



## Full wwPDB EM Validation Report ⓘ

Apr 21, 2026 – 04:49 PM JST

PDB ID : 9K4S / pdb\_00009k4s  
EMDB ID : EMD-62068  
Title : Structure of substrate-engaged 26S proteasome RP-CP subcomplex in state EB.2  
Authors : Wu, Z.; Chen, E.; Mao, Y.  
Deposited on : 2024-10-21  
Resolution : 4.70 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](mailto: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>.

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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

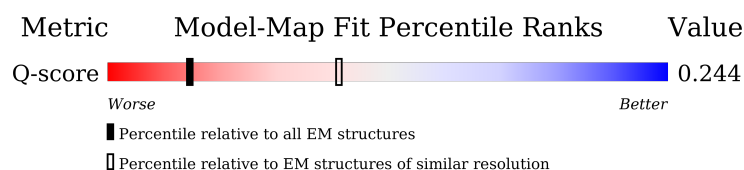
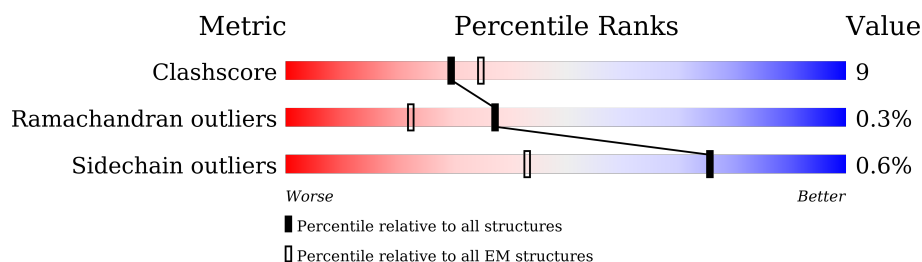
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.70 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	1989 ( 4.20 - 5.20 )

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  $\geq 3$ , 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	x	76	
33	y	76	
34	v	28	

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 107468 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	406	Total	C	N	O	S	0	0
			3164	1992	555	600	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	397	Total	C	N	O	S	0	0
			3099	1953	525	606	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	381	Total	C	N	O	S	0	0
			2978	1872	536	554	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	389	Total	C	N	O	S	0	0
			3097	1947	552	581	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	415	Total	C	N	O	S	0	0
			3251	2038	561	634	18		

- 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	240	Total	C	N	O	S	0	0
			1867	1187	312	355	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
			1801	1149	304	342	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	248	Total	C	N	O	S	0	0
			1933	1222	330	371	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	1166	327	363	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	238	Total	C	N	O	S	0	0
			1813	1139	302	361	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	240	Total	C	N	O	S	0	0
			1876	1175	338	352	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	242	Total	C	N	O	S	0	0
			1890	1200	323	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	818	Total	C	N	O	S	0	0
			6373	4047	1084	1197	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	444	Total	C	N	O	S	0	0
			3612	2301	645	653	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		

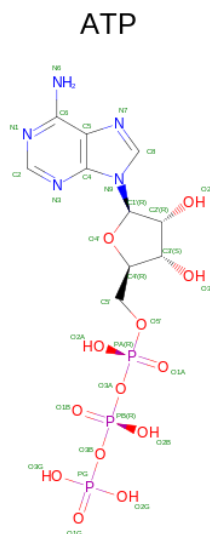
- Molecule 33 is a protein called Ubiquitin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	x	76	Total	C	N	O	S	0	0
			601	378	105	117	1		
33	y	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	v	28	Total	C	N	O	0	0
			143	86	29	28		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).

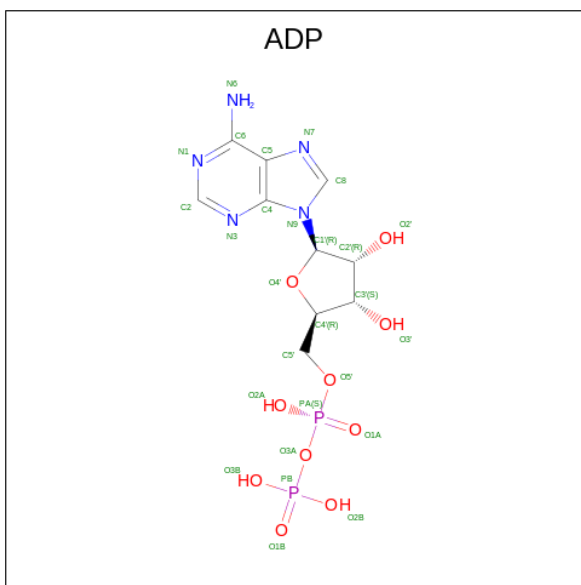


Mol	Chain	Residues	Atoms					AltConf
35	A	1	Total 31	C 10	N 5	O 13	P 3	0
35	D	1	Total 31	C 10	N 5	O 13	P 3	0
35	F	1	Total 31	C 10	N 5	O 13	P 3	0

- 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 1 1	0
36	D	1	Total Mg 1 1	0
36	F	1	Total Mg 1 1	0

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ) (labeled as "Ligand of Interest" by depositor).



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

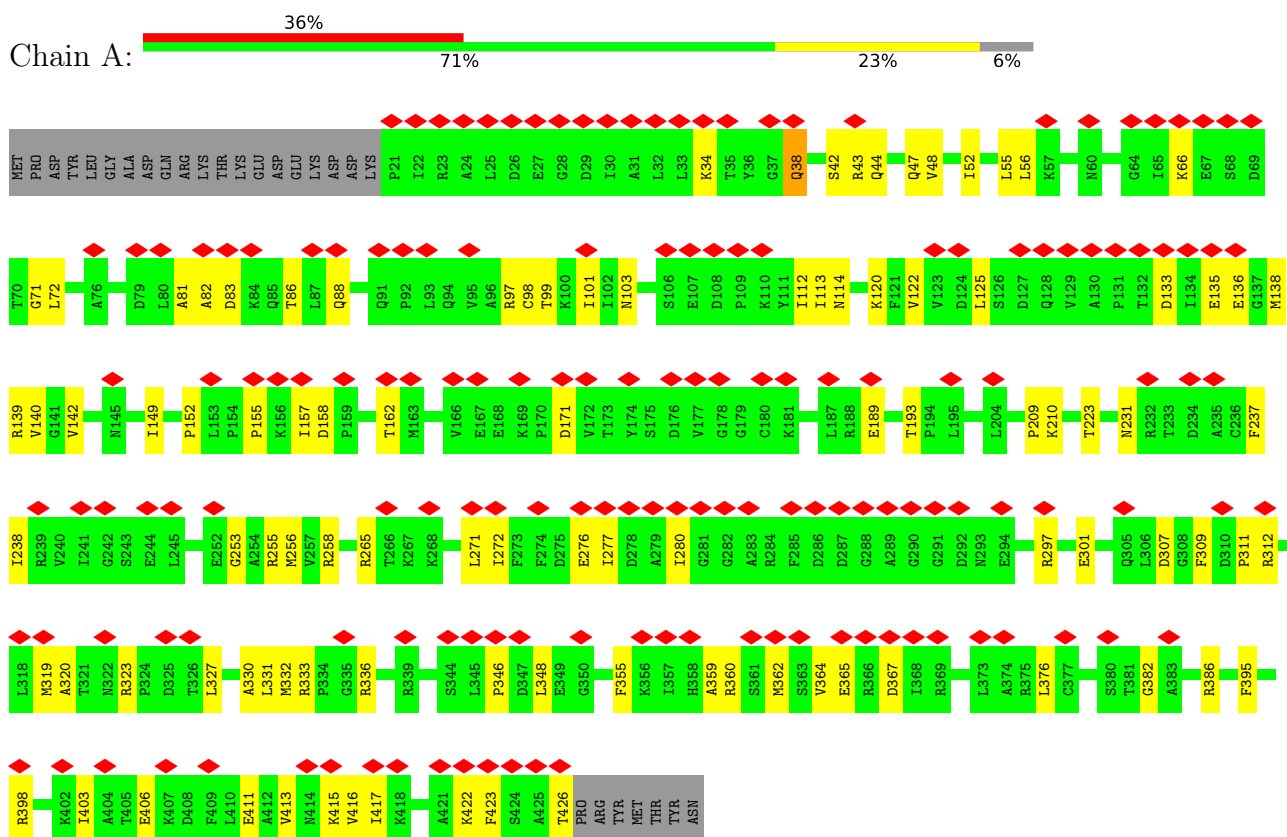
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

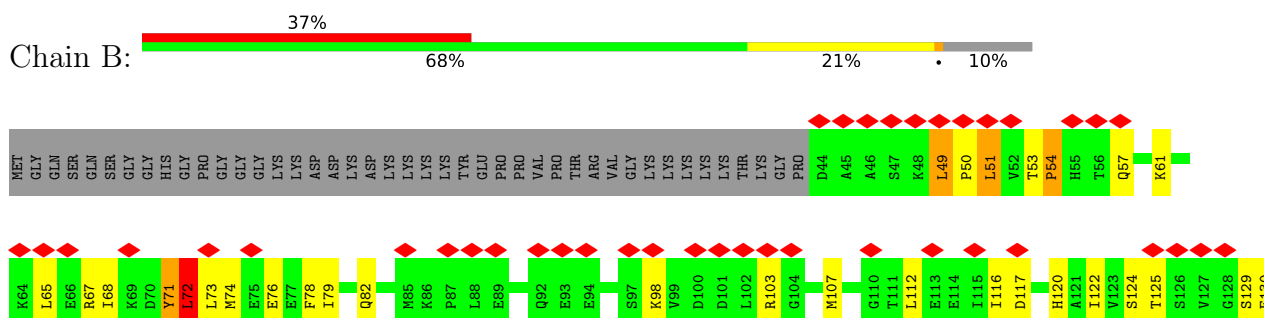
### 3 Residue-property plots

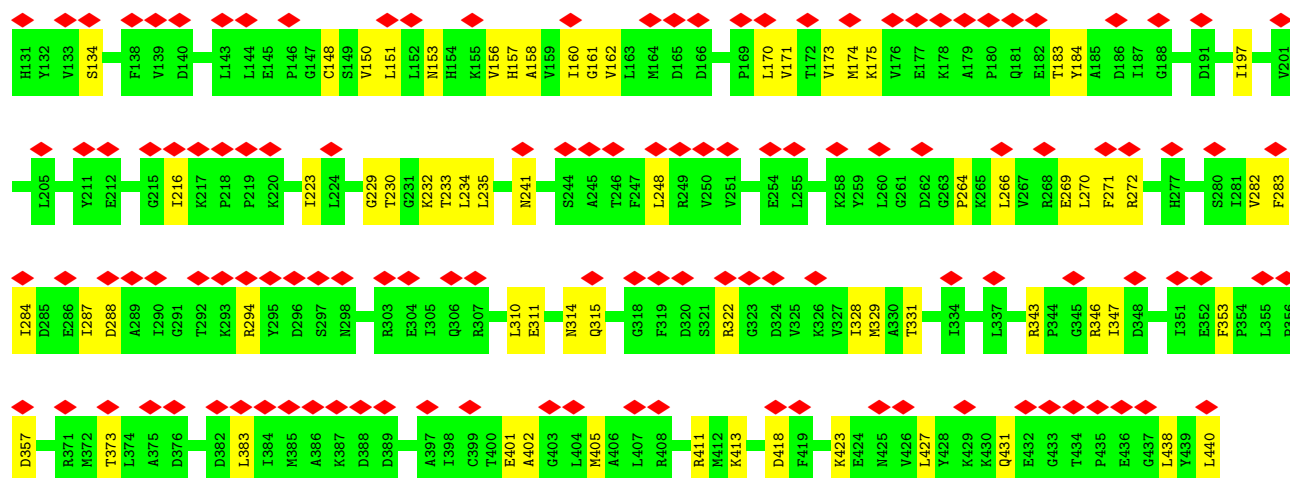
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



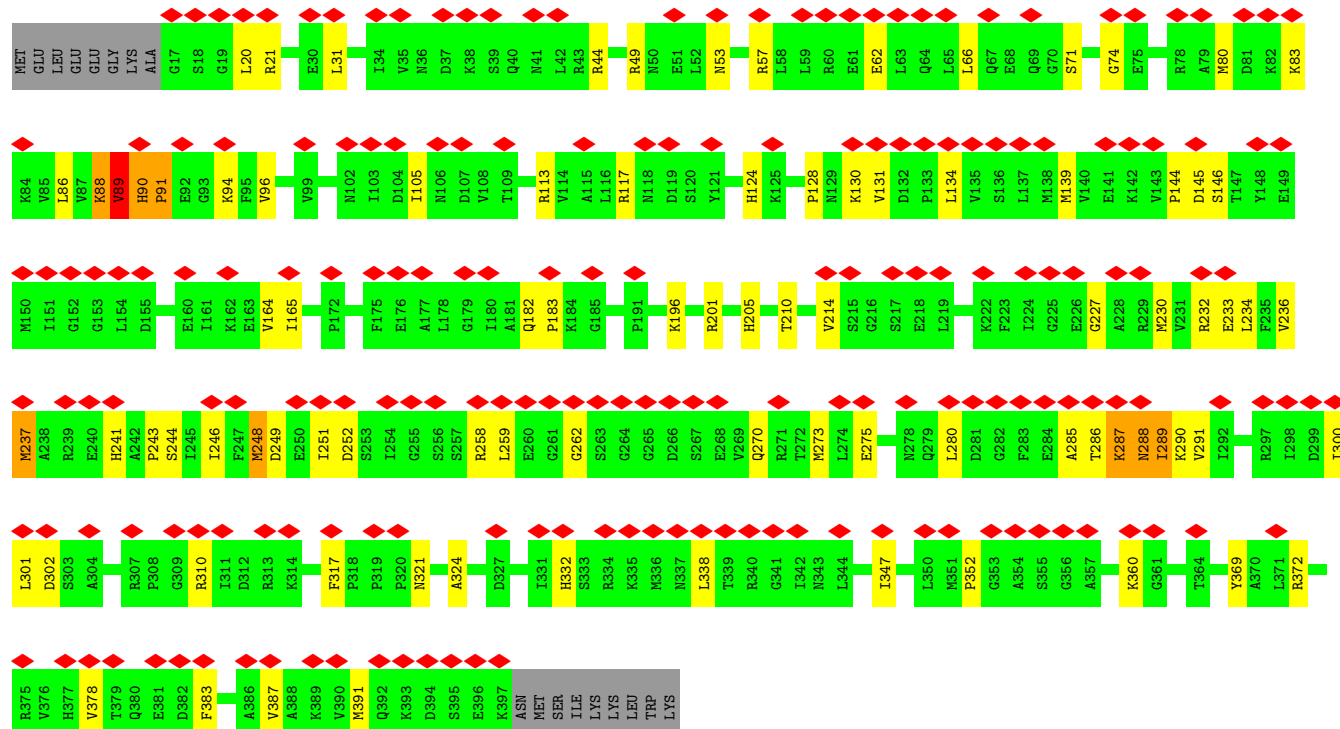
#### • Molecule 2: 26S proteasome regulatory subunit 4





