



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 05:04 AM UTC

PDB ID : 6MSE / pdb_00006mse
EMDB ID : EMD-9218
Title : Cryo-EM structures and dynamics of substrate-engaged human 26S proteasome
Authors : Mao, Y.D.
Deposited on : 2018-10-16
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

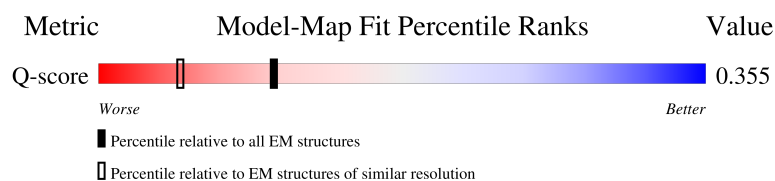
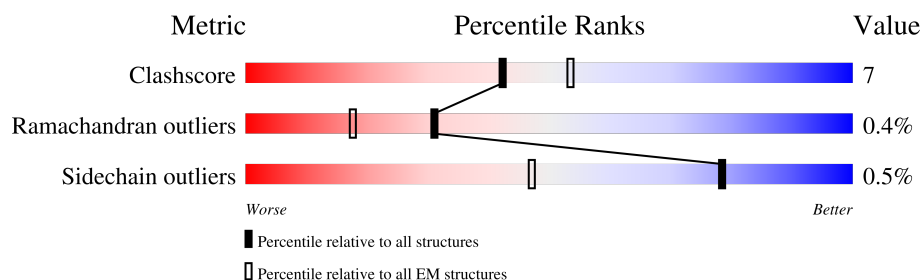
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	50% 68% 17% 15%
2	V	533	66% 64% 26% 10%
3	W	456	47% 75% 24%
4	X	422	50% 82% 9% 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	u	76	
20	v	28	
21	G	245	
21	g	245	
22	H	233	
22	h	233	
23	I	260	
23	i	260	
24	J	247	
24	j	247	
25	K	240	

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

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 105062 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	812	Total	C	N	O	S	0	0
			6334	4023	1078	1189	44		

- 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	393	Total	C	N	O	S	0	0
			3067	1930	539	581	17		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	395	Total	C	N	O	S	0	0
			3086	1946	523	602	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	381	Total	C	N	O	S	0	0
			2978	1872	536	554	16		

- 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
			3039	1923	524	579	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	415	Total	C	N	O	S	0	0
			3251	2038	561	634	18		

- Molecule 19 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	u	76	Total	C	N	O	S	0	0
			603	378	107	117	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	63	ARG	LYS	conflict	UNP P0CG47

- Molecule 20 is a protein called substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	v	28	Total	C	N	O	0	0
			143	86	29	28		

- Molecule 21 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		
21	g	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 22 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		
22	h	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 23 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		
23	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 24 is a protein called Proteasome subunit alpha type-7.

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

- Molecule 25 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 26 is a protein called Proteasome subunit alpha type-1.

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

- Molecule 27 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 28 is a protein called Proteasome subunit beta type-6.

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

- Molecule 29 is a protein called Proteasome subunit beta type-7.

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

- Molecule 30 is a protein called Proteasome subunit beta type-3.

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

- Molecule 31 is a protein called Proteasome subunit beta type-2.

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

- Molecule 32 is a protein called Proteasome subunit beta type-5.

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

- Molecule 33 is a protein called Proteasome subunit beta type-1.

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

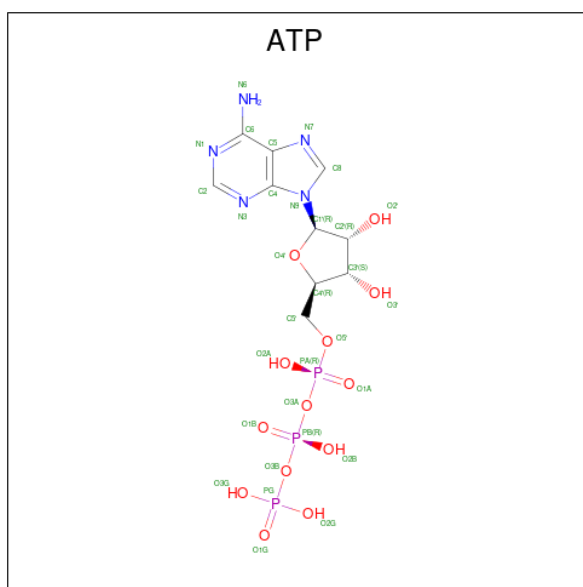
- Molecule 34 is a protein called Proteasome subunit beta type-4.

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

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

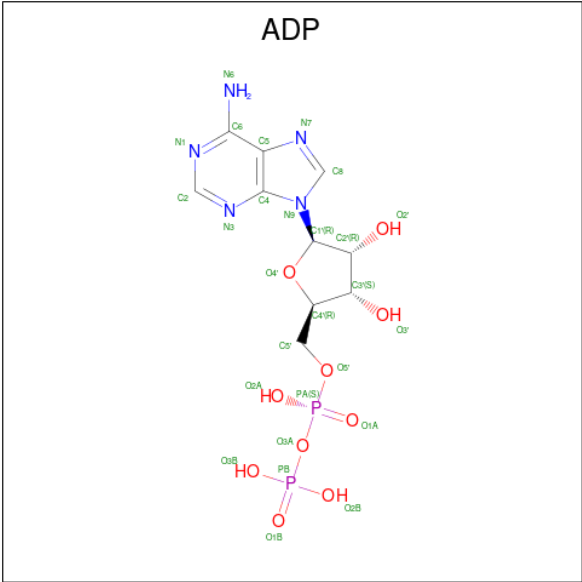


Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	F	1	Total	Mg	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

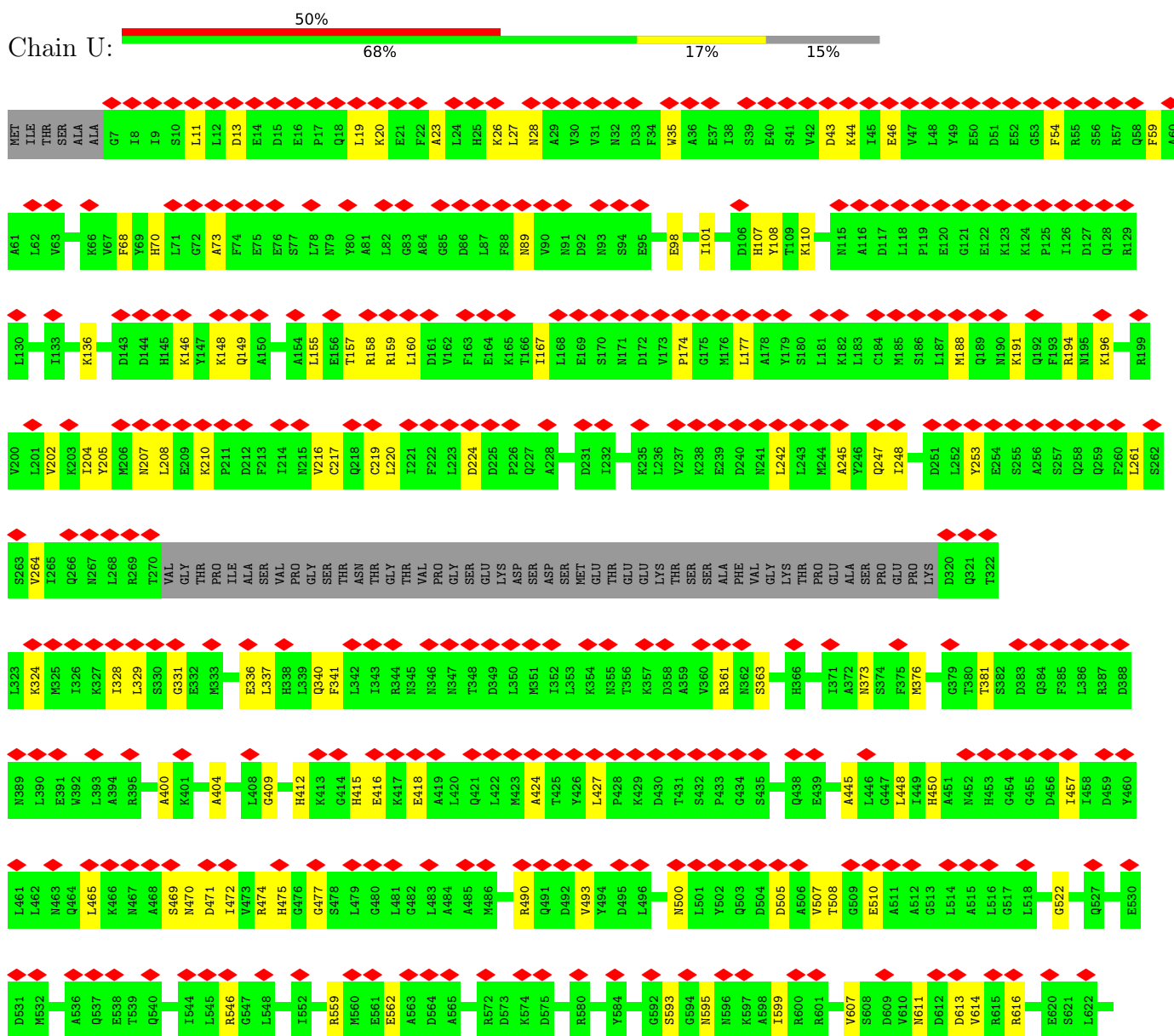


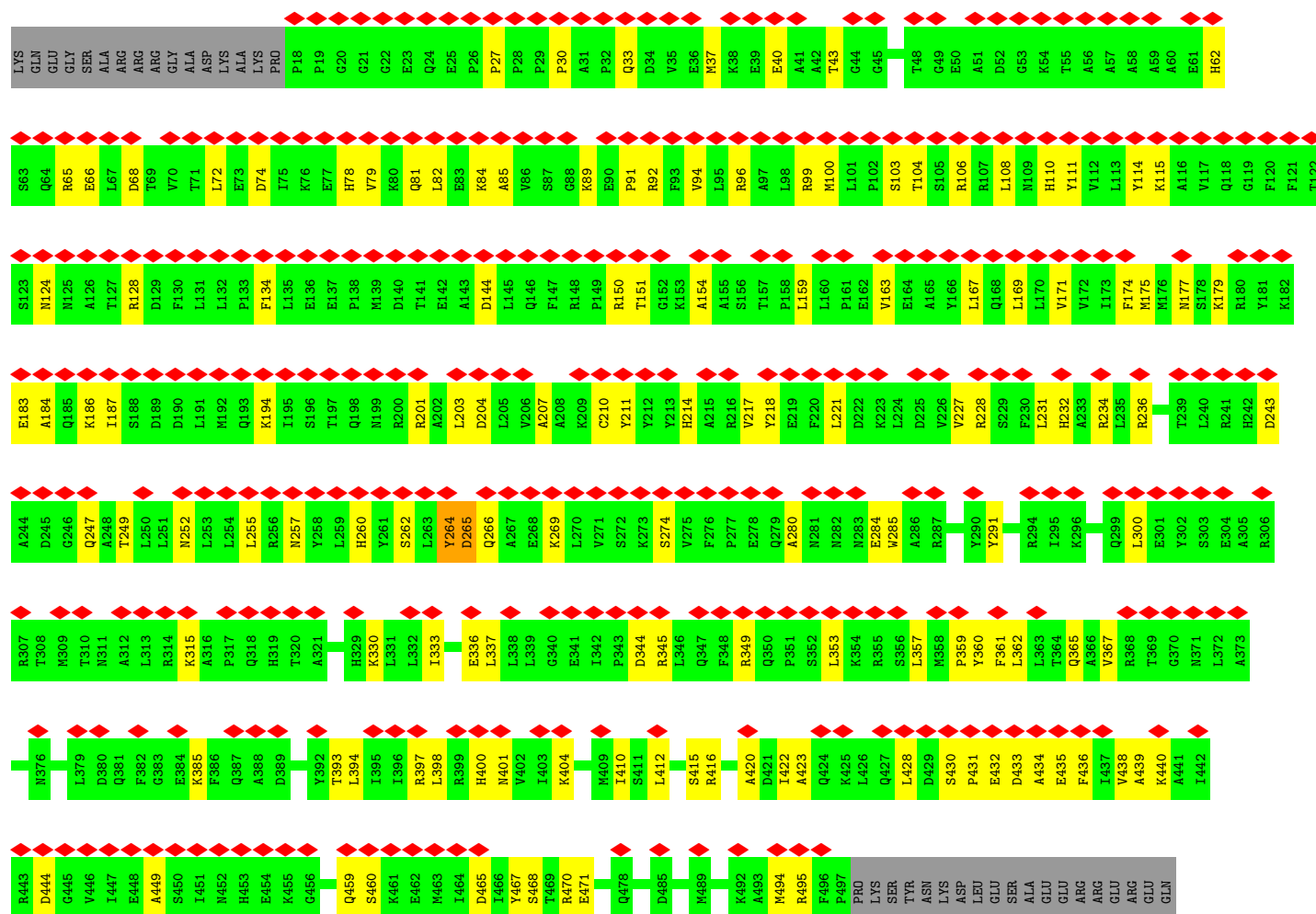
Mol	Chain	Residues	Atoms					AltConf
38	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
38	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

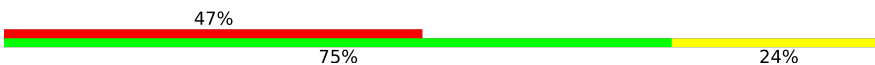
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1

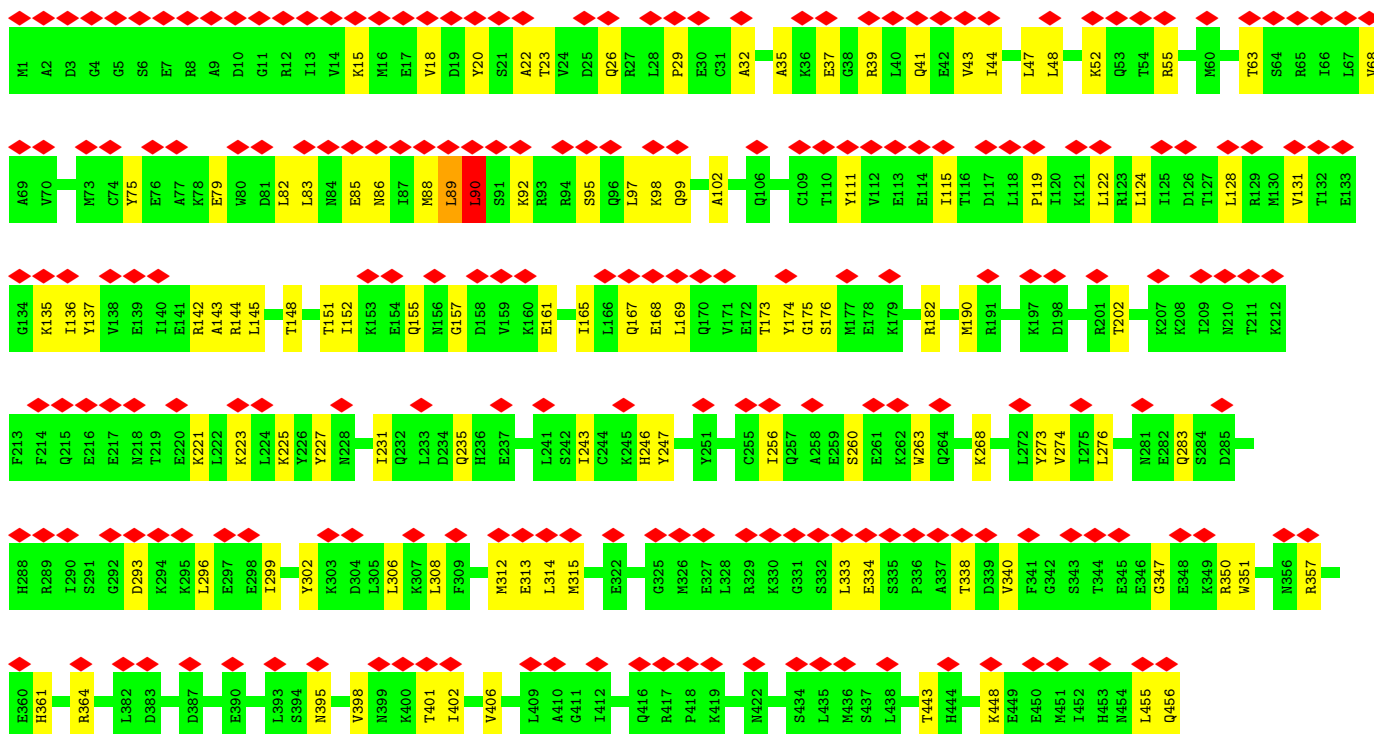




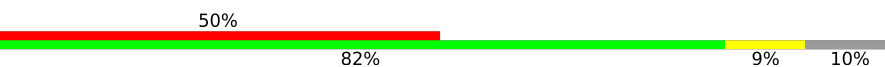
GLN
ASP
LEU
GLU
PHE
ALA
LYS
GLU
MET
GLU
ALA
ASP
ASP
ASP
SER
PHE
PRO

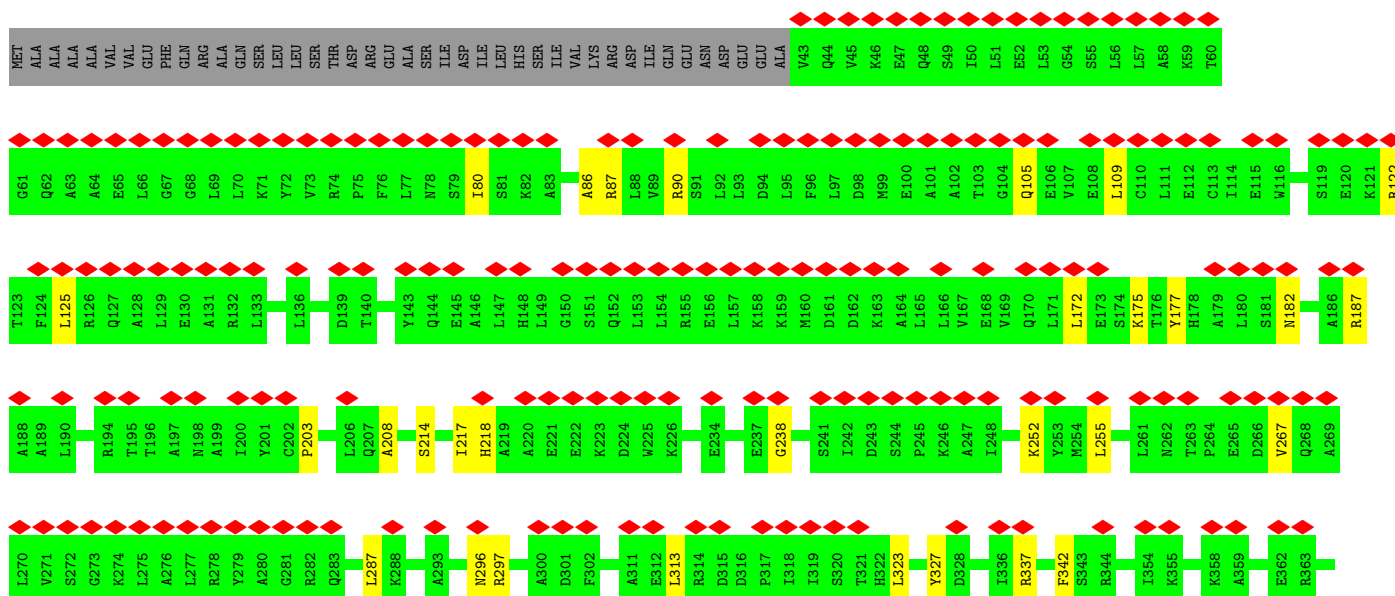
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 



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

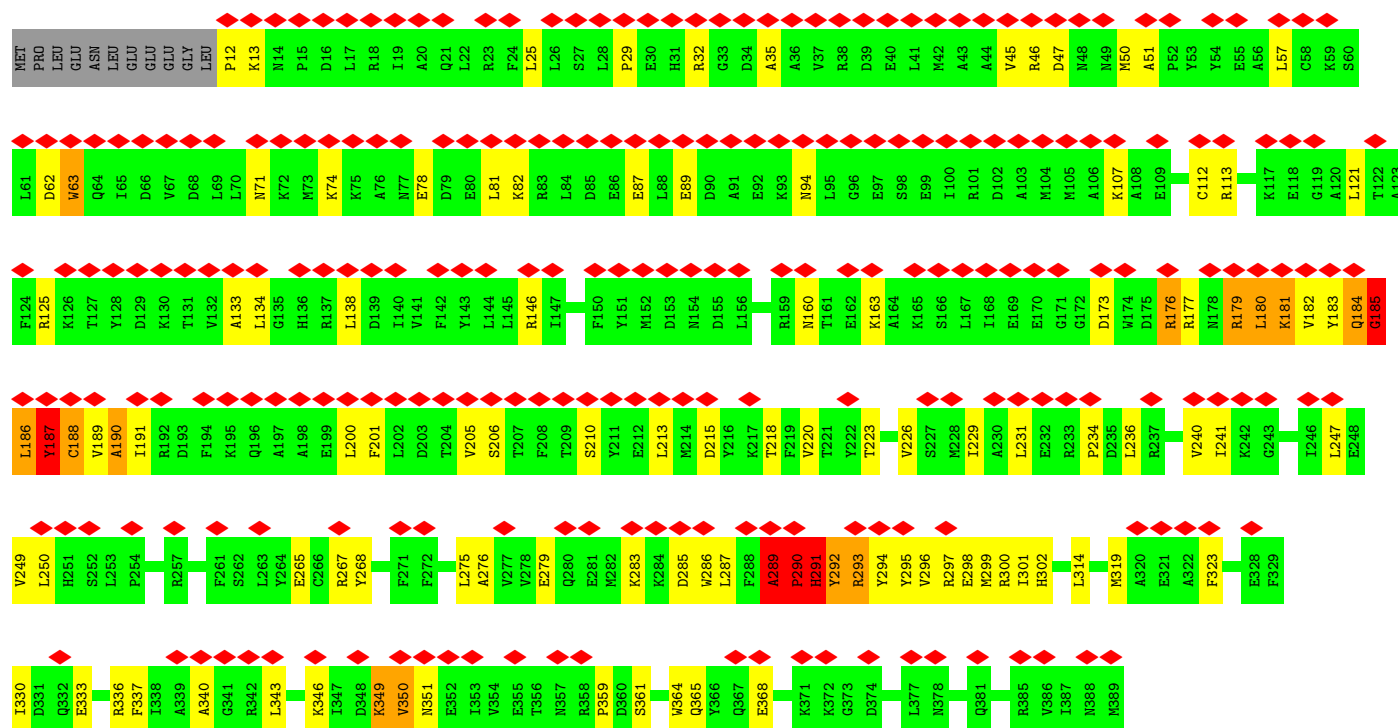
Chain X: 





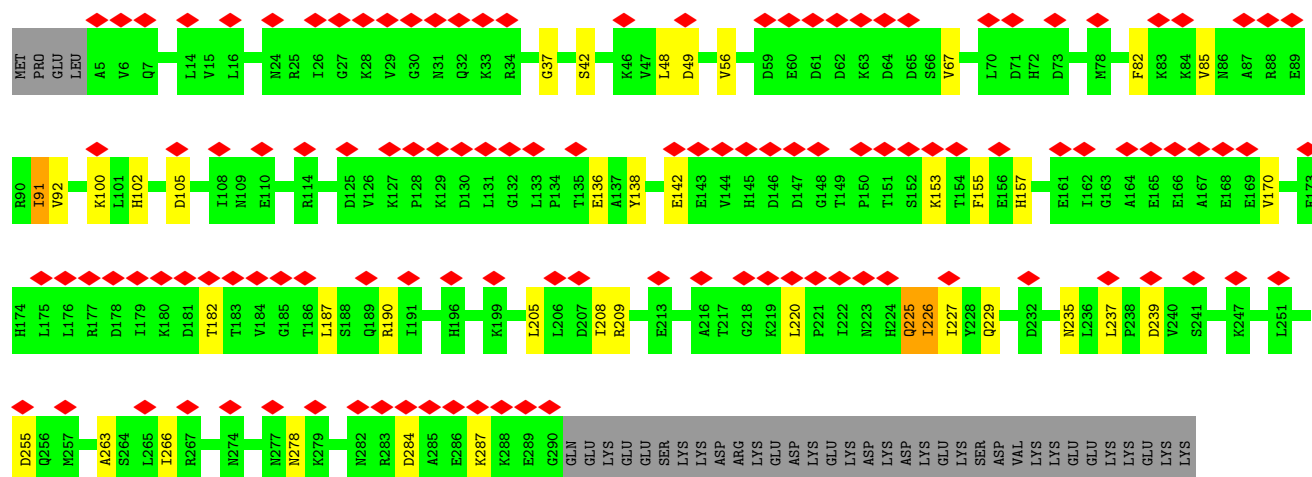
- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 62% 69% 24%

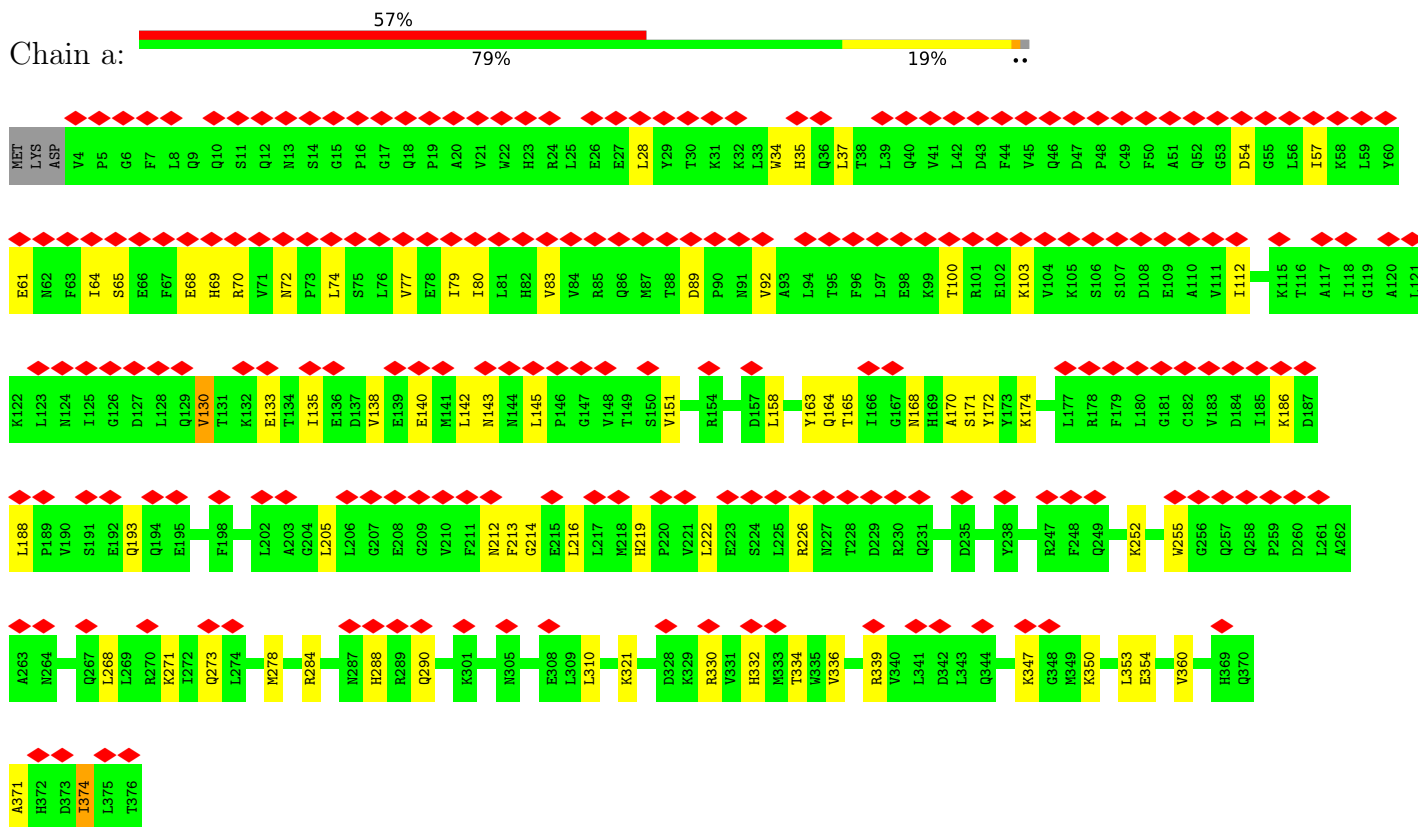


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7

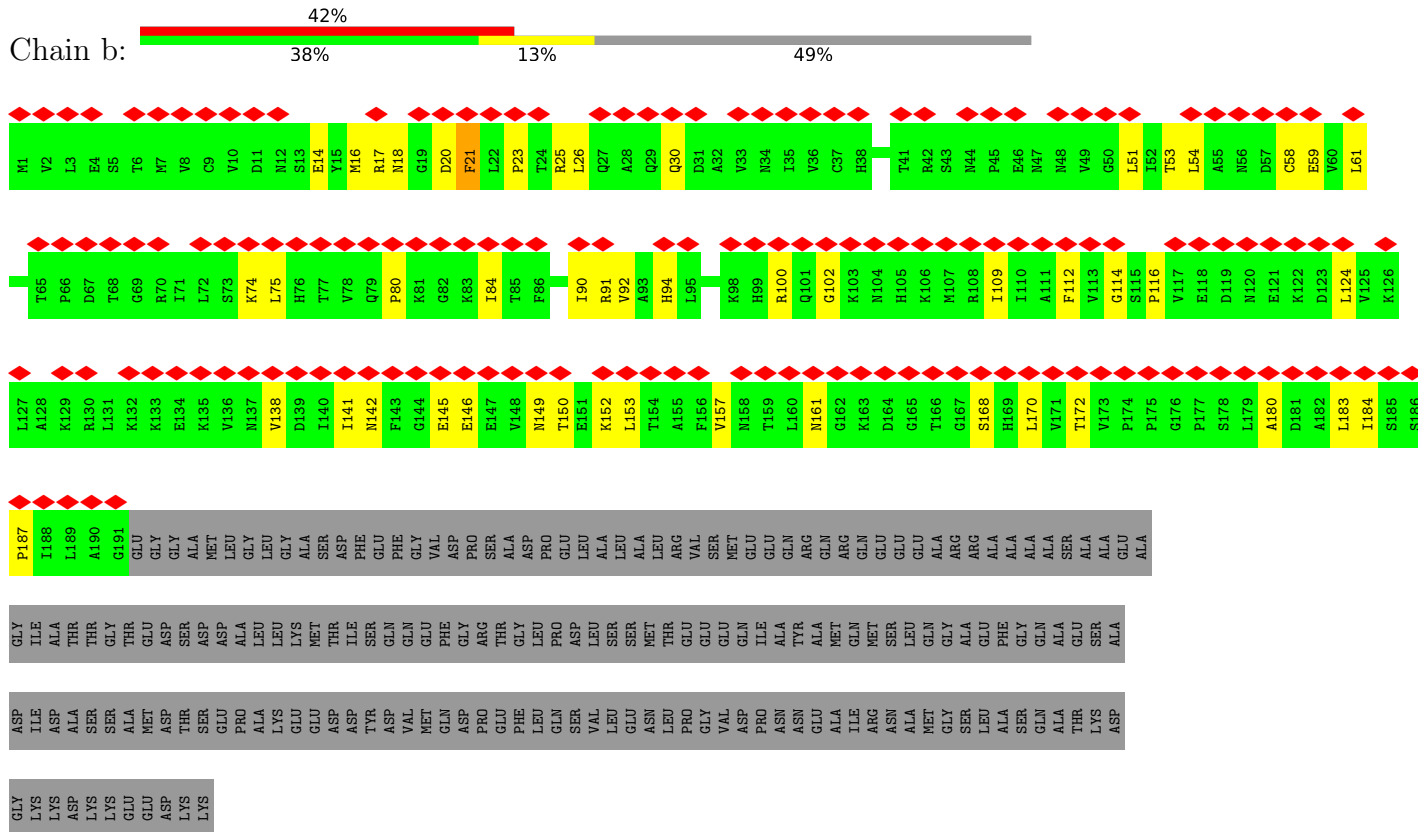
Chain Z: 37% 76% 11% 12%



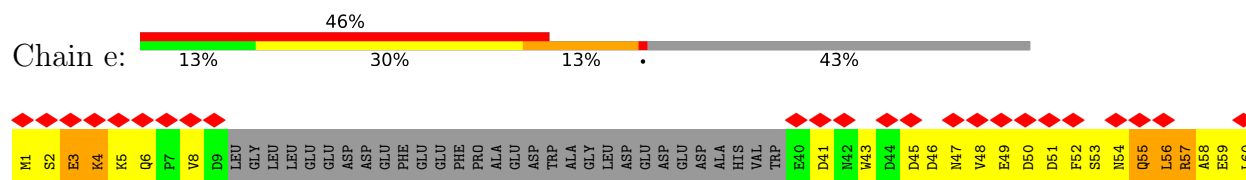
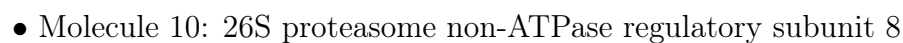
- Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

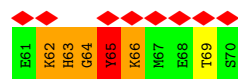


- Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

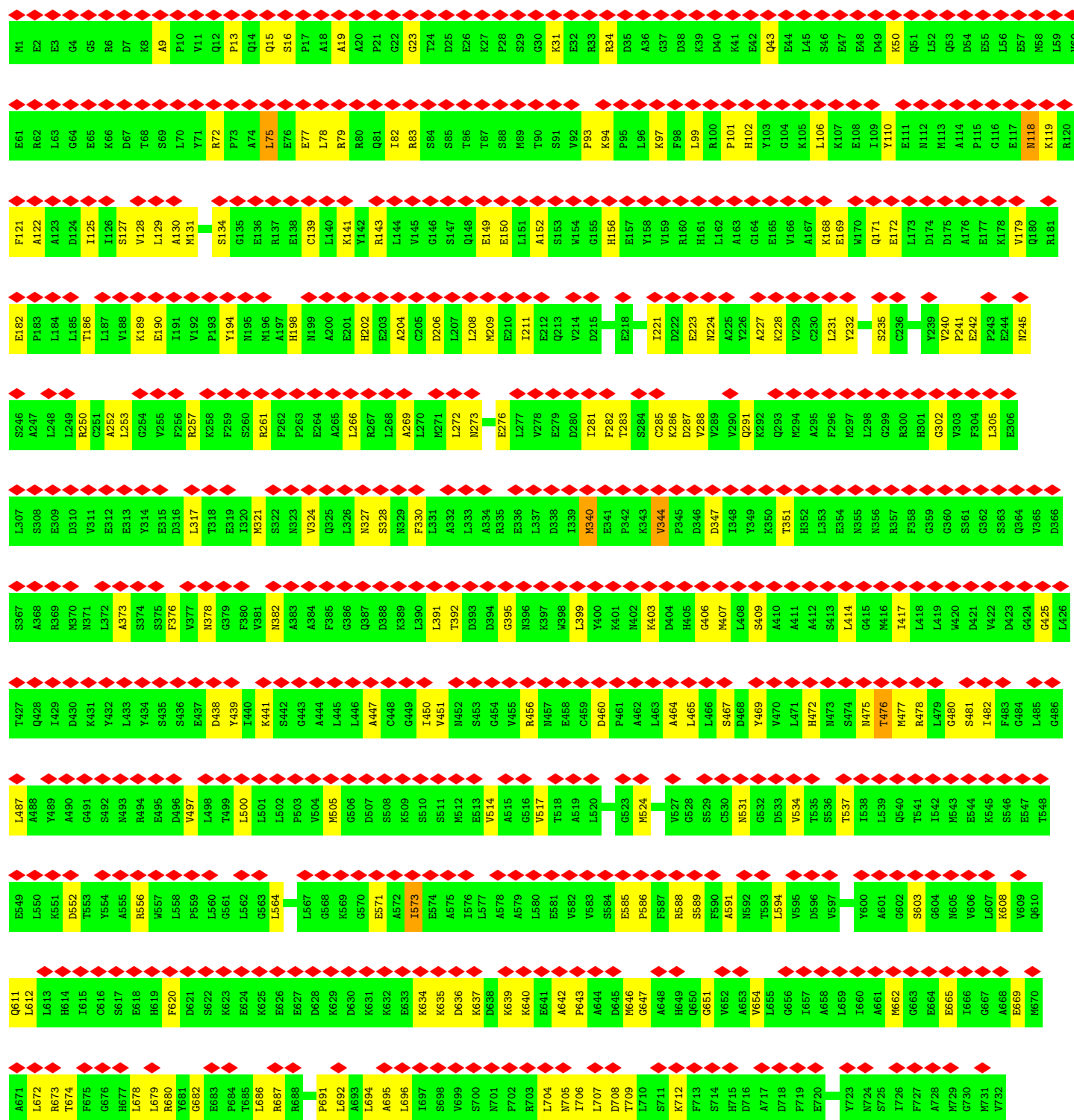
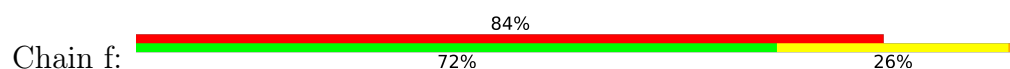


