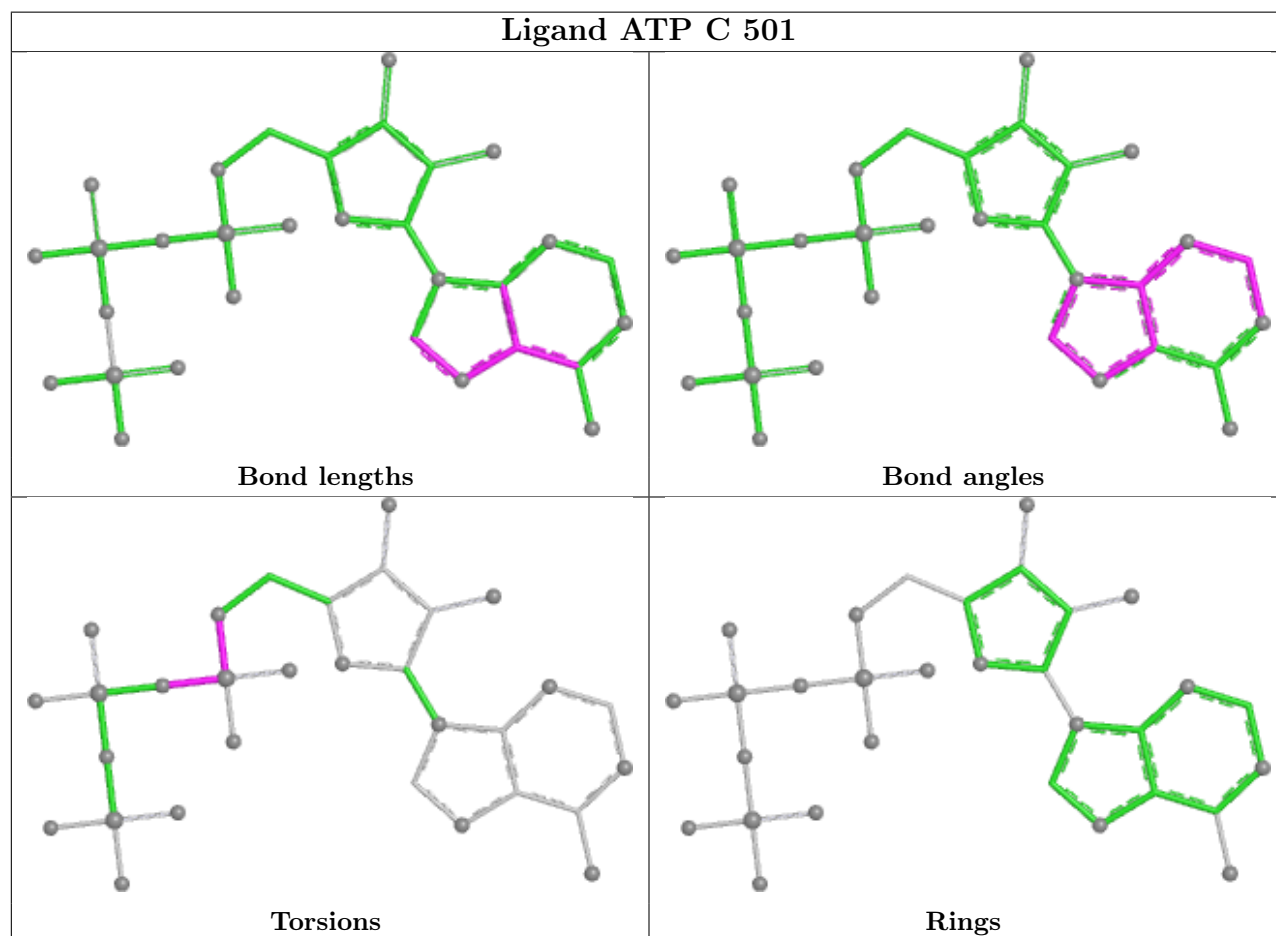
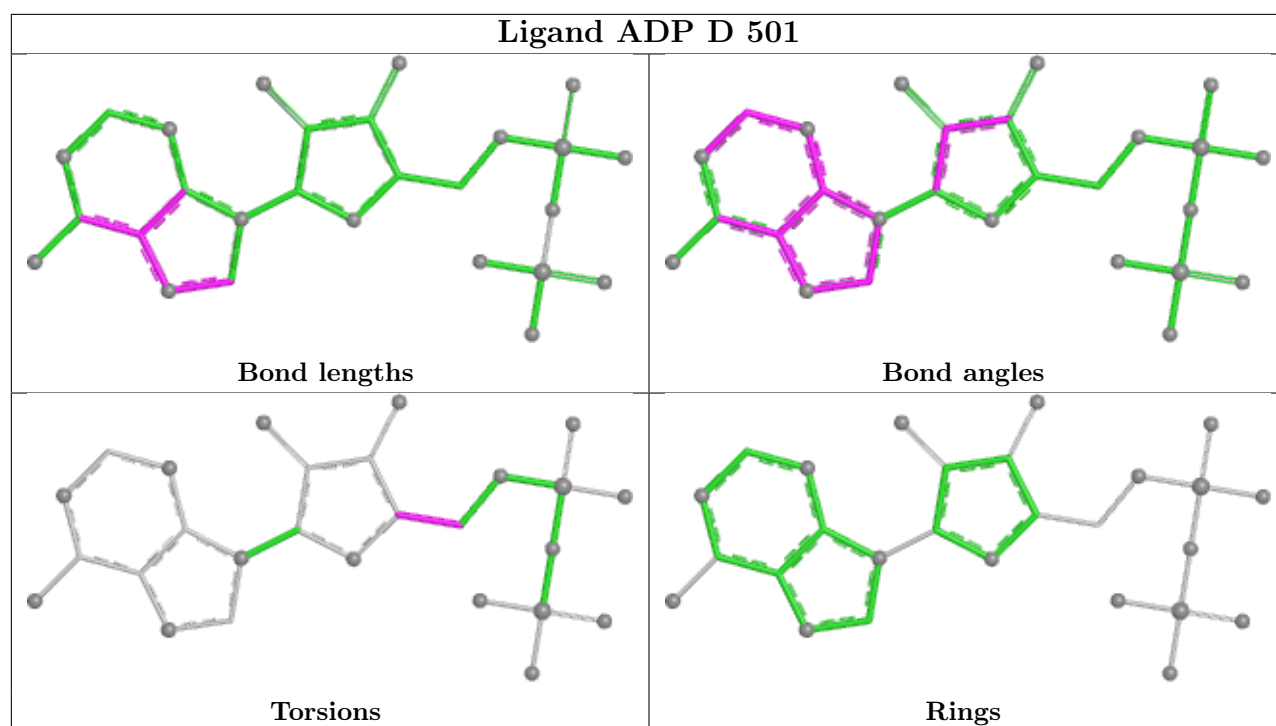
Mol	Chain	Res	Type	Atoms
35	C	501	ATP	C5'-O5'-PA-O1A
35	C	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C3'-C4'-C5'-O5'
35	F	501	ATP	O4'-C4'-C5'-O5'
35	C	501	ATP	PB-O3A-PA-O1A
35	F	501	ATP	PB-O3A-PA-O1A
35	C	501	ATP	PB-O3A-PA-O2A
35	F	501	ATP	PB-O3A-PA-O2A
37	D	501	ADP	O4'-C4'-C5'-O5'
35	B	501	ATP	PA-O3A-PB-O2B