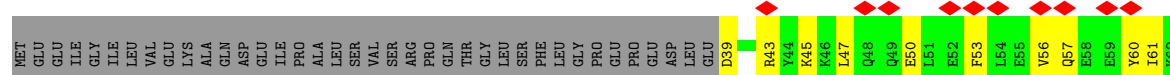
• Molecule 3: 26S proteasome regulatory subunit 8

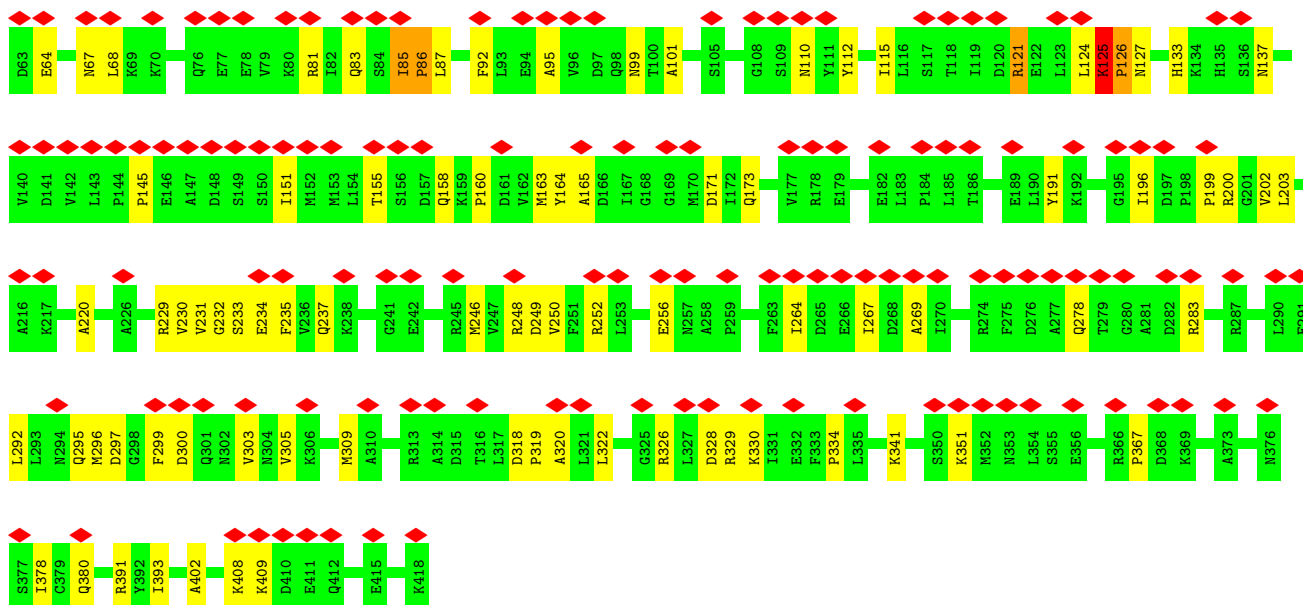
Chain C: 48% 74% 20%



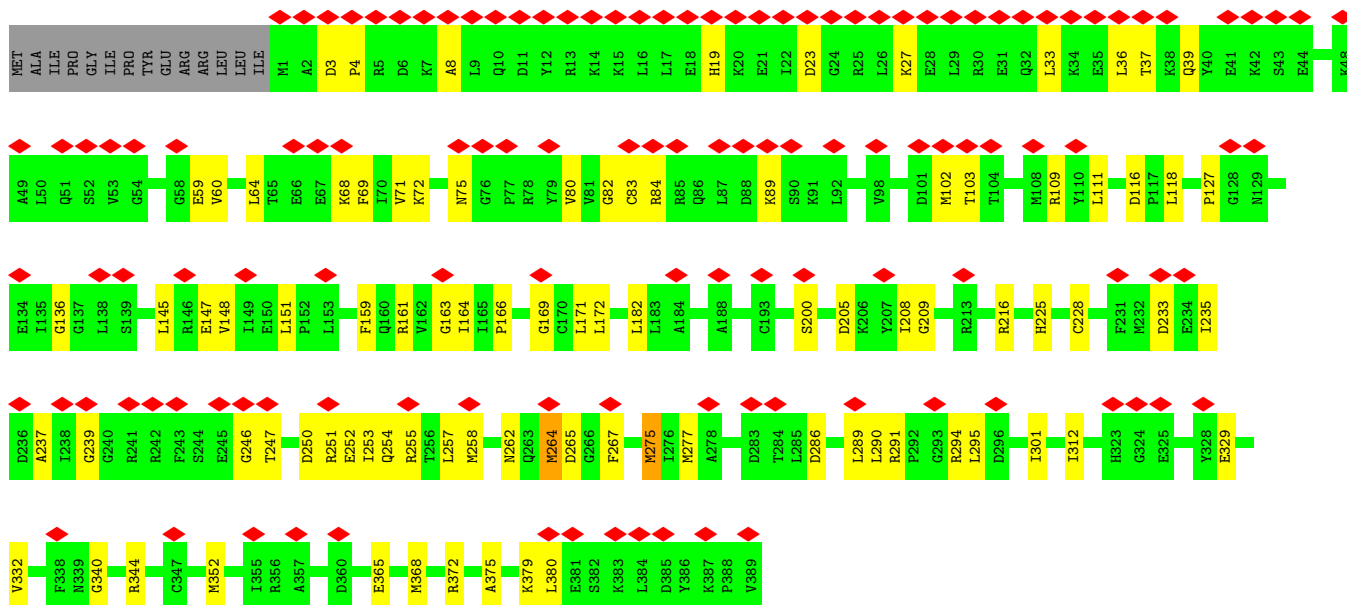
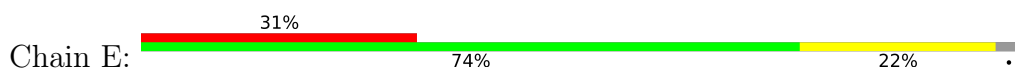
• Molecule 4: 26S proteasome regulatory subunit 6B

Chain D: 36% 68% 22% 9%

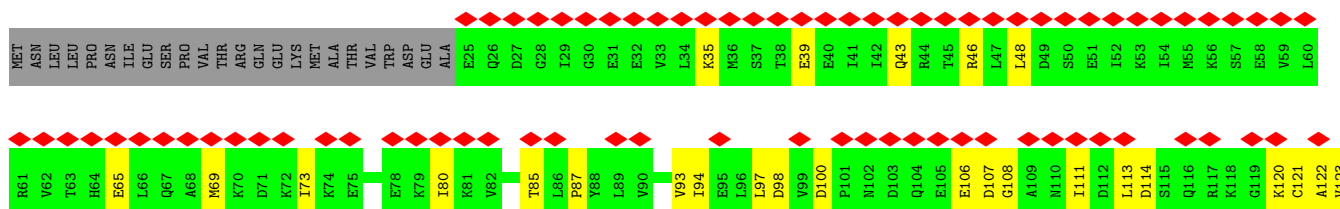
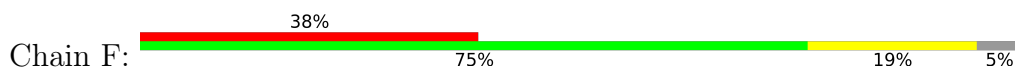


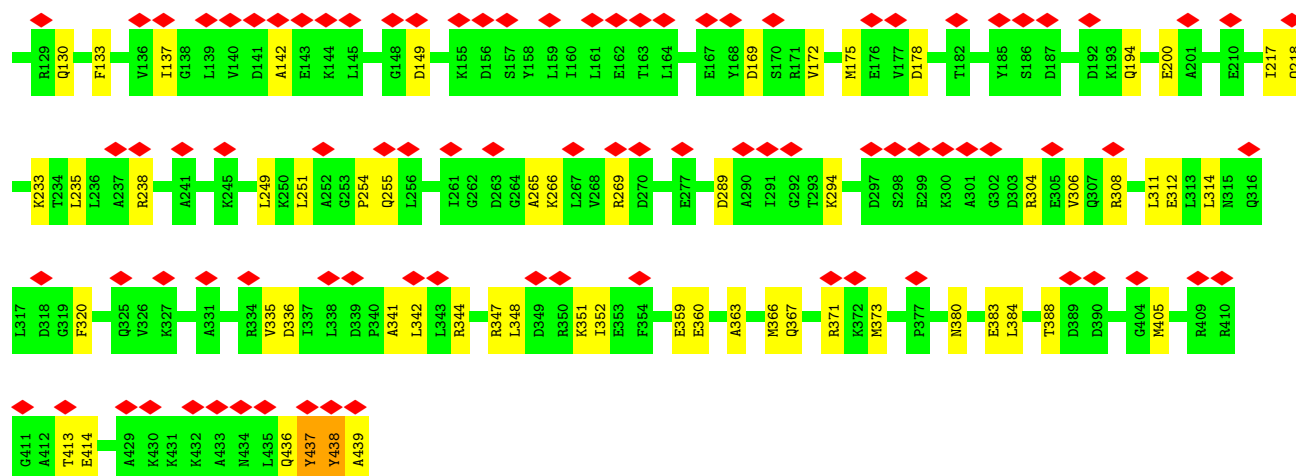


• Molecule 5: Proteasome 26S subunit, ATPase 6

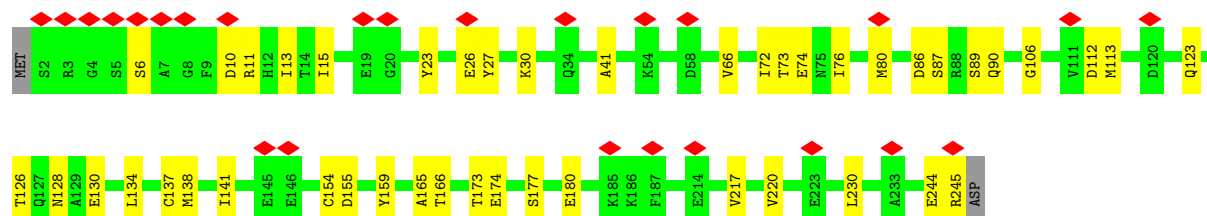
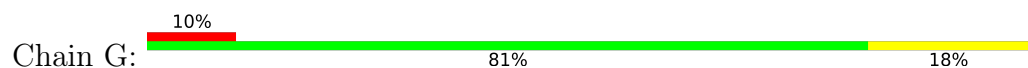


• Molecule 6: 26S proteasome regulatory subunit 6A

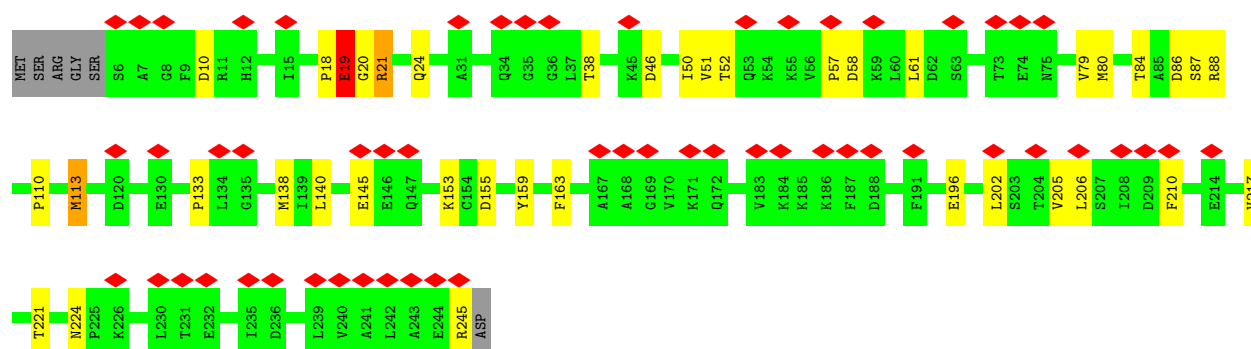
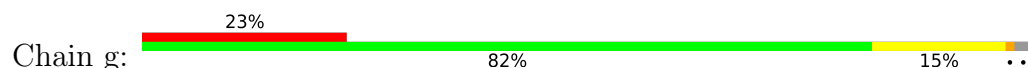




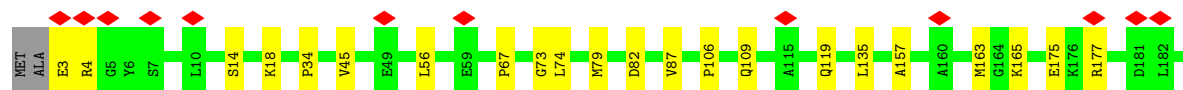
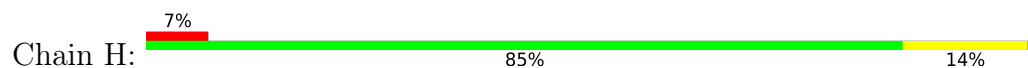
• Molecule 7: Proteasome subunit alpha type-6