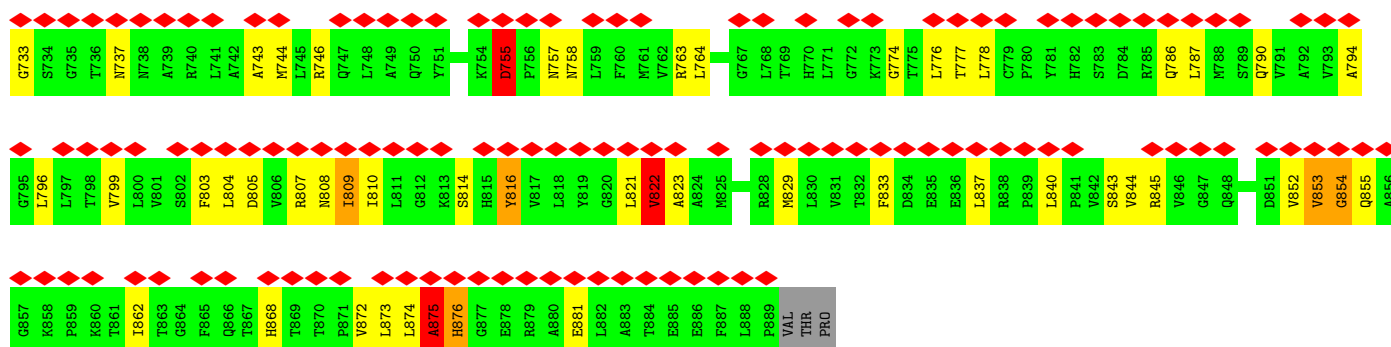
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14



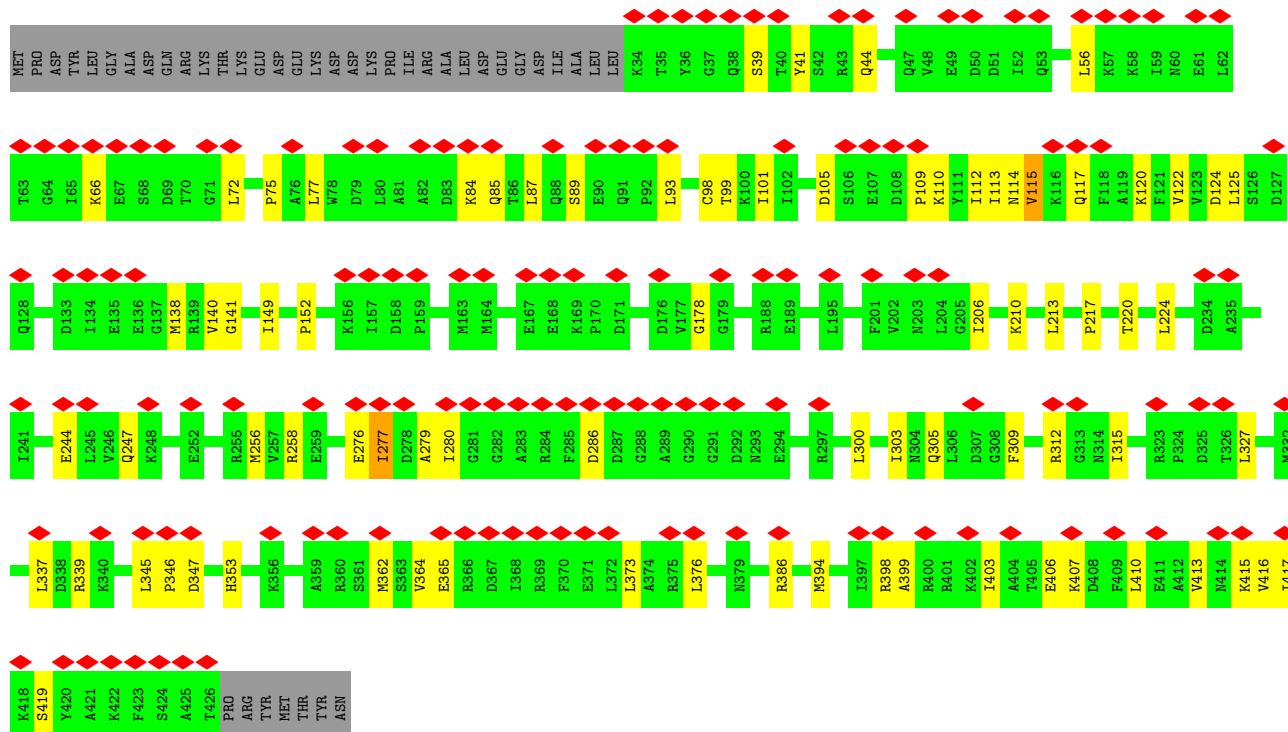
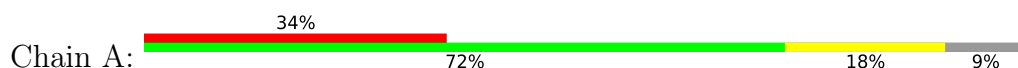


• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2

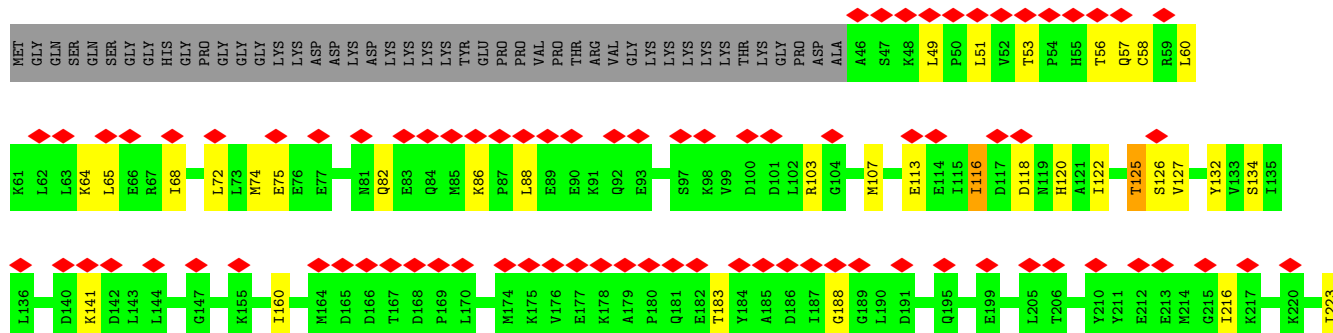
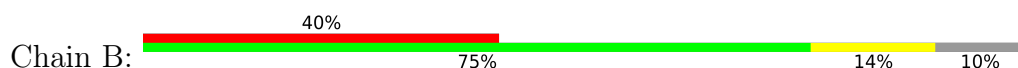


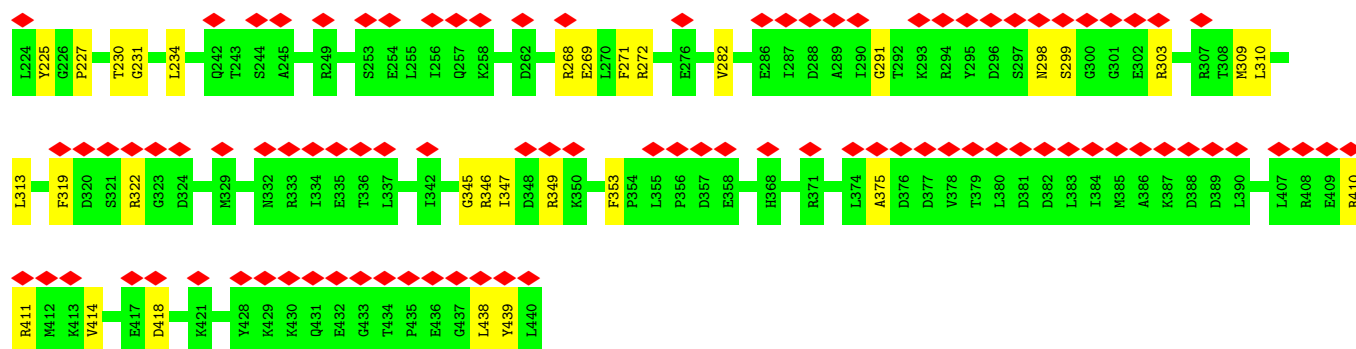


• Molecule 13: 26S proteasome regulatory subunit 7

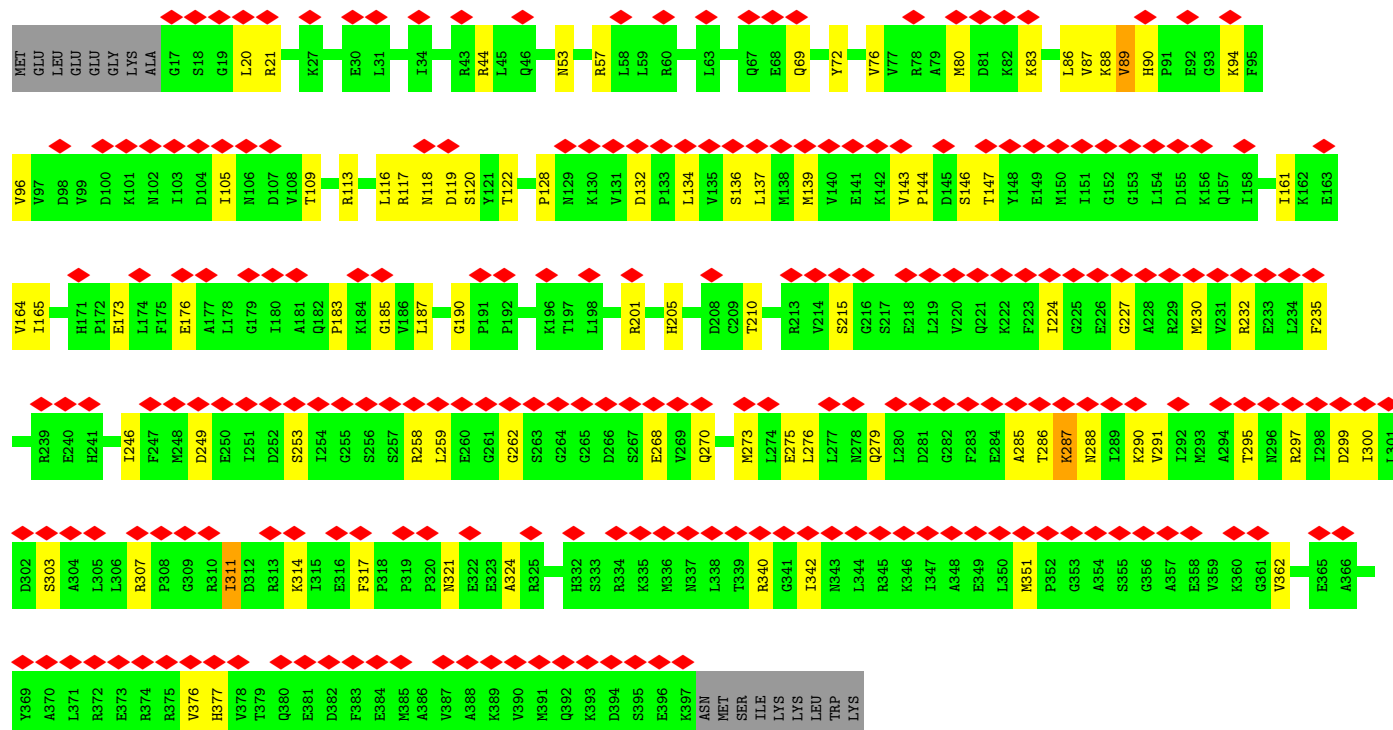


• Molecule 14: 26S proteasome regulatory subunit 4

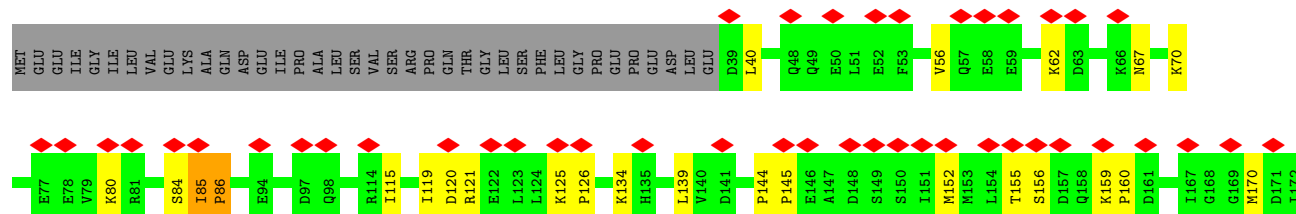
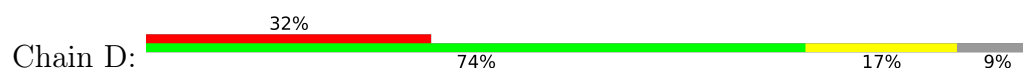


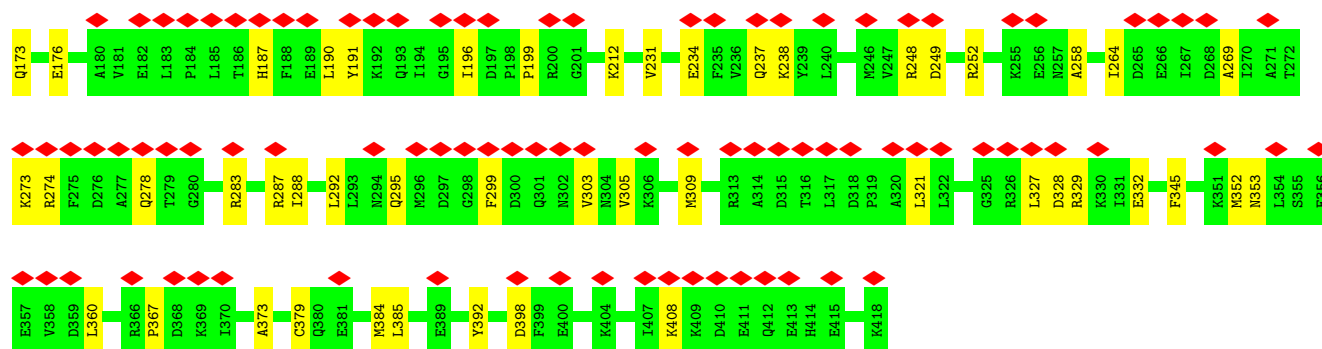


• Molecule 15: 26S proteasome regulatory subunit 8



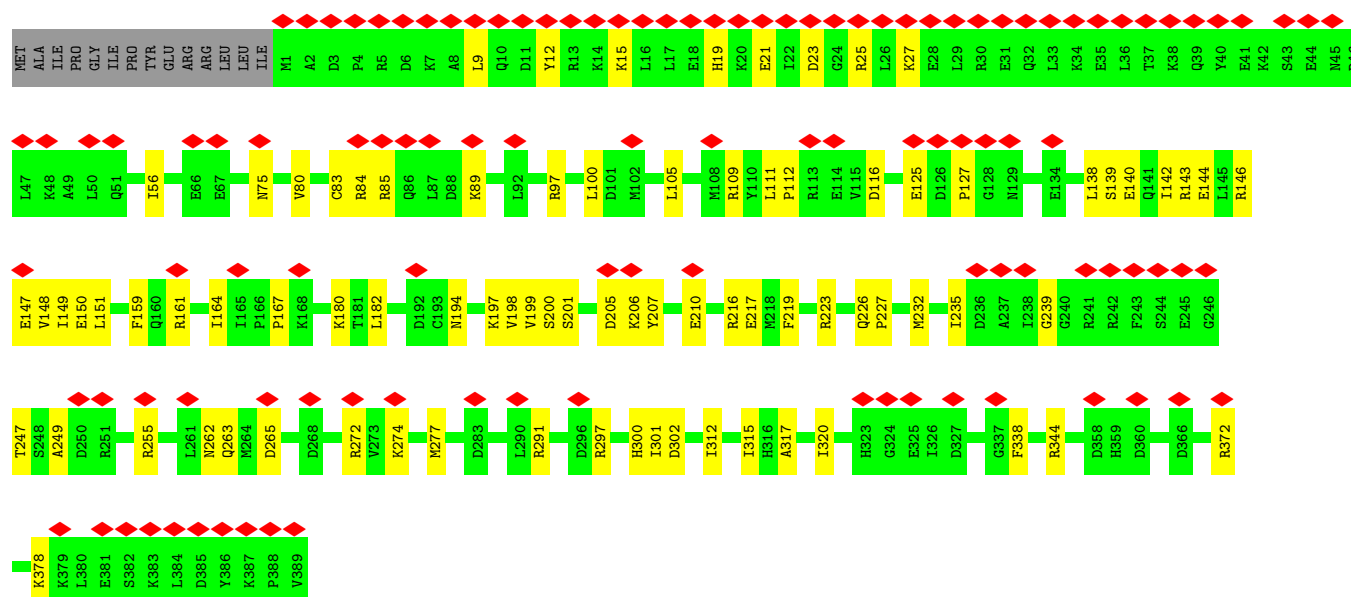
• Molecule 16: 26S proteasome regulatory subunit 6B





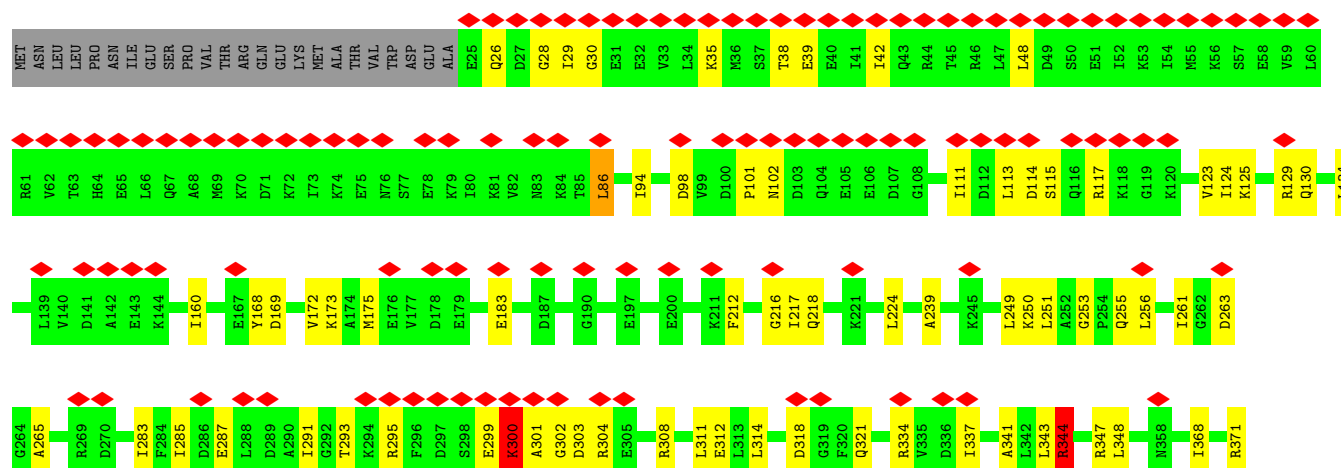
• Molecule 17: 26S proteasome regulatory subunit 10B

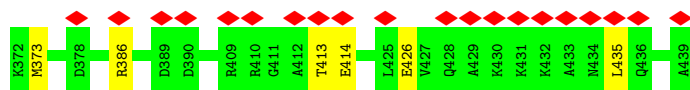
Chain E: 28% 76% 21%



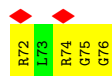
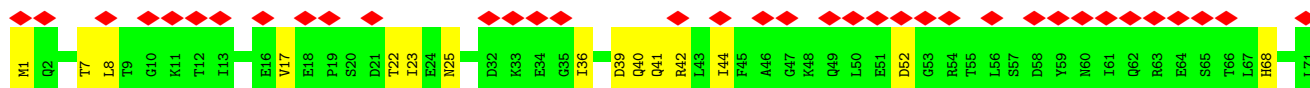
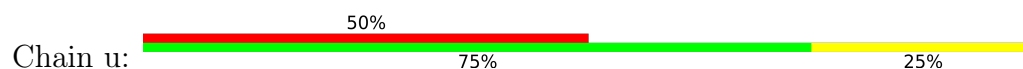
• Molecule 18: 26S proteasome regulatory subunit 6A

Chain F: 32% 76% 18% 5%

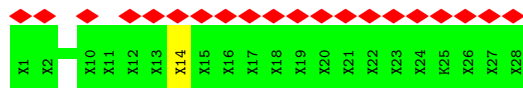




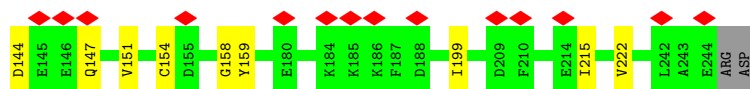
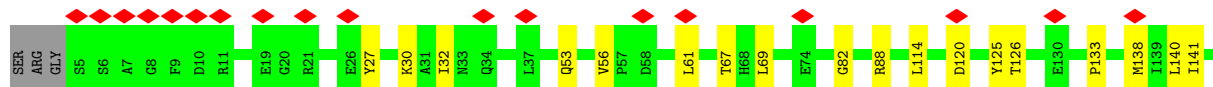
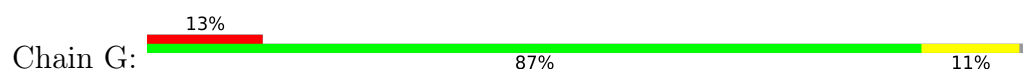
- Molecule 19: Ubiquitin



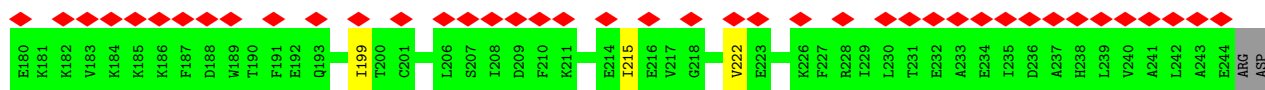
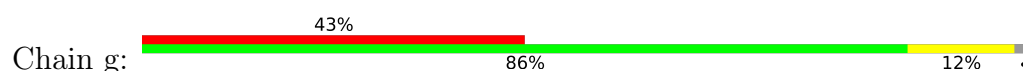
- Molecule 20: substrate



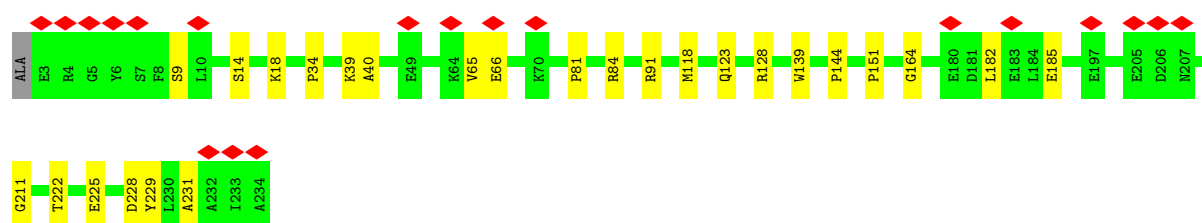
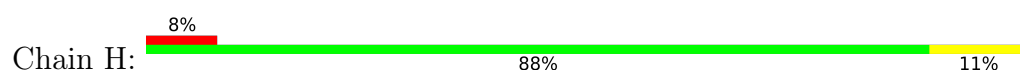
- Molecule 21: Proteasome subunit alpha type-6



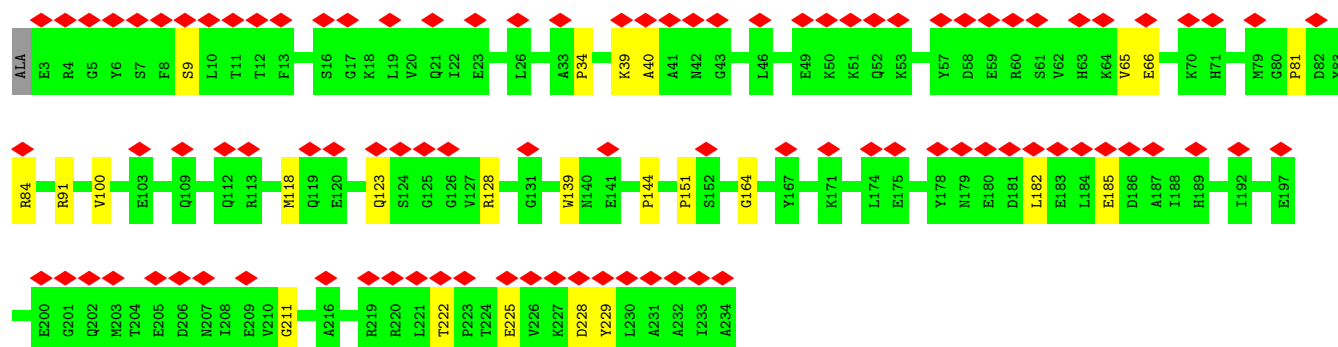
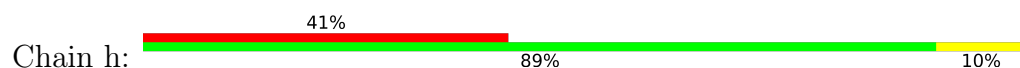
- Molecule 21: Proteasome subunit alpha type-6



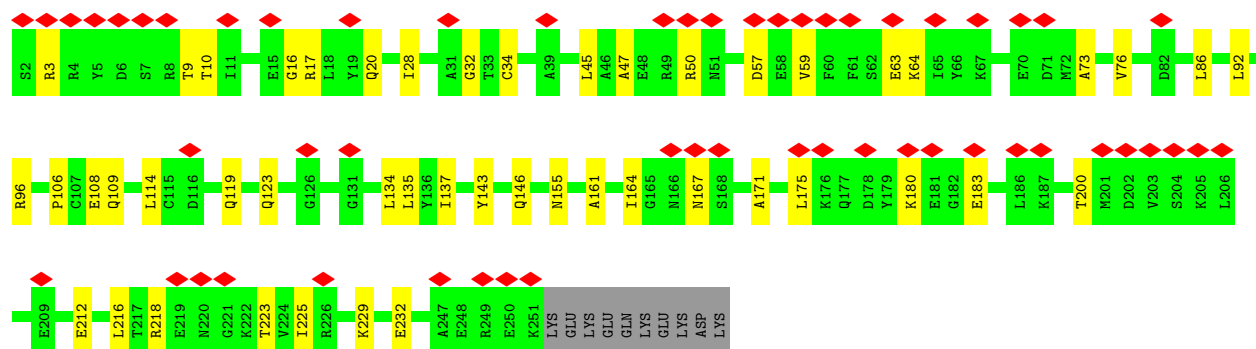
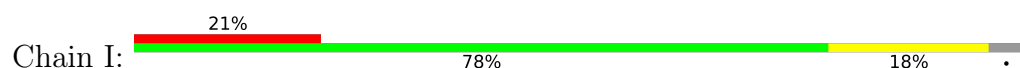
- Molecule 22: Proteasome subunit alpha type-2



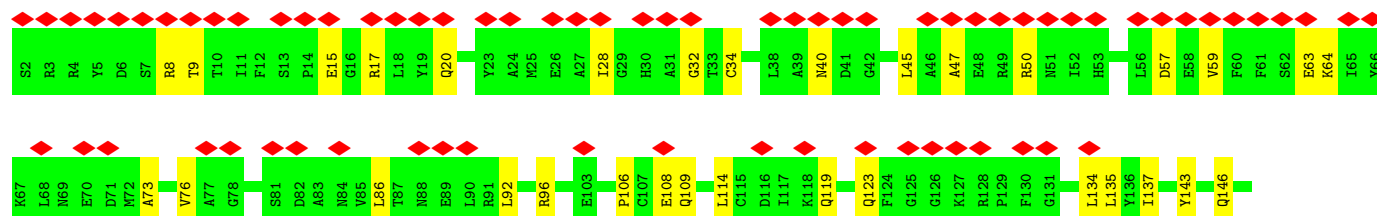
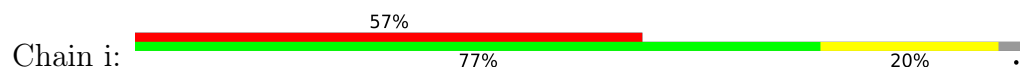
• Molecule 22: Proteasome subunit alpha type-2

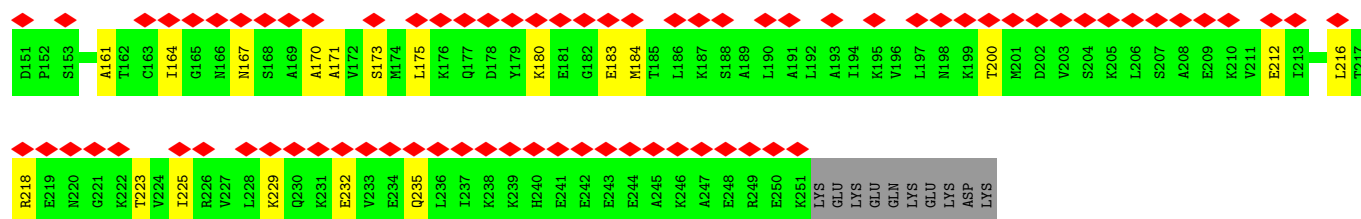


• Molecule 23: Proteasome subunit alpha type-4

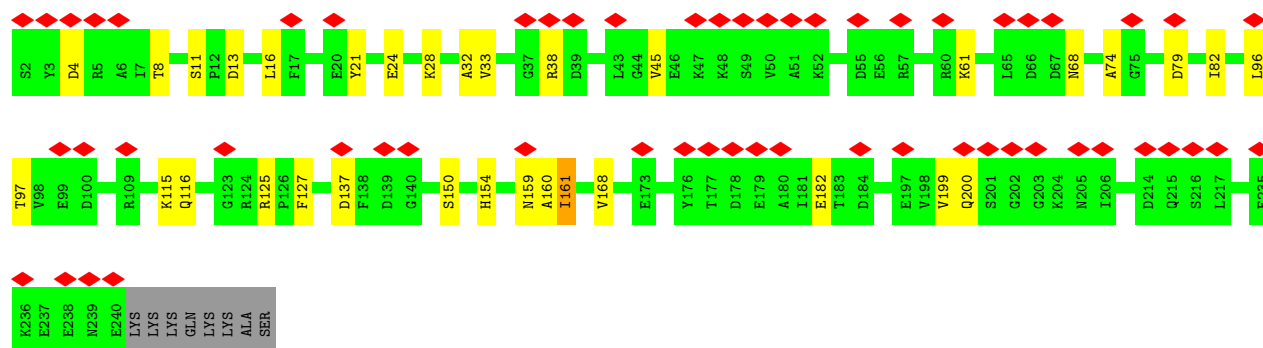
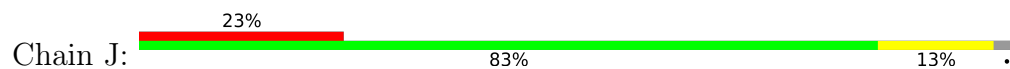


• Molecule 23: Proteasome subunit alpha type-4

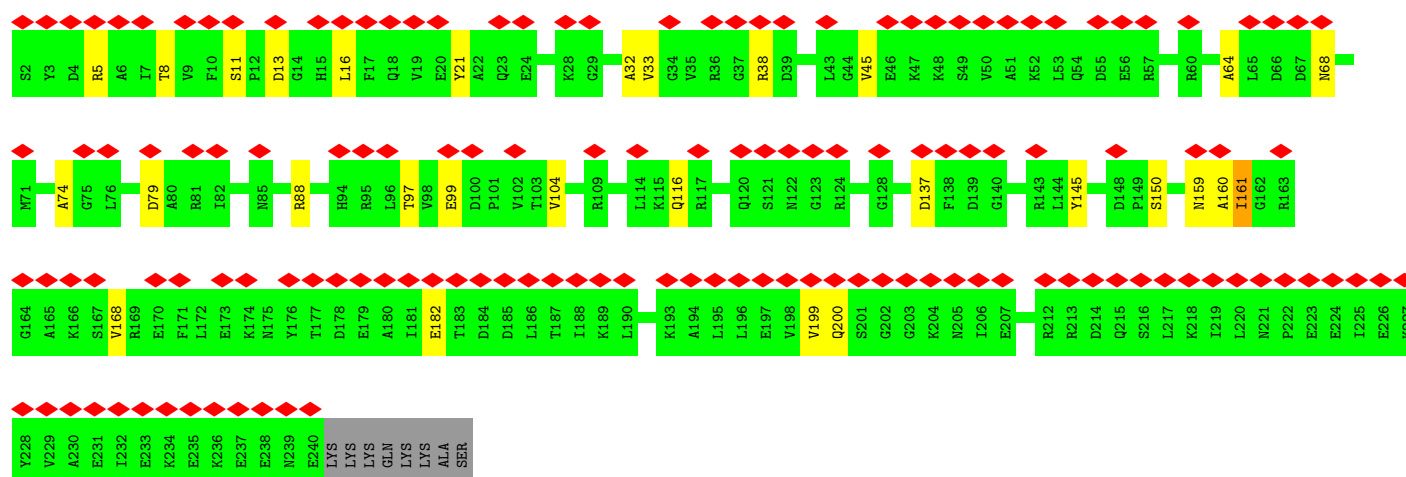
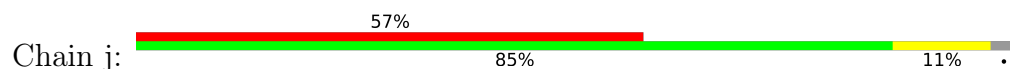




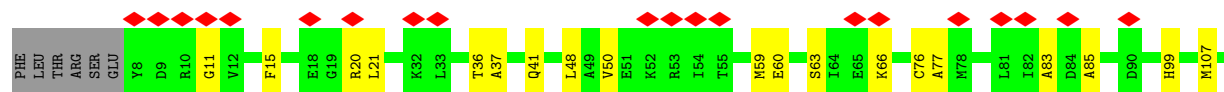
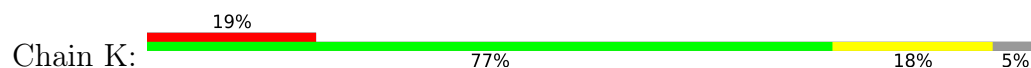
• Molecule 24: Proteasome subunit alpha type-7