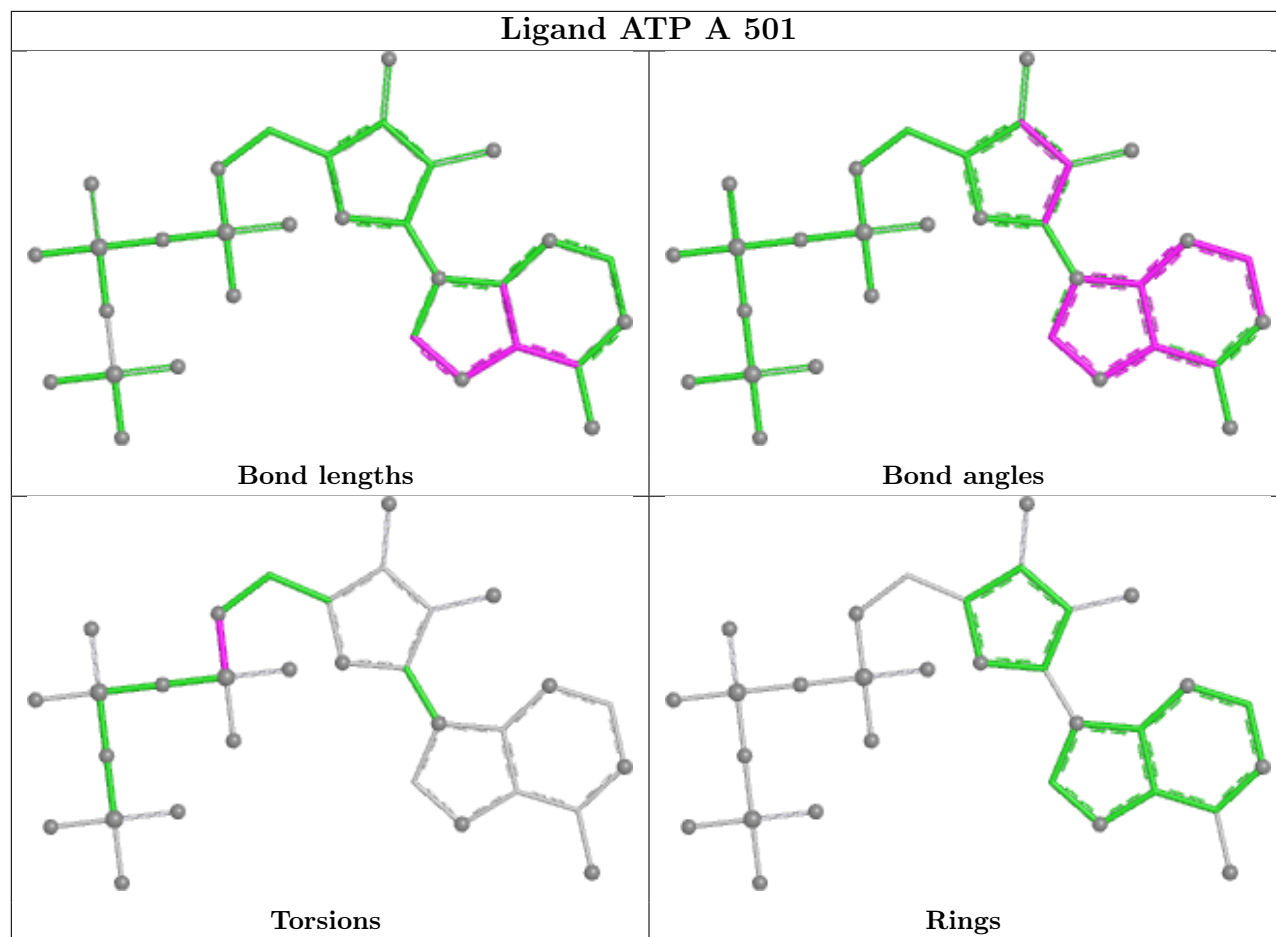
There are no ring outliers.