• Molecule 7: Proteasome subunit alpha type-6



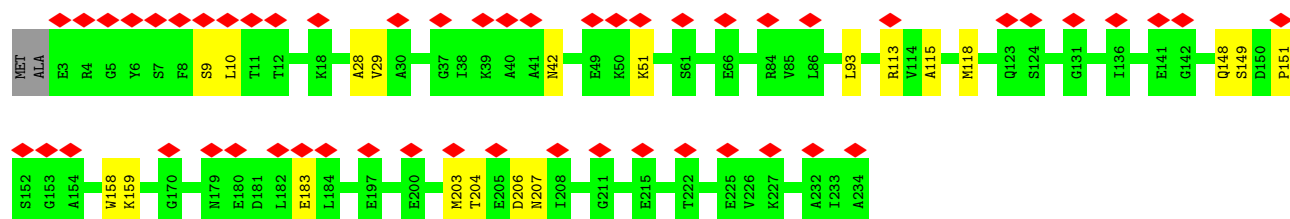
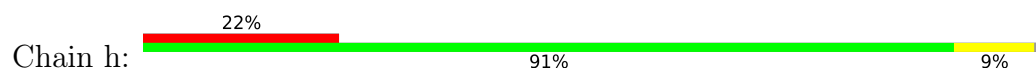
• Molecule 8: Proteasome subunit alpha type-2



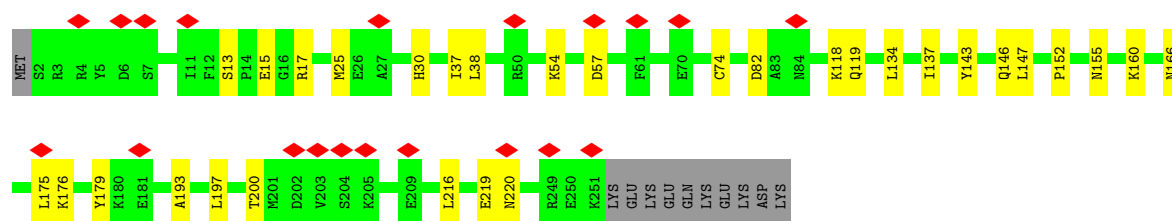
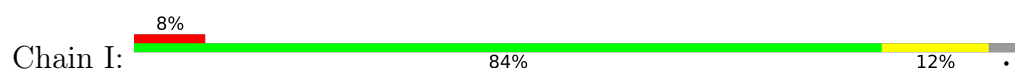




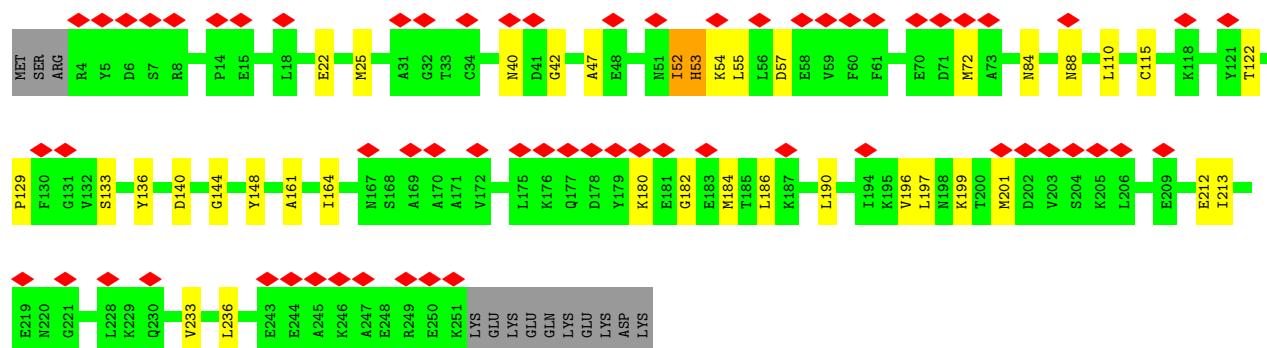
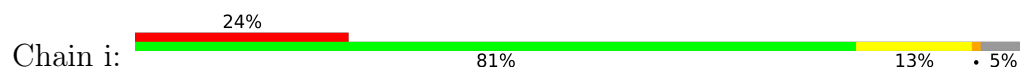
• Molecule 8: Proteasome subunit alpha type-2



• Molecule 9: Proteasome subunit alpha type-4

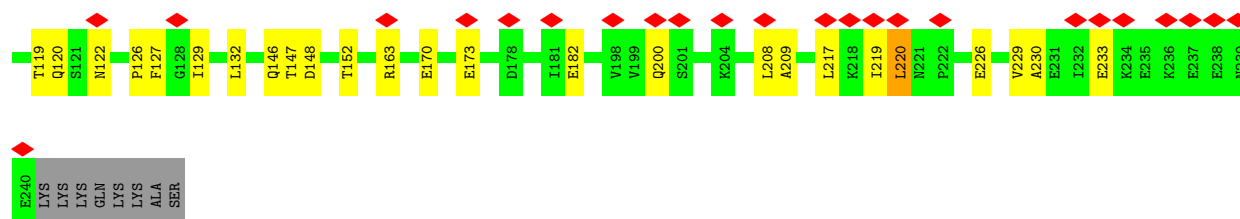


• Molecule 9: Proteasome subunit alpha type-4



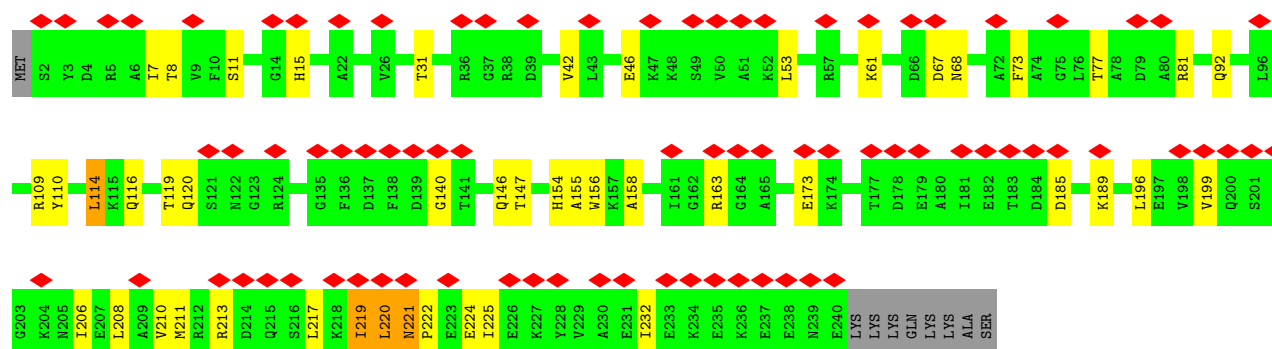
• Molecule 10: Proteasome subunit alpha type-7





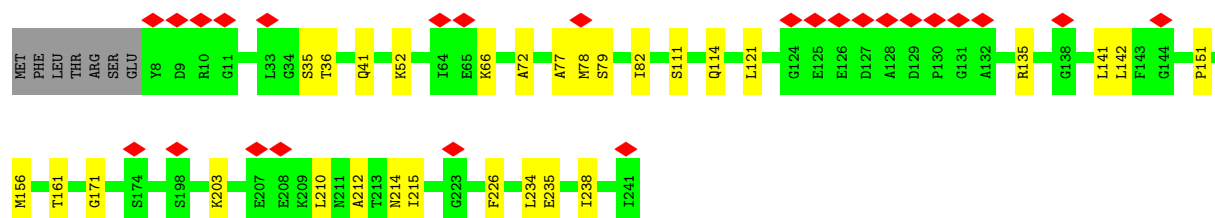
• Molecule 10: Proteasome subunit alpha type-7

Chain j: 33% 77% 17%



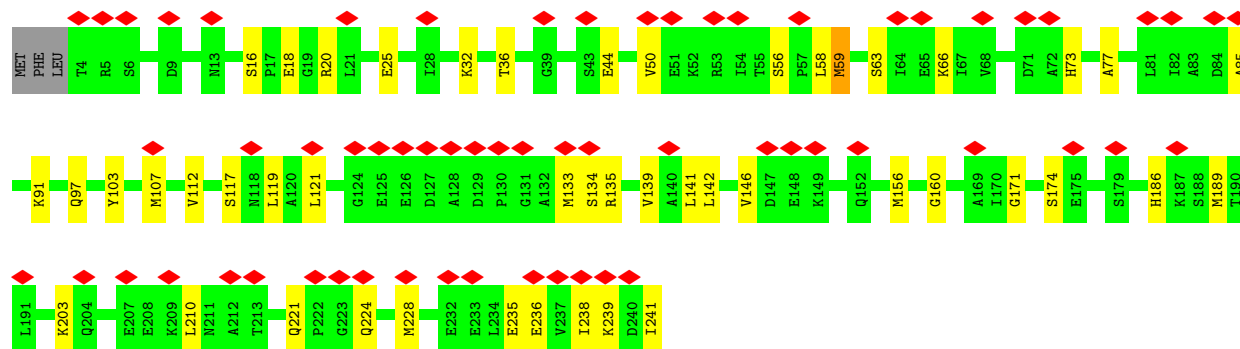
• Molecule 11: Proteasome subunit alpha type-5

Chain K: 10% 85% 12%

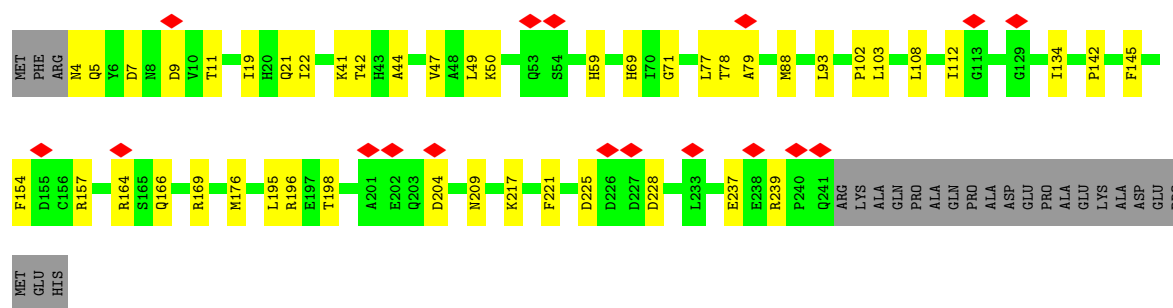
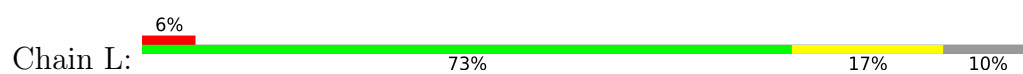


• Molecule 11: Proteasome subunit alpha type-5

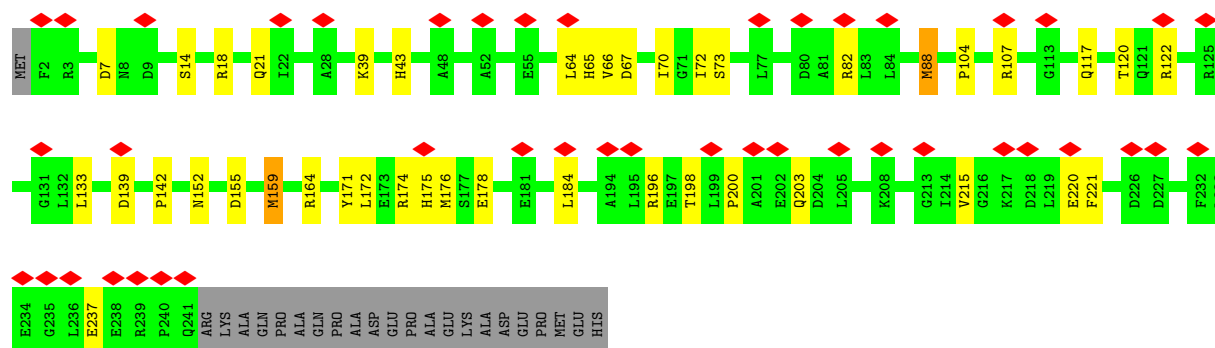
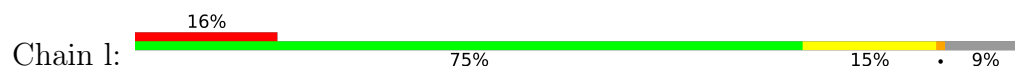
Chain k: 26% 79% 19%



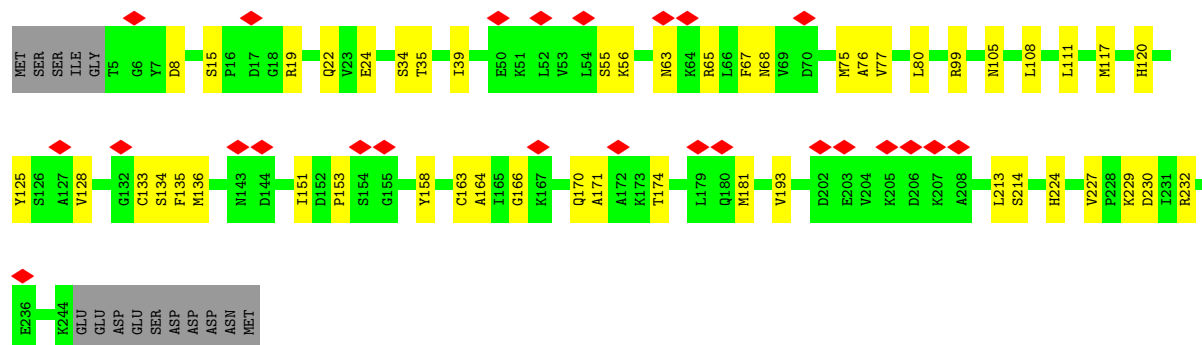
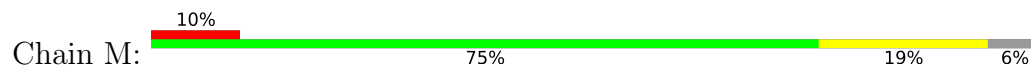
• Molecule 12: Proteasome subunit alpha type-1



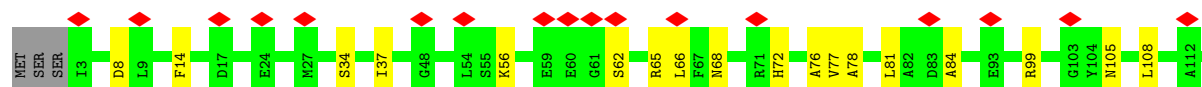
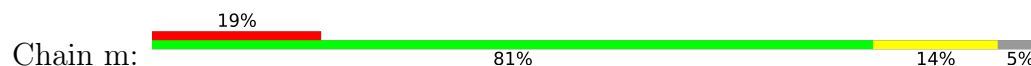
• Molecule 12: Proteasome subunit alpha type-1