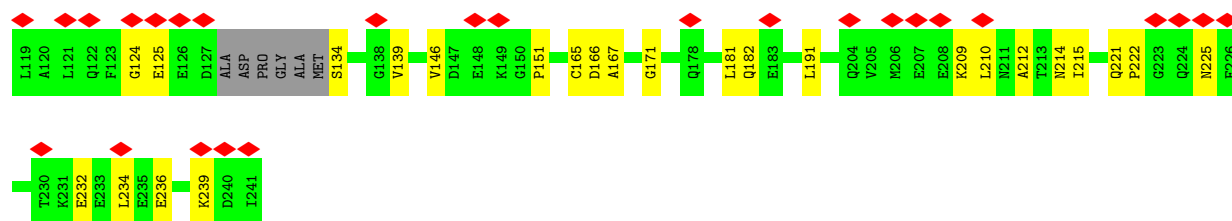


• Molecule 24: Proteasome subunit alpha type-7



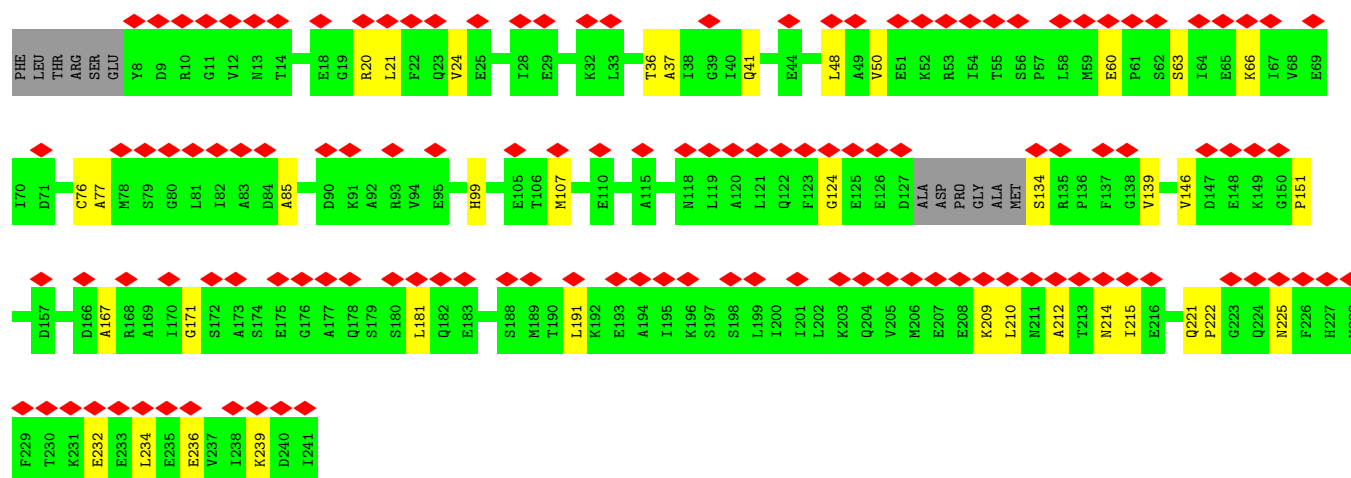
• Molecule 25: Proteasome subunit alpha type-5





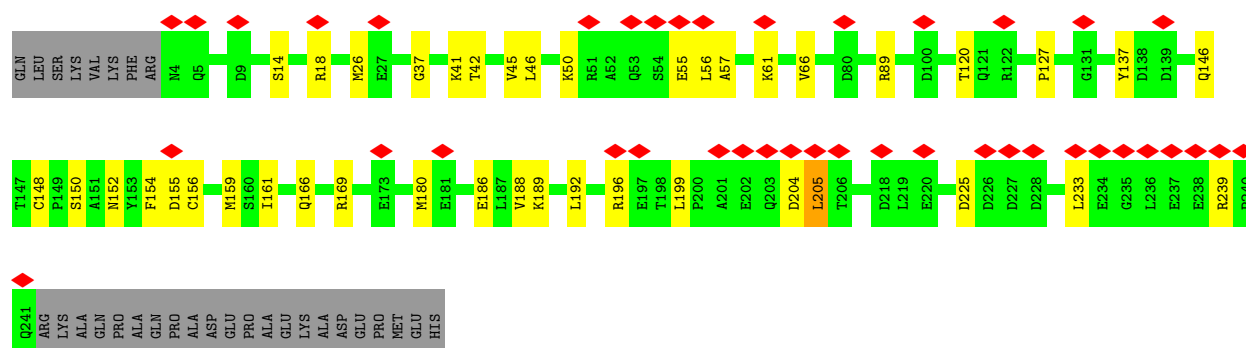
• Molecule 25: Proteasome subunit alpha type-5

Chain k: 53% 80% 15% 5%



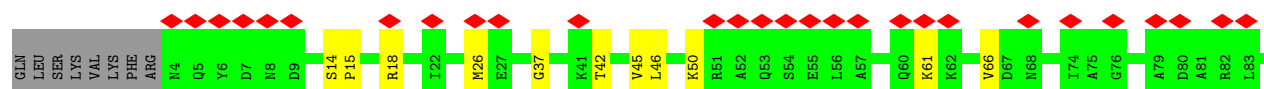
• Molecule 26: Proteasome subunit alpha type-1

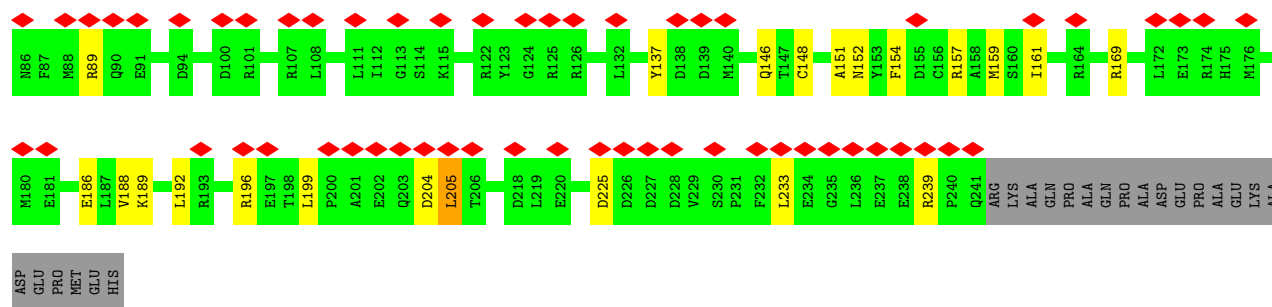
Chain L: 15% 74% 15% 11%



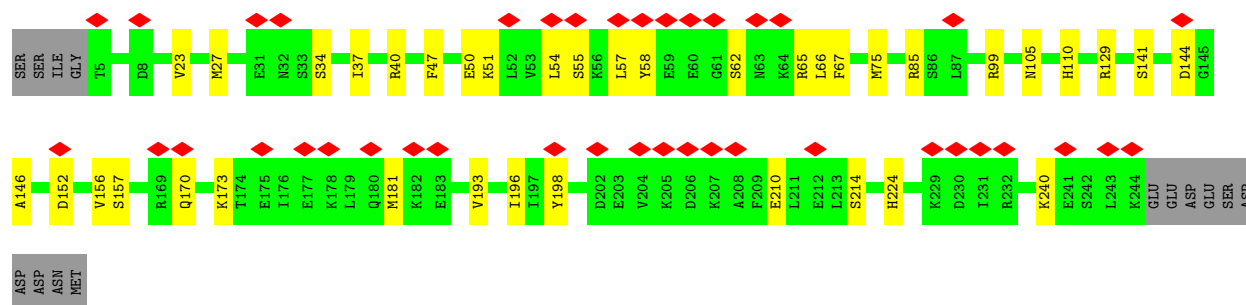
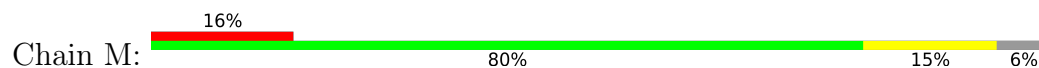
• Molecule 26: Proteasome subunit alpha type-1

Chain I: 32% 76% 12% 11%

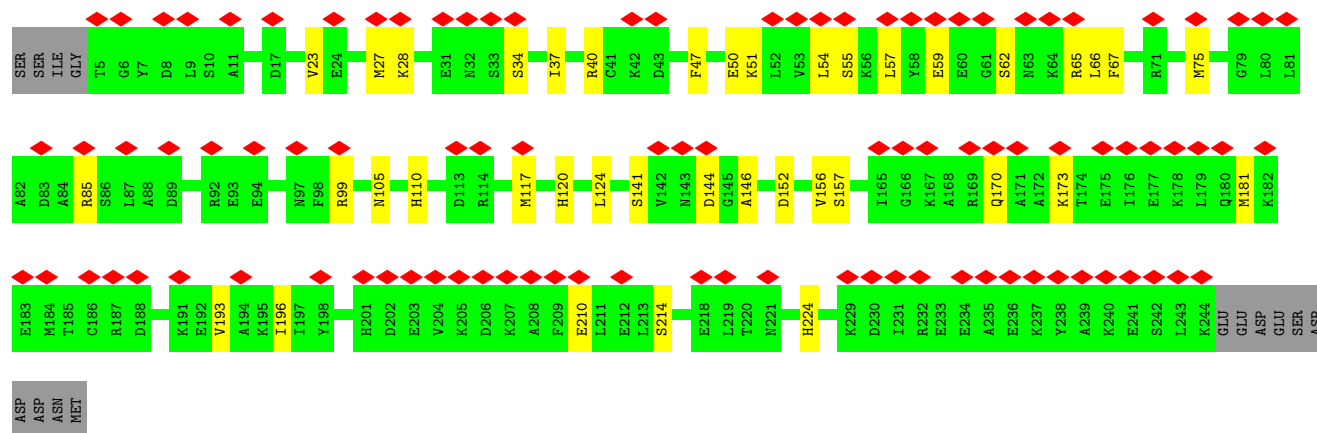
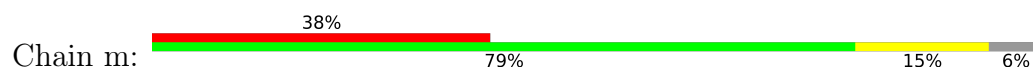




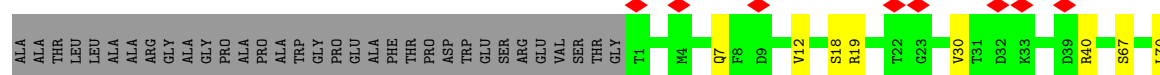
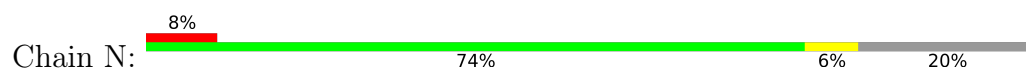
• Molecule 27: Proteasome subunit alpha type-3

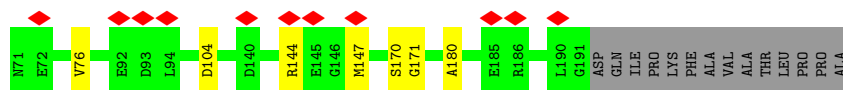


• Molecule 27: Proteasome subunit alpha type-3

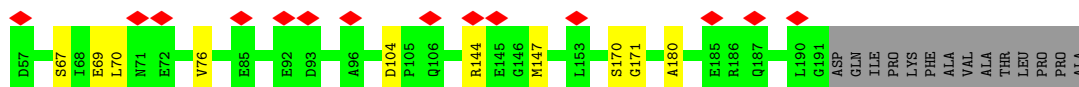


• Molecule 28: Proteasome subunit beta type-6

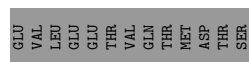
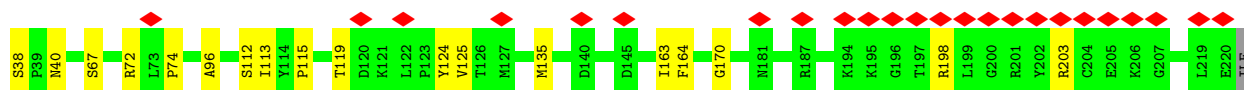
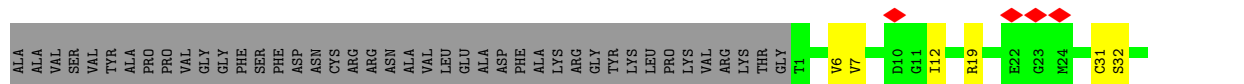




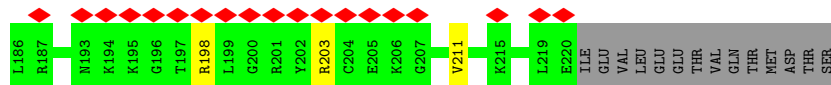
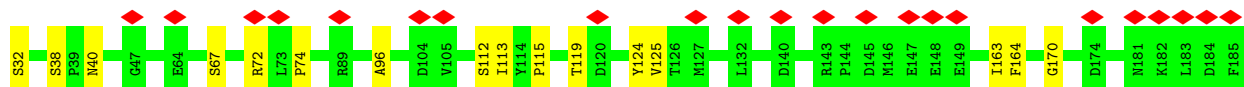
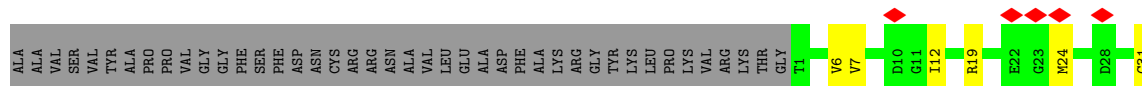
- Molecule 28: Proteasome subunit beta type-6



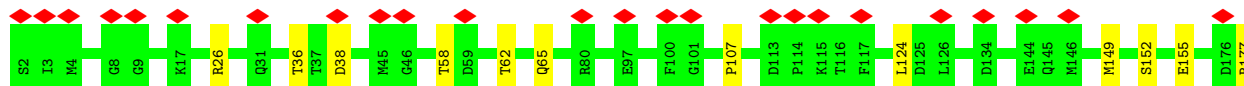
- Molecule 29: Proteasome subunit beta type-7



- Molecule 29: Proteasome subunit beta type-7

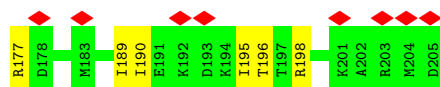
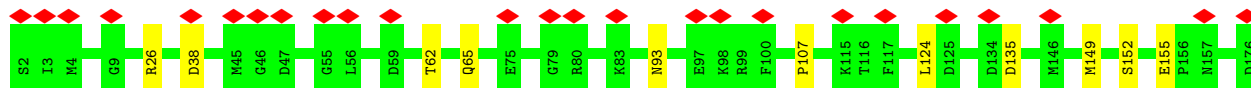
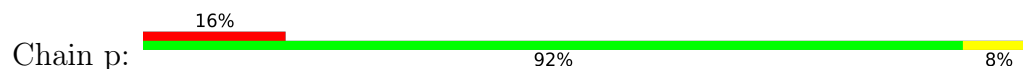


- Molecule 30: Proteasome subunit beta type-3

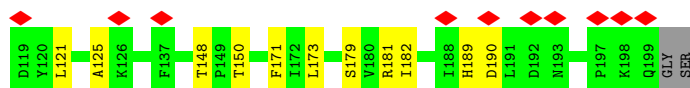
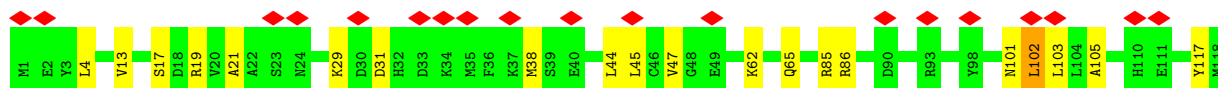
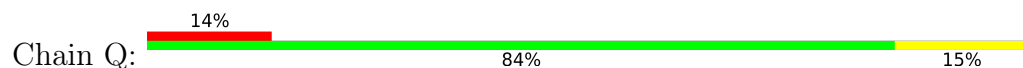




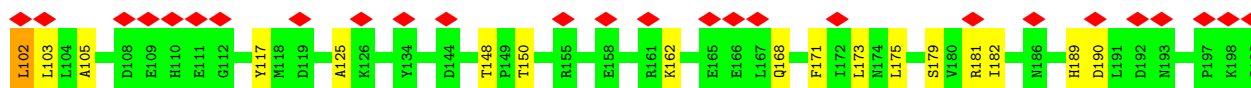
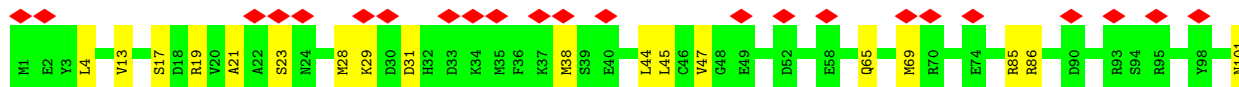
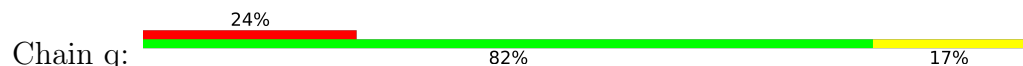
- Molecule 30: Proteasome subunit beta type-3



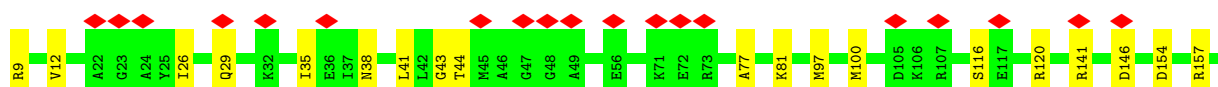
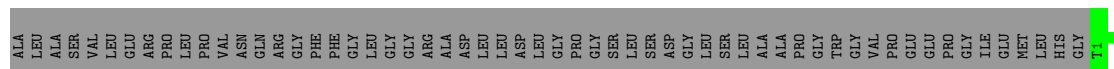
- Molecule 31: Proteasome subunit beta type-2

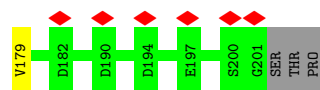


- Molecule 31: Proteasome subunit beta type-2

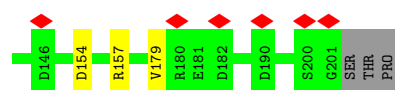
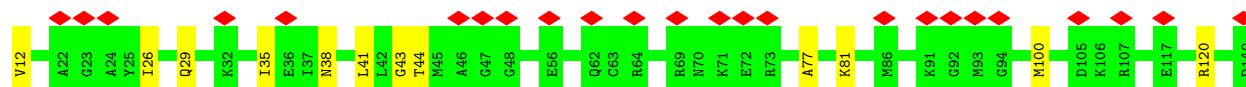
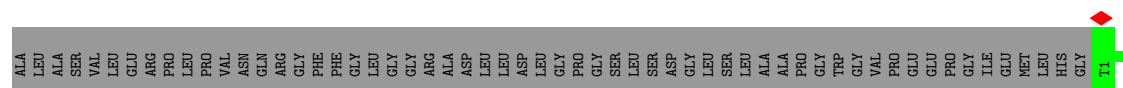


- Molecule 32: Proteasome subunit beta type-5

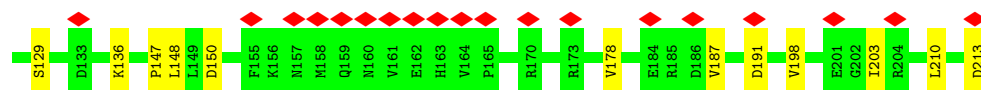
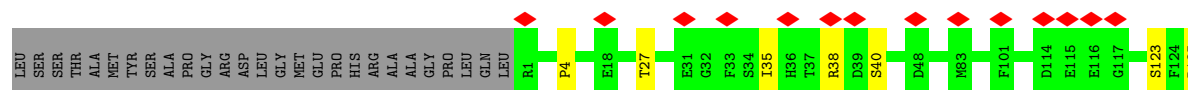
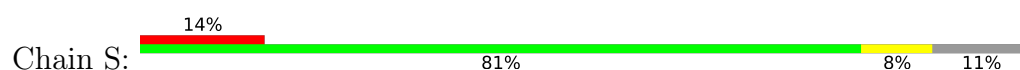




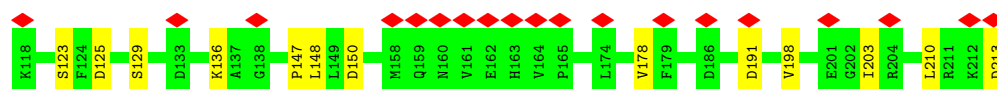
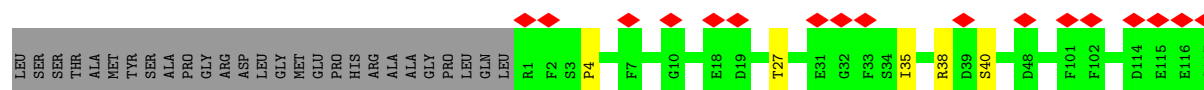
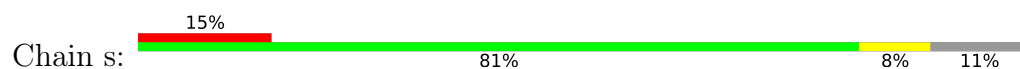
- Molecule 32: Proteasome subunit beta type-5



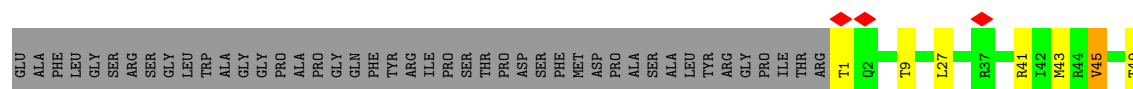
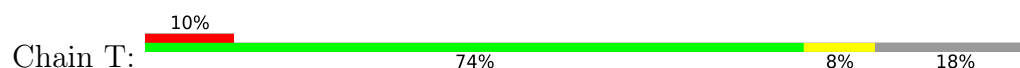
- Molecule 33: Proteasome subunit beta type-1

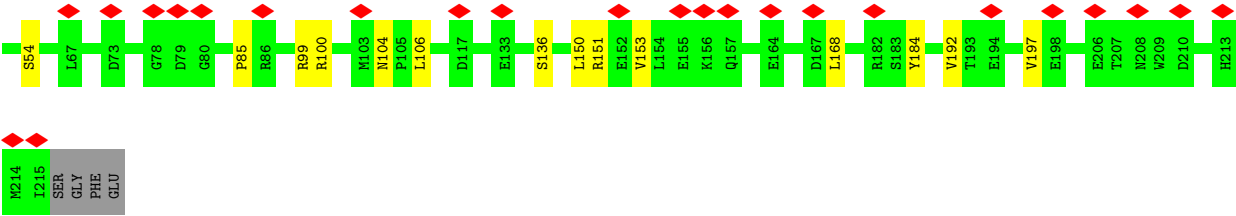


- Molecule 33: Proteasome subunit beta type-1

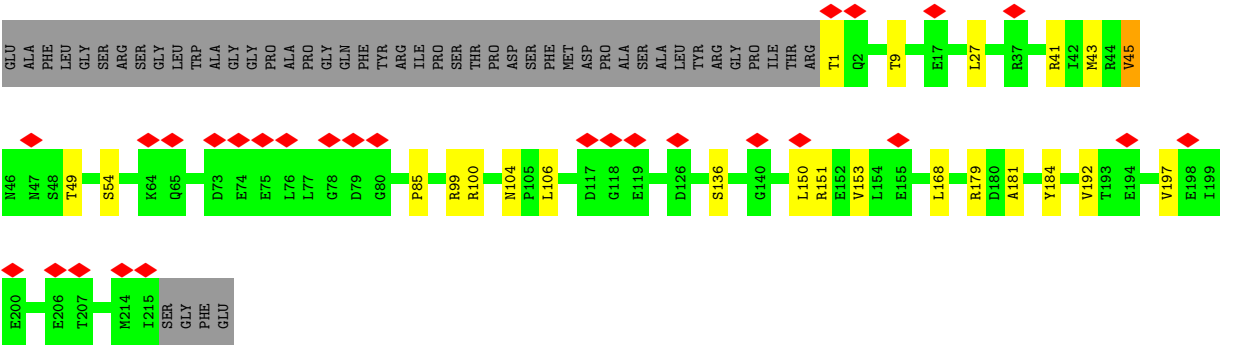


- Molecule 34: Proteasome subunit beta type-4





• Molecule 34: 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	242965	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	0.016	Depositor
Minimum map value	-0.004	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: ATP, MG, ADP, ZN

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	0.22	0/6449	0.55	3/8729 (0.0%)
2	V	0.30	1/3929 (0.0%)	0.73	1/5309 (0.0%)
3	W	0.25	0/3751	0.65	2/5042 (0.0%)
4	X	0.21	0/3053	0.50	0/4115
5	Y	0.59	8/3173 (0.3%)	0.98	23/4273 (0.5%)
6	Z	0.25	0/2324	0.68	0/3150
7	a	0.25	0/3053	0.64	3/4133 (0.1%)
8	b	0.23	0/1478	0.61	0/2001
9	c	0.27	0/2302	0.65	0/3110
10	d	0.25	0/2162	0.62	0/2919
11	e	1.12	3/338 (0.9%)	2.24	15/450 (3.3%)
12	f	0.28	0/6980	0.75	8/9433 (0.1%)
13	A	0.26	0/3117	0.64	0/4207
14	B	0.26	0/3131	0.58	0/4227
15	C	0.24	0/3017	0.65	3/4058 (0.1%)
16	D	0.26	0/3089	0.55	0/4168
17	E	0.26	0/3145	0.55	0/4233
18	F	0.28	1/3292 (0.0%)	0.53	0/4435
19	u	0.26	0/609	0.65	2/819 (0.2%)
20	v	0.02	0/8	0.05	0/8
21	G	0.23	0/1859	0.51	0/2523
21	g	0.23	0/1859	0.51	0/2523
22	H	0.24	0/1743	0.48	0/2372
22	h	0.24	0/1743	0.48	0/2372
23	I	0.22	0/1942	0.51	0/2628
23	i	0.22	0/1942	0.52	0/2628
24	J	0.22	0/1728	0.54	1/2358 (0.0%)
24	j	0.22	0/1728	0.54	1/2358 (0.0%)
25	K	0.22	0/1747	0.48	0/2364
25	k	0.22	0/1747	0.48	0/2364
26	L	0.26	0/1885	0.55	0/2552
26	l	0.26	0/1885	0.55	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	M	0.24	0/1891	0.54	0/2552
27	m	0.24	0/1891	0.54	0/2552
28	N	0.21	0/1454	0.41	0/1967
28	n	0.21	0/1454	0.41	0/1967
29	O	0.22	0/1670	0.40	0/2265
29	o	0.22	0/1670	0.40	0/2265
30	P	0.22	0/1614	0.41	0/2177
30	p	0.22	0/1614	0.41	0/2177
31	Q	0.26	0/1603	0.51	0/2174
31	q	0.26	0/1603	0.51	0/2174
32	R	0.22	0/1579	0.36	0/2134
32	r	0.22	0/1579	0.36	0/2134
33	S	0.22	0/1671	0.40	0/2253
33	s	0.22	0/1671	0.40	0/2253
34	T	0.23	0/1700	0.43	0/2305
34	t	0.23	0/1700	0.43	0/2305
All	All	0.27	13/106572 (0.0%)	0.59	62/144067 (0.0%)

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	1
2	V	0	3
3	W	0	2
5	Y	0	12
6	Z	0	2
7	a	0	1
8	b	0	2
9	c	0	2
10	d	0	2
11	e	0	5
12	f	0	11
13	A	0	3
14	B	0	1
15	C	0	3
16	D	0	6
18	F	0	2
21	G	0	1
21	g	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	J	0	1
24	j	0	1
25	K	0	1
25	k	0	1
34	T	0	1
34	t	0	1
All	All	0	66

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	184	GLN	CA-C	10.26	1.65	1.52
5	Y	184	GLN	N-CA	8.23	1.54	1.46
5	Y	186	LEU	CA-C	7.89	1.60	1.52
5	Y	185	GLY	CA-C	7.88	1.62	1.51
11	e	64	GLY	CA-C	6.56	1.61	1.51
5	Y	292	TYR	CA-CB	6.52	1.60	1.52
5	Y	291	HIS	C-N	6.36	1.41	1.33
5	Y	289	ALA	C-N	6.04	1.48	1.33
11	e	64	GLY	N-CA	6.03	1.54	1.45
5	Y	185	GLY	N-CA	5.97	1.54	1.45
18	F	86	LEU	C-N	5.79	1.39	1.33
2	V	471	GLU	C-N	5.23	1.40	1.34
11	e	63	HIS	CA-C	5.13	1.59	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	185	GLY	CA-C-N	14.68	144.78	122.17
5	Y	185	GLY	C-N-CA	14.68	144.78	122.17
11	e	63	HIS	CA-C-N	13.50	147.86	121.41
11	e	63	HIS	C-N-CA	13.50	147.86	121.41
11	e	63	HIS	CB-CA-C	12.66	135.61	110.42
5	Y	292	TYR	CA-CB-CG	11.22	134.09	113.90
11	e	63	HIS	N-CA-CB	-11.17	91.61	110.49
11	e	63	HIS	CA-CB-CG	11.17	124.97	113.80
11	e	57	ARG	CG-CD-NE	10.19	134.41	112.00
5	Y	291	HIS	N-CA-C	9.52	131.07	110.80
11	e	53	SER	N-CA-C	9.01	127.49	114.16
19	u	75	GLY	CA-C-N	-8.36	106.65	121.70
19	u	75	GLY	C-N-CA	-8.36	106.65	121.70
1	U	472	ILE	N-CA-C	-7.90	105.79	113.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	j	21	TYR	N-CA-C	-7.38	105.19	114.56
24	J	21	TYR	N-CA-C	-7.35	105.22	114.56
5	Y	185	GLY	N-CA-C	7.33	130.56	113.18
5	Y	189	VAL	N-CA-C	7.04	116.46	106.53
11	e	64	GLY	O-C-N	-6.97	113.64	122.70
5	Y	292	TYR	N-CA-CB	6.94	121.46	110.49
5	Y	184	GLN	CA-C-N	6.93	135.00	121.41
5	Y	184	GLN	C-N-CA	6.93	135.00	121.41
1	U	873	PRO	CA-C-N	6.93	134.77	121.54
1	U	873	PRO	C-N-CA	6.93	134.77	121.54
5	Y	191	ILE	CA-C-N	6.84	130.70	120.17
5	Y	191	ILE	C-N-CA	6.84	130.70	120.17
11	e	64	GLY	N-CA-C	6.63	128.90	113.18
5	Y	187	TYR	CA-C-N	6.61	134.16	121.54
5	Y	187	TYR	C-N-CA	6.61	134.16	121.54
5	Y	290	PRO	N-CA-C	6.60	126.07	112.47
15	C	285	ALA	CA-C-N	6.25	133.47	121.54
15	C	285	ALA	C-N-CA	6.25	133.47	121.54
5	Y	184	GLN	N-CA-C	5.99	122.65	113.19
11	e	65	TYR	CB-CA-C	-5.78	98.92	110.42
5	Y	186	LEU	N-CA-C	5.78	119.86	112.12
11	e	65	TYR	N-CA-C	5.77	123.09	110.80
12	f	874	LEU	CA-C-N	-5.76	115.58	122.44
12	f	874	LEU	C-N-CA	-5.76	115.58	122.44
15	C	147	THR	N-CA-C	-5.73	100.34	109.96
5	Y	186	LEU	CA-CB-CG	5.71	136.28	116.30
12	f	875	ALA	CA-C-N	5.71	132.44	121.54
12	f	875	ALA	C-N-CA	5.71	132.44	121.54
5	Y	289	ALA	N-CA-C	5.67	122.35	109.81
5	Y	187	TYR	N-CA-C	5.58	118.92	107.69
11	e	49	GLU	CA-C-O	-5.50	114.14	120.24
11	e	65	TYR	CA-CB-CG	5.47	123.75	113.90
7	a	374	ILE	N-CA-C	-5.45	107.51	112.96
7	a	165	THR	CA-C-N	5.44	128.20	120.53
7	a	165	THR	C-N-CA	5.44	128.20	120.53
12	f	868	HIS	CA-C-N	5.33	131.71	121.54
12	f	868	HIS	C-N-CA	5.33	131.71	121.54
5	Y	186	LEU	CB-CA-C	-5.32	102.42	111.26
5	Y	291	HIS	CA-C-N	-5.32	114.34	122.21
5	Y	291	HIS	C-N-CA	-5.32	114.34	122.21
11	e	66	LYS	N-CA-C	5.28	118.01	109.83
12	f	822	VAL	CA-C-N	5.28	131.62	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	f	822	VAL	C-N-CA	5.28	131.62	121.54
3	W	90	LEU	CA-C-N	5.20	131.48	121.54
3	W	90	LEU	C-N-CA	5.20	131.48	121.54
2	V	27	PRO	N-CA-C	5.19	117.03	110.70
11	e	56	LEU	CA-CB-CG	5.17	134.39	116.30
5	Y	190	ALA	CB-CA-C	-5.07	104.55	112.31

There are no chirality outliers.

All (66) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	A	115	VAL	Peptide
13	A	345	LEU	Peptide
13	A	39	SER	Peptide
14	B	116	ILE	Peptide
15	C	146	SER	Peptide
15	C	287	LYS	Peptide
15	C	89	VAL	Peptide
16	D	125	LYS	Peptide
16	D	126	PRO	Peptide
16	D	258	ALA	Peptide
16	D	273	LYS	Peptide
16	D	408	LYS	Peptide
16	D	85	ILE	Peptide
18	F	343	LEU	Peptide
18	F	344	ARG	Peptide
21	G	222	VAL	Peptide
24	J	199	VAL	Peptide
25	K	232	GLU	Peptide
34	T	45	VAL	Peptide
1	U	873	PRO	Peptide
2	V	264	TYR	Peptide
2	V	344	ASP	Peptide
2	V	82	LEU	Peptide
3	W	137	TYR	Peptide
3	W	313	GLU	Peptide
5	Y	173	ASP	Peptide
5	Y	179	ARG	Peptide
5	Y	180	LEU	Peptide
5	Y	181	LYS	Peptide
5	Y	185	GLY	Peptide
5	Y	187	TYR	Peptide

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Mol	Chain	Res	Type	Group
5	Y	293	ARG	Peptide
5	Y	294	TYR	Peptide
5	Y	349	LYS	Peptide
5	Y	51	ALA	Peptide
5	Y	62	ASP	Peptide
5	Y	87	GLU	Peptide
6	Z	225	GLN	Peptide
6	Z	239	ASP	Peptide
7	a	164	GLN	Peptide
8	b	149	ASN	Peptide
8	b	21	PHE	Peptide
9	c	185	ASN	Peptide
9	c	266	THR	Peptide
10	d	198	LEU	Peptide
10	d	201	ASN	Peptide
11	e	4	LYS	Peptide
11	e	43	TRP	Peptide
11	e	55	GLN	Peptide
11	e	60	LEU	Peptide
11	e	62	LYS	Peptide
12	f	340	MET	Peptide
12	f	620	PHE	Peptide
12	f	642	ALA	Peptide
12	f	712	LYS	Peptide
12	f	737	ASN	Peptide
12	f	755	ASP	Peptide
12	f	807	ARG	Peptide
12	f	816	TYR	Peptide
12	f	822	VAL	Peptide
12	f	854	GLY	Peptide
12	f	875	ALA	Peptide
21	g	222	VAL	Peptide
24	j	199	VAL	Peptide
25	k	232	GLU	Peptide
34	t	45	VAL	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	6334	0	6366	97	0
2	V	3852	0	3893	99	0
3	W	3703	0	3822	73	0
4	X	3009	0	3113	22	0
5	Y	3115	0	3120	102	0
6	Z	2281	0	2312	28	0
7	a	2995	0	3012	42	0
8	b	1458	0	1505	28	0
9	c	2260	0	2276	39	0
10	d	2116	0	2146	39	0
11	e	334	0	294	51	0
12	f	6866	0	6866	154	0
13	A	3067	0	3100	56	0
14	B	3086	0	3134	46	0
15	C	2978	0	3075	51	0
16	D	3039	0	3075	43	0
17	E	3097	0	3174	65	0
18	F	3251	0	3318	58	0
19	u	603	0	629	14	0
20	v	143	0	44	1	0
21	G	1826	0	1796	16	0
21	g	1826	0	1796	19	0
22	H	1708	0	1594	17	0
22	h	1708	0	1594	16	0
23	I	1912	0	1851	30	0
23	i	1912	0	1851	29	0
24	J	1704	0	1517	22	0
24	j	1704	0	1517	16	0
25	K	1722	0	1673	29	0
25	k	1722	0	1673	20	0
26	L	1850	0	1822	31	0
26	l	1850	0	1822	22	0
27	M	1856	0	1814	26	0
27	m	1856	0	1814	28	0
28	N	1430	0	1398	10	0
28	n	1430	0	1398	9	0
29	O	1643	0	1644	15	0
29	o	1643	0	1644	16	0
30	P	1585	0	1598	12	0
30	p	1585	0	1598	13	0
31	Q	1570	0	1547	19	0
31	q	1570	0	1547	22	0
32	R	1548	0	1499	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	r	1548	0	1499	8	0
33	S	1641	0	1618	15	0
33	s	1641	0	1618	13	0
34	T	1667	0	1628	15	0
34	t	1667	0	1628	16	0
35	c	1	0	0	0	0
36	A	31	0	12	1	0
36	D	31	0	12	2	0
36	F	31	0	12	0	0
37	A	1	0	0	0	0
37	D	1	0	0	0	0
37	F	1	0	0	0	0
38	B	27	0	12	3	0
38	E	27	0	12	2	0
All	All	105062	0	104332	1392	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 7.