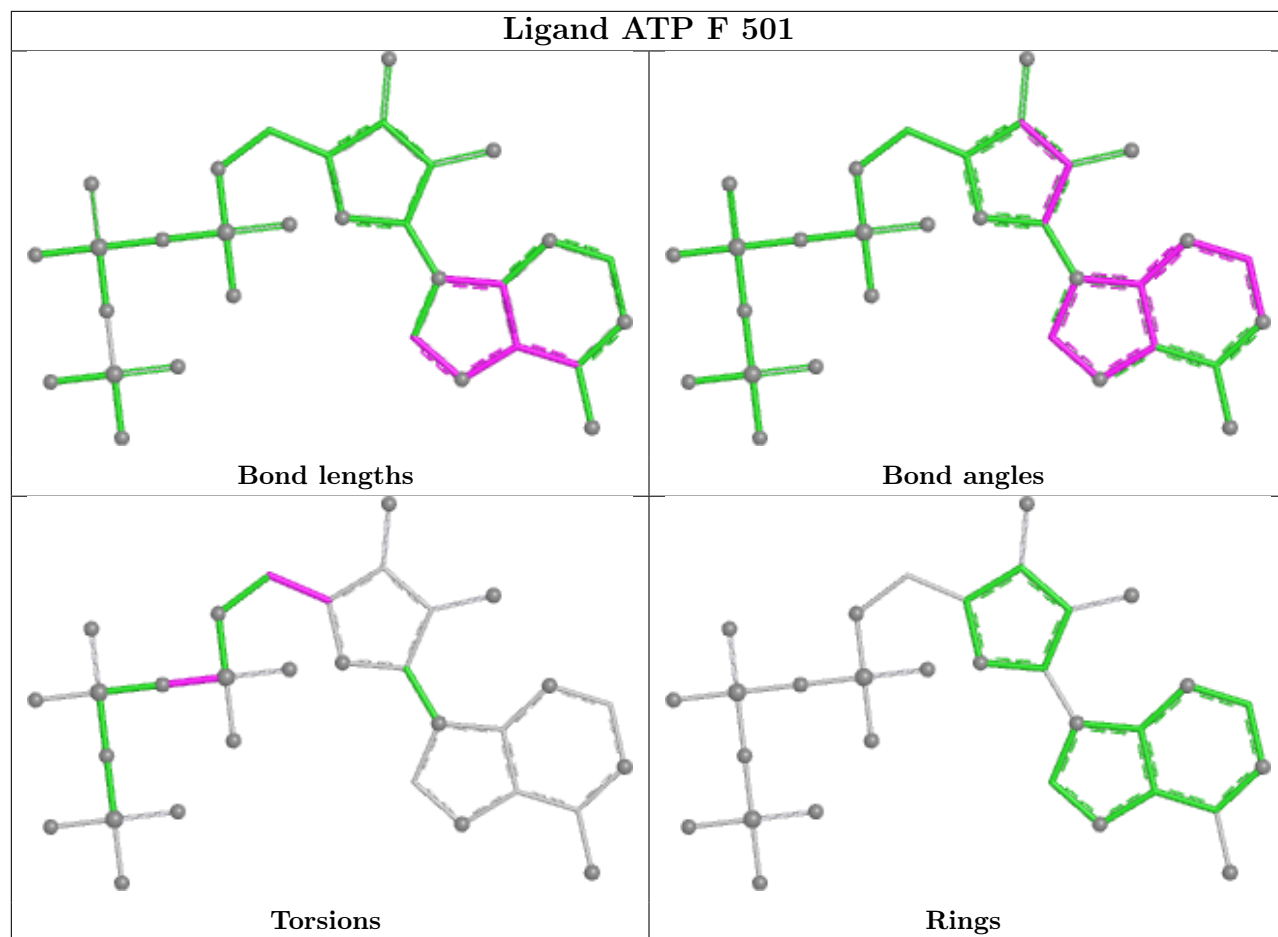
4 monomers are involved in 6 short contacts:

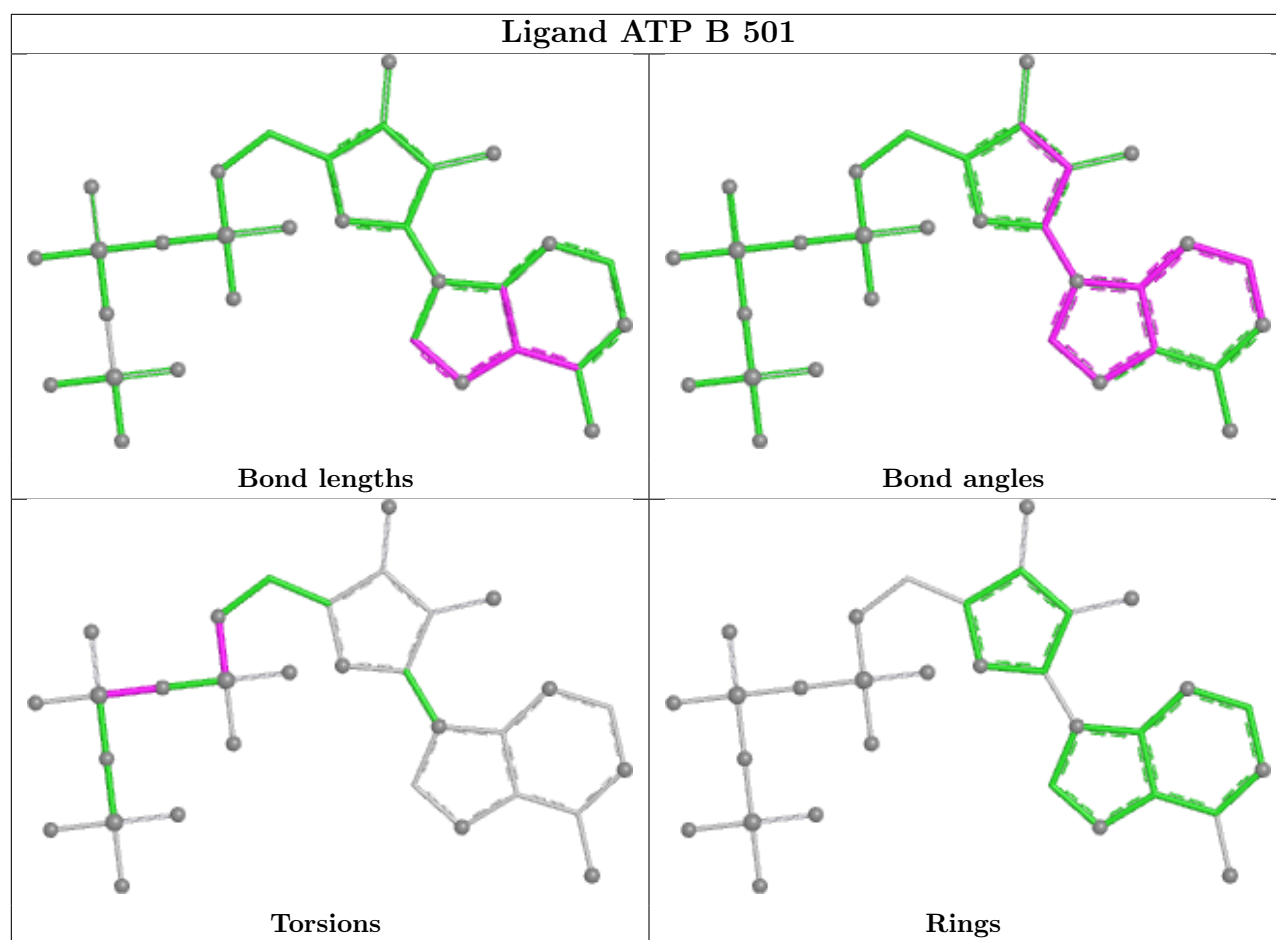
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	C	501	ATP	2	0
35	A	501	ATP	1	0
35	F	501	ATP	1	0
35	B	501	ATP	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

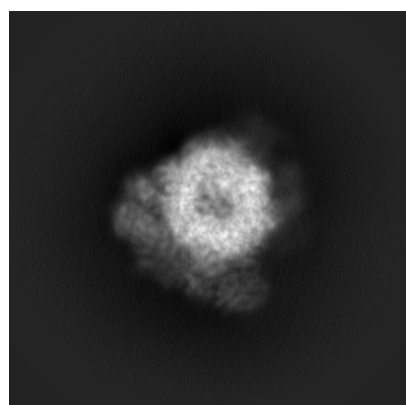
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9222. These allow visual inspection of the internal detail of the map and identification of artifacts.

