



Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 07:19 PM JST

PDB ID : 9K4K / pdb_00009k4k
EMDB ID : EMD-62062
Title : Structure of substrate-engaged human 26S proteasome RP-CP subcomplex in state EA1.1
Authors : Wu, Z.; Chen, E.; Mao, Y.
Deposited on : 2024-10-21
Resolution : 4.00 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:

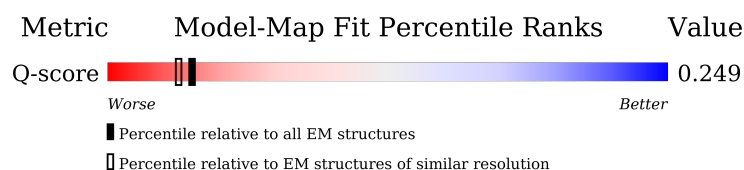
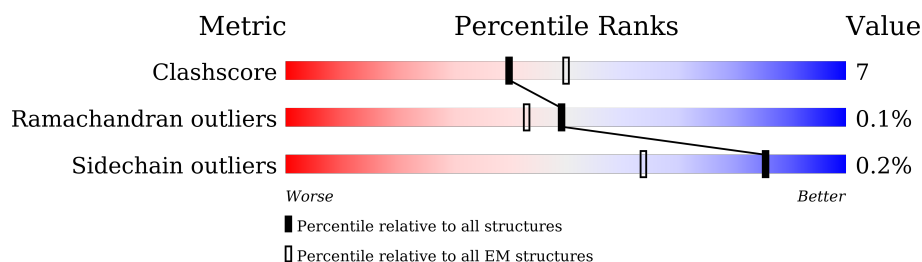
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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 4.00 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	7587 (3.50 - 4.50)

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	A	433	
2	B	440	
3	C	398	
4	D	418	

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Mol	Chain	Length	Quality of chain
5	E	403	
6	F	439	
7	G	246	
7	g	246	
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	

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Mol	Chain	Length	Quality of chain
18	r	263	
19	S	241	
19	s	241	
20	T	264	
20	t	264	
21	U	953	
22	V	534	
23	W	456	
24	X	422	
25	Y	389	
26	Z	324	
27	a	376	
28	b	377	
29	c	310	
30	d	350	
31	e	70	
32	f	908	
33	u	76	
33	v	76	
33	w	76	
34	y	5	
34	z	5	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 107223 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 regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	413	Total	C	N	O	S	0	0
			3240	2042	567	613	18		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	388	Total	C	N	O	S	0	0
			3042	1915	519	593	15		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	363	Total	C	N	O	S	0	0
			2864	1808	515	525	16		

- Molecule 4 is a protein called 26S proteasome regulatory subunit 6B.

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

- Molecule 5 is a protein called Proteasome 26S subunit, ATPase 6.

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

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

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

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	244	Total	C	N	O	S	0	0
			1889	1198	316	362	13		
7	g	244	Total	C	N	O	S	0	0
			1880	1193	318	356	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1805	1152	305	342	6		
8	h	232	Total	C	N	O	S	0	0
			1805	1154	307	338	6		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	1	0
			1958	1236	336	376	10		
9	i	250	Total	C	N	O	S	0	0
			1955	1234	336	375	10		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1880	1179	333	363	5		
10	j	239	Total	C	N	O	S	0	0
			1861	1168	332	356	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1777	1117	295	354	11		
11	k	234	Total	C	N	O	S	0	0
			1782	1119	295	357	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1866	1169	336	350	11		
12	l	238	Total	C	N	O	S	0	0
			1861	1165	335	350	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1876	1191	321	353	11		
13	m	240	Total	C	N	O	S	0	0
			1881	1193	321	356	11		

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	202	Total	C	N	O	S	0	0
			1514	949	258	295	12		
14	n	202	Total	C	N	O	S	0	0
			1510	947	258	293	12		

- Molecule 15 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	220	Total	C	N	O	S	0	0
			1649	1038	279	320	12		
15	o	220	Total	C	N	O	S	0	0
			1659	1044	283	320	12		

- Molecule 16 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1587	1010	264	294	19		
16	p	204	Total	C	N	O	S	0	0
			1591	1013	265	294	19		

- Molecule 17 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	199	Total	C	N	O	S	0	0
			1588	1017	270	292	9		

- Molecule 18 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		
18	r	201	Total	C	N	O	S	0	0
			1559	982	274	294	9		

- Molecule 19 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1641	1041	281	309	10		
19	s	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 20 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	216	Total	C	N	O	S	0	0
			1683	1062	291	318	12		
20	t	216	Total	C	N	O	S	0	0
			1687	1064	291	320	12		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	868	Total	C	N	O	S	0	0
			6787	4303	1153	1285	46		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	472	Total	C	N	O	S	0	0
			3754	2387	673	681	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	441	Total	C	N	O	S	0	0
			3596	2277	613	682	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	389	Total	C	N	O	S	0	0
			3202	2041	545	598	18		

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

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

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

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

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

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

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

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

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

- Molecule 31 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	50	Total	C	N	O	0	0
			425	260	65	100		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	844	Total	C	N	O	S	0	0
			6529	4126	1108	1250	45		

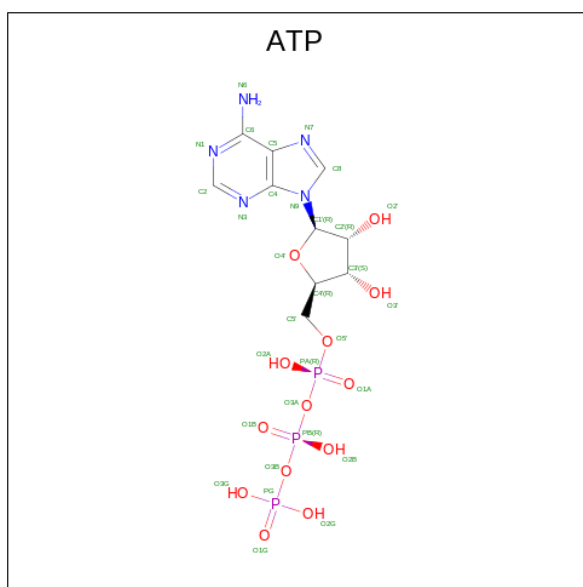
- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	v	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	w	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 34 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	y	5	Total	C	N	O	0	0
			25	15	5	5		
34	z	5	Total	C	N	O	0	0
			25	15	5	5		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

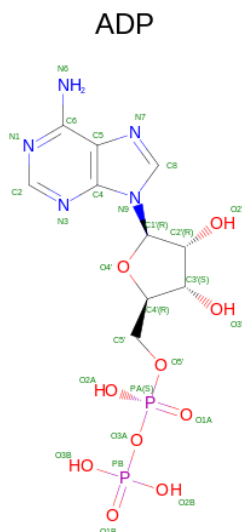


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

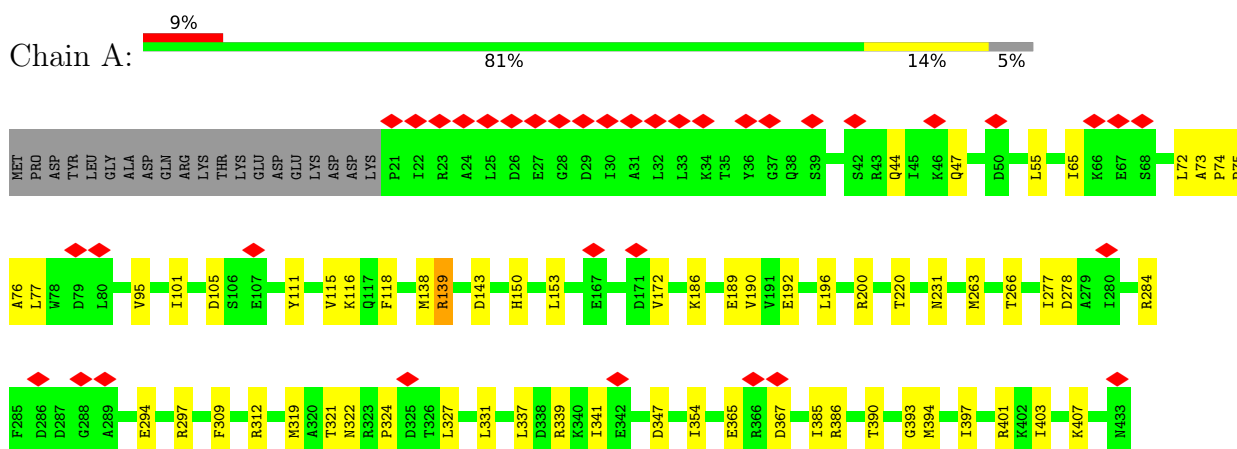
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

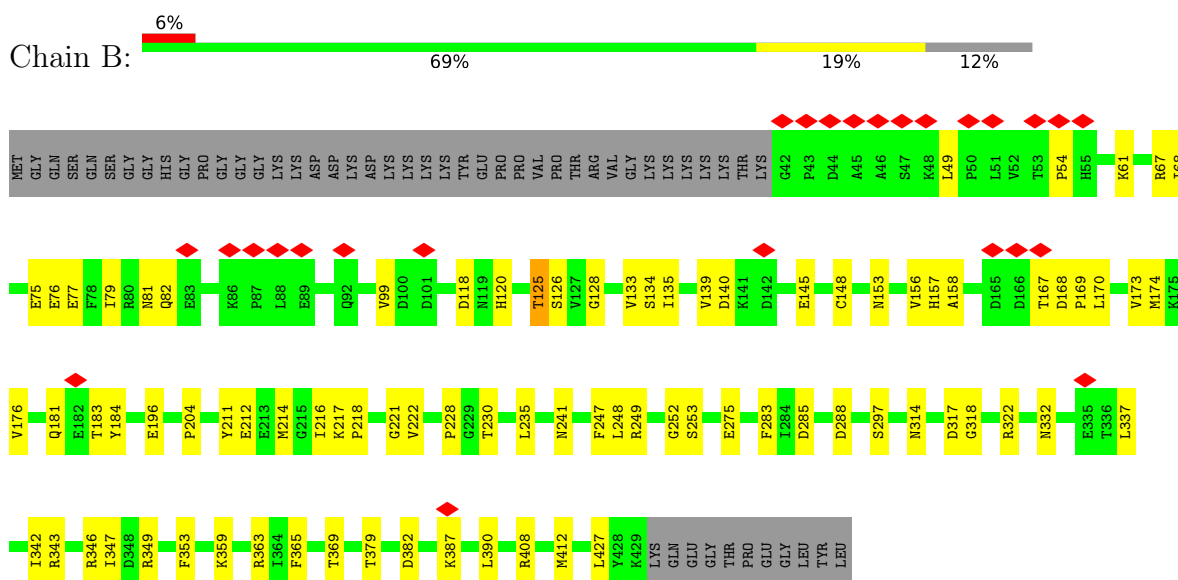
3 Residue-property plots

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

- Molecule 1: 26S proteasome regulatory subunit 7

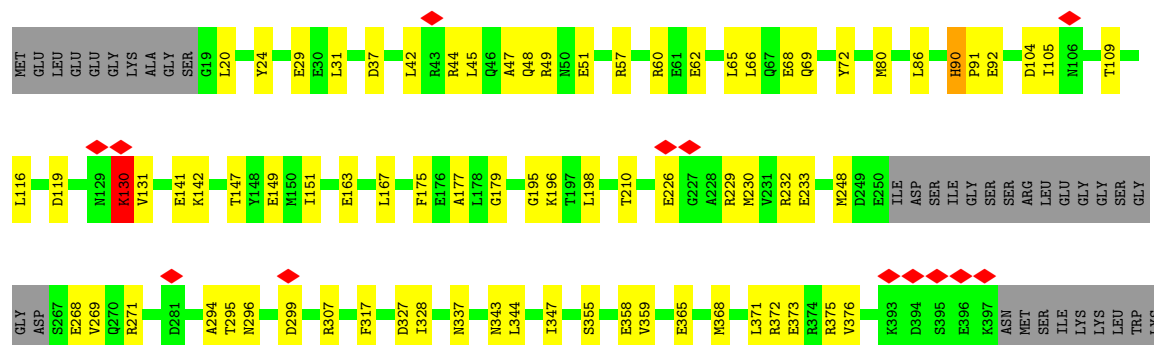


- Molecule 2: 26S proteasome regulatory subunit 4

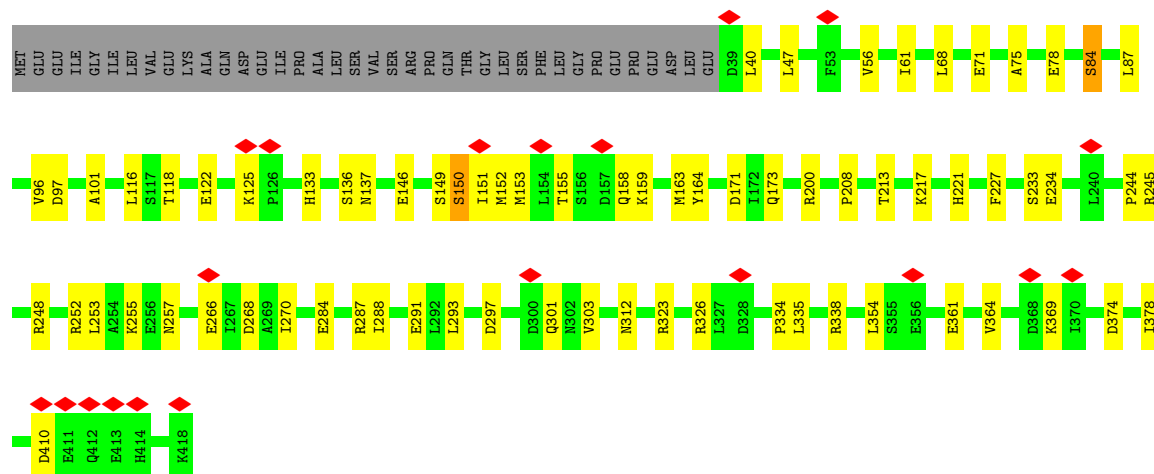
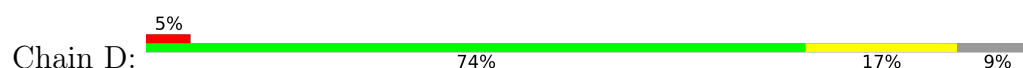


- Molecule 3: 26S proteasome regulatory subunit 8

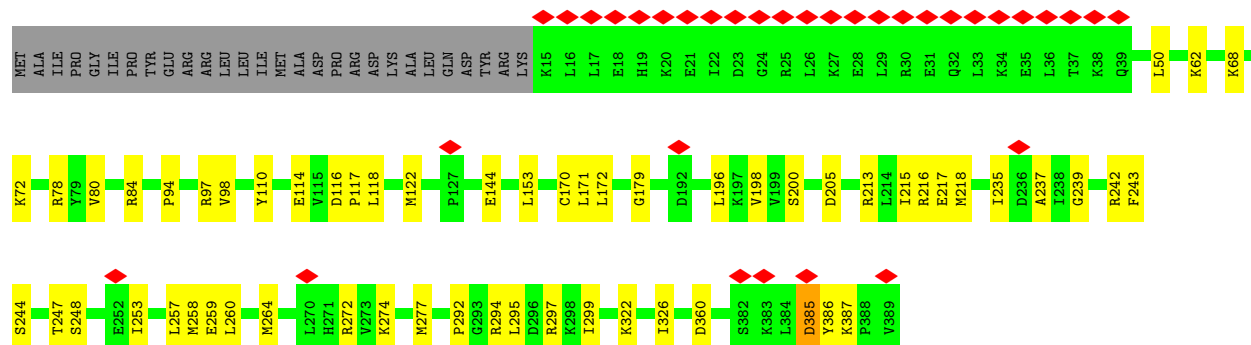
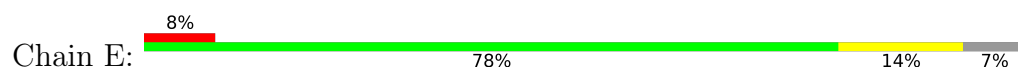




• Molecule 4: 26S proteasome regulatory subunit 6B

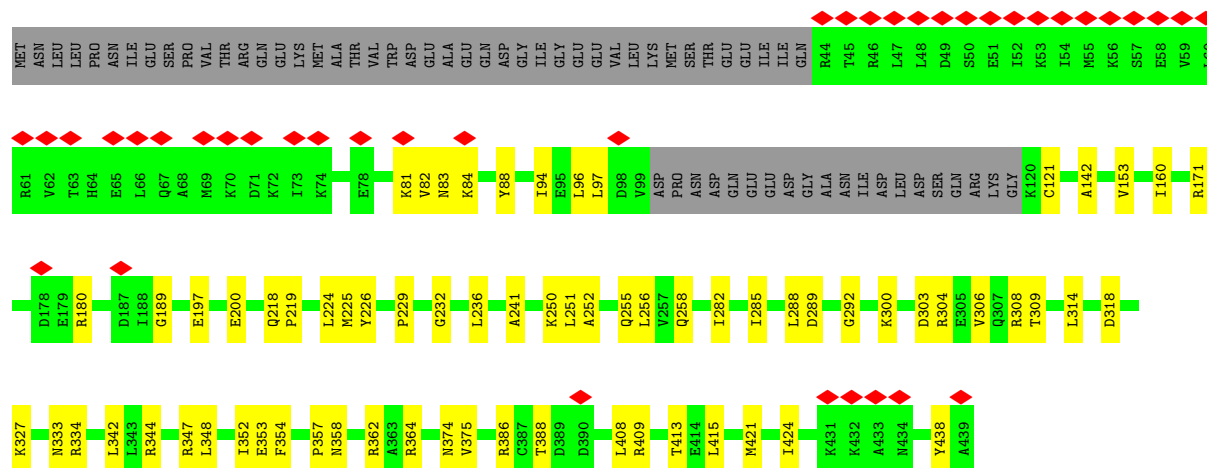


• Molecule 5: Proteasome 26S subunit, ATPase 6

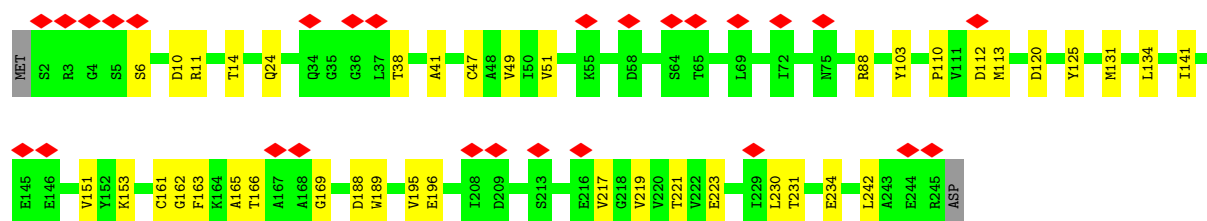
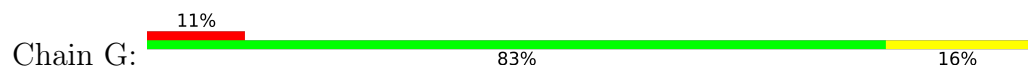


• Molecule 6: 26S proteasome regulatory subunit 6A

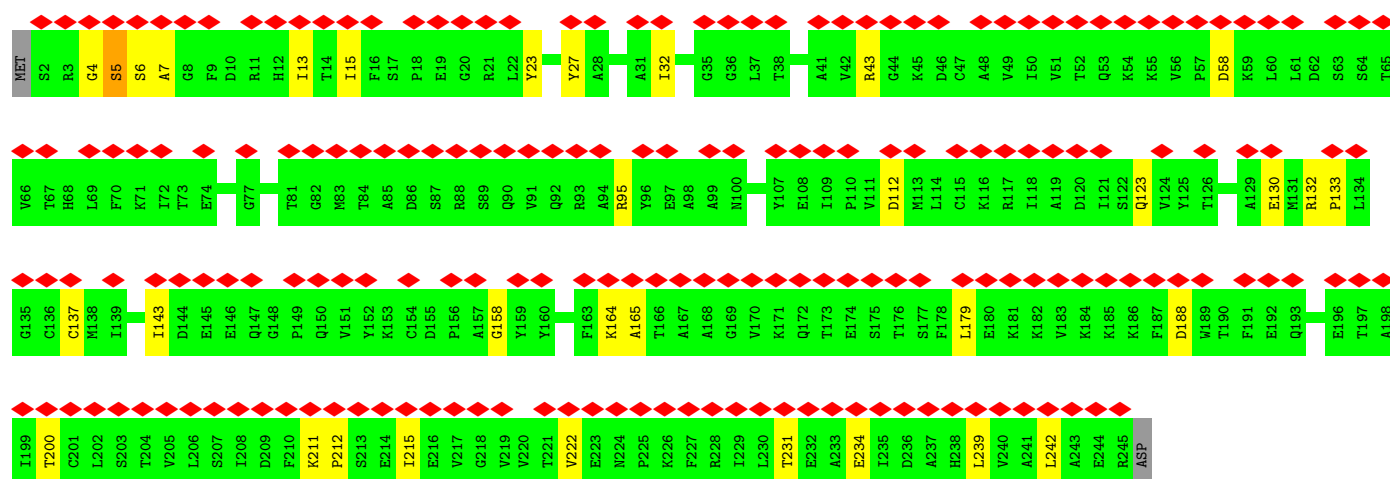
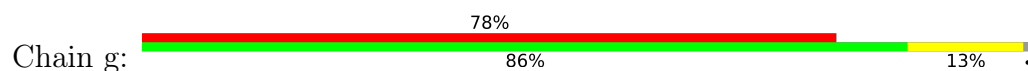




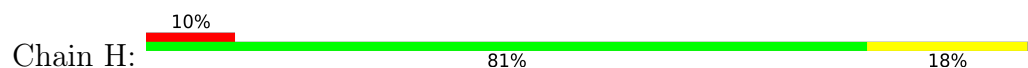
• Molecule 7: Proteasome subunit alpha type-6

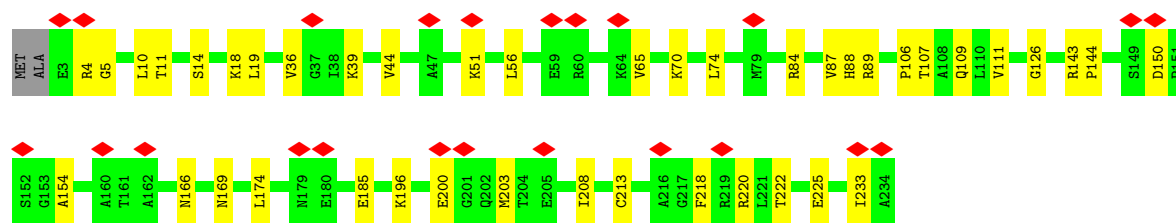


• Molecule 7: Proteasome subunit alpha type-6

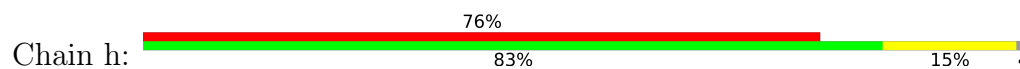


• Molecule 8: Proteasome subunit alpha type-2

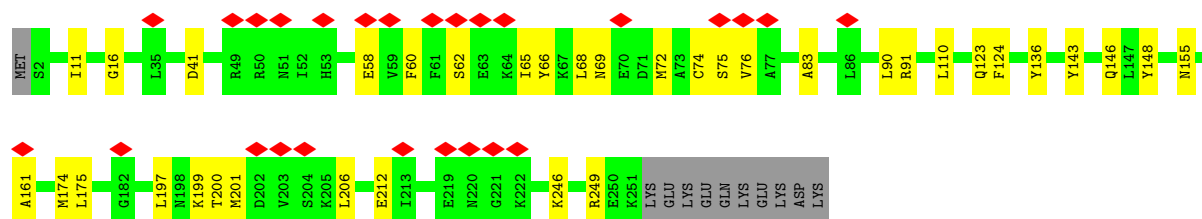
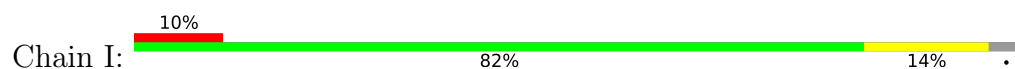




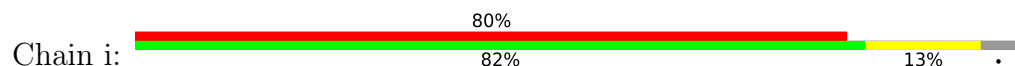
• Molecule 8: Proteasome subunit alpha type-2

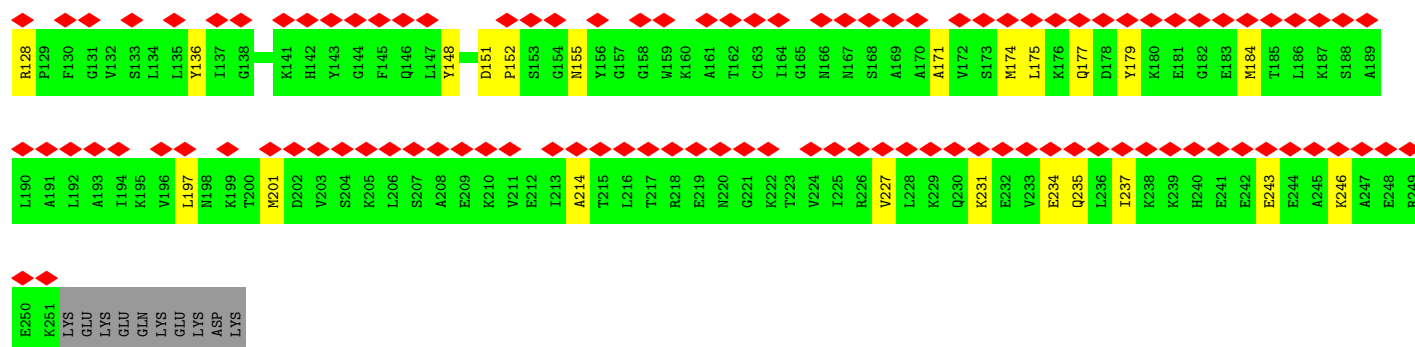


• Molecule 9: Proteasome subunit alpha type-4

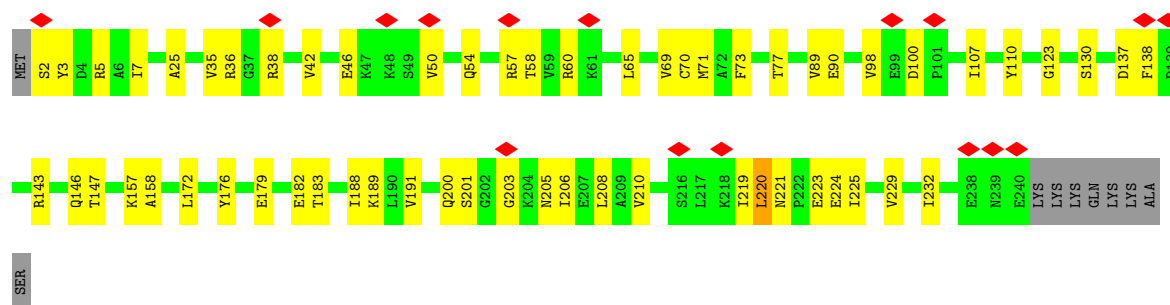


• Molecule 9: Proteasome subunit alpha type-4

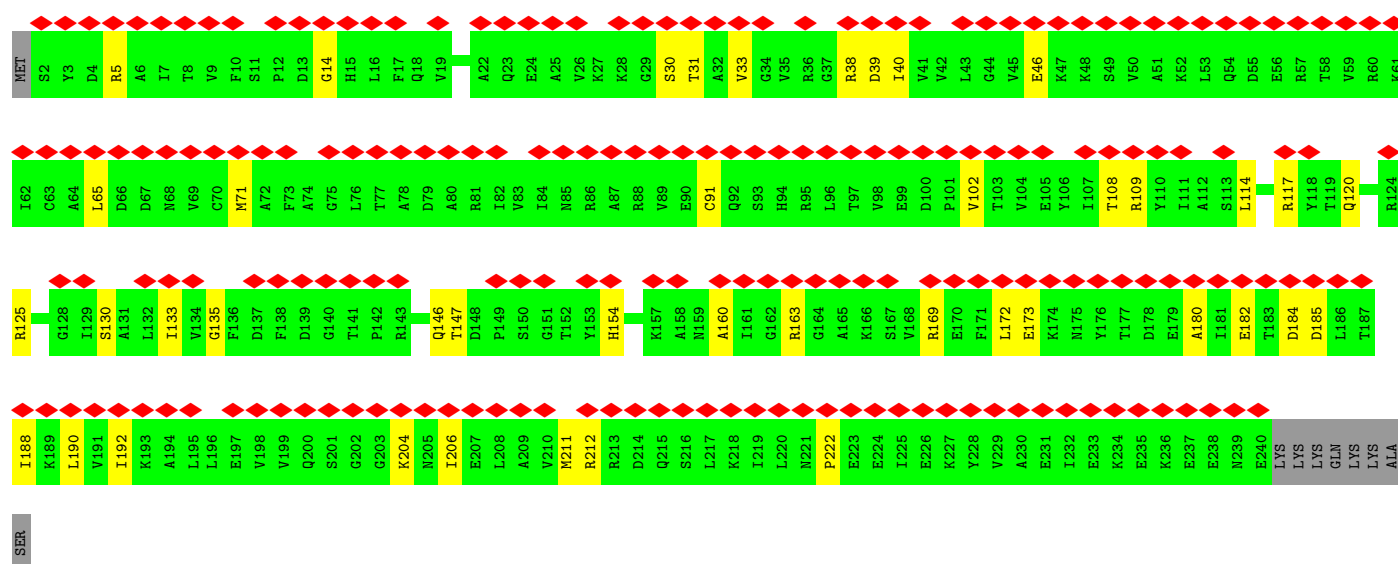
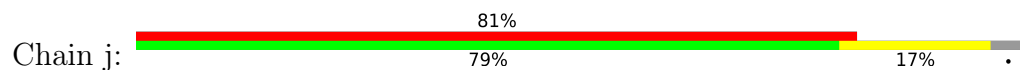




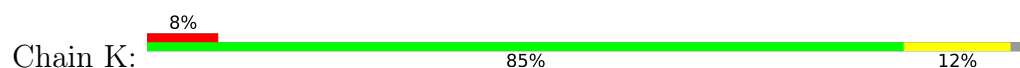
- Molecule 10: Proteasome subunit alpha type-7

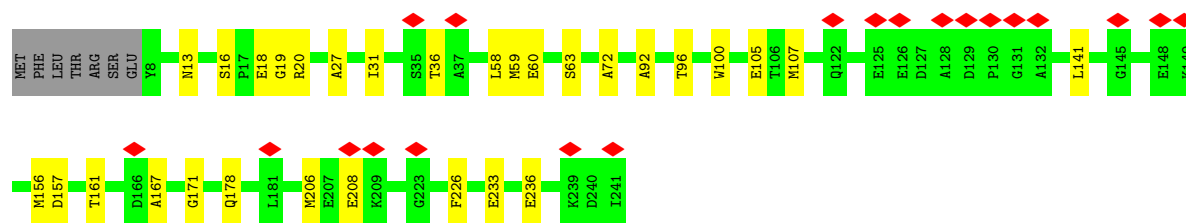


- Molecule 10: Proteasome subunit alpha type-7

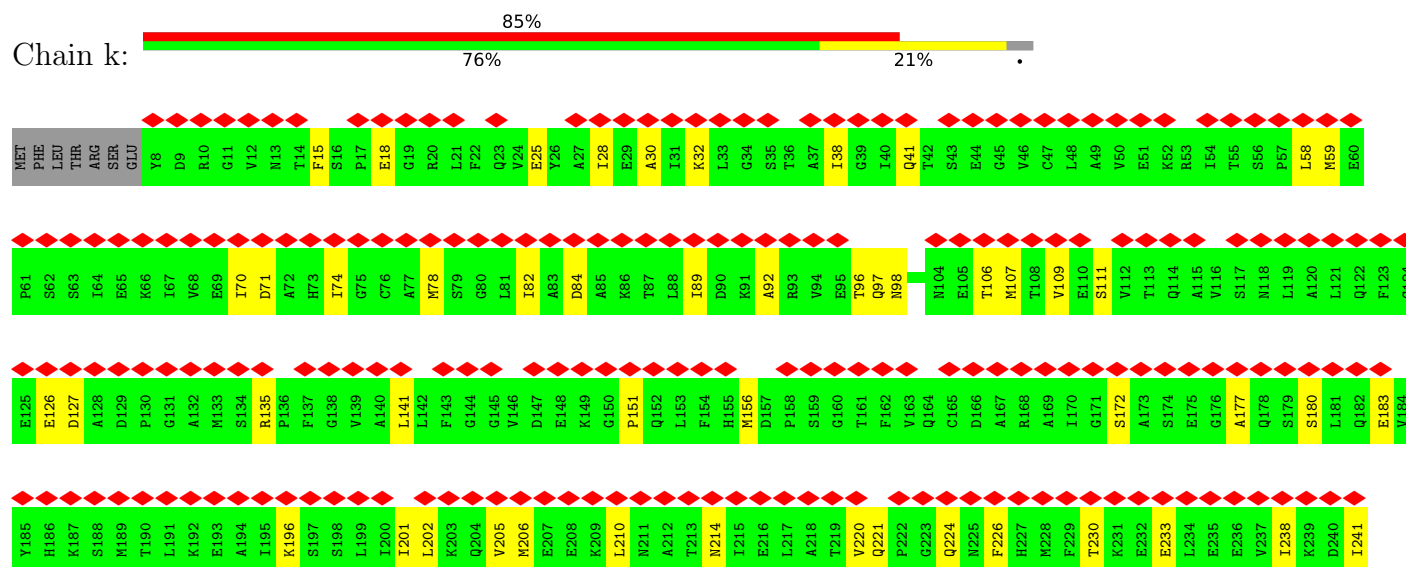


- Molecule 11: Proteasome subunit alpha type-5

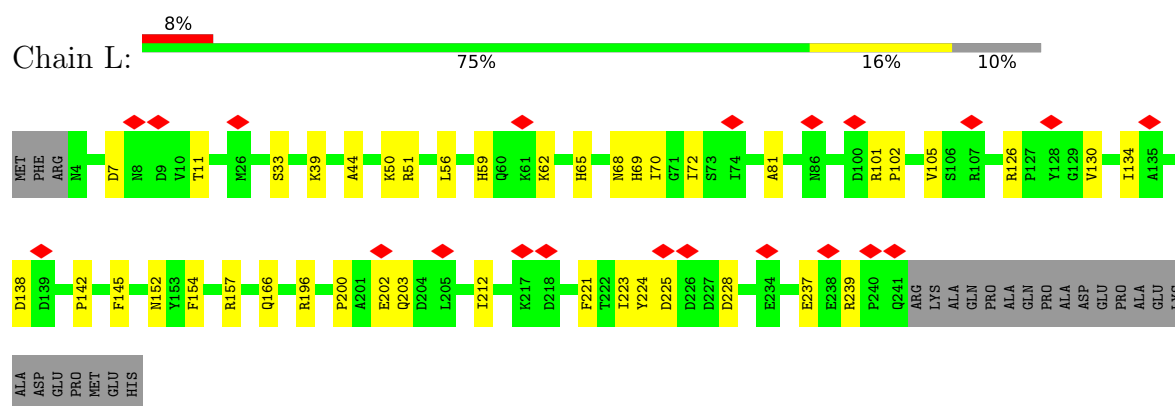




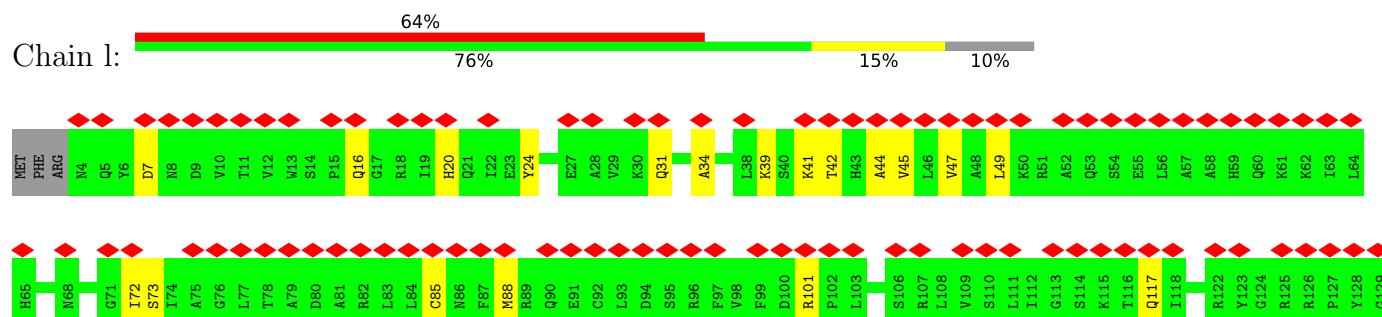
• Molecule 11: Proteasome subunit alpha type-5