All (1392) 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:206:LYS:HE2	18:F:263:ASP:OD2	1.62	0.97
17:E:206:LYS:HE3	18:F:263:ASP:OD1	1.65	0.96
17:E:206:LYS:CE	18:F:263:ASP:OD1	2.30	0.79
5:Y:177:ARG:HA	5:Y:180:LEU:HB2	1.68	0.76
5:Y:184:GLN:HB2	11:e:66:LYS:HB3	1.67	0.75
2:V:432:GLU:HB2	11:e:6:GLN:HB3	1.70	0.73
2:V:266:GLN:HG3	2:V:269:LYS:HZ3	1.54	0.73
17:E:205:ASP:O	18:F:261:ILE:CD1	2.38	0.72
23:i:143:TYR:HB2	23:i:146:GLN:HE21	1.55	0.72
5:Y:186:LEU:N	11:e:64:GLY:H	1.88	0.71
3:W:293:ASP:HB3	3:W:296:LEU:HB2	1.73	0.70
23:I:143:TYR:HB2	23:I:146:GLN:HE21	1.55	0.70
11:e:45:ASP:HA	11:e:48:VAL:HB	1.73	0.70
15:C:139:MET:HE2	15:C:215:SER:H	1.57	0.70
3:W:41:GLN:HG3	3:W:92:LYS:HD2	1.74	0.69
17:E:205:ASP:O	18:F:261:ILE:HD11	1.93	0.69
17:E:206:LYS:HE2	18:F:263:ASP:CG	2.18	0.69
2:V:285:TRP:HD1	2:V:315:LYS:HE2	1.58	0.68
24:j:38:ARG:HH12	24:j:182:GLU:HA	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:238:LYS:HD3	17:E:207:TYR:CD1	2.28	0.68
12:f:276:GLU:O	12:f:286:LYS:NZ	2.25	0.68
12:f:829:MET:H	12:f:845:ARG:HB3	1.58	0.68
3:W:135:LYS:HD3	3:W:144:ARG:HE	1.57	0.68
12:f:704:LEU:HA	12:f:707:LEU:HB2	1.74	0.68
1:U:337:LEU:HD21	1:U:789:ILE:HG21	1.77	0.67
5:Y:182:VAL:HG13	5:Y:186:LEU:HD13	1.74	0.67
12:f:571:GLU:HG3	12:f:573:ILE:H	1.58	0.67
12:f:673:ARG:HH22	12:f:709:THR:HA	1.60	0.67
2:V:79:VAL:HG13	2:V:81:GLN:H	1.60	0.67
15:C:227:GLY:HA2	15:C:230:MET:HE2	1.75	0.67
24:J:38:ARG:HH12	24:J:182:GLU:HA	1.59	0.67
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.77	0.67
24:J:68:ASN:HD21	24:J:137:ASP:HA	1.60	0.67
15:C:340:ARG:NH1	15:C:342:ILE:O	2.29	0.66
2:V:91:PRO:HG3	2:V:124:ASN:HB2	1.77	0.66
16:D:248:ARG:HG2	16:D:295:GLN:HE22	1.61	0.66
13:A:114:ASN:HB3	13:A:120:LYS:HG2	1.77	0.66
2:V:345:ARG:HH22	2:V:353:LEU:HD11	1.61	0.66
4:X:297:ARG:HH11	4:X:337:ARG:HH21	1.44	0.66
15:C:262:GLY:HA2	15:C:270:GLN:HE22	1.58	0.66
3:W:340:VAL:HA	3:W:350:ARG:HH11	1.60	0.66
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.76	0.66
24:J:4:ASP:HB3	25:K:125:GLU:HB3	1.79	0.65
14:B:313:LEU:O	14:B:346:ARG:NH1	2.29	0.65
24:j:68:ASN:HD21	24:j:137:ASP:HA	1.60	0.65
5:Y:287:LEU:HD12	11:e:57:ARG:H	1.61	0.65
2:V:365:GLN:HE21	11:e:41:ASP:H	1.44	0.65
5:Y:292:TYR:HB3	11:e:55:GLN:H	1.62	0.65
12:f:340:MET:SD	12:f:757:ASN:ND2	2.70	0.65
5:Y:287:LEU:HB2	11:e:57:ARG:HB2	1.79	0.65
19:u:72:ARG:HD3	19:u:74:ARG:HD2	1.78	0.65
12:f:586:PRO:HA	12:f:589:SER:HB2	1.78	0.64
2:V:255:LEU:HD22	2:V:291:TYR:HB3	1.80	0.64
5:Y:184:GLN:N	11:e:64:GLY:O	2.29	0.64
12:f:127:SER:HA	12:f:131:MET:HB2	1.79	0.64
17:E:206:LYS:CE	18:F:263:ASP:CG	2.70	0.64
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.31	0.64
13:A:277:ILE:HG22	13:A:280:ILE:HD12	1.80	0.64
17:E:198:VAL:HG12	17:E:200:SER:H	1.61	0.64
23:I:34:CYS:HB2	23:I:164:ILE:HD12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:218:ARG:NH1	23:i:223:THR:OG1	2.31	0.64
3:W:169:LEU:O	3:W:182:ARG:NH1	2.31	0.64
13:A:365:GLU:HB3	13:A:406:GLU:HG2	1.80	0.64
1:U:804:SER:HA	1:U:892:LEU:HA	1.79	0.63
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.80	0.63
23:I:218:ARG:NH1	23:I:223:THR:OG1	2.31	0.63
3:W:347:GLY:O	3:W:351:TRP:N	2.30	0.63
27:M:55:SER:H	27:M:57:LEU:HD23	1.64	0.63
23:i:8:ARG:HE	24:j:5:ARG:HH21	1.46	0.62
27:m:55:SER:H	27:m:57:LEU:HD23	1.64	0.62
13:A:99:THR:HG22	13:A:115:VAL:HA	1.81	0.62
13:A:258:ARG:HG3	13:A:305:GLN:HE22	1.63	0.62
27:M:214:SER:OG	27:M:224:HIS:NE2	2.31	0.62
18:F:224:LEU:HB2	18:F:348:LEU:HD23	1.80	0.62
1:U:642:GLU:O	15:C:53:ASN:ND2	2.33	0.62
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.82	0.62
34:T:192:VAL:HG12	34:T:197:VAL:HG22	1.82	0.62
2:V:495:ARG:HB2	15:C:44:ARG:HG3	1.80	0.62
13:A:72:LEU:HD11	14:B:103:ARG:HH22	1.63	0.62
6:Z:187:LEU:HD23	9:c:293:THR:HG22	1.82	0.62
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.81	0.62
19:u:23:ILE:HB	19:u:52:ASP:HA	1.81	0.62
23:i:34:CYS:HB2	23:i:164:ILE:HD12	1.80	0.62
2:V:214:HIS:HE1	2:V:227:VAL:HG21	1.65	0.62
3:W:136:ILE:HG13	3:W:143:ALA:HB3	1.80	0.62
5:Y:179:ARG:HB3	5:Y:182:VAL:HG23	1.81	0.61
34:t:192:VAL:HG12	34:t:197:VAL:HG22	1.82	0.61
26:L:186:GLU:HA	26:L:189:LYS:HG2	1.83	0.61
1:U:465:LEU:HD11	1:U:477:GLY:HA3	1.82	0.61
12:f:171:GLN:HG3	12:f:179:VAL:HG22	1.83	0.61
18:F:295:ARG:HH22	18:F:311:LEU:HD21	1.63	0.61
26:l:186:GLU:HA	26:l:189:LYS:HG2	1.83	0.61
18:F:175:MET:HA	18:F:250:LYS:HE3	1.83	0.61
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.83	0.60
2:V:423:ALA:HB2	2:V:434:ALA:HB2	1.83	0.60
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.83	0.60
12:f:875:ALA:O	12:f:876:HIS:ND1	2.34	0.60
1:U:11:LEU:HD13	1:U:26:LYS:HD2	1.83	0.60
5:Y:183:TYR:N	11:e:64:GLY:O	2.34	0.60
2:V:359:PRO:HG2	2:V:385:LYS:HG2	1.83	0.60
5:Y:187:TYR:HA	11:e:63:HIS:CG	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:111:ARG:HB3	10:d:114:GLU:HB2	1.82	0.60
12:f:441:LYS:HB2	12:f:477:MET:HE1	1.82	0.60
9:c:115:HIS:HB3	9:c:118:PHE:HB2	1.83	0.60
25:K:36:THR:HA	25:K:171:GLY:HA3	1.84	0.60
12:f:125:ILE:HD13	12:f:129:LEU:HB2	1.82	0.60
17:E:235:ILE:HD11	17:E:277:MET:HB3	1.82	0.60
12:f:556:ARG:HD3	12:f:786:GLN:HB2	1.84	0.60
13:A:41:TYR:HB2	13:A:44:GLN:HB3	1.83	0.60
1:U:149:GLN:NE2	15:C:20:LEU:O	2.33	0.60
5:Y:361:SER:O	5:Y:365:GLN:NE2	2.34	0.60
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.84	0.60
3:W:223:LYS:NZ	3:W:227:TYR:OH	2.34	0.59
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.84	0.59
3:W:312:MET:HG2	3:W:314:LEU:HA	1.84	0.59
5:Y:292:TYR:HB2	5:Y:295:TYR:H	1.66	0.59
5:Y:293:ARG:HA	11:e:52:PHE:CG	2.38	0.59
17:E:21:GLU:OE2	17:E:25:ARG:NH2	2.35	0.59
1:U:23:ALA:O	1:U:27:LEU:N	2.36	0.59
16:D:353:ASN:ND2	16:D:392:TYR:O	2.36	0.59
12:f:106:LEU:HB2	12:f:141:LYS:HD2	1.85	0.59
17:E:226:GLN:HG3	17:E:272:ARG:HD2	1.85	0.59
25:K:212:ALA:HA	25:K:234:LEU:HD22	1.85	0.59
1:U:160:LEU:HD21	1:U:196:LYS:HB3	1.85	0.59
7:a:188:LEU:HG	7:a:193:GLN:HE21	1.67	0.59
8:b:54:LEU:HD13	8:b:84:ILE:HG13	1.85	0.59
16:D:278:GLN:HE22	16:D:283:ARG:HD3	1.67	0.59
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.84	0.59
17:E:97:ARG:NH2	17:E:112:PRO:O	2.36	0.59
27:m:214:SER:OG	27:m:224:HIS:NE2	2.31	0.59
3:W:124:LEU:HD13	3:W:151:THR:HG22	1.83	0.59
15:C:321:ASN:H	15:C:324:ALA:HB3	1.66	0.59
5:Y:205:VAL:HG11	15:C:376:VAL:HG23	1.84	0.59
12:f:862:ILE:O	12:f:876:HIS:NE2	2.35	0.59
2:V:265:ASP:O	2:V:269:LYS:NZ	2.35	0.58
2:V:416:ARG:HG3	2:V:459:GLN:HB3	1.84	0.58
5:Y:29:PRO:HB2	5:Y:32:ARG:HB3	1.85	0.58
12:f:288:VAL:HA	12:f:291:GLN:HG2	1.83	0.58
12:f:378:ASN:HD21	12:f:392:THR:HG22	1.67	0.58
34:T:99:ARG:HG2	34:T:106:LEU:HG	1.84	0.58
25:k:36:THR:HA	25:k:171:GLY:HA3	1.84	0.58
2:V:92:ARG:HE	2:V:114:TYR:HB2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:416:ARG:NH1	5:Y:351:ASN:OD1	2.36	0.58
16:D:170:MET:HG2	16:D:173:GLN:HB2	1.85	0.58
16:D:352:MET:HE1	16:D:379:CYS:HB3	1.85	0.58
17:E:344:ARG:NH1	38:E:401:ADP:O3'	2.36	0.58
12:f:594:LEU:O	12:f:635:LYS:NZ	2.35	0.58
25:K:222:PRO:O	25:K:225:ASN:ND2	2.36	0.58
29:O:203:ARG:NH2	30:P:155:GLU:OE1	2.36	0.58
33:S:38:ARG:HH12	34:T:151:ARG:HD3	1.68	0.58
2:V:167:LEU:HD12	2:V:169:LEU:H	1.68	0.58
7:a:212:ASN:OD1	7:a:213:PHE:N	2.37	0.58
12:f:240:VAL:HG13	12:f:257:ARG:HE	1.67	0.58
14:B:107:MET:HB2	15:C:96:VAL:HB	1.84	0.58
25:k:222:PRO:O	25:k:225:ASN:ND2	2.36	0.58
15:C:83:LYS:HG2	15:C:105:ILE:HD11	1.85	0.58
18:F:35:LYS:HB2	18:F:38:THR:HB	1.86	0.58
7:a:140:GLU:O	7:a:143:ASN:ND2	2.37	0.58
27:m:51:LYS:NZ	27:m:62:SER:O	2.36	0.58
1:U:613:ASP:OD1	1:U:616:ARG:NH2	2.33	0.58
12:f:682:GLY:HA3	12:f:687:ARG:HH11	1.68	0.58
17:E:216:ARG:HG3	17:E:263:GLN:HE22	1.68	0.58
27:M:51:LYS:NZ	27:M:62:SER:O	2.36	0.58
3:W:276:LEU:HA	3:W:357:ARG:HG3	1.85	0.58
3:W:448:LYS:HD2	6:Z:100:LYS:HD2	1.84	0.58
4:X:122:ARG:HD2	4:X:125:LEU:HB2	1.85	0.58
29:o:203:ARG:NH2	30:p:155:GLU:OE1	2.37	0.58
2:V:128:ARG:HD3	2:V:171:VAL:HG21	1.86	0.58
2:V:470:ARG:HH12	10:d:242:LEU:HD21	1.67	0.58
7:a:278:MET:O	7:a:339:ARG:NH2	2.36	0.57
5:Y:57:LEU:HA	5:Y:63:TRP:HE1	1.69	0.57
8:b:25:ARG:NH2	8:b:145:GLU:OE1	2.31	0.57
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.69	0.57
24:j:99:GLU:OE2	32:r:81:LYS:NZ	2.37	0.57
25:k:76:CYS:SG	25:k:77:ALA:N	2.78	0.57
25:k:212:ALA:HA	25:k:234:LEU:HD22	1.85	0.57
23:I:106:PRO:HD2	23:I:109:GLN:HE21	1.69	0.57
27:M:40:ARG:NH1	27:M:146:ALA:O	2.36	0.57
1:U:798:PRO:O	1:U:880:ASN:ND2	2.37	0.57
23:I:47:ALA:HB3	23:I:212:GLU:HB3	1.86	0.57
5:Y:223:THR:HA	5:Y:226:VAL:HG12	1.87	0.57
10:d:174:ILE:HG23	11:e:2:SER:H	1.69	0.57
10:d:174:ILE:HG12	11:e:1:MET:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:e:56:LEU:HB2	11:e:59:GLU:HB3	1.86	0.57
12:f:209:MET:HG3	12:f:211:ILE:H	1.70	0.57
14:B:230:THR:HG21	14:B:353:PHE:HB3	1.86	0.57
17:E:199:VAL:HG23	17:E:201:SER:H	1.69	0.57
34:t:99:ARG:HG2	34:t:106:LEU:HG	1.85	0.57
1:U:13:ASP:OD1	1:U:44:LYS:NZ	2.38	0.57
25:K:76:CYS:SG	25:K:77:ALA:N	2.78	0.57
33:S:38:ARG:NH2	29:o:164:PHE:O	2.37	0.57
25:k:41:GLN:NE2	25:k:151:PRO:O	2.37	0.57
10:d:122:LEU:HB3	10:d:125:LYS:HB2	1.86	0.57
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.86	0.57
28:N:40:ARG:NH1	28:N:180:ALA:O	2.37	0.57
13:A:56:LEU:HD12	14:B:72:LEU:HD21	1.85	0.57
18:F:113:LEU:HD13	18:F:117:ARG:HH12	1.69	0.57
21:g:144:ASP:HB3	21:g:147:GLN:HB2	1.86	0.57
4:X:90:ARG:HH21	4:X:125:LEU:HA	1.70	0.57
13:A:210:LYS:HB3	13:A:312:ARG:HH21	1.70	0.57
17:E:205:ASP:OD2	17:E:210:GLU:HB3	2.05	0.57
5:Y:289:ALA:O	11:e:57:ARG:NH1	2.38	0.57
12:f:171:GLN:HE21	12:f:179:VAL:HG13	1.70	0.56
10:d:131:VAL:HA	10:d:134:LYS:HB3	1.88	0.56
23:i:47:ALA:HB3	23:i:212:GLU:HB3	1.86	0.56
28:n:40:ARG:NH1	28:n:180:ALA:O	2.37	0.56
1:U:559:ARG:HB3	1:U:562:GLU:HB2	1.86	0.56
4:X:87:ARG:HH11	22:H:231:ALA:HB2	1.70	0.56
4:X:406:ASN:HA	4:X:409:LYS:HZ1	1.69	0.56
5:Y:220:VAL:HG11	5:Y:249:VAL:HG21	1.85	0.56
10:d:140:GLU:HA	10:d:143:LEU:HB2	1.87	0.56
15:C:132:ASP:O	15:C:136:SER:N	2.39	0.56
21:G:144:ASP:HB3	21:G:147:GLN:HB2	1.86	0.56
25:K:41:GLN:NE2	25:K:151:PRO:O	2.37	0.56
25:K:236:GLU:HA	25:K:239:LYS:HE3	1.86	0.56
2:V:33:GLN:HE21	2:V:85:ALA:HA	1.70	0.56
12:f:110:TYR:OH	12:f:118:ASN:ND2	2.38	0.56
12:f:378:ASN:OD1	12:f:382:ASN:ND2	2.38	0.56
21:G:159:TYR:HB3	22:H:81:PRO:HG3	1.86	0.56
22:H:118:MET:HE2	22:H:151:PRO:HA	1.88	0.56
24:j:74:ALA:HB2	24:j:161:ILE:HD13	1.87	0.56
1:U:19:LEU:O	1:U:23:ALA:N	2.38	0.56
10:d:32:GLU:OE1	10:d:47:GLN:NE2	2.37	0.56
15:C:185:GLY:HA3	15:C:311:ILE:HG22	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:106:PRO:HD2	23:i:109:GLN:HE21	1.69	0.56
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.87	0.56
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.39	0.56
9:c:136:LEU:HD11	19:u:7:THR:HG21	1.88	0.56
27:m:40:ARG:NH1	27:m:146:ALA:O	2.36	0.56
3:W:308:LEU:O	3:W:361:HIS:NE2	2.39	0.56
5:Y:240:VAL:HG23	5:Y:241:ILE:HG13	1.88	0.56
10:d:188:LYS:HD2	10:d:221:ASN:HD21	1.71	0.56
31:Q:117:TYR:HB3	31:Q:125:ALA:HB3	1.88	0.56
25:K:166:ASP:HB2	26:L:56:LEU:HB2	1.88	0.56
25:k:236:GLU:HA	25:k:239:LYS:HE3	1.86	0.56
30:p:65:GLN:OE1	31:q:86:ARG:NH2	2.39	0.56
1:U:770:TRP:O	9:c:177:THR:OG1	2.24	0.56
8:b:51:LEU:HD11	8:b:61:LEU:HB2	1.87	0.56
1:U:245:ALA:O	1:U:324:LYS:NZ	2.39	0.56
12:f:198:HIS:O	12:f:202:HIS:N	2.39	0.56
13:A:112:ILE:HG12	13:A:122:VAL:HG22	1.87	0.56
22:H:222:THR:OG1	22:H:225:GLU:OE1	2.24	0.56
22:h:118:MET:HE2	22:h:151:PRO:HA	1.88	0.56
1:U:177:LEU:O	1:U:205:TYR:OH	2.24	0.55
7:a:347:LYS:HA	7:a:350:LYS:HZ2	1.71	0.55
2:V:94:VAL:HG11	2:V:134:PHE:HB3	1.87	0.55
21:g:132:ARG:HD3	27:m:124:LEU:HD23	1.87	0.55
5:Y:81:LEU:HG	5:Y:107:LYS:HD2	1.89	0.55
3:W:83:LEU:HG	3:W:89:LEU:H	1.71	0.55
4:X:177:TYR:HB3	4:X:182:ASN:HB3	1.88	0.55
10:d:121:ARG:HG3	10:d:122:LEU:HG	1.89	0.55
15:C:183:PRO:O	15:C:290:LYS:NZ	2.40	0.55
2:V:432:GLU:HB3	11:e:8:VAL:H	1.71	0.55
3:W:32:ALA:O	3:W:86:ASN:ND2	2.39	0.55
3:W:173:THR:HG23	3:W:182:ARG:HH11	1.70	0.55
3:W:268:LYS:HD3	3:W:299:ILE:HG12	1.89	0.55
1:U:522:GLY:O	1:U:559:ARG:NH2	2.40	0.55
3:W:443:THR:HG22	6:Z:229:GLN:HE22	1.72	0.55
9:c:282:ARG:NH2	16:D:120:ASP:OD1	2.37	0.55
5:Y:32:ARG:HH22	5:Y:35:ALA:HB3	1.71	0.55
9:c:89:PRO:HG2	19:u:44:ILE:HD11	1.89	0.55
14:B:269:GLU:OE2	14:B:272:ARG:NH1	2.39	0.55
15:C:69:GLN:HB3	15:C:118:ASN:HD21	1.71	0.55
1:U:607:VAL:O	16:D:67:ASN:ND2	2.40	0.55
5:Y:364:TRP:NE1	5:Y:368:GLU:OE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.89	0.55
12:f:552:ASP:HB3	12:f:556:ARG:HG3	1.88	0.55
15:C:164:VAL:HG13	15:C:165:ILE:HG13	1.88	0.55
10:d:183:GLU:OE2	10:d:215:TRP:NE1	2.40	0.55
1:U:475:HIS:NE2	1:U:507:VAL:O	2.29	0.55
17:E:148:VAL:HG13	17:E:149:ILE:HG13	1.87	0.55
1:U:898:CYS:SG	1:U:899:ARG:N	2.80	0.54
5:Y:180:LEU:HA	5:Y:183:TYR:HD2	1.72	0.54
12:f:705:ASN:HB3	12:f:787:LEU:HD21	1.88	0.54
16:D:212:LYS:NZ	36:D:501:ATP:O1G	2.40	0.54
18:F:39:GLU:HA	18:F:42:ILE:HB	1.89	0.54
21:G:53:GLN:HA	21:G:215:ILE:HA	1.89	0.54
31:q:117:TYR:HB3	31:q:125:ALA:HB3	1.88	0.54
1:U:35:TRP:HE3	1:U:70:HIS:HB2	1.72	0.54
3:W:274:VAL:O	3:W:283:GLN:NE2	2.41	0.54
9:c:96:LEU:HD12	19:u:8:LEU:HD22	1.88	0.54
12:f:505:MET:HE3	12:f:537:THR:HG22	1.89	0.54
12:f:378:ASN:O	12:f:382:ASN:ND2	2.40	0.54
12:f:695:ALA:O	13:A:85:GLN:NE2	2.40	0.54
17:E:372:ARG:HD3	27:M:170:GLN:HB3	1.90	0.54
33:S:35:ILE:HB	34:T:151:ARG:HH12	1.72	0.54
22:h:222:THR:OG1	22:h:225:GLU:OE1	2.24	0.54
2:V:89:LYS:HD3	2:V:92:ARG:HH12	1.71	0.54
12:f:150:GLU:O	12:f:156:HIS:ND1	2.40	0.54
21:g:144:ASP:OD2	29:o:72:ARG:NH2	2.41	0.54
21:g:158:GLY:O	22:h:84:ARG:NH2	2.40	0.54
1:U:107:HIS:HA	1:U:110:LYS:HE3	1.89	0.54
1:U:328:ILE:HG13	1:U:329:LEU:HG	1.87	0.54
10:d:162:SER:OG	10:d:164:THR:OG1	2.21	0.54
24:J:74:ALA:HB2	24:J:161:ILE:HD13	1.88	0.54
1:U:768:GLN:HB2	1:U:775:LEU:HD12	1.89	0.54
2:V:33:GLN:NE2	2:V:84:LYS:O	2.41	0.54
5:Y:176:ARG:O	5:Y:180:LEU:N	2.40	0.54
5:Y:340:ALA:O	11:e:47:ASN:ND2	2.40	0.54
7:a:290:GLN:HA	7:a:332:HIS:HA	1.89	0.54
12:f:252:ALA:O	12:f:257:ARG:NH1	2.41	0.54
16:D:234:GLU:O	16:D:237:GLN:NE2	2.41	0.54
26:L:205:LEU:HD13	26:L:233:LEU:HD22	1.90	0.54
33:s:123:SER:HB3	33:s:136:LYS:HG3	1.90	0.54
2:V:440:LYS:O	2:V:444:ASP:N	2.40	0.54
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.89	0.54
3:W:55:ARG:HH12	3:W:79:GLU:HG3	1.71	0.54
16:D:199:PRO:HB3	16:D:328:ASP:HB2	1.90	0.54
26:L:156:CYS:HA	27:M:58:TYR:HA	1.90	0.54
26:l:205:LEU:HD13	26:l:233:LEU:HD22	1.90	0.54
2:V:349:ARG:HA	2:V:353:LEU:HD23	1.89	0.54
5:Y:186:LEU:H	11:e:64:GLY:H	1.54	0.54
12:f:202:HIS:ND1	12:f:242:GLU:OE2	2.40	0.54
18:F:386:ARG:HB3	26:L:166:GLN:HE22	1.73	0.54
33:S:150:ASP:OD2	30:p:177:ARG:NH2	2.38	0.54
2:V:106:ARG:O	2:V:110:HIS:ND1	2.42	0.53
5:Y:231:LEU:HG	5:Y:236:LEU:HB2	1.89	0.53
14:B:125:THR:OG1	14:B:126:SER:N	2.41	0.53
23:I:3:ARG:HH12	25:K:11:GLY:HA2	1.73	0.53
26:L:42:THR:O	26:L:137:TYR:OH	2.27	0.53
22:h:65:VAL:HG11	22:h:211:GLY:HA3	1.90	0.53
1:U:376:MET:HA	1:U:739:ALA:HA	1.91	0.53
3:W:98:LYS:HG2	3:W:136:ILE:HA	1.90	0.53
12:f:139:CYS:O	12:f:143:ARG:NH1	2.41	0.53
22:H:65:VAL:HG11	22:H:211:GLY:HA3	1.89	0.53
2:V:100:MET:O	2:V:104:THR:N	2.41	0.53
12:f:125:ILE:HD11	12:f:128:VAL:HB	1.89	0.53
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.88	0.53
15:C:88:LYS:HB2	15:C:94:LYS:HG2	1.90	0.53
24:J:96:LEU:HD12	31:Q:62:LYS:HG3	1.91	0.53
26:l:42:THR:O	26:l:137:TYR:OH	2.27	0.53
18:F:111:ILE:HG12	18:F:113:LEU:H	1.73	0.53
30:P:149:MET:HE3	33:s:147:PRO:HB2	1.89	0.53
3:W:63:THR:HA	3:W:68:VAL:HG22	1.90	0.53
7:a:35:HIS:NE2	8:b:14:GLU:O	2.41	0.53
9:c:111:TRP:NE1	9:c:130:GLN:OE1	2.39	0.53
19:u:44:ILE:HB	19:u:68:HIS:HB2	1.90	0.53
26:l:14:SER:HB2	26:l:18:ARG:H	1.74	0.53
5:Y:187:TYR:HA	11:e:63:HIS:CD2	2.43	0.53
5:Y:268:TYR:HB3	5:Y:323:PHE:HD1	1.73	0.53
10:d:256:ILE:O	16:D:62:LYS:NZ	2.38	0.53
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.91	0.53
15:C:20:LEU:HD12	15:C:21:ARG:HG3	1.91	0.53
30:P:65:GLN:OE1	31:Q:86:ARG:NH2	2.42	0.53
31:Q:148:THR:HG22	31:Q:150:THR:H	1.74	0.53
3:W:227:TYR:HB3	3:W:246:HIS:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:187:ARG:HE	4:X:217:ILE:HG22	1.74	0.53
5:Y:25:LEU:HD13	5:Y:286:TRP:HA	1.91	0.53
5:Y:296:VAL:O	5:Y:300:ARG:N	2.39	0.53
17:E:205:ASP:O	18:F:261:ILE:HD12	2.09	0.53
23:I:32:GLY:H	23:I:50:ARG:HH21	1.56	0.53
21:g:53:GLN:HA	21:g:215:ILE:HA	1.89	0.53
2:V:433:ASP:HA	2:V:436:PHE:HD2	1.73	0.53
4:X:296:ASN:O	4:X:337:ARG:NH1	2.41	0.53
30:P:62:THR:OG1	31:Q:85:ARG:NH2	2.41	0.53
26:I:152:ASN:HA	27:m:85:ARG:HH22	1.73	0.53
1:U:217:CYS:HB2	1:U:248:ILE:HD12	1.91	0.53
1:U:469:SER:OG	1:U:470:ASN:N	2.41	0.53
9:c:54:MET:O	9:c:77:GLN:NE2	2.42	0.53
12:f:680:ARG:HD2	12:f:763:ARG:HA	1.90	0.53
16:D:238:LYS:HB3	17:E:207:TYR:HB3	1.91	0.53
17:E:97:ARG:HE	17:E:111:LEU:HB2	1.74	0.53
33:S:123:SER:HB3	33:S:136:LYS:HG3	1.90	0.53
21:g:159:TYR:HB3	22:h:81:PRO:HG3	1.90	0.53
1:U:177:LEU:HD23	1:U:205:TYR:HE1	1.74	0.53
3:W:15:LYS:HA	3:W:18:VAL:HB	1.91	0.53
5:Y:185:GLY:H	11:e:64:GLY:C	2.16	0.53
5:Y:231:LEU:HD12	5:Y:234:PRO:HG2	1.91	0.53
18:F:251:LEU:HD23	18:F:285:ILE:HG12	1.91	0.53
26:L:14:SER:HB2	26:L:18:ARG:H	1.74	0.53
29:o:198:ARG:NH2	30:p:152:SER:O	2.42	0.53
2:V:494:MET:O	6:Z:278:ASN:ND2	2.41	0.52
4:X:177:TYR:O	4:X:182:ASN:N	2.41	0.52
17:E:235:ILE:O	17:E:239:GLY:N	2.40	0.52
12:f:77:GLU:OE1	12:f:79:ARG:NH1	2.42	0.52
29:O:164:PHE:O	33:s:38:ARG:NH2	2.43	0.52
28:n:18:SER:HB2	28:n:30:VAL:HA	1.91	0.52
12:f:149:GLU:HG3	12:f:152:ALA:HB2	1.92	0.52
16:D:119:ILE:O	16:D:121:ARG:NH1	2.41	0.52
18:F:293:THR:HA	18:F:337:ILE:HG22	1.91	0.52
2:V:432:GLU:HA	11:e:6:GLN:HE21	1.75	0.52
8:b:16:MET:HA	8:b:25:ARG:HD2	1.91	0.52
9:c:141:VAL:HG22	9:c:161:ARG:HD3	1.90	0.52
14:B:49:LEU:HD13	14:B:51:LEU:H	1.75	0.52
18:F:299:GLU:N	18:F:299:GLU:OE2	2.42	0.52
1:U:20:LYS:HB3	1:U:54:PHE:HD1	1.73	0.52
8:b:21:PHE:HD2	8:b:25:ARG:HG2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:872:VAL:HG21	12:f:881:GLU:H	1.74	0.52
14:B:223:ILE:HG13	14:B:347:ILE:HG21	1.90	0.52
16:D:283:ARG:HB3	16:D:287:ARG:HH11	1.73	0.52
4:X:86:ALA:HB2	4:X:122:ARG:HH12	1.75	0.52
9:c:124:GLY:O	9:c:128:ASN:ND2	2.43	0.52
14:B:319:PHE:O	14:B:322:ARG:NH1	2.43	0.52
16:D:231:VAL:HG13	17:E:262:ASN:HD22	1.74	0.52
33:s:198:VAL:HG22	33:s:203:ILE:HG12	1.92	0.52
2:V:467:TYR:OH	6:Z:255:ASP:OD1	2.28	0.52
12:f:373:ALA:HB2	12:f:744:MET:HA	1.92	0.52
13:A:89:SER:HA	13:A:93:LEU:HD23	1.91	0.52
15:C:187:LEU:HB3	15:C:314:LYS:HG2	1.91	0.52
5:Y:290:PRO:HD2	11:e:57:ARG:HB3	1.90	0.52
23:i:32:GLY:H	23:i:50:ARG:HH21	1.56	0.52
31:q:148:THR:HG22	31:q:150:THR:H	1.74	0.52
6:Z:263:ALA:HB1	9:c:288:VAL:HG13	1.92	0.52
13:A:206:ILE:HG22	18:F:373:MET:HE2	1.91	0.52
23:I:45:LEU:HD11	23:I:137:ILE:HG12	1.92	0.52
33:S:198:VAL:HG22	33:S:203:ILE:HG12	1.92	0.52
27:m:141:SER:HB3	27:m:144:ASP:HB2	1.92	0.52
3:W:145:LEU:HA	3:W:148:THR:HG22	1.92	0.52
5:Y:186:LEU:H	11:e:64:GLY:CA	2.22	0.52
15:C:258:ARG:HG3	15:C:259:LEU:H	1.74	0.52
27:M:141:SER:HB3	27:M:144:ASP:HB2	1.92	0.52
28:N:18:SER:HB2	28:N:30:VAL:HA	1.91	0.52
4:X:323:LEU:O	4:X:327:TYR:N	2.43	0.51
29:o:31:CYS:SG	29:o:32:SER:N	2.83	0.51
14:B:231:GLY:N	38:B:501:ADP:O2A	2.41	0.51
17:E:247:THR:HG22	17:E:249:ALA:H	1.75	0.51
25:k:209:LYS:O	25:k:214:ASN:ND2	2.44	0.51
6:Z:42:SER:HB3	6:Z:49:ASP:HB3	1.92	0.51
13:A:413:VAL:HA	13:A:416:VAL:HG22	1.93	0.51
3:W:35:ALA:HB2	3:W:48:LEU:HD21	1.92	0.51
6:Z:142:GLU:OE2	6:Z:153:LYS:NZ	2.44	0.51
7:a:273:GLN:HB3	7:a:310:LEU:HD11	1.92	0.51
7:a:360:VAL:HG22	9:c:308:VAL:HG13	1.91	0.51
12:f:564:LEU:HD22	12:f:776:LEU:HG	1.92	0.51
17:E:127:PRO:HD2	18:F:321:GLN:HG2	1.91	0.51
25:K:209:LYS:O	25:K:214:ASN:ND2	2.44	0.51
26:l:26:MET:HE1	26:l:148:CYS:HB2	1.92	0.51
26:l:50:LYS:HE2	26:l:61:LYS:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:p:135:ASP:OD1	30:p:135:ASP:N	2.44	0.51
5:Y:134:LEU:O	5:Y:138:LEU:N	2.43	0.51
6:Z:48:LEU:HD21	6:Z:92:VAL:HG21	1.92	0.51
11:e:46:ASP:O	11:e:50:ASP:N	2.43	0.51
12:f:837:LEU:HB2	13:A:362:MET:HA	1.92	0.51
25:K:124:GLY:O	25:K:134:SER:N	2.44	0.51
1:U:643:SER:O	15:C:57:ARG:NH2	2.44	0.51
2:V:186:LYS:HZ2	2:V:234:ARG:HH11	1.58	0.51
2:V:218:TYR:HA	2:V:221:LEU:HG	1.92	0.51
14:B:227:PRO:O	14:B:230:THR:OG1	2.26	0.51
1:U:219:CYS:SG	1:U:220:LEU:N	2.83	0.51
26:L:120:THR:O	27:M:129:ARG:NH1	2.35	0.51
31:Q:44:LEU:HD12	31:Q:102:LEU:HD12	1.93	0.51
25:k:50:VAL:HG11	25:k:66:LYS:HB2	1.93	0.51
2:V:214:HIS:HA	2:V:217:VAL:HB	1.93	0.51
9:c:79:GLY:HA2	9:c:84:VAL:HA	1.93	0.51
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.92	0.51
12:f:257:ARG:HG2	12:f:272:LEU:HD13	1.93	0.51
12:f:777:THR:HG22	12:f:803:PHE:HA	1.93	0.51
14:B:188:GLY:H	38:B:501:ADP:HN62	1.59	0.51
21:G:114:LEU:HD22	21:G:140:LEU:HD21	1.93	0.51
2:V:415:SER:HB2	5:Y:346:LYS:HB3	1.92	0.51
5:Y:215:ASP:OD1	5:Y:218:THR:OG1	2.28	0.51
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.44	0.51
14:B:411:ARG:NH2	14:B:418:ASP:OD1	2.44	0.51
25:k:191:LEU:HD21	25:k:221:GLN:HE21	1.76	0.51
31:q:44:LEU:HD12	31:q:102:LEU:HD12	1.93	0.51
2:V:440:LYS:NZ	10:d:148:TYR:OH	2.29	0.51
3:W:37:GLU:HB3	3:W:39:ARG:HG2	1.93	0.51
3:W:221:LYS:HA	3:W:225:LYS:HD3	1.93	0.51
7:a:216:LEU:HA	7:a:219:HIS:HB2	1.93	0.51
13:A:415:LYS:O	13:A:419:SER:N	2.38	0.51
18:F:183:GLU:HB3	18:F:239:ALA:HA	1.92	0.51
19:u:1:MET:N	19:u:17:VAL:O	2.36	0.51
19:u:39:ASP:O	19:u:42:ARG:NH2	2.44	0.51
25:k:124:GLY:O	25:k:134:SER:N	2.44	0.51
2:V:211:TYR:HA	2:V:214:HIS:HB3	1.92	0.50
6:Z:138:TYR:HB3	6:Z:155:PHE:HB3	1.92	0.50
9:c:131:GLN:HA	9:c:134:GLU:HG2	1.93	0.50
12:f:425:GLY:HA3	12:f:451:VAL:HG11	1.93	0.50
23:I:86:LEU:HD22	23:I:114:LEU:HD11	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:73:ALA:HB3	23:i:137:ILE:HD11	1.93	0.50
1:U:510:GLU:OE2	1:U:546:ARG:NH2	2.44	0.50
10:d:18:LYS:O	10:d:22:GLU:N	2.39	0.50
22:H:66:GLU:OE2	22:H:91:ARG:NH2	2.44	0.50
26:l:189:LYS:HA	26:l:192:LEU:HG	1.93	0.50
7:a:130:VAL:HA	7:a:133:GLU:HB2	1.92	0.50
9:c:151:VAL:HG13	9:c:153:GLY:H	1.76	0.50
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.93	0.50
12:f:253:LEU:HD11	12:f:272:LEU:HB3	1.93	0.50
14:B:234:LEU:HD11	38:B:501:ADP:H2'	1.93	0.50