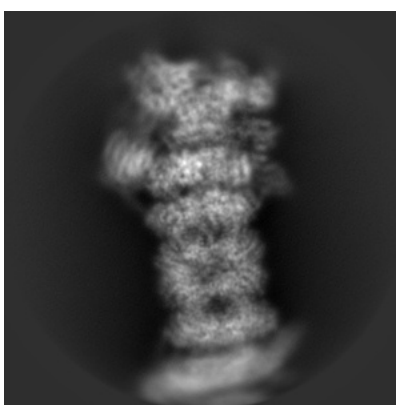
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

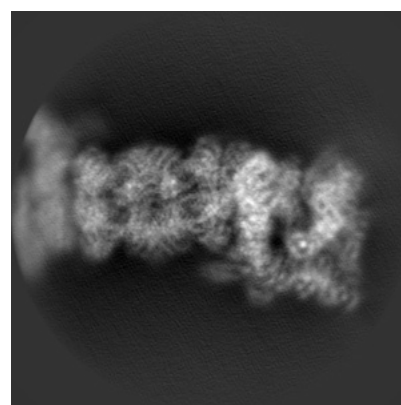
6.1.1 Primary map



X



Y

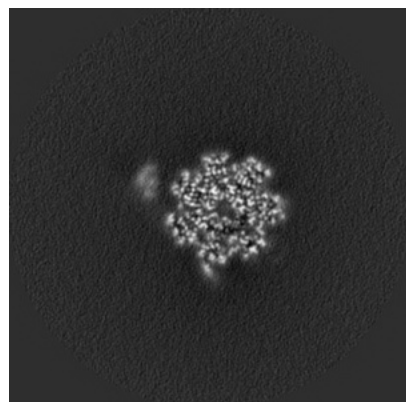


Z

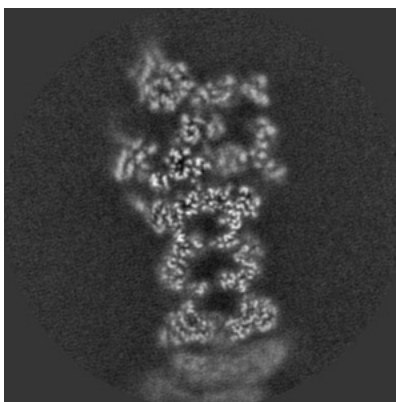
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

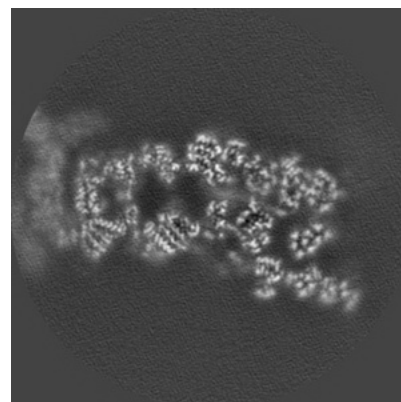
6.2.1 Primary map



X Index: 300



Y Index: 300

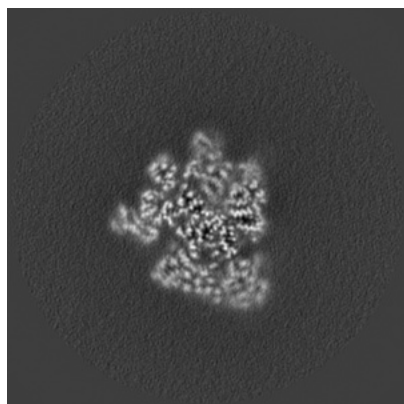


Z Index: 300

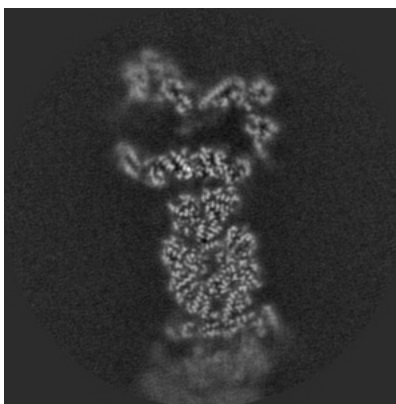
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

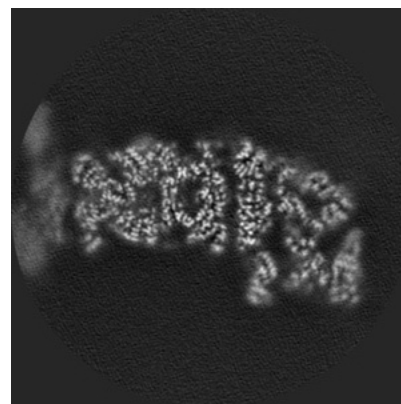
6.3.1 Primary map



X Index: 369



Y Index: 274

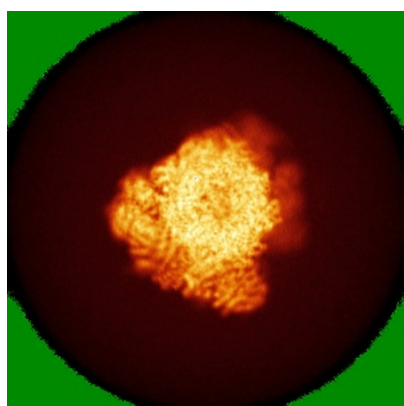


Z Index: 273

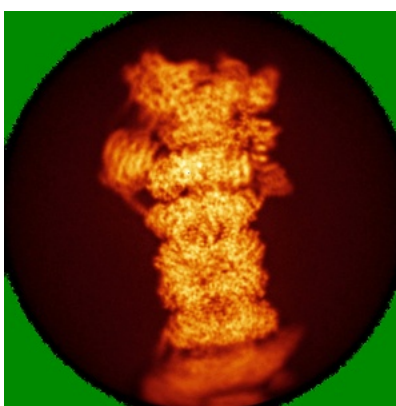
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