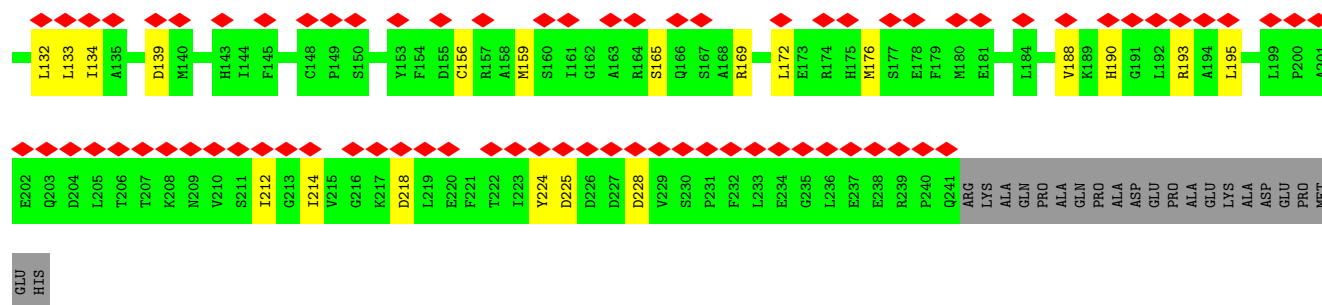


• Molecule 12: Proteasome subunit alpha type-1

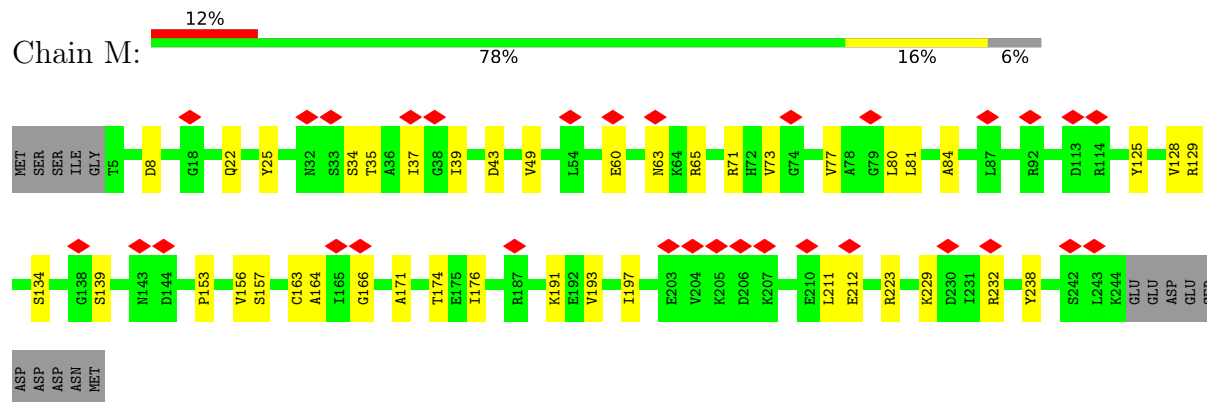


• Molecule 12: Proteasome subunit alpha type-1

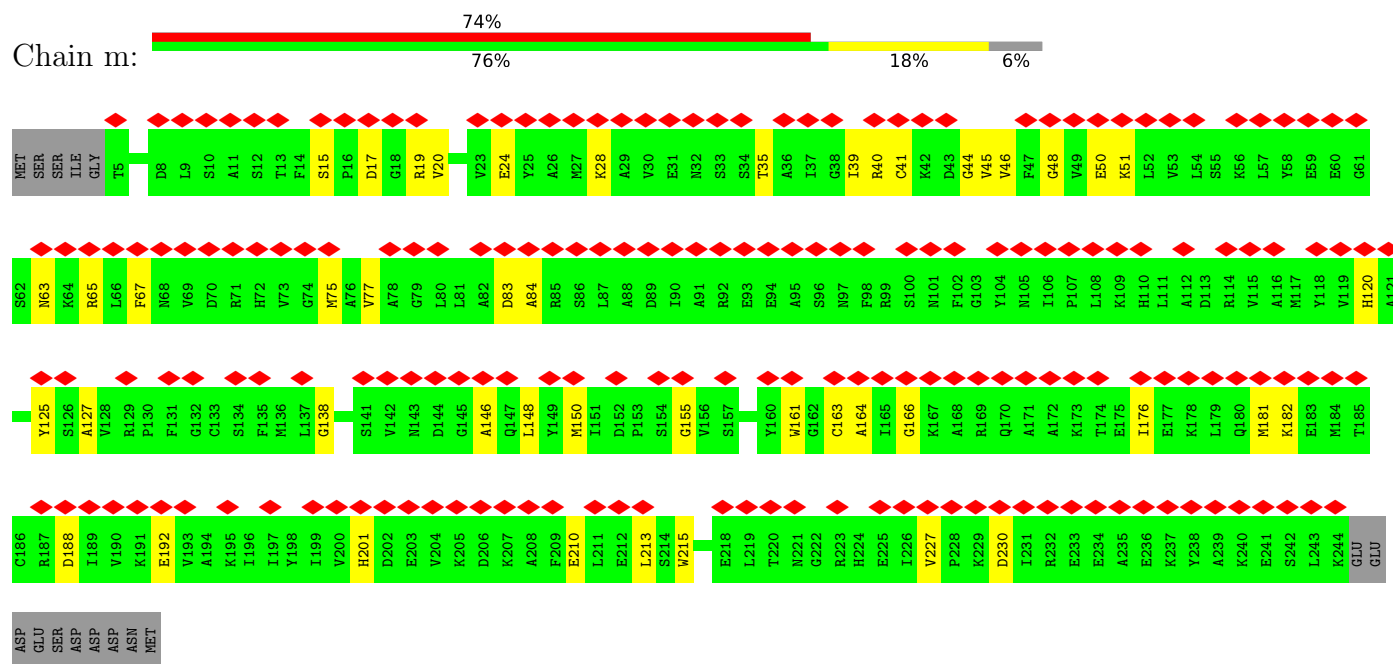




- Molecule 13: Proteasome subunit alpha type-3

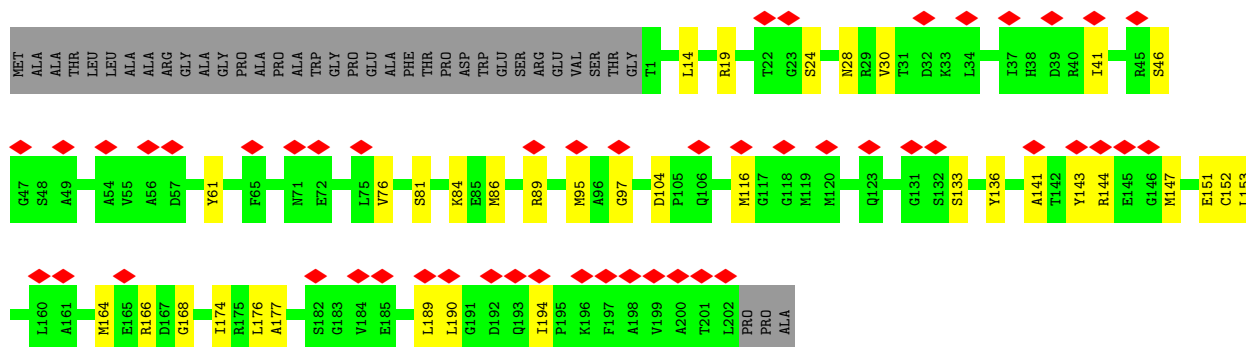


- Molecule 13: Proteasome subunit alpha type-3

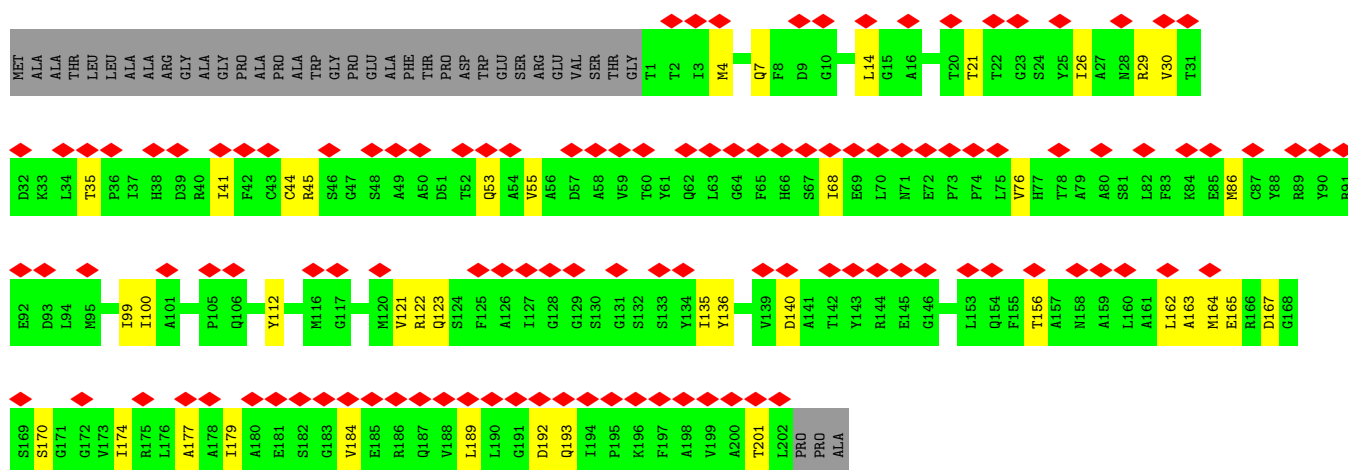


- Molecule 14: Proteasome subunit beta type-6

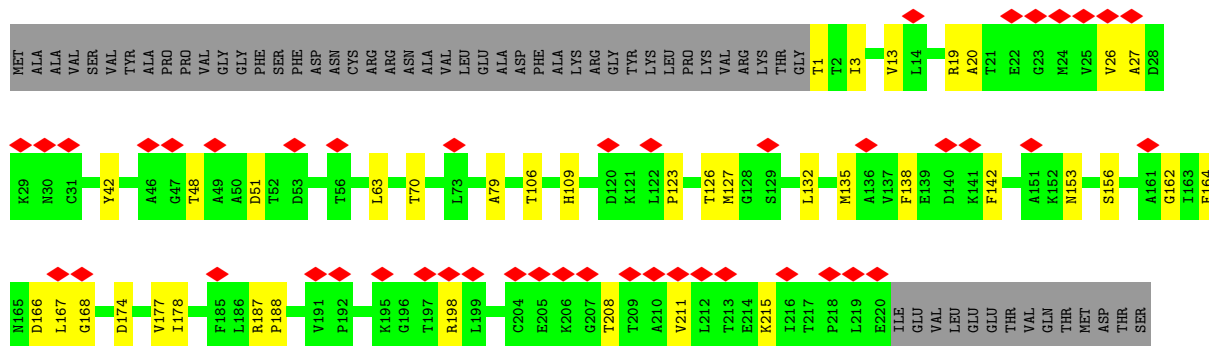




• Molecule 14: Proteasome subunit beta type-6

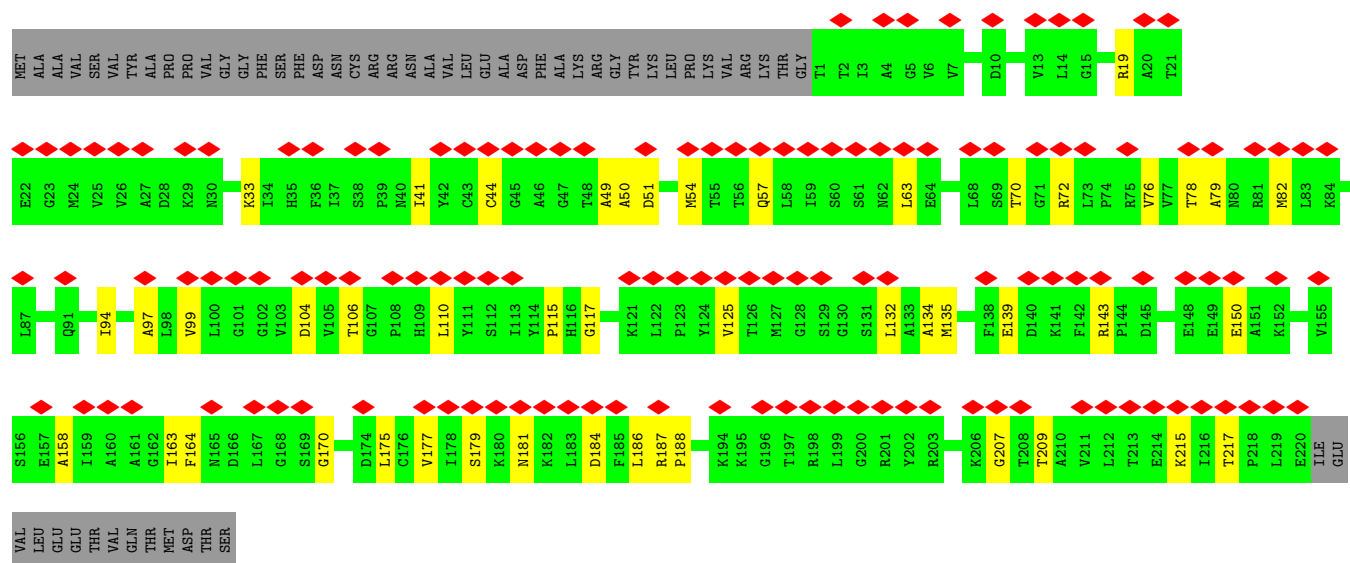


• Molecule 15: Proteasome subunit beta type-7

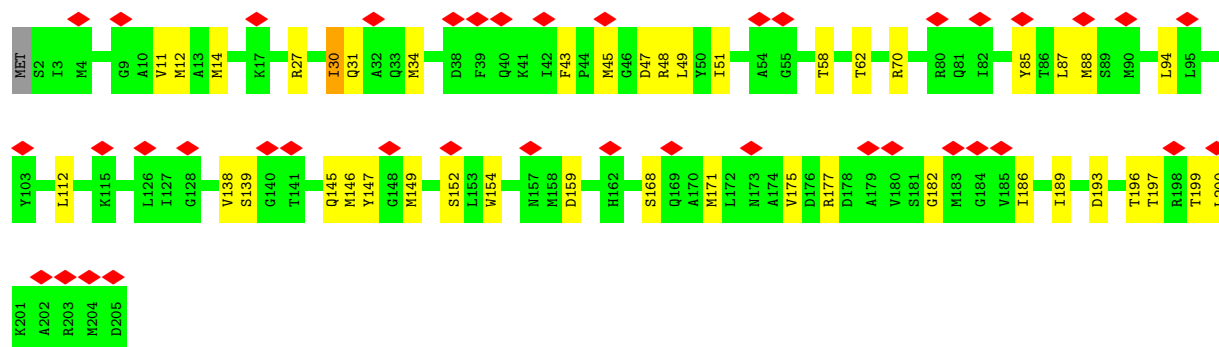
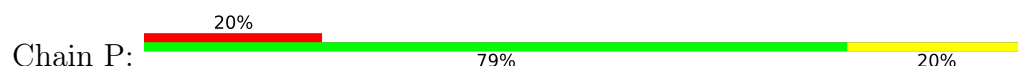


• Molecule 15: Proteasome subunit beta type-7

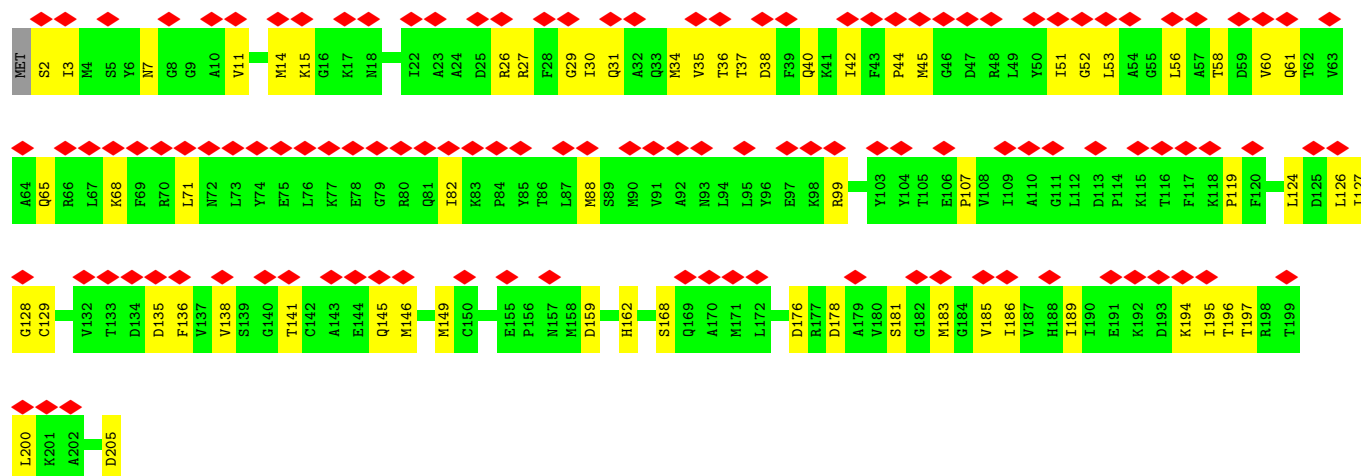




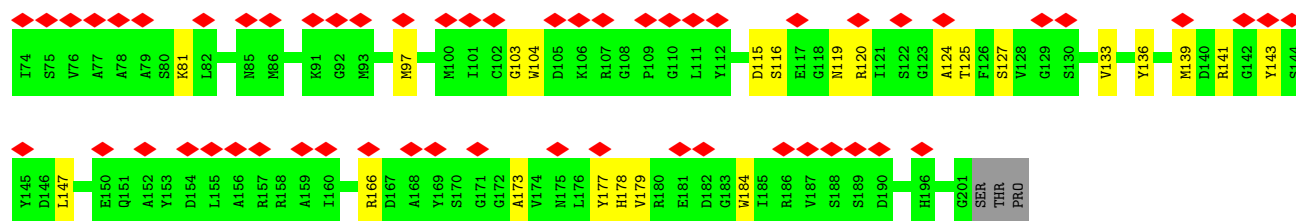
• Molecule 16: Proteasome subunit beta type-3



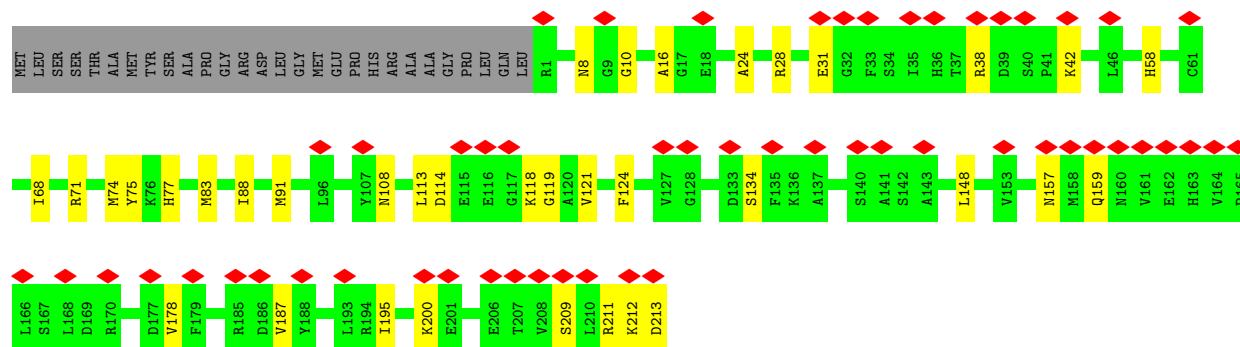
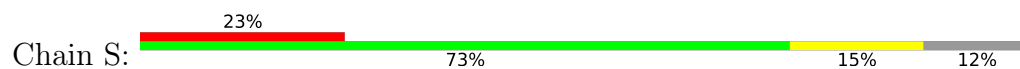
• Molecule 16: Proteasome subunit beta type-3



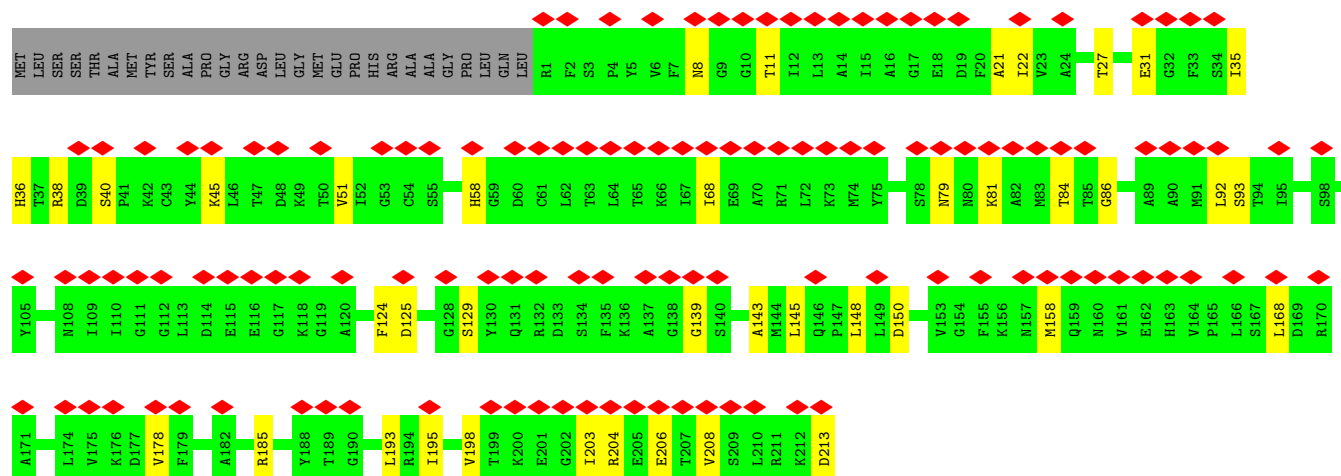
	K7	F8	H9	G11	V14	A15	A16	D17	S13	T21	A22	G23	A24	A27	S28	Q29	V31	K32	K33	I35	E36	I37	L41	L42	G43	T44	M45	A46	G47	G48	S53	F54	W55	E56	I65	Y66	E57	L68	R69	N70	K71	E72	R73	NET	ALA	LEU	ALA	SER	VAL	LEU	GLU	ARG	PRO	LEU	PRO	VAL	ASN	GLN	ARG	GLY	PHE	PHE	GLY	LEU	GLY	GLY	ASP	ALA	ASP	LEU	LEU	ASP	LEU	GLY	PRO	GLY	SER	SER	LEU	SER	ASP	GLY	LEU	GLY	SER	TRP	GLY	GLY	VAL	PRO	GLU	GLU	PRO	GLY	ILE	GLU	MET	LEU	HIS	GLY	T1
--	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	----



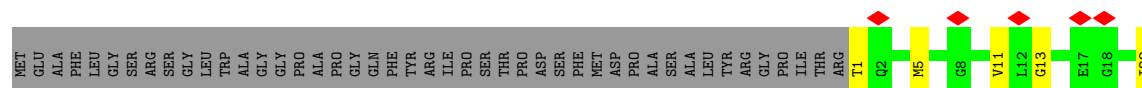
• Molecule 19: Proteasome subunit beta type-1

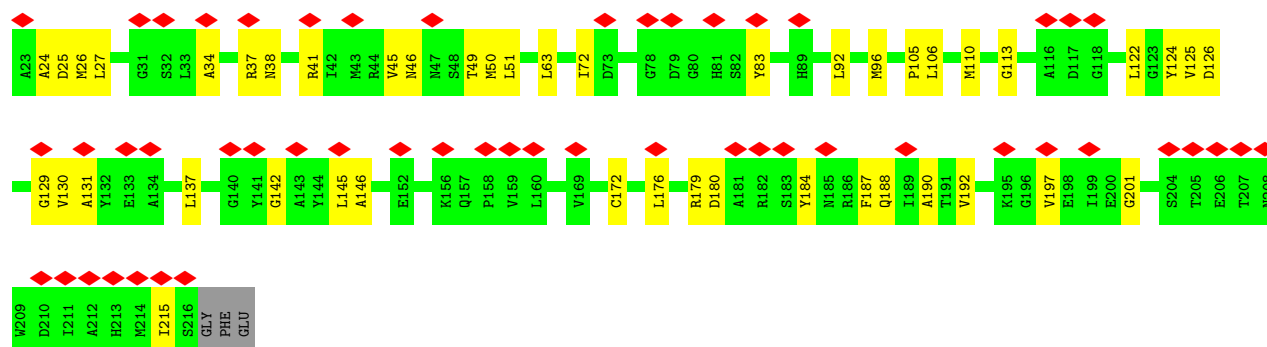


• Molecule 19: Proteasome subunit beta type-1

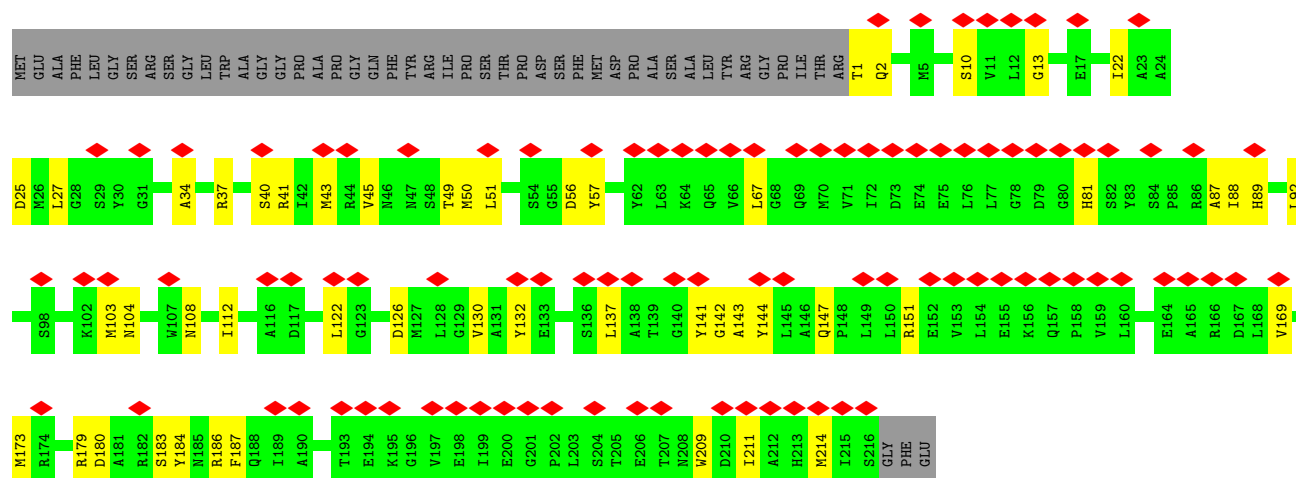


• Molecule 20: Proteasome subunit beta type-4

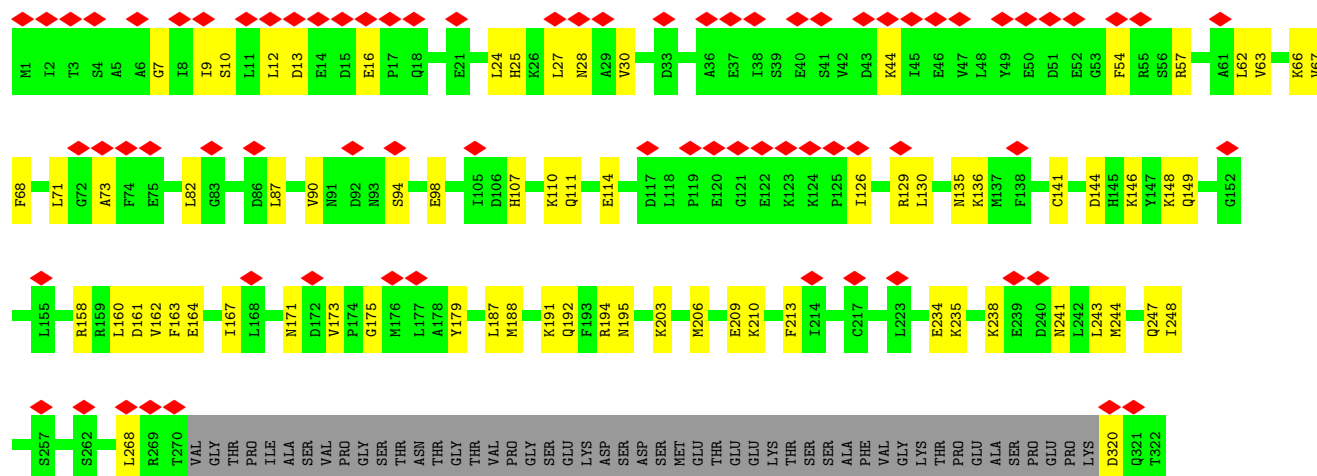




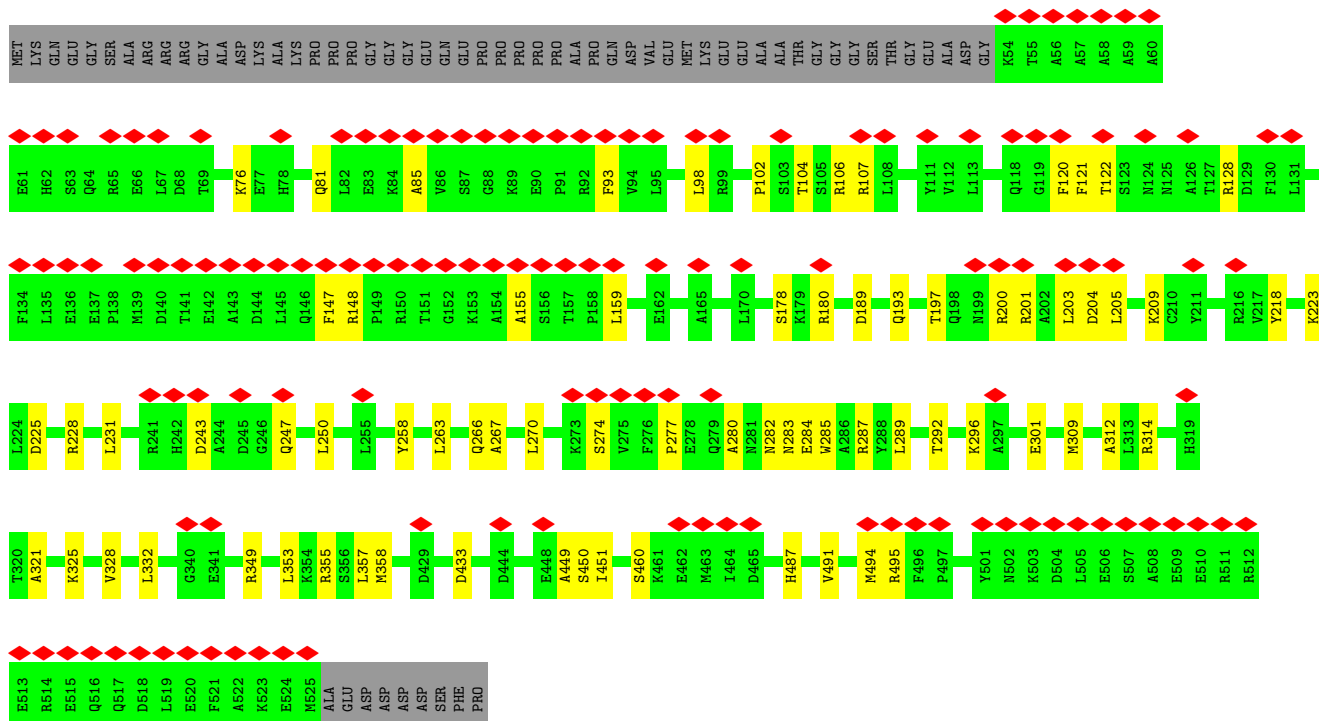
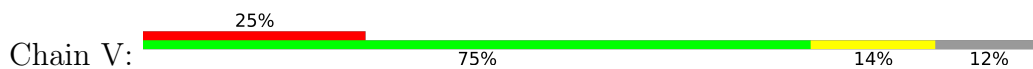
• Molecule 20: Proteasome subunit beta type-4



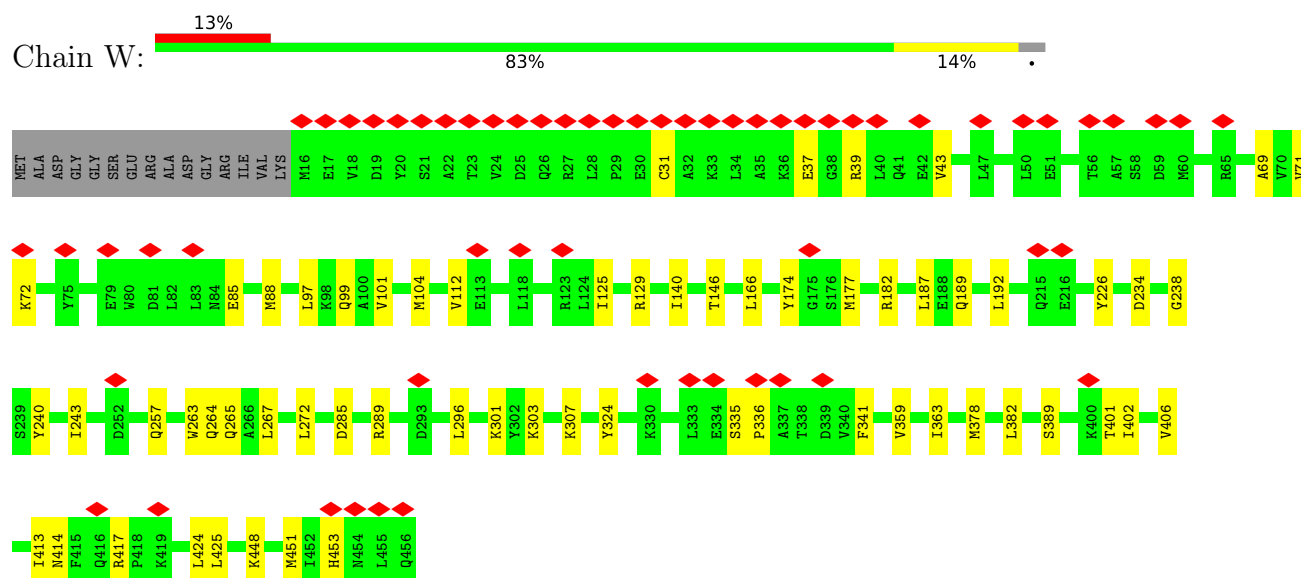
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1



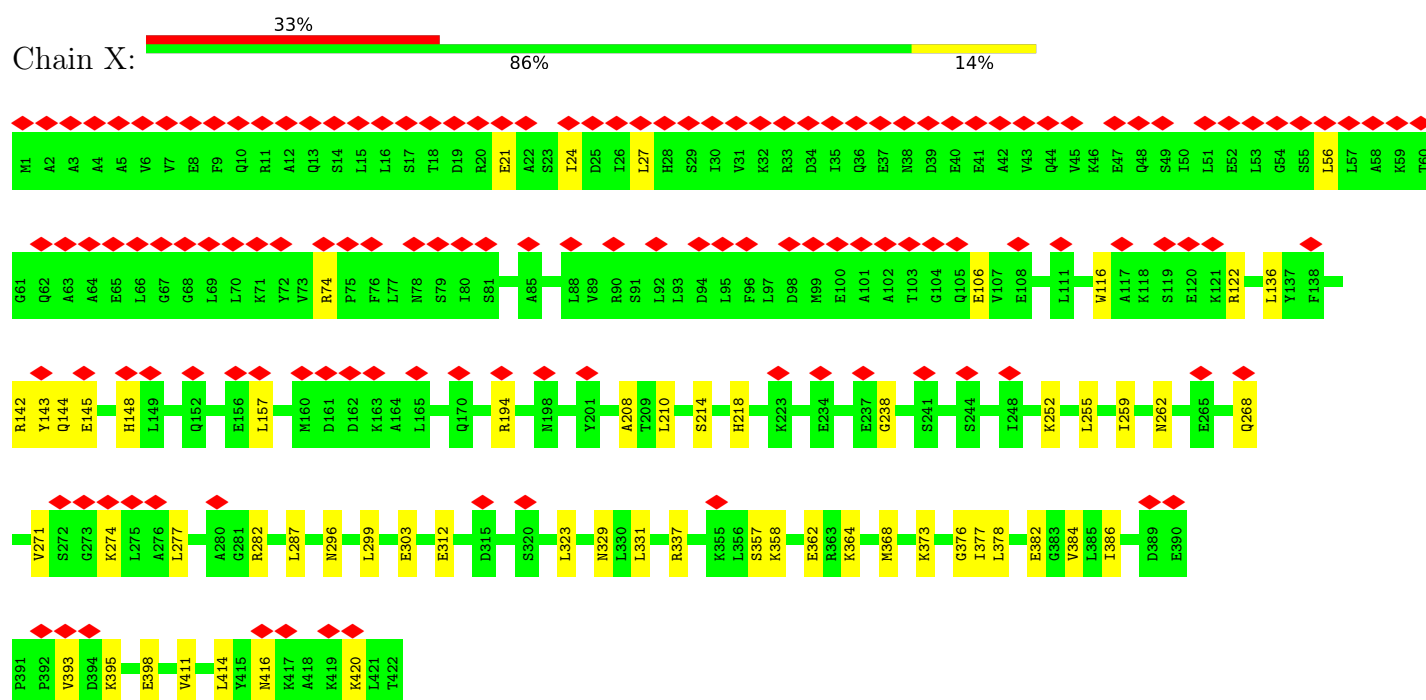
- Molecule 22: 26S proteasome non-ATPase regulatory subunit 3



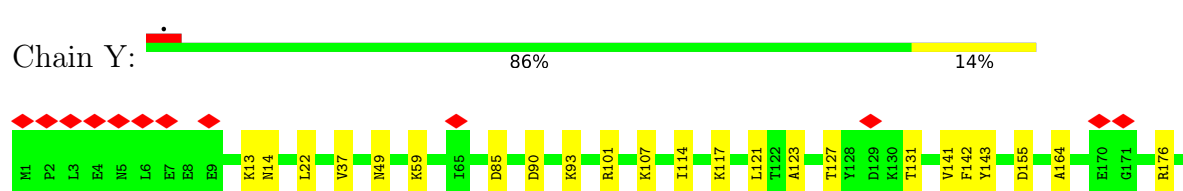
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 12