18:F:368:ILE:HG23	18:F:371:ARG:HH22	1.75	0.50
25:K:48:LEU:HD21	25:K:77:ALA:HB2	1.92	0.50
23:i:45:LEU:HD11	23:i:137:ILE:HG12	1.92	0.50
1:U:780:SER:HA	1:U:783:TYR:HD2	1.75	0.50
5:Y:184:GLN:HE21	5:Y:200:LEU:HD12	1.76	0.50
12:f:50:LYS:HA	13:A:399:ALA:HA	1.94	0.50
25:K:50:VAL:HG11	25:K:66:LYS:HB2	1.93	0.50
6:Z:225:GLN:HG3	6:Z:226:ILE:HG13	1.93	0.50
6:Z:284:ASP:HA	6:Z:287:LYS:HG2	1.94	0.50
8:b:100:ARG:NH1	8:b:102:GLY:O	2.45	0.50
9:c:50:PRO:HG3	17:E:84:ARG:HG2	1.93	0.50
12:f:23:GLY:HA3	12:f:34:ARG:HH22	1.77	0.50
22:h:66:GLU:OE2	22:h:91:ARG:NH2	2.44	0.50
25:k:48:LEU:HD21	25:k:77:ALA:HB2	1.93	0.50
28:n:67:SER:HA	28:n:70:LEU:HD12	1.94	0.50
3:W:144:ARG:NH1	16:D:392:TYR:OH	2.43	0.50
4:X:313:LEU:HD11	4:X:323:LEU:HD21	1.94	0.50
5:Y:292:TYR:CZ	5:Y:296:VAL:HB	2.47	0.50
6:Z:136:GLU:OE2	6:Z:157:HIS:ND1	2.45	0.50
15:C:117:ARG:HG2	15:C:119:ASP:H	1.76	0.50
23:I:73:ALA:HB3	23:I:137:ILE:HD11	1.93	0.50
26:L:50:LYS:HE2	26:L:61:LYS:HA	1.92	0.50
26:l:151:ALA:O	27:m:85:ARG:NH2	2.45	0.50
34:t:27:LEU:HD22	34:t:184:TYR:HB2	1.93	0.50
3:W:231:ILE:O	3:W:235:GLN:N	2.44	0.50
12:f:228:LYS:HB3	12:f:231:LEU:HD13	1.94	0.50
25:K:191:LEU:HD21	25:K:221:GLN:HE21	1.76	0.50
30:P:189:ILE:HG23	30:P:196:THR:HB	1.94	0.50
1:U:204:ILE:HA	1:U:207:ASN:HB2	1.94	0.50
12:f:373:ALA:HA	12:f:376:PHE:HD2	1.76	0.50
13:A:213:LEU:HD12	13:A:337:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:u:40:GLN:HA	19:u:72:ARG:HB2	1.94	0.50
21:G:88:ARG:NH1	27:M:157:SER:O	2.38	0.50
26:L:189:LYS:HA	26:L:192:LEU:HG	1.93	0.50
2:V:201:ARG:HH21	2:V:243:ASP:H	1.60	0.50
5:Y:247:LEU:HD12	5:Y:250:LEU:HD11	1.94	0.50
9:c:175:ARG:HG3	9:c:181:LEU:HD21	1.93	0.50
13:A:394:MET:HE2	14:B:349:ARG:HH22	1.75	0.50
15:C:161:ILE:HG23	15:C:165:ILE:HD12	1.94	0.50
16:D:86:PRO:HB2	16:D:134:LYS:HE3	1.94	0.50
28:N:67:SER:HA	28:N:70:LEU:HD12	1.94	0.50
34:T:27:LEU:HD22	34:T:184:TYR:HB2	1.93	0.50
23:i:108:GLU:OE2	23:i:146:GLN:NE2	2.43	0.50
6:Z:237:LEU:HD12	9:c:310:LYS:HE2	1.93	0.49
9:c:52:GLU:OE1	19:u:76:GLY:N	2.45	0.49
12:f:327:ASN:HD22	12:f:330:PHE:HB3	1.77	0.49
13:A:394:MET:O	13:A:398:ARG:N	2.37	0.49
17:E:146:ARG:NH1	17:E:150:GLU:OE1	2.45	0.49
25:K:167:ALA:H	26:L:56:LEU:HD13	1.76	0.49
26:L:26:MET:HE1	26:L:148:CYS:HB2	1.92	0.49
21:g:114:LEU:HD22	21:g:140:LEU:HD21	1.93	0.49
23:i:86:LEU:HD22	23:i:114:LEU:HD11	1.93	0.49
5:Y:121:LEU:HB2	5:Y:125:ARG:HH12	1.76	0.49
5:Y:298:GLU:O	5:Y:302:HIS:N	2.43	0.49
7:a:65:SER:HA	7:a:68:GLU:HB2	1.92	0.49
12:f:524:MET:HA	12:f:776:LEU:HD23	1.95	0.49
18:F:94:ILE:HD12	18:F:123:VAL:HG12	1.94	0.49
22:H:39:LYS:HE2	22:H:144:PRO:HG2	1.94	0.49
23:I:229:LYS:N	23:I:232:GLU:OE2	2.45	0.49
30:p:189:ILE:HG23	30:p:196:THR:HB	1.94	0.49
1:U:146:LYS:HE2	1:U:148:LYS:HB2	1.94	0.49
8:b:30:GLN:HG3	8:b:75:LEU:HD13	1.93	0.49
10:d:55:LEU:HB2	10:d:78:LEU:HD21	1.93	0.49
7:a:268:LEU:HD23	7:a:271:LYS:HD3	1.95	0.49
8:b:142:ASN:HD22	8:b:172:THR:HA	1.78	0.49
13:A:140:VAL:HG12	13:A:152:PRO:HA	1.93	0.49
23:I:123:GLN:HE22	24:J:82:ILE:HG13	1.77	0.49
12:f:438:ASP:HA	12:f:477:MET:HE2	1.94	0.49
13:A:339:ARG:NH1	18:F:426:GLU:OE2	2.46	0.49
15:C:187:LEU:HD11	15:C:295:THR:HG22	1.94	0.49
4:X:105:GLN:HB3	4:X:109:LEU:HD13	1.93	0.49
17:E:140:GLU:OE1	17:E:143:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:M:37:ILE:HD11	27:M:193:VAL:HG13	1.94	0.49
29:O:198:ARG:NH2	30:P:152:SER:O	2.46	0.49
1:U:220:LEU:O	1:U:224:ASP:N	2.46	0.49
1:U:400:ALA:O	1:U:404:ALA:N	2.45	0.49
2:V:85:ALA:O	2:V:89:LYS:NZ	2.46	0.49
8:b:180:ALA:HA	8:b:183:LEU:HD13	1.94	0.49
10:d:78:LEU:HD13	10:d:98:LEU:HD21	1.95	0.49
18:F:435:LEU:HD12	25:K:20:ARG:HE	1.78	0.49
22:H:9:SER:OG	22:H:123:GLN:O	2.30	0.49
27:M:152:ASP:OD1	27:M:156:VAL:N	2.46	0.49
2:V:151:THR:HA	2:V:154:ALA:HB3	1.94	0.49
2:V:264:TYR:O	2:V:266:GLN:N	2.46	0.49
8:b:161:ASN:ND2	8:b:168:SER:O	2.46	0.49
10:d:56:GLU:HG2	10:d:98:LEU:HD22	1.95	0.49
12:f:662:MET:HB3	14:B:82:GLN:HG3	1.94	0.49
12:f:665:GLU:HG2	12:f:669:GLU:HG3	1.95	0.49
12:f:691:PRO:HA	12:f:694:LEU:HB2	1.95	0.49
21:G:158:GLY:O	22:H:84:ARG:NH2	2.45	0.49
25:K:182:GLN:NE2	26:L:55:GLU:OE1	2.46	0.49
21:g:138:MET:HB3	21:g:154:CYS:HB3	1.94	0.49
7:a:290:GLN:HG2	7:a:330:ARG:HB3	1.95	0.49
22:h:9:SER:OG	22:h:123:GLN:O	2.30	0.49
27:m:152:ASP:OD1	27:m:156:VAL:N	2.46	0.49
1:U:341:PHE:HZ	1:U:883:ARG:HB3	1.78	0.49
3:W:95:SER:O	3:W:99:GLN:NE2	2.46	0.49
7:a:135:ILE:HG12	7:a:158:LEU:HD13	1.95	0.49
12:f:469:TYR:O	12:f:472:HIS:ND1	2.33	0.49
13:A:224:LEU:HD11	36:A:501:ATP:H2'	1.94	0.49
14:B:438:LEU:HD12	23:I:155:ASN:HD21	1.78	0.49
16:D:249:ASP:OD1	16:D:252:ARG:NH2	2.45	0.49
23:I:16:GLY:HA3	24:J:24:GLU:HB2	1.95	0.49
30:p:26:ARG:HH21	30:p:38:ASP:HA	1.78	0.49
31:q:21:ALA:HB3	31:q:29:LYS:HB3	1.95	0.49
33:S:4:PRO:O	34:T:100:ARG:NH2	2.44	0.48
23:i:171:ALA:HB2	23:i:200:THR:HG21	1.95	0.48
1:U:490:ARG:HB2	1:U:493:VAL:HG12	1.95	0.48
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.94	0.48
5:Y:50:MET:HE2	5:Y:74:LYS:HB3	1.95	0.48
5:Y:292:TYR:CE2	5:Y:296:VAL:HB	2.49	0.48
26:l:196:ARG:HH21	26:l:239:ARG:HG3	1.79	0.48
30:p:62:THR:OG1	31:q:85:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:90:LEU:HB2	3:W:97:LEU:HD12	1.93	0.48
5:Y:210:SER:H	5:Y:213:LEU:HB2	1.78	0.48
13:A:125:LEU:HA	13:A:149:ILE:HB	1.94	0.48
23:I:17:ARG:HB3	24:J:28:LYS:HE3	1.94	0.48
24:j:11:SER:OG	24:j:13:ASP:OD1	2.31	0.48
27:m:37:ILE:HD11	27:m:193:VAL:HG13	1.94	0.48
2:V:179:LYS:HD3	2:V:210:CYS:HB2	1.95	0.48
2:V:280:ALA:HB1	2:V:284:GLU:HB3	1.96	0.48
12:f:189:LYS:HG2	12:f:190:GLU:HG2	1.95	0.48
12:f:640:LYS:HD3	12:f:651:GLY:HA3	1.94	0.48
16:D:321:LEU:HB3	16:D:327:LEU:HD12	1.96	0.48
18:F:318:ASP:OD2	18:F:344:ARG:NH2	2.46	0.48
28:N:144:ARG:H	28:N:147:MET:HE3	1.77	0.48
21:g:67:THR:HG22	21:g:69:LEU:H	1.78	0.48
22:h:39:LYS:HE2	22:h:144:PRO:HG2	1.94	0.48
5:Y:276:ALA:HA	5:Y:279:GLU:HB3	1.95	0.48
21:G:138:MET:HB3	21:G:154:CYS:HB3	1.94	0.48
23:I:171:ALA:HB2	23:I:200:THR:HG21	1.95	0.48
24:J:116:GLN:NE2	24:J:150:SER:O	2.46	0.48
34:T:43:MET:HE3	34:T:45:VAL:HG22	1.95	0.48
5:Y:291:HIS:HB3	11:e:54:ASN:N	2.29	0.48
7:a:321:LYS:O	7:a:334:THR:OG1	2.29	0.48
13:A:312:ARG:HB2	13:A:315:ILE:HD13	1.95	0.48
31:Q:21:ALA:HB3	31:Q:29:LYS:HB3	1.95	0.48
30:p:190:ILE:HG22	30:p:195:ILE:HG23	1.96	0.48
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.95	0.48
14:B:56:THR:HG23	14:B:58:CYS:H	1.79	0.48
23:i:92:LEU:HD22	23:i:96:ARG:HH21	1.78	0.48
24:j:116:GLN:NE2	24:j:150:SER:O	2.46	0.48
29:o:7:VAL:HG22	29:o:12:ILE:HG12	1.95	0.48
2:V:108:LEU:HA	2:V:111:TYR:HD2	1.79	0.48
2:V:394:LEU:O	2:V:398:LEU:N	2.47	0.48
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.95	0.48
7:a:371:ALA:HA	7:a:374:ILE:HD13	1.96	0.48
10:d:238:PRO:HA	10:d:241:GLU:HG2	1.95	0.48
12:f:465:LEU:O	12:f:481:SER:OG	2.31	0.48
14:B:60:LEU:HB3	14:B:64:LYS:HZ3	1.79	0.48
29:O:113:ILE:HG12	29:O:119:THR:HG22	1.96	0.48
2:V:183:GLU:OE2	2:V:211:TYR:OH	2.31	0.48
3:W:83:LEU:HA	3:W:88:MET:HA	1.94	0.48
10:d:47:GLN:O	10:d:51:ALA:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:43:GLN:HG3	12:f:121:PHE:HB2	1.96	0.48
16:D:269:ALA:HB1	17:E:255:ARG:HG2	1.96	0.48
3:W:155:GLN:NE2	3:W:161:GLU:OE1	2.47	0.48
12:f:130:ALA:O	12:f:134:SER:N	2.42	0.48
12:f:227:ALA:HB3	12:f:232:TYR:HB2	1.96	0.48
12:f:643:PRO:HB2	12:f:646:MET:HB3	1.96	0.48
30:P:190:ILE:HG22	30:P:195:ILE:HG23	1.96	0.48
33:S:147:PRO:HB2	30:p:149:MET:HE3	1.95	0.48
23:i:229:LYS:N	23:i:232:GLU:OE2	2.45	0.48
2:V:92:ARG:HG2	2:V:96:ARG:HH22	1.78	0.47
2:V:204:ASP:OD1	2:V:234:ARG:NH2	2.47	0.47
2:V:440:LYS:H	11:e:4:LYS:NZ	2.12	0.47
10:d:52:ARG:HH12	10:d:92:SER:HB3	1.79	0.47
12:f:75:LEU:HD12	12:f:78:LEU:HD13	1.96	0.47
12:f:223:GLU:HA	14:B:60:LEU:HD21	1.96	0.47
12:f:673:ARG:NH1	12:f:708:ASP:OD2	2.47	0.47
17:E:23:ASP:OD2	17:E:27:LYS:NZ	2.46	0.47
29:O:7:VAL:HG22	29:O:12:ILE:HG12	1.95	0.47
30:P:26:ARG:HH21	30:P:38:ASP:HA	1.78	0.47
1:U:242:LEU:HA	1:U:245:ALA:HB3	1.96	0.47
5:Y:94:ASN:HD21	14:B:410:ARG:HD2	1.79	0.47
5:Y:186:LEU:N	11:e:63:HIS:H	2.12	0.47
13:A:300:LEU:HD23	13:A:303:ILE:HD12	1.95	0.47
17:E:75:ASN:HD22	18:F:130:GLN:HG2	1.79	0.47
21:G:67:THR:HG22	21:G:69:LEU:H	1.78	0.47
23:I:92:LEU:HD22	23:I:96:ARG:HH21	1.78	0.47
34:T:45:VAL:HB	34:T:49:THR:HG23	1.97	0.47
28:n:144:ARG:H	28:n:147:MET:HE3	1.77	0.47
29:o:113:ILE:HG12	29:o:119:THR:HG22	1.96	0.47
1:U:89:ASN:O	1:U:136:LYS:NZ	2.45	0.47
5:Y:133:ALA:HB2	15:C:205:HIS:CE1	2.49	0.47
12:f:833:PHE:HB2	12:f:840:LEU:HD22	1.96	0.47
18:F:341:ALA:O	18:F:347:ARG:NH1	2.48	0.47
21:g:126:THR:O	22:h:128:ARG:NH1	2.41	0.47
2:V:37:MET:HG2	2:V:115:LYS:HE2	1.96	0.47
5:Y:285:ASP:OD2	5:Y:287:LEU:HD22	2.15	0.47
13:A:286:ASP:OD2	18:F:334:ARG:NH2	2.47	0.47
17:E:300:HIS:NE2	17:E:302:ASP:OD1	2.47	0.47
33:s:38:ARG:HH12	34:t:151:ARG:HD3	1.79	0.47
10:d:199:PHE:O	10:d:205:LYS:NZ	2.37	0.47
13:A:386:ARG:HH22	14:B:345:GLY:HA2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:264:ILE:HD12	16:D:309:MET:HE2	1.97	0.47
5:Y:295:TYR:O	5:Y:299:MET:N	2.40	0.47
6:Z:187:LEU:HA	6:Z:190:ARG:HB2	1.95	0.47
15:C:113:ARG:NH2	15:C:128:PRO:O	2.37	0.47
15:C:190:GLY:HA3	15:C:317:PHE:HB2	1.96	0.47
1:U:373:ASN:HA	1:U:376:MET:HG2	1.95	0.47
2:V:179:LYS:O	2:V:183:GLU:N	2.43	0.47
3:W:312:MET:HG3	3:W:315:MET:HG2	1.95	0.47
3:W:361:HIS:HA	3:W:364:ARG:HH11	1.79	0.47
5:Y:293:ARG:HB2	11:e:56:LEU:HG	1.96	0.47
9:c:59:GLY:HA3	9:c:69:VAL:HA	1.97	0.47
15:C:246:ILE:HB	15:C:291:VAL:HG12	1.95	0.47
23:I:108:GLU:OE2	23:I:146:GLN:NE2	2.43	0.47
34:T:1:THR:N	34:T:104:ASN:OD1	2.48	0.47
34:t:1:THR:N	34:t:104:ASN:OD1	2.48	0.47
34:t:43:MET:HE3	34:t:45:VAL:HG22	1.95	0.47
1:U:772:TRP:HD1	1:U:775:LEU:HB2	1.79	0.47
2:V:440:LYS:NZ	10:d:144:MET:O	2.44	0.47
12:f:72:ARG:HH12	12:f:83:ARG:HA	1.80	0.47
33:S:125:ASP:OD1	33:S:129:SER:N	2.48	0.47
25:k:167:ALA:HB3	25:k:181:LEU:HD21	1.97	0.47
17:E:109:ARG:NH2	18:F:114:ASP:O	2.42	0.47
24:J:116:GLN:HE21	25:K:83:ALA:HB3	1.79	0.47
33:s:4:PRO:O	34:t:100:ARG:NH2	2.47	0.47
33:s:125:ASP:OD1	33:s:129:SER:N	2.48	0.47
5:Y:359:PRO:HB2	5:Y:364:TRP:HB2	1.97	0.47
7:a:205:LEU:O	7:a:271:LYS:NZ	2.47	0.47
12:f:608:LYS:HA	12:f:611:GLN:HG2	1.97	0.47
12:f:743:ALA:HA	12:f:746:ARG:HH21	1.79	0.47
17:E:139:SER:HA	17:E:142:ILE:HD12	1.96	0.47
32:R:141:ARG:NH2	31:q:162:LYS:O	2.48	0.47
33:S:213:ASP:OD2	29:o:19:ARG:NH2	2.47	0.47
21:g:120:ASP:OD1	22:h:84:ARG:NH1	2.48	0.47
2:V:65:ARG:HD3	2:V:68:ASP:HB2	1.97	0.46
3:W:406:VAL:HG23	4:X:342:PHE:HB3	1.96	0.46
5:Y:275:LEU:HD11	5:Y:296:VAL:HG13	1.97	0.46
7:a:100:THR:HA	7:a:103:LYS:HG2	1.97	0.46
12:f:224:ASN:OD1	12:f:235:SER:OG	2.28	0.46
12:f:281:ILE:HA	12:f:282:PHE:HA	1.58	0.46
12:f:758:ASN:HB2	12:f:809:ILE:HG21	1.97	0.46
18:F:101:PRO:HA	18:F:115:SER:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:K:167:ALA:HB3	25:K:181:LEU:HD21	1.97	0.46
28:N:76:VAL:HG23	28:N:104:ASP:HB2	1.97	0.46
27:m:66:LEU:HD13	27:m:214:SER:HB2	1.97	0.46
2:V:171:VAL:O	2:V:175:MET:N	2.35	0.46
5:Y:349:LYS:HG3	5:Y:350:VAL:HG13	1.97	0.46
8:b:109:ILE:HB	8:b:138:VAL:HG22	1.97	0.46
15:C:72:TYR:HB2	15:C:116:LEU:HB3	1.96	0.46
27:M:170:GLN:HA	27:M:173:LYS:HE2	1.98	0.46
31:q:19:ARG:HH21	31:q:31:ASP:HB2	1.80	0.46
1:U:500:ASN:OD1	1:U:508:THR:OG1	2.28	0.46
2:V:128:ARG:HB3	2:V:171:VAL:HG11	1.97	0.46
3:W:119:PRO:HA	3:W:122:LEU:HB2	1.97	0.46
5:Y:185:GLY:O	11:e:62:LYS:HG3	2.15	0.46
5:Y:226:VAL:HA	5:Y:229:ILE:HD13	1.97	0.46
13:A:347:ASP:N	13:A:347:ASP:OD1	2.49	0.46
17:E:84:ARG:O	17:E:85:ARG:NE	2.43	0.46
31:Q:19:ARG:HH21	31:Q:31:ASP:HB2	1.80	0.46
1:U:599:ILE:HG23	16:D:56:VAL:HG21	1.97	0.46
2:V:247:GLN:HE21	2:V:274:SER:HB3	1.80	0.46
3:W:174:TYR:HB3	17:E:161:ARG:HG3	1.98	0.46
3:W:190:MET:HB2	3:W:202:THR:HG23	1.96	0.46
5:Y:333:GLU:HG3	5:Y:336:ARG:HH21	1.79	0.46
12:f:202:HIS:CE1	12:f:241:PRO:HB2	2.49	0.46
12:f:407:MET:HE3	12:f:439:TYR:HB2	1.97	0.46
14:B:120:HIS:HA	14:B:134:SER:HA	1.96	0.46
21:g:89:SER:OG	27:m:117:MET:SD	2.73	0.46
22:h:139:TRP:HA	22:h:144:PRO:HA	1.98	0.46
7:a:100:THR:HG22	7:a:103:LYS:HE2	1.97	0.46
15:C:249:ASP:OD1	15:C:249:ASP:N	2.46	0.46
17:E:147:GLU:HG3	17:E:151:LEU:HD12	1.98	0.46
17:E:205:ASP:OD2	17:E:210:GLU:CB	2.63	0.46
17:E:338:PHE:HA	17:E:378:LYS:HZ1	1.79	0.46
26:L:196:ARG:HH21	26:L:239:ARG:HG3	1.79	0.46
26:l:146:GLN:HE22	26:l:159:MET:HE2	1.80	0.46
32:r:26:ILE:HG21	32:r:29:GLN:HE21	1.80	0.46
3:W:455:LEU:HA	3:W:456:GLN:HA	1.68	0.46
8:b:53:THR:HG22	8:b:59:GLU:H	1.80	0.46
10:d:217:LEU:HB2	10:d:222:TYR:HE1	1.81	0.46
12:f:852:VAL:O	12:f:854:GLY:N	2.48	0.46
24:J:32:ALA:HB2	24:J:45:VAL:HG23	1.97	0.46
23:i:57:ASP:HB3	23:i:59:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:m:170:GLN:HA	27:m:173:LYS:HE2	1.98	0.46
28:n:19:ARG:NH1	28:n:170:SER:O	2.48	0.46
31:q:103:LEU:HB3	31:q:117:TYR:HA	1.98	0.46
1:U:191:LYS:HD2	1:U:194:ARG:HH11	1.80	0.46
1:U:688:LEU:HB3	1:U:713:TYR:HE1	1.81	0.46
3:W:115:ILE:HG12	3:W:119:PRO:HG2	1.98	0.46
10:d:48:LEU:HA	10:d:51:ALA:HB3	1.96	0.46
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.96	0.46
15:C:72:TYR:N	15:C:116:LEU:O	2.47	0.46
15:C:143:VAL:O	15:C:201:ARG:NH2	2.49	0.46
16:D:173:GLN:NE2	16:D:332:GLU:O	2.49	0.46
21:G:144:ASP:OD2	29:O:72:ARG:NH2	2.43	0.46
26:L:225:ASP:N	26:L:225:ASP:OD1	2.47	0.46
28:N:19:ARG:NH1	28:N:170:SER:O	2.48	0.46
33:S:35:ILE:O	34:T:151:ARG:NH2	2.38	0.46
21:g:86:ASP:OD1	27:m:120:HIS:NE2	2.49	0.46
25:k:37:ALA:HB2	25:k:50:VAL:HG23	1.98	0.46
28:n:76:VAL:HG23	28:n:104:ASP:HB2	1.97	0.46
34:t:45:VAL:HB	34:t:49:THR:HG23	1.97	0.46
1:U:336:GLU:O	1:U:340:GLN:N	2.48	0.46
5:Y:184:GLN:HG2	5:Y:200:LEU:HB3	1.98	0.46
9:c:151:VAL:HG21	16:D:80:LYS:HB2	1.97	0.46
13:A:247:GLN:HE22	13:A:256:MET:HE3	1.81	0.46
17:E:205:ASP:OD2	17:E:210:GLU:HG3	2.16	0.46
23:I:180:LYS:HD2	23:I:183:GLU:HB2	1.98	0.46
33:S:27:THR:HB	33:S:40:SER:H	1.81	0.46
25:k:210:LEU:HD11	25:k:215:ILE:HG12	1.97	0.46
5:Y:184:GLN:HB3	5:Y:201:PHE:HE1	1.81	0.46
12:f:778:LEU:HA	12:f:803:PHE:HB3	1.98	0.46
17:E:205:ASP:OD2	17:E:210:GLU:CG	2.63	0.46
17:E:265:ASP:OD2	17:E:291:ARG:NH2	2.48	0.46
1:U:68:PHE:HB3	1:U:73:ALA:HB3	1.97	0.46
1:U:341:PHE:HD1	1:U:881:PRO:HB2	1.81	0.46
2:V:435:GLU:HA	2:V:438:VAL:HG23	1.98	0.46
5:Y:78:GLU:HG3	5:Y:82:LYS:HD2	1.97	0.46
5:Y:314:LEU:HD21	5:Y:319:MET:HE3	1.98	0.46
18:F:169:ASP:HB3	18:F:172:VAL:HG23	1.98	0.46
26:L:146:GLN:HE22	26:L:159:MET:HE2	1.80	0.46
34:T:136:SER:HB2	34:T:150:LEU:HD13	1.97	0.46
23:i:216:LEU:HD12	23:i:225:ILE:HG12	1.97	0.46
2:V:184:ALA:HA	2:V:187:ILE:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:227:VAL:O	2:V:231:LEU:N	2.37	0.45
3:W:82:LEU:HD22	3:W:90:LEU:HA	1.98	0.45
5:Y:206:SER:HB2	11:e:69:THR:HA	1.98	0.45
10:d:170:LEU:HA	10:d:173:THR:HG22	1.98	0.45
17:E:197:LYS:HZ3	17:E:199:VAL:HG12	1.82	0.45
31:Q:13:VAL:HG11	31:Q:105:ALA:HB1	1.99	0.45
34:T:49:THR:HB	34:T:85:PRO:HG3	1.99	0.45
26:l:45:VAL:HG11	26:l:188:VAL:HG22	1.99	0.45
1:U:695:MET:HE3	1:U:695:MET:HB2	1.84	0.45
2:V:400:HIS:HA	10:d:145:GLU:HG3	1.97	0.45
3:W:55:ARG:NH1	3:W:75:TYR:O	2.49	0.45
5:Y:13:LYS:NZ	5:Y:112:CYS:SG	2.83	0.45
5:Y:220:VAL:HA	5:Y:223:THR:HG22	1.97	0.45
9:c:75:MET:SD	9:c:75:MET:N	2.90	0.45
12:f:764:LEU:HD11	12:f:774:GLY:HA3	1.98	0.45
17:E:9:LEU:HD11	18:F:29:ILE:HG12	1.98	0.45
23:I:57:ASP:HB3	23:I:59:VAL:HG13	1.97	0.45
23:I:216:LEU:HD12	23:I:225:ILE:HG12	1.97	0.45
27:M:34:SER:OG	27:M:65:ARG:NH2	2.43	0.45
31:Q:181:ARG:NH1	31:Q:190:ASP:OD1	2.49	0.45
24:j:32:ALA:HB2	24:j:45:VAL:HG23	1.97	0.45
26:l:66:VAL:HA	26:l:89:ARG:HE	1.81	0.45
34:t:136:SER:HB2	34:t:150:LEU:HD13	1.97	0.45
1:U:643:SER:O	1:U:649:ARG:NH1	2.43	0.45
3:W:142:ARG:NH2	3:W:176:SER:O	2.49	0.45
5:Y:265:GLU:OE1	5:Y:267:ARG:NH2	2.49	0.45
14:B:86:LYS:O	14:B:88:LEU:N	2.48	0.45
17:E:144:GLU:O	17:E:297:ARG:NH2	2.49	0.45
18:F:304:ARG:O	18:F:308:ARG:NH1	2.50	0.45
22:H:139:TRP:HA	22:H:144:PRO:HA	1.98	0.45
24:J:11:SER:OG	24:J:13:ASP:OD1	2.31	0.45
27:M:66:LEU:HD13	27:M:214:SER:HB2	1.97	0.45
31:q:171:PHE:HB3	31:q:173:LEU:H	1.81	0.45
31:q:181:ARG:NH1	31:q:190:ASP:OD1	2.49	0.45
2:V:144:ASP:HB2	2:V:150:ARG:HH21	1.82	0.45
2:V:262:SER:HB2	10:d:120:GLU:HG3	1.98	0.45
3:W:124:LEU:O	3:W:128:LEU:N	2.44	0.45
10:d:197:ILE:HG22	11:e:5:LYS:HG2	1.98	0.45
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.98	0.45
12:f:324:VAL:O	12:f:328:SER:N	2.48	0.45
14:B:74:MET:HE2	14:B:74:MET:HB3	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:M:99:ARG:NH2	27:M:105:ASN:OD1	2.50	0.45
29:O:31:CYS:SG	29:O:32:SER:N	2.83	0.45
31:Q:103:LEU:HB3	31:Q:117:TYR:HA	1.98	0.45
1:U:913:ILE:H	1:U:913:ILE:HG13	1.65	0.45
3:W:55:ARG:HH11	3:W:75:TYR:HB3	1.81	0.45
6:Z:209:ARG:HB3	7:a:353:LEU:HD12	1.97	0.45
7:a:89:ASP:HB3	7:a:92:VAL:HG22	1.99	0.45
12:f:344:VAL:HG11	12:f:391:LEU:HG	1.97	0.45
12:f:531:ASN:HD22	12:f:534:VAL:HB	1.81	0.45
15:C:144:PRO:O	15:C:205:HIS:ND1	2.50	0.45
16:D:115:ILE:HG22	16:D:139:LEU:HB2	1.99	0.45
17:E:167:PRO:O	17:E:274:LYS:NZ	2.49	0.45
21:G:126:THR:O	22:H:128:ARG:NH1	2.41	0.45
31:q:13:VAL:HG11	31:q:105:ALA:HB1	1.99	0.45
3:W:43:VAL:O	3:W:47:LEU:N	2.43	0.45
12:f:403:LYS:HG3	12:f:406:GLY:H	1.82	0.45
25:K:210:LEU:HD11	25:K:215:ILE:HG12	1.97	0.45
26:L:45:VAL:HG11	26:L:188:VAL:HG22	1.99	0.45
26:L:66:VAL:HA	26:L:89:ARG:HE	1.81	0.45
32:R:26:ILE:HG21	32:R:29:GLN:HE21	1.80	0.45
29:o:67:SER:HB3	29:o:74:PRO:HG3	1.99	0.45
33:s:191:ASP:O	33:s:210:LEU:N	2.49	0.45
1:U:70:HIS:HA	2:V:236:ARG:HH22	1.80	0.45
2:V:194:LYS:H	2:V:194:LYS:HD2	1.82	0.45
5:Y:181:LYS:C	11:e:65:TYR:HA	2.41	0.45
7:a:61:GLU:HG3	7:a:79:ILE:HD13	1.98	0.45
9:c:49:VAL:HG23	9:c:148:ILE:HD11	1.99	0.45
12:f:240:VAL:O	12:f:257:ARG:NH2	2.38	0.45
12:f:253:LEU:HA	12:f:257:ARG:HD3	1.99	0.45
12:f:395:GLY:O	12:f:399:LEU:N	2.43	0.45
12:f:464:ALA:O	12:f:467:SER:OG	2.34	0.45
12:f:705:ASN:OD1	12:f:706:ILE:N	2.46	0.45
13:A:66:LYS:HD2	13:A:75:PRO:HG3	1.99	0.45
13:A:217:PRO:O	13:A:220:THR:OG1	2.32	0.45
13:A:376:LEU:HB3	13:A:417:ILE:HD11	1.99	0.45
15:C:351:MET:HE1	15:C:362:VAL:HG21	1.99	0.45
17:E:180:LYS:HG2	17:E:301:ILE:HD12	1.98	0.45
28:N:7:GLN:HA	28:N:12:VAL:HA	1.99	0.45
31:Q:171:PHE:HB3	31:Q:173:LEU:H	1.81	0.45
27:m:51:LYS:O	27:m:210:GLU:N	2.48	0.45
27:m:99:ARG:NH2	27:m:105:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:r:38:ASN:HD22	32:r:41:LEU:HD12	1.82	0.45
3:W:302:TYR:O	3:W:306:LEU:N	2.50	0.45
7:a:186:LYS:HB3	7:a:193:GLN:HE22	1.81	0.45
13:A:105:ASP:HB2	13:A:110:LYS:HB2	1.98	0.45
14:B:65:LEU:HD23	14:B:68:ILE:HD12	1.99	0.45
18:F:98:ASP:N	18:F:98:ASP:OD1	2.50	0.45
18:F:265:ALA:HA	18:F:312:GLU:HG2	1.98	0.45
24:J:96:LEU:O	32:R:81:LYS:NZ	2.47	0.45
33:s:35:ILE:HB	34:t:151:ARG:HH12	1.81	0.45
1:U:714:SER:HA	1:U:717:ILE:HG22	1.98	0.45
1:U:801:GLN:HB3	1:U:877:LEU:HD22	1.98	0.45
2:V:99:ARG:HB3	2:V:103:SER:HB2	1.99	0.45
3:W:99:GLN:HA	3:W:102:ALA:HB3	1.98	0.45
7:a:80:ILE:HD12	7:a:83:VAL:HB	1.99	0.45
9:c:291:LEU:O	9:c:295:ASN:ND2	2.50	0.45
13:A:407:LYS:HA	13:A:410:LEU:HB2	1.97	0.45
17:E:194:ASN:ND2	17:E:227:PRO:O	2.49	0.45
18:F:124:ILE:HD11	18:F:160:ILE:HD11	1.97	0.45
34:t:49:THR:HB	34:t:85:PRO:HG3	1.98	0.45
1:U:632:GLN:O	1:U:635:SER:OG	2.34	0.45
3:W:231:ILE:HG21	3:W:247:TYR:HE1	1.82	0.45
5:Y:279:GLU:HG3	5:Y:283:LYS:HE3	1.98	0.45
10:d:148:TYR:HB2	11:e:3:GLU:HA	1.99	0.45
12:f:478:ARG:HG3	12:f:514:VAL:HG11	1.98	0.45
13:A:244:GLU:HA	14:B:268:ARG:HH22	1.81	0.45
16:D:85:ILE:HG23	17:E:80:VAL:HG12	1.99	0.45
16:D:139:LEU:HA	16:D:139:LEU:HD23	1.75	0.45
23:I:161:ALA:HB1	23:I:175:LEU:HD13	1.99	0.45
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.82	0.44
6:Z:82:PHE:HA	6:Z:85:VAL:HG12	1.98	0.44
12:f:692:LEU:HD13	13:A:77:LEU:HD12	1.99	0.44
15:C:253:SER:HB3	15:C:300:ILE:HD11	1.99	0.44
16:D:384:MET:HE2	17:E:159:PHE:HD1	1.81	0.44
26:L:204:ASP:HB3	26:L:239:ARG:HH22	1.82	0.44
31:Q:47:VAL:O	31:Q:101:ASN:N	2.48	0.44
33:S:191:ASP:O	33:S:210:LEU:N	2.49	0.44
2:V:357:LEU:O	2:V:361:PHE:N	2.39	0.44
7:a:28:LEU:HD23	7:a:37:LEU:HA	1.98	0.44
9:c:196:LEU:HA	9:c:197:ASN:HA	1.59	0.44
23:i:119:GLN:HE22	24:j:79:ASP:HA	1.82	0.44
1:U:445:ALA:HA	1:U:448:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:649:ARG:HD3	15:C:57:ARG:HH22	1.82	0.44
2:V:92:ARG:O	2:V:96:ARG:NH1	2.51	0.44
2:V:337:LEU:HD22	2:V:367:VAL:HG21	1.99	0.44
5:Y:287:LEU:HD12	11:e:58:ALA:H	1.83	0.44
9:c:269:GLN:HA	9:c:272:ILE:HG22	1.99	0.44
10:d:152:PHE:HB2	10:d:199:PHE:HE2	1.83	0.44
12:f:269:ALA:O	12:f:273:ASN:N	2.42	0.44
12:f:816:TYR:HB3	12:f:821:LEU:HD13	1.98	0.44
15:C:80:MET:HE1	15:C:86:LEU:HB2	2.00	0.44
17:E:12:TYR:OH	18:F:28:GLY:O	2.35	0.44
25:K:99:HIS:HB2	25:K:107:MET:HE3	1.99	0.44
27:M:47:PHE:HB2	27:M:214:SER:HB3	2.00	0.44
29:O:67:SER:HB3	29:O:74:PRO:HG3	1.99	0.44
34:T:41:ARG:HH21	34:T:54:SER:HA	1.82	0.44
26:l:146:GLN:HE21	26:l:154:PHE:HD2	1.65	0.44
29:o:163:ILE:HG23	29:o:170:GLY:HA2	1.99	0.44
34:t:41:ARG:HH21	34:t:54:SER:HA	1.82	0.44
2:V:68:ASP:O	2:V:72:LEU:N	2.51	0.44
2:V:257:ASN:HA	2:V:260:HIS:HB3	1.99	0.44
2:V:423:ALA:HA	2:V:428:LEU:HD23	1.99	0.44
7:a:284:ARG:NH2	7:a:288:HIS:O	2.44	0.44
13:A:258:ARG:HH22	18:F:255:GLN:HA	1.83	0.44
13:A:416:VAL:HA	13:A:419:SER:HB2	1.99	0.44
15:C:235:PHE:HD2	15:C:279:GLN:HG2	1.81	0.44
16:D:176:GLU:OE2	16:D:329:ARG:NH1	2.51	0.44
17:E:116:ASP:HB2	17:E:217:GLU:HG2	1.99	0.44
32:R:38:ASN:HD22	32:R:41:LEU:HD12	1.82	0.44
21:g:56:VAL:HG13	21:g:61:LEU:HD22	1.99	0.44
23:i:170:ALA:O	23:i:173:SER:OG	2.33	0.44
24:j:88:ARG:NH1	31:q:69:MET:O	2.50	0.44
33:s:27:THR:HB	33:s:40:SER:H	1.81	0.44
1:U:636:VAL:HG23	1:U:637:VAL:HG23	2.00	0.44
3:W:243:ILE:O	3:W:273:TYR:OH	2.27	0.44
5:Y:292:TYR:CB	11:e:54:ASN:H	2.31	0.44
6:Z:205:LEU:HA	6:Z:208:ILE:HG22	2.00	0.44
8:b:90:ILE:O	8:b:94:HIS:N	2.51	0.44
13:A:101:ILE:HD12	13:A:138:MET:HB3	2.00	0.44
13:A:114:ASN:HA	13:A:120:LYS:HA	2.00	0.44
14:B:299:SER:HA	14:B:303:ARG:HB2	1.99	0.44
19:u:36:ILE:HB	19:u:41:GLN:HE21	1.82	0.44
26:L:146:GLN:HE21	26:L:154:PHE:HD2	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:r:77:ALA:O	32:r:120:ARG:NH2	2.51	0.44
6:Z:182:THR:HG22	16:D:70:LYS:HE2	2.00	0.44
7:a:252:LYS:HD2	7:a:255:TRP:CD1	2.52	0.44