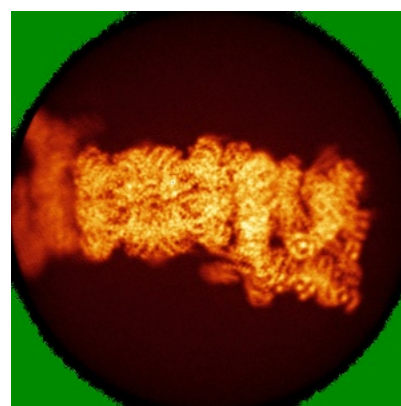
6.4.1 Primary map



X



Y

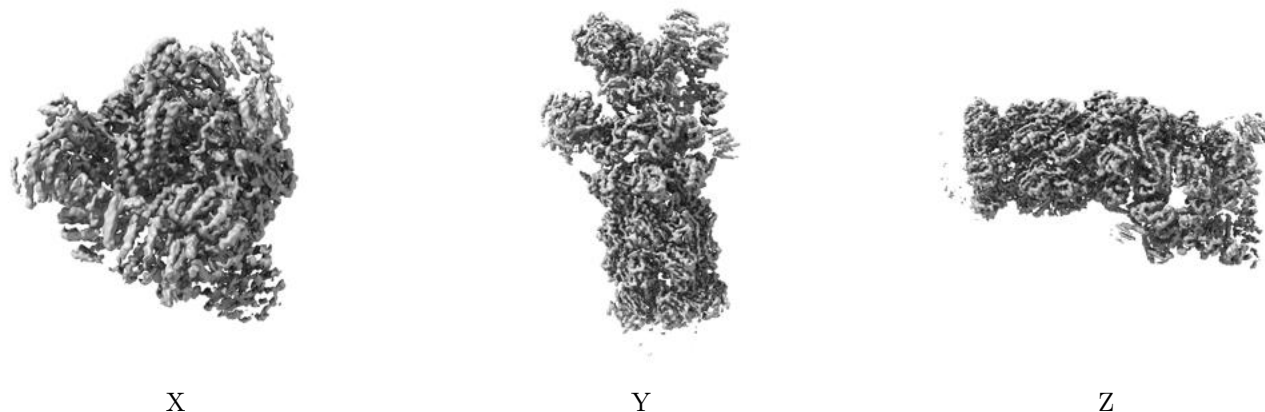


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

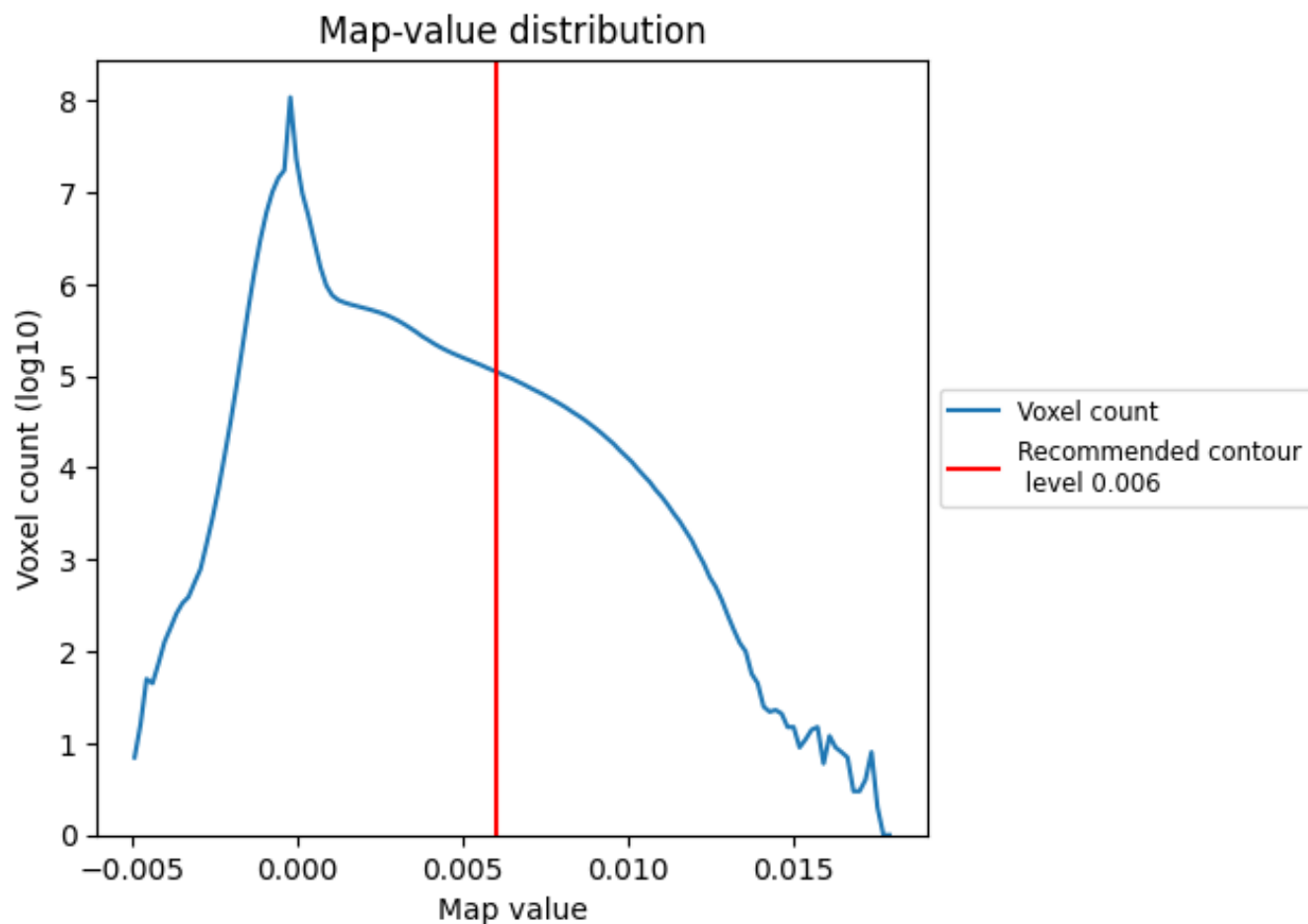
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