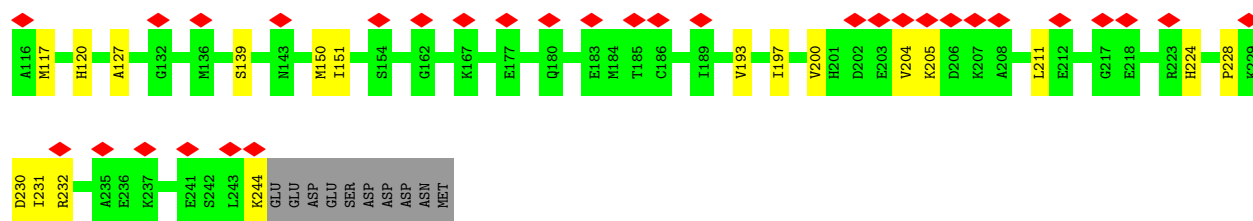


• Molecule 13: Proteasome subunit alpha type-3

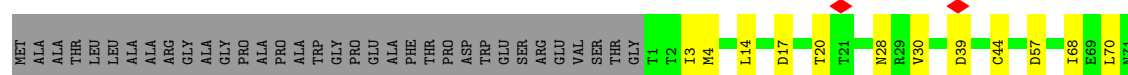


• Molecule 13: Proteasome subunit alpha type-3

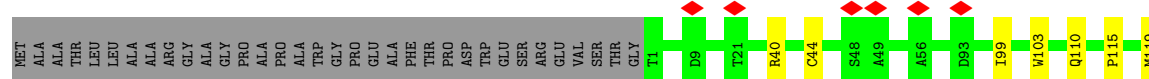
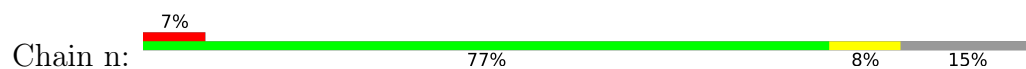




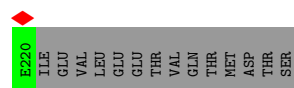
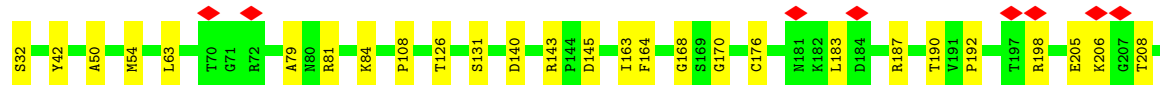
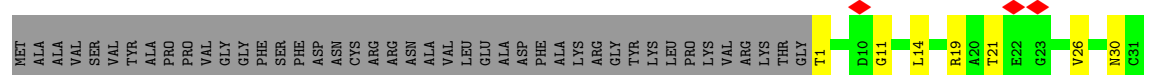
• Molecule 14: Proteasome subunit beta type-6



• Molecule 14: Proteasome subunit beta type-6

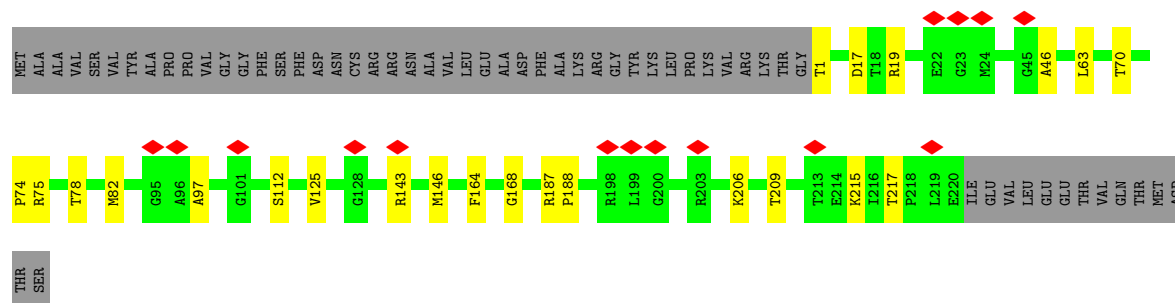


• Molecule 15: Proteasome subunit beta type-7

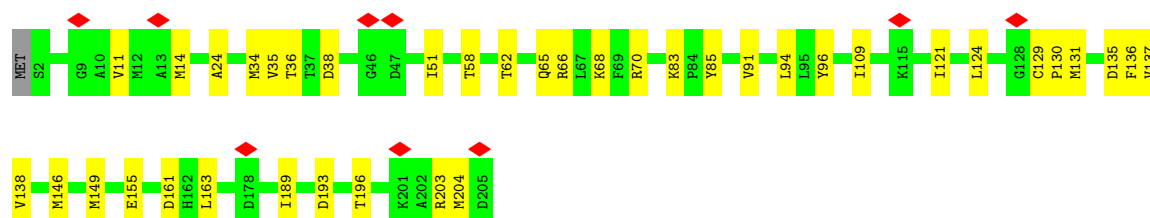
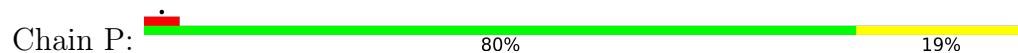


• Molecule 15: Proteasome subunit beta type-7

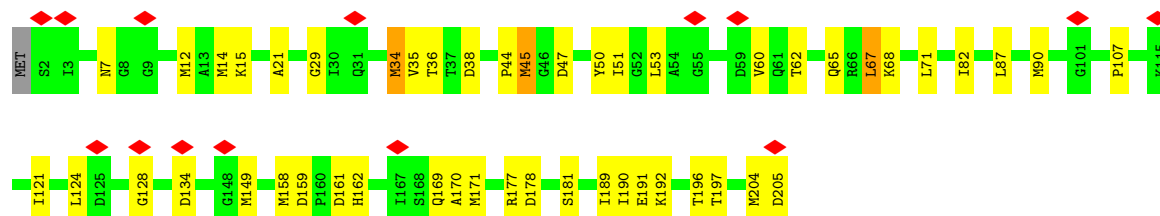
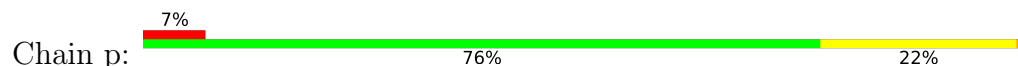




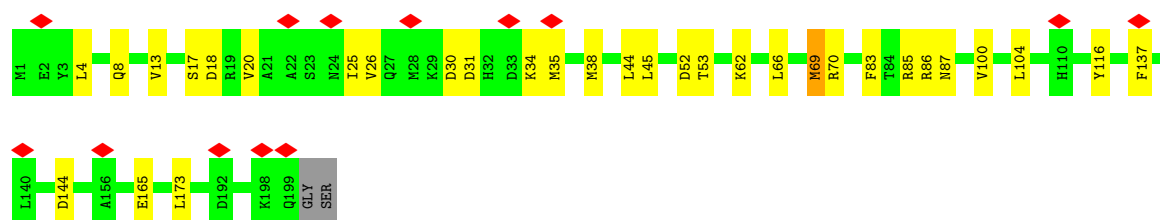
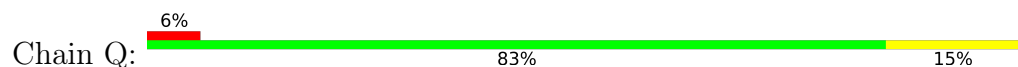
• Molecule 16: Proteasome subunit beta type-3



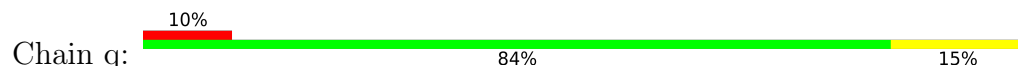
• Molecule 16: Proteasome subunit beta type-3

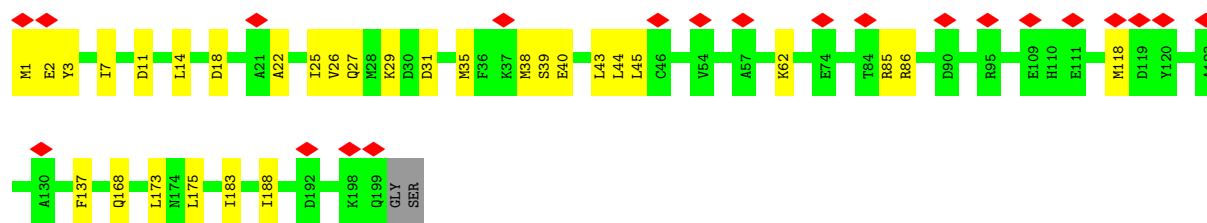


• Molecule 17: Proteasome subunit beta type-2

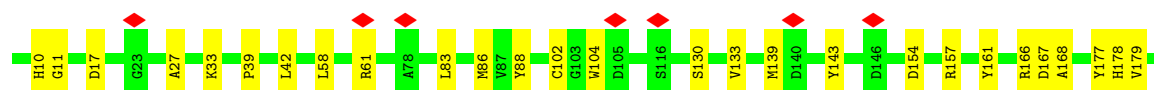
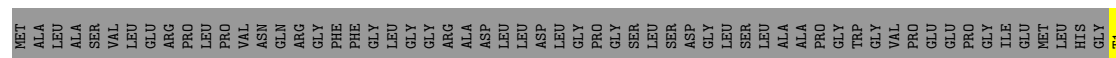


• Molecule 17: Proteasome subunit beta type-2

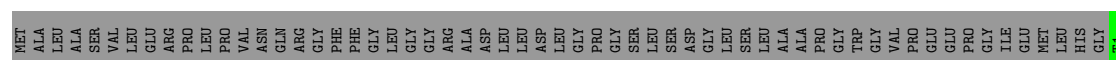




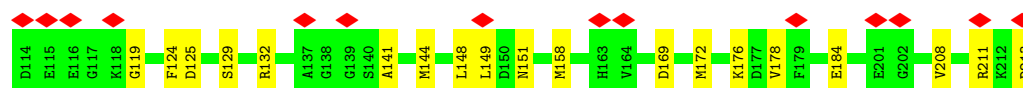
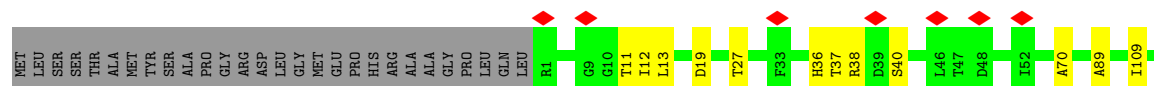
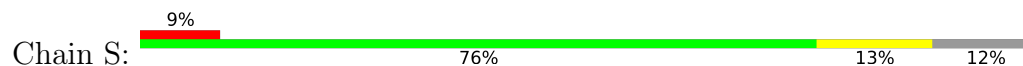
• Molecule 18: Proteasome subunit beta type-5



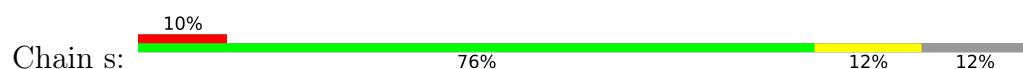
• Molecule 18: Proteasome subunit beta type-5