10:d:199:PHE:HD1	10:d:199:PHE:HA	1.73	0.44
17:E:312:ILE:HA	17:E:315:ILE:HD12	1.99	0.44
28:N:19:ARG:HH11	28:N:171:GLY:HA3	1.82	0.44
29:O:96:ALA:H	29:O:115:PRO:HB3	1.83	0.44
23:i:180:LYS:HD2	23:i:183:GLU:HB2	1.98	0.44
26:l:196:ARG:HA	26:l:199:LEU:HD12	1.99	0.44
27:m:47:PHE:HB2	27:m:214:SER:HB3	2.00	0.44
29:o:112:SER:HB3	29:o:125:VAL:HG11	1.99	0.44
1:U:643:SER:HA	15:C:53:ASN:HD21	1.82	0.44
2:V:401:ASN:HD22	2:V:404:LYS:HB2	1.83	0.44
5:Y:186:LEU:H	11:e:64:GLY:N	2.16	0.44
5:Y:289:ALA:C	11:e:57:ARG:HD3	2.43	0.44
5:Y:349:LYS:O	5:Y:351:ASN:N	2.51	0.44
9:c:175:ARG:HE	9:c:181:LEU:HD11	1.83	0.44
12:f:414:LEU:HD23	12:f:417:ILE:HD12	2.00	0.44
12:f:612:LEU:HD21	12:f:636:ASP:HA	1.98	0.44
15:C:273:MET:HA	15:C:276:LEU:HD12	2.00	0.44
25:K:37:ALA:HB2	25:K:50:VAL:HG23	1.98	0.44
26:l:225:ASP:OD1	26:l:225:ASP:N	2.47	0.44
1:U:381:THR:HG22	1:U:412:HIS:HA	1.98	0.44
1:U:415:HIS:CD2	1:U:418:GLU:H	2.35	0.44
1:U:471:ASP:HA	1:U:474:ARG:HB2	2.00	0.44
1:U:611:ASN:HB3	1:U:614:VAL:HG12	2.00	0.44
1:U:765:VAL:HG11	1:U:778:PHE:HD2	1.83	0.44
4:X:401:LEU:HA	4:X:404:ILE:HD12	1.99	0.44
7:a:72:ASN:HD21	7:a:74:LEU:HD12	1.83	0.44
12:f:647:GLY:O	12:f:651:GLY:N	2.51	0.44
12:f:674:THR:O	12:f:678:LEU:N	2.38	0.44
14:B:271:PHE:HE1	14:B:282:VAL:HG11	1.81	0.44
14:B:375:ALA:H	14:B:414:VAL:HB	1.83	0.44
17:E:56:ILE:HB	17:E:100:LEU:HB2	1.99	0.44
29:O:112:SER:HB3	29:O:125:VAL:HG11	1.99	0.44
23:i:9:THR:HG22	23:i:20:GLN:HE21	1.83	0.44
28:n:19:ARG:HH11	28:n:171:GLY:HA3	1.82	0.44
31:q:38:MET:O	31:q:65:GLN:NE2	2.50	0.44
1:U:202:VAL:HB	1:U:216:VAL:HG23	1.99	0.44
4:X:214:SER:O	4:X:218:HIS:ND1	2.36	0.44
12:f:169:GLU:HA	12:f:172:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:250:ARG:NH1	12:f:285:CYS:SG	2.91	0.44
12:f:414:LEU:HA	12:f:417:ILE:HD12	1.98	0.44
12:f:460:ASP:HB2	12:f:464:ALA:H	1.83	0.44
13:A:279:ALA:HB2	14:B:310:LEU:HD23	2.00	0.44
29:O:163:ILE:HG23	29:O:170:GLY:HA2	1.99	0.44
31:Q:38:MET:O	31:Q:65:GLN:NE2	2.50	0.44
23:i:161:ALA:HB1	23:i:175:LEU:HD13	1.99	0.44
1:U:188:MET:HG2	1:U:194:ARG:HB2	2.00	0.43
2:V:333:ILE:HA	2:V:336:GLU:HB2	1.99	0.43
5:Y:297:ARG:HD3	5:Y:337:PHE:CE1	2.53	0.43
12:f:194:TYR:O	12:f:198:HIS:N	2.44	0.43
12:f:305:LEU:HB2	12:f:317:LEU:HD22	2.00	0.43
12:f:755:ASP:N	12:f:755:ASP:OD1	2.50	0.43
1:U:43:ASP:HA	1:U:46:GLU:HB3	2.00	0.43
2:V:40:GLU:HA	2:V:43:THR:HB	2.00	0.43
3:W:334:GLU:OE2	3:W:338:THR:OG1	2.35	0.43
7:a:222:LEU:HD12	7:a:226:ARG:HE	1.82	0.43
9:c:226:MET:SD	9:c:226:MET:N	2.92	0.43
12:f:873:LEU:HG	12:f:875:ALA:H	1.82	0.43
14:B:51:LEU:HD11	14:B:53:THR:HG22	2.00	0.43
18:F:129:ARG:HH21	20:v:14:UNK:CB	2.31	0.43
21:G:56:VAL:HG13	21:G:61:LEU:HD22	1.99	0.43
23:I:135:LEU:HG	23:I:164:ILE:HD11	2.00	0.43
1:U:361:ARG:HG3	1:U:363:SER:H	1.83	0.43
5:Y:290:PRO:N	11:e:57:ARG:HD3	2.34	0.43
8:b:26:LEU:HD11	8:b:80:PRO:HG3	1.99	0.43
12:f:206:ASP:OD2	12:f:245:ASN:ND2	2.52	0.43
13:A:117:GLN:NE2	14:B:127:VAL:O	2.42	0.43
13:A:312:ARG:HD2	13:A:315:ILE:HB	1.99	0.43
15:C:297:ARG:HH21	15:C:299:ASP:HB2	1.83	0.43
30:P:58:THR:OG1	31:Q:121:LEU:O	2.28	0.43
28:n:7:GLN:HA	28:n:12:VAL:HA	1.99	0.43
5:Y:292:TYR:HB2	5:Y:295:TYR:HB3	2.00	0.43
12:f:476:THR:O	12:f:480:GLY:N	2.43	0.43
13:A:277:ILE:H	13:A:277:ILE:HG13	1.57	0.43
14:B:118:ASP:O	14:B:141:LYS:NZ	2.49	0.43
15:C:224:ILE:HG12	15:C:268:GLU:HG2	2.01	0.43
16:D:191:TYR:HA	16:D:196:ILE:HD12	1.99	0.43
17:E:83:CYS:HB2	17:E:89:LYS:HE2	2.01	0.43
1:U:772:TRP:CD1	1:U:775:LEU:HB2	2.53	0.43
3:W:20:TYR:O	3:W:23:THR:OG1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:252:LYS:HA	7:a:255:TRP:HD1	1.82	0.43
12:f:704:LEU:O	12:f:708:ASP:N	2.48	0.43
12:f:733:GLY:O	12:f:746:ARG:NH1	2.41	0.43
16:D:385:LEU:HD23	16:D:398:ASP:HA	1.99	0.43
18:F:212:PHE:O	18:F:216:GLY:N	2.43	0.43
18:F:249:LEU:HD23	18:F:283:ILE:HG12	1.99	0.43
18:F:256:LEU:HD12	18:F:291:ILE:HD13	2.00	0.43
18:F:413:THR:OG1	18:F:414:GLU:OE1	2.37	0.43
25:K:20:ARG:HG3	25:K:21:LEU:H	1.83	0.43
32:R:77:ALA:O	32:R:120:ARG:NH2	2.51	0.43
25:k:85:ALA:HB2	25:k:139:VAL:HG21	2.00	0.43
26:l:204:ASP:HB3	26:l:239:ARG:HH22	1.82	0.43
27:m:110:HIS:CE1	28:n:69:GLU:HG2	2.54	0.43
1:U:70:HIS:CD2	2:V:236:ARG:HH12	2.37	0.43
2:V:449:ALA:HB2	2:V:460:SER:HB3	1.99	0.43
3:W:131:VAL:HG13	3:W:144:ARG:HD3	2.00	0.43
6:Z:102:HIS:N	6:Z:105:ASP:OD2	2.41	0.43
7:a:170:ALA:O	7:a:174:LYS:N	2.41	0.43
8:b:61:LEU:HD23	8:b:74:LYS:HD2	2.01	0.43
12:f:102:HIS:CE1	12:f:106:LEU:HG	2.54	0.43
12:f:696:LEU:HD22	13:A:85:GLN:HB2	2.01	0.43
14:B:103:ARG:HB2	14:B:160:ILE:HD13	2.00	0.43
14:B:439:TYR:HE2	24:J:61:LYS:HE3	1.82	0.43
23:i:76:VAL:HG23	23:i:134:LEU:HB3	2.00	0.43
1:U:885:MET:HG2	1:U:887:ALA:H	1.83	0.43
4:X:255:LEU:HD22	4:X:267:VAL:HG13	2.00	0.43
4:X:255:LEU:HB2	4:X:287:LEU:HD13	2.01	0.43
14:B:113:GLU:HB3	14:B:122:ILE:HG23	2.00	0.43
14:B:291:GLY:HA2	14:B:309:MET:HG3	2.01	0.43
18:F:124:ILE:HD12	18:F:134:LEU:HD21	2.00	0.43
18:F:253:GLY:HA3	18:F:287:GLU:HG2	1.99	0.43
18:F:311:LEU:HD23	18:F:314:LEU:HD12	2.01	0.43
19:u:22:THR:OG1	19:u:25:ASN:ND2	2.52	0.43
23:I:9:THR:HG22	23:I:20:GLN:HE21	1.83	0.43
23:I:167:ASN:ND2	23:I:200:THR:O	2.50	0.43
31:Q:4:LEU:HD22	31:Q:45:LEU:HD13	2.00	0.43
31:q:4:LEU:HD22	31:q:45:LEU:HD13	2.00	0.43
31:q:17:SER:OG	31:q:179:SER:OG	2.36	0.43
1:U:98:GLU:HA	1:U:101:ILE:HG12	2.01	0.43
3:W:175:GLY:HA2	17:E:161:ARG:NH1	2.34	0.43
7:a:34:TRP:HZ3	7:a:64:ILE:HG23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:167:MET:HE3	9:c:170:LEU:HD23	2.00	0.43
12:f:603:SER:HB2	12:f:639:LYS:HZ2	1.82	0.43
13:A:406:GLU:O	13:A:410:LEU:N	2.39	0.43
25:K:85:ALA:HB2	25:K:139:VAL:HG21	2.00	0.43
26:l:157:ARG:NE	27:m:59:GLU:OE2	2.52	0.43
1:U:261:LEU:HA	1:U:264:VAL:HG12	2.00	0.43
1:U:416:GLU:OE1	1:U:450:HIS:NE2	2.50	0.43
1:U:424:ALA:HA	1:U:427:LEU:HD13	2.01	0.43
2:V:330:LYS:O	2:V:360:TYR:OH	2.26	0.43
2:V:439:ALA:H	11:e:4:LYS:HZ3	1.66	0.43
6:Z:37:GLY:HA2	6:Z:56:VAL:HG12	2.01	0.43
6:Z:226:ILE:HG13	6:Z:226:ILE:H	1.60	0.43
10:d:103:LEU:HD23	10:d:136:PRO:HB2	2.00	0.43
12:f:182:GLU:OE2	12:f:186:THR:OG1	2.35	0.43
12:f:283:THR:O	12:f:287:ASP:N	2.41	0.43
16:D:144:PRO:HA	16:D:145:PRO:HD3	1.84	0.43
22:H:185:GLU:O	22:H:229:TYR:OH	2.36	0.43
30:P:177:ARG:NH2	33:s:150:ASP:OD2	2.46	0.43
31:Q:17:SER:OG	31:Q:179:SER:OG	2.36	0.43
21:g:141:ILE:HG22	21:g:151:VAL:HG22	2.01	0.43
23:i:135:LEU:HG	23:i:164:ILE:HD11	2.00	0.43
27:m:67:PHE:HB2	27:m:75:MET:HB2	2.01	0.43
31:q:168:GLN:NE2	31:q:175:LEU:O	2.49	0.43
1:U:593:SER:OG	1:U:595:ASN:ND2	2.52	0.43
2:V:249:THR:HG22	2:V:284:GLU:HG3	2.00	0.43
5:Y:45:VAL:HG23	5:Y:46:ARG:HD3	2.01	0.43
6:Z:235:ASN:HD21	7:a:336:VAL:H	1.65	0.43
9:c:34:SER:HB3	9:c:70:ILE:HA	2.01	0.43
15:C:173:GLU:HA	15:C:176:GLU:HB2	2.01	0.43
22:h:100:VAL:HG13	30:p:93:ASN:HD22	1.84	0.43
25:k:20:ARG:HG3	25:k:21:LEU:H	1.83	0.43
29:o:96:ALA:H	29:o:115:PRO:HB3	1.83	0.43
2:V:228:ARG:O	2:V:232:HIS:ND1	2.34	0.42
2:V:465:ASP:HA	2:V:468:SER:HB3	2.00	0.42
5:Y:291:HIS:O	11:e:56:LEU:N	2.52	0.42
8:b:25:ARG:NH1	8:b:114:GLY:O	2.52	0.42
12:f:31:LYS:HE3	12:f:82:ILE:HG21	2.01	0.42
17:E:317:ALA:HA	17:E:320:ILE:HD12	2.00	0.42
26:L:204:ASP:OD1	26:L:204:ASP:N	2.52	0.42
22:h:185:GLU:O	22:h:229:TYR:OH	2.36	0.42
23:i:63:GLU:CD	23:i:64:LYS:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:167:ASN:ND2	23:i:200:THR:O	2.50	0.42
25:k:99:HIS:HB2	25:k:107:MET:HE3	1.99	0.42
27:m:181:MET:HE3	27:m:181:MET:HB3	1.74	0.42
30:p:107:PRO:HG2	30:p:124:LEU:HB2	2.01	0.42
31:q:47:VAL:O	31:q:101:ASN:N	2.48	0.42
34:t:9:THR:O	34:t:41:ARG:NH2	2.51	0.42
1:U:208:LEU:HD23	1:U:210:LYS:H	1.85	0.42
5:Y:190:ALA:HB2	11:e:63:HIS:CG	2.55	0.42
7:a:138:VAL:O	7:a:142:LEU:N	2.51	0.42
12:f:810:ILE:HG22	12:f:855:GLN:HA	2.00	0.42
13:A:84:LYS:HA	13:A:87:LEU:HD13	2.01	0.42
18:F:26:GLN:O	18:F:30:GLY:N	2.47	0.42
18:F:300:LYS:HB2	18:F:301:ALA:H	1.62	0.42
21:G:141:ILE:HG22	21:G:151:VAL:HG22	2.01	0.42
26:L:199:LEU:HD13	26:L:204:ASP:HA	2.01	0.42
27:M:181:MET:HB3	27:M:181:MET:HE3	1.74	0.42
29:O:6:VAL:HG23	29:O:124:TYR:HB3	2.01	0.42
30:P:107:PRO:HG2	30:P:124:LEU:HB2	2.01	0.42
33:S:148:LEU:HD23	33:S:178:VAL:HG12	2.01	0.42
21:g:32:ILE:HA	21:g:82:GLY:HA2	2.01	0.42
2:V:420:ALA:HA	2:V:431:PRO:HB3	2.00	0.42
16:D:288:ILE:O	16:D:292:LEU:N	2.46	0.42
21:G:32:ILE:HA	21:G:82:GLY:HA2	2.01	0.42
24:J:33:VAL:HG11	24:J:168:VAL:HG11	2.02	0.42
26:L:196:ARG:HA	26:L:199:LEU:HD12	1.99	0.42
34:t:153:VAL:HG21	34:t:168:LEU:HD11	2.01	0.42
1:U:409:GLY:HA3	1:U:445:ALA:HB1	2.01	0.42
3:W:395:ASN:HA	3:W:398:VAL:HG22	2.00	0.42
4:X:252:LYS:HA	4:X:287:LEU:HD11	2.01	0.42
5:Y:297:ARG:HA	5:Y:300:ARG:HB2	2.01	0.42
8:b:58:CYS:HB3	8:b:92:VAL:HG11	2.02	0.42
8:b:184:ILE:HA	8:b:187:PRO:HD2	2.01	0.42
9:c:189:ILE:HD12	9:c:192:LEU:HD11	2.01	0.42
12:f:77:GLU:HB2	12:f:79:ARG:HH12	1.83	0.42
12:f:347:ASP:O	12:f:351:THR:OG1	2.34	0.42
15:C:134:LEU:HD22	15:C:230:MET:HA	2.02	0.42
16:D:155:THR:OG1	16:D:156:SER:N	2.53	0.42
16:D:159:LYS:HA	16:D:160:PRO:HD3	1.86	0.42
26:L:148:CYS:SG	26:L:150:SER:OG	2.66	0.42
34:T:153:VAL:HG21	34:T:168:LEU:HD11	2.01	0.42
26:l:199:LEU:HD13	26:l:204:ASP:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:r:44:THR:HG21	32:r:100:MET:HE3	2.01	0.42
1:U:28:ASN:HB3	1:U:59:PHE:HZ	1.83	0.42
2:V:439:ALA:HB3	11:e:4:LYS:HA	2.01	0.42
23:I:76:VAL:HG23	23:I:134:LEU:HB3	2.00	0.42
23:I:119:GLN:HE22	24:J:79:ASP:HA	1.83	0.42
25:K:165:CYS:HA	26:L:57:ALA:HA	2.02	0.42
26:L:41:LYS:NZ	26:L:180:MET:O	2.44	0.42
26:L:159:MET:HE1	26:L:169:ARG:HE	1.84	0.42
32:R:44:THR:HG21	32:R:100:MET:HE3	2.01	0.42
25:k:60:GLU:OE1	25:k:63:SER:N	2.53	0.42
29:o:6:VAL:HG23	29:o:124:TYR:HB3	2.01	0.42
16:D:303:VAL:HG12	16:D:305:VAL:HG23	2.01	0.42
27:M:54:LEU:HB2	27:M:57:LEU:HG	2.02	0.42
22:h:34:PRO:HA	22:h:164:GLY:HA3	2.02	0.42
1:U:646:PRO:HA	1:U:649:ARG:HB2	2.00	0.42
2:V:74:ASP:O	2:V:78:HIS:NE2	2.52	0.42
3:W:82:LEU:HD22	3:W:90:LEU:HG	2.02	0.42
3:W:152:ILE:HD11	3:W:165:ILE:HB	2.01	0.42
5:Y:186:LEU:N	11:e:65:TYR:H	2.18	0.42
12:f:406:GLY:HA2	12:f:409:SER:HB2	2.02	0.42
12:f:852:VAL:HG22	12:f:853:VAL:HG13	2.00	0.42
22:H:34:PRO:HA	22:H:164:GLY:HA3	2.02	0.42
23:I:63:GLU:CD	23:I:64:LYS:H	2.27	0.42
24:J:159:ASN:OD1	24:J:160:ALA:N	2.53	0.42
21:g:84:THR:HB	27:m:156:VAL:HG22	2.01	0.42
24:j:8:THR:HG22	24:j:16:LEU:HD22	2.01	0.42
1:U:788:VAL:HG12	1:U:909:GLY:HA2	2.00	0.42
5:Y:47:ASP:OD1	5:Y:113:ARG:NH1	2.52	0.42
6:Z:170:VAL:HA	9:c:152:LYS:HA	2.01	0.42
8:b:116:PRO:HA	8:b:146:GLU:HA	2.01	0.42
10:d:203:PRO:HG2	10:d:205:LYS:H	1.85	0.42
13:A:362:MET:HG3	13:A:364:VAL:HG13	2.01	0.42
15:C:117:ARG:HD3	15:C:120:SER:HB2	2.02	0.42
24:J:8:THR:HG22	24:J:16:LEU:HD22	2.01	0.42
27:M:50:GLU:O	27:M:65:ARG:NH2	2.52	0.42
32:R:9:ARG:NH2	32:R:146:ASP:OD1	2.48	0.42
32:R:154:ASP:OD1	32:R:157:ARG:NH1	2.52	0.42
33:s:148:LEU:HD23	33:s:178:VAL:HG12	2.01	0.42
1:U:253:TYR:CZ	1:U:331:GLY:HA3	2.55	0.42
1:U:450:HIS:HB2	1:U:457:ILE:HG21	2.02	0.42
2:V:361:PHE:HD2	2:V:362:LEU:HD22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:312:MET:HG2	3:W:315:MET:H	1.84	0.42
6:Z:225:GLN:O	6:Z:227:ILE:N	2.53	0.42
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.01	0.42
12:f:241:PRO:O	12:f:245:ASN:N	2.43	0.42
12:f:261:ARG:HG2	12:f:266:LEU:HD13	2.02	0.42
12:f:777:THR:OG1	12:f:805:ASP:OD2	2.33	0.42
17:E:182:LEU:HD22	38:E:401:ADP:H2'	2.01	0.42
21:g:88:ARG:NH1	27:m:157:SER:O	2.38	0.42
23:i:15:GLU:OE1	23:i:17:ARG:NE	2.39	0.42
24:j:159:ASN:OD1	24:j:160:ALA:N	2.53	0.42
26:l:37:GLY:HA2	26:l:46:LEU:HA	2.01	0.42
26:l:159:MET:HE1	26:l:169:ARG:HE	1.84	0.42
2:V:300:LEU:HD11	10:d:116:HIS:CD2	2.55	0.42
2:V:345:ARG:HH12	2:V:353:LEU:HD21	1.85	0.42
3:W:260:SER:HA	3:W:263:TRP:HE3	1.85	0.42
5:Y:292:TYR:HB3	11:e:54:ASN:H	1.84	0.42
12:f:77:GLU:O	12:f:79:ARG:NH1	2.53	0.42
12:f:94:LYS:HE2	12:f:110:TYR:HB2	2.00	0.42
12:f:843:SER:OG	12:f:844:VAL:N	2.52	0.42
13:A:276:GLU:HB3	14:B:310:LEU:HD21	2.02	0.42
17:E:125:GLU:HG3	18:F:321:GLN:HE22	1.84	0.42
24:J:32:ALA:HB3	24:J:161:ILE:HD11	2.02	0.42
25:K:146:VAL:HG22	25:K:151:PRO:HB3	2.02	0.42
23:i:40:ASN:OD1	23:i:184:MET:N	2.40	0.42
26:l:15:PRO:O	27:m:28:LYS:NZ	2.36	0.42
2:V:393:THR:O	2:V:397:ARG:NH2	2.53	0.41
3:W:52:LYS:HZ3	3:W:90:LEU:HD11	1.85	0.41
5:Y:297:ARG:HG3	11:e:51:ASP:HA	2.02	0.41
16:D:373:ALA:HA	36:D:501:ATP:H1'	2.02	0.41
26:L:152:ASN:HA	27:M:85:ARG:HH22	1.85	0.41
26:L:155:ASP:HB3	27:M:62:SER:HB2	2.02	0.41
27:M:51:LYS:O	27:M:210:GLU:N	2.48	0.41
31:Q:182:ILE:HG23	31:Q:189:HIS:HB2	2.02	0.41
25:k:146:VAL:HG22	25:k:151:PRO:HB3	2.02	0.41
32:r:12:VAL:HB	32:r:179:VAL:HB	2.02	0.41
32:r:35:ILE:N	32:r:43:GLY:O	2.52	0.41
32:r:154:ASP:OD1	32:r:157:ARG:NH1	2.52	0.41
1:U:791:LEU:O	1:U:914:LEU:N	2.44	0.41
3:W:22:ALA:O	3:W:26:GLN:N	2.51	0.41
3:W:111:TYR:O	3:W:115:ILE:N	2.40	0.41
10:d:2:TYR:HE1	10:d:50:LEU:HD22	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:814:SER:OG	12:f:822:VAL:O	2.38	0.41
22:H:40:ALA:HB1	22:H:182:LEU:HB2	2.02	0.41
32:R:35:ILE:N	32:R:43:GLY:O	2.52	0.41
1:U:247:GLN:HG3	1:U:904:LYS:HD2	2.02	0.41
4:X:208:ALA:HB2	4:X:238:GLY:HA3	2.02	0.41
12:f:9:ALA:HA	12:f:13:PRO:HD2	2.02	0.41
12:f:15:GLN:O	12:f:19:ALA:N	2.49	0.41
12:f:382:ASN:HB3	12:f:417:ILE:HG23	2.01	0.41
15:C:117:ARG:HB3	15:C:122:THR:H	1.85	0.41
21:G:120:ASP:OD1	22:H:84:ARG:NH1	2.54	0.41
23:I:10:THR:HG22	24:J:125:ARG:HB2	2.01	0.41
23:I:119:GLN:NE2	23:I:123:GLN:HE21	2.19	0.41
25:K:60:GLU:OE1	25:K:63:SER:N	2.53	0.41
27:M:23:VAL:HG12	27:M:27:MET:HE3	2.02	0.41
27:M:110:HIS:NE2	28:N:70:LEU:HD23	2.36	0.41
24:j:32:ALA:HB3	24:j:161:ILE:HD11	2.02	0.41
27:m:50:GLU:O	27:m:65:ARG:NH2	2.52	0.41
27:m:54:LEU:HB2	27:m:57:LEU:HG	2.02	0.41
2:V:62:HIS:O	2:V:66:GLU:N	2.50	0.41
5:Y:71:ASN:HA	5:Y:74:LYS:HG2	2.02	0.41
5:Y:176:ARG:HG3	5:Y:180:LEU:HD13	2.01	0.41
6:Z:67:VAL:HG11	8:b:91:ARG:HG3	2.01	0.41
9:c:80:THR:HA	18:F:113:LEU:HD23	2.02	0.41
12:f:634:LYS:HA	12:f:637:LYS:HZ3	1.85	0.41
18:F:301:ALA:O	18:F:303:ASP:N	2.54	0.41
29:O:135:MET:SD	34:t:179:ARG:NH2	2.93	0.41
31:q:23:SER:HB2	31:q:28:MET:HE2	2.02	0.41
1:U:696:ILE:HG22	1:U:737:LEU:HA	2.01	0.41
3:W:29:PRO:HA	3:W:32:ALA:HB3	2.02	0.41
7:a:163:TYR:CG	7:a:172:TYR:HB2	2.56	0.41
12:f:171:GLN:HG2	12:f:208:LEU:HD21	2.01	0.41
27:m:23:VAL:HG12	27:m:27:MET:HE3	2.02	0.41
1:U:505:ASP:HB3	1:U:508:THR:HG22	2.02	0.41
14:B:291:GLY:HA3	14:B:309:MET:HE2	2.02	0.41
15:C:303:SER:O	15:C:307:ARG:N	2.54	0.41
16:D:152:MET:SD	16:D:152:MET:N	2.94	0.41
16:D:187:HIS:HB3	16:D:190:LEU:HD12	2.01	0.41
17:E:198:VAL:HB	17:E:232:MET:HG2	2.02	0.41
17:E:219:PHE:O	17:E:223:ARG:N	2.53	0.41
22:H:225:GLU:HA	22:H:228:ASP:HB2	2.03	0.41
24:J:154:HIS:NE2	25:K:59:MET:SD	2.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:M:67:PHE:HB2	27:M:75:MET:HB2	2.01	0.41
29:o:211:VAL:HG11	30:p:198:ARG:HD3	2.02	0.41
5:Y:186:LEU:N	11:e:64:GLY:N	2.64	0.41
10:d:179:ALA:HB1	10:d:213:ARG:HG3	2.03	0.41
13:A:124:ASP:OD1	13:A:125:LEU:N	2.53	0.41
17:E:19:HIS:CD2	18:F:48:LEU:HD22	2.56	0.41
25:K:15:PHE:HE2	26:L:127:PRO:HD2	1.85	0.41
29:o:38:SER:OG	29:o:40:ASN:OD1	2.32	0.41
5:Y:185:GLY:C	11:e:63:HIS:H	2.28	0.41
5:Y:205:VAL:HG13	15:C:377:HIS:CE1	2.56	0.41
7:a:34:TRP:HD1	8:b:18:ASN:HA	1.84	0.41
14:B:223:ILE:HG22	14:B:225:TYR:HD1	1.86	0.41
21:G:125:TYR:HB3	21:G:133:PRO:HA	2.03	0.41
29:O:38:SER:OG	29:O:40:ASN:OD1	2.32	0.41
1:U:157:THR:HG23	1:U:159:ARG:H	1.86	0.41
2:V:410:ILE:HD13	2:V:422:ILE:HG13	2.03	0.41
2:V:412:LEU:O	5:Y:346:LYS:NZ	2.46	0.41
3:W:82:LEU:HA	3:W:85:GLU:HG2	2.02	0.41
3:W:155:GLN:HG2	3:W:157:GLY:H	1.84	0.41
3:W:268:LYS:HG3	3:W:333:LEU:HD11	2.02	0.41
5:Y:12:PRO:HB2	5:Y:13:LYS:H	1.60	0.41
6:Z:209:ARG:HH22	7:a:354:GLU:HG2	1.86	0.41
10:d:164:THR:HA	10:d:167:ILE:HG12	2.03	0.41
12:f:168:LYS:HD3	12:f:204:ALA:HB1	2.01	0.41
12:f:654:VAL:HG22	14:B:75:GLU:HB2	2.03	0.41
13:A:327:LEU:HD13	13:A:327:LEU:HA	1.90	0.41
16:D:384:MET:HE1	17:E:164:ILE:HB	2.03	0.41
18:F:94:ILE:HD11	18:F:125:LYS:HB2	2.02	0.41
22:h:40:ALA:HB1	22:h:182:LEU:HB2	2.02	0.41
24:j:33:VAL:HG11	24:j:168:VAL:HG11	2.02	0.41
24:j:104:VAL:HG13	24:j:145:TYR:HE2	1.86	0.41
27:m:34:SER:OG	27:m:65:ARG:NH2	2.43	0.41
1:U:167:ILE:HB	1:U:177:LEU:HD11	2.02	0.41
1:U:701:ILE:HG21	1:U:810:THR:HG22	2.02	0.41
8:b:124:LEU:HD21	8:b:152:LYS:HB3	2.03	0.41
9:c:88:ASP:N	9:c:88:ASP:OD1	2.54	0.41
9:c:139:ARG:H	9:c:139:ARG:HD2	1.85	0.41
12:f:16:SER:HA	12:f:19:ALA:HB3	2.03	0.41
14:B:56:THR:OG1	14:B:57:GLN:N	2.54	0.41
18:F:299:GLU:N	18:F:299:GLU:CD	2.79	0.41
21:G:27:TYR:HA	21:G:30:LYS:HZ3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:H:14:SER:HG	22:H:18:LYS:H	1.67	0.41
26:L:37:GLY:HA2	26:L:46:LEU:HA	2.01	0.41
33:S:187:VAL:HG21	29:o:24:MET:HE3	2.03	0.41
24:j:64:ALA:O	24:j:88:ARG:NH1	2.54	0.41
1:U:155:LEU:O	1:U:158:ARG:NH1	2.53	0.40
2:V:174:PHE:HD1	2:V:177:ASN:HD22	1.69	0.40
2:V:401:ASN:HA	2:V:404:LYS:HB2	2.02	0.40
3:W:44:ILE:HA	3:W:47:LEU:HD12	2.02	0.40
3:W:131:VAL:HG22	3:W:144:ARG:HG3	2.03	0.40
5:Y:185:GLY:H	11:e:65:TYR:N	2.18	0.40
5:Y:187:TYR:H	11:e:64:GLY:HA3	1.86	0.40
8:b:150:THR:HB	8:b:153:LEU:HB2	2.04	0.40
9:c:135:ALA:HB3	19:u:36:ILE:HD11	2.03	0.40
12:f:679:LEU:HD12	12:f:686:LEU:HD13	2.03	0.40
13:A:98:CYS:HA	13:A:141:GLY:HA2	2.03	0.40
16:D:345:PHE:HB3	16:D:360:LEU:HD21	2.01	0.40
17:E:12:TYR:HA	17:E:15:LYS:HB2	2.04	0.40
18:F:217:ILE:HG13	18:F:218:GLN:H	1.86	0.40
32:R:12:VAL:HB	32:R:179:VAL:HB	2.02	0.40
34:T:9:THR:O	34:T:41:ARG:NH2	2.51	0.40
23:i:119:GLN:NE2	23:i:123:GLN:HE21	2.19	0.40
25:k:21:LEU:HD13	25:k:24:VAL:HB	2.04	0.40
2:V:430:SER:HA	2:V:431:PRO:HD3	1.93	0.40
6:Z:91:ILE:H	6:Z:91:ILE:HG13	1.59	0.40
8:b:20:ASP:OD2	8:b:25:ARG:NH2	2.44	0.40
8:b:112:PHE:HE1	8:b:141:ILE:HD12	1.86	0.40
12:f:460:ASP:OD1	12:f:460:ASP:N	2.52	0.40
13:A:101:ILE:HA	13:A:113:ILE:HG12	2.02	0.40
13:A:362:MET:HE3	14:B:216:ILE:HD11	2.03	0.40
18:F:168:TYR:HB2	18:F:173:LYS:HE2	2.04	0.40
31:Q:102:LEU:HD22	31:Q:103:LEU:H	1.86	0.40
22:h:225:GLU:HA	22:h:228:ASP:HB2	2.03	0.40
31:q:182:ILE:HG23	31:q:189:HIS:HB2	2.02	0.40
2:V:159:LEU:O	2:V:163:VAL:N	2.50	0.40
4:X:407:MET:HA	4:X:410:VAL:HG22	2.02	0.40
5:Y:188:CYS:H	11:e:63:HIS:C	2.29	0.40
9:c:197:ASN:ND2	9:c:200:TYR:O	2.54	0.40
12:f:221:ILE:HD12	12:f:224:ASN:HB2	2.03	0.40
13:A:178:GLY:HA3	13:A:353:HIS:HD2	1.87	0.40
15:C:76:VAL:HA	15:C:87:VAL:HG22	2.04	0.40
21:g:125:TYR:HB3	21:g:133:PRO:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:232:GLU:HA	23:i:235:GLN:HG2	2.04	0.40
3:W:273:TYR:HA	3:W:276:LEU:HB2	2.03	0.40
5:Y:13:LYS:HE3	5:Y:146:ARG:NH1	2.36	0.40
7:a:70:ARG:HG3	8:b:17:ARG:HD2	2.04	0.40
7:a:168:ASN:ND2	7:a:171:SER:OG	2.55	0.40
9:c:52:GLU:OE1	19:u:76:GLY:HA2	2.21	0.40
12:f:321:MET:HE3	12:f:456:ARG:HG3	2.04	0.40
15:C:232:ARG:HH12	15:C:275:GLU:HB3	1.86	0.40
15:C:286:THR:O	15:C:288:ASN:N	2.54	0.40
24:J:115:LYS:HG3	24:J:127:PHE:HD2	1.87	0.40
27:M:198:TYR:CZ	27:M:240:LYS:HG2	2.57	0.40
28:N:19:ARG:HH21	34:t:181:ALA:HA	1.87	0.40
29:O:19:ARG:NH2	33:s:213:ASP:OD2	2.55	0.40
30:P:36:THR:OG1	30:P:38:ASP:OD1	2.33	0.40
32:R:97:MET:O	32:R:116:SER:N	2.55	0.40
31:q:102:LEU:HD22	31:q:103:LEU:H	1.86	0.40
31:q:171:PHE:HD1	31:q:171:PHE:HA	1.78	0.40
2:V:203:LEU:O	2:V:207:ALA:N	2.44	0.40
10:d:51:ALA:HA	10:d:54:ILE:HG12	2.02	0.40
14:B:116:ILE:HD12	14:B:132:TYR:HE1	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	806/953 (85%)	748 (93%)	55 (7%)	3 (0%)	30	60
2	V	478/533 (90%)	412 (86%)	65 (14%)	1 (0%)	43	71
3	W	454/456 (100%)	409 (90%)	45 (10%)	0	100	100
4	X	378/422 (90%)	362 (96%)	15 (4%)	1 (0%)	36	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	Y	376/389 (97%)	317 (84%)	51 (14%)	8 (2%)	5	26
6	Z	284/324 (88%)	251 (88%)	32 (11%)	1 (0%)	30	60
7	a	371/376 (99%)	334 (90%)	35 (9%)	2 (0%)	24	55
8	b	189/377 (50%)	168 (89%)	20 (11%)	1 (0%)	24	55
9	c	285/309 (92%)	256 (90%)	29 (10%)	0	100	100
10	d	255/349 (73%)	213 (84%)	41 (16%)	1 (0%)	30	60
11	e	36/70 (51%)	16 (44%)	18 (50%)	2 (6%)	1	9
12	f	887/892 (99%)	714 (80%)	164 (18%)	9 (1%)	12	40
13	A	391/433 (90%)	335 (86%)	53 (14%)	3 (1%)	16	45
14	B	393/440 (89%)	343 (87%)	50 (13%)	0	100	100
15	C	379/398 (95%)	334 (88%)	42 (11%)	3 (1%)	16	45
16	D	378/418 (90%)	330 (87%)	43 (11%)	5 (1%)	9	35
17	E	387/403 (96%)	349 (90%)	38 (10%)	0	100	100
18	F	413/439 (94%)	374 (91%)	36 (9%)	3 (1%)	18	49
19	u	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
20	v	1/28 (4%)	0	1 (100%)	0	100	100
21	G	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
21	g	238/245 (97%)	225 (94%)	13 (6%)	0	100	100
22	H	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
22	h	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
23	I	248/260 (95%)	228 (92%)	20 (8%)	0	100	100
23	i	248/260 (95%)	227 (92%)	21 (8%)	0	100	100
24	J	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	16	45
24	j	237/247 (96%)	216 (91%)	19 (8%)	2 (1%)	16	45
25	K	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
25	k	224/240 (93%)	211 (94%)	13 (6%)	0	100	100
26	L	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
26	l	236/268 (88%)	222 (94%)	14 (6%)	0	100	100
27	M	238/254 (94%)	216 (91%)	22 (9%)	0	100	100
27	m	238/254 (94%)	215 (90%)	23 (10%)	0	100	100
28	N	189/238 (79%)	184 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	n	189/238 (79%)	184 (97%)	5 (3%)	0	100	100
29	O	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
29	o	218/276 (79%)	209 (96%)	9 (4%)	0	100	100
30	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
30	p	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
31	Q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
31	q	197/201 (98%)	182 (92%)	15 (8%)	0	100	100
32	R	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
32	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100
33	S	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
33	s	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
34	T	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
34	t	213/263 (81%)	207 (97%)	6 (3%)	0	100	100
All	All	13375/14947 (90%)	12160 (91%)	1168 (9%)	47 (0%)	31	60