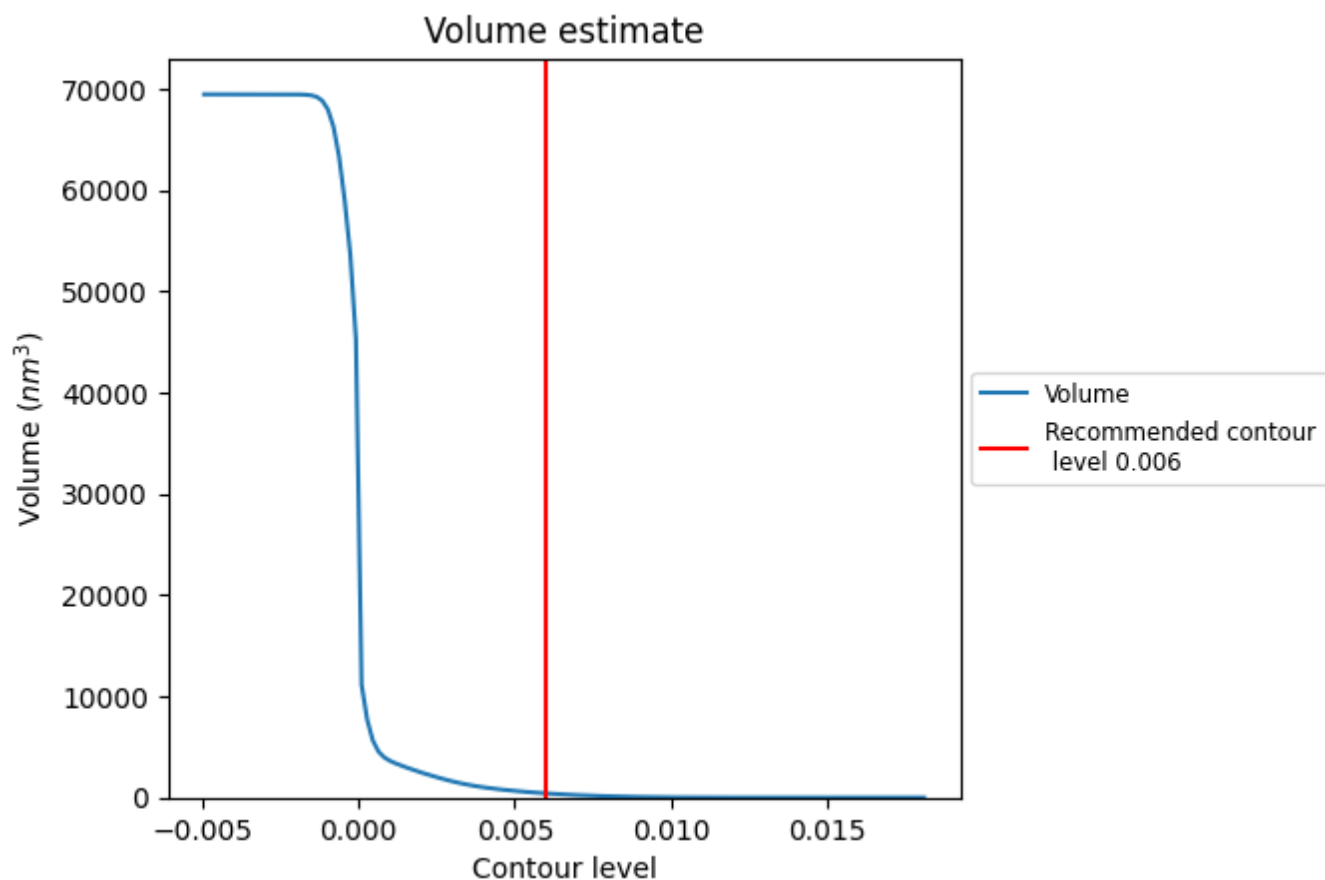
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

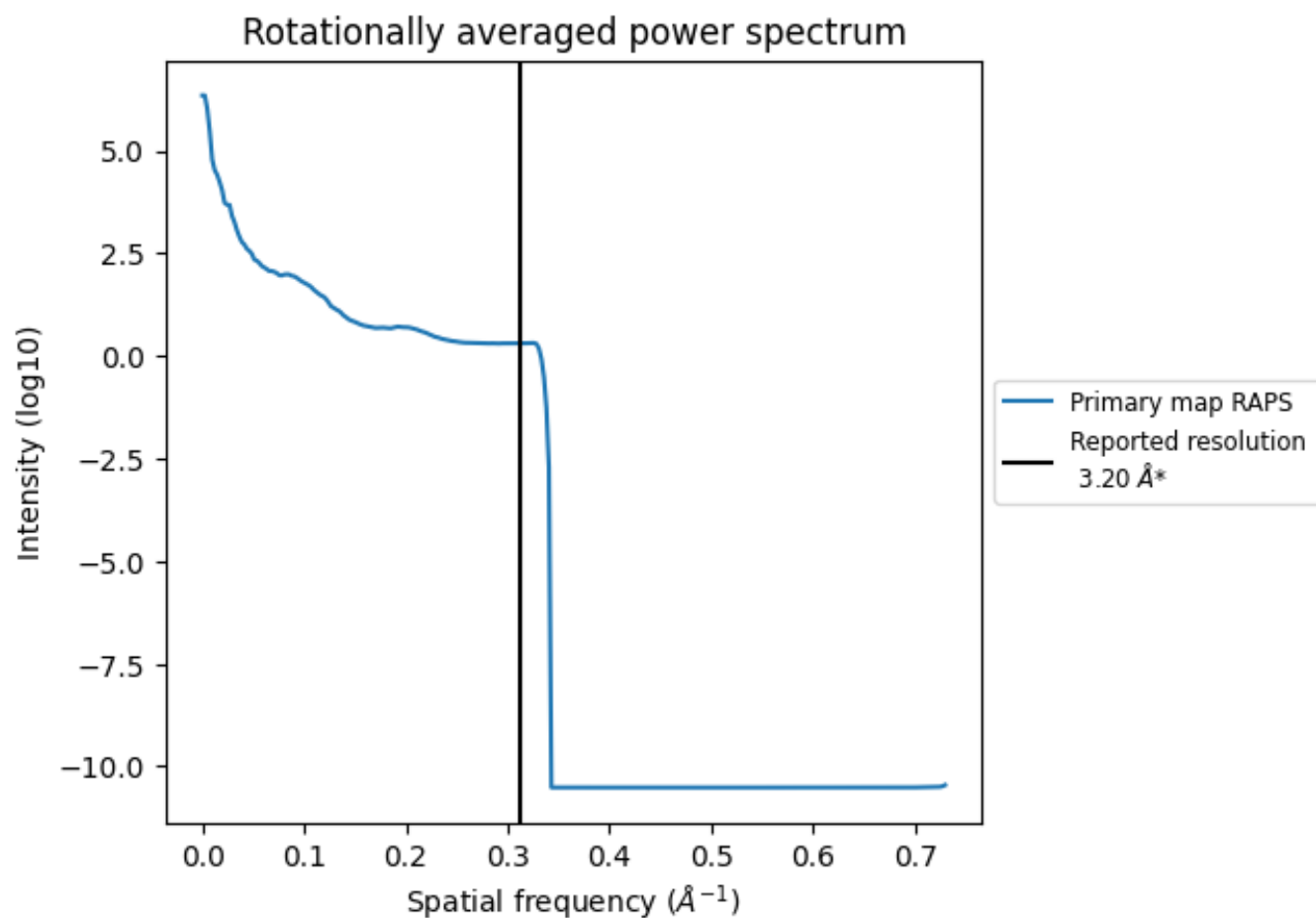
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 414 nm³; this corresponds to an approximate mass of 374 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