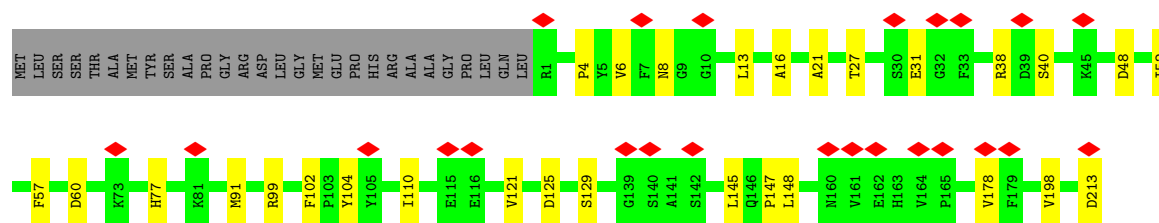


• Molecule 19: Proteasome subunit beta type-1

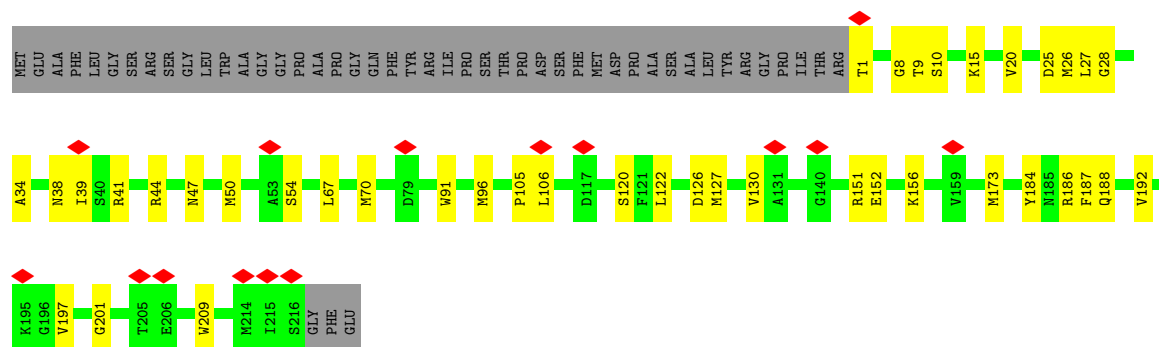


• Molecule 19: Proteasome subunit beta type-1

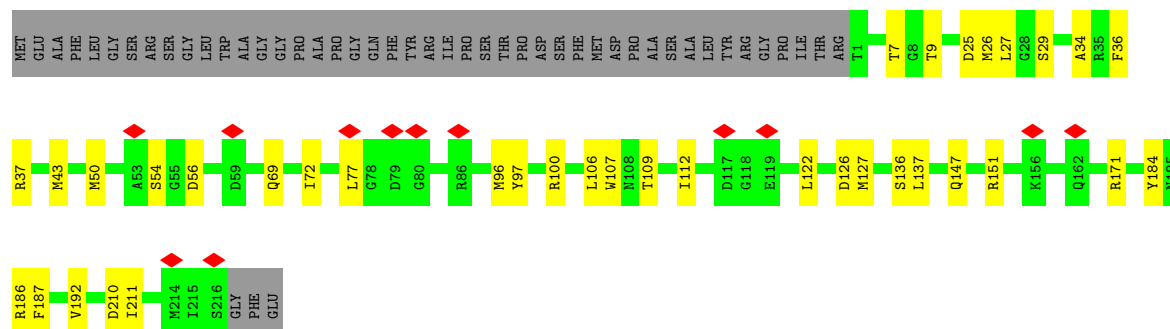




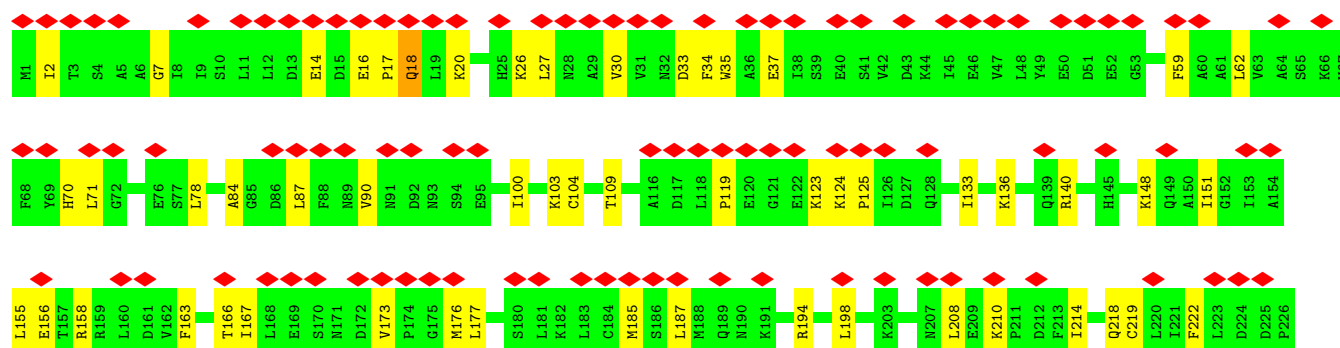
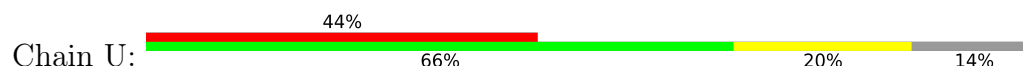
- Molecule 20: Proteasome subunit beta type-4

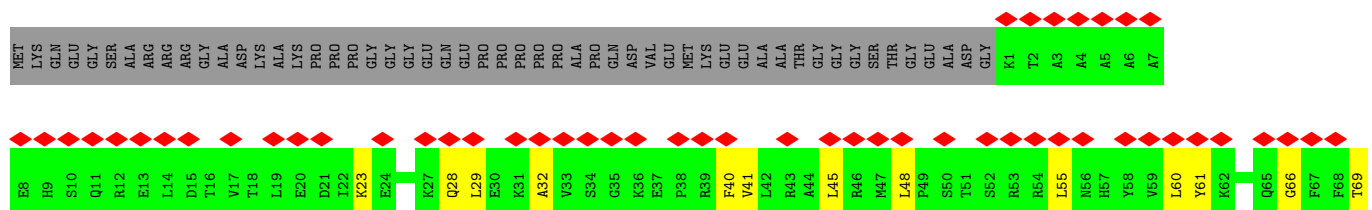
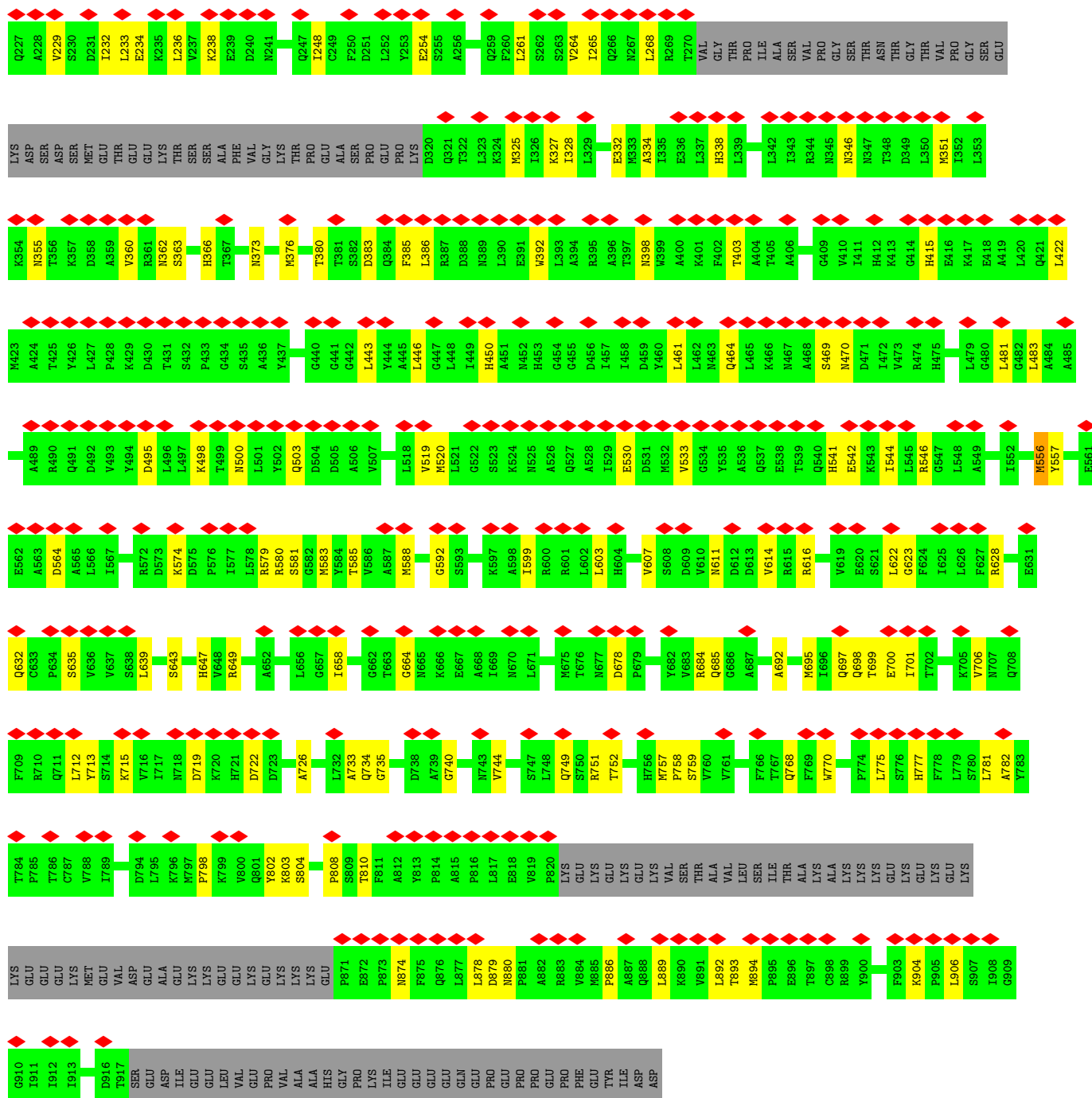


- Molecule 20: Proteasome subunit beta type-4

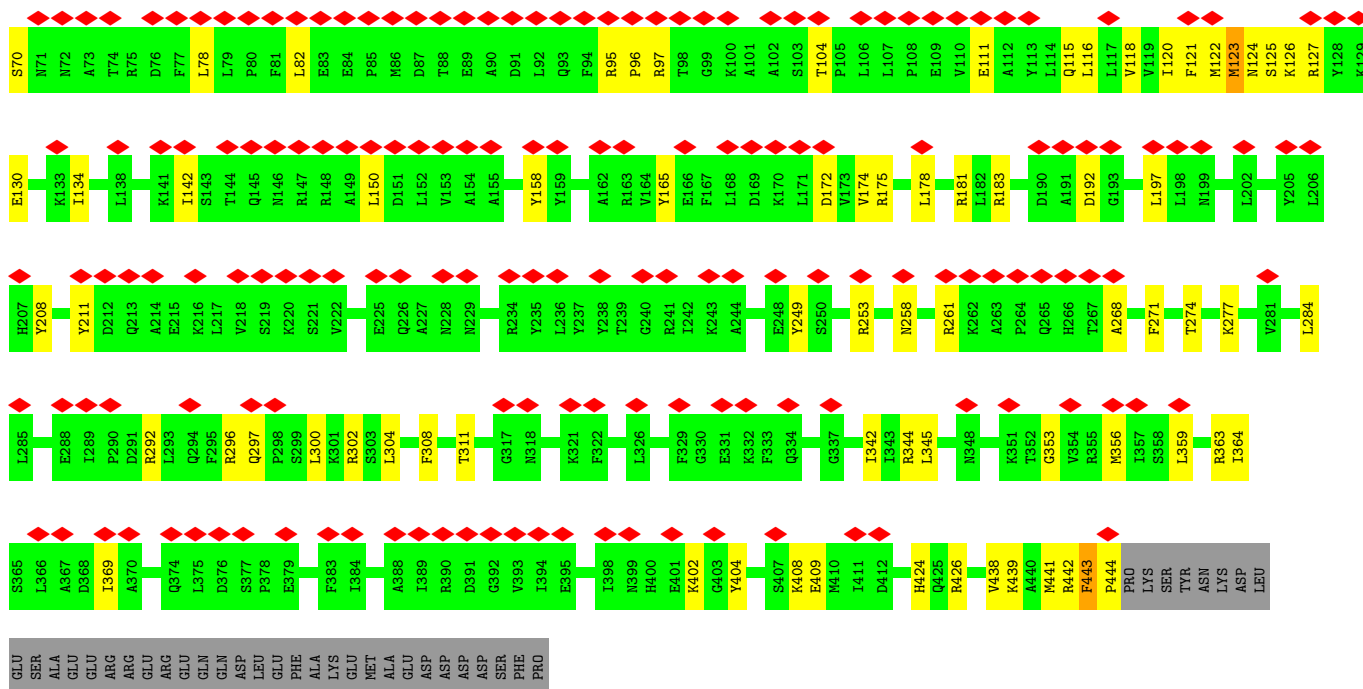


- Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

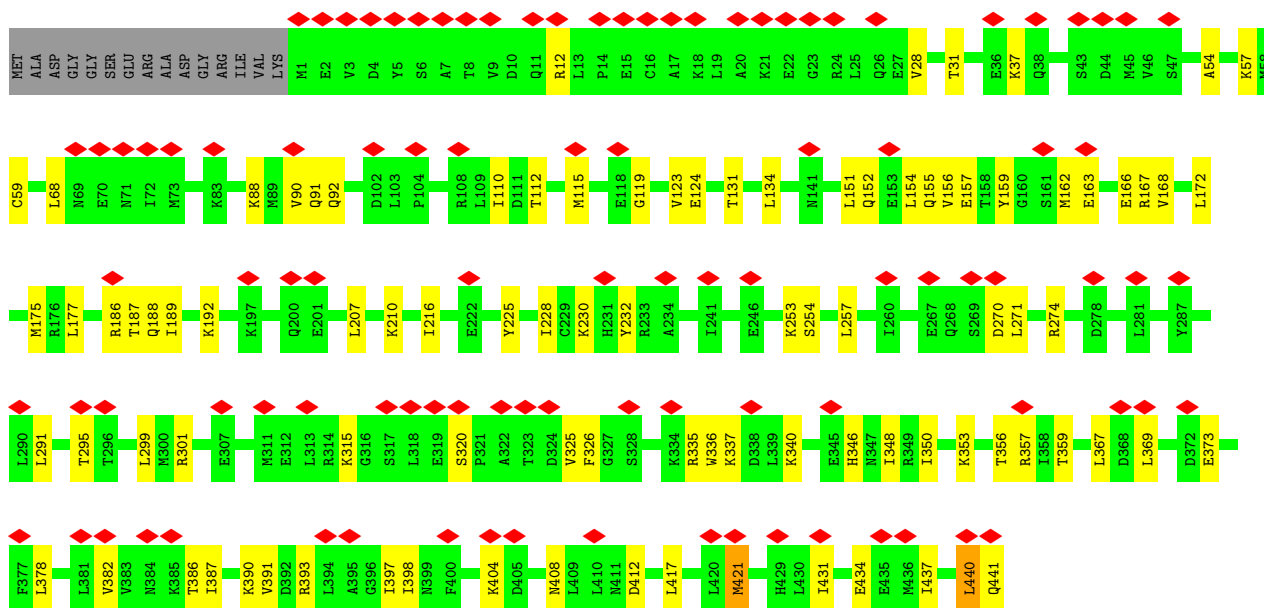
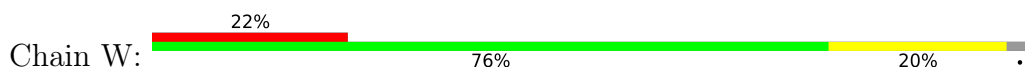




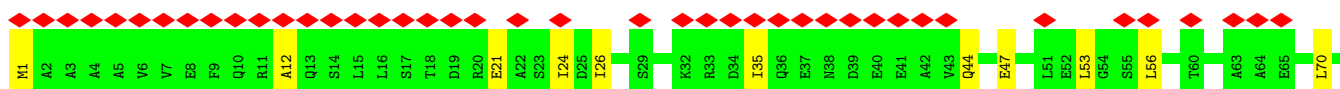
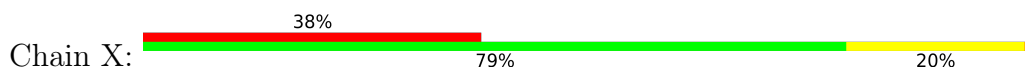