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	e	65	TYR
12	f	808	ASN
12	f	853	VAL
1	U	874	ASN
5	Y	89	GLU
5	Y	290	PRO
5	Y	350	VAL
6	Z	226	ILE
13	A	346	PRO
18	F	302	GLY
5	Y	176	ARG
5	Y	188	CYS
7	a	69	HIS
12	f	118	ASN
12	f	476	THR
12	f	876	HIS
16	D	86	PRO
18	F	344	ARG
1	U	873	PRO

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Mol	Chain	Res	Type
2	V	265	ASP
5	Y	63	TRP
5	Y	291	HIS
11	e	3	GLU
12	f	823	ALA
16	D	299	PHE
18	F	300	LYS
24	J	97	THR
24	J	200	GLN
24	j	97	THR
24	j	200	GLN
13	A	309	PHE
15	C	90	HIS
15	C	287	LYS
16	D	84	SER
16	D	274	ARG
12	f	475	ASN
10	d	203	PRO
12	f	809	ILE
13	A	109	PRO
15	C	89	VAL
4	X	203	PRO
8	b	23	PRO
5	Y	289	ALA
16	D	367	PRO
1	U	174	PRO
7	a	214	GLY
12	f	755	ASP

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	692/816 (85%)	689 (100%)	3 (0%)	84	84
2	V	414/459 (90%)	414 (100%)	0	100	100
3	W	416/416 (100%)	413 (99%)	3 (1%)	76	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	327/362 (90%)	326 (100%)	1 (0%)	86	86
5	Y	334/344 (97%)	332 (99%)	2 (1%)	78	81
6	Z	257/295 (87%)	254 (99%)	3 (1%)	63	75
7	a	333/336 (99%)	329 (99%)	4 (1%)	63	75
8	b	167/312 (54%)	167 (100%)	0	100	100
9	c	252/267 (94%)	251 (100%)	1 (0%)	84	84
10	d	231/293 (79%)	231 (100%)	0	100	100
11	e	38/63 (60%)	38 (100%)	0	100	100
12	f	745/748 (100%)	740 (99%)	5 (1%)	76	80
13	A	332/372 (89%)	329 (99%)	3 (1%)	70	78
14	B	344/385 (89%)	341 (99%)	3 (1%)	70	78
15	C	326/346 (94%)	322 (99%)	4 (1%)	63	75
16	D	333/366 (91%)	332 (100%)	1 (0%)	86	86
17	E	341/353 (97%)	339 (99%)	2 (1%)	78	81
18	F	357/379 (94%)	354 (99%)	3 (1%)	73	79
19	u	68/68 (100%)	68 (100%)	0	100	100
20	v	1/1 (100%)	1 (100%)	0	100	100
21	G	193/209 (92%)	192 (100%)	1 (0%)	81	83
21	g	193/209 (92%)	192 (100%)	1 (0%)	81	83
22	H	164/190 (86%)	164 (100%)	0	100	100
22	h	164/190 (86%)	164 (100%)	0	100	100
23	I	193/220 (88%)	192 (100%)	1 (0%)	81	83
23	i	193/220 (88%)	192 (100%)	1 (0%)	81	83
24	J	152/210 (72%)	151 (99%)	1 (1%)	76	80
24	j	152/210 (72%)	151 (99%)	1 (1%)	76	80
25	K	186/202 (92%)	186 (100%)	0	100	100
25	k	186/202 (92%)	186 (100%)	0	100	100
26	L	198/229 (86%)	196 (99%)	2 (1%)	68	76
26	l	198/229 (86%)	196 (99%)	2 (1%)	68	76
27	M	192/211 (91%)	191 (100%)	1 (0%)	81	83
27	m	192/211 (91%)	191 (100%)	1 (0%)	81	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	N	148/180 (82%)	148 (100%)	0	100	100
28	n	148/180 (82%)	148 (100%)	0	100	100
29	O	177/227 (78%)	177 (100%)	0	100	100
29	o	177/227 (78%)	177 (100%)	0	100	100
30	P	172/173 (99%)	172 (100%)	0	100	100
30	p	172/173 (99%)	172 (100%)	0	100	100
31	Q	164/171 (96%)	163 (99%)	1 (1%)	78	81
31	q	164/171 (96%)	163 (99%)	1 (1%)	78	81
32	R	153/201 (76%)	153 (100%)	0	100	100
32	r	153/201 (76%)	153 (100%)	0	100	100
33	S	174/198 (88%)	174 (100%)	0	100	100
33	s	174/198 (88%)	174 (100%)	0	100	100
34	T	175/214 (82%)	175 (100%)	0	100	100
34	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11190/12651 (88%)	11138 (100%)	52 (0%)	78	83

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	629	THR
1	U	775	LEU
1	U	913	ILE
3	W	89	LEU
3	W	90	LEU
3	W	256	ILE
4	X	80	ILE
5	Y	291	HIS
5	Y	330	ILE
6	Z	91	ILE
6	Z	220	LEU
6	Z	266	ILE
7	a	112	ILE
7	a	130	VAL
7	a	145	LEU
7	a	151	VAL
9	c	156	VAL
12	f	75	LEU

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Mol	Chain	Res	Type
12	f	344	VAL
12	f	573	ILE
12	f	672	LEU
12	f	822	VAL
13	A	277	ILE
13	A	373	LEU
13	A	403	ILE
14	B	125	THR
14	B	183	THR
14	B	298	ASN
15	C	109	THR
15	C	137	LEU
15	C	210	THR
15	C	311	ILE
16	D	40	LEU
17	E	105	LEU
17	E	138	LEU
18	F	86	LEU
18	F	102	ASN
18	F	300	LYS
21	G	199	ILE
23	I	28	ILE
24	J	161	ILE
26	L	161	ILE
26	L	205	LEU
27	M	196	ILE
31	Q	102	LEU
21	g	199	ILE
23	i	28	ILE
24	j	161	ILE
26	l	161	ILE
26	l	205	LEU
27	m	196	ILE
31	q	102	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (208) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	70	HIS
1	U	111	GLN
1	U	171	ASN
1	U	345	ASN

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Mol	Chain	Res	Type
1	U	377	HIS
1	U	389	ASN
1	U	415	HIS
1	U	491	GLN
1	U	595	ASN
1	U	647	HIS
1	U	698	GLN
1	U	768	GLN
2	V	33	GLN
2	V	146	GLN
2	V	168	GLN
2	V	177	ASN
2	V	214	HIS
2	V	242	HIS
2	V	247	GLN
2	V	319	HIS
3	W	41	GLN
3	W	106	GLN
3	W	235	GLN
4	X	170	GLN
4	X	198	ASN
4	X	213	GLN
4	X	292	GLN
4	X	296	ASN
4	X	329	ASN
4	X	333	GLN
4	X	334	ASN
4	X	349	HIS
4	X	380	GLN
4	X	406	ASN
5	Y	136	HIS
5	Y	178	ASN
5	Y	184	GLN
5	Y	291	HIS
6	Z	77	ASN
6	Z	96	HIS
6	Z	102	HIS
6	Z	229	GLN
6	Z	231	GLN
7	a	18	GLN
7	a	23	HIS
7	a	129	GLN

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Mol	Chain	Res	Type
7	a	143	ASN
7	a	168	ASN
7	a	193	GLN
7	a	227	ASN
7	a	258	GLN
7	a	264	ASN
7	a	369	HIS
8	b	169	HIS
9	c	77	GLN
9	c	92	GLN
9	c	128	ASN
9	c	183	HIS
9	c	199	HIS
9	c	254	ASN
9	c	256	ASN
9	c	287	HIS
10	d	96	HIS
10	d	116	HIS
10	d	128	GLN
10	d	228	GLN
11	e	6	GLN
11	e	55	GLN
12	f	43	GLN
12	f	112	ASN
12	f	118	ASN
12	f	171	GLN
12	f	245	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	747	GLN
12	f	752	HIS
12	f	766	GLN
12	f	786	GLN
12	f	808	ASN
12	f	848	GLN

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Mol	Chain	Res	Type
13	A	44	GLN
13	A	54	GLN
13	A	165	GLN
13	A	197	HIS
13	A	247	GLN
13	A	304	ASN
13	A	305	GLN
13	A	353	HIS
13	A	358	HIS
14	B	57	GLN
14	B	84	GLN
14	B	131	HIS
14	B	195	GLN
14	B	277	HIS
14	B	298	ASN
14	B	368	HIS
15	C	50	ASN
15	C	53	ASN
15	C	69	GLN
15	C	124	HIS
15	C	270	GLN
15	C	278	ASN
16	D	57	GLN
16	D	98	GLN
16	D	187	HIS
16	D	295	GLN
16	D	301	GLN
17	E	220	ASN
17	E	226	GLN
17	E	254	GLN
17	E	262	ASN
17	E	263	GLN
17	E	271	HIS
17	E	316	HIS
17	E	339	ASN
17	E	364	GLN
18	F	92	ASN
18	F	102	ASN
18	F	110	ASN
18	F	255	GLN
18	F	315	ASN
18	F	417	HIS

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Mol	Chain	Res	Type
19	u	25	ASN
19	u	41	GLN
19	u	49	GLN
21	G	33	ASN
21	G	75	ASN
21	G	90	GLN
21	G	193	GLN
22	H	71	HIS
22	H	102	GLN
22	H	109	GLN
22	H	166	ASN
22	H	169	ASN
23	I	20	GLN
23	I	30	HIS
23	I	119	GLN
23	I	123	GLN
23	I	149	GLN
24	J	18	GLN
24	J	68	ASN
24	J	85	ASN
24	J	116	GLN
25	K	41	GLN
25	K	99	HIS
25	K	114	GLN
25	K	155	HIS
25	K	164	GLN
25	K	214	ASN
25	K	225	ASN
26	L	90	GLN
26	L	146	GLN
26	L	190	HIS
27	M	32	ASN
28	N	158	ASN
29	O	116	HIS
30	P	93	ASN
31	Q	71	ASN
31	Q	82	ASN
31	Q	99	HIS
32	R	29	GLN
32	R	38	ASN
33	S	151	ASN
33	S	159	GLN

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Mol	Chain	Res	Type
34	T	69	GLN
21	g	90	GLN
21	g	193	GLN
22	h	71	HIS
22	h	102	GLN
22	h	109	GLN
23	i	20	GLN
23	i	30	HIS
23	i	119	GLN
23	i	123	GLN
23	i	149	GLN
24	j	18	GLN
24	j	68	ASN
24	j	116	GLN
25	k	41	GLN
25	k	99	HIS
25	k	114	GLN
25	k	155	HIS
25	k	164	GLN
25	k	214	ASN
25	k	225	ASN
26	l	21	GLN
26	l	90	GLN
26	l	146	GLN
27	m	32	ASN
27	m	97	ASN
28	n	158	ASN
29	o	116	HIS
30	p	93	ASN
31	q	71	ASN
31	q	82	ASN
32	r	29	GLN
32	r	38	ASN
33	s	151	ASN
34	t	69	GLN
34	t	81	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 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$
36	ATP	A	501	37	32,33,33	1.29	5 (15%)	48,52,52	1.83	9 (18%)
36	ATP	D	501	37	32,33,33	1.32	3 (9%)	48,52,52	1.99	9 (18%)
38	ADP	E	401	-	28,29,29	1.36	4 (14%)	43,45,45	1.96	9 (20%)
38	ADP	B	501	-	28,29,29	1.37	4 (14%)	43,45,45	1.91	8 (18%)
36	ATP	F	501	37	32,33,33	1.30	4 (12%)	48,52,52	1.89	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
36	ATP	A	501	37	-	0/22/38/38	0/3/3/3
36	ATP	D	501	37	-	7/22/38/38	0/3/3/3
38	ADP	E	401	-	-	3/16/32/32	0/3/3/3
38	ADP	B	501	-	-	3/16/32/32	0/3/3/3
36	ATP	F	501	37	-	3/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	501	ATP	C5-C4	4.70	1.47	1.39
36	F	501	ATP	C5-C4	4.58	1.47	1.39
38	B	501	ADP	C5-C4	4.55	1.47	1.39
38	E	401	ADP	C5-C4	4.44	1.47	1.39
36	A	501	ATP	C5-C4	4.39	1.46	1.39
36	D	501	ATP	C5-N7	-2.77	1.34	1.39
38	B	501	ADP	C5-N7	-2.70	1.34	1.39
38	E	401	ADP	C5-N7	-2.66	1.34	1.39
36	F	501	ATP	C5-N7	-2.64	1.34	1.39
36	A	501	ATP	C5-N7	-2.50	1.34	1.39
36	A	501	ATP	C5-C6	2.50	1.48	1.41
38	E	401	ADP	C5-C6	2.49	1.47	1.41
36	D	501	ATP	C5-C6	2.49	1.47	1.41
36	F	501	ATP	C5-C6	2.47	1.47	1.41
38	B	501	ADP	C5-C6	2.41	1.47	1.41
36	A	501	ATP	C4-N9	-2.13	1.33	1.37
36	A	501	ATP	C8-N7	2.06	1.35	1.31
36	F	501	ATP	C8-N7	2.02	1.35	1.31
38	B	501	ADP	C8-N7	2.02	1.35	1.31
38	E	401	ADP	C8-N7	2.01	1.35	1.31

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	D	501	ATP	C5-C4-N3	-7.06	117.00	126.72
38	E	401	ADP	C5-C4-N3	-6.59	117.64	126.72
36	F	501	ATP	C5-C4-N3	-6.58	117.65	126.72
38	B	501	ADP	C5-C4-N3	-6.23	118.14	126.72
36	A	501	ATP	C5-C4-N3	-5.96	118.51	126.72
36	D	501	ATP	N3-C4-N9	5.88	137.18	127.17
36	F	501	ATP	N3-C4-N9	5.63	136.74	127.17
38	E	401	ADP	N3-C4-N9	5.42	136.38	127.17
38	B	501	ADP	N3-C4-N9	5.15	135.92	127.17
36	A	501	ATP	N3-C4-N9	4.88	135.46	127.17
36	D	501	ATP	C2-N3-C4	4.16	121.99	111.83
36	F	501	ATP	C2-N3-C4	4.00	121.59	111.83
38	E	401	ADP	C2-N3-C4	3.96	121.51	111.83
36	A	501	ATP	C2-N3-C4	3.71	120.90	111.83
38	B	501	ADP	C2-N3-C4	3.68	120.81	111.83
36	D	501	ATP	N3-C2-N1	-3.31	123.57	128.58
36	F	501	ATP	N3-C2-N1	-3.30	123.59	128.58
36	A	501	ATP	C4-C5-N7	-3.26	106.85	110.58
38	E	401	ADP	N3-C2-N1	-3.15	123.81	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	501	ATP	N3-C2-N1	-3.14	123.83	128.58
38	E	401	ADP	C4-C5-N7	-3.12	107.01	110.58
36	D	501	ATP	C3'-C2'-C1'	3.06	107.25	101.46
38	B	501	ADP	C4-C5-N7	-3.03	107.12	110.58
38	B	501	ADP	C3'-C2'-C1'	3.02	107.18	101.46
38	B	501	ADP	N3-C2-N1	-2.95	124.12	128.58
36	A	501	ATP	C4-N9-C8	2.90	108.78	105.74
36	F	501	ATP	C4-C5-N7	-2.88	107.29	110.58
38	E	401	ADP	C3'-C2'-C1'	2.88	106.92	101.46
36	D	501	ATP	C4-C5-N7	-2.83	107.34	110.58
36	A	501	ATP	C3'-C2'-C1'	2.80	106.77	101.46
36	D	501	ATP	C1'-N9-C8	-2.79	120.89	127.09
36	F	501	ATP	C4-N9-C8	2.58	108.45	105.74
36	F	501	ATP	C3'-C2'-C1'	2.47	106.14	101.46
36	A	501	ATP	C5-N7-C8	2.42	107.25	103.45
38	B	501	ADP	C4-N9-C8	2.41	108.27	105.74
38	E	401	ADP	C4-N9-C8	2.38	108.24	105.74
38	E	401	ADP	C5-N7-C8	2.37	107.18	103.45
38	B	501	ADP	C5-N7-C8	2.37	107.17	103.45
36	F	501	ATP	C5-N7-C8	2.33	107.11	103.45
36	A	501	ATP	C2'-C1'-N9	-2.25	107.70	113.30
36	D	501	ATP	C5-N7-C8	2.16	106.84	103.45
36	F	501	ATP	C1'-N9-C8	-2.13	122.36	127.09
36	D	501	ATP	C4-N9-C1'	2.06	131.44	126.63
38	E	401	ADP	C1'-N9-C8	-2.02	122.60	127.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	D	501	ATP	C5'-O5'-PA-O3A
36	D	501	ATP	C3'-C4'-C5'-O5'
36	F	501	ATP	C5'-O5'-PA-O1A
36	F	501	ATP	C5'-O5'-PA-O2A
36	F	501	ATP	C5'-O5'-PA-O3A
38	B	501	ADP	C5'-O5'-PA-O1A
38	B	501	ADP	C5'-O5'-PA-O2A
38	B	501	ADP	C5'-O5'-PA-O3A
38	E	401	ADP	C5'-O5'-PA-O1A
36	D	501	ATP	C4'-C5'-O5'-PA
36	D	501	ATP	O4'-C4'-C5'-O5'
38	E	401	ADP	C3'-C4'-C5'-O5'

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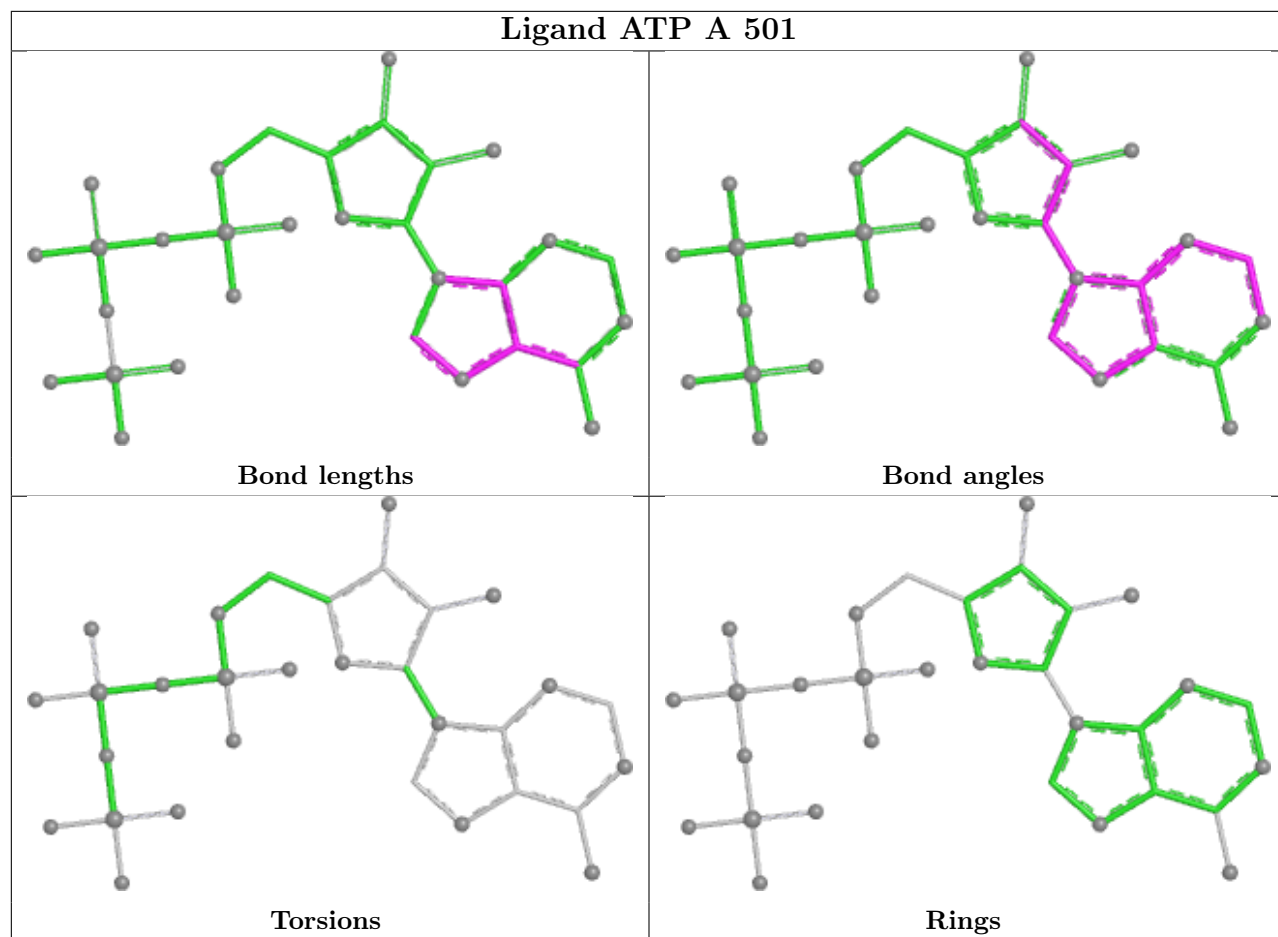
Mol	Chain	Res	Type	Atoms
38	E	401	ADP	O4'-C4'-C5'-O5'
36	D	501	ATP	C5'-O5'-PA-O1A
36	D	501	ATP	C2'-C1'-N9-C4
36	D	501	ATP	C2'-C1'-N9-C8

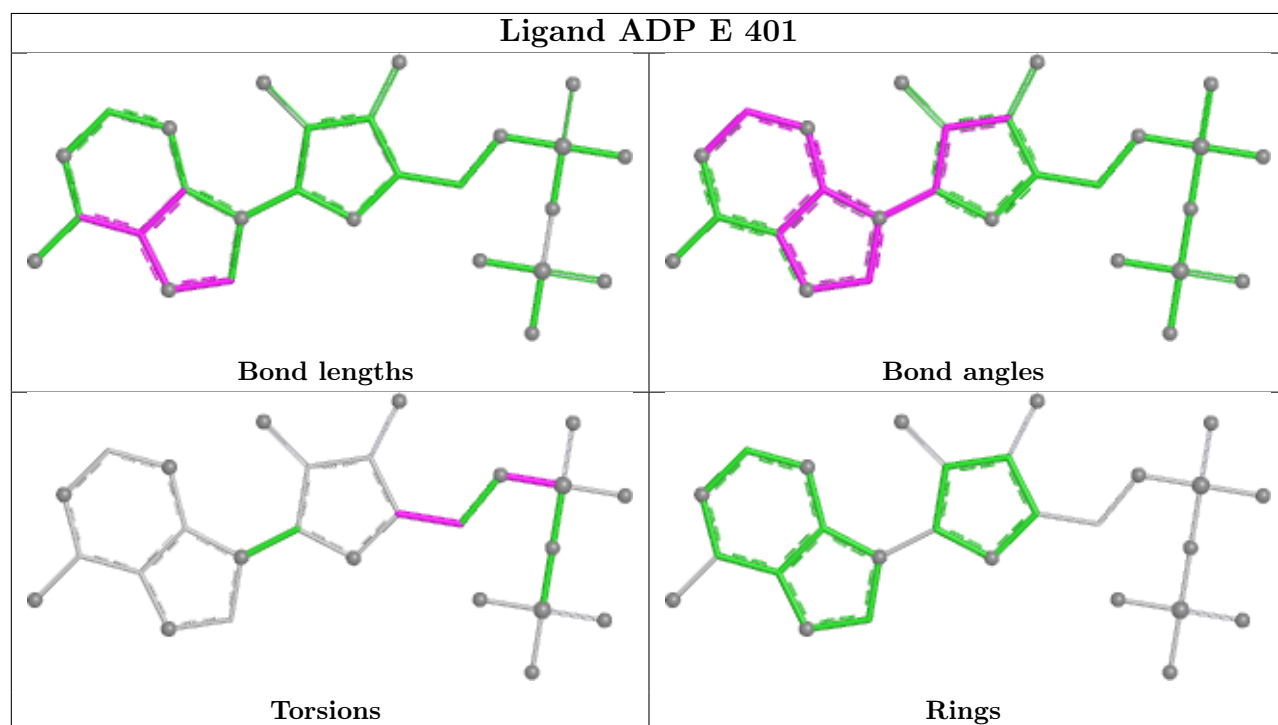
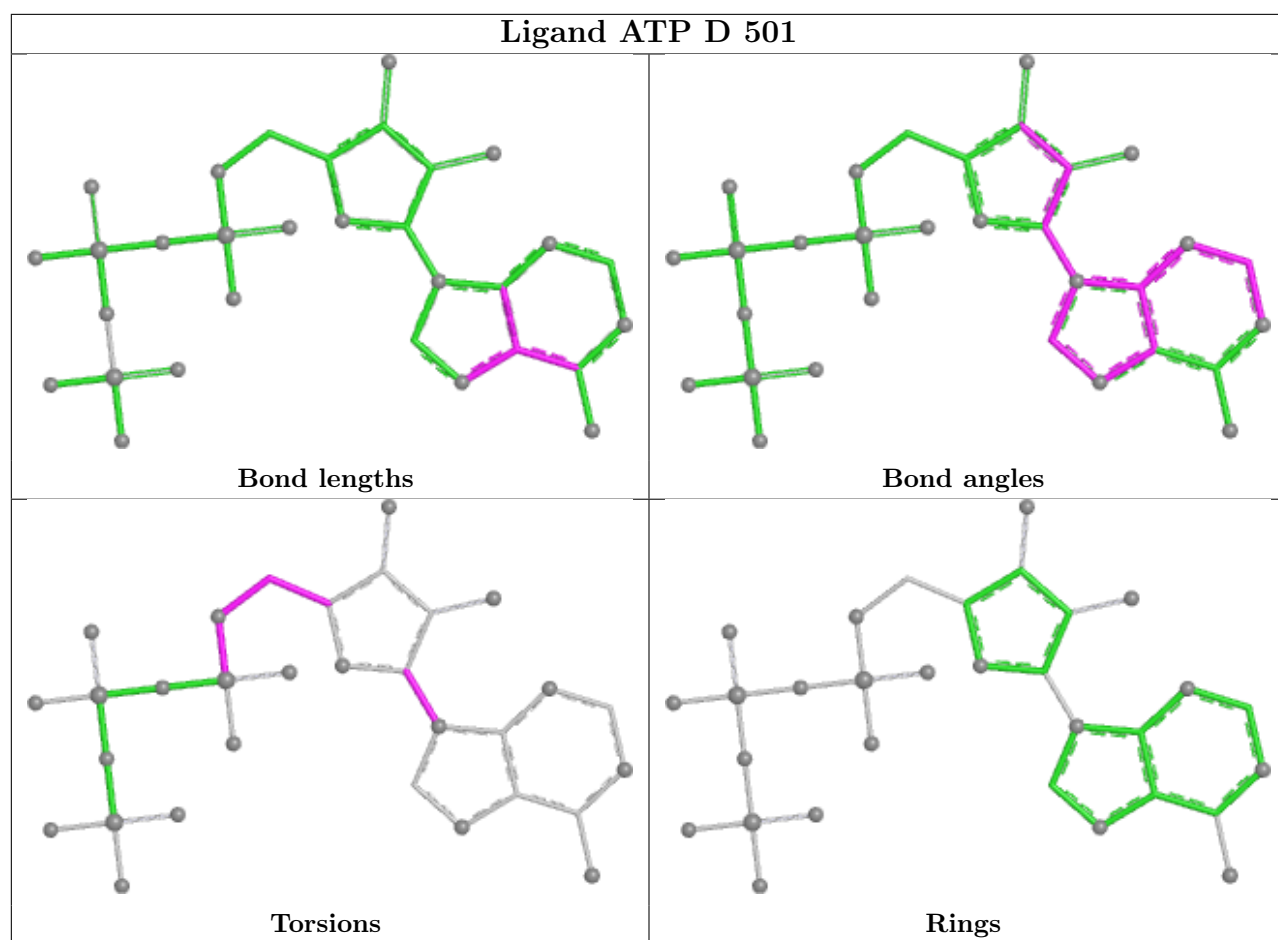
There are no ring outliers.