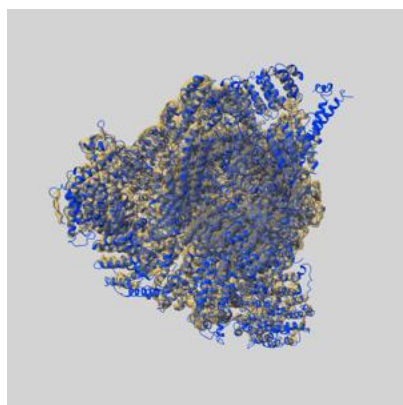
8 Fourier-Shell correlation ⓘ

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

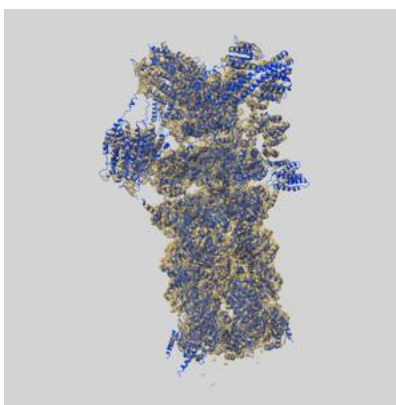
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9222 and PDB model 6MSK. Per-residue inclusion information can be found in section [3](#) on page [12](#).

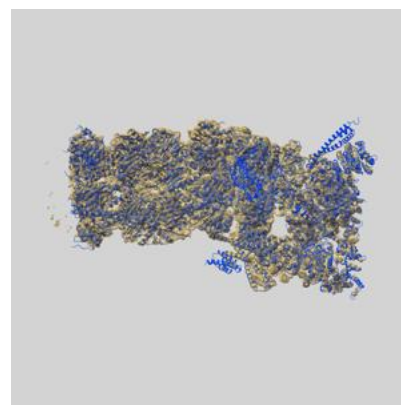
9.1 Map-model overlay [i](#)



X



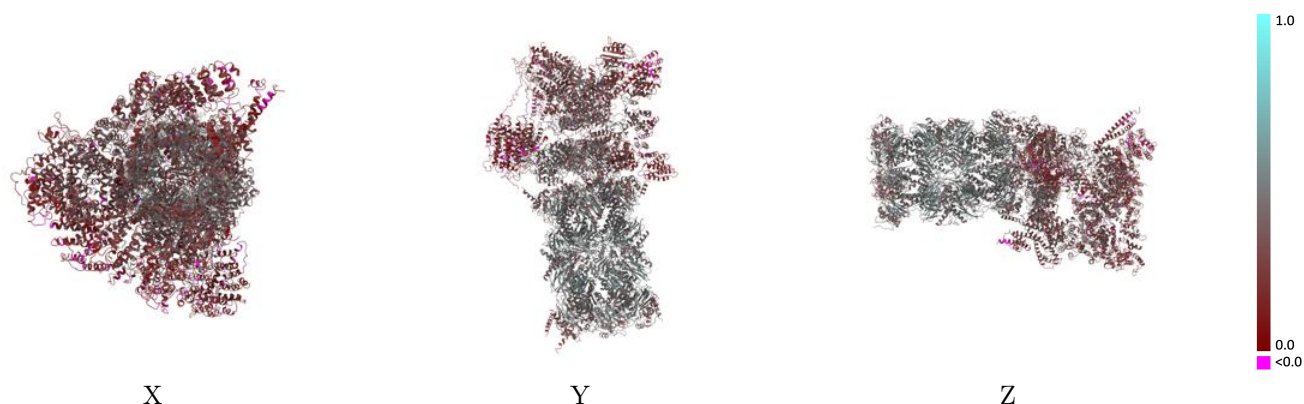
Y



Z

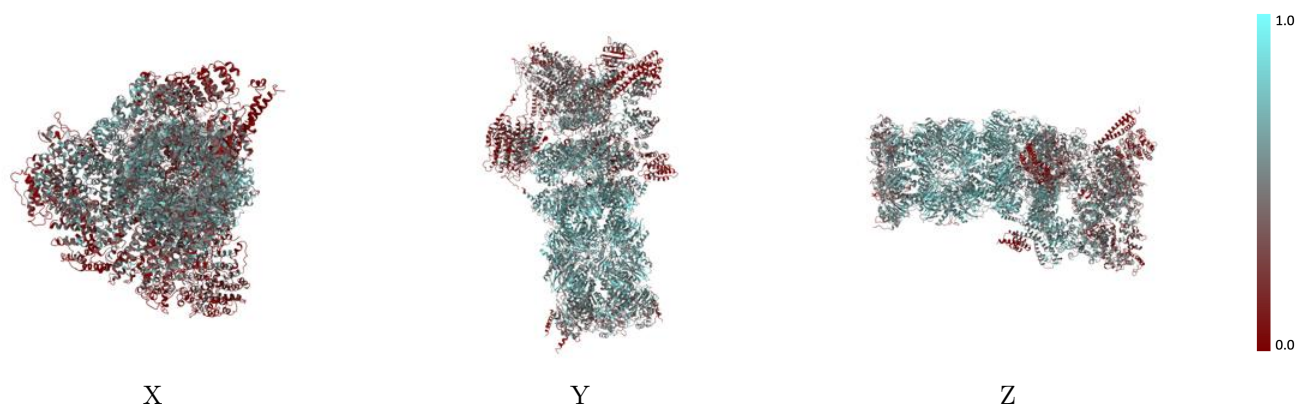
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