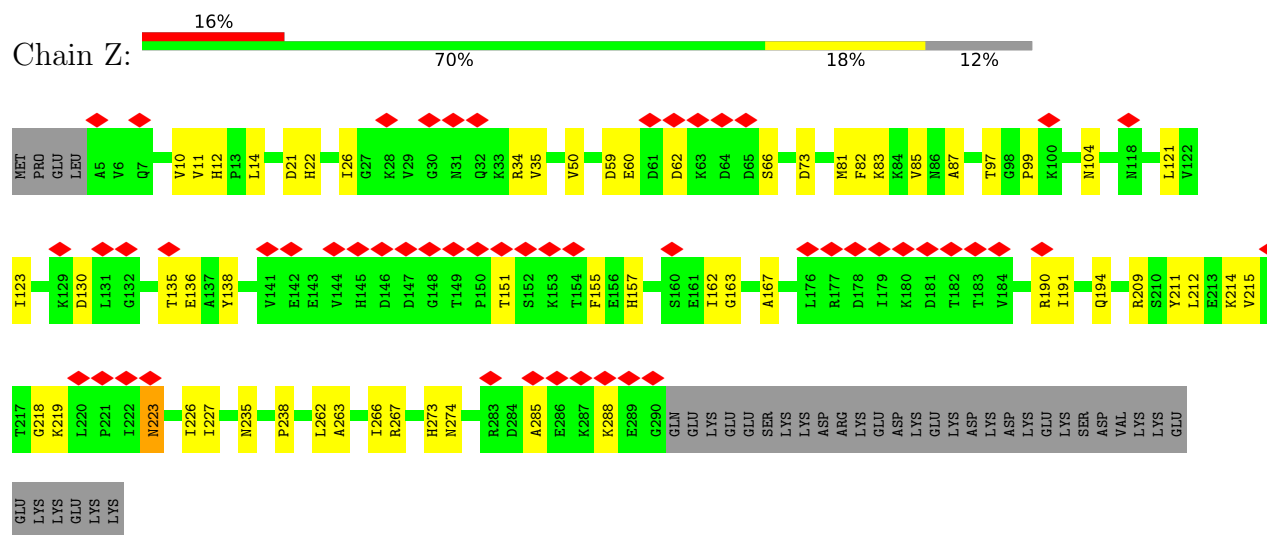
- Molecule 24: 26S proteasome non-ATPase regulatory subunit 11



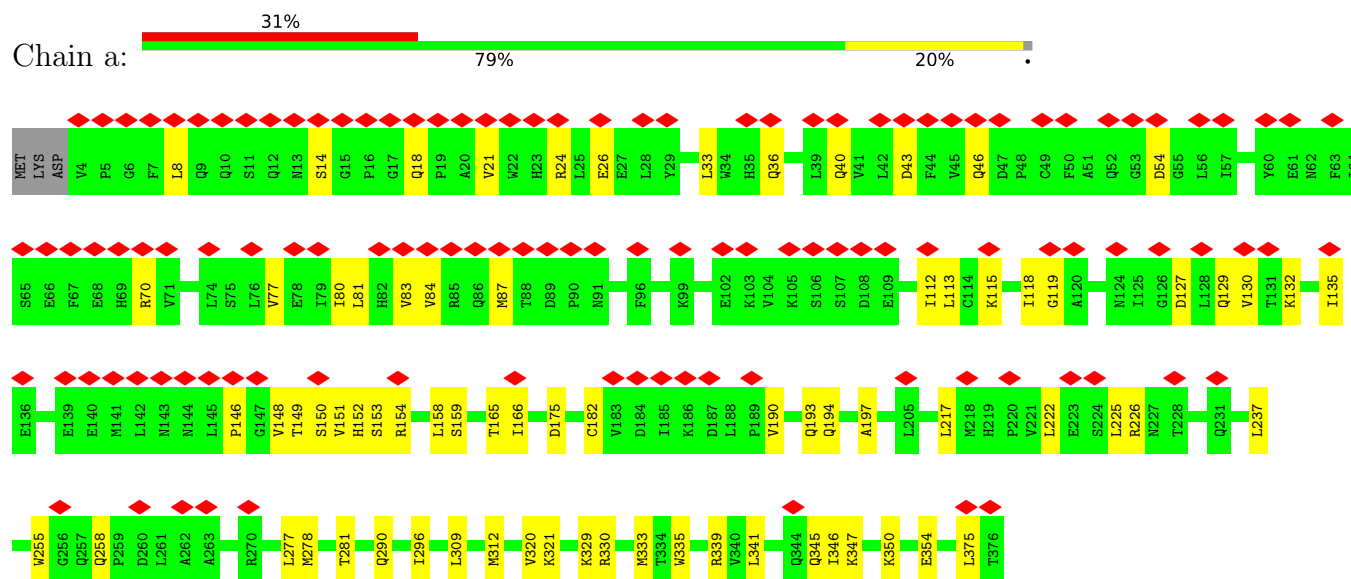
- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6



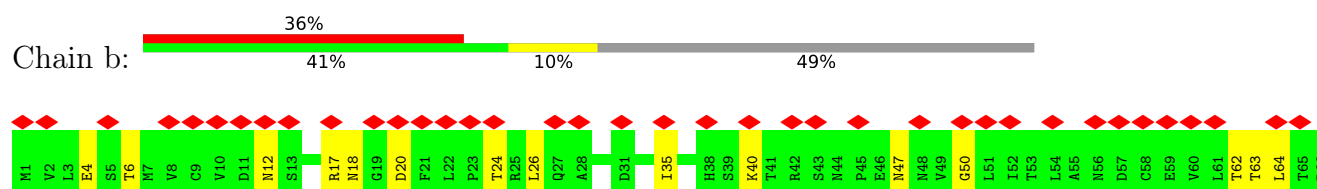
- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

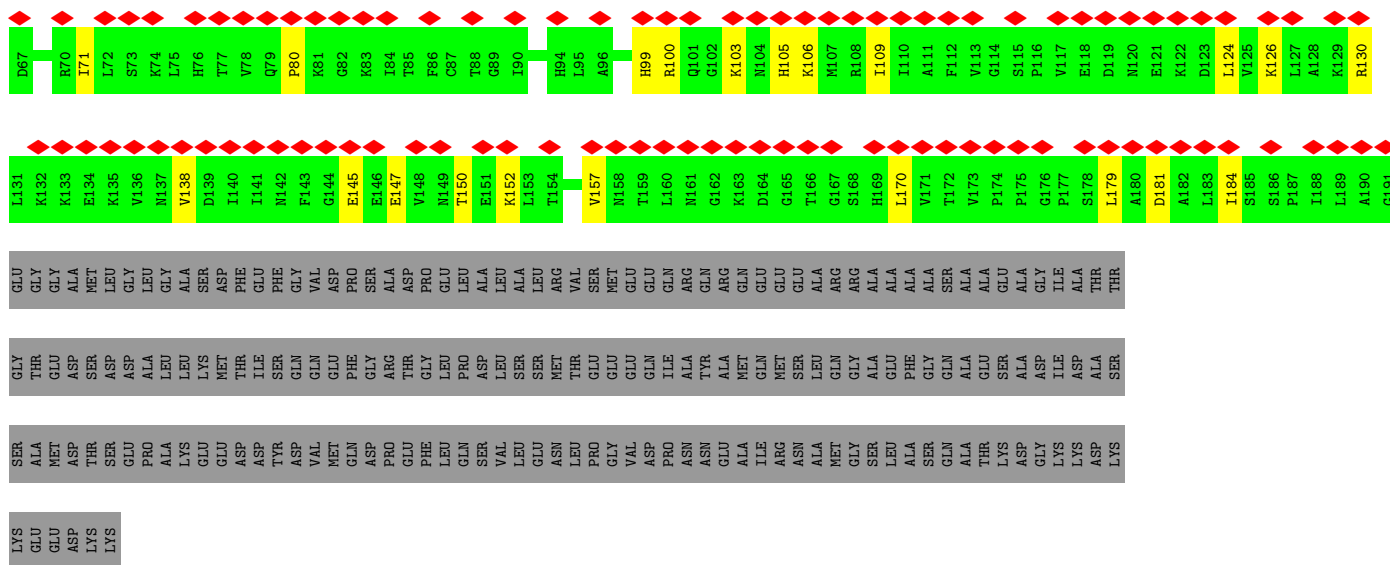


- Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

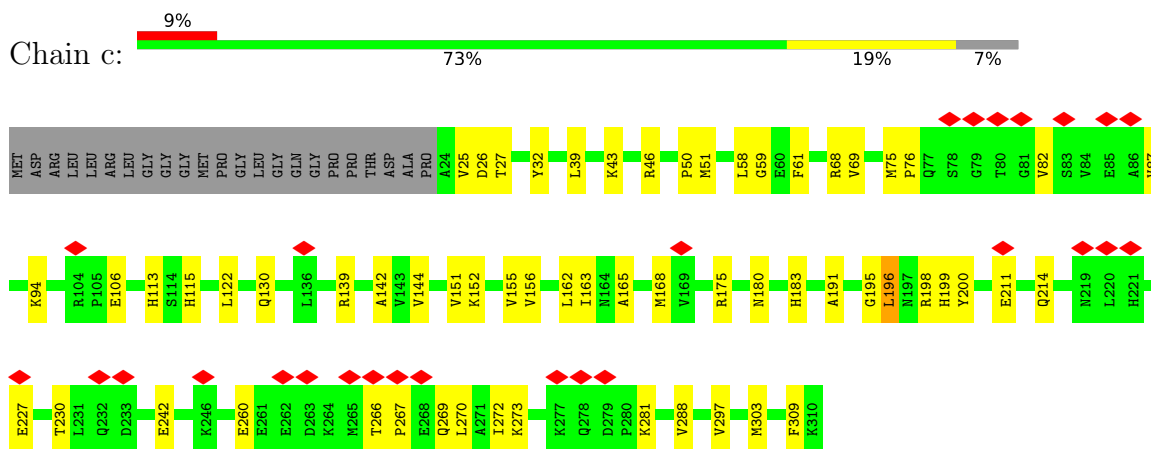


- Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

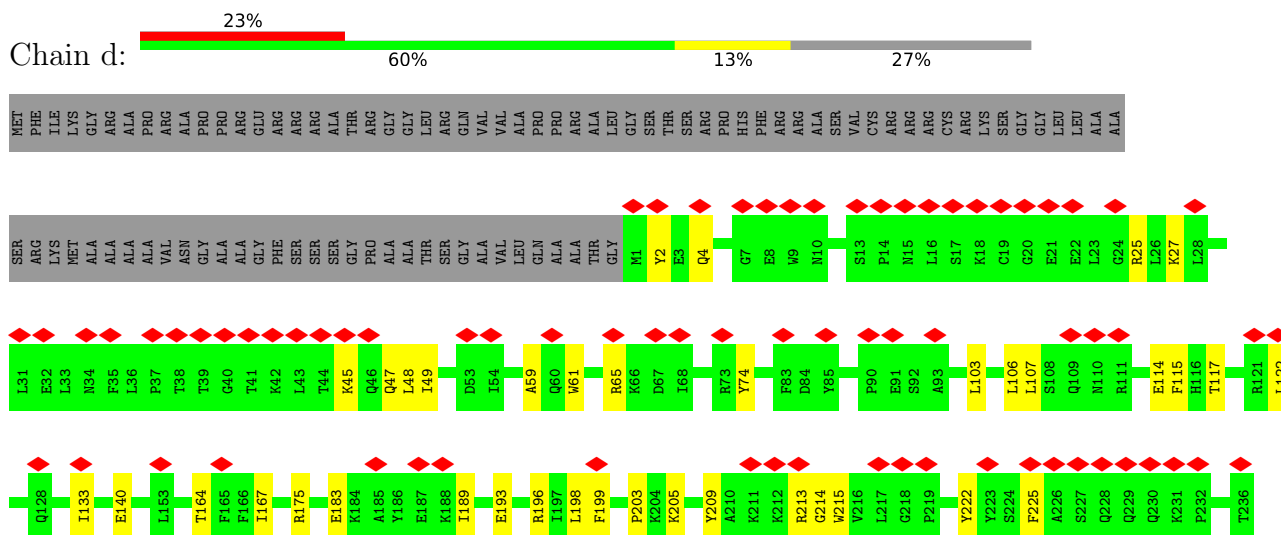




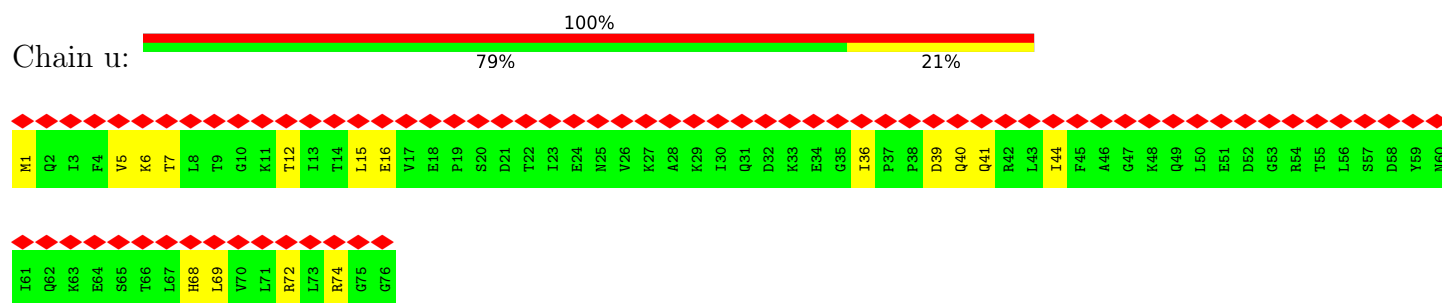
- Molecule 29: 26S proteasome non-ATPase regulatory subunit 14



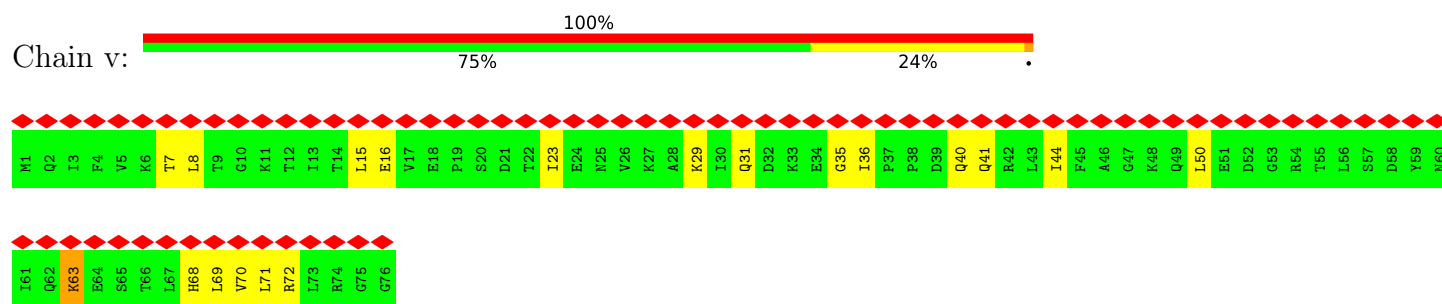
- Molecule 30: 26S proteasome non-ATPase regulatory subunit 8



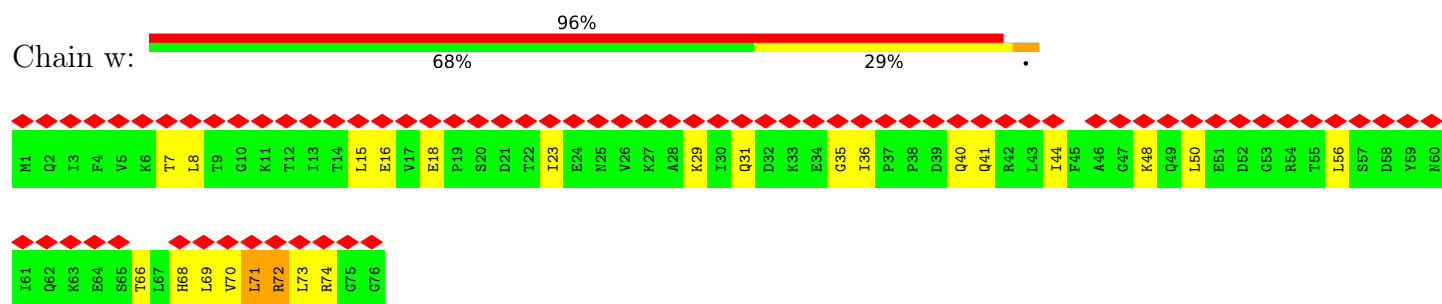
● Molecule 33: Ubiquitin



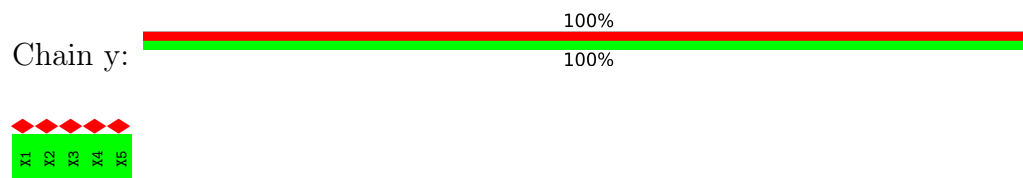
● Molecule 33: Ubiquitin



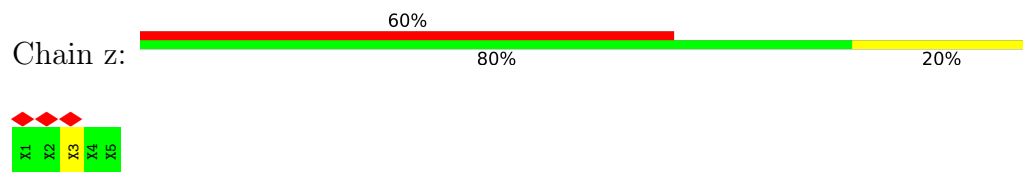
● Molecule 33: Ubiquitin



● Molecule 34: Substrate



● Molecule 34: Substrate



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43620	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.016	Depositor
Minimum map value	-0.005	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00465	Depositor
Map size (\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 (\AA)	0.685, 0.685, 0.685	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ATP, 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	A	0.21	0/3294	0.50	0/4447
2	B	0.21	0/3086	0.51	0/4164
3	C	0.20	0/2902	0.51	0/3904
4	D	0.25	0/3089	0.54	0/4168
5	E	0.20	0/2904	0.53	2/3924 (0.1%)
6	F	0.20	0/2896	0.47	0/3912
7	G	0.15	0/1923	0.42	0/2601
7	g	0.19	0/1914	0.46	0/2590
8	H	0.17	0/1844	0.40	0/2499
8	h	0.17	0/1844	0.39	0/2497
9	I	0.15	0/1991	0.42	0/2685
9	i	0.16	0/1985	0.46	0/2677
10	J	0.20	0/1906	0.47	0/2573
10	j	0.15	0/1887	0.43	0/2549
11	K	0.15	0/1804	0.43	0/2436
11	k	0.19	0/1809	0.43	0/2444
12	L	0.14	0/1901	0.37	0/2570
12	l	0.15	0/1896	0.37	0/2565
13	M	0.14	0/1911	0.39	0/2573
13	m	0.14	0/1916	0.40	0/2580
14	N	0.14	0/1540	0.37	0/2085
14	n	0.16	0/1536	0.39	0/2080
15	O	0.16	0/1676	0.42	0/2271
15	o	0.15	0/1686	0.43	0/2282
16	P	0.18	0/1616	0.53	2/2180 (0.1%)
16	p	0.17	0/1620	0.45	0/2184
17	Q	0.12	0/1621	0.35	0/2194
17	q	0.13	0/1621	0.37	0/2194
18	R	0.13	0/1590	0.37	0/2147
18	r	0.16	0/1590	0.42	0/2147
19	S	0.16	0/1671	0.48	0/2252
19	s	0.15	0/1684	0.42	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	T	0.15	0/1716	0.42	0/2323
20	t	0.15	0/1720	0.39	0/2328
21	U	0.19	0/6903	0.51	2/9324 (0.0%)
22	V	0.17	0/3824	0.44	0/5170
23	W	0.16	0/3644	0.43	0/4901
24	X	0.17	0/3381	0.44	0/4558
25	Y	0.18	0/3261	0.46	0/4393
26	Z	0.19	0/2324	0.53	0/3150
27	a	0.20	0/3053	0.55	0/4133
28	b	0.19	0/1478	0.52	0/2001
29	c	0.25	0/2302	0.63	1/3110 (0.0%)
30	d	0.21	0/2162	0.55	0/2919
31	e	0.24	0/437	0.57	0/595
32	f	0.23	0/6640	0.55	1/8988 (0.0%)
33	u	0.13	0/607	0.33	0/816
33	v	0.15	0/607	0.41	0/816
33	w	0.15	0/607	0.39	0/816
All	All	0.18	0/108819	0.47	8/146983 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	155	VAL	N-CA-C	-10.11	102.85	112.96
5	E	385	ASP	CA-C-N	5.15	131.38	121.54
5	E	385	ASP	C-N-CA	5.15	131.38	121.54
16	P	30	ILE	CA-C-N	5.15	128.55	120.82
16	P	30	ILE	C-N-CA	5.15	128.55	120.82
21	U	427	LEU	CA-C-N	5.14	125.19	119.32
21	U	427	LEU	C-N-CA	5.14	125.19	119.32
32	f	670	MET	CA-CB-CG	-5.02	104.05	114.10

There are no chirality outliers.

There are no planarity outliers.