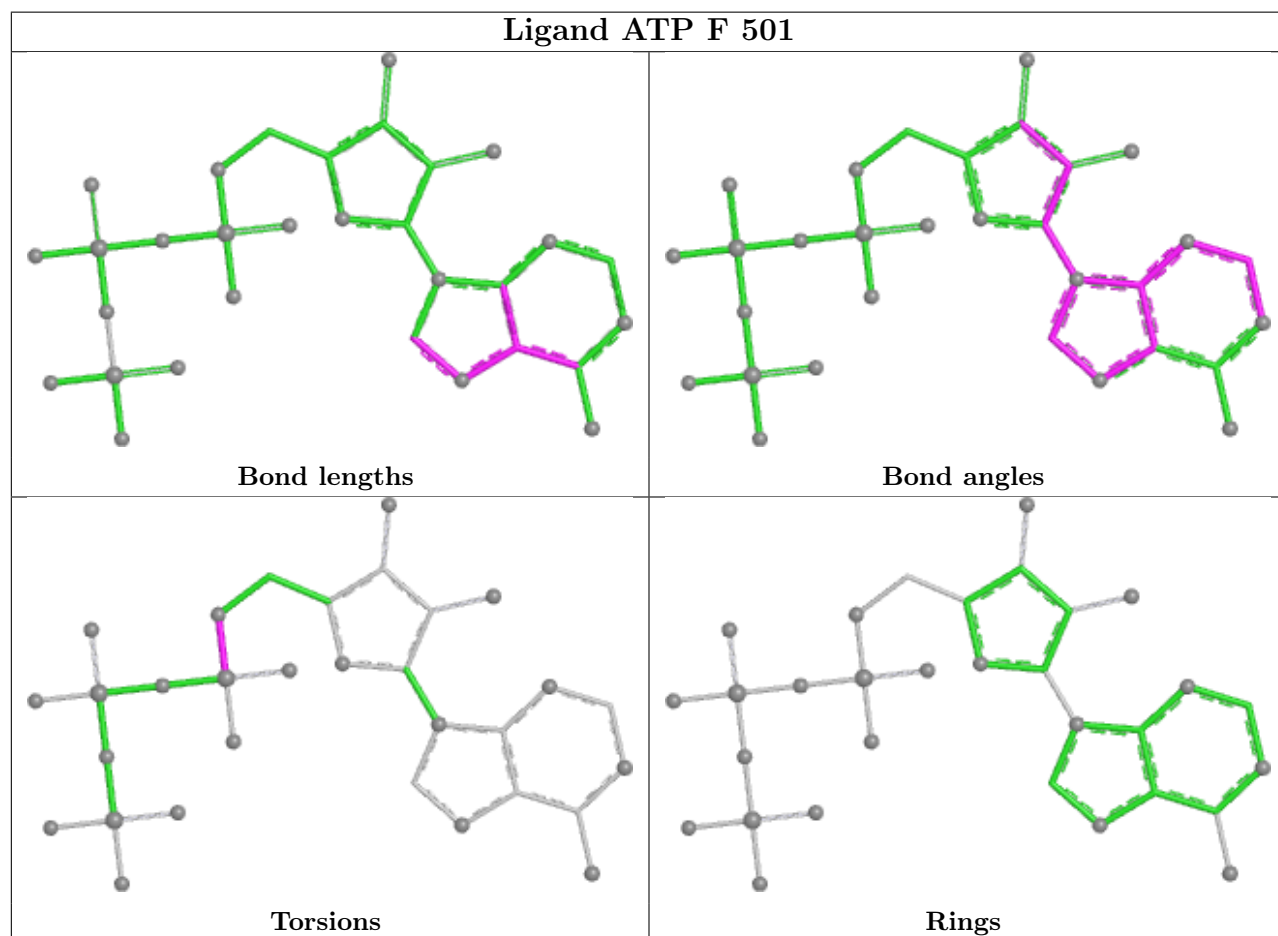
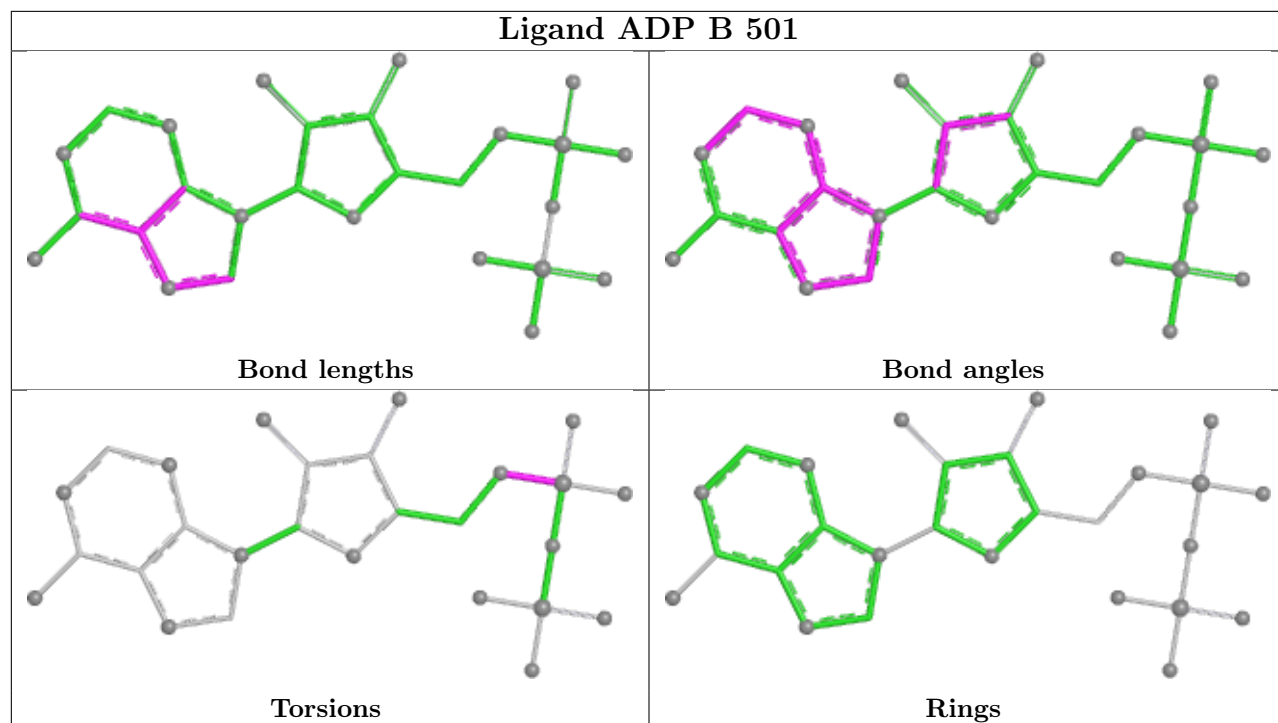
4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	A	501	ATP	1	0
36	D	501	ATP	2	0
38	E	401	ADP	2	0
38	B	501	ADP	3	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.

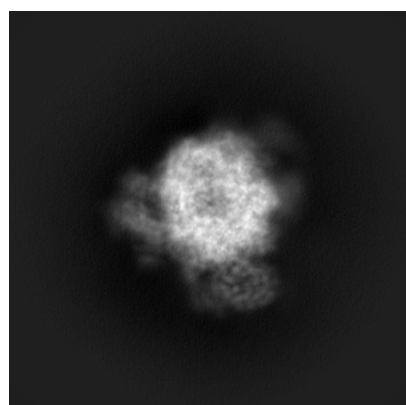
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9218. These allow visual inspection of the internal detail of the map and identification of artifacts.

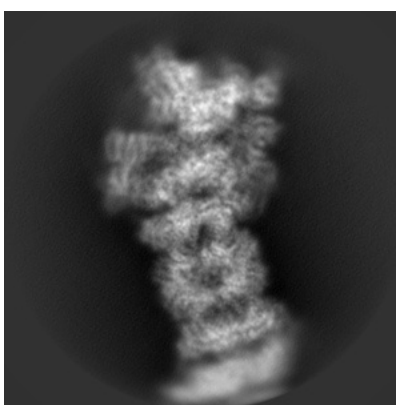
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

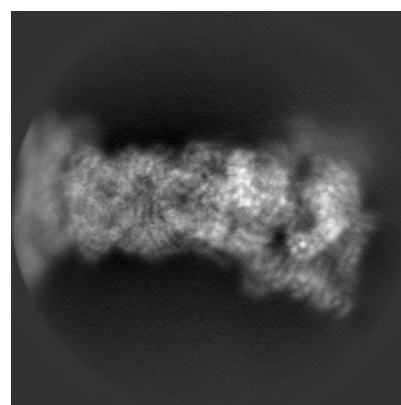
6.1.1 Primary map



X



Y

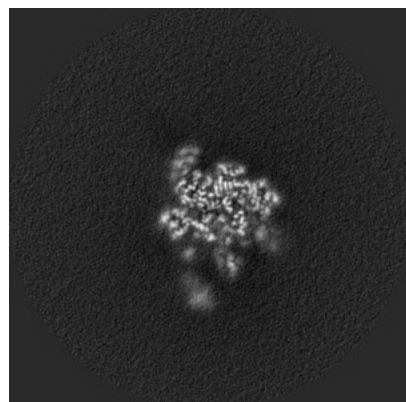


Z

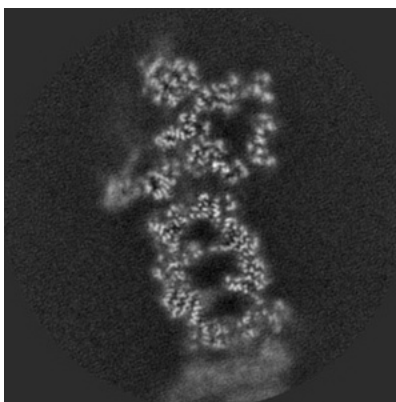
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

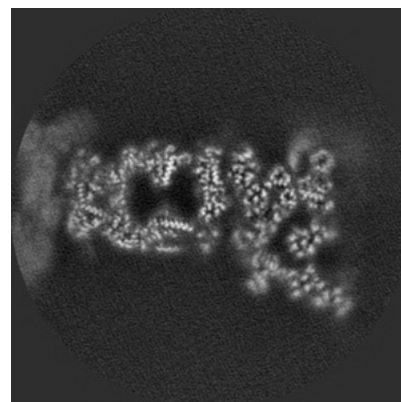
6.2.1 Primary map



X Index: 300



Y Index: 300

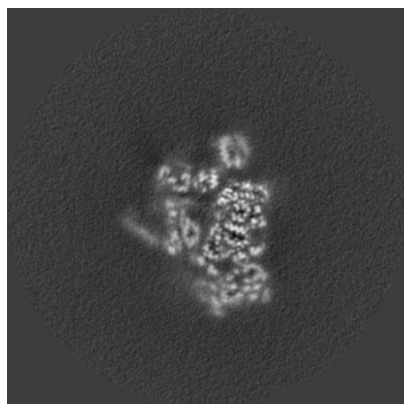


Z Index: 300

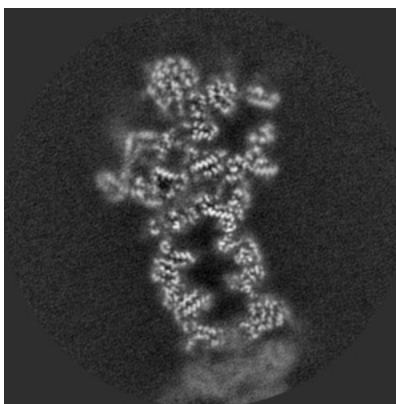
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

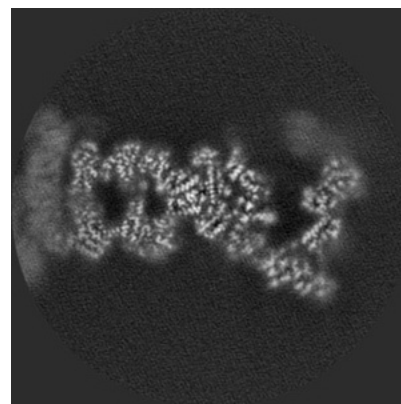
6.3.1 Primary map



X Index: 344



Y Index: 313

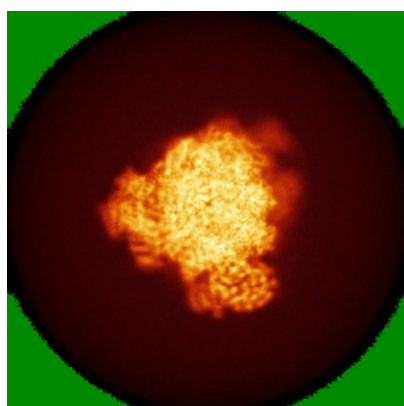


Z Index: 335

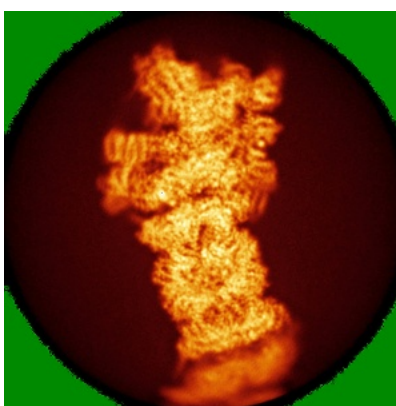
The images above show the largest variance slices of the map in three orthogonal directions.

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

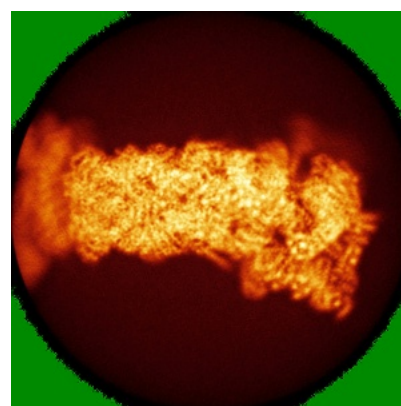
6.4.1 Primary map



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.

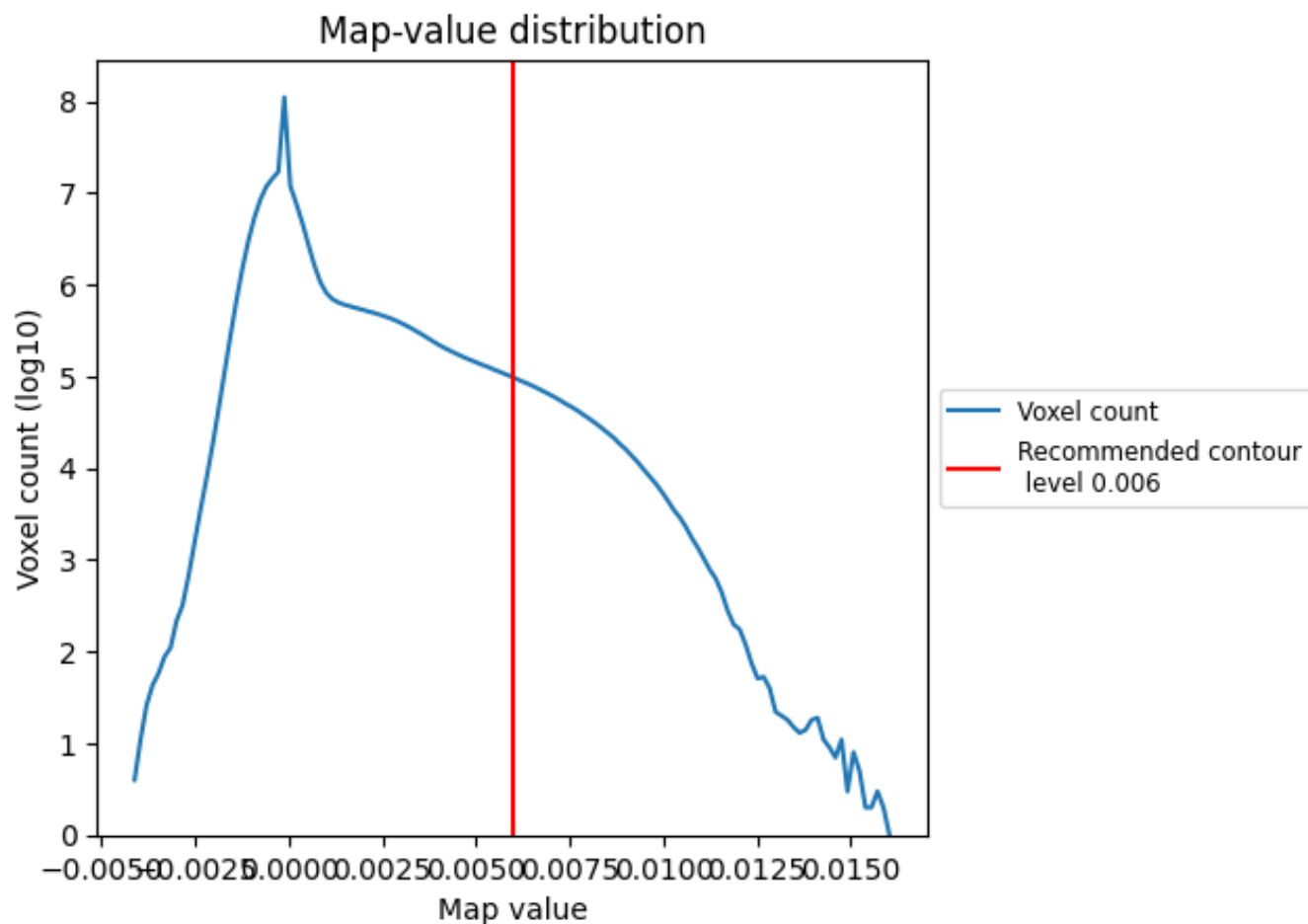
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

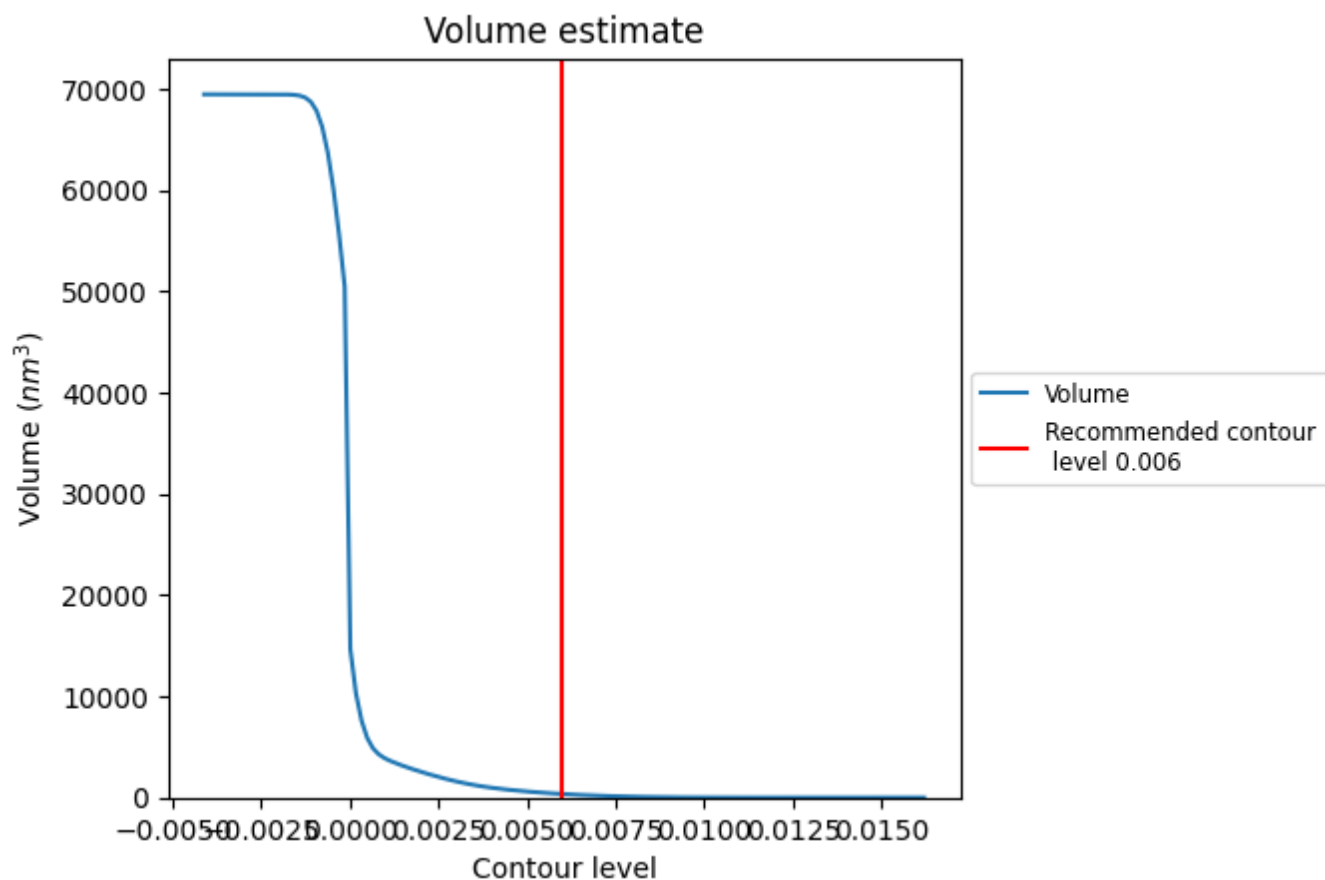
This section contains the results of statistical analysis of the map.

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.

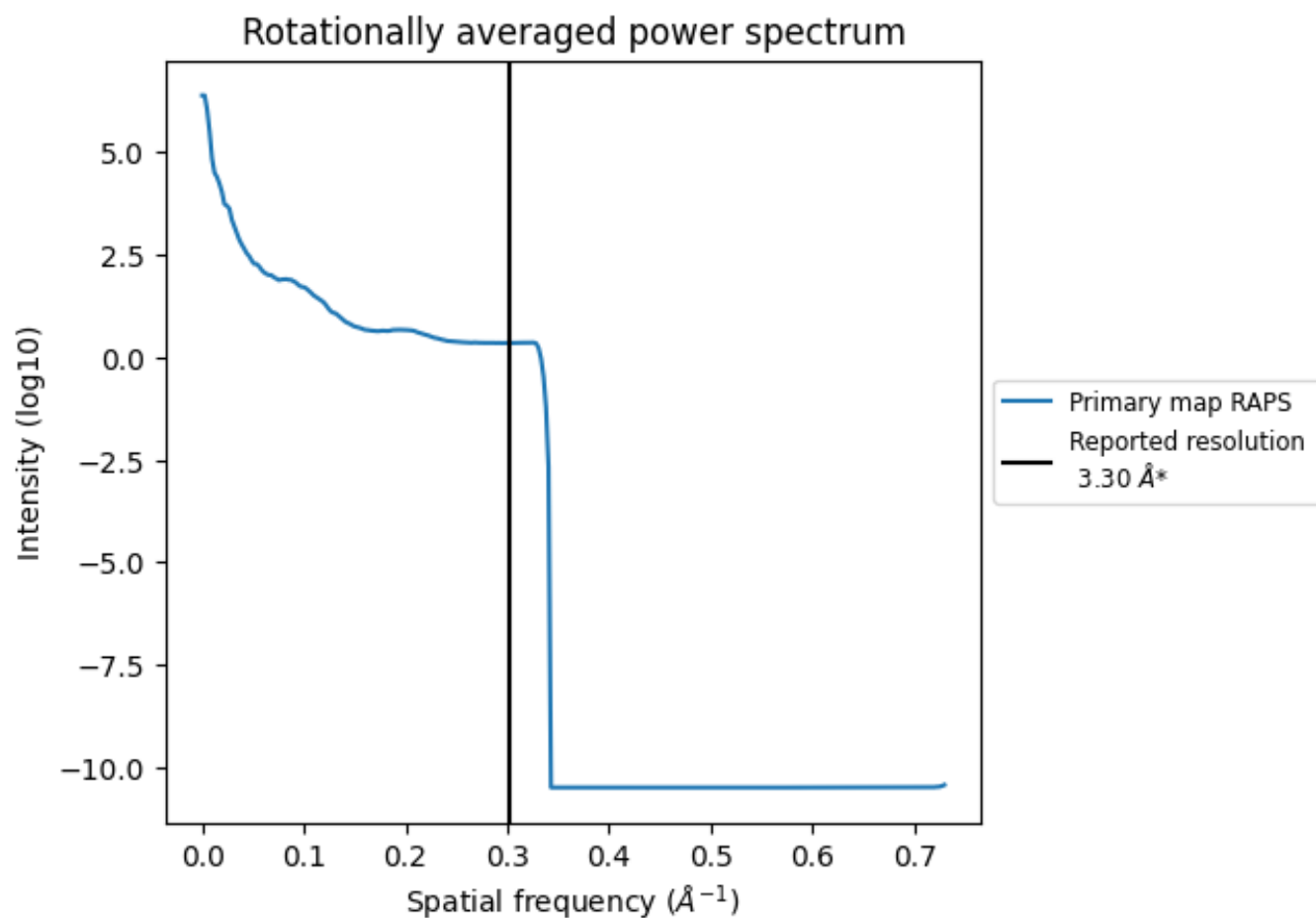
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 350 nm³; this corresponds to an approximate mass of 316 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 0.303 Å⁻¹

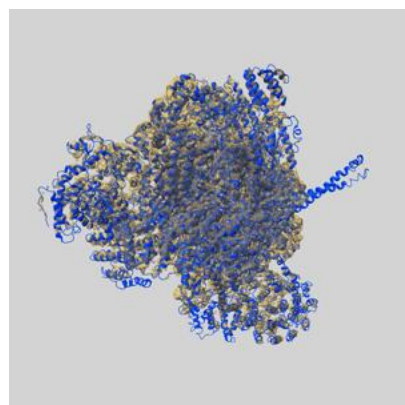
8 Fourier-Shell correlation

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

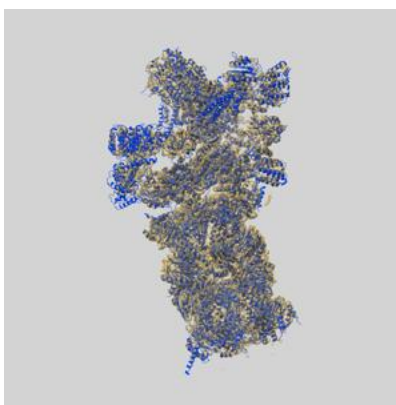
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-9218 and PDB model 6MSE. Per-residue inclusion information can be found in section 3 on page 13.

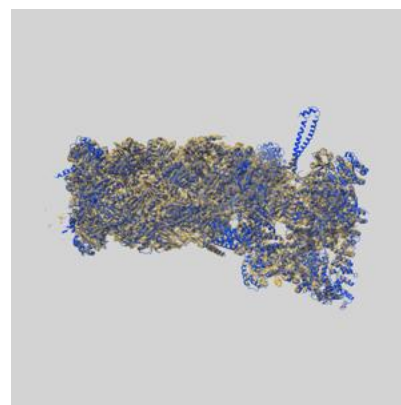
9.1 Map-model overlay [i](#)



X



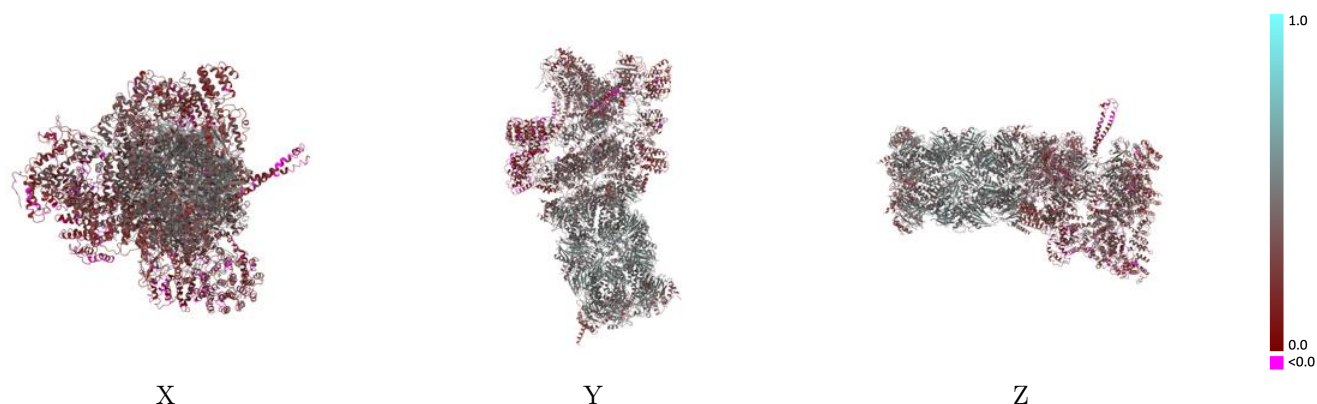
Y



Z

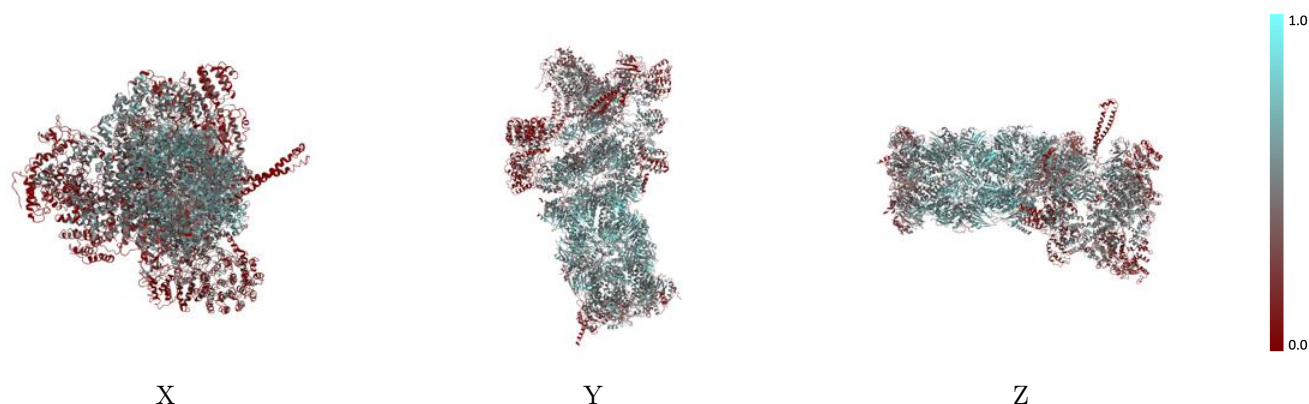
The images above show the 3D surface view of the map at the recommended contour level 0.006 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



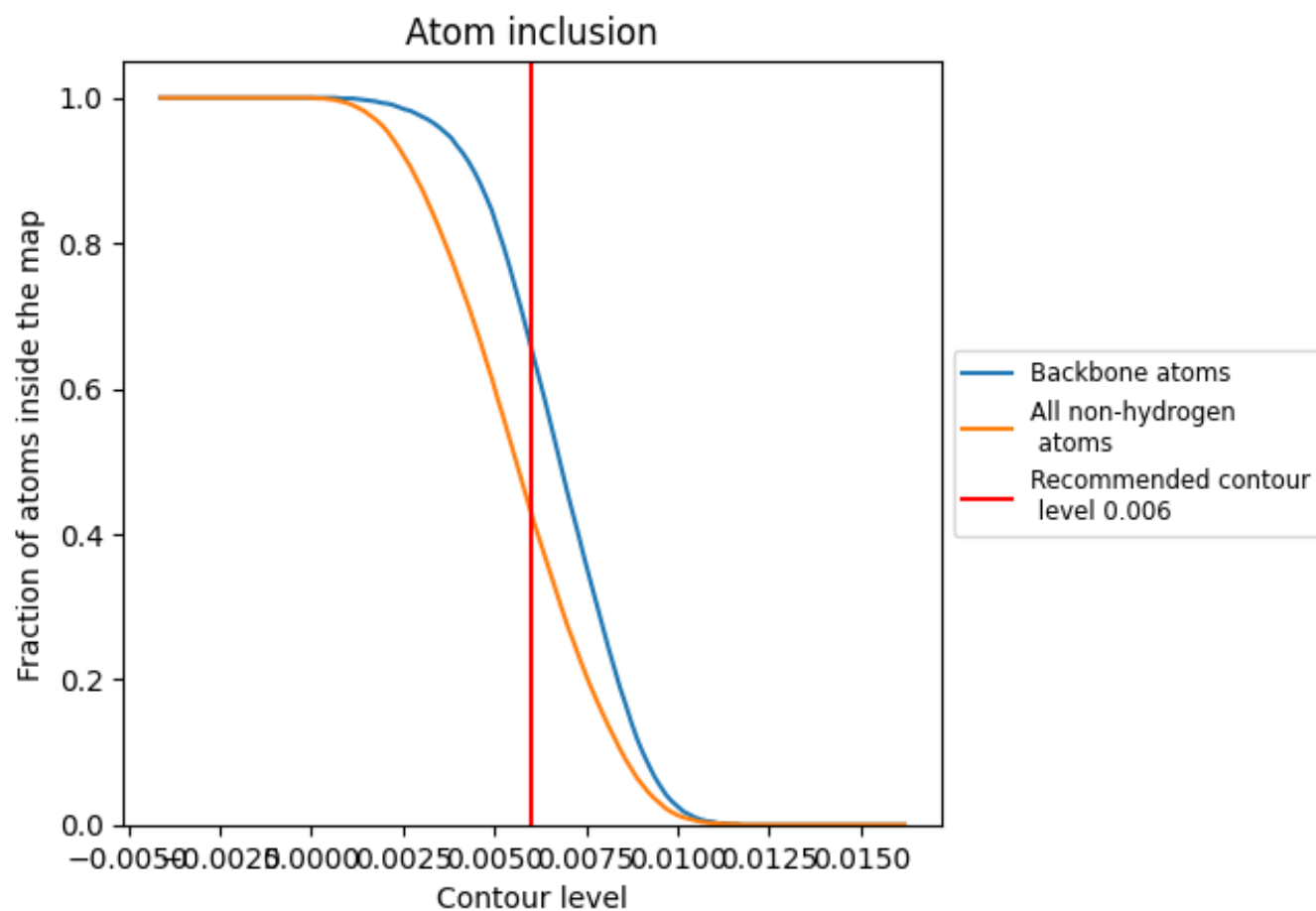
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 43% 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	 0.4290	 0.3550
A	 0.4580	 0.3390
B	 0.4140	 0.3210
C	 0.3400	 0.2970
D	 0.4810	 0.3710
E	 0.4870	 0.3650
F	 0.4560	 0.3530
G	 0.5960	 0.4380
H	 0.6250	 0.4410
I	 0.5590	 0.4010
J	 0.5320	 0.4010
K	 0.5250	 0.4120
L	 0.5830	 0.4330
M	 0.5600	 0.4060
N	 0.6290	 0.4730
O	 0.5980	 0.4690
P	 0.6030	 0.4800
Q	 0.5880	 0.4490
R	 0.6260	 0.4810
S	 0.5680	 0.4790
T	 0.6250	 0.4790
U	 0.3490	 0.2980
V	 0.2460	 0.2070
W	 0.3920	 0.2490
X	 0.3600	 0.3020
Y	 0.2940	 0.2070
Z	 0.4290	 0.3590
a	 0.3340	 0.2620
b	 0.2140	 0.2880
c	 0.4650	 0.3730
d	 0.1510	 0.2060
e	 0.1760	 0.0300
f	 0.1610	 0.1760
g	 0.4240	 0.4320
h	 0.4280	 0.4300



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Chain	Atom inclusion	Q-score
i	 0.3430	 0.3770
j	 0.3260	 0.3800
k	 0.3780	 0.3940
l	 0.4730	 0.4310
m	 0.4410	 0.4120
n	 0.5840	 0.4840
o	 0.5270	 0.4760
p	 0.5520	 0.4810
q	 0.5320	 0.4560
r	 0.5850	 0.4920
s	 0.5460	 0.4780
t	 0.6080	 0.4860
u	 0.3830	 0.3900
v	 0.2520	 0.3740