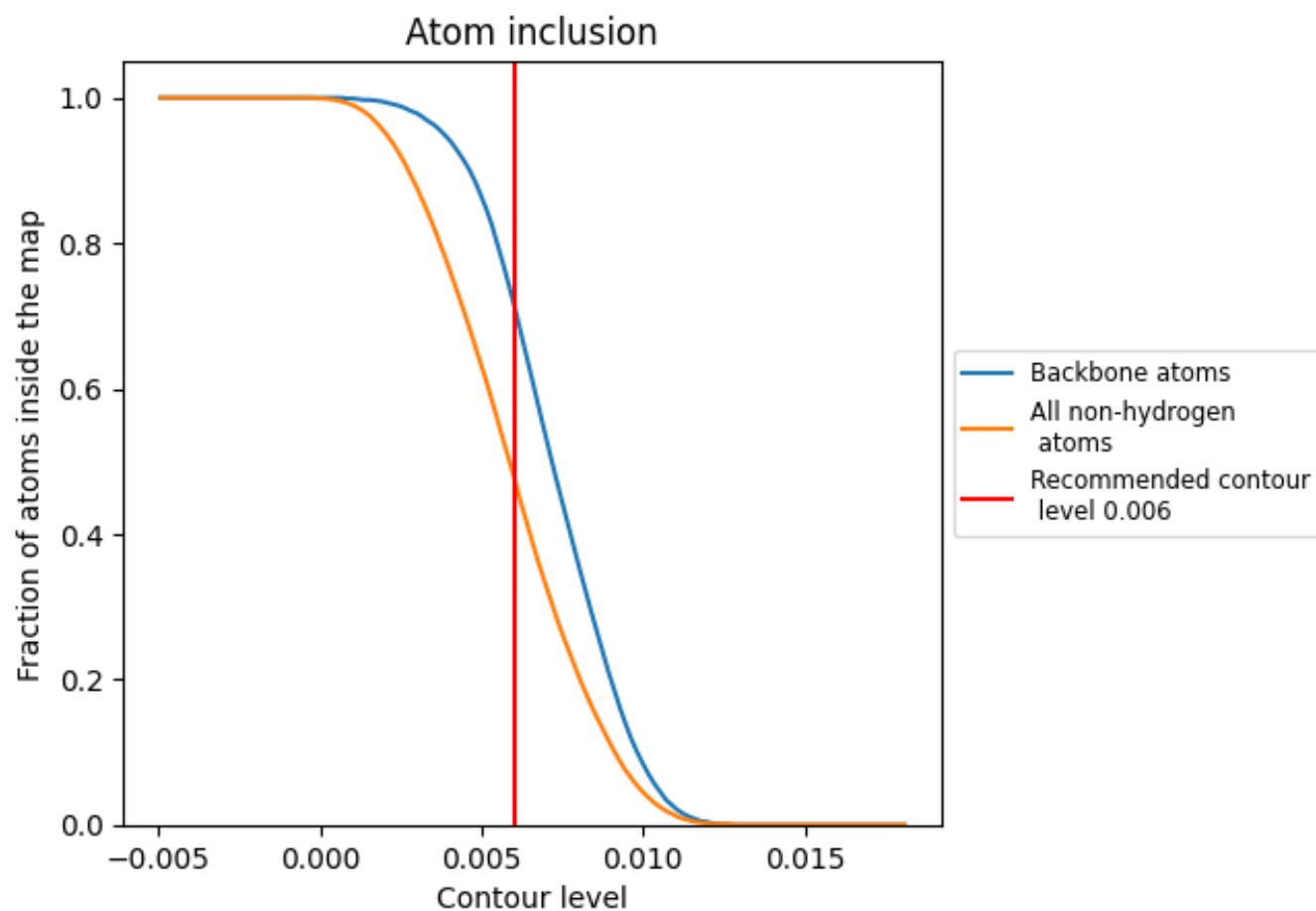
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.006).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 48% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4800	 0.3550
A	 0.5110	 0.3670
B	 0.5060	 0.3540
C	 0.5670	 0.3740
D	 0.5510	 0.3600
E	 0.2520	 0.2210
F	 0.4420	 0.3240
G	 0.6380	 0.4290
H	 0.6810	 0.4480
I	 0.6260	 0.4150
J	 0.6210	 0.4190
K	 0.6240	 0.4300
L	 0.6550	 0.4470
M	 0.6260	 0.4200
N	 0.6620	 0.4650
O	 0.6350	 0.4620
P	 0.6600	 0.4810
Q	 0.6510	 0.4610
R	 0.6800	 0.4780
S	 0.6210	 0.4710
T	 0.6570	 0.4700
U	 0.3420	 0.2650
V	 0.3360	 0.2260
W	 0.3360	 0.2390
X	 0.4560	 0.3010
Y	 0.5410	 0.3010
Z	 0.4070	 0.3110
a	 0.3350	 0.2510
b	 0.2480	 0.2570
c	 0.3930	 0.3120
d	 0.2700	 0.2220
e	 0.3580	 0.2290
f	 0.2380	 0.1820
g	 0.4810	 0.4330
h	 0.4950	 0.4390



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Chain	Atom inclusion	Q-score
i	 0.4320	 0.4040
j	 0.4030	 0.3860
k	 0.4720	 0.4140
l	 0.5350	 0.4460
m	 0.5170	 0.4140
n	 0.6270	 0.4770
o	 0.5940	 0.4690
p	 0.6070	 0.4790
q	 0.6020	 0.4740
r	 0.6500	 0.4880
s	 0.5970	 0.4840
t	 0.6510	 0.4800
v	 0.1500	 0.3230