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	A	3240	0	3286	46	0
2	B	3042	0	3101	63	0
3	C	2864	0	2971	54	0
4	D	3039	0	3076	50	0
5	E	2860	0	2828	42	0
6	F	2858	0	2852	49	0
7	G	1889	0	1885	28	0
7	g	1880	0	1875	21	0
8	H	1805	0	1784	23	0
8	h	1805	0	1798	27	0
9	I	1958	0	1960	22	0
9	i	1955	0	1955	22	0
10	J	1880	0	1892	38	0
10	j	1861	0	1865	27	0
11	K	1777	0	1762	20	0
11	k	1782	0	1766	34	0
12	L	1866	0	1852	29	0
12	l	1861	0	1839	24	0
13	M	1876	0	1861	28	0
13	m	1881	0	1868	29	0
14	N	1514	0	1487	27	0
14	n	1510	0	1483	27	0
15	O	1649	0	1659	28	0
15	o	1659	0	1681	32	0
16	P	1587	0	1598	30	0
16	p	1591	0	1609	42	0
17	Q	1588	0	1584	28	0
17	q	1588	0	1584	30	0
18	R	1559	0	1523	26	0
18	r	1559	0	1523	23	0
19	S	1641	0	1639	27	0
19	s	1654	0	1656	28	0
20	T	1683	0	1662	36	0
20	t	1687	0	1666	38	0
21	U	6787	0	6858	123	0
22	V	3754	0	3749	50	0
23	W	3596	0	3713	35	0
24	X	3335	0	3435	37	0
25	Y	3202	0	3204	36	0
26	Z	2281	0	2312	44	0
27	a	2995	0	3012	52	0
28	b	1458	0	1505	23	0
29	c	2260	0	2276	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	d	2116	0	2146	28	0
31	e	425	0	328	10	0
32	f	6529	0	6541	109	0
33	u	601	0	629	10	0
33	v	601	0	626	14	0
33	w	601	0	629	31	0
34	y	25	0	8	0	0
34	z	25	0	9	1	0
35	A	31	0	12	1	0
35	B	31	0	12	2	0
35	D	31	0	12	1	0
35	E	31	0	12	3	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	E	1	0	0	0	0
36	F	1	0	0	0	0
37	C	27	0	12	1	0
37	F	27	0	12	1	0
38	c	1	0	0	0	0
All	All	107223	0	107482	1529	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 (1529) 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)
33:w:71:LEU:CD1	33:w:72:ARG:H	1.18	1.52
33:w:71:LEU:HD12	33:w:72:ARG:N	1.06	1.37
33:w:71:LEU:HD12	33:w:72:ARG:CA	1.88	1.04
7:g:130:GLU:HG2	8:h:5:GLY:HA2	1.51	0.91
4:D:151:ILE:HG22	4:D:152:MET:HG2	1.54	0.88
33:w:71:LEU:CD1	33:w:72:ARG:N	1.96	0.86
33:w:71:LEU:CG	33:w:72:ARG:H	1.91	0.83
2:B:68:ILE:HG12	32:f:670:MET:HE1	1.60	0.80
32:f:459:CYS:O	33:w:66:THR:HG21	1.82	0.80
9:i:175:LEU:O	9:i:179:TYR:HB2	1.84	0.78
32:f:43:GLN:HE21	32:f:43:GLN:N	1.82	0.77
1:A:297:ARG:HH12	6:F:306:VAL:HG21	1.51	0.76
33:v:23:ILE:HD13	33:v:50:LEU:HB3	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:w:23:ILE:HD13	33:w:50:LEU:HB3	1.68	0.74
13:m:19:ARG:HH12	13:m:24:GLU:HB2	1.52	0.74
10:J:221:ASN:HD21	10:J:223:GLU:HB3	1.52	0.74
22:V:247:GLN:HG3	22:V:277:PRO:HG3	1.70	0.73
4:D:163:MET:HE3	4:D:164:TYR:H	1.55	0.72
21:U:556:MET:HE2	21:U:559:ARG:HD3	1.71	0.72
5:E:198:VAL:HG12	5:E:200:SER:H	1.55	0.72
33:v:7:THR:HG22	33:v:69:LEU:HD23	1.72	0.71
1:A:294:GLU:HA	1:A:297:ARG:HE	1.55	0.71
28:b:4:GLU:HA	28:b:106:LYS:H	1.55	0.71
33:u:44:ILE:HB	33:u:68:HIS:HB2	1.73	0.71
23:W:448:LYS:HA	23:W:451:MET:HE3	1.72	0.70
20:t:22:ILE:HG12	20:t:50:MET:HE1	1.72	0.70
1:A:390:THR:HA	2:B:216:ILE:HD11	1.72	0.70
32:f:670:MET:HA	32:f:673:ARG:HG3	1.72	0.69
33:w:7:THR:HG22	33:w:69:LEU:HD23	1.72	0.69
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.58	0.68
27:a:14:SER:HB2	27:a:18:GLN:HG2	1.76	0.68
21:U:402:PHE:HB2	21:U:437:TYR:HB3	1.74	0.68
7:G:88:ARG:HH22	13:M:156:VAL:HA	1.57	0.68
10:J:221:ASN:HD22	10:J:224:GLU:HG3	1.58	0.68
18:R:139:MET:O	18:R:143:TYR:HB2	1.94	0.68
5:E:253:ILE:HG13	6:F:308:ARG:HH22	1.59	0.68
17:q:45:LEU:HB2	17:q:103:LEU:HB2	1.75	0.67
25:Y:14:ASN:HB2	25:Y:143:TYR:HE1	1.59	0.67
4:D:244:PRO:HB3	4:D:291:GLU:HG3	1.76	0.67
16:P:48:ARG:HD3	16:P:112:LEU:HD12	1.77	0.67
15:O:215:LYS:HB3	16:P:197:THR:HB	1.76	0.67
27:a:24:ARG:HH12	27:a:40:GLN:HG2	1.58	0.67
27:a:129:GLN:HG2	27:a:130:VAL:HG23	1.76	0.66
30:d:246:VAL:HA	30:d:249:TYR:CD2	2.30	0.66
26:Z:97:THR:HG23	26:Z:99:PRO:HD3	1.76	0.65
26:Z:263:ALA:HB1	29:c:288:VAL:HG23	1.77	0.65
21:U:834:SER:HB2	21:U:836:THR:HG23	1.78	0.64
4:D:293:LEU:HD12	4:D:326:ARG:HH11	1.62	0.64
20:t:67:LEU:HD11	20:t:88:ILE:HD12	1.79	0.64
3:C:230:MET:HG3	3:C:232:ARG:H	1.63	0.64
4:D:159:LYS:HD2	4:D:221:HIS:HA	1.80	0.64
7:G:41:ALA:HB3	7:G:166:THR:HB	1.79	0.64
12:L:134:ILE:HB	12:L:145:PHE:HB2	1.80	0.64
4:D:56:VAL:HG22	21:U:600:ARG:HE	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:MET:HE1	3:C:86:LEU:HB2	1.78	0.64
32:f:402:ASN:HB2	32:f:407:MET:HB3	1.78	0.64
6:F:318:ASP:HB3	6:F:347:ARG:HG2	1.80	0.64
17:q:143:LEU:O	17:q:147:TYR:HB2	1.98	0.64
17:q:21:ALA:HB3	17:q:29:LYS:HB3	1.80	0.63
1:A:55:LEU:HD11	2:B:76:GLU:HG2	1.79	0.63
20:T:110:MET:HB2	20:T:125:VAL:HB	1.80	0.63
21:U:68:PHE:HB3	21:U:73:ALA:HB3	1.80	0.63
13:M:35:THR:HA	13:M:166:GLY:HA3	1.79	0.63
27:a:33:LEU:HD13	27:a:36:GLN:HB2	1.81	0.63
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.80	0.63
8:h:39:LYS:HG3	8:h:44:VAL:HG22	1.81	0.63
20:t:43:MET:HB3	20:t:51:LEU:HB3	1.79	0.63
21:U:694:ILE:HG23	21:U:695:MET:HG2	1.81	0.63
6:F:251:LEU:HD21	6:F:256:LEU:HD11	1.79	0.63
32:f:655:LEU:HD11	32:f:800:LEU:HD13	1.81	0.63
27:a:83:VAL:HG12	27:a:87:MET:HE2	1.81	0.62
29:c:168:MET:HE1	29:c:199:HIS:HA	1.79	0.62
23:W:414:ASN:HB2	23:W:417:ARG:HG3	1.81	0.62
10:j:192:ILE:HD12	10:j:206:ILE:HD12	1.80	0.62
25:Y:101:ARG:HD3	25:Y:131:THR:HG22	1.80	0.62
16:p:11:VAL:HG11	16:p:52:GLY:HA3	1.81	0.62
3:C:147:THR:HG23	3:C:149:GLU:H	1.63	0.62
30:d:114:GLU:HA	30:d:117:THR:HG22	1.81	0.62
33:w:44:ILE:HB	33:w:68:HIS:HB2	1.81	0.62
10:j:114:LEU:HA	10:j:117:ARG:HE	1.63	0.62
10:J:89:VAL:HG22	17:Q:66:LEU:HD11	1.80	0.62
21:U:241:ASN:HD21	21:U:244:MET:HE3	1.64	0.62
8:h:81:PRO:HA	8:h:84:ARG:HE	1.65	0.62
12:l:34:ALA:HB3	12:l:49:LEU:HD12	1.82	0.62
33:v:44:ILE:HB	33:v:68:HIS:HB2	1.81	0.62
30:d:238:PRO:O	30:d:242:LEU:HB2	1.99	0.62
27:a:321:LYS:HB2	27:a:335:TRP:HB3	1.81	0.62
32:f:779:CYS:SG	32:f:785:ARG:NH1	2.73	0.62
21:U:234:GLU:HG2	21:U:238:LYS:HE3	1.80	0.62
21:U:54:PHE:HB3	21:U:57:ARG:HB2	1.82	0.61
26:Z:85:VAL:HA	29:c:76:PRO:HB3	1.83	0.61
9:i:174:MET:HA	9:i:177:GLN:HG3	1.80	0.61
9:i:234:GLU:HA	9:i:237:ILE:HG12	1.82	0.61
21:U:475:HIS:HE1	21:U:507:VAL:HG22	1.66	0.61
27:a:281:THR:HG21	27:a:333:MET:HE2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:320:ILE:HA	32:f:325:GLN:HE22	1.64	0.61
2:B:387:LYS:HG2	2:B:390:LEU:HB3	1.83	0.61
33:w:44:ILE:O	33:w:68:HIS:N	2.33	0.61
7:G:113:MET:HE3	15:O:70:THR:HA	1.83	0.61
21:U:126:ILE:HD12	21:U:130:LEU:HD11	1.82	0.61
27:a:33:LEU:HA	28:b:18:ASN:HD22	1.64	0.61
32:f:320:ILE:O	32:f:323:ASN:ND2	2.34	0.61
8:h:3:GLU:HG2	13:m:127:ALA:HB3	1.82	0.61
11:k:74:ILE:HG12	11:k:109:VAL:HG22	1.83	0.61
15:o:44:CYS:HB2	15:o:99:VAL:HB	1.81	0.61
16:P:145:GLN:NE2	19:s:143:ALA:HB1	2.16	0.61
17:Q:104:LEU:HB3	17:Q:116:TYR:HB2	1.83	0.61
33:w:72:ARG:O	33:w:73:LEU:HD23	2.01	0.61
33:v:36:ILE:O	33:v:41:GLN:NE2	2.34	0.60
5:E:235:ILE:HD12	5:E:277:MET:HG2	1.83	0.60
20:T:63:LEU:HD21	20:T:106:LEU:HD13	1.82	0.60
30:d:213:ARG:NH1	30:d:214:GLY:O	2.35	0.60
21:U:360:VAL:HG22	21:U:392:TRP:HE1	1.65	0.60
19:s:11:THR:HA	19:s:139:GLY:HA3	1.83	0.60
33:w:36:ILE:O	33:w:41:GLN:NE2	2.34	0.60
3:C:62:GLU:HB2	3:C:66:LEU:HD23	1.82	0.60
20:T:176:LEU:O	20:T:180:ASP:HB3	2.02	0.60
21:U:613:ASP:HA	21:U:616:ARG:HD3	1.84	0.60
32:f:569:LYS:HE3	32:f:572:ALA:HB3	1.82	0.60
13:m:45:VAL:HG11	13:m:138:GLY:HA3	1.83	0.60
16:p:189:ILE:HB	16:p:196:THR:HB	1.83	0.60
8:H:106:PRO:HB2	8:H:109:GLN:HG2	1.82	0.60
20:T:11:VAL:HG13	20:T:24:ALA:HB2	1.83	0.60
16:P:58:THR:O	17:Q:85:ARG:NH2	2.35	0.60
26:Z:285:ALA:HA	26:Z:288:LYS:HE3	1.84	0.60
20:T:122:LEU:HG	20:T:137:LEU:HD12	1.84	0.59
32:f:389:LYS:HE3	32:f:428:GLN:HG2	1.84	0.59
8:h:93:LEU:HD13	8:h:113:ARG:HB3	1.84	0.59
10:j:38:ARG:HH22	10:j:182:GLU:HA	1.67	0.59
3:C:130:LYS:HD2	3:C:131:VAL:H	1.68	0.59
10:j:109:ARG:NH2	18:r:70:ASN:OD1	2.33	0.59
16:p:14:MET:HG3	16:p:136:PHE:HB3	1.82	0.59
20:t:92:LEU:HD12	20:t:112:ILE:HD11	1.84	0.59
10:j:130:SER:HB3	10:j:146:GLN:HE22	1.66	0.59
15:o:78:THR:HG22	15:o:82:MET:HE1	1.84	0.59
26:Z:81:MET:HE1	29:c:94:LYS:HD2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:206:MET:HE1	11:k:210:LEU:HD22	1.83	0.59
27:a:77:VAL:HG21	27:a:113:LEU:HD13	1.85	0.59
10:j:154:HIS:HB3	11:k:59:MET:HE1	1.83	0.59
13:m:150:MET:HE3	13:m:163:CYS:HB3	1.84	0.59
6:F:224:LEU:HB2	6:F:348:LEU:HD23	1.84	0.59
17:Q:183:ILE:HG12	17:Q:188:ILE:HG12	1.84	0.59
1:A:76:ALA:HA	32:f:680:ARG:HD3	1.83	0.59
7:g:123:GLN:NE2	8:h:82:ASP:OD1	2.35	0.59
12:l:7:ASP:HB3	12:l:20:HIS:HD1	1.67	0.59
6:F:282:ILE:HG22	6:F:327:LYS:HB2	1.85	0.59
16:p:44:PRO:O	16:p:68:LYS:NZ	2.36	0.59
25:Y:13:LYS:HG2	25:Y:212:GLU:HB2	1.85	0.59
3:C:44:ARG:HG3	22:V:495:ARG:HD3	1.85	0.58
32:f:367:SER:O	32:f:371:ASN:ND2	2.36	0.58
3:C:57:ARG:NH2	21:U:643:SER:O	2.36	0.58
27:a:112:ILE:HD12	27:a:151:VAL:HG11	1.84	0.58
28:b:124:LEU:HD21	28:b:152:LYS:HB3	1.85	0.58
32:f:668:ALA:HA	32:f:697:ILE:HD11	1.85	0.58
4:D:87:LEU:HB3	5:E:80:VAL:HB	1.86	0.58
5:E:322:LYS:HD3	5:E:326:ILE:HG13	1.86	0.58
12:L:44:ALA:HB2	12:L:142:PRO:HB3	1.85	0.58
16:P:189:ILE:HB	16:P:196:THR:HB	1.86	0.58
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.36	0.58
6:F:252:ALA:HB3	6:F:255:GLN:HB2	1.85	0.58
33:v:44:ILE:O	33:v:68:HIS:N	2.33	0.58
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.35	0.58
7:G:221:THR:HG22	7:G:223:GLU:H	1.67	0.58
14:n:14:LEU:HB2	14:n:177:ALA:HB3	1.83	0.58
15:o:177:VAL:HB	15:o:184:ASP:HB2	1.85	0.58
4:D:116:LEU:HD23	4:D:118:THR:H	1.69	0.58
4:D:149:SER:O	4:D:150:SER:C	2.46	0.58
14:N:95:MET:HA	14:N:116:MET:HE1	1.86	0.58
14:N:164:MET:HE1	14:N:194:ILE:HD13	1.86	0.58
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.86	0.58
22:V:121:PHE:O	22:V:128:ARG:NH1	2.37	0.58
12:l:73:SER:HB3	12:l:133:LEU:HB2	1.85	0.58
19:s:45:LYS:HA	19:s:51:VAL:HG22	1.86	0.58
1:A:73:ALA:HA	2:B:140:ASP:HB3	1.86	0.58
32:f:83:ARG:NH1	32:f:153:SER:OG	2.37	0.58
32:f:304:PHE:HA	32:f:321:MET:HE2	1.85	0.58
2:B:75:GLU:OE2	32:f:677:HIS:ND1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:B:501:ATP:H5'1	3:C:307:ARG:HH12	1.69	0.58
17:Q:143:LEU:O	17:Q:147:TYR:HB2	2.03	0.58
21:U:111:GLN:NE2	21:U:114:GLU:OE1	2.37	0.58
32:f:562:LEU:HD21	32:f:576:ILE:HG21	1.85	0.58
7:g:32:ILE:HD13	7:g:137:CYS:HB2	1.86	0.58
33:w:71:LEU:HD12	33:w:72:ARG:C	2.28	0.58
11:K:100:TRP:O	18:R:57:ARG:NH2	2.35	0.58
21:U:416:GLU:OE1	21:U:450:HIS:NE2	2.36	0.58
17:q:43:LEU:HG	17:q:188:ILE:HD13	1.86	0.58
21:U:452:ASN:H	21:U:486:MET:HE1	1.69	0.57
22:V:349:ARG:NH2	31:e:37:HIS:O	2.37	0.57
32:f:137:ARG:NH2	32:f:165:GLU:OE1	2.36	0.57
13:m:45:VAL:HG23	13:m:146:ALA:HB1	1.85	0.57
33:v:40:GLN:HG2	33:v:72:ARG:HB3	1.86	0.57
21:U:896:GLU:O	21:U:901:GLN:NE2	2.37	0.57
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.85	0.57
30:d:122:LEU:HD11	30:d:133:ILE:HG21	1.86	0.57
9:i:231:LYS:O	9:i:235:GLN:NE2	2.35	0.57
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.86	0.57
23:W:140:ILE:HG12	23:W:177:MET:HB3	1.85	0.57
24:X:414:LEU:HD21	26:Z:273:HIS:HD2	1.68	0.57
15:O:3:ILE:HD11	15:O:127:MET:HE2	1.87	0.57
28:b:179:LEU:HD23	28:b:181:ASP:H	1.69	0.57
32:f:548:THR:HA	32:f:551:LYS:HE3	1.86	0.57
16:p:7:ASN:ND2	16:p:29:GLY:O	2.37	0.57
17:Q:19:ARG:NH1	17:Q:179:SER:OG	2.37	0.57
24:X:296:ASN:O	24:X:337:ARG:NH1	2.37	0.57
8:h:196:LYS:HG3	8:h:203:MET:HE1	1.87	0.57
16:P:85:TYR:HA	16:P:88:MET:HE2	1.87	0.57
19:s:193:LEU:HB3	19:s:208:VAL:HB	1.86	0.57
2:B:253:SER:O	3:C:271:ARG:NH2	2.38	0.57
9:i:243:GLU:HA	9:i:246:LYS:HG2	1.86	0.57
11:k:18:GLU:O	12:l:31:GLN:NE2	2.36	0.57
33:v:40:GLN:HE22	33:v:71:LEU:HB3	1.69	0.57
6:F:236:LEU:HD12	6:F:354:PHE:HZ	1.68	0.57
29:c:270:LEU:HA	29:c:273:LYS:HG2	1.86	0.57
32:f:827:PRO:HB2	32:f:829:MET:HG2	1.87	0.57
14:n:55:VAL:HG13	14:n:86:MET:HG2	1.86	0.57
2:B:174:MET:HE1	2:B:248:LEU:HD13	1.87	0.57
28:b:109:ILE:HB	28:b:138:VAL:HG22	1.87	0.57
18:r:10:HIS:O	18:r:178:HIS:NE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:43:PHE:HB3	16:P:45:MET:HE3	1.86	0.56
20:T:45:VAL:HG21	20:T:51:LEU:HD23	1.87	0.56
21:U:770:TRP:HA	29:c:180:ASN:HB3	1.87	0.56
30:d:164:THR:HA	30:d:167:ILE:HG12	1.87	0.56
19:s:36:HIS:HD1	20:t:132:TYR:HH	1.52	0.56
20:t:37:ARG:O	20:t:186:ARG:NH1	2.38	0.56
21:U:628:ARG:NH2	21:U:753:GLY:O	2.38	0.56
32:f:861:THR:HB	32:f:879:ARG:HH11	1.69	0.56
35:E:401:ATP:O3G	6:F:344:ARG:NH1	2.38	0.56
6:F:421:MET:HA	6:F:424:ILE:HD12	1.86	0.56
10:J:36:ARG:O	10:J:176:TYR:OH	2.23	0.56
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.86	0.56
21:U:596:ASN:HA	21:U:599:ILE:HG22	1.87	0.56
22:V:231:LEU:HD11	22:V:250:LEU:HD22	1.87	0.56
22:V:450:SER:OG	22:V:451:ILE:N	2.39	0.56
7:g:95:ARG:HD3	14:n:68:ILE:HG22	1.86	0.56
10:j:146:GLN:NE2	10:j:147:THR:O	2.38	0.56
18:r:179:VAL:HG22	18:r:184:TRP:HB3	1.86	0.56
33:w:16:GLU:O	33:w:29:LYS:NZ	2.29	0.56
4:D:233:SER:OG	5:E:259:GLU:OE1	2.22	0.56
4:D:270:ILE:HD12	4:D:288:ILE:HG21	1.87	0.56
5:E:122:MET:HE1	5:E:196:LEU:HB3	1.86	0.56
20:T:188:GLN:HG3	20:T:201:GLY:HA3	1.87	0.56
21:U:413:LYS:HD2	21:U:780:SER:HB2	1.87	0.56
23:W:71:VAL:HG21	23:W:104:MET:HB2	1.87	0.56
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.87	0.56
4:D:338:ARG:HD2	4:D:364:VAL:HG12	1.88	0.56
14:N:24:SER:HG	20:t:141:TYR:HH	1.54	0.56
21:U:243:LEU:HG	21:U:913:ILE:HG12	1.88	0.56
23:W:129:ARG:NH1	23:W:146:THR:OG1	2.38	0.56
32:f:285:CYS:O	32:f:291:GLN:NE2	2.39	0.56
32:f:445:LEU:HG	32:f:466:LEU:HD13	1.87	0.56
12:l:212:ILE:HB	12:l:224:TYR:HB2	1.87	0.56
2:B:212:GLU:HB3	32:f:865:PHE:HZ	1.70	0.56
6:F:374:ASN:ND2	6:F:413:THR:O	2.39	0.56
32:f:845:ARG:HH22	32:f:865:PHE:HD2	1.53	0.56
7:g:5:SER:HA	7:g:23:TYR:OH	2.06	0.56
26:Z:190:ARG:HH12	29:c:297:VAL:HG22	1.69	0.56
33:w:7:THR:HA	33:w:69:LEU:HB3	1.87	0.56
14:N:14:LEU:HB2	14:N:177:ALA:HB3	1.88	0.56
26:Z:35:VAL:HB	26:Z:97:THR:HB	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:43:GLN:N	32:f:43:GLN:NE2	2.52	0.56
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.86	0.56
33:w:72:ARG:C	33:w:73:LEU:HG	2.29	0.56
10:J:146:GLN:NE2	10:J:147:THR:O	2.39	0.56
3:C:60:ARG:NH2	4:D:71:GLU:OE2	2.39	0.56
33:v:7:THR:HA	33:v:69:LEU:HB3	1.87	0.56
2:B:196:GLU:OE2	2:B:349:ARG:NH1	2.39	0.55
19:S:38:ARG:NH2	15:o:164:PHE:O	2.40	0.55
19:S:113:LEU:HD13	19:S:200:LYS:HZ2	1.71	0.55
22:V:287:ARG:NH1	31:e:21:GLU:OE2	2.39	0.55
15:o:63:LEU:HD11	15:o:79:ALA:HB2	1.88	0.55
19:s:68:ILE:HD11	19:s:92:LEU:HD13	1.87	0.55
33:w:71:LEU:O	33:w:72:ARG:NH1	2.39	0.55
16:P:12:MET:HE1	16:P:138:VAL:HA	1.89	0.55
32:f:398:TRP:HA	32:f:401:LYS:HD3	1.87	0.55
16:P:146:MET:HA	16:P:149:MET:HE2	1.88	0.55
28:b:62:THR:HG21	28:b:71:ILE:HG13	1.89	0.55
33:w:40:GLN:HE21	33:w:72:ARG:CZ	2.20	0.55
26:Z:235:ASN:HD21	27:a:335:TRP:HA	1.71	0.55
13:m:77:VAL:HG11	13:m:84:ALA:HB1	1.89	0.55
1:A:324:PRO:HA	1:A:327:LEU:HD13	1.89	0.55
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.88	0.55
14:N:46:SER:OG	14:N:97:GLY:O	2.24	0.55
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.88	0.55
19:S:159:GLN:NE2	15:o:207:GLY:O	2.40	0.55
15:o:50:ALA:HB2	16:p:129:CYS:HB2	1.88	0.55
16:p:126:LEU:HG	16:p:127:ILE:HG23	1.88	0.55
6:F:232:GLY:HA2	37:F:501:ADP:H5'2	1.86	0.55
8:H:74:LEU:HD12	8:H:87:VAL:HG22	1.89	0.55
21:U:576:PRO:HB3	21:U:611:ASN:HD22	1.72	0.55
23:W:401:THR:HG23	23:W:402:ILE:HD12	1.87	0.55
14:N:166:ARG:NH1	20:t:34:ALA:O	2.40	0.55
22:V:243:ASP:O	22:V:247:GLN:NE2	2.40	0.55
29:c:267:PRO:HA	29:c:270:LEU:HD23	1.88	0.55
32:f:459:CYS:O	33:w:66:THR:CG2	2.53	0.55
16:p:194:LYS:NZ	16:p:196:THR:OG1	2.36	0.55
32:f:531:ASN:O	32:f:565:ASN:ND2	2.37	0.55
18:r:14:VAL:HB	18:r:177:TYR:HB2	1.88	0.55
9:I:68:LEU:HD22	9:I:90:LEU:HD22	1.88	0.55
23:W:234:ASP:O	23:W:238:GLY:N	2.37	0.55
24:X:255:LEU:HD12	24:X:287:LEU:HD13	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:191:ALA:O	29:c:196:LEU:HB3	2.07	0.55
9:i:45:LEU:HD13	9:i:75:SER:HB2	1.89	0.55
15:o:215:LYS:HB3	16:p:197:THR:HB	1.88	0.55
21:U:126:ILE:HB	21:U:130:LEU:HD21	1.89	0.54
12:l:225:ASP:H	12:l:228:ASP:HB2	1.71	0.54
17:q:22:ALA:HA	17:q:28:MET:H	1.72	0.54
5:E:237:ALA:HB1	6:F:308:ARG:HG3	1.90	0.54
5:E:260:LEU:HD23	5:E:264:MET:HE2	1.89	0.54
17:Q:143:LEU:O	17:Q:147:TYR:CB	2.56	0.54
21:U:887:ALA:O	21:U:890:LYS:NZ	2.40	0.54
12:L:68:ASN:O	12:L:221:PHE:N	2.40	0.54
6:F:358:ASN:O	6:F:362:ARG:NH1	2.40	0.54
15:O:138:PHE:O	15:O:142:PHE:HB2	2.07	0.54
23:W:424:LEU:HG	23:W:425:LEU:HD12	1.89	0.54
2:B:412:MET:HE1	3:C:177:ALA:HB1	1.88	0.54
21:U:90:VAL:HG12	21:U:136:LYS:HE2	1.89	0.54
3:C:151:ILE:HD12	3:C:198:LEU:HD13	1.88	0.54
10:J:189:LYS:HA	10:J:232:ILE:HD11	1.90	0.54
24:X:208:ALA:HB2	24:X:238:GLY:HA3	1.90	0.54
32:f:83:ARG:O	32:f:87:THR:OG1	2.25	0.54
12:l:117:GLN:NE2	13:m:83:ASP:OD1	2.40	0.54
1:A:172:VAL:O	1:A:231:ASN:ND2	2.36	0.54
4:D:84:SER:O	5:E:68:LYS:NZ	2.40	0.54
26:Z:10:VAL:HG13	26:Z:163:GLY:HA3	1.89	0.54
26:Z:26:ILE:HD11	26:Z:35:VAL:HG22	1.90	0.54
32:f:654:VAL:HA	32:f:657:ILE:HD12	1.89	0.54
9:i:60:PHE:HE1	9:i:63:GLU:HG3	1.72	0.54
9:i:151:ASP:OD1	9:i:155:ASN:N	2.40	0.54
16:p:15:LYS:HE2	16:p:119:PRO:HB2	1.90	0.54
24:X:299:LEU:HD21	24:X:331:LEU:HA	1.89	0.54
20:T:126:ASP:OD1	20:T:130:VAL:N	2.39	0.54
22:V:122:THR:HG21	22:V:155:ALA:HB1	1.90	0.54
22:V:147:PHE:O	22:V:148:ARG:NH1	2.41	0.54
28:b:50:GLY:H	28:b:64:LEU:HD12	1.72	0.54
30:d:175:ARG:HH22	30:d:199:PHE:HB3	1.73	0.54
14:n:100:ILE:HB	14:n:112:TYR:HB2	1.89	0.54
17:q:143:LEU:O	17:q:147:TYR:CB	2.56	0.54
10:J:208:LEU:HD22	10:J:220:LEU:HG	1.90	0.53
22:V:280:ALA:HB1	22:V:284:GLU:HB2	1.89	0.53
24:X:194:ARG:HG2	24:X:210:LEU:HD21	1.90	0.53
27:a:290:GLN:O	27:a:330:ARG:NH2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:35:ILE:HD11	28:b:184:ILE:HD11	1.89	0.53
18:r:97:MET:HB3	18:r:116:SER:HB3	1.89	0.53
19:s:21:ALA:HB3	19:s:198:VAL:HB	1.89	0.53
1:A:73:ALA:HB2	2:B:140:ASP:H	1.73	0.53
19:S:209:SER:OG	19:S:212:LYS:NZ	2.41	0.53
22:V:289:LEU:HB3	22:V:312:ALA:HB2	1.91	0.53
29:c:51:MET:HA	29:c:82:VAL:HG22	1.89	0.53
10:j:5:ARG:NH2	11:k:126:GLU:OE1	2.41	0.53
2:B:408:ARG:NH1	3:C:163:GLU:OE2	2.42	0.53
3:C:365:GLU:HA	3:C:368:MET:HE2	1.90	0.53
5:E:84:ARG:HG2	29:c:50:PRO:HG3	1.89	0.53
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.89	0.53
17:Q:173:LEU:HD23	17:q:173:LEU:HD23	1.90	0.53
3:C:175:PHE:O	3:C:179:GLY:N	2.41	0.53
26:Z:12:HIS:ND1	26:Z:50:VAL:O	2.39	0.53
27:a:194:GLN:HB2	27:a:226:ARG:HG2	1.91	0.53
17:q:53:THR:HG22	17:q:100:VAL:HG12	1.91	0.53
1:A:401:ARG:HH12	1:A:407:LYS:HZ2	1.56	0.53
10:J:35:VAL:HG13	10:J:176:TYR:HE2	1.74	0.53
19:S:71:ARG:HD2	19:S:74:MET:HE2	1.91	0.53
21:U:580:ARG:NH2	21:U:768:GLN:OE1	2.41	0.53
25:Y:328:GLU:OE2	31:e:62:LYS:NZ	2.40	0.53
14:n:53:GLN:NE2	15:o:117:GLY:O	2.42	0.53
15:o:54:MET:HA	15:o:57:GLN:HG2	1.89	0.53
33:u:36:ILE:O	33:u:41:GLN:NE2	2.42	0.53
4:D:122:GLU:O	4:D:125:LYS:NZ	2.32	0.53
26:Z:138:TYR:HB3	26:Z:155:PHE:HB3	1.91	0.53
27:a:197:ALA:HB2	27:a:222:LEU:HD22	1.91	0.53
30:d:2:TYR:O	30:d:25:ARG:NH2	2.40	0.53
3:C:72:TYR:N	3:C:116:LEU:O	2.40	0.53
10:J:38:ARG:HH12	10:J:183:THR:HA	1.73	0.53
12:L:39:LYS:HD2	12:L:142:PRO:HB2	1.90	0.53
30:d:205:LYS:HZ2	30:d:209:TYR:HE2	1.56	0.53
17:q:19:ARG:HD2	17:q:179:SER:HB3	1.91	0.53
20:t:122:LEU:HG	20:t:137:LEU:HD12	1.90	0.53
7:G:49:VAL:HG22	7:G:219:VAL:HG22	1.91	0.53
16:P:70:ARG:HD2	16:P:94:LEU:HD12	1.90	0.53
32:f:140:LEU:HD23	32:f:165:GLU:HB3	1.91	0.53
13:m:50:GLU:OE2	13:m:201:HIS:ND1	2.41	0.53
33:v:16:GLU:O	33:v:29:LYS:NZ	2.29	0.53
7:G:120:ASP:OD1	8:H:84:ARG:NH1	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:174:MET:HE3	9:I:199:LYS:HG2	1.90	0.53
10:J:98:VAL:HG12	10:J:100:ASP:HB2	1.89	0.53
14:N:174:ILE:HB	14:N:189:LEU:HB2	1.90	0.53
32:f:785:ARG:NH2	32:f:876:HIS:O	2.42	0.53
16:p:185:VAL:HG11	16:p:200:LEU:HD12	1.91	0.53
19:s:35:ILE:O	20:t:151:ARG:NH2	2.42	0.53
1:A:139:ARG:HB2	1:A:153:LEU:HB2	1.91	0.53
3:C:373:GLU:HG3	3:C:375:ARG:HG3	1.90	0.53
9:I:90:LEU:HD21	9:I:110:LEU:HD21	1.91	0.53
18:R:174:VAL:HG21	18:R:195:LEU:HD11	1.90	0.53
21:U:167:ILE:O	21:U:171:ASN:ND2	2.37	0.53
21:U:469:SER:OG	21:U:470:ASN:N	2.41	0.53
19:s:8:ASN:ND2	19:s:31:GLU:OE2	2.42	0.53
11:K:107:MET:SD	11:K:107:MET:N	2.82	0.52
14:N:19:ARG:NH1	14:N:168:GLY:O	2.42	0.52
15:O:162:GLY:O	15:O:166:ASP:HB2	2.09	0.52
19:S:211:ARG:NH2	19:S:213:ASP:OD2	2.41	0.52
21:U:24:LEU:HD23	21:U:27:LEU:HD11	1.91	0.52
21:U:701:ILE:HG21	21:U:810:THR:HA	1.91	0.52
22:V:85:ALA:HB2	22:V:93:PHE:HB2	1.89	0.52
18:R:131:GLY:HA2	18:R:134:TYR:HD2	1.74	0.52
22:V:449:ALA:HB3	22:V:460:SER:HA	1.92	0.52
27:a:309:LEU:HA	27:a:312:MET:HE2	1.90	0.52
18:r:125:THR:HB	18:r:139:MET:HE1	1.90	0.52
20:t:89:HIS:HB2	20:t:112:ILE:HG21	1.90	0.52
33:u:7:THR:HG22	33:u:69:LEU:HD23	1.90	0.52
20:T:27:LEU:HD22	20:T:184:TYR:HB2	1.91	0.52
32:f:797:LEU:HD13	32:f:800:LEU:HD11	1.91	0.52
32:f:828:ARG:HD3	32:f:873:LEU:HD22	1.92	0.52
9:i:90:LEU:HD21	9:i:114:LEU:HB3	1.91	0.52
9:i:123:GLN:HA	10:j:125:ARG:HE	1.73	0.52
11:k:38:ILE:HD12	11:k:202:LEU:HG	1.90	0.52
2:B:153:ASN:HD22	2:B:156:VAL:HG22	1.72	0.52
7:g:143:ILE:HD12	7:g:222:VAL:HG13	1.91	0.52
3:C:344:LEU:HA	3:C:347:ILE:HD12	1.92	0.52
11:K:141:LEU:HB2	11:K:156:MET:HB3	1.92	0.52
18:R:195:LEU:HD23	18:R:198:LYS:HE3	1.90	0.52
19:S:58:HIS:HD2	20:T:131:ALA:H	1.57	0.52
24:X:376:GLY:O	25:Y:358:ARG:NH2	2.42	0.52
8:H:51:LYS:NZ	8:H:200:GLU:O	2.43	0.52
21:U:900:TYR:HB3	21:U:914:LEU:HG	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:217:LEU:HD21	32:f:229:VAL:HG11	1.92	0.52
8:h:34:PRO:HA	8:h:164:GLY:HA3	1.92	0.52
10:j:65:LEU:HD21	10:j:71:MET:HE2	1.91	0.52
27:a:112:ILE:HB	27:a:151:VAL:HG21	1.91	0.52
9:i:171:ALA:HA	9:i:174:MET:HE2	1.91	0.52
33:v:15:LEU:HD22	33:v:29:LYS:HG2	1.92	0.52
21:U:530:GLU:HA	21:U:533:VAL:HG12	1.91	0.52
15:o:19:ARG:O	15:o:33:LYS:NZ	2.39	0.52
18:r:18:SER:OG	18:r:173:ALA:N	2.40	0.52
33:w:15:LEU:HD22	33:w:29:LYS:HG2	1.92	0.52
21:U:160:LEU:HA	21:U:163:PHE:HB3	1.92	0.52
23:W:174:TYR:O	23:W:182:ARG:NH2	2.43	0.52
27:a:159:SER:OG	27:a:175:ASP:OD2	2.25	0.52
28:b:24:THR:HG22	28:b:26:LEU:H	1.75	0.52
29:c:211:GLU:HA	29:c:214:GLN:HB2	1.92	0.52
21:U:9:ILE:HD12	21:U:12:LEU:HD12	1.91	0.52
21:U:173:VAL:HG12	21:U:175:GLY:H	1.74	0.52
8:H:143:ARG:HH11	8:H:144:PRO:HD2	1.74	0.51
14:N:190:LEU:HD13	20:t:209:TRP:HB2	1.91	0.51
8:h:34:PRO:HD2	8:h:49:GLU:HB3	1.92	0.51
15:o:175:LEU:HB2	15:o:186:LEU:HB2	1.91	0.51
2:B:135:ILE:HG22	2:B:139:VAL:HG11	1.93	0.51
3:C:69:GLN:NE2	3:C:119:ASP:OD2	2.42	0.51
3:C:248:MET:HE2	3:C:269:VAL:HG13	1.92	0.51
10:J:221:ASN:ND2	10:J:223:GLU:HB3	2.25	0.51
13:M:197:ILE:HG21	13:M:211:LEU:HD13	1.91	0.51
18:R:133:VAL:HG21	17:q:137:PHE:HB3	1.91	0.51
22:V:258:TYR:HE2	22:V:270:LEU:HD12	1.75	0.51
23:W:101:VAL:HA	23:W:104:MET:SD	2.50	0.51
23:W:240:TYR:HA	23:W:243:ILE:HD12	1.91	0.51
24:X:411:VAL:HG13	25:Y:383:LEU:HD22	1.91	0.51
32:f:151:LEU:HD21	32:f:162:LEU:HD23	1.92	0.51
32:f:369:ARG:NH1	32:f:756:PRO:O	2.44	0.51
8:h:45:VAL:HG23	8:h:212:ILE:HG22	1.92	0.51
33:w:8:LEU:HD11	33:w:70:VAL:HG22	1.92	0.51
16:P:62:THR:OG1	17:Q:85:ARG:NH2	2.42	0.51
21:U:13:ASP:OD1	21:U:44:LYS:NZ	2.42	0.51
21:U:107:HIS:HA	21:U:110:LYS:HE3	1.92	0.51
26:Z:73:ASP:H	28:b:63:THR:HG21	1.74	0.51
13:m:50:GLU:O	13:m:65:ARG:NH1	2.42	0.51
1:A:284:ARG:O	6:F:334:ARG:NH1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:161:ALA:HB1	9:I:175:LEU:HD13	1.92	0.51
21:U:808:PRO:HB3	21:U:874:ASN:HA	1.92	0.51
29:c:75:MET:HE2	29:c:87:VAL:HG12	1.92	0.51
15:o:70:THR:O	15:o:72:ARG:NH1	2.43	0.51
8:H:65:VAL:O	8:H:220:ARG:NH1	2.44	0.51
15:O:19:ARG:NH2	19:s:213:ASP:OD2	2.44	0.51
16:P:138:VAL:HG11	16:P:147:TYR:HE1	1.75	0.51
17:Q:22:ALA:HA	17:Q:28:MET:H	1.74	0.51
17:Q:162:LYS:O	18:r:141:ARG:NH2	2.44	0.51
28:b:6:THR:HG21	28:b:40:LYS:HG3	1.93	0.51
32:f:171:GLN:NE2	32:f:210:GLU:O	2.43	0.51
16:p:71:LEU:HD11	16:p:82:ILE:HG21	1.91	0.51
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.43	0.51
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.43	0.51
7:g:43:ARG:HH21	7:g:164:LYS:HG2	1.74	0.51
16:p:26:ARG:HH11	16:p:186:ILE:HB	1.75	0.51
4:D:153:MET:HG3	4:D:227:PHE:HD2	1.75	0.51
30:d:47:GLN:HG2	30:d:48:LEU:HG	1.92	0.51
13:m:35:THR:HA	13:m:166:GLY:HA3	1.92	0.51
33:v:8:LEU:HD11	33:v:70:VAL:HG22	1.92	0.51
2:B:67:ARG:HH21	32:f:239:TYR:HA	1.76	0.51
9:I:197:LEU:HA	9:I:200:THR:HG22	1.93	0.51
18:R:144:SER:OG	18:R:145:TYR:N	2.43	0.51
18:r:41:LEU:HD23	18:r:103:GLY:HA3	1.93	0.51
4:D:97:ASP:HA	29:c:272:ILE:HD12	1.93	0.51
7:G:38:THR:HA	7:G:169:GLY:HA3	1.92	0.51
17:q:4:LEU:HD22	17:q:45:LEU:HD23	1.93	0.51
19:s:84:THR:HG22	19:s:86:GLY:H	1.75	0.51
19:s:93:SER:HB2	19:s:124:PHE:HE2	1.75	0.51
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.92	0.51
8:H:39:LYS:HG3	8:H:44:VAL:HG22	1.92	0.51
15:O:138:PHE:O	15:O:142:PHE:CB	2.59	0.51
9:i:214:ALA:HA	9:i:227:VAL:HA	1.92	0.51
14:n:21:THR:HG22	14:n:26:ILE:HA	1.93	0.51
14:n:174:ILE:HB	14:n:189:LEU:HB2	1.91	0.51
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.37	0.50
27:a:43:ASP:HA	27:a:46:GLN:HG2	1.91	0.50
13:m:15:SER:OG	13:m:17:ASP:OD1	2.28	0.50
20:t:10:SER:OG	20:t:142:GLY:N	2.43	0.50
2:B:387:LYS:HB3	2:B:390:LEU:HD23	1.92	0.50
7:G:88:ARG:HH12	13:M:157:SER:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:159:ASP:N	16:P:159:ASP:OD1	2.43	0.50
21:U:780:SER:HA	21:U:783:TYR:HD2	1.77	0.50
32:f:83:ARG:NH2	32:f:150:GLU:OE2	2.44	0.50
11:k:41:GLN:NE2	11:k:151:PRO:O	2.45	0.50
11:K:167:ALA:O	11:K:178:GLN:NE2	2.44	0.50
22:V:102:PRO:O	22:V:106:ARG:NH1	2.43	0.50
25:Y:85:ASP:OD1	25:Y:107:LYS:NZ	2.40	0.50
27:a:193:GLN:HB3	27:a:225:LEU:HD21	1.93	0.50
27:a:347:LYS:HD2	27:a:350:LYS:HD3	1.92	0.50
32:f:77:GLU:OE2	32:f:80:ARG:NH2	2.38	0.50
8:h:65:VAL:O	8:h:220:ARG:NH1	2.45	0.50
10:j:173:GLU:HG2	11:k:58:LEU:HD23	1.93	0.50
17:q:25:ILE:HG22	17:q:26:VAL:HG13	1.93	0.50
17:q:37:LYS:O	17:q:61:GLN:NE2	2.44	0.50
20:t:169:VAL:HG12	20:t:173:MET:HE1	1.92	0.50
1:A:394:MET:HG2	2:B:349:ARG:HH22	1.77	0.50
11:K:36:THR:HA	11:K:171:GLY:HA3	1.93	0.50
12:L:203:GLN:O	12:L:239:ARG:NH2	2.44	0.50
26:Z:121:LEU:HD11	26:Z:138:TYR:HD2	1.76	0.50
27:a:119:GLY:HA3	27:a:158:LEU:HD11	1.92	0.50
5:E:215:ILE:HA	5:E:218:MET:SD	2.50	0.50
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.28	0.50
21:U:376:MET:HA	21:U:739:ALA:HA	1.92	0.50
23:W:359:VAL:O	23:W:363:ILE:HG12	2.12	0.50
32:f:384:ALA:HA	32:f:419:LEU:HB3	1.94	0.50
13:M:34:SER:HB3	13:M:65:ARG:HH12	1.76	0.50
17:q:181:ARG:HG2	17:q:190:ASP:HA	1.92	0.50
21:U:666:LYS:HA	21:U:669:ILE:HD12	1.93	0.50
24:X:252:LYS:HG2	24:X:287:LEU:HD11	1.94	0.50
24:X:282:ARG:NH2	24:X:312:GLU:OE1	2.45	0.50
30:d:183:GLU:HA	30:d:215:TRP:HE1	1.77	0.50
32:f:860:LYS:NZ	32:f:862:ILE:O	2.35	0.50
10:j:40:ILE:HG22	10:j:212:ARG:HG2	1.94	0.50
2:B:77:GLU:OE2	2:B:81:ASN:ND2	2.43	0.50
3:C:328:ILE:HG22	3:C:359:VAL:HG11	1.93	0.50
6:F:96:LEU:HD11	6:F:142:ALA:HB1	1.94	0.50
21:U:146:LYS:HE2	21:U:148:LYS:HD3	1.94	0.50
11:k:210:LEU:HD12	11:k:238:ILE:HD11	1.93	0.50
12:l:101:ARG:HH22	20:t:87:ALA:HB2	1.77	0.50
16:p:27:ARG:HB2	16:p:183:MET:HB2	1.93	0.50
12:L:72:ILE:HG22	12:L:134:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:43:ASP:OD1	13:M:43:ASP:N	2.44	0.50
21:U:381:THR:HG22	21:U:412:HIS:HA	1.93	0.50
30:d:237:ILE:HG13	30:d:238:PRO:HD3	1.93	0.50
17:q:19:ARG:HD3	17:q:177:THR:HG22	1.93	0.50
20:t:56:ASP:O	20:t:108:ASN:ND2	2.43	0.50
16:P:146:MET:HG2	16:P:149:MET:HE2	1.94	0.49
21:U:235:LYS:HA	21:U:238:LYS:HD2	1.94	0.49
21:U:805:ASN:OD1	21:U:893:THR:OG1	2.29	0.49
24:X:144:GLN:OE1	24:X:148:HIS:NE2	2.42	0.49
13:m:46:VAL:HG13	13:m:215:TRP:HB3	1.93	0.49
20:t:25:ASP:OD1	20:t:41:ARG:NH2	2.42	0.49
1:A:277:ILE:HG22	1:A:321:THR:HB	1.94	0.49
1:A:278:ASP:N	1:A:278:ASP:OD1	2.43	0.49
5:E:72:LYS:HB2	5:E:78:ARG:HG2	1.95	0.49
10:J:57:ARG:HG3	10:J:60:ARG:HH12	1.78	0.49
23:W:37:GLU:OE1	23:W:39:ARG:NH1	2.45	0.49
23:W:264:GLN:OE1	23:W:335:SER:OG	2.30	0.49
8:h:3:GLU:OE1	13:m:125:TYR:HB2	2.12	0.49
13:m:215:TRP:CD1	13:m:227:VAL:HG22	2.48	0.49
20:T:50:MET:HE3	20:T:190:ALA:HB1	1.93	0.49
20:T:145:LEU:HD12	20:T:176:LEU:HD23	1.94	0.49
25:Y:196:GLN:HA	25:Y:199:GLU:HG3	1.93	0.49
10:j:180:ALA:HB1	10:j:190:LEU:HD11	1.93	0.49
33:u:1:MET:N	33:u:16:GLU:OE2	2.42	0.49
3:C:355:SER:OG	3:C:358:GLU:OE1	2.29	0.49
4:D:75:ALA:HA	4:D:78:GLU:HB2	1.93	0.49
9:I:65:ILE:HG12	9:I:75:SER:HB2	1.94	0.49
12:L:70:ILE:HD11	12:L:105:VAL:HG22	1.94	0.49
16:P:168:SER:HA	16:P:171:MET:HE2	1.94	0.49
21:U:27:LEU:HA	21:U:30:VAL:HG22	1.95	0.49
22:V:284:GLU:OE2	22:V:287:ARG:NH2	2.44	0.49
27:a:150:SER:O	27:a:154:ARG:NH1	2.44	0.49
27:a:341:LEU:HD13	27:a:345:GLN:HB2	1.94	0.49
29:c:59:GLY:HA3	29:c:69:VAL:HA	1.95	0.49
32:f:379:GLY:HA3	32:f:416:MET:HE3	1.93	0.49
10:j:91:CYS:HA	10:j:102:VAL:HG11	1.93	0.49
19:s:45:LYS:HE3	19:s:203:ILE:HD12	1.93	0.49
1:A:192:GLU:HB2	1:A:196:LEU:HD13	1.94	0.49
5:E:385:ASP:OD2	5:E:387:LYS:NZ	2.34	0.49
12:L:33:SER:OG	12:L:62:LYS:NZ	2.40	0.49
25:Y:90:ASP:HA	25:Y:93:LYS:HD2	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:143:ARG:HH22	9:i:59:VAL:HG22	1.78	0.49
12:l:165:SER:OG	12:l:169:ARG:NH1	2.46	0.49
2:B:221:GLY:HA3	2:B:347:ILE:HA	1.93	0.49
2:B:297:SER:OG	3:C:268:GLU:OE2	2.29	0.49
6:F:288:LEU:O	6:F:292:GLY:N	2.44	0.49
15:O:164:PHE:O	19:s:38:ARG:NH2	2.46	0.49
22:V:225:ASP:OD1	22:V:228:ARG:NH1	2.45	0.49
24:X:214:SER:O	24:X:218:HIS:ND1	2.34	0.49
27:a:255:TRP:O	27:a:258:GLN:NE2	2.45	0.49
27:a:320:VAL:HG22	27:a:333:MET:HE1	1.95	0.49
30:d:215:TRP:H	30:d:225:PHE:HE1	1.59	0.49
16:p:88:MET:HG2	16:p:124:LEU:HD11	1.94	0.49
1:A:220:THR:N	35:A:501:ATP:O1B	2.42	0.49
2:B:54:PRO:HD2	2:B:61:LYS:HG3	1.94	0.49
3:C:163:GLU:HA	3:C:167:LEU:HD13	1.94	0.49
3:C:196:LYS:HD2	3:C:294:ALA:HB1	1.95	0.49
4:D:97:ASP:OD1	4:D:97:ASP:N	2.45	0.49
7:G:110:PRO:HG2	7:G:113:MET:HB2	1.95	0.49
11:K:72:ALA:O	11:K:226:PHE:N	2.44	0.49
12:L:157:ARG:NH2	13:M:60:GLU:OE1	2.45	0.49
16:P:186:ILE:HA	16:P:199:THR:HG22	1.95	0.49
21:U:540:GLN:HB3	29:c:68:ARG:HH22	1.77	0.49
23:W:267:LEU:HD21	23:W:296:LEU:HA	1.95	0.49
3:C:31:LEU:HD22	4:D:47:LEU:HB3	1.94	0.49
5:E:170:CYS:HB3	5:E:297:ARG:HB3	1.94	0.49
11:K:13:ASN:HB3	12:L:126:ARG:HB3	1.94	0.49
21:U:571:CYS:SG	21:U:601:ARG:NH1	2.85	0.49
22:V:263:LEU:HD22	22:V:266:GLN:HE22	1.77	0.49
27:a:70:ARG:HE	28:b:17:ARG:HB3	1.77	0.49
28:b:12:ASN:HB2	28:b:80:PRO:HA	1.94	0.49
14:n:192:ASP:OD1	14:n:192:ASP:N	2.45	0.49
17:q:102:LEU:HB2	17:q:118:MET:HB2	1.94	0.49
20:t:126:ASP:OD1	20:t:130:VAL:N	2.45	0.49
20:T:124:TYR:HB2	20:T:137:LEU:HD13	1.95	0.49
21:U:440:GLY:HA2	21:U:473:VAL:HG13	1.95	0.49
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.95	0.49
27:a:135:ILE:HD11	27:a:159:SER:HB3	1.94	0.49
32:f:419:LEU:HD11	32:f:825:MET:HE1	1.95	0.49
11:k:220:VAL:HG22	11:k:226:PHE:HD1	1.78	0.49
13:m:19:ARG:NH1	13:m:20:VAL:O	2.46	0.49
2:B:212:GLU:HB3	32:f:865:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:143:TYR:O	14:N:144:ARG:NH1	2.40	0.49
18:R:38:ASN:OD1	18:R:41:LEU:N	2.46	0.49
21:U:268:LEU:HD23	21:U:325:MET:HB3	1.93	0.49
21:U:475:HIS:CE1	21:U:507:VAL:HG22	2.46	0.49
22:V:120:PHE:HB3	22:V:159:LEU:HD11	1.95	0.49
26:Z:167:ALA:HB2	29:c:46:ARG:HG2	1.95	0.49
32:f:323:ASN:HB3	32:f:326:LEU:HB2	1.95	0.49
32:f:411:ALA:HB2	32:f:440:ILE:HD13	1.95	0.49
4:D:133:HIS:HB3	4:D:137:ASN:H	1.78	0.48
16:P:145:GLN:HE22	19:s:143:ALA:HB1	1.77	0.48
21:U:94:SER:HA	21:U:98:GLU:HG3	1.93	0.48
21:U:580:ARG:HD2	21:U:613:ASP:HB3	1.95	0.48
26:Z:14:LEU:HD22	29:c:43:LYS:HD3	1.95	0.48
29:c:130:GLN:HG3	29:c:142:ALA:HB2	1.95	0.48
12:l:41:LYS:HG3	12:l:42:THR:HG23	1.95	0.48
18:r:179:VAL:HA	18:r:184:TRP:HA	1.95	0.48
20:t:40:SER:O	20:t:57:TYR:OH	2.30	0.48
1:A:65:ILE:HG22	1:A:75:PRO:HD2	1.95	0.48
1:A:386:ARG:HH11	1:A:390:THR:HG21	1.77	0.48
4:D:374:ASP:HB3	5:E:292:PRO:HG2	1.95	0.48
12:L:81:ALA:HB2	12:L:130:VAL:HG21	1.95	0.48
12:L:202:GLU:OE2	12:L:203:GLN:NE2	2.44	0.48
18:R:39:PRO:HA	18:R:184:TRP:HE1	1.78	0.48
32:f:68:THR:HA	32:f:71:TYR:HB2	1.95	0.48
20:t:2:GLN:NE2	20:t:103:MET:O	2.46	0.48
4:D:96:VAL:H	4:D:101:ALA:HA	1.78	0.48
4:D:255:LYS:HZ3	4:D:303:VAL:HG21	1.78	0.48
5:E:247:THR:OG1	5:E:248:SER:N	2.45	0.48
13:M:39:ILE:HD12	13:M:193:VAL:HG22	1.95	0.48
21:U:744:VAL:HA	21:U:785:PRO:HA	1.96	0.48
21:U:791:LEU:O	21:U:914:LEU:N	2.45	0.48
22:V:314:ARG:HH11	25:Y:385:ARG:HD3	1.78	0.48
16:p:124:LEU:HD23	16:p:128:GLY:HA2	1.94	0.48
2:B:183:THR:OG1	2:B:184:TYR:N	2.45	0.48
6:F:83:ASN:OD1	6:F:88:TYR:OH	2.31	0.48
12:L:65:HIS:O	19:S:77:HIS:NE2	2.46	0.48
21:U:68:PHE:HA	21:U:71:LEU:HB3	1.95	0.48
12:l:39:LYS:HA	12:l:44:ALA:HA	1.96	0.48
16:p:56:LEU:HD11	17:q:121:LEU:HD13	1.95	0.48
16:p:58:THR:O	17:q:85:ARG:NH2	2.46	0.48
33:v:36:ILE:HB	33:v:41:GLN:HE21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:50:LEU:HD13	6:F:82:VAL:HG11	1.94	0.48
5:E:144:GLU:OE2	5:E:297:ARG:NH1	2.47	0.48
17:Q:21:ALA:O	17:Q:28:MET:N	2.46	0.48
27:a:278:MET:HG2	27:a:339:ARG:HH22	1.78	0.48
19:s:168:LEU:HD21	19:s:204:ARG:HH21	1.79	0.48
2:B:173:VAL:HG21	3:C:233:GLU:HG3	1.96	0.48
3:C:90:HIS:CE1	3:C:92:GLU:HB2	2.49	0.48
10:J:179:GLU:HA	10:J:182:GLU:HG2	1.95	0.48
21:U:898:CYS:SG	21:U:899:ARG:N	2.86	0.48
25:Y:362:LYS:O	25:Y:366:TYR:N	2.47	0.48
10:j:31:THR:OG1	10:j:163:ARG:O	2.30	0.48
16:p:138:VAL:HG11	16:p:146:MET:HB3	1.96	0.48
1:A:101:ILE:HD11	1:A:111:TYR:HB3	1.96	0.48
3:C:20:LEU:HD22	21:U:149:GLN:HG3	1.95	0.48
12:L:196:ARG:NH1	12:L:237:GLU:O	2.46	0.48
13:M:37:ILE:HD11	13:M:193:VAL:HG13	1.96	0.48
17:Q:36:PHE:HB2	17:Q:44:LEU:HB3	1.96	0.48
21:U:345:ASN:O	21:U:743:ASN:ND2	2.46	0.48
23:W:31:CYS:HA	23:W:43:VAL:HG11	1.96	0.48
27:a:127:ASP:OD1	27:a:127:ASP:N	2.45	0.48
29:c:32:TYR:HB2	29:c:68:ARG:HG3	1.95	0.48
30:d:2:TYR:HA	30:d:4:GLN:HE22	1.77	0.48
2:B:145:GLU:HG2	2:B:148:CYS:HB2	1.94	0.48
6:F:180:ARG:NH1	6:F:241:ALA:O	2.45	0.48
12:L:50:LYS:HB3	12:L:59:HIS:HB3	1.96	0.48
21:U:680:VAL:HB	21:U:683:VAL:HG12	1.96	0.48
23:W:265:GLN:HE21	23:W:336:PRO:HD2	1.79	0.48
26:Z:191:ILE:HG21	27:a:375:LEU:HD22	1.94	0.48
9:i:118:LYS:HE2	9:i:152:PRO:HA	1.95	0.48
16:p:2:SER:OG	16:p:3:ILE:N	2.45	0.48
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.96	0.48
4:D:200:ARG:HH22	4:D:301:GLN:H	1.62	0.48
4:D:208:PRO:HB3	4:D:312:ASN:HD21	1.78	0.48
4:D:293:LEU:HD12	4:D:326:ARG:NH1	2.27	0.48
5:E:62:LYS:HA	5:E:94:PRO:HB3	1.96	0.48
6:F:303:ASP:OD1	6:F:303:ASP:N	2.46	0.48
23:W:85:GLU:HA	23:W:88:MET:HE2	1.95	0.48
11:k:97:GLN:HB3	18:r:61:ARG:HG2	1.95	0.48
33:w:71:LEU:CD1	33:w:72:ARG:O	2.61	0.48
2:B:249:ARG:HG3	2:B:283:PHE:HD2	1.77	0.48
4:D:155:THR:H	4:D:158:GLN:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:73:VAL:HG22	13:M:139:SER:HB2	1.95	0.48
15:O:126:THR:OG1	15:O:135:MET:HB2	2.14	0.48
18:R:179:VAL:HA	18:R:184:TRP:HA	1.95	0.48
24:X:364:LYS:HD2	24:X:364:LYS:HA	1.69	0.48
32:f:771:LEU:HG	32:f:776:LEU:HB2	1.96	0.48
15:o:143:ARG:NH2	15:o:150:GLU:OE1	2.47	0.48
16:p:53:LEU:HG	16:p:107:PRO:HB3	1.96	0.48
17:q:183:ILE:HG12	17:q:188:ILE:HG12	1.96	0.48
6:F:226:TYR:CZ	6:F:353:GLU:HB3	2.49	0.47
10:J:157:LYS:NZ	11:K:59:MET:O	2.47	0.47
14:N:30:VAL:HG11	20:t:211:ILE:HG23	1.96	0.47
19:S:114:ASP:OD1	19:S:118:LYS:N	2.44	0.47
21:U:320:ASP:O	21:U:324:LYS:N	2.47	0.47
26:Z:212:LEU:HD11	27:a:350:LYS:HA	1.95	0.47
32:f:539:LEU:HD12	32:f:542:ILE:HD11	1.94	0.47
7:g:215:ILE:HD11	7:g:239:LEU:HD11	1.96	0.47
19:s:58:HIS:HB3	20:t:130:VAL:HG13	1.96	0.47
4:D:171:ASP:OD1	4:D:171:ASP:N	2.47	0.47
12:L:65:HIS:HB2	12:L:223:ILE:HD11	1.96	0.47
21:U:175:GLY:O	21:U:179:TYR:N	2.47	0.47
25:Y:117:LYS:HE2	25:Y:121:LEU:HD11	1.96	0.47
2:B:76:GLU:HA	2:B:79:ILE:HG22	1.95	0.47
3:C:37:ASP:OD1	3:C:37:ASP:N	2.47	0.47
35:D:501:ATP:O2G	5:E:294:ARG:NH1	2.45	0.47
6:F:438:TYR:O	12:L:51:ARG:NH2	2.47	0.47
7:G:14:THR:HG22	7:G:24:GLN:HB3	1.96	0.47
13:M:49:VAL:HB	13:M:212:GLU:HB3	1.96	0.47
14:N:24:SER:OG	20:t:141:TYR:OH	2.28	0.47
15:O:13:VAL:HG22	15:O:177:VAL:HG13	1.97	0.47
20:T:37:ARG:NH1	14:n:165:GLU:OE2	2.45	0.47
32:f:99:LEU:HA	32:f:102:HIS:HB2	1.95	0.47
15:o:217:THR:HB	16:p:195:ILE:HB	1.96	0.47
16:p:40:GLN:NE2	16:p:42:ILE:O	2.46	0.47
20:t:1:THR:N	20:t:104:ASN:OD1	2.39	0.47
33:w:36:ILE:HB	33:w:41:GLN:HE21	1.78	0.47
1:A:190:VAL:HG21	1:A:339:ARG:HG3	1.96	0.47
2:B:222:VAL:HG22	2:B:349:ARG:HB2	1.95	0.47
7:G:231:THR:OG1	7:G:234:GLU:OE1	2.24	0.47
12:L:200:PRO:O	12:L:239:ARG:NH2	2.40	0.47
16:P:14:MET:HE2	16:P:154:TRP:HD1	1.79	0.47
9:I:41:ASP:OD1	9:I:41:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:18:GLU:OE2	11:K:20:ARG:NE	2.48	0.47
15:O:19:ARG:NH1	15:O:167:LEU:O	2.47	0.47
21:U:247:GLN:OE1	21:U:913:ILE:N	2.47	0.47
22:V:204:ASP:OD1	22:V:204:ASP:N	2.48	0.47
26:Z:11:VAL:O	26:Z:163:GLY:N	2.45	0.47
32:f:862:ILE:HG12	32:f:879:ARG:HB3	1.96	0.47
19:s:195:ILE:HD12	19:s:206:GLU:HB3	1.95	0.47
3:C:368:MET:HA	3:C:371:LEU:HG	1.96	0.47
6:F:306:VAL:O	6:F:309:THR:OG1	2.32	0.47
18:R:130:SER:OG	18:R:167:ASP:OD2	2.29	0.47
19:S:58:HIS:NE2	20:T:131:ALA:O	2.46	0.47
8:h:35:SER:N	8:h:163:MET:O	2.45	0.47
13:m:230:ASP:OD1	13:m:230:ASP:N	2.48	0.47
10:J:158:ALA:HB3	11:K:58:LEU:HD13	1.95	0.47
11:K:157:ASP:OD1	11:K:161:THR:N	2.45	0.47
12:L:152:ASN:HD21	13:M:81:LEU:HD12	1.79	0.47
15:O:174:ASP:OD2	15:O:187:ARG:NH1	2.48	0.47
16:P:193:ASP:OD1	16:P:193:ASP:N	2.47	0.47
20:T:27:LEU:HD11	20:T:34:ALA:HB1	1.96	0.47
21:U:346:ASN:HD21	21:U:348:THR:HG23	1.79	0.47