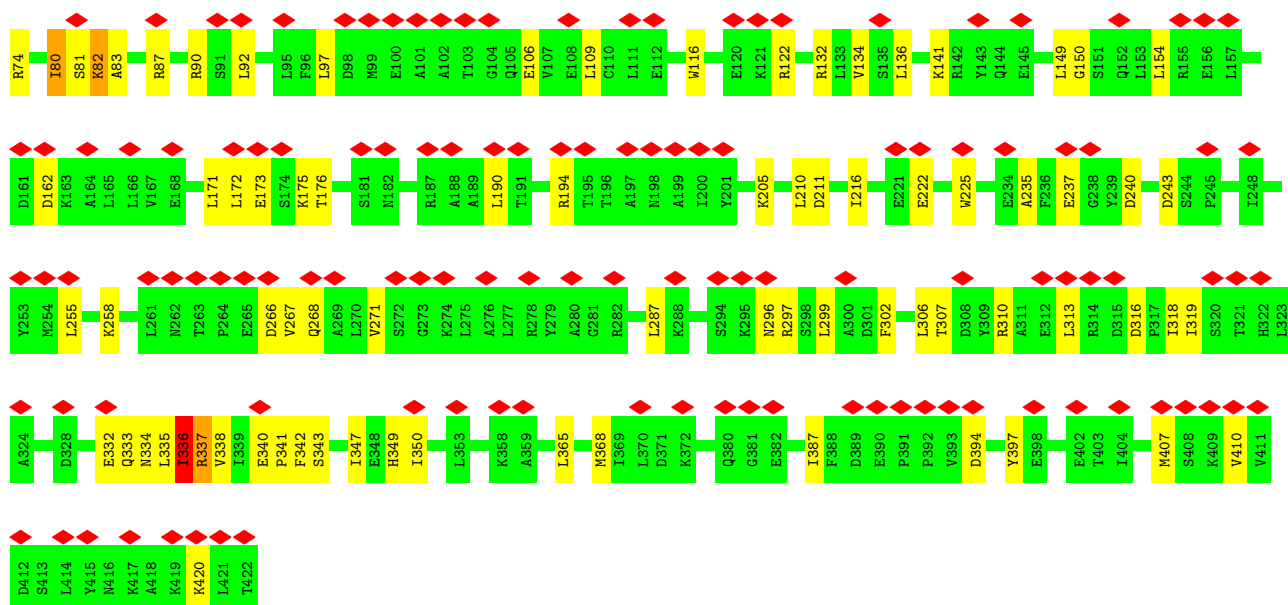


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

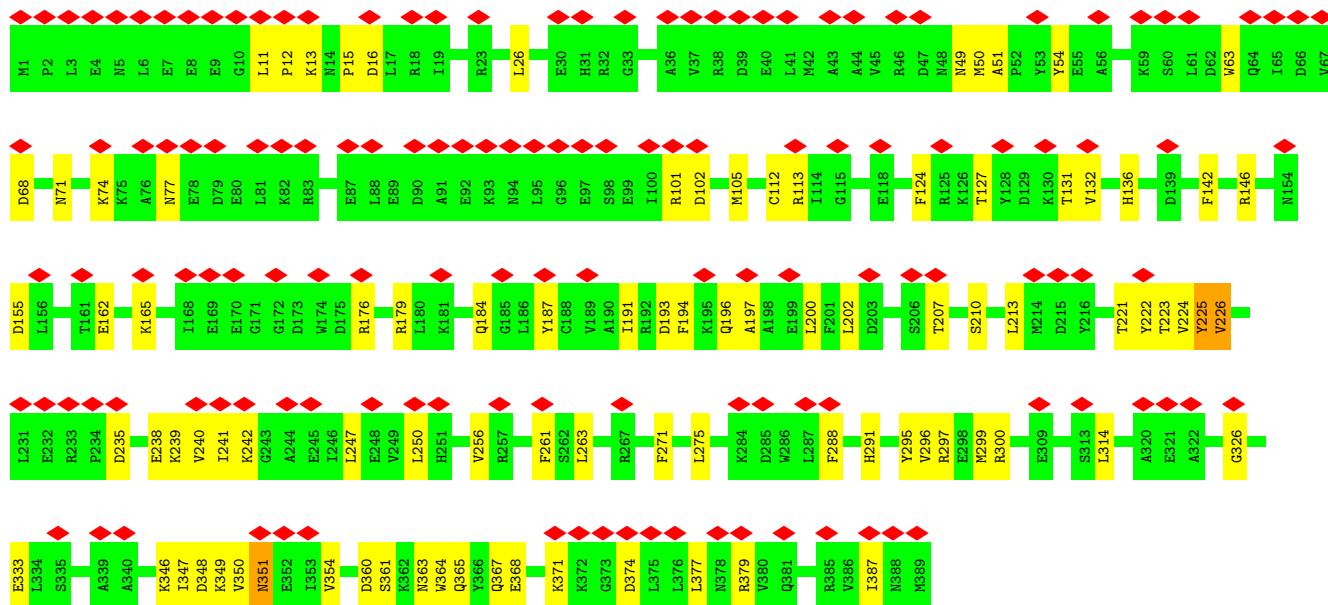
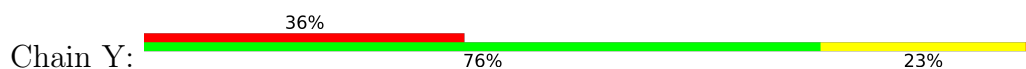


• Molecule 24: 26S proteasome non-ATPase regulatory subunit 11

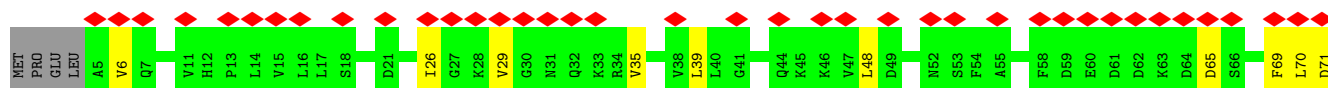
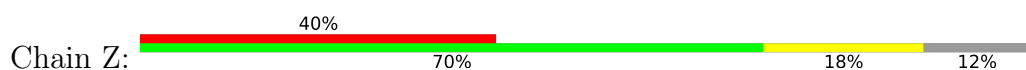


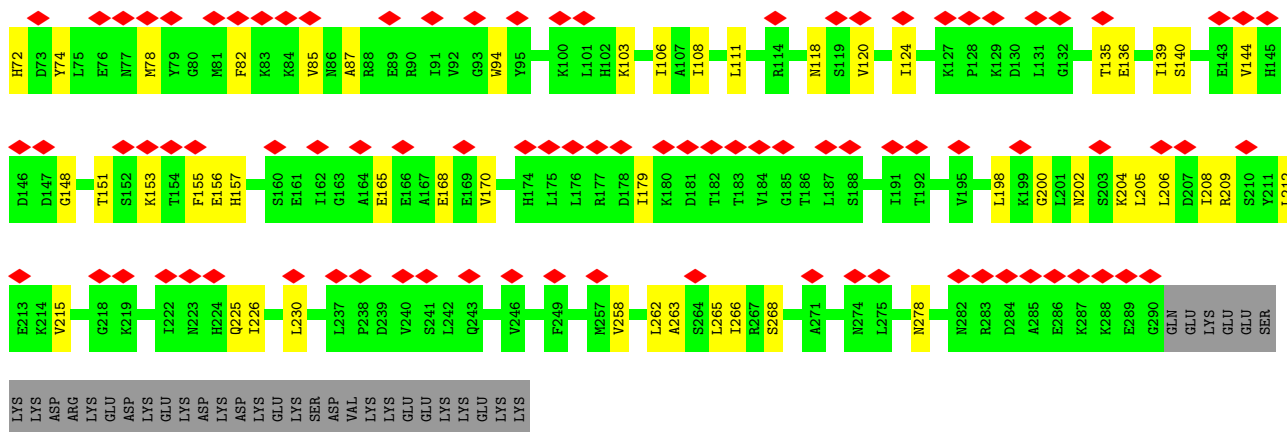


- Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

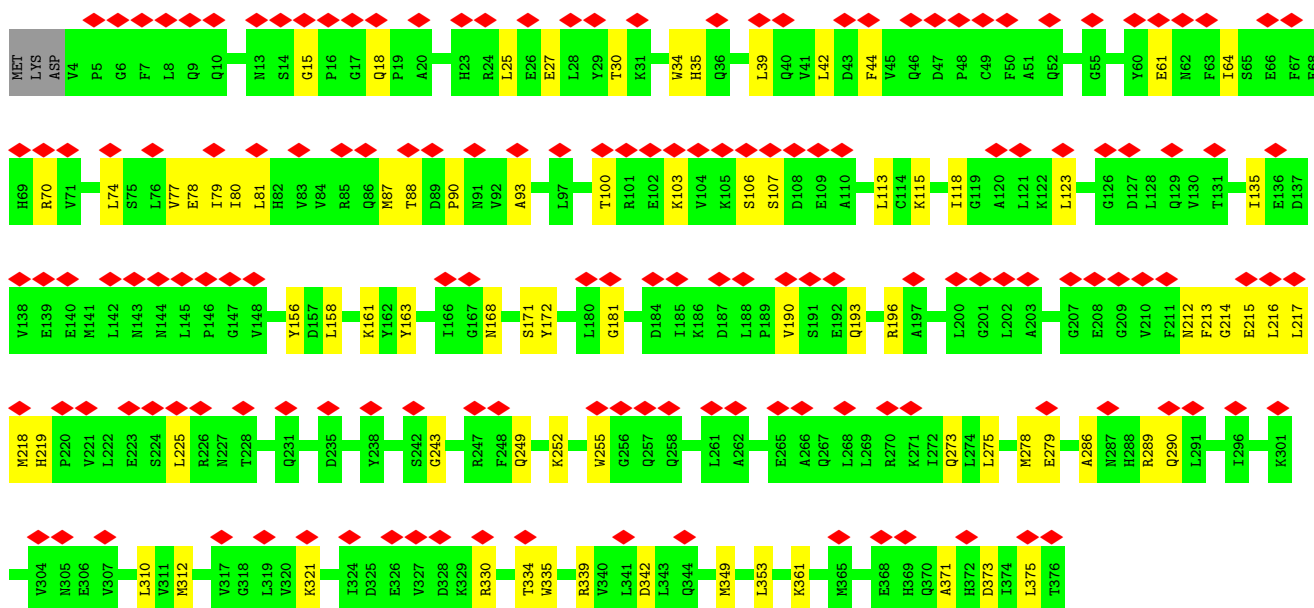
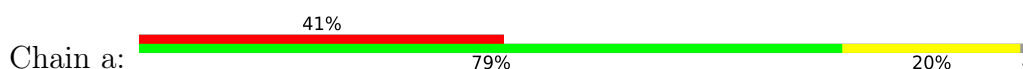


- Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

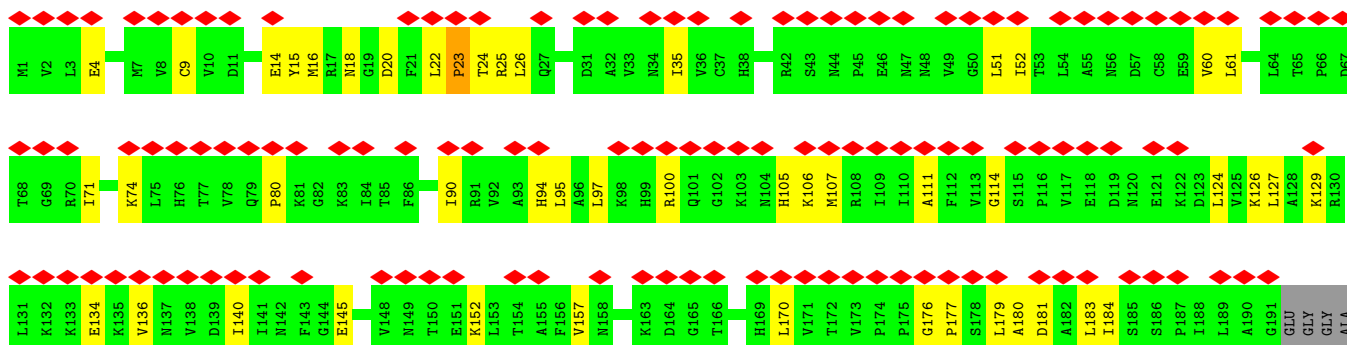
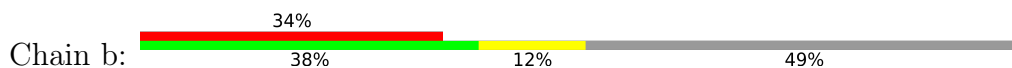




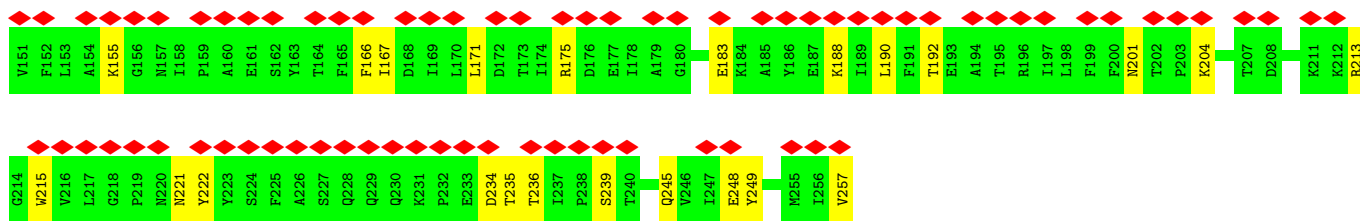
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13



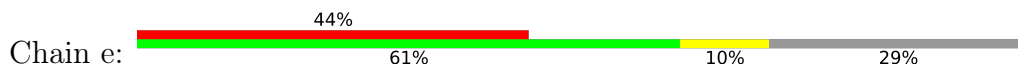
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4