21:U:451:ALA:O	21:U:453:HIS:ND1	2.42	0.47
22:V:200:ARG:HB3	22:V:203:LEU:HB2	1.97	0.47
24:X:299:LEU:O	24:X:303:GLU:N	2.41	0.47
27:a:54:ASP:N	27:a:54:ASP:OD1	2.45	0.47
29:c:25:VAL:HG23	29:c:175:ARG:HA	1.97	0.47
30:d:107:LEU:HD11	30:d:140:GLU:HB3	1.96	0.47
32:f:894:LEU:HA	32:f:898:VAL:HG21	1.97	0.47
9:i:79:ILE:HG22	9:i:82:ASP:H	1.80	0.47
10:j:38:ARG:NH1	10:j:182:GLU:O	2.39	0.47
10:j:120:GLN:HG3	11:k:135:ARG:HG2	1.96	0.47
13:m:39:ILE:HD11	13:m:176:ILE:HG12	1.97	0.47
13:m:120:HIS:HB2	13:m:155:GLY:HA3	1.95	0.47
14:n:35:THR:OG1	14:n:45:ARG:NE	2.44	0.47
15:o:179:SER:OG	15:o:181:ASN:OD1	2.29	0.47
33:u:6:LYS:HA	33:u:12:THR:HA	1.96	0.47
33:u:40:GLN:HG2	33:u:72:ARG:HD3	1.97	0.47
1:A:319:MET:HE1	1:A:337:LEU:HG	1.97	0.47
7:G:10:ASP:OD1	7:G:10:ASP:N	2.46	0.47
15:O:211:VAL:HA	16:P:200:LEU:HD22	1.97	0.47
18:R:18:SER:OG	18:R:173:ALA:N	2.47	0.47
21:U:583:MET:SD	21:U:605:VAL:HG11	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:4:GLU:OE2	28:b:47:ASN:ND2	2.45	0.47
12:l:72:ILE:HD12	12:l:134:ILE:HG12	1.97	0.47
20:t:13:GLY:HA2	20:t:22:ILE:HG22	1.96	0.47
33:u:7:THR:HA	33:u:69:LEU:HB3	1.97	0.47
5:E:179:GLY:N	35:E:401:ATP:O1B	2.41	0.47
14:N:86:MET:HG2	14:N:89:ARG:NH1	2.30	0.47
26:Z:214:LYS:HA	26:Z:218:GLY:HA3	1.95	0.47
29:c:27:THR:HB	29:c:175:ARG:HB3	1.97	0.47
11:k:78:MET:HE1	11:k:82:ILE:HG22	1.97	0.47
13:m:40:ARG:HB2	13:m:148:LEU:HB2	1.96	0.47
1:A:143:ASP:HB3	1:A:150:HIS:CE1	2.50	0.47
3:C:42:LEU:HD12	3:C:45:LEU:HD11	1.95	0.47
16:P:12:MET:HE1	16:P:139:SER:H	1.80	0.47
20:T:192:VAL:HG13	20:T:197:VAL:HG22	1.96	0.47
22:V:283:ASN:HB3	31:e:19:PHE:HE1	1.80	0.47
27:a:277:LEU:HD21	27:a:296:ILE:HG23	1.97	0.47
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.97	0.47
19:s:79:ASN:HB3	19:s:81:LYS:HG2	1.97	0.47
3:C:48:GLN:NE2	3:C:51:GLU:OE2	2.48	0.46
21:U:346:ASN:HD22	21:U:347:ASN:N	2.13	0.46
25:Y:316:LEU:HB3	25:Y:354:VAL:HG23	1.97	0.46
26:Z:59:ASP:HB2	28:b:99:HIS:CE1	2.49	0.46
32:f:449:GLY:HA2	32:f:488:ALA:HB2	1.97	0.46
17:q:41:LYS:HG2	17:q:107:TYR:HB3	1.97	0.46
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.49	0.46
18:r:127:SER:HB3	18:r:136:TYR:HE1	1.80	0.46
33:w:71:LEU:HD11	33:w:72:ARG:O	2.15	0.46
4:D:173:GLN:HE22	4:D:334:PRO:HD2	1.81	0.46
4:D:268:ASP:HB2	5:E:258:MET:HE1	1.96	0.46
7:G:125:TYR:HD2	7:G:134:LEU:HD22	1.79	0.46
13:M:8:ASP:HB2	13:M:25:TYR:HE2	1.78	0.46
14:N:147:MET:HE2	14:N:152:CYS:HA	1.97	0.46
14:N:166:ARG:NH2	14:n:140:ASP:OD2	2.46	0.46
18:R:139:MET:HE1	18:R:155:LEU:HG	1.97	0.46
24:X:142:ARG:NH1	24:X:145:GLU:OE2	2.42	0.46
25:Y:233:ARG:HH12	25:Y:264:TYR:HA	1.80	0.46
25:Y:314:LEU:HD23	25:Y:319:MET:HE2	1.96	0.46
29:c:266:THR:HG23	29:c:269:GLN:HB2	1.98	0.46
32:f:694:LEU:HA	32:f:697:ILE:HG22	1.97	0.46
8:h:139:TRP:CD1	8:h:215:GLU:HA	2.50	0.46
3:C:368:MET:HB3	3:C:372:ARG:HH21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:97:LEU:HB2	6:F:121:CYS:HB2	1.98	0.46
7:G:112:ASP:OD1	7:G:112:ASP:N	2.49	0.46
8:H:166:ASN:OD1	8:H:169:ASN:ND2	2.42	0.46
13:M:163:CYS:SG	13:M:164:ALA:N	2.89	0.46
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.97	0.46
20:T:13:GLY:HA2	20:T:22:ILE:HA	1.98	0.46
30:d:193:GLU:OE2	30:d:196:ARG:NH2	2.47	0.46
32:f:394:ASP:OD1	32:f:394:ASP:N	2.46	0.46
32:f:425:GLY:HA3	32:f:451:VAL:HG21	1.97	0.46
12:l:72:ILE:HD11	12:l:132:LEU:HD13	1.97	0.46
14:n:164:MET:SD	14:n:170:SER:HB3	2.55	0.46
15:o:104:ASP:OD1	15:o:106:THR:OG1	2.28	0.46
2:B:133:VAL:HG11	2:B:157:HIS:HB2	1.97	0.46
3:C:62:GLU:HA	3:C:65:LEU:HB3	1.96	0.46
16:P:27:ARG:HE	16:P:34:MET:HE1	1.79	0.46
21:U:690:ALA:O	21:U:694:ILE:HB	2.16	0.46
27:a:190:VAL:HA	27:a:193:GLN:HB2	1.96	0.46
30:d:175:ARG:HD3	30:d:198:LEU:HD22	1.97	0.46
32:f:696:LEU:HD12	32:f:800:LEU:HD21	1.97	0.46
7:G:51:VAL:HG23	7:G:217:VAL:HG22	1.98	0.46
26:Z:209:ARG:HH12	27:a:354:GLU:HA	1.80	0.46
27:a:115:LYS:HA	27:a:118:ILE:HD12	1.97	0.46
29:c:26:ASP:OD1	29:c:26:ASP:N	2.48	0.46
29:c:113:HIS:HE1	29:c:115:HIS:CD2	2.33	0.46
31:e:30:LEU:HD22	31:e:34:GLU:HB3	1.98	0.46
7:g:231:THR:OG1	7:g:234:GLU:OE1	2.26	0.46
12:l:172:LEU:HB3	12:l:176:MET:HE3	1.96	0.46
15:o:51:ASP:OD2	16:p:99:ARG:NH2	2.47	0.46
15:o:217:THR:N	16:p:195:ILE:O	2.42	0.46
2:B:228:PRO:HB3	2:B:332:ASN:HD22	1.79	0.46
5:E:98:VAL:HG12	5:E:110:TYR:HA	1.98	0.46
5:E:215:ILE:HD13	5:E:260:LEU:HD12	1.96	0.46
14:N:147:MET:HE3	14:N:151:GLU:HG2	1.97	0.46
26:Z:62:ASP:N	26:Z:62:ASP:OD1	2.48	0.46
31:e:54:ASN:OD1	31:e:57:ARG:NH2	2.48	0.46
8:h:36:VAL:HG13	8:h:174:LEU:HD11	1.97	0.46
1:A:116:LYS:NZ	2:B:128:GLY:O	2.44	0.46
3:C:47:ALA:HB3	22:V:495:ARG:HH21	1.81	0.46
8:H:4:ARG:HE	8:H:5:GLY:H	1.64	0.46
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	1.97	0.46
20:T:126:ASP:OD1	20:T:129:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:203:LYS:HG3	21:U:206:MET:HE2	1.96	0.46
22:V:193:GLN:O	22:V:197:THR:OG1	2.33	0.46
22:V:325:LYS:HA	22:V:328:VAL:HG12	1.98	0.46
9:i:136:TYR:HB2	9:i:148:TYR:HB2	1.98	0.46
11:k:210:LEU:HA	11:k:214:ASN:HD21	1.80	0.46
1:A:105:ASP:OD1	1:A:105:ASP:N	2.48	0.46
5:E:97:ARG:HH12	5:E:114:GLU:HB2	1.81	0.46
5:E:117:PRO:HD3	6:F:94:ILE:HG23	1.98	0.46
9:I:16:GLY:HA3	10:J:25:ALA:HB2	1.98	0.46
9:I:66:TYR:HB3	9:I:91:ARG:HH21	1.81	0.46
10:J:5:ARG:O	10:J:123:GLY:N	2.48	0.46
17:Q:11:ASP:N	17:Q:11:ASP:OD1	2.48	0.46
18:R:21:THR:HA	18:R:27:ALA:H	1.79	0.46
24:X:268:GLN:HA	24:X:271:VAL:HG22	1.97	0.46
26:Z:34:ARG:HH12	26:Z:60:GLU:HG3	1.81	0.46
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.98	0.46
27:a:165:THR:HG22	27:a:166:ILE:H	1.81	0.46
32:f:103:TYR:HD1	32:f:106:LEU:HD12	1.81	0.46
32:f:845:ARG:NH2	32:f:865:PHE:HD2	2.14	0.46
10:j:160:ALA:O	10:j:169:ARG:NH2	2.49	0.46
11:k:141:LEU:H	11:k:156:MET:HB2	1.80	0.46
1:A:393:GLY:HA2	2:B:214:MET:HE2	1.98	0.46
22:V:353:LEU:HB3	22:V:357:LEU:HD12	1.98	0.46
24:X:398:GLU:OE1	25:Y:365:GLN:NE2	2.49	0.46
32:f:655:LEU:HD22	32:f:804:LEU:HD11	1.98	0.46
2:B:317:ASP:HB2	2:B:346:ARG:HG2	1.96	0.46
3:C:29:GLU:HB2	22:V:201:ARG:HE	1.81	0.46
10:J:42:VAL:HG22	10:J:210:VAL:HG12	1.97	0.46
27:a:132:LYS:O	27:a:135:ILE:N	2.49	0.46
7:g:130:GLU:CG	8:h:5:GLY:HA2	2.37	0.46
11:k:84:ASP:OD1	11:k:135:ARG:NH2	2.49	0.46
1:A:186:LYS:HE3	1:A:341:ILE:HG22	1.98	0.45
4:D:234:GLU:OE2	5:E:216:ARG:NH1	2.49	0.45
5:E:295:LEU:HD23	5:E:295:LEU:HA	1.83	0.45
6:F:197:GLU:HA	6:F:200:GLU:HG3	1.99	0.45
16:P:49:LEU:HD21	16:P:87:LEU:HD22	1.98	0.45
22:V:98:LEU:HD22	22:V:209:LYS:HD3	1.98	0.45
23:W:453:HIS:CE1	26:Z:219:LYS:HD2	2.51	0.45
8:h:123:GLN:OE1	9:i:128:ARG:NE	2.49	0.45
11:k:196:LYS:HG3	11:k:241:ILE:HD11	1.99	0.45
13:m:163:CYS:SG	13:m:164:ALA:N	2.88	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:167:ASP:HB3	14:n:170:SER:HB2	1.98	0.45
11:K:16:SER:OG	11:K:19:GLY:N	2.49	0.45
12:L:11:THR:HA	13:M:129:ARG:HD3	1.98	0.45
18:R:192:VAL:HA	18:R:195:LEU:HD12	1.98	0.45
19:S:10:GLY:HA3	19:S:42:LYS:HE2	1.98	0.45
19:S:28:ARG:NH1	19:S:187:VAL:O	2.48	0.45
20:T:1:THR:N	20:T:105:PRO:O	2.49	0.45
21:U:213:PHE:HB3	21:U:248:ILE:HD13	1.98	0.45
21:U:549:ALA:O	21:U:581:SER:OG	2.31	0.45
21:U:681:ASN:OD1	21:U:682:TYR:N	2.49	0.45
21:U:725:MET:SD	21:U:725:MET:N	2.89	0.45
26:Z:130:ASP:OD1	26:Z:130:ASP:N	2.48	0.45
12:l:16:GLN:O	13:m:28:LYS:NZ	2.45	0.45
2:B:217:LYS:HD2	2:B:218:PRO:HD2	1.97	0.45
7:G:49:VAL:HG11	7:G:195:VAL:HG22	1.97	0.45
9:I:68:LEU:HD11	9:I:74:CYS:HB3	1.98	0.45
18:R:19:ARG:NH1	16:p:205:ASP:O	2.48	0.45
21:U:82:LEU:O	21:U:129:ARG:NE	2.50	0.45
32:f:492:SER:HB2	32:f:494:ARG:HD3	1.99	0.45
6:F:225:MET:SD	6:F:352:ILE:HG13	2.56	0.45
8:H:150:ASP:OD1	8:H:154:ALA:N	2.50	0.45
22:V:491:VAL:HA	22:V:494:MET:HB2	1.98	0.45
26:Z:151:THR:HG23	27:a:146:PRO:HB2	1.97	0.45
29:c:151:VAL:HG23	29:c:152:LYS:H	1.82	0.45
19:s:145:LEU:HD22	19:s:178:VAL:HB	1.97	0.45
3:C:299:ASP:OD1	3:C:299:ASP:N	2.48	0.45
35:E:401:ATP:O2A	6:F:344:ARG:NH1	2.50	0.45
8:H:222:THR:OG1	8:H:225:GLU:OE1	2.25	0.45
10:J:71:MET:HE1	10:J:73:PHE:HB3	1.97	0.45
13:M:229:LYS:HA	13:M:232:ARG:HG2	1.99	0.45
14:N:116:MET:HB3	20:T:5:MET:HG3	1.98	0.45
32:f:193:PRO:HA	32:f:196:MET:HG2	1.97	0.45
32:f:683:GLU:HB2	32:f:686:LEU:HD13	1.99	0.45
15:o:187:ARG:HA	15:o:188:PRO:HA	1.80	0.45
17:q:47:VAL:HG23	17:q:101:ASN:HB2	1.98	0.45
19:s:36:HIS:ND1	20:t:132:TYR:OH	2.42	0.45
3:C:90:HIS:HB2	3:C:91:PRO:HD2	1.99	0.45
10:J:69:VAL:HG11	10:J:107:ILE:HD11	1.98	0.45
13:M:77:VAL:HG11	13:M:84:ALA:HB1	1.98	0.45
18:R:59:LEU:HD22	18:R:83:LEU:HB2	1.98	0.45
20:T:25:ASP:HA	20:T:187:PHE:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:223:LYS:O	22:V:225:ASP:N	2.50	0.45
22:V:282:ASN:HA	22:V:285:TRP:HB2	1.97	0.45
29:c:58:LEU:HG	29:c:106:GLU:HB2	1.97	0.45
32:f:216:MET:HA	32:f:219:LYS:HD3	1.98	0.45
7:g:188:ASP:OD1	7:g:188:ASP:N	2.47	0.45
15:o:49:ALA:HB2	34:z:3:UNK:H	1.81	0.45
18:r:115:ASP:OD1	18:r:119:ASN:N	2.46	0.45
19:s:125:ASP:OD1	19:s:129:SER:N	2.49	0.45
33:w:72:ARG:O	33:w:73:LEU:CD2	2.65	0.45
4:D:146:GLU:O	4:D:252:ARG:NH2	2.48	0.45
10:J:130:SER:OG	10:J:147:THR:O	2.32	0.45
17:Q:18:ASP:OD1	17:Q:18:ASP:N	2.49	0.45
17:Q:166:GLU:HA	17:Q:169:LYS:HG2	1.99	0.45
22:V:309:MET:HE1	22:V:332:LEU:HA	1.97	0.45
29:c:303:MET:O	30:d:239:SER:OG	2.33	0.45
7:g:58:ASP:OD1	7:g:58:ASP:N	2.50	0.45
14:n:121:VAL:HG13	14:n:123:GLN:NE2	2.31	0.45
33:w:40:GLN:HE22	33:w:72:ARG:HB2	1.81	0.45
1:A:95:VAL:HG23	2:B:133:VAL:HG12	1.99	0.45
2:B:252:GLY:N	2:B:285:ASP:O	2.43	0.45
6:F:362:ARG:NE	6:F:388:THR:O	2.49	0.45
16:P:175:VAL:HB	16:P:182:GLY:HA2	1.98	0.45
19:S:88:ILE:HG12	19:S:91:MET:HE2	1.99	0.45
21:U:187:LEU:O	21:U:188:MET:HE2	2.17	0.45
21:U:602:LEU:HD21	21:U:621:SER:HB3	1.99	0.45
23:W:112:VAL:HG11	23:W:125:ILE:HD11	1.98	0.45
25:Y:333:GLU:HA	25:Y:336:ARG:HE	1.81	0.45
28:b:17:ARG:HG2	28:b:80:PRO:HG2	1.98	0.45
32:f:266:LEU:HD11	32:f:278:VAL:HG13	1.99	0.45
16:p:178:ASP:HB3	16:p:181:SER:HB2	1.99	0.45
33:u:72:ARG:HH21	33:u:74:ARG:HD2	1.80	0.45
20:T:215:ILE:HD11	14:n:30:VAL:HB	1.98	0.45
21:U:560:MET:HE1	21:U:590:TYR:HA	1.99	0.45
25:Y:332:GLN:HG3	25:Y:336:ARG:HH21	1.82	0.45
26:Z:135:THR:HG21	26:Z:162:ILE:HD11	1.98	0.45
32:f:298:LEU:O	32:f:302:GLY:N	2.50	0.45
11:k:25:GLU:HA	11:k:28:ILE:HD12	1.99	0.45
11:k:180:SER:HA	11:k:183:GLU:HG3	1.97	0.45
12:l:85:CYS:HA	12:l:88:MET:HG2	1.97	0.45
1:A:143:ASP:OD1	1:A:143:ASP:N	2.50	0.45
10:J:158:ALA:HB1	10:J:172:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:296:LYS:O	22:V:301:GLU:N	2.47	0.45
32:f:253:LEU:HD21	32:f:281:ILE:HD11	1.98	0.45
7:g:13:ILE:HG13	7:g:15:ILE:HG12	1.99	0.45
19:s:22:ILE:HD11	19:s:168:LEU:HD12	1.98	0.45
1:A:347:ASP:OD1	1:A:347:ASP:N	2.43	0.44
2:B:49:LEU:HD12	2:B:49:LEU:HA	1.83	0.44
2:B:82:GLN:HG2	32:f:681:TYR:HB3	1.98	0.44
5:E:153:LEU:HD13	5:E:272:ARG:HD2	2.00	0.44
5:E:171:LEU:HD22	5:E:295:LEU:HD13	1.99	0.44
5:E:213:ARG:NH1	5:E:217:GLU:OE2	2.50	0.44
12:L:101:ARG:HH21	20:T:83:TYR:HE1	1.64	0.44
14:N:81:SER:HA	14:N:84:LYS:HG2	1.99	0.44
18:R:29:GLN:HB3	18:R:172:GLY:HA2	1.99	0.44
21:U:786:THR:HG21	21:U:886:PRO:HG3	1.99	0.44
24:X:106:GLU:HB3	24:X:136:LEU:HD21	1.99	0.44
24:X:393:VAL:HB	25:Y:362:LYS:HD3	1.99	0.44
27:a:8:LEU:HD11	27:a:26:GLU:HB3	1.99	0.44
29:c:165:ALA:HA	29:c:168:MET:HG2	1.99	0.44
11:k:127:ASP:N	11:k:127:ASP:OD1	2.50	0.44
11:k:221:GLN:OE1	11:k:224:GLN:NE2	2.50	0.44
12:L:138:ASP:OD1	12:L:138:ASP:N	2.50	0.44
19:S:16:ALA:HB1	19:S:119:GLY:HA3	2.00	0.44
23:W:166:LEU:HG	23:W:189:GLN:HG2	1.99	0.44
26:Z:238:PRO:HG2	29:c:309:PHE:HB3	2.00	0.44
27:a:217:LEU:HD13	27:a:237:LEU:HB3	2.00	0.44
29:c:27:THR:OG1	29:c:175:ARG:NH2	2.50	0.44
32:f:658:ALA:HB2	32:f:693:ALA:HB1	1.98	0.44
2:B:181:GLN:O	2:B:241:ASN:ND2	2.50	0.44
6:F:229:PRO:HB3	6:F:333:ASN:HD22	1.81	0.44
6:F:251:LEU:HD23	6:F:285:ILE:HG12	1.99	0.44
14:N:153:LEU:HD22	14:N:176:LEU:HD13	1.99	0.44
32:f:589:SER:HB3	32:f:649:HIS:CE1	2.52	0.44
15:o:209:THR:HG21	16:p:168:SER:HB2	2.00	0.44
2:B:235:LEU:HD13	2:B:353:PHE:HZ	1.82	0.44
3:C:45:LEU:HD13	4:D:61:ILE:HB	1.99	0.44
3:C:142:LYS:NZ	4:D:297:ASP:OD1	2.42	0.44
4:D:410:ASP:OD1	4:D:410:ASP:N	2.44	0.44
5:E:172:LEU:HD23	5:E:299:ILE:HB	2.00	0.44
6:F:289:ASP:OD1	6:F:289:ASP:N	2.50	0.44
22:V:98:LEU:HD11	22:V:205:LEU:HB3	1.99	0.44
27:a:36:GLN:NE2	28:b:145:GLU:OE2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:c:162:LEU:HA	29:c:200:TYR:HB3	1.99	0.44
32:f:127:SER:OG	32:f:139:CYS:O	2.34	0.44
10:j:204:LYS:NZ	10:j:222:PRO:O	2.50	0.44
11:k:15:PHE:HD2	12:l:24:TYR:HB3	1.82	0.44
12:l:156:CYS:HB3	12:l:159:MET:HE1	1.99	0.44
15:o:97:ALA:HB2	15:o:115:PRO:HD3	1.98	0.44
16:p:145:GLN:O	16:p:149:MET:HG2	2.17	0.44
2:B:230:THR:N	35:B:501:ATP:O2B	2.50	0.44
2:B:275:GLU:HG3	2:B:322:ARG:HH21	1.82	0.44
6:F:81:LYS:HG2	6:F:84:LYS:HE3	2.00	0.44
6:F:225:MET:HE2	6:F:354:PHE:CZ	2.53	0.44
15:O:20:ALA:O	15:O:27:ALA:N	2.41	0.44
22:V:189:ASP:OD1	22:V:218:TYR:OH	2.33	0.44
22:V:433:ASP:OD1	22:V:433:ASP:N	2.50	0.44
25:Y:127:THR:O	25:Y:131:THR:N	2.50	0.44
32:f:560:LEU:O	32:f:564:LEU:N	2.40	0.44
11:k:180:SER:HB3	11:k:201:ILE:HG12	2.00	0.44
12:l:190:HIS:HA	12:l:193:ARG:HD2	1.99	0.44
14:n:135:ILE:HD13	14:n:163:ALA:HB2	1.99	0.44
16:p:61:GLN:HE22	17:q:124:LEU:H	1.66	0.44
1:A:365:GLU:HG2	1:A:367:ASP:H	1.82	0.44
2:B:365:PHE:O	2:B:369:THR:OG1	2.24	0.44
3:C:49:ARG:HD3	4:D:61:ILE:HD12	2.00	0.44
4:D:266:GLU:HG3	5:E:258:MET:HG3	2.00	0.44
4:D:284:GLU:OE1	4:D:287:ARG:NH2	2.51	0.44
8:H:36:VAL:HG13	8:H:174:LEU:HD11	2.00	0.44
14:N:133:SER:HA	14:N:136:TYR:CD2	2.52	0.44
23:W:301:LYS:HB3	23:W:324:TYR:HE2	1.82	0.44
23:W:378:MET:HE1	23:W:389:SER:HB3	2.00	0.44
27:a:18:GLN:HA	27:a:21:VAL:HG22	2.00	0.44
27:a:290:GLN:HG2	27:a:330:ARG:HE	1.82	0.44
7:G:188:ASP:OD1	7:G:189:TRP:N	2.51	0.44
21:U:388:ASP:OD1	21:U:388:ASP:N	2.50	0.44
21:U:512:ALA:O	21:U:516:LEU:HB2	2.18	0.44
21:U:802:TYR:HB3	21:U:895:PRO:HB3	1.99	0.44
24:X:274:LYS:HA	24:X:277:LEU:HB2	1.99	0.44
11:k:96:THR:HA	11:k:107:MET:HE1	2.00	0.44
15:o:41:ILE:HG12	15:o:76:VAL:HG22	2.00	0.44
1:A:74:PRO:HG2	1:A:77:LEU:HD13	2.00	0.44
2:B:343:ARG:HE	2:B:346:ARG:HH11	1.65	0.44
3:C:195:GLY:N	37:C:501:ADP:O2A	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:70:LYS:O	8:H:218:PHE:N	2.41	0.44
13:M:8:ASP:O	13:M:22:GLN:NE2	2.44	0.44
21:U:490:ARG:HH11	21:U:491:GLN:H	1.66	0.44
32:f:345:PRO:HA	32:f:348:ILE:HD12	2.00	0.44
32:f:404:ASP:OD1	32:f:404:ASP:N	2.50	0.44
14:n:4:MET:HE1	14:n:156:THR:HG23	1.99	0.44
33:u:39:ASP:N	33:u:39:ASP:OD1	2.50	0.44
11:K:105:GLU:OE2	19:S:75:TYR:OH	2.25	0.44
13:M:125:TYR:HB2	13:M:128:VAL:HG22	1.98	0.44
18:R:19:ARG:O	18:R:33:LYS:NZ	2.51	0.44
19:S:88:ILE:HA	19:S:91:MET:HE2	2.00	0.44
20:T:38:ASN:HD21	14:n:201:THR:HA	1.83	0.44
21:U:629:THR:HA	21:U:630:PRO:HD3	1.87	0.44
25:Y:123:ALA:O	25:Y:127:THR:OG1	2.29	0.44
30:d:103:LEU:HD12	30:d:106:LEU:HD11	2.00	0.44
8:H:11:THR:HG22	8:H:19:LEU:HD22	2.00	0.43
9:I:136:TYR:HB2	9:I:148:TYR:HB2	2.00	0.43
15:O:187:ARG:HA	15:O:188:PRO:HA	1.83	0.43
20:T:50:MET:O	20:T:113:GLY:N	2.46	0.43
23:W:285:ASP:OD1	23:W:289:ARG:NH2	2.51	0.43
30:d:215:TRP:HE3	30:d:222:TYR:HB3	1.83	0.43
32:f:233:LEU:HD22	32:f:248:LEU:HB2	2.00	0.43
3:C:24:TYR:OH	4:D:40:LEU:O	2.35	0.43
3:C:337:ASN:ND2	3:C:376:VAL:O	2.51	0.43
7:G:131:MET:SD	7:G:131:MET:N	2.91	0.43
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.82	0.43
9:I:123:GLN:HG3	9:I:124:PHE:HD1	1.82	0.43
10:J:46:GLU:HA	10:J:206:ILE:HG22	1.99	0.43
10:J:100:ASP:HB3	10:J:138:PHE:HZ	1.83	0.43
19:S:157:ASN:ND2	16:p:176:ASP:OD2	2.38	0.43
21:U:885:MET:HE3	21:U:888:GLN:HG3	2.00	0.43
23:W:359:VAL:HG23	23:W:382:LEU:HD22	2.00	0.43
32:f:290:VAL:HG12	32:f:294:MET:HE1	2.00	0.43
32:f:686:LEU:O	32:f:690:VAL:HG23	2.18	0.43
7:g:200:THR:HB	7:g:242:LEU:HD11	1.99	0.43
14:n:179:ILE:HG23	14:n:184:VAL:HG22	2.01	0.43
15:o:163:ILE:HG12	15:o:170:GLY:HA2	1.99	0.43
3:C:141:GLU:O	4:D:323:ARG:NH1	2.51	0.43
7:G:47:CYS:HB3	7:G:221:THR:HG23	2.00	0.43
16:P:11:VAL:O	16:P:12:MET:HE2	2.18	0.43
17:Q:19:ARG:HH21	17:Q:31:ASP:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:46:ALA:HB3	18:R:98:GLY:HA3	2.00	0.43
19:S:8:ASN:ND2	19:S:31:GLU:OE2	2.51	0.43
26:Z:21:ASP:OD1	26:Z:22:HIS:N	2.51	0.43
7:g:23:TYR:HB3	7:g:27:TYR:CZ	2.53	0.43
8:h:145:TYR:HE1	9:i:59:VAL:HG11	1.83	0.43
10:j:135:GLY:HA2	10:j:211:MET:HE1	1.99	0.43
1:A:115:VAL:HG21	1:A:118:PHE:HB2	2.00	0.43
6:F:386:ARG:HE	12:L:166:GLN:NE2	2.17	0.43
7:G:103:TYR:HB2	14:N:61:TYR:CD1	2.53	0.43
9:I:69:ASN:OD1	9:I:72:MET:N	2.44	0.43
16:P:51:ILE:HD11	16:P:87:LEU:HD21	2.00	0.43
25:Y:275:LEU:HD21	25:Y:296:VAL:HG13	2.01	0.43
7:g:112:ASP:OD1	7:g:112:ASP:N	2.50	0.43
10:j:185:ASP:OD1	10:j:185:ASP:N	2.50	0.43
11:k:107:MET:HB3	11:k:111:SER:HB2	1.99	0.43
33:w:40:GLN:NE2	33:w:72:ARG:HB2	2.33	0.43
4:D:253:LEU:O	4:D:257:ASN:HB2	2.17	0.43
4:D:335:LEU:HD23	4:D:369:LYS:HB2	2.00	0.43
6:F:171:ARG:NH1	6:F:258:GLN:OE1	2.51	0.43
11:K:107:MET:HE2	11:K:107:MET:HB2	1.89	0.43
20:T:142:GLY:HA2	20:T:176:LEU:HD21	2.01	0.43
8:h:34:PRO:HG3	8:h:165:LYS:HG2	2.00	0.43
14:n:189:LEU:HD22	14:n:193:GLN:HB3	2.00	0.43
17:q:41:LYS:NZ	17:q:185:LYS:O	2.48	0.43
20:t:25:ASP:HA	20:t:187:PHE:HA	2.01	0.43
1:A:72:LEU:HD11	2:B:99:VAL:HG11	2.00	0.43
2:B:288:ASP:N	2:B:288:ASP:OD1	2.51	0.43
2:B:379:THR:OG1	2:B:382:ASP:OD2	2.36	0.43
5:E:242:ARG:HD3	5:E:242:ARG:HA	1.89	0.43
8:H:185:GLU:HB2	24:X:122:ARG:HH21	1.83	0.43
12:L:212:ILE:HB	12:L:224:TYR:HB3	2.00	0.43
19:S:108:ASN:HB2	19:S:124:PHE:HB2	2.01	0.43
26:Z:215:VAL:HG22	27:a:346:ILE:HD12	2.00	0.43
30:d:59:ALA:HB2	30:d:74:TYR:HB3	2.00	0.43
32:f:757:ASN:O	32:f:761:MET:HG2	2.18	0.43
14:n:7:GLN:OE1	14:n:122:ARG:NH2	2.50	0.43
14:n:41:ILE:HG12	14:n:76:VAL:HG22	2.01	0.43
16:p:135:ASP:OD1	16:p:135:ASP:N	2.51	0.43
3:C:327:ASP:N	3:C:327:ASP:OD1	2.52	0.43
10:J:2:SER:OG	10:J:3:TYR:N	2.45	0.43
15:O:106:THR:OG1	15:O:109:HIS:NE2	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:153:ASN:O	15:O:156:SER:N	2.51	0.43
21:U:462:LEU:HG	21:U:496:LEU:HD21	2.00	0.43
24:X:262:ASN:HD21	24:X:329:ASN:HD21	1.65	0.43
24:X:377:ILE:HG22	24:X:386:ILE:HB	2.00	0.43
26:Z:262:LEU:O	26:Z:266:ILE:HG12	2.19	0.43
29:c:195:GLY:O	29:c:199:HIS:N	2.52	0.43
30:d:115:PHE:CZ	30:d:140:GLU:HG2	2.54	0.43
12:l:47:VAL:HG12	12:l:195:LEU:HD22	1.99	0.43
15:o:51:ASP:HB3	15:o:94:ILE:HG23	2.00	0.43
20:t:143:ALA:HA	20:t:147:GLN:HB2	1.99	0.43
8:H:107:THR:O	8:H:111:VAL:HG23	2.19	0.43
9:I:62:SER:OG	9:I:212:GLU:OE2	2.35	0.43
13:M:39:ILE:HD11	13:M:176:ILE:HG12	2.01	0.43
15:O:26:VAL:O	19:s:185:ARG:NH1	2.50	0.43
15:O:42:TYR:HB2	15:O:178:ILE:HD11	2.00	0.43
22:V:263:LEU:O	22:V:267:ALA:HB2	2.19	0.43
22:V:321:ALA:HB2	31:e:19:PHE:H	1.83	0.43
23:W:187:LEU:HD21	23:W:226:TYR:HB2	2.00	0.43
26:Z:83:LYS:NZ	26:Z:87:ALA:O	2.40	0.43
32:f:341:GLU:HA	32:f:342:PRO:HD3	1.88	0.43
11:k:230:THR:HG23	11:k:233:GLU:H	1.84	0.43
18:r:97:MET:O	18:r:116:SER:N	2.52	0.43
7:G:153:LYS:HB3	7:G:163:PHE:CE1	2.54	0.43
10:J:220:LEU:HD12	10:J:225:ILE:CG1	2.49	0.43
15:O:1:THR:N	15:O:168:GLY:O	2.52	0.43
17:Q:13:VAL:HG23	17:Q:113:PRO:HB2	2.01	0.43
21:U:135:ASN:OD1	21:U:136:LYS:N	2.52	0.43
21:U:524:LYS:HB3	21:U:559:ARG:HE	1.84	0.43
21:U:725:MET:HE3	29:c:183:HIS:HB3	2.01	0.43
22:V:104:THR:HG22	22:V:107:ARG:HH21	1.82	0.43
22:V:355:ARG:HA	22:V:358:MET:HE1	2.00	0.43
27:a:149:THR:HA	27:a:152:HIS:HB3	2.01	0.43
32:f:59:LEU:HD21	32:f:78:LEU:HB2	2.01	0.43
16:p:53:LEU:HB3	16:p:60:VAL:HG22	2.01	0.43
18:r:81:LYS:HE3	18:r:120:ARG:CZ	2.49	0.43
3:C:62:GLU:O	3:C:66:LEU:HB2	2.19	0.43
4:D:245:ARG:HA	4:D:248:ARG:HG2	2.00	0.43
6:F:153:VAL:HG22	6:F:160:ILE:HG22	1.98	0.43
11:K:27:ALA:O	11:K:31:ILE:HG12	2.19	0.43
21:U:759:SER:HA	21:U:782:ALA:HA	2.01	0.43
23:W:272:LEU:HD22	23:W:341:PHE:HE2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:148:VAL:HG13	27:a:152:HIS:HB2	2.00	0.43
32:f:496:ASP:OD1	32:f:497:VAL:N	2.51	0.43
10:j:33:VAL:HG13	10:j:172:LEU:HD11	2.01	0.43
15:o:134:ALA:HB1	15:o:158:ALA:HB1	2.01	0.43
16:p:34:MET:HE2	16:p:37:THR:HG22	2.01	0.43
16:p:159:ASP:OD1	16:p:162:HIS:ND1	2.52	0.43
2:B:133:VAL:HB	2:B:158:ALA:HA	1.99	0.42
2:B:314:ASN:O	2:B:318:GLY:N	2.52	0.42
4:D:68:LEU:HD23	4:D:68:LEU:HA	1.86	0.42
6:F:189:GLY:HA3	6:F:364:ARG:HG2	2.01	0.42
7:G:196:GLU:HG3	7:G:242:LEU:HD12	2.01	0.42
9:I:11:ILE:HG22	10:J:7:ILE:HG23	2.01	0.42
9:I:201:MET:HB2	9:I:206:LEU:HD21	2.01	0.42
10:J:201:SER:HB2	10:J:205:ASN:HD21	1.83	0.42
19:S:16:ALA:HB3	19:S:134:SER:HA	2.01	0.42
21:U:141:CYS:HA	21:U:144:ASP:HB3	2.01	0.42
21:U:247:GLN:HE22	21:U:912:ILE:HA	1.84	0.42
7:g:211:LYS:HD2	7:g:212:PRO:HD2	2.00	0.42
10:j:30:SER:HB3	10:j:46:GLU:HB3	2.01	0.42
33:v:31:GLN:O	33:v:35:GLY:N	2.51	0.42
33:v:40:GLN:NE2	33:v:72:ARG:O	2.46	0.42
9:I:246:LYS:HG2	9:I:249:ARG:HH21	1.84	0.42
22:V:270:LEU:O	22:V:274:SER:OG	2.31	0.42
23:W:69:ALA:HA	23:W:72:LYS:HG2	2.01	0.42
26:Z:123:ILE:HB	26:Z:136:GLU:HB3	2.01	0.42
13:m:188:ASP:O	13:m:192:GLU:HG2	2.19	0.42
16:p:45:MET:HE1	16:p:51:ILE:HB	2.01	0.42
33:u:5:VAL:HG21	33:u:15:LEU:HD12	2.00	0.42
1:A:138:MET:HE3	1:A:153:LEU:O	2.18	0.42
1:A:309:PHE:HB3	6:F:250:LYS:HE2	2.01	0.42
21:U:16:GLU:HB3	30:d:27:LYS:HZ3	1.84	0.42
21:U:636:VAL:HG23	21:U:637:VAL:HG23	2.02	0.42
24:X:21:GLU:HA	24:X:24:ILE:HG22	2.01	0.42
24:X:362:GLU:HG2	24:X:378:LEU:HD21	2.00	0.42
25:Y:22:LEU:HD22	25:Y:37:VAL:HG13	2.01	0.42
26:Z:274:ASN:OD1	29:c:281:LYS:NZ	2.44	0.42
7:g:165:ALA:HB1	7:g:179:LEU:HD13	2.02	0.42
11:k:32:LYS:HA	11:k:172:SER:HA	2.00	0.42
13:m:48:GLY:HA2	13:m:213:LEU:HD23	2.02	0.42
2:B:204:PRO:HG3	2:B:211:TYR:HE2	1.84	0.42
5:E:116:ASP:HB3	5:E:217:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:318:ASP:OD2	6:F:344:ARG:NH2	2.52	0.42
15:O:208:THR:HG23	19:s:158:MET:HG3	2.00	0.42
21:U:336:GLU:HA	21:U:339:LEU:HB3	2.01	0.42
22:V:487:HIS:CE1	26:Z:267:ARG:HH21	2.37	0.42
26:Z:223:ASN:HB3	26:Z:227:ILE:HG23	2.00	0.42
28:b:100:ARG:CZ	28:b:105:HIS:HB2	2.49	0.42
32:f:348:ILE:HD13	32:f:381:VAL:HG21	2.01	0.42
32:f:688:ARG:HG2	32:f:720:GLU:HB2	2.01	0.42
14:n:44:CYS:HB2	14:n:99:ILE:HB	2.01	0.42
2:B:176:VAL:HG21	2:B:247:PHE:HD2	1.85	0.42
6:F:357:PRO:O	6:F:362:ARG:NH1	2.53	0.42
10:J:42:VAL:HG11	10:J:191:VAL:HG21	2.01	0.42
10:J:203:GLY:HA2	10:J:229:VAL:HG21	2.02	0.42
19:S:58:HIS:HB3	20:T:130:VAL:HG22	2.01	0.42
21:U:63:VAL:O	21:U:67:VAL:N	2.47	0.42
21:U:664:GLY:HA2	21:U:695:MET:HE1	2.02	0.42
24:X:27:LEU:HD12	24:X:56:LEU:HD12	2.02	0.42
25:Y:49:ASN:HB2	25:Y:114:ILE:HG22	2.01	0.42
25:Y:141:VAL:HG11	25:Y:164:ALA:HB2	2.01	0.42
27:a:148:VAL:HG22	27:a:151:VAL:HG12	2.02	0.42
32:f:438:ASP:OD1	32:f:438:ASP:N	2.49	0.42
32:f:803:PHE:CD1	32:f:810:ILE:HG13	2.54	0.42
32:f:830:LEU:HD23	32:f:844:VAL:HG21	2.02	0.42
9:i:38:LEU:O	9:i:179:TYR:OH	2.30	0.42
11:k:71:ASP:OD2	11:k:106:THR:OG1	2.32	0.42
14:n:29:ARG:NH2	15:o:139:GLU:OE1	2.52	0.42
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.53	0.42
1:A:189:GLU:OE2	6:F:409:ARG:NH2	2.43	0.42
3:C:295:THR:OG1	3:C:296:ASN:N	2.52	0.42
5:E:116:ASP:O	5:E:118:LEU:N	2.52	0.42
12:L:225:ASP:H	12:L:228:ASP:HB2	1.85	0.42
17:Q:104:LEU:HB2	17:Q:118:MET:HE1	2.01	0.42
18:R:76:VAL:HG21	18:R:110:GLY:HA3	2.02	0.42
18:R:97:MET:HB2	18:R:116:SER:N	2.34	0.42
18:R:139:MET:HE3	18:R:159:ALA:HB2	2.00	0.42
21:U:203:LYS:HA	21:U:206:MET:HE2	2.01	0.42
25:Y:347:ILE:HG22	25:Y:354:VAL:HG13	2.02	0.42
32:f:300:ARG:HD2	32:f:300:ARG:HA	1.83	0.42
32:f:600:TYR:CE2	32:f:608:LYS:HE3	2.55	0.42
8:h:65:VAL:HG22	8:h:75:VAL:HG23	2.02	0.42
9:i:197:LEU:HB3	9:i:201:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:35:MET:HG3	17:q:45:LEU:HG	2.01	0.42
9:I:58:GLU:HB2	9:I:60:PHE:HE1	1.85	0.42
15:O:162:GLY:O	15:O:166:ASP:CB	2.68	0.42
21:U:554:LEU:HD11	21:U:761:VAL:HG13	2.00	0.42
23:W:257:GLN:HA	23:W:263:TRP:HB3	2.00	0.42
24:X:143:TYR:HD2	24:X:144:GLN:HG2	1.83	0.42
28:b:126:LYS:O	28:b:130:ARG:HG2	2.20	0.42
32:f:845:ARG:HH21	32:f:866:GLN:C	2.26	0.42
20:t:45:VAL:HB	20:t:49:THR:HB	2.01	0.42
1:A:263:MET:O	1:A:266:THR:OG1	2.35	0.42
2:B:168:ASP:HB2	2:B:169:PRO:HD2	2.02	0.42
4:D:213:THR:HG22	4:D:217:LYS:HE3	2.02	0.42
11:K:92:ALA:O	11:K:96:THR:HG23	2.20	0.42
20:T:26:MET:HB2	20:T:188:GLN:HE22	1.85	0.42
22:V:349:ARG:HH11	31:e:41:ASP:CG	2.28	0.42
27:a:153:SER:OG	27:a:182:CYS:SG	2.63	0.42
32:f:100:ARG:NH2	32:f:132:THR:O	2.53	0.42
16:p:38:ASP:OD1	16:p:38:ASP:N	2.52	0.42
17:q:52:ASP:HB3	17:q:98:TYR:HD1	1.85	0.42
15:O:132:LEU:HD22	20:t:144:TYR:HB3	2.01	0.42
17:Q:37:LYS:HA	17:Q:43:LEU:HD23	2.02	0.42
21:U:160:LEU:O	21:U:164:GLU:N	2.46	0.42
21:U:801:GLN:HB3	21:U:877:LEU:HD22	2.01	0.42
22:V:81:GLN:HB3	22:V:93:PHE:HB3	2.01	0.42
24:X:382:GLU:HG2	24:X:384:VAL:HG23	2.02	0.42
32:f:178:LYS:HA	32:f:181:ARG:HB2	2.02	0.42
8:h:195:LEU:HD23	8:h:195:LEU:HA	1.92	0.42
15:o:110:LEU:HD21	15:o:125:VAL:HG22	2.02	0.42
5:E:360:ASP:N	5:E:360:ASP:OD1	2.53	0.42
11:K:233:GLU:HA	11:K:236:GLU:HB3	2.02	0.42
15:O:48:THR:HB	15:O:51:ASP:HB2	2.02	0.42
17:Q:48:GLY:HA3	17:Q:100:VAL:HA	2.02	0.42
22:V:76:LYS:HB3	22:V:147:PHE:HZ	1.85	0.42
25:Y:290:PRO:HB3	31:e:39:TRP:HH2	1.85	0.42
11:k:70:ILE:HD11	11:k:89:ILE:HD12	2.02	0.42
2:B:168:ASP:OD2	2:B:170:LEU:HD23	2.20	0.41
4:D:338:ARG:NH2	4:D:361:GLU:OE2	2.53	0.41
6:F:218:GLN:NE2	6:F:219:PRO:O	2.53	0.41
7:G:161:CYS:SG	7:G:162:GLY:N	2.93	0.41
13:M:191:LYS:HB3	13:M:238:TYR:CD2	2.55	0.41
18:R:20:ALA:HB3	18:R:31:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:147:LEU:HB3	18:R:152:ALA:HB2	2.02	0.41
21:U:7:GLY:O	21:U:10:SER:OG	2.33	0.41
24:X:74:ARG:HH22	24:X:116:TRP:HB2	1.85	0.41
28:b:20:ASP:OD1	28:b:20:ASP:N	2.53	0.41
30:d:45:LYS:O	30:d:49:ILE:N	2.45	0.41
14:n:121:VAL:O	14:n:123:GLN:NE2	2.51	0.41
1:A:312:ARG:H	1:A:312:ARG:HG2	1.70	0.41
16:P:30:ILE:HG22	16:P:31:GLN:H	1.85	0.41
19:S:24:ALA:HB2	19:S:195:ILE:HG23	2.03	0.41
19:S:58:HIS:CD2	20:T:131:ALA:H	2.37	0.41
19:S:83:MET:SD	19:S:83:MET:N	2.93	0.41
23:W:97:LEU:HG	23:W:99:GLN:H	1.84	0.41
24:X:414:LEU:HD23	24:X:414:LEU:HA	1.92	0.41
30:d:189:ILE:HG23	30:d:193:GLU:HB3	2.02	0.41
13:m:67:PHE:HB2	13:m:75:MET:HE3	2.02	0.41
17:q:8:GLN:O	17:q:147:TYR:OH	2.24	0.41
3:C:68:GLU:O	4:D:136:SER:OG	2.38	0.41
3:C:226:GLU:OE2	3:C:229:ARG:NH1	2.50	0.41
5:E:243:PHE:HE2	6:F:304:ARG:HE	1.69	0.41
20:T:46:ASN:OD1	20:T:49:THR:N	2.53	0.41
21:U:191:LYS:HE3	21:U:195:ASN:HB3	2.02	0.41
21:U:377:HIS:HD2	21:U:380:THR:HG21	1.84	0.41
23:W:406:VAL:HG23	23:W:413:ILE:HG22	2.01	0.41
24:X:259:ILE:HD13	24:X:259:ILE:HA	1.93	0.41
12:l:139:ASP:HB2	20:t:81:HIS:CE1	2.55	0.41
18:r:9:ARG:NH2	18:r:147:LEU:O	2.52	0.41
1:A:331:LEU:O	1:A:337:LEU:HD13	2.21	0.41
2:B:359:LYS:N	10:J:200:GLN:OE1	2.54	0.41
8:H:14:SER:HG	8:H:18:LYS:H	1.66	0.41
8:H:203:MET:HB2	8:H:208:ILE:HD11	2.03	0.41
15:O:135:MET:SD	20:t:179:ARG:HG3	2.60	0.41
17:Q:5:ILE:HD11	17:Q:143:LEU:HD11	2.02	0.41
23:W:166:LEU:HD22	23:W:192:LEU:HD12	2.02	0.41
25:Y:127:THR:O	25:Y:131:THR:HG23	2.21	0.41
28:b:100:ARG:HH21	28:b:103:LYS:HA	1.84	0.41
32:f:291:GLN:HA	32:f:294:MET:HE2	2.02	0.41
32:f:333:LEU:HD22	32:f:829:MET:SD	2.60	0.41
9:i:184:MET:SD	9:i:184:MET:N	2.94	0.41
13:m:51:LYS:O	13:m:210:GLU:N	2.46	0.41
19:s:27:THR:HB	19:s:40:SER:H	1.86	0.41
1:A:200:ARG:HB3	6:F:408:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.56	0.41
12:L:7:ASP:OD1	12:L:7:ASP:N	2.53	0.41
14:N:141:ALA:O	14:N:144:ARG:NH2	2.54	0.41
19:S:16:ALA:HB2	19:S:121:VAL:HG23	2.02	0.41
21:U:894:MET:HE3	21:U:896:GLU:HB3	2.02	0.41
27:a:81:LEU:HA	27:a:84:VAL:HG12	2.03	0.41
32:f:298:LEU:HB3	32:f:321:MET:HE1	2.02	0.41
11:k:238:ILE:HD12	11:k:238:ILE:HA	1.92	0.41
12:l:45:VAL:HG22	12:l:214:ILE:HG12	2.02	0.41
17:q:29:LYS:HE3	17:q:32:HIS:HA	2.02	0.41
33:w:71:LEU:CD1	33:w:72:ARG:C	2.93	0.41
5:E:244:SER:HB2	6:F:300:LYS:HA	2.02	0.41
14:N:166:ARG:HG2	14:n:136:TYR:HB3	2.03	0.41
21:U:161:ASP:OD1	21:U:162:VAL:N	2.52	0.41
22:V:178:SER:HB3	22:V:180:ARG:CZ	2.50	0.41
24:X:323:LEU:HD23	24:X:323:LEU:HA	1.89	0.41
24:X:357:SER:OG	24:X:358:LYS:N	2.54	0.41
26:Z:211:TYR:CE2	26:Z:226:ILE:HG12	2.55	0.41
30:d:203:PRO:HB2	30:d:205:LYS:H	1.84	0.41
32:f:701:ASN:HB2	32:f:876:HIS:CD2	2.55	0.41
7:g:143:ILE:HD13	7:g:143:ILE:HA	1.90	0.41
10:j:14:GLY:HA3	11:k:30:ALA:HB2	2.02	0.41
13:m:41:CYS:N	13:m:44:GLY:O	2.47	0.41
20:t:92:LEU:HD23	20:t:92:LEU:HA	1.91	0.41
2:B:118:ASP:OD1	2:B:118:ASP:N	2.54	0.41
2:B:337:LEU:HD11	2:B:342:ILE:HD11	2.02	0.41
3:C:196:LYS:HG2	3:C:317:PHE:CD2	2.55	0.41
4:D:374:ASP:O	4:D:378:ILE:HG12	2.20	0.41
14:N:28:ASN:HA	20:t:179:ARG:HH12	1.86	0.41
21:U:63:VAL:HA	21:U:66:LYS:HB3	2.03	0.41
21:U:367:THR:HA	21:U:370:VAL:HG12	2.02	0.41
25:Y:381:GLN:HG2	25:Y:385:ARG:HH11	1.85	0.41
8:H:10:LEU:HG	8:H:126:GLY:HA2	2.03	0.41
15:O:123:PRO:HB3	20:t:214:MET:HE3	2.03	0.41
19:S:68:ILE:HD11	19:S:91:MET:HE3	2.01	0.41
22:V:289:LEU:HA	22:V:292:THR:HG22	2.03	0.41
25:Y:198:ALA:HB2	25:Y:226:VAL:HG22	2.03	0.41
29:c:61:PHE:HZ	29:c:139:ARG:HB2	1.86	0.41
32:f:482:ILE:HD12	32:f:518:THR:HG23	2.02	0.41
16:p:141:THR:OG1	16:p:178:ASP:OD2	2.38	0.41
33:w:31:GLN:O	33:w:35:GLY:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:H	1:A:139:ARG:HG2	1.43	0.41
1:A:321:THR:OG1	1:A:322:ASN:N	2.54	0.41
2:B:120:HIS:HB3	2:B:134:SER:HA	2.03	0.41
2:B:275:GLU:OE2	2:B:322:ARG:NE	2.39	0.41
5:E:205:ASP:OD1	5:E:205:ASP:N	2.53	0.41
6:F:375:VAL:HG22	6:F:415:LEU:HD12	2.03	0.41
7:G:141:ILE:HG22	7:G:151:VAL:HG22	2.02	0.41
7:G:217:VAL:HB	7:G:230:LEU:HB2	2.02	0.41
8:H:88:HIS:CD2	8:H:89:ARG:HH21	2.39	0.41
9:I:76:VAL:HG11	9:I:83:ALA:HB1	2.03	0.41
12:L:69:HIS:CE1	12:L:102:PRO:HB3	2.55	0.41
12:L:154:PHE:HD1	13:M:63:ASN:HD21	1.68	0.41
16:P:177:ARG:NH2	19:s:150:ASP:OD2	2.49	0.41
17:Q:45:LEU:HB2	17:Q:103:LEU:HB2	2.03	0.41
20:T:92:LEU:HD22	20:T:96:MET:HE1	2.02	0.41
21:U:62:LEU:HD22	21:U:87:LEU:HD22	2.02	0.41
21:U:241:ASN:ND2	21:U:244:MET:HE3	2.34	0.41
21:U:505:ASP:HB3	21:U:508:THR:HG22	2.03	0.41
24:X:157:LEU:HD23	24:X:157:LEU:HA	1.85	0.41
24:X:368:MET:HE1	24:X:373:LYS:HD2	2.03	0.41
24:X:395:LYS:HB2	29:c:242:GLU:HG2	2.02	0.41
25:Y:142:PHE:HE2	25:Y:176:ARG:HD2	1.86	0.41
25:Y:155:ASP:N	25:Y:155:ASP:OD1	2.53	0.41
26:Z:190:ARG:HH21	26:Z:194:GLN:HG3	1.85	0.41
29:c:113:HIS:CE1	29:c:144:VAL:HG12	2.56	0.41
32:f:253:LEU:HD12	32:f:268:LEU:HB2	2.03	0.41
7:g:132:ARG:HA	7:g:133:PRO:HD3	1.83	0.41
11:k:177:ALA:HB2	11:k:205:VAL:HG11	2.02	0.41
12:l:45:VAL:HG11	12:l:188:VAL:HG22	2.02	0.41
15:o:132:LEU:HA	15:o:135:MET:HG3	2.03	0.41
18:r:7:LYS:HD2	18:r:124:ALA:HA	2.01	0.41
18:r:11:GLY:HA2	18:r:104:TRP:HZ3	1.85	0.41
33:w:18:GLU:O	33:w:56:LEU:HD12	2.21	0.41
1:A:397:ILE:HD13	2:B:211:TYR:HD1	1.85	0.41
6:F:314:LEU:HD21	6:F:342:LEU:HB3	2.03	0.41
11:K:60:GLU:HB3	11:K:63:SER:HB3	2.03	0.41
21:U:567:ILE:HD12	21:U:586:VAL:HB	2.03	0.41
21:U:617:ALA:O	21:U:621:SER:OG	2.32	0.41
25:Y:59:LYS:HE3	25:Y:59:LYS:HB3	1.87	0.41
27:a:329:LYS:HE2	27:a:329:LYS:HB2	1.83	0.41
29:c:122:LEU:HB2	29:c:200:TYR:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:371:ASN:O	32:f:375:SER:OG	2.33	0.41
8:h:38:ILE:HD12	8:h:191:ALA:HB2	2.02	0.41
10:j:39:ASP:OD1	10:j:39:ASP:N	2.53	0.41
13:m:51:LYS:HD2	13:m:63:ASN:HB2	2.01	0.41
17:q:171:PHE:HE2	17:q:173:LEU:HD12	1.86	0.41
18:r:139:MET:O	18:r:143:TYR:HB2	2.21	0.41
20:t:180:ASP:HB3	20:t:183:SER:HB3	2.03	0.41
2:B:363:ARG:HD2	2:B:363:ARG:HA	1.89	0.40
3:C:343:ASN:C	3:C:343:ASN:HD22	2.28	0.40
4:D:155:THR:HG23	4:D:159:LYS:HE2	2.04	0.40
7:G:6:SER:OG	7:G:11:ARG:NH1	2.54	0.40
9:I:148:TYR:HE1	10:J:58:THR:HG21	1.86	0.40
10:J:188:ILE:HA	10:J:191:VAL:HG22	2.02	0.40
11:K:206:MET:SD	11:K:208:GLU:N	2.94	0.40
14:N:41:ILE:HD12	14:N:76:VAL:HG22	2.03	0.40
15:O:198:ARG:NH1	16:P:152:SER:O	2.54	0.40
21:U:25:HIS:HA	21:U:28:ASN:ND2	2.36	0.40
21:U:158:ARG:NH2	21:U:192:GLN:OE1	2.50	0.40
23:W:125:ILE:HD13	23:W:125:ILE:HA	1.95	0.40
25:Y:300:ARG:HH21	31:e:52:PHE:HB2	1.84	0.40
26:Z:14:LEU:HD11	29:c:39:LEU:HD22	2.03	0.40
30:d:248:GLU:OE1	30:d:251:ARG:NH1	2.54	0.40
32:f:67:ASP:OD2	32:f:69:SER:OG	2.33	0.40
32:f:785:ARG:HH22	32:f:876:HIS:CD2	2.39	0.40
20:t:51:LEU:HD13	20:t:112:ILE:HD13	2.02	0.40
2:B:387:LYS:HE3	2:B:427:LEU:HD22	2.04	0.40
5:E:239:GLY:HA2	5:E:257:LEU:HD12	2.03	0.40
10:J:137:ASP:OD2	10:J:143:ARG:NE	2.49	0.40
13:M:71:ARG:HH11	13:M:223:ARG:HH12	1.68	0.40
13:M:80:LEU:HD12	13:M:80:LEU:HA	1.95	0.40
13:M:171:ALA:HA	13:M:174:THR:HG22	2.03	0.40
14:N:104:ASP:OD1	14:N:104:ASP:N	2.53	0.40
21:U:585:THR:O	21:U:589:ALA:CB	2.69	0.40
28:b:147:GLU:HG2	28:b:150:THR:HA	2.02	0.40
29:c:227:GLU:O	29:c:230:THR:OG1	2.35	0.40
30:d:61:TRP:O	30:d:65:ARG:HG2	2.20	0.40
32:f:222:ASP:HB3	32:f:225:ALA:HB3	2.03	0.40
8:h:51:LYS:NZ	8:h:200:GLU:O	2.55	0.40
10:j:108:THR:HG23	10:j:133:ILE:HD12	2.03	0.40
10:j:184:ASP:O	10:j:188:ILE:HG12	2.20	0.40
12:l:218:ASP:OD1	12:l:218:ASP:N	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:p:30:ILE:HG22	16:p:31:GLN:H	1.86	0.40
3:C:104:ASP:OD1	3:C:105:ILE:N	2.53	0.40
8:H:196:LYS:HZ1	8:H:233:ILE:HG21	1.86	0.40
17:Q:41:LYS:HD3	17:Q:107:TYR:HD2	1.86	0.40
20:T:146:ALA:HB1	20:T:172:CYS:HB3	2.02	0.40
20:T:179:ARG:HD3	20:T:179:ARG:HA	1.90	0.40
23:W:265:GLN:NE2	23:W:336:PRO:HD2	2.35	0.40
23:W:303:LYS:HG2	23:W:307:LYS:NZ	2.36	0.40
25:Y:244:ALA:HA	25:Y:247:LEU:HB3	2.04	0.40
8:h:102:GLN:NE2	15:o:57:GLN:OE1	2.48	0.40
8:h:119:GLN:HG3	9:i:81:SER:HB2	2.02	0.40
13:m:161:TRP:CD2	13:m:182:LYS:HE2	2.55	0.40
1:A:354:ILE:HG22	1:A:385:ILE:HG21	2.04	0.40
10:J:65:LEU:H	10:J:70:CYS:HA	1.86	0.40
16:P:47:ASP:OD1	16:P:47:ASP:N	2.53	0.40
21:U:191:LYS:HA	21:U:194:ARG:HB3	2.04	0.40
21:U:209:GLU:HG2	21:U:210:LYS:HG2	2.04	0.40
21:U:401:LYS:HB3	21:U:438:GLN:HB2	2.04	0.40
21:U:516:LEU:HG	21:U:532:MET:HE2	2.04	0.40
21:U:658:ILE:HD13	21:U:763:VAL:HG21	2.03	0.40
22:V:270:LEU:HD23	22:V:270:LEU:HA	1.90	0.40
24:X:416:ASN:HA	24:X:420:LYS:HE2	2.03	0.40
32:f:292:LYS:HE3	32:f:899:ILE:HD13	2.04	0.40
7:g:158:GLY:O	8:h:84:ARG:NH2	2.55	0.40
11:k:70:ILE:HD12	11:k:92:ALA:HB3	2.04	0.40
13:m:181:MET:HE3	13:m:181:MET:HB3	1.97	0.40
15:o:175:LEU:O	15:o:186:LEU:N	2.54	0.40
2:B:125:THR:OG1	2:B:126:SER:N	2.54	0.40
7:G:88:ARG:NH2	13:M:156:VAL:HA	2.32	0.40
13:M:71:ARG:NH2	20:T:72:ILE:HA	2.37	0.40
14:N:141:ALA:HB2	14:n:162:LEU:HD11	2.03	0.40
21:U:536:ALA:HB1	21:U:545:LEU:HD23	2.04	0.40
26:Z:66:SER:HA	26:Z:104:ASN:HD21	1.87	0.40
29:c:163:ILE:HG23	29:c:200:TYR:HA	2.03	0.40
29:c:260:GLU:N	29:c:260:GLU:OE1	2.54	0.40
32:f:268:LEU:HA	32:f:271:MET:HG2	2.03	0.40
32:f:294:MET:HA	32:f:297:MET:HG3	2.04	0.40
11:k:98:ASN:OD1	18:r:61:ARG:NH2	2.54	0.40
17:q:139:THR:HA	17:q:142:ILE:HD12	2.04	0.40
33:w:48:LYS:HB2	33:w:48:LYS:HE2	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	411/433 (95%)	370 (90%)	41 (10%)	0	100	100
2	B	386/440 (88%)	358 (93%)	27 (7%)	1 (0%)	36	70
3	C	359/398 (90%)	333 (93%)	24 (7%)	2 (1%)	21	57
4	D	378/418 (90%)	336 (89%)	40 (11%)	2 (0%)	24	60
5	E	373/403 (93%)	341 (91%)	31 (8%)	1 (0%)	36	70
6	F	372/439 (85%)	342 (92%)	30 (8%)	0	100	100
7	G	242/246 (98%)	231 (96%)	11 (4%)	0	100	100
7	g	242/246 (98%)	224 (93%)	15 (6%)	3 (1%)	10	42
8	H	230/234 (98%)	219 (95%)	11 (5%)	0	100	100
8	h	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
9	I	249/261 (95%)	241 (97%)	8 (3%)	0	100	100
9	i	248/261 (95%)	240 (97%)	8 (3%)	0	100	100
10	J	237/248 (96%)	226 (95%)	11 (5%)	0	100	100
10	j	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
11	K	232/241 (96%)	218 (94%)	14 (6%)	0	100	100
11	k	232/241 (96%)	224 (97%)	8 (3%)	0	100	100
12	L	236/263 (90%)	230 (98%)	6 (2%)	0	100	100
12	l	236/263 (90%)	229 (97%)	7 (3%)	0	100	100
13	M	238/255 (93%)	233 (98%)	5 (2%)	0	100	100
13	m	238/255 (93%)	228 (96%)	10 (4%)	0	100	100
14	N	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
14	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
15	O	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
15	o	218/277 (79%)	208 (95%)	10 (5%)	0	100	100
16	P	202/205 (98%)	188 (93%)	14 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
17	Q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
17	q	197/201 (98%)	191 (97%)	6 (3%)	0	100	100
18	R	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
18	r	199/263 (76%)	191 (96%)	8 (4%)	0	100	100
19	S	211/241 (88%)	201 (95%)	10 (5%)	0	100	100
19	s	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
20	T	214/264 (81%)	206 (96%)	8 (4%)	0	100	100
20	t	214/264 (81%)	207 (97%)	7 (3%)	0	100	100
21	U	864/953 (91%)	797 (92%)	67 (8%)	0	100	100
22	V	470/534 (88%)	450 (96%)	20 (4%)	0	100	100
23	W	439/456 (96%)	431 (98%)	8 (2%)	0	100	100
24	X	420/422 (100%)	396 (94%)	24 (6%)	0	100	100
25	Y	387/389 (100%)	365 (94%)	22 (6%)	0	100	100
26	Z	284/324 (88%)	255 (90%)	29 (10%)	0	100	100
27	a	371/376 (99%)	339 (91%)	32 (9%)	0	100	100
28	b	189/377 (50%)	171 (90%)	18 (10%)	0	100	100
29	c	285/310 (92%)	247 (87%)	37 (13%)	1 (0%)	30	65
30	d	255/350 (73%)	217 (85%)	38 (15%)	0	100	100
31	e	48/70 (69%)	41 (85%)	5 (10%)	2 (4%)	2	21
32	f	840/908 (92%)	800 (95%)	40 (5%)	0	100	100
33	u	74/76 (97%)	73 (99%)	1 (1%)	0	100	100
33	v	74/76 (97%)	71 (96%)	2 (3%)	1 (1%)	9	39
33	w	74/76 (97%)	70 (95%)	3 (4%)	1 (1%)	9	39
All	All	13562/15104 (90%)	12761 (94%)	787 (6%)	14 (0%)	49	81

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	167	THR
3	C	130	LYS
3	C	90	HIS
5	E	386	TYR
7	g	4	GLY

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Mol	Chain	Res	Type
7	g	5	SER
33	w	71	LEU
4	D	150	SER
31	e	41	ASP
33	v	63	LYS
4	D	84	SER
29	c	156	VAL
7	g	7	ALA
31	e	48	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	352/372 (95%)	350 (99%)	2 (1%)	78	81
2	B	341/385 (89%)	340 (100%)	1 (0%)	86	85
3	C	314/346 (91%)	311 (99%)	3 (1%)	68	76
4	D	333/366 (91%)	332 (100%)	1 (0%)	86	85
5	E	298/353 (84%)	297 (100%)	1 (0%)	86	85
6	F	296/379 (78%)	296 (100%)	0	100	100
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	201 (100%)	1 (0%)	81	82
8	H	188/191 (98%)	188 (100%)	0	100	100
8	h	188/191 (98%)	186 (99%)	2 (1%)	65	74
9	I	207/221 (94%)	207 (100%)	0	100	100
9	i	206/221 (93%)	206 (100%)	0	100	100
10	J	201/211 (95%)	199 (99%)	2 (1%)	68	76
10	j	196/211 (93%)	196 (100%)	0	100	100
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	195/203 (96%)	195 (100%)	0	100	100
12	L	202/224 (90%)	202 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	l	201/224 (90%)	201 (100%)	0	100	100
13	M	196/212 (92%)	196 (100%)	0	100	100
13	m	198/212 (93%)	198 (100%)	0	100	100
14	N	157/181 (87%)	157 (100%)	0	100	100
14	n	156/181 (86%)	156 (100%)	0	100	100
15	O	179/228 (78%)	179 (100%)	0	100	100
15	o	181/228 (79%)	181 (100%)	0	100	100
16	P	172/174 (99%)	172 (100%)	0	100	100
16	p	173/174 (99%)	173 (100%)	0	100	100
17	Q	168/171 (98%)	168 (100%)	0	100	100
17	q	168/171 (98%)	168 (100%)	0	100	100
18	R	156/202 (77%)	156 (100%)	0	100	100
18	r	156/202 (77%)	156 (100%)	0	100	100
19	S	175/199 (88%)	175 (100%)	0	100	100
19	s	178/199 (89%)	178 (100%)	0	100	100
20	T	178/215 (83%)	178 (100%)	0	100	100
20	t	179/215 (83%)	179 (100%)	0	100	100
21	U	742/816 (91%)	741 (100%)	1 (0%)	88	89
22	V	391/460 (85%)	391 (100%)	0	100	100
23	W	406/416 (98%)	406 (100%)	0	100	100
24	X	362/362 (100%)	362 (100%)	0	100	100
25	Y	344/344 (100%)	344 (100%)	0	100	100
26	Z	257/295 (87%)	256 (100%)	1 (0%)	84	84
27	a	333/336 (99%)	333 (100%)	0	100	100
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	250 (99%)	2 (1%)	73	77
30	d	231/294 (79%)	231 (100%)	0	100	100
31	e	44/63 (70%)	44 (100%)	0	100	100
32	f	711/763 (93%)	707 (99%)	4 (1%)	78	81
33	u	68/68 (100%)	68 (100%)	0	100	100
33	v	68/68 (100%)	67 (98%)	1 (2%)	57	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	w	68/68 (100%)	66 (97%)	2 (3%)	37 58
All	All	11532/12818 (90%)	11508 (100%)	24 (0%)	85 87