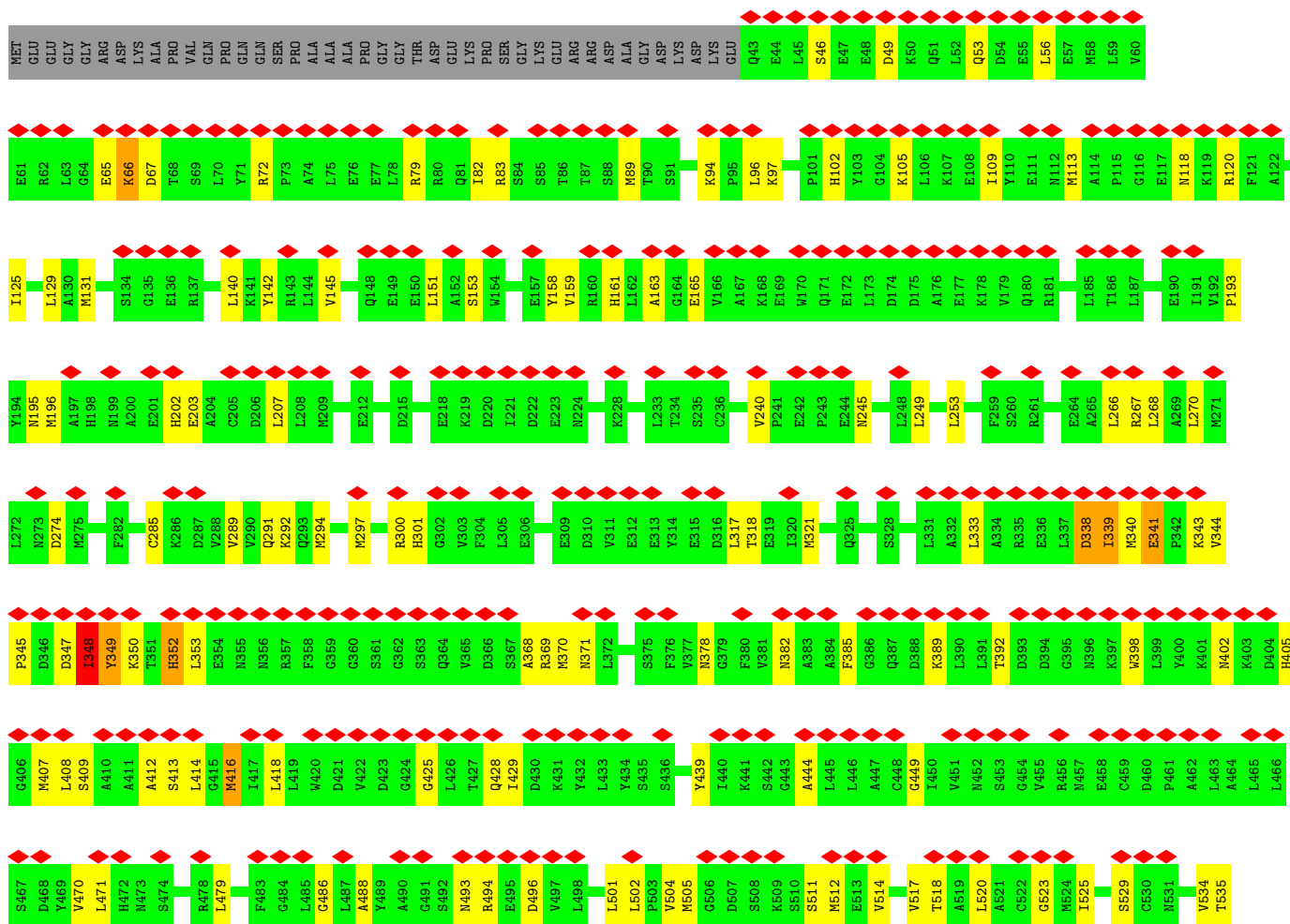


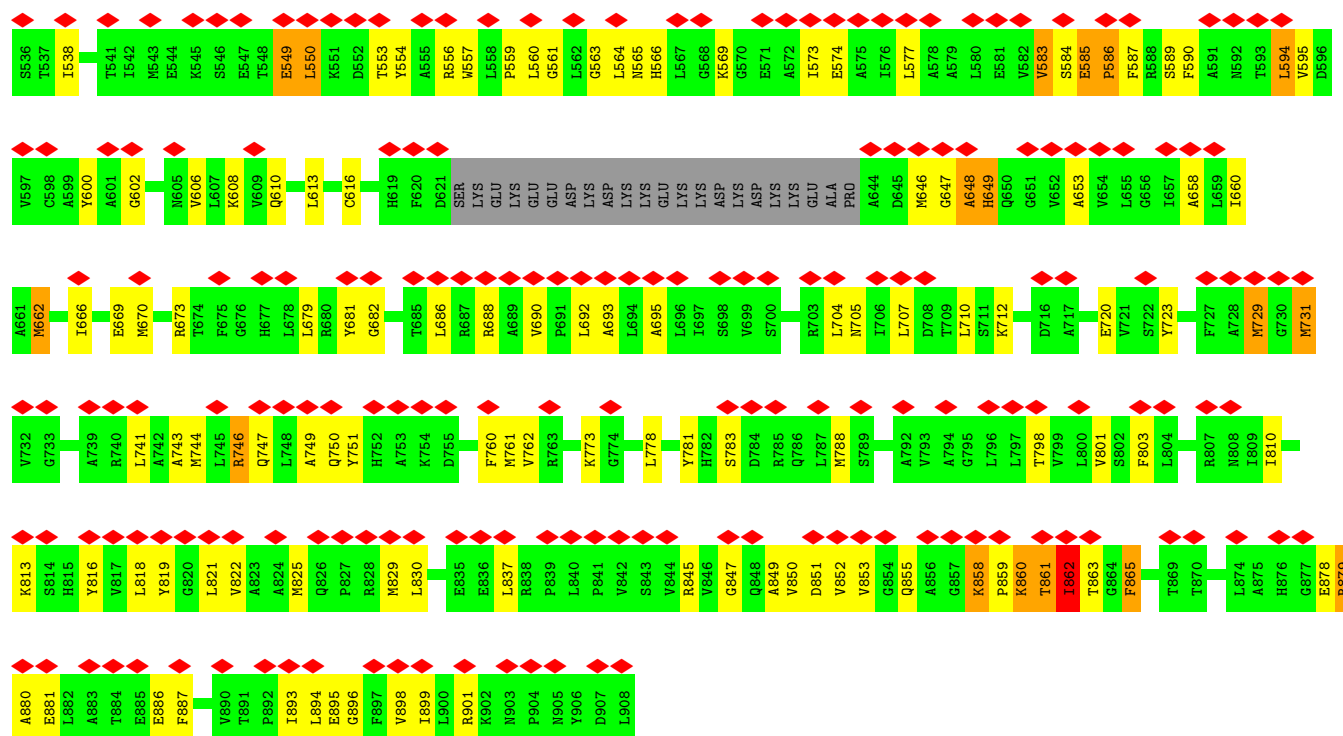


• Molecule 31: 26S proteasome complex subunit SEM1

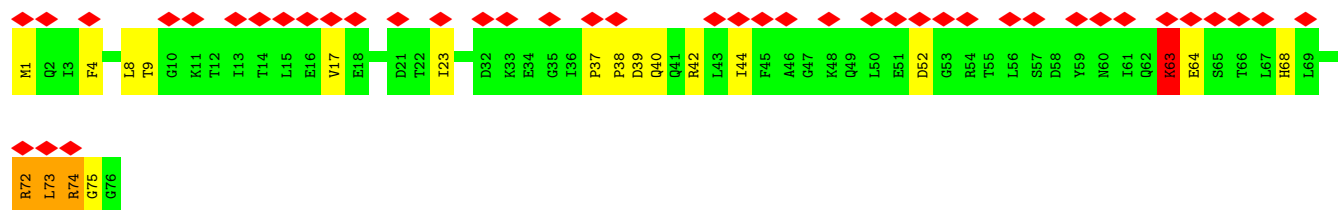
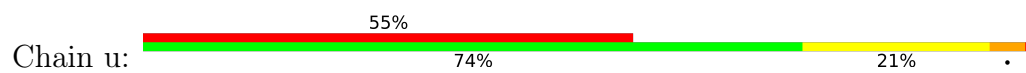


• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

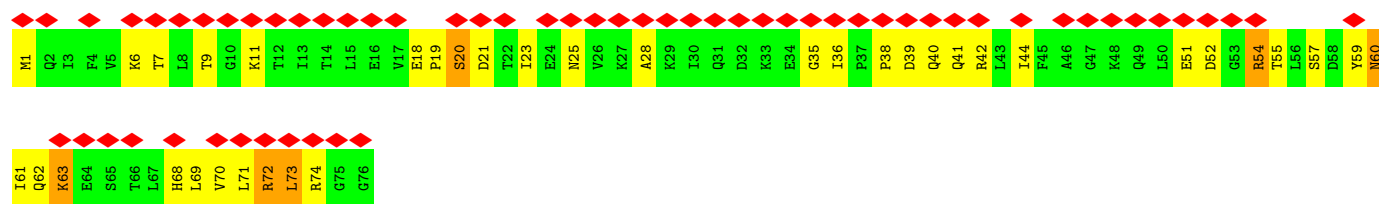
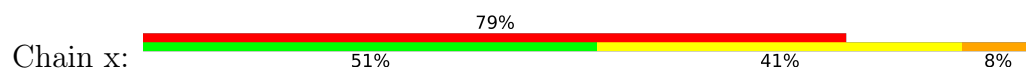




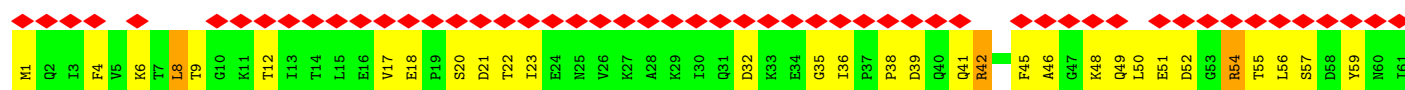
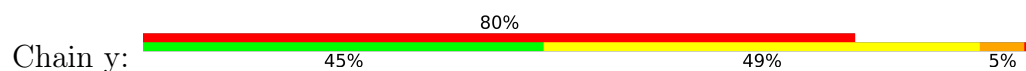
### • Molecule 33: Ubiquitin

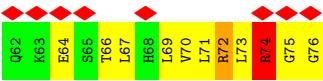


### • Molecule 33: Ubiquitin

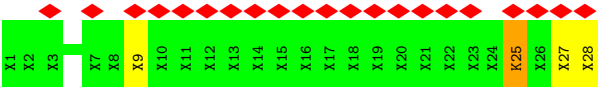
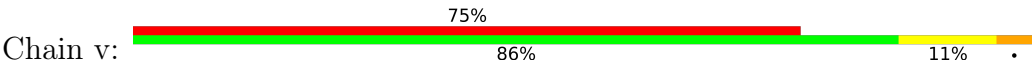


### • Molecule 33: Ubiquitin





● Molecule 34: Substrate



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9754	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	0.013	Depositor
Minimum map value	-0.005	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00452	Depositor
Map size (Å)	411.0, 411.0, 411.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.685, 0.685, 0.685	Depositor



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.23	0/3215	0.57	0/4340
2	B	0.26	0/3144	0.57	2/4245 (0.0%)
3	C	0.29	1/3017 (0.0%)	0.59	4/4058 (0.1%)
4	D	0.26	0/3089	0.54	1/4168 (0.0%)
5	E	0.26	0/3145	0.58	4/4233 (0.1%)
6	F	0.22	0/3292	0.53	0/4435
7	G	0.21	0/1923	0.44	0/2601
7	g	0.25	0/1901	0.52	3/2572 (0.1%)
8	H	0.21	0/1844	0.44	0/2499
8	h	0.24	0/1840	0.53	0/2495
9	I	0.19	0/1991	0.46	0/2685
9	i	0.23	0/1963	0.44	0/2650
10	J	0.27	0/1906	0.52	0/2573
10	j	0.24	0/1887	0.48	1/2553 (0.0%)
11	K	0.18	0/1804	0.43	0/2436
11	k	0.22	1/1841 (0.1%)	0.45	1/2486 (0.0%)
12	L	0.26	0/1901	0.47	0/2570
12	l	0.25	0/1911	0.45	2/2584 (0.1%)
13	M	0.20	0/1911	0.45	0/2573
13	m	0.18	0/1925	0.45	0/2592
14	N	0.23	0/1540	0.44	0/2085
14	n	0.19	0/1536	0.40	0/2080
15	O	0.20	0/1676	0.42	0/2271
15	o	0.21	0/1686	0.43	0/2282
16	P	0.26	0/1616	0.57	0/2180
16	p	0.38	1/1620 (0.1%)	0.59	4/2184 (0.2%)
17	Q	0.27	1/1621 (0.1%)	0.43	2/2194 (0.1%)
17	q	0.20	0/1621	0.39	0/2194
18	R	0.18	0/1590	0.44	0/2147
18	r	0.21	0/1590	0.43	0/2147
19	S	0.18	0/1671	0.42	0/2252
19	s	0.19	0/1684	0.44	0/2268

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.21	0/1716	0.46	0/2323
20	t	0.21	0/1720	0.45	0/2328
21	U	0.24	1/6488 (0.0%)	0.49	0/8782
22	V	0.20	0/3681	0.47	1/4969 (0.0%)
23	W	0.24	1/3644 (0.0%)	0.52	1/4901 (0.0%)
24	X	0.24	0/3381	0.51	1/4558 (0.0%)
25	Y	0.20	0/3261	0.49	1/4393 (0.0%)
26	Z	0.23	0/2324	0.56	0/3150
27	a	0.22	0/3053	0.54	0/4133
28	b	0.23	0/1478	0.53	0/2001
29	c	0.27	0/2302	0.60	0/3110
30	d	0.25	0/2162	0.59	0/2919
31	e	0.18	0/437	0.48	0/595
32	f	0.45	3/6640 (0.0%)	0.81	19/8988 (0.2%)
33	u	0.19	0/607	0.43	1/816 (0.1%)
33	x	0.61	0/607	1.01	0/816
33	y	0.54	0/607	1.00	0/816
34	v	0.02	0/8	0.05	0/8
All	All	0.26	9/109017 (0.0%)	0.53	48/147238 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	p	45	MET	SD-CE	-7.65	1.60	1.79
17	Q	69	MET	SD-CE	-5.80	1.65	1.79
32	f	729	MET	SD-CE	-5.66	1.65	1.79
11	k	59	MET	SD-CE	-5.62	1.65	1.79
21	U	556	MET	SD-CE	-5.51	1.65	1.79
3	C	248	MET	SD-CE	-5.42	1.66	1.79
32	f	731	MET	SD-CE	-5.32	1.66	1.79
32	f	594	LEU	CG-CD2	-5.20	1.35	1.52
23	W	421	MET	SD-CE	-5.06	1.66	1.79

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	731	MET	CG-SD-CE	-14.79	68.36	100.90
3	C	248	MET	CG-SD-CE	-9.68	79.61	100.90
23	W	421	MET	CG-SD-CE	-9.16	80.75	100.90
32	f	550	LEU	CB-CG-CD1	-9.03	83.61	110.70
32	f	865	PHE	N-CA-C	8.57	122.70	108.73
16	p	45	MET	CB-CG-SD	-8.12	88.35	112.70