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	ARG
1	A	403	ILE
2	B	125	THR
3	C	109	THR
3	C	130	LYS
3	C	210	THR
4	D	354	LEU
5	E	274	LYS
10	J	219	ILE
10	J	220	LEU
21	U	542	GLU
26	Z	223	ASN
29	c	196	LEU
29	c	198	ARG
32	f	43	GLN
32	f	68	THR
32	f	673	ARG
32	f	828	ARG
7	g	6	SER
8	h	3	GLU
8	h	4	ARG
33	v	63	LYS
33	w	72	ARG
33	w	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (113) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
2	B	57	GLN
2	B	207	HIS
3	C	32	GLN
3	C	48	GLN
3	C	90	HIS
3	C	278	ASN

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Mol	Chain	Res	Type
4	D	173	GLN
4	D	257	ASN
4	D	312	ASN
5	E	75	ASN
5	E	129	ASN
5	E	226	GLN
5	E	263	GLN
5	E	280	ASN
6	F	417	HIS
7	G	33	ASN
7	G	53	GLN
8	H	109	GLN
9	I	109	GLN
9	I	142	HIS
9	I	146	GLN
10	J	18	GLN
10	J	54	GLN
10	J	175	ASN
10	J	205	ASN
10	J	221	ASN
11	K	41	GLN
11	K	204	GLN
12	L	31	GLN
12	L	166	GLN
12	L	175	HIS
16	P	145	GLN
16	P	169	GLN
16	P	173	ASN
17	Q	168	GLN
18	R	70	ASN
18	R	175	ASN
20	T	38	ASN
20	T	162	GLN
21	U	28	ASN
21	U	340	GLN
21	U	355	ASN
21	U	463	ASN
21	U	475	HIS
21	U	525	ASN
21	U	540	GLN
21	U	604	HIS
21	U	718	ASN

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Mol	Chain	Res	Type
21	U	734	GLN
21	U	743	ASN
21	U	749	GLN
22	V	282	ASN
22	V	326	GLN
22	V	401	ASN
22	V	473	GLN
23	W	53	GLN
23	W	86	ASN
23	W	232	GLN
23	W	362	ASN
24	X	170	GLN
24	X	296	ASN
24	X	329	ASN
24	X	333	GLN
24	X	380	GLN
24	X	416	ASN
25	Y	48	ASN
25	Y	94	ASN
25	Y	273	GLN
27	a	18	GLN
27	a	164	GLN
27	a	194	GLN
27	a	219	HIS
27	a	257	GLN
27	a	258	GLN
27	a	337	GLN
28	b	27	GLN
28	b	34	ASN
28	b	94	HIS
29	c	30	GLN
29	c	113	HIS
29	c	128	ASN
29	c	199	HIS
30	d	135	HIS
32	f	51	GLN
32	f	323	ASN
32	f	327	ASN
32	f	382	ASN
32	f	758	ASN
7	g	33	ASN
7	g	75	ASN

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Mol	Chain	Res	Type
7	g	128	ASN
9	i	102	GLN
10	j	23	GLN
10	j	92	GLN
10	j	146	GLN
10	j	154	HIS
10	j	175	ASN
11	k	23	GLN
11	k	97	GLN
11	k	118	ASN
11	k	122	GLN
11	k	224	GLN
14	n	53	GLN
16	p	93	ASN
16	p	173	ASN
17	q	101	ASN
18	r	10	HIS
18	r	85	ASN
19	s	151	ASN
33	v	41	GLN
33	w	40	GLN
33	w	41	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	ATP	B	501	36	29,33,33	0.32	0	44,52,52	0.49	1 (2%)
35	ATP	D	501	36	29,33,33	0.33	0	44,52,52	0.53	0
37	ADP	F	501	36	27,29,29	1.35	4 (14%)	42,45,45	1.95	9 (21%)
37	ADP	C	501	-	27,29,29	1.35	4 (14%)	42,45,45	2.01	10 (23%)
35	ATP	A	501	36	29,33,33	0.30	0	44,52,52	0.47	1 (2%)
35	ATP	E	401	36	29,33,33	0.31	0	44,52,52	0.45	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	B	501	36	-	7/22/38/38	0/3/3/3
35	ATP	D	501	36	-	9/22/38/38	0/3/3/3
37	ADP	F	501	36	-	10/16/32/32	0/3/3/3
37	ADP	C	501	-	-	3/16/32/32	0/3/3/3
35	ATP	A	501	36	-	3/22/38/38	0/3/3/3
35	ATP	E	401	36	-	5/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	F	501	ADP	C5-C4	4.49	1.47	1.39
37	C	501	ADP	C5-C4	4.46	1.47	1.39
37	C	501	ADP	C5-C6	2.60	1.48	1.41
37	F	501	ADP	C5-C6	2.56	1.48	1.41
37	C	501	ADP	C5-N7	-2.37	1.34	1.39
37	F	501	ADP	C5-N7	-2.35	1.34	1.39
37	F	501	ADP	C8-N7	2.34	1.36	1.31
37	C	501	ADP	C8-N7	2.33	1.36	1.31

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	C	501	ADP	C5-C4-N3	-6.43	118.36	126.75
37	F	501	ADP	C5-C4-N3	-6.30	118.54	126.75
37	C	501	ADP	N3-C4-N9	5.08	135.45	127.08
37	F	501	ADP	N3-C4-N9	4.84	135.06	127.08
37	C	501	ADP	C2-N3-C4	3.90	120.97	111.75
37	F	501	ADP	PA-O3A-PB	-3.78	119.84	132.83
37	F	501	ADP	C2-N3-C4	3.66	120.39	111.75
37	C	501	ADP	PA-O3A-PB	-3.62	120.41	132.83
37	F	501	ADP	C4-C5-N7	-3.25	106.66	110.62
37	C	501	ADP	C4-C5-N7	-3.18	106.75	110.62
37	C	501	ADP	N3-C2-N1	-3.04	123.85	128.60
37	C	501	ADP	C5-N7-C8	2.73	107.39	103.51
37	C	501	ADP	C3'-C2'-C1'	2.68	106.52	101.43
37	F	501	ADP	C5-N7-C8	2.65	107.27	103.51
37	F	501	ADP	N3-C2-N1	-2.62	124.51	128.60
37	C	501	ADP	C4-N9-C8	2.51	108.44	105.73
37	F	501	ADP	C3'-C2'-C1'	2.32	105.84	101.43
37	F	501	ADP	C4-N9-C8	2.32	108.24	105.73
35	A	501	ATP	PB-O3B-PG	2.04	139.84	132.83
35	E	401	ATP	PB-O3B-PG	2.02	139.75	132.83
35	B	501	ATP	PB-O3B-PG	2.01	139.73	132.83
37	C	501	ADP	C6-C5-N7	2.01	135.76	132.02

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	B	501	ATP	PB-O3B-PG-O3G
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	D	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	O4'-C4'-C5'-O5'
35	D	501	ATP	O4'-C1'-N9-C8
35	D	501	ATP	O4'-C1'-N9-C4
35	E	401	ATP	C5'-O5'-PA-O2A
37	C	501	ADP	O4'-C4'-C5'-O5'
37	C	501	ADP	C3'-C4'-C5'-O5'
37	F	501	ADP	PA-O3A-PB-O2B
37	F	501	ADP	C5'-O5'-PA-O1A
37	F	501	ADP	C5'-O5'-PA-O3A
37	F	501	ADP	O4'-C4'-C5'-O5'
37	F	501	ADP	C3'-C4'-C5'-O5'
37	F	501	ADP	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
35	E	401	ATP	C5'-O5'-PA-O3A
35	E	401	ATP	PA-O3A-PB-O2B
35	D	501	ATP	C5'-O5'-PA-O1A
35	D	501	ATP	C5'-O5'-PA-O2A
35	E	401	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	PB-O3B-PG-O1G
35	D	501	ATP	PA-O3A-PB-O1B
37	C	501	ADP	PB-O3A-PA-O2A
37	F	501	ADP	C2'-C1'-N9-C4
35	B	501	ATP	PA-O3A-PB-O1B
35	D	501	ATP	PG-O3B-PB-O2B
37	F	501	ADP	O4'-C1'-N9-C8
37	F	501	ADP	PA-O3A-PB-O1B
37	F	501	ADP	PA-O3A-PB-O3B
35	B	501	ATP	C5'-O5'-PA-O3A
35	A	501	ATP	PG-O3B-PB-O1B
35	A	501	ATP	PG-O3B-PB-O2B
35	B	501	ATP	PA-O3A-PB-O2B
35	D	501	ATP	PG-O3B-PB-O1B
35	E	401	ATP	PA-O3A-PB-O1B
35	A	501	ATP	C5'-O5'-PA-O1A

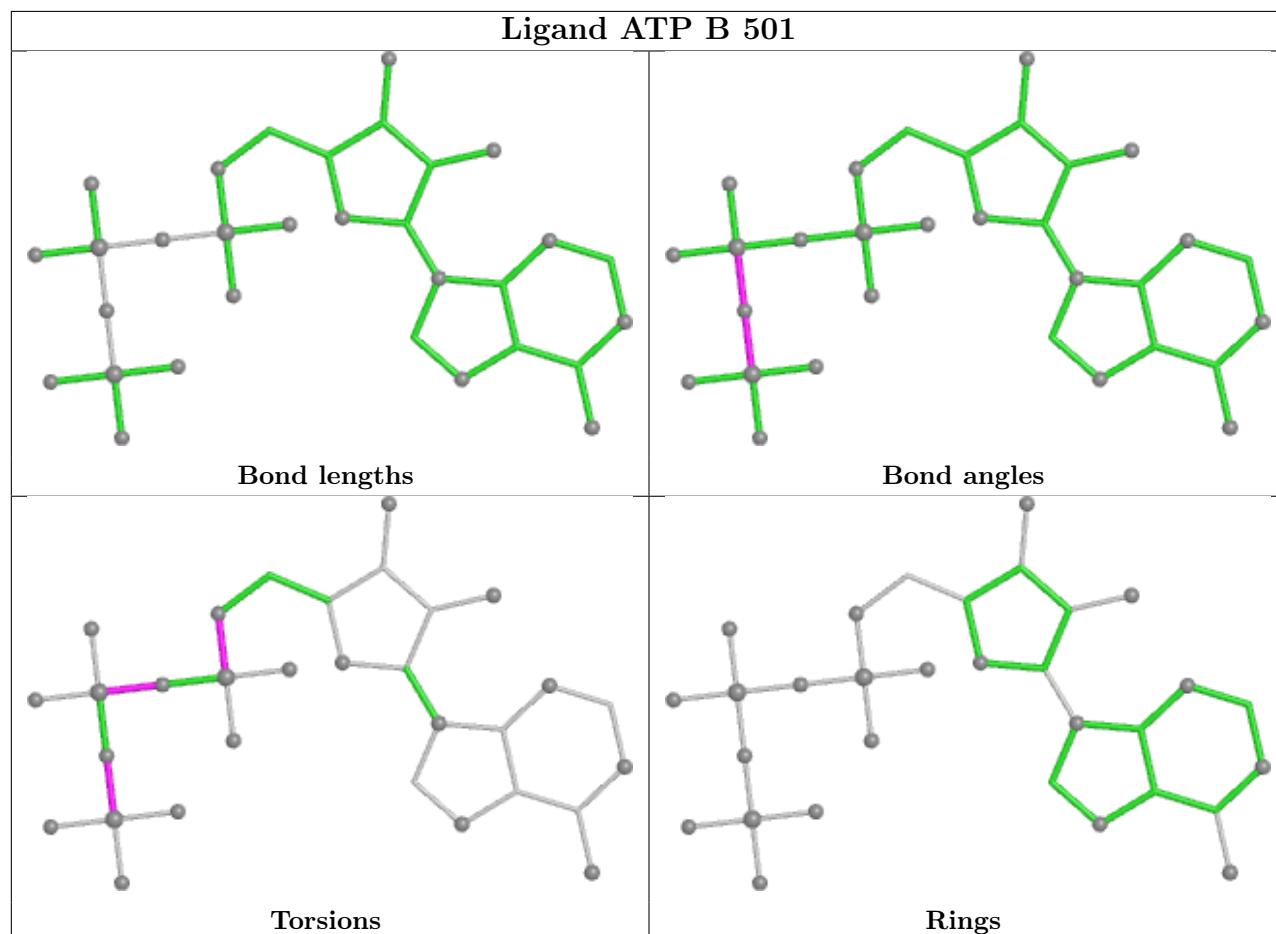
There are no ring outliers.

6 monomers are involved in 9 short contacts:

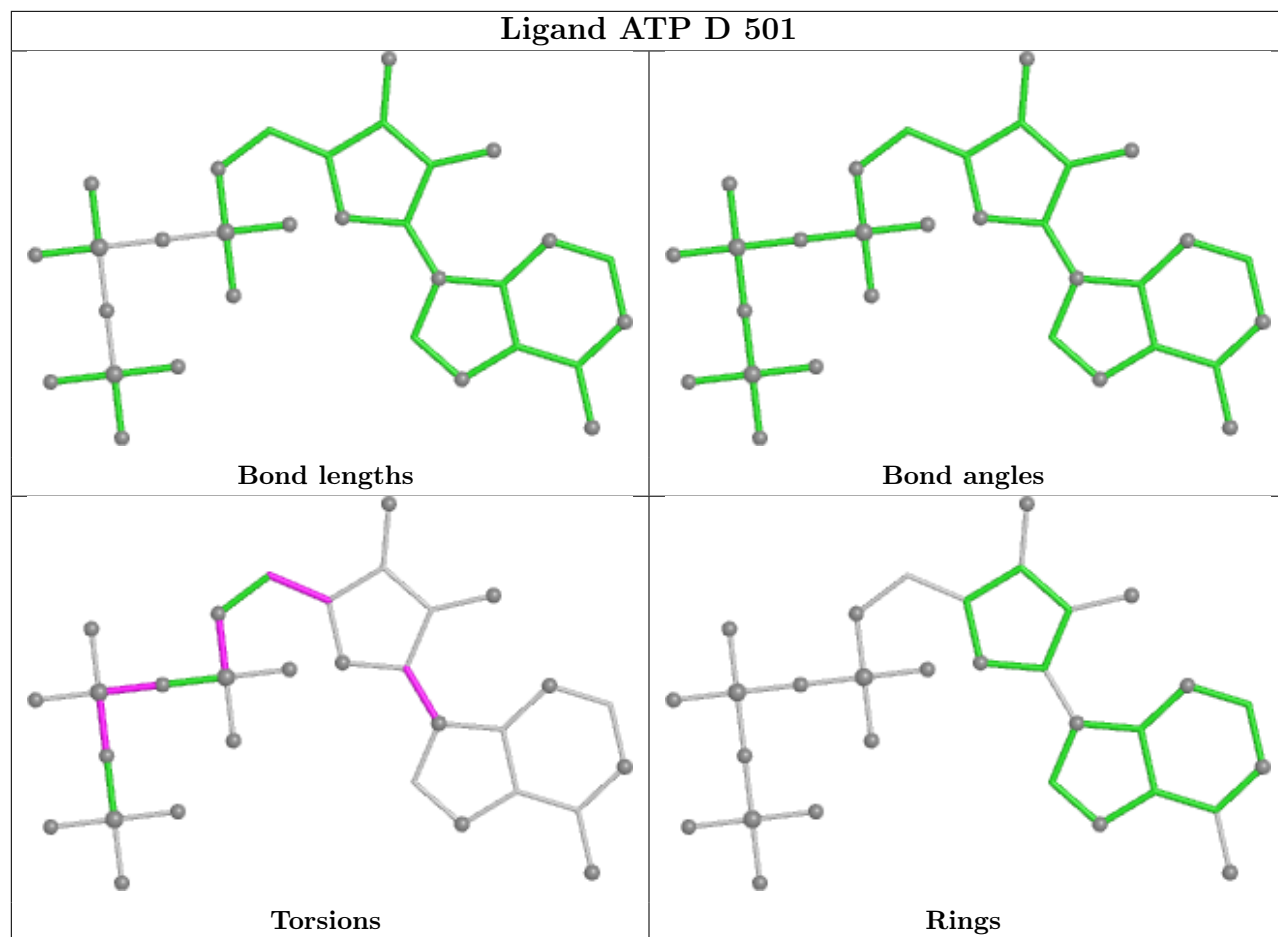
Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B	501	ATP	2	0
35	D	501	ATP	1	0
37	F	501	ADP	1	0
37	C	501	ADP	1	0
35	A	501	ATP	1	0
35	E	401	ATP	3	0

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

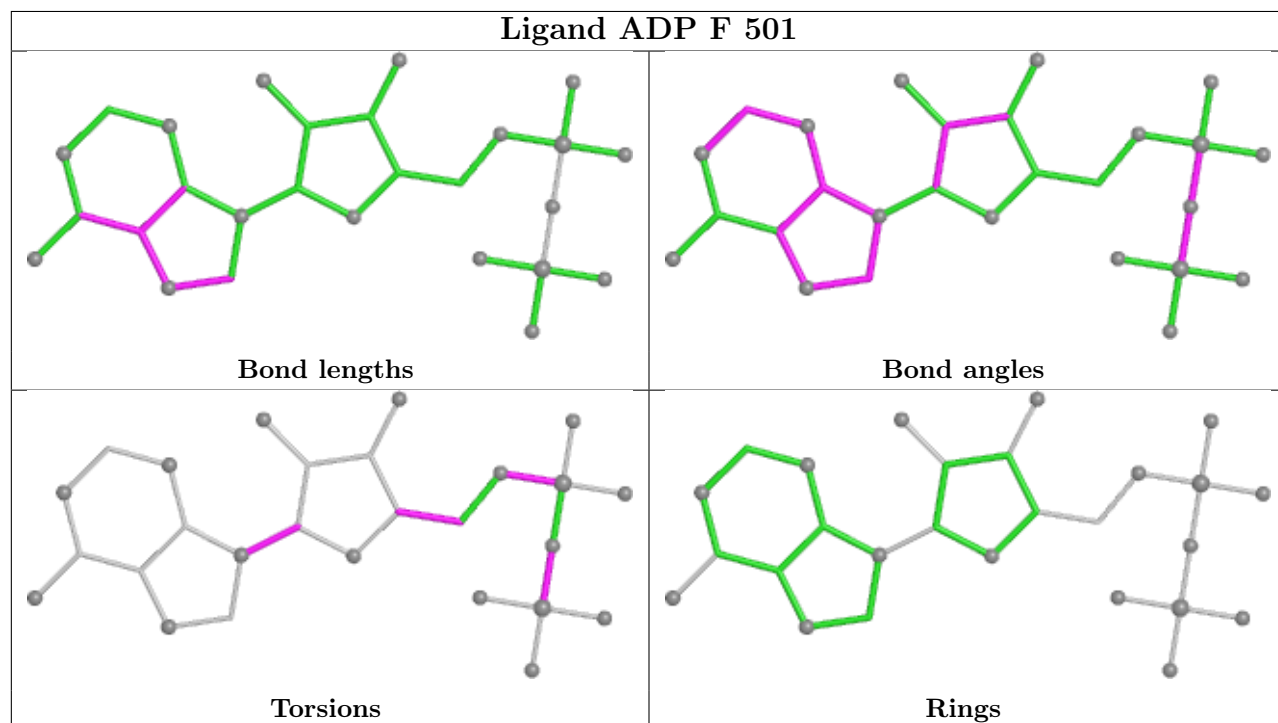
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

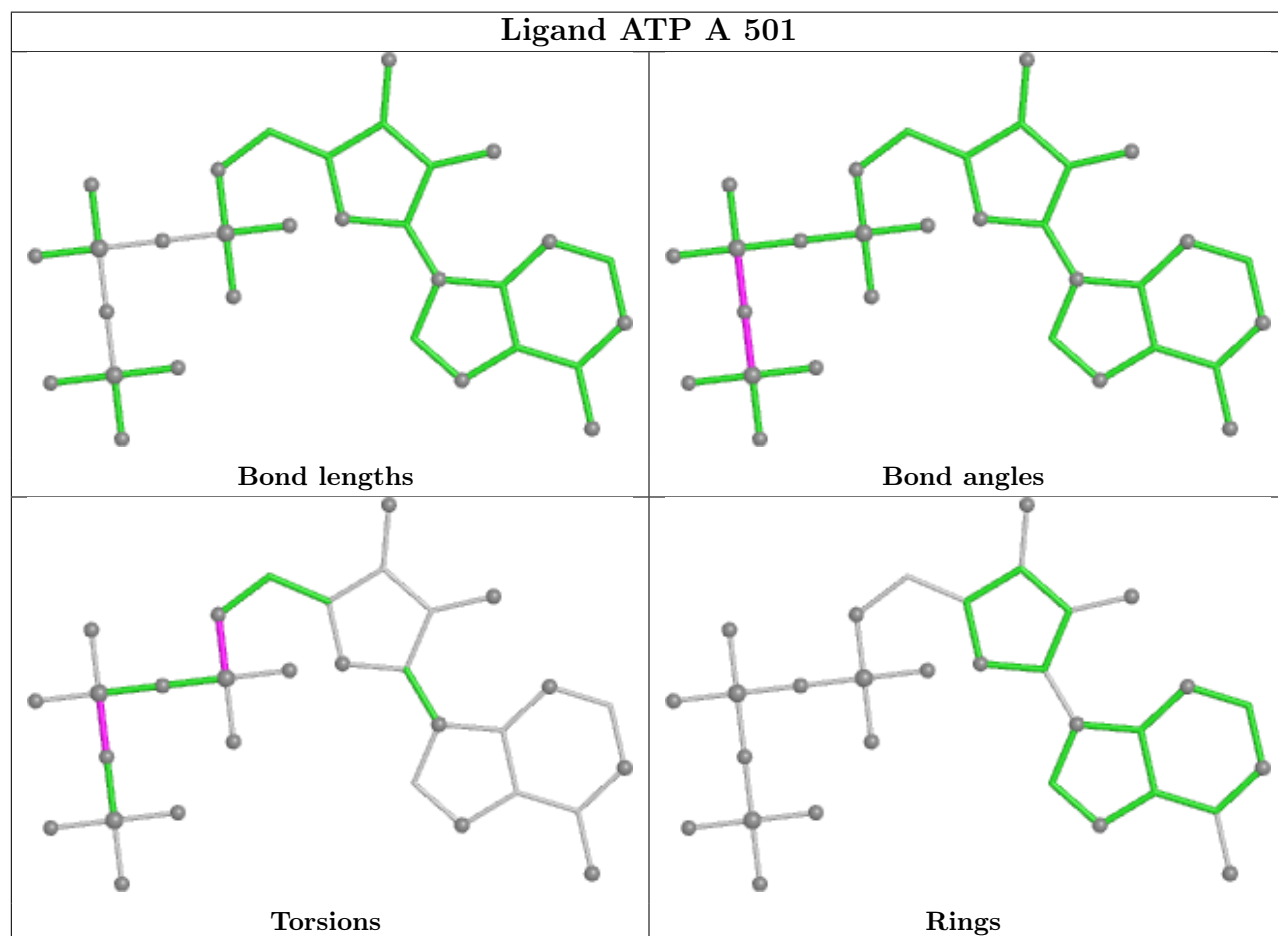
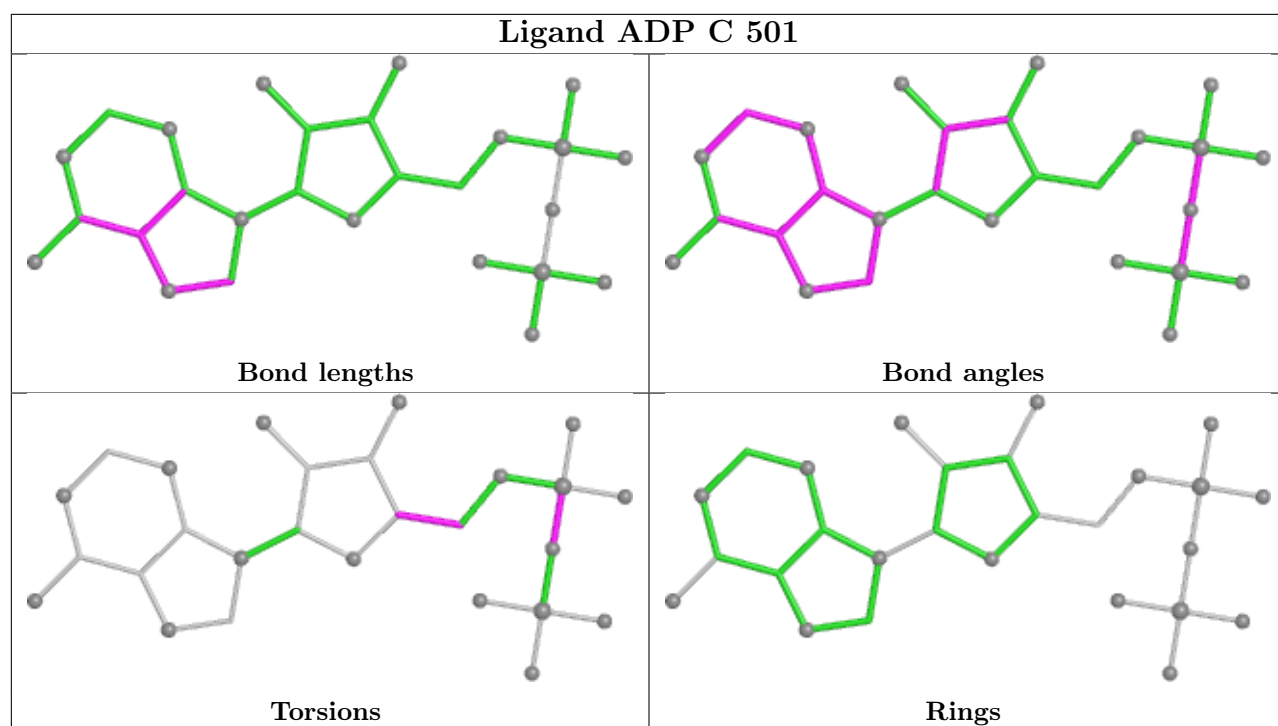


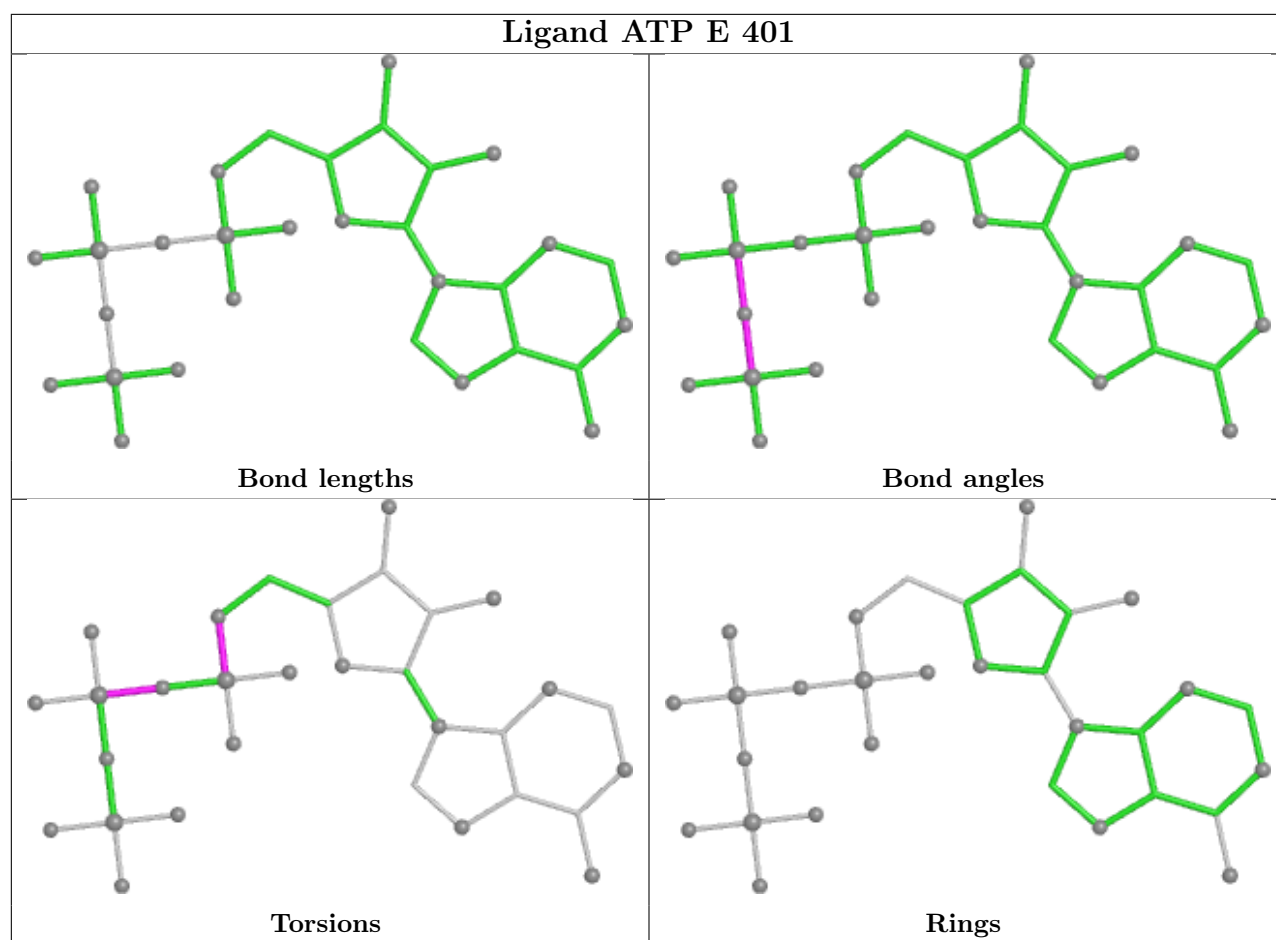
Ligand ATP D 501



Ligand ADP F 501







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.

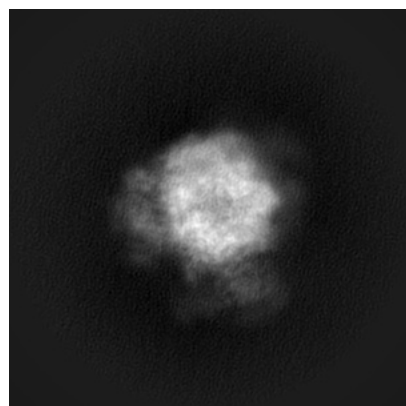
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62062. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

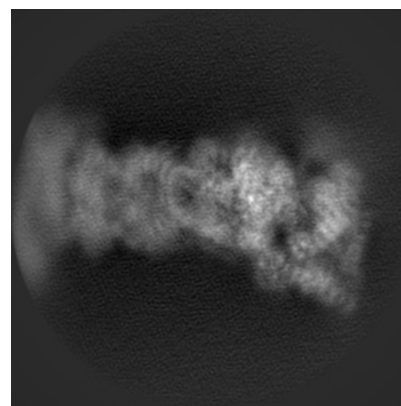
6.1.1 Primary map



X

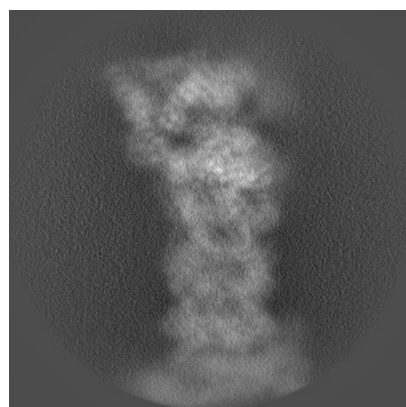


Y

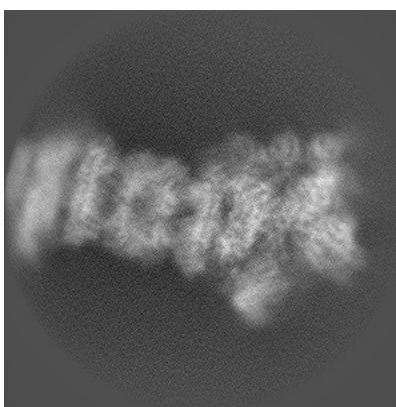


Z

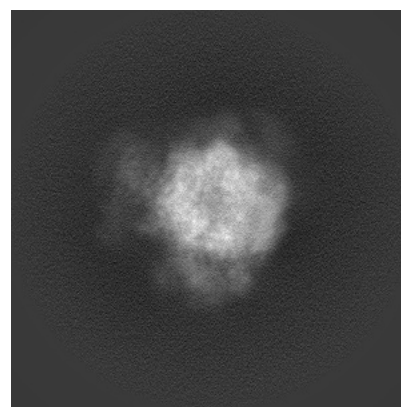
6.1.2 Raw map



X



Y

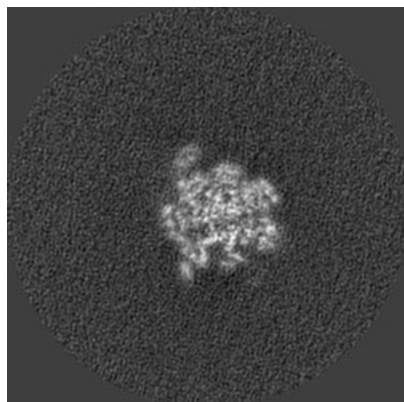


Z

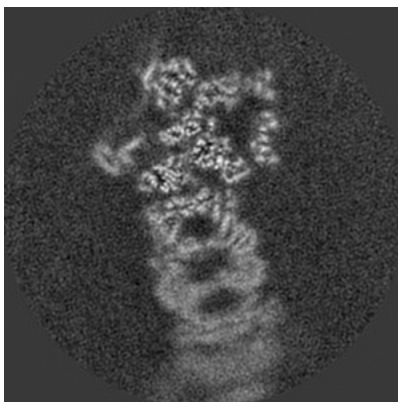
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

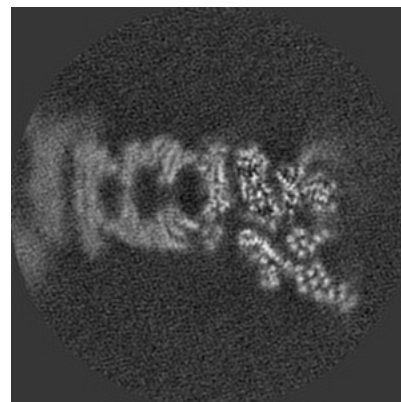
6.2.1 Primary map



X Index: 300

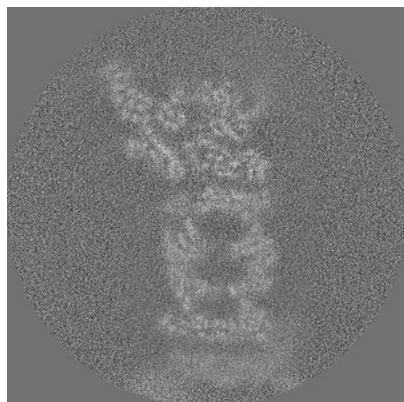


Y Index: 300

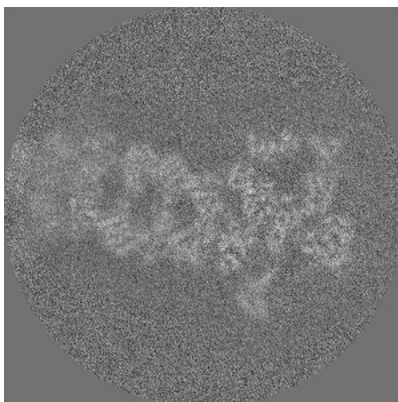


Z Index: 300

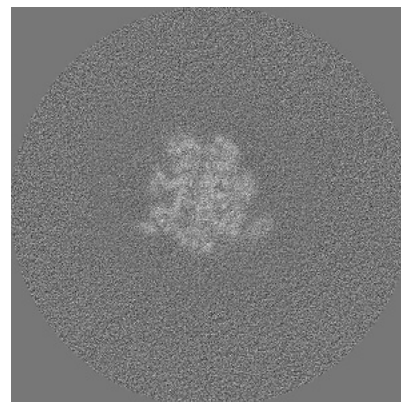
6.2.2 Raw map



X Index: 300



Y Index: 300

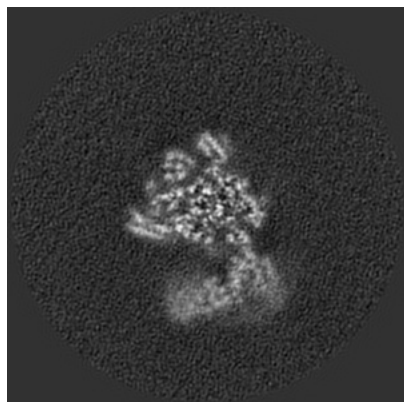


Z Index: 300

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

6.3 Largest variance slices [i](#)

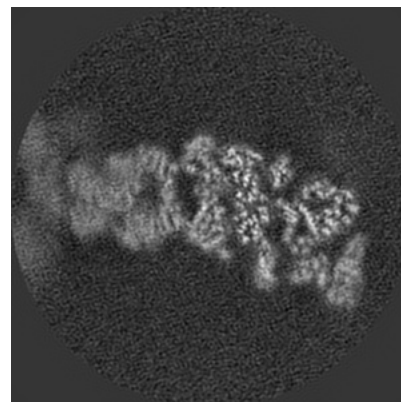
6.3.1 Primary map



X Index: 371

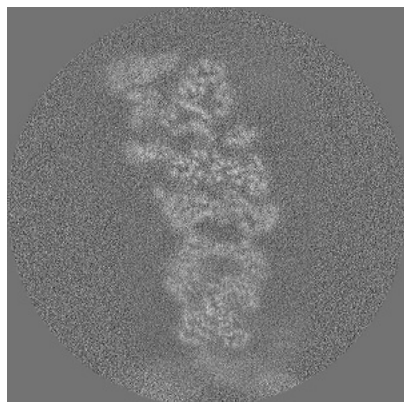


Y Index: 314

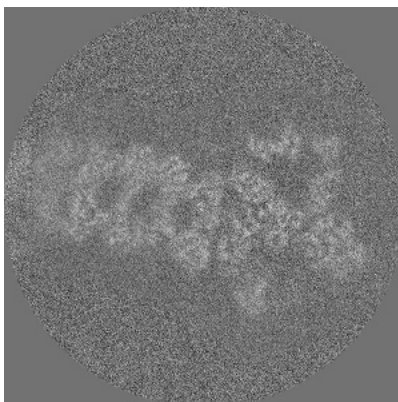


Z Index: 274

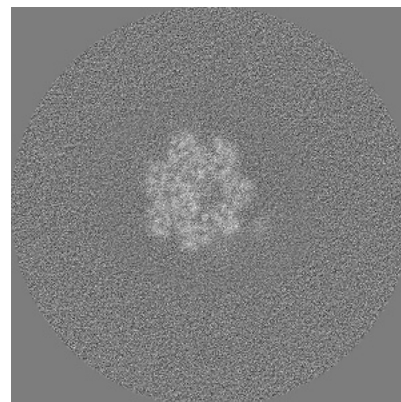
6.3.2 Raw map



X Index: 274



Y Index: 293

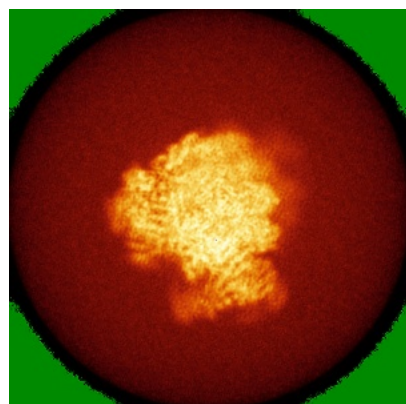


Z Index: 289

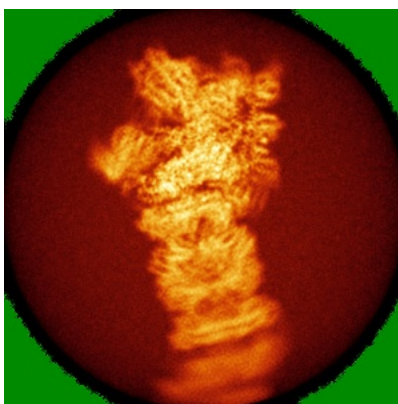
The images above show the largest variance slices of the map in three orthogonal directions.

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

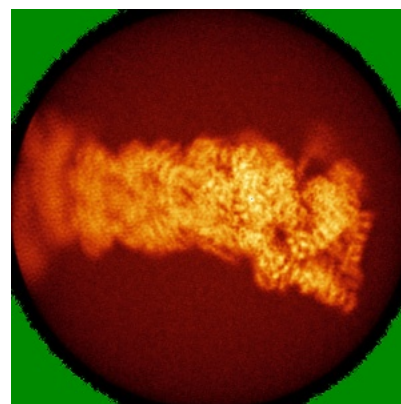
6.4.1 Primary map



X

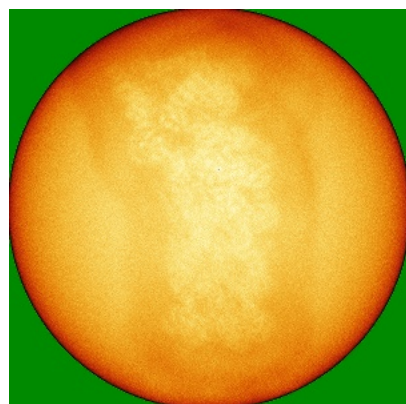


Y

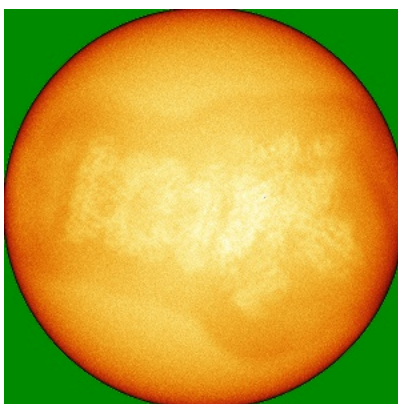


Z

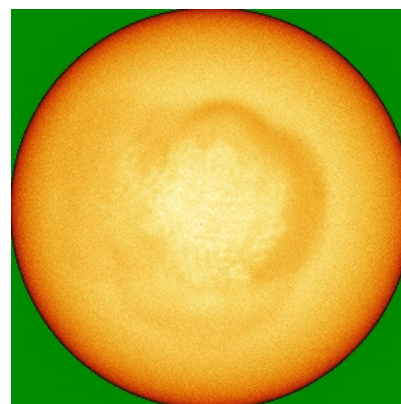
6.4.2 Raw map



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.

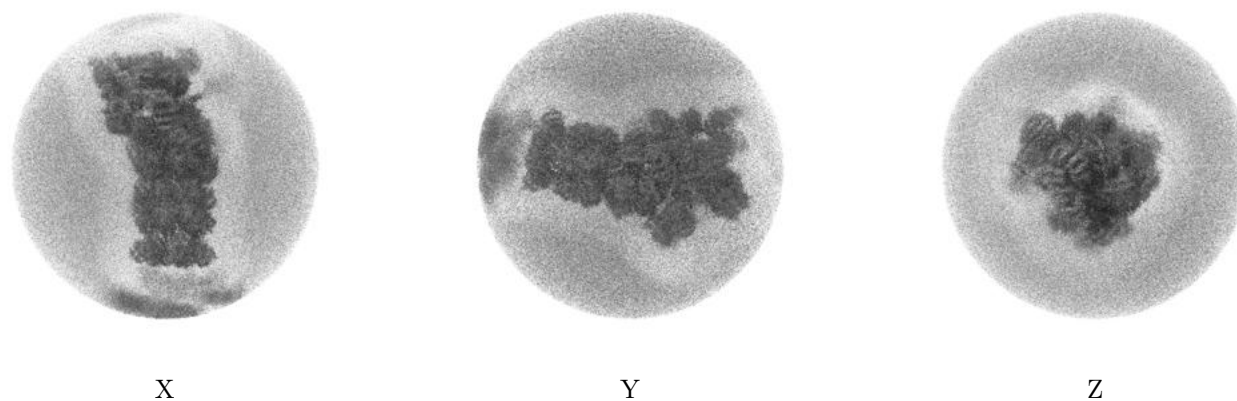
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00465. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

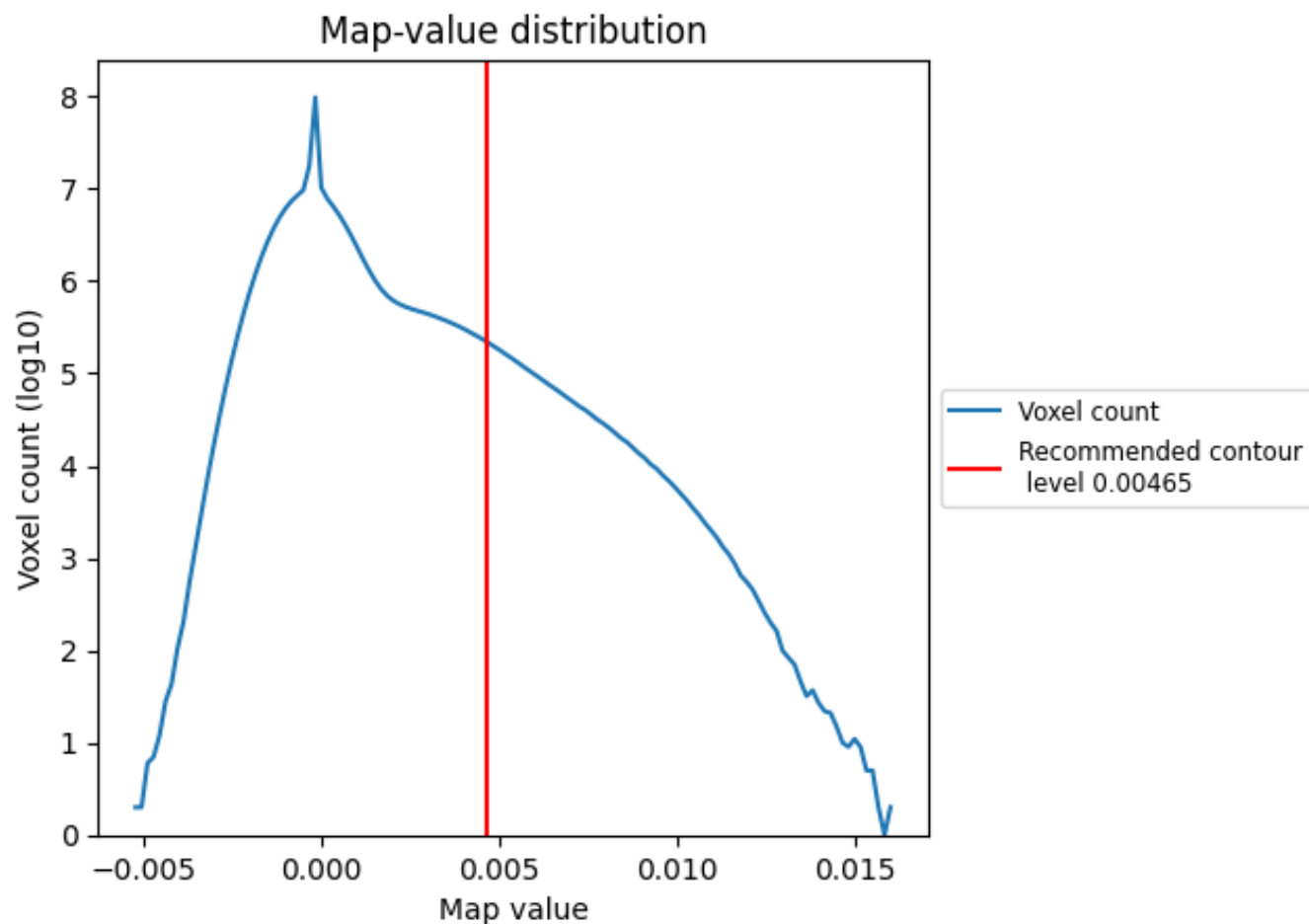
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

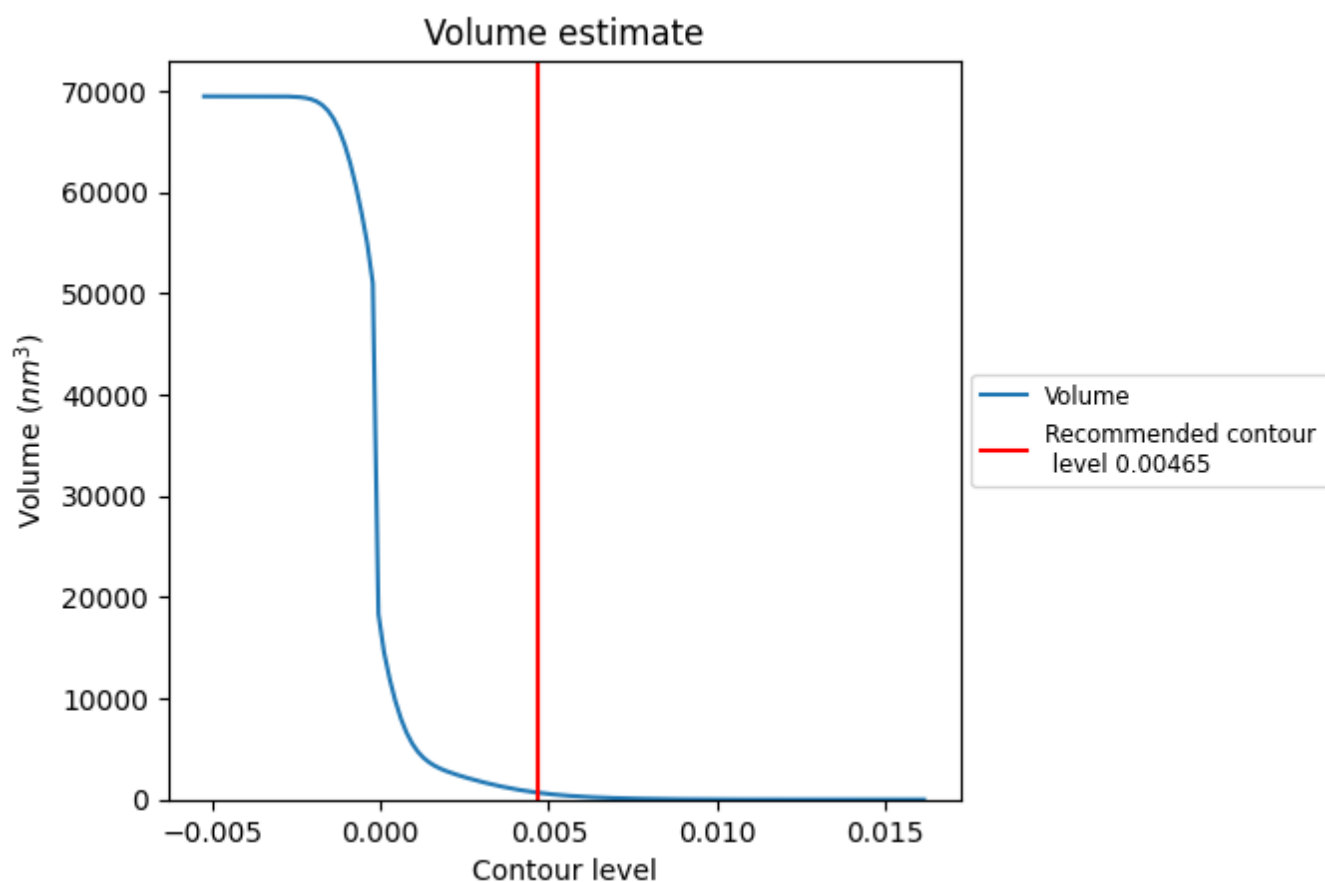
This section contains the results of statistical analysis of the map.

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.

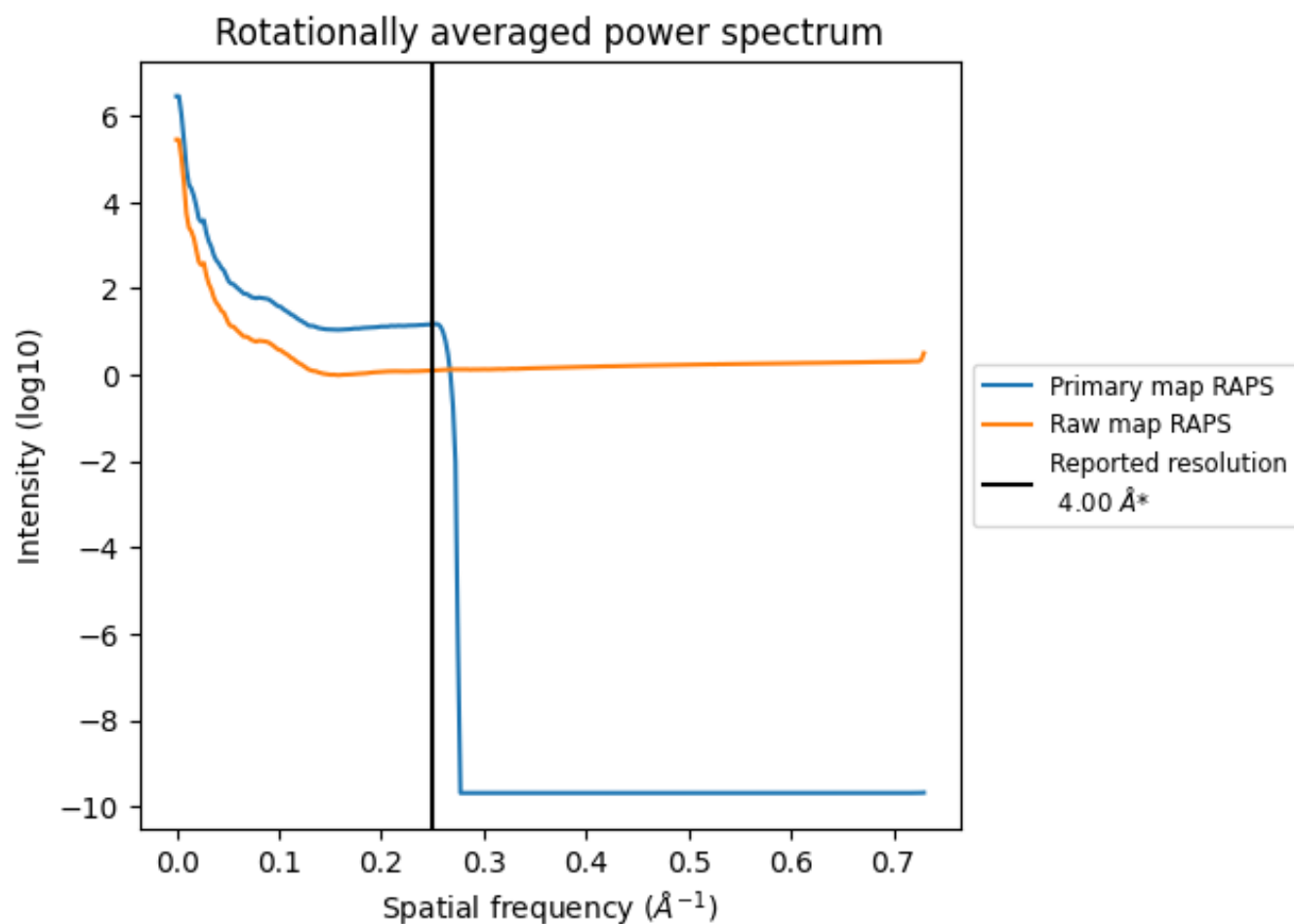
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 694 nm³; this corresponds to an approximate mass of 627 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 ⓘ

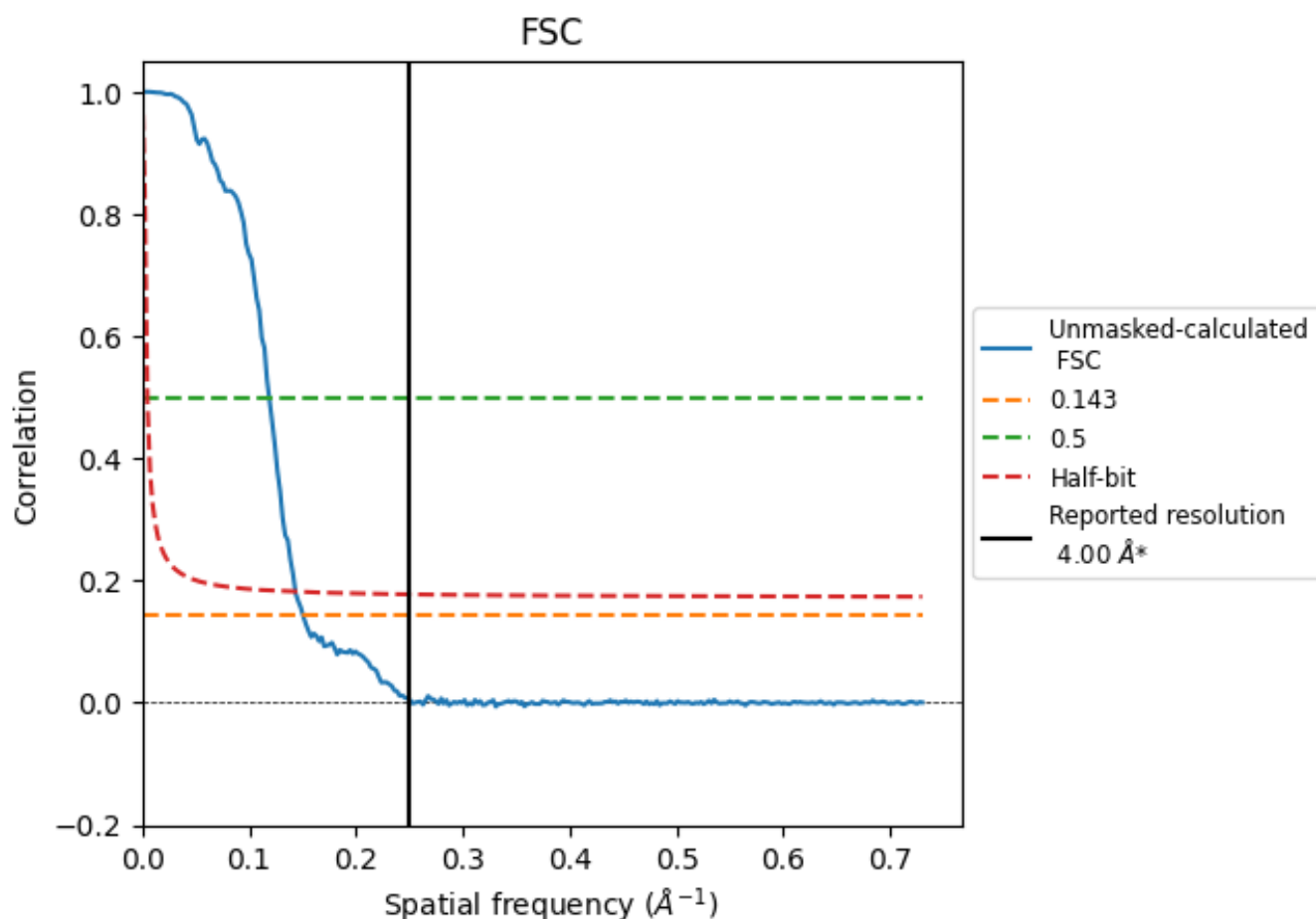


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 \AA^{-1}

8.2 Resolution estimates [i](#)

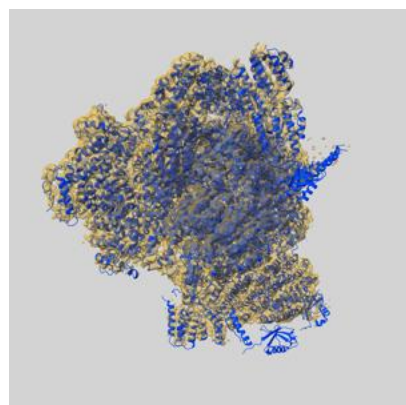
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.65	8.41	6.98

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.65 differs from the reported value 4.0 by more than 10 %

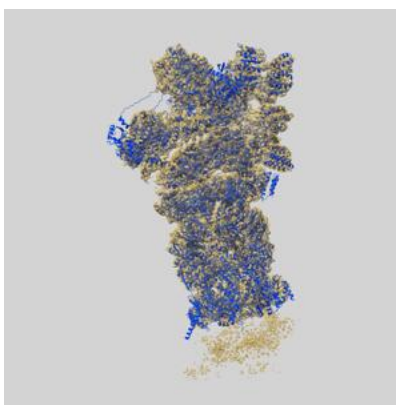
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62062 and PDB model 9K4K. Per-residue inclusion information can be found in section 3 on page 13.

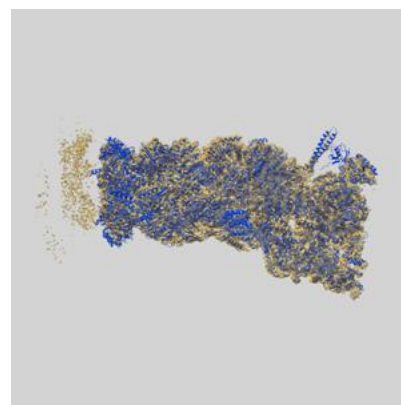
9.1 Map-model overlay [i](#)



X



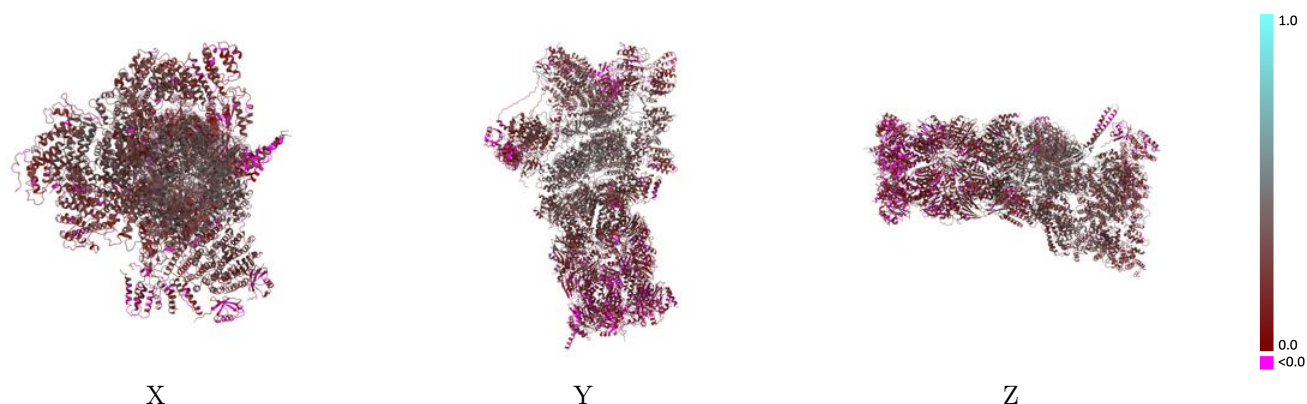
Y



Z

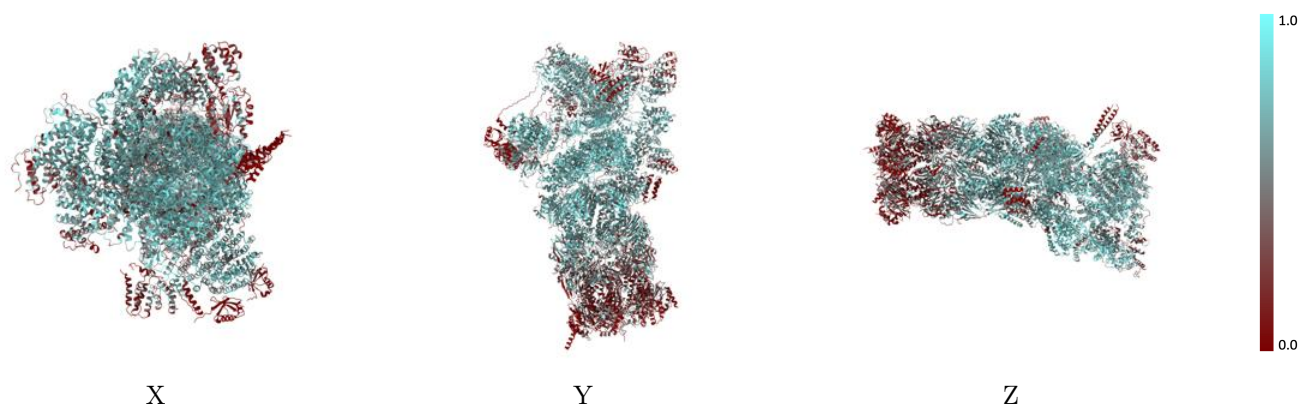
The images above show the 3D surface view of the map at the recommended contour level 0.00465 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



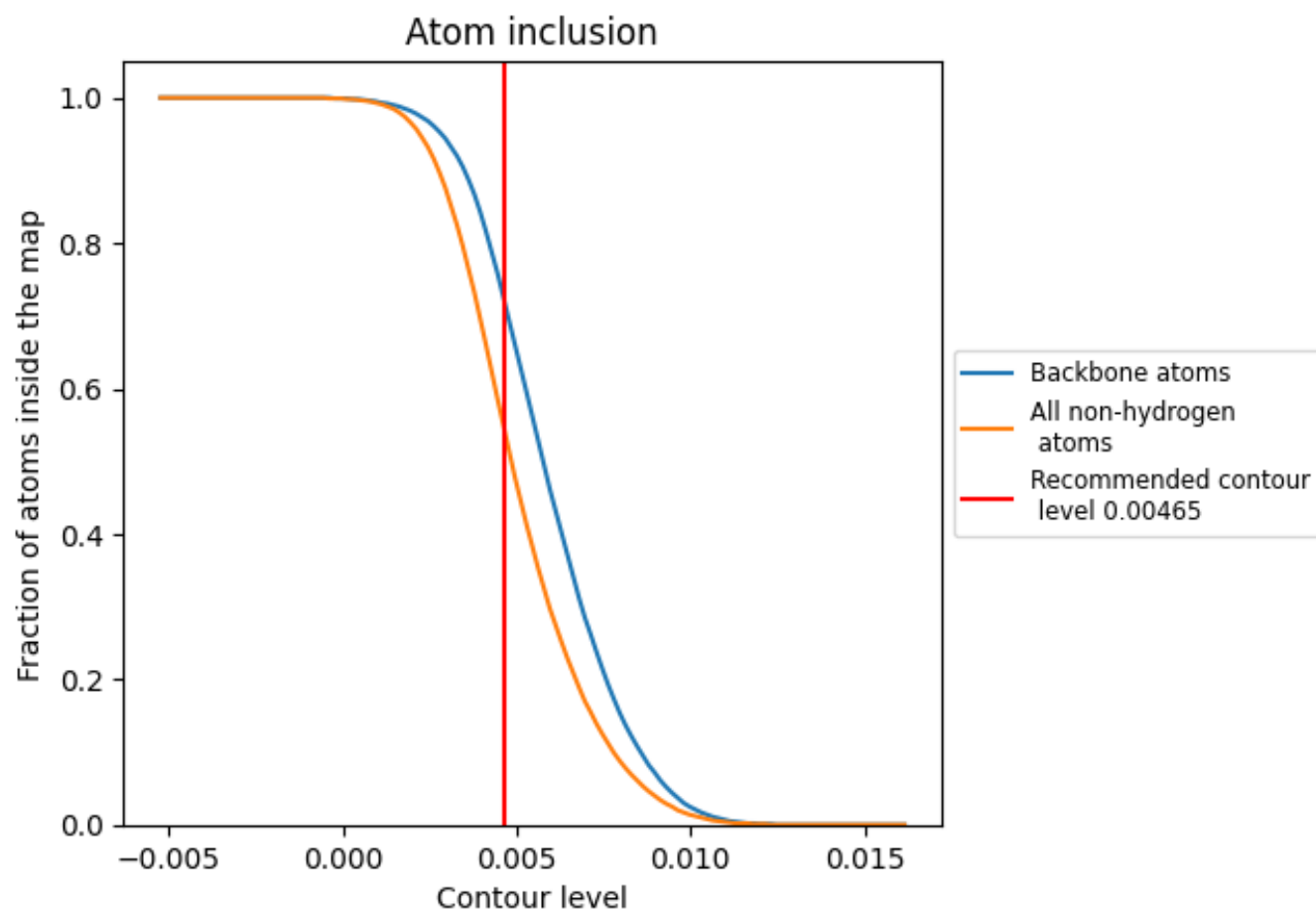
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00465).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 54% 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 (0.00465) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5430	 0.2490
A	 0.7140	 0.3640
B	 0.7170	 0.3550
C	 0.7510	 0.3760
D	 0.7200	 0.3630
E	 0.7410	 0.3700
F	 0.7140	 0.3680
G	 0.6670	 0.2870
H	 0.6920	 0.3020
I	 0.6780	 0.2930
J	 0.6920	 0.3120
K	 0.6670	 0.3250
L	 0.7040	 0.3280
M	 0.6620	 0.2830
N	 0.5800	 0.2010
O	 0.6090	 0.2220
P	 0.5980	 0.2230
Q	 0.6120	 0.2330
R	 0.6200	 0.2440
S	 0.5530	 0.2270
T	 0.5550	 0.2110
U	 0.5940	 0.2570
V	 0.5660	 0.2670
W	 0.6270	 0.2900
X	 0.5120	 0.2730
Y	 0.7560	 0.3230
Z	 0.6130	 0.2770
a	 0.5170	 0.2210
b	 0.2870	 0.1920
c	 0.6690	 0.3270
d	 0.5280	 0.2100
e	 0.5300	 0.2750
f	 0.5560	 0.2230
g	 0.2180	 0.1260
h	 0.2260	 0.1290



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Chain	Atom inclusion	Q-score
i	 0.1770	 0.1280
j	 0.1850	 0.1120
k	 0.1550	 0.1230
l	 0.2760	 0.1450
m	 0.2180	 0.1270
n	 0.3740	 0.1670
o	 0.3530	 0.1500
p	 0.3750	 0.1680
q	 0.4110	 0.1670
r	 0.4480	 0.1720
s	 0.3490	 0.1360
t	 0.4380	 0.1650
u	 0.0020	 0.0450
v	 0.0000	 0.0380
w	 0.0690	 0.0390
y	 0.0800	 0.1200
z	 0.4000	 0.1070