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	f	416	MET	CG-SD-CE	-7.72	83.91	100.90
32	f	662	MET	CG-SD-CE	-7.28	84.89	100.90
32	f	647	GLY	CA-C-N	7.26	130.33	120.38
32	f	647	GLY	C-N-CA	7.26	130.33	120.38
32	f	648	ALA	CB-CA-C	-7.18	98.47	110.68
17	Q	69	MET	CB-CG-SD	-7.16	91.23	112.70
32	f	729	MET	CG-SD-CE	-6.75	86.05	100.90
3	C	237	MET	CB-CG-SD	6.64	132.61	112.70
2	B	72	LEU	N-CA-C	-6.58	104.35	112.38
5	E	264	MET	CG-SD-CE	-6.54	86.52	100.90
32	f	89	MET	CA-C-N	6.50	137.95	126.45
32	f	89	MET	C-N-CA	6.50	137.95	126.45
11	k	59	MET	CG-SD-CE	-6.33	86.98	100.90
12	l	159	MET	CG-SD-CE	-6.16	87.36	100.90
16	p	34	MET	CG-SD-CE	-5.99	87.72	100.90
12	l	88	MET	CG-SD-CE	-5.86	88.02	100.90
32	f	879	ARG	CB-CA-C	5.85	119.39	109.50
24	X	340	GLU	N-CA-C	5.82	121.54	113.45
32	f	352	HIS	N-CA-C	-5.81	104.86	111.07
16	p	67	LEU	CD1-CG-CD2	-5.81	98.02	110.80
7	g	113	MET	CG-SD-CE	-5.74	88.27	100.90
32	f	583	VAL	CA-C-N	5.69	132.41	121.54
32	f	583	VAL	C-N-CA	5.69	132.41	121.54
4	D	125	LYS	N-CA-C	5.53	122.04	109.81
7	g	210	PHE	CA-C-N	5.52	132.74	121.48
7	g	210	PHE	C-N-CA	5.52	132.74	121.48
16	p	67	LEU	CB-CG-CD1	-5.51	94.16	110.70
32	f	549	GLU	CA-C-N	-5.49	111.41	121.52
32	f	549	GLU	C-N-CA	-5.49	111.41	121.52
2	B	49	LEU	CD1-CG-CD2	5.39	122.67	110.80
5	E	209	GLY	CA-C-N	5.30	131.67	121.54
5	E	209	GLY	C-N-CA	5.30	131.67	121.54
22	V	123	MET	CB-CG-SD	5.30	128.60	112.70
25	Y	225	TYR	N-CA-C	-5.22	107.57	114.04
17	Q	69	MET	CA-CB-CG	-5.18	103.73	114.10
32	f	729	MET	CB-CG-SD	-5.13	97.30	112.70
5	E	275	MET	CG-SD-CE	-5.11	89.66	100.90
10	j	114	LEU	CD1-CG-CD2	-5.10	99.57	110.80
32	f	649	HIS	N-CA-CB	-5.06	102.68	110.16
3	C	237	MET	N-CA-CB	5.05	118.63	110.40
33	u	63	LYS	N-CA-C	5.03	116.98	109.59
3	C	237	MET	CA-CB-CG	5.00	124.10	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	3164	0	3200	87	0
2	B	3099	0	3143	97	0
3	C	2978	0	3075	70	0
4	D	3039	0	3075	72	0
5	E	3097	0	3174	66	0
6	F	3251	0	3318	66	0
7	G	1889	0	1885	30	0
7	g	1867	0	1867	32	0
8	H	1805	0	1784	21	0
8	h	1801	0	1773	14	0
9	I	1958	0	1960	21	0
9	i	1933	0	1923	23	0
10	J	1880	0	1892	35	0
10	j	1861	0	1846	36	0
11	K	1777	0	1762	18	0
11	k	1813	0	1796	34	0
12	L	1866	0	1852	31	0
12	l	1876	0	1856	29	0
13	M	1876	0	1861	32	0
13	m	1890	0	1880	24	0
14	N	1514	0	1487	25	0
14	n	1510	0	1483	12	0
15	O	1649	0	1659	23	0
15	o	1659	0	1681	16	0
16	P	1587	0	1598	29	0
16	p	1591	0	1609	42	0
17	Q	1588	0	1584	26	0
17	q	1588	0	1584	21	0
18	R	1559	0	1523	26	0
18	r	1559	0	1523	16	0
19	S	1641	0	1639	19	0
19	s	1654	0	1656	21	0
20	T	1683	0	1662	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	t	1687	0	1666	29	0
21	U	6373	0	6409	124	0
22	V	3612	0	3685	64	0
23	W	3596	0	3716	71	0
24	X	3335	0	3435	72	0
25	Y	3202	0	3204	60	0
26	Z	2281	0	2312	49	0
27	a	2995	0	3012	50	0
28	b	1458	0	1505	35	0
29	c	2260	0	2276	63	0
30	d	2116	0	2146	35	0
31	e	425	0	331	6	0
32	f	6529	0	6541	278	0
33	u	601	0	627	36	0
33	x	601	0	627	94	0
33	y	601	0	629	115	0
34	v	143	0	46	3	0
35	A	31	0	12	3	0
35	D	31	0	12	0	0
35	F	31	0	12	5	0
36	A	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	B	27	0	12	3	0
37	E	27	0	12	4	0
38	c	1	0	0	0	0
All	All	107468	0	107837	1988	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 9.

All (1988) 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:x:63:LYS:NZ	33:y:76:GLY:C	1.67	1.48
33:u:4:PHE:CE2	33:u:64:GLU:HG2	1.58	1.38
33:x:60:ASN:CA	33:y:8:LEU:HD12	1.55	1.36
33:x:60:ASN:HA	33:y:8:LEU:CD1	1.54	1.36
1:A:360:ARG:CD	32:f:858:LYS:HD2	1.56	1.36
33:x:60:ASN:HB3	33:y:8:LEU:CB	1.56	1.33
32:f:862:ILE:CD1	32:f:879:ARG:HB3	1.59	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:57:SER:CB	33:y:73:LEU:HD12	1.66	1.26
3:C:90:HIS:CB	3:C:91:PRO:HD3	1.63	1.24
33:x:60:ASN:CB	33:y:8:LEU:HB2	1.67	1.24
3:C:90:HIS:HB3	3:C:91:PRO:CD	1.66	1.22
2:B:68:ILE:HA	32:f:670:MET:CE	1.73	1.18
32:f:862:ILE:HD11	32:f:879:ARG:CB	1.74	1.17
33:u:4:PHE:HE2	33:u:64:GLU:CG	1.59	1.14
1:A:360:ARG:HD3	32:f:858:LYS:CD	1.80	1.11
2:B:68:ILE:HA	32:f:670:MET:HE1	1.13	1.09
33:y:48:LYS:HG3	33:y:49:GLN:H	0.96	1.08
33:x:20:SER:HA	33:y:73:LEU:HD21	1.20	1.08
33:u:63:LYS:HE3	33:u:64:GLU:CB	1.85	1.07
7:g:21:ARG:HH11	7:g:21:ARG:CG	1.67	1.06
32:f:723:TYR:CG	32:f:761:MET:HE1	1.91	1.05
32:f:723:TYR:HB3	32:f:761:MET:CE	1.85	1.05
33:x:57:SER:HB2	33:y:73:LEU:HD12	1.05	1.04
32:f:723:TYR:HB3	32:f:761:MET:HE1	1.39	1.03
32:f:723:TYR:HA	32:f:761:MET:SD	1.97	1.03
33:x:20:SER:HA	33:y:73:LEU:CD2	1.87	1.03
33:u:63:LYS:HE3	33:u:64:GLU:HB2	1.37	1.02
7:g:21:ARG:HG2	7:g:21:ARG:NH1	1.65	1.02
33:x:60:ASN:CB	33:y:8:LEU:CD1	2.38	1.02
2:B:71:TYR:OH	32:f:606:VAL:HG12	1.59	1.01
33:x:20:SER:CA	33:y:73:LEU:HD21	1.91	1.01
33:x:60:ASN:CA	33:y:8:LEU:CD1	2.25	1.01
7:g:21:ARG:HH11	7:g:21:ARG:HG2	0.85	1.00
33:u:63:LYS:CE	33:u:64:GLU:HB3	1.90	1.00
3:C:90:HIS:HB3	3:C:91:PRO:HD3	1.00	1.00
32:f:862:ILE:HG13	32:f:881:GLU:OE2	1.61	1.00
3:C:90:HIS:CG	3:C:91:PRO:HD3	1.97	0.99
33:u:63:LYS:HE2	33:u:64:GLU:HB3	1.44	0.99
33:x:63:LYS:HZ2	33:y:76:GLY:C	1.44	0.98
33:y:48:LYS:HG3	33:y:49:GLN:N	1.73	0.97
32:f:723:TYR:CB	32:f:761:MET:HE1	1.94	0.96
33:x:57:SER:HB2	33:y:73:LEU:CD1	1.94	0.96
33:x:57:SER:OG	33:y:73:LEU:HA	1.65	0.96
32:f:585:GLU:HB2	32:f:586:PRO:HD2	1.44	0.96
33:x:60:ASN:HB3	33:y:8:LEU:CD1	1.94	0.96
33:u:64:GLU:O	33:u:64:GLU:CD	2.08	0.95
33:y:48:LYS:CG	33:y:49:GLN:H	1.78	0.95
28:b:22:LEU:HB2	28:b:23:PRO:HD3	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:57:SER:CB	33:y:73:LEU:CD1	2.44	0.94
33:x:57:SER:CB	33:y:73:LEU:HA	1.99	0.93
33:x:19:PRO:HB2	33:y:74:ARG:H	1.34	0.93
33:x:19:PRO:C	33:y:73:LEU:HD11	1.93	0.93
33:u:42:ARG:HH12	33:u:72:ARG:HG3	1.31	0.92
2:B:82:GLN:HG2	32:f:681:TYR:CG	2.04	0.92
33:y:6:LYS:NZ	33:y:12:THR:HB	1.84	0.92
33:x:60:ASN:CB	33:y:8:LEU:HD12	2.00	0.92
23:W:326:PHE:HE1	23:W:336:TRP:HA	1.33	0.91
33:u:4:PHE:HE2	33:u:64:GLU:HG2	0.77	0.91
4:D:127:ASN:HB3	4:D:252:ARG:HH11	1.33	0.91
33:y:73:LEU:O	33:y:74:ARG:HB2	1.68	0.91
33:x:63:LYS:CE	33:y:76:GLY:C	2.43	0.90
33:y:6:LYS:HG2	33:y:66:THR:CG2	2.01	0.90
33:x:60:ASN:HA	33:y:8:LEU:HD12	0.91	0.89
33:u:63:LYS:CE	33:u:64:GLU:CB	2.47	0.89
33:x:19:PRO:HG2	33:y:74:ARG:HA	1.51	0.89
32:f:855:GLN:HE22	32:f:861:THR:CG2	1.84	0.89
32:f:862:ILE:HD11	32:f:879:ARG:HB3	0.92	0.89
33:x:73:LEU:H	33:x:73:LEU:HD23	1.39	0.88
2:B:71:TYR:OH	32:f:606:VAL:CG1	2.21	0.88
32:f:339:ILE:HG13	32:f:773:LYS:HD3	1.55	0.88
7:g:20:GLY:HA3	8:h:28:ALA:HB2	1.56	0.88
33:x:19:PRO:O	33:y:73:LEU:HD11	1.73	0.88
29:c:54:MET:HE1	33:u:75:GLY:N	1.89	0.88
2:B:71:TYR:OH	32:f:606:VAL:CB	2.22	0.87
32:f:550:LEU:HD21	32:f:586:PRO:HB2	1.55	0.87
5:E:264:MET:HE1	5:E:275:MET:HE3	1.55	0.86
25:Y:222:TYR:O	25:Y:226:VAL:HG12	1.75	0.86
33:y:6:LYS:HG2	33:y:66:THR:HG23	1.57	0.86
33:u:42:ARG:NH1	33:u:72:ARG:HG3	1.89	0.86
6:F:175:MET:HE1	6:F:251:LEU:HB2	1.58	0.86
1:A:360:ARG:HD3	32:f:858:LYS:HD2	0.87	0.86
33:y:8:LEU:CD2	33:y:70:VAL:HA	2.06	0.86
32:f:852:VAL:HG21	32:f:859:PRO:HB3	1.55	0.85
2:B:71:TYR:HH	32:f:606:VAL:HG12	1.39	0.85
24:X:47:GLU:OE2	24:X:80:ILE:HD13	1.77	0.85
24:X:82:LYS:O	24:X:82:LYS:HD2	1.77	0.85
32:f:723:TYR:CA	32:f:761:MET:SD	2.65	0.84
2:B:68:ILE:CA	32:f:670:MET:HE1	2.03	0.84
33:x:20:SER:HA	33:y:73:LEU:HD11	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:60:ASN:HB3	33:y:8:LEU:CG	2.08	0.84
33:x:60:ASN:HB3	33:y:8:LEU:HB2	0.84	0.83
32:f:289:VAL:HG21	32:f:901:ARG:HD3	1.57	0.83
33:x:63:LYS:CE	33:x:63:LYS:H	1.92	0.83
7:g:20:GLY:CA	8:h:28:ALA:HB2	2.09	0.82
33:y:6:LYS:CG	33:y:66:THR:CG2	2.58	0.81
32:f:850:VAL:HB	32:f:861:THR:HB	1.62	0.80
32:f:723:TYR:CB	32:f:761:MET:CE	2.55	0.80
33:x:20:SER:CA	33:y:73:LEU:HD11	2.12	0.80
33:x:20:SER:HA	33:y:73:LEU:CG	2.12	0.80
32:f:855:GLN:HE22	32:f:861:THR:HG22	1.46	0.79
33:x:57:SER:HB3	33:y:73:LEU:CD1	2.11	0.79
14:N:17:ASP:HB3	14:N:164:MET:HE1	1.64	0.79
3:C:90:HIS:CB	3:C:91:PRO:CD	2.38	0.78
33:x:20:SER:HA	33:y:73:LEU:CD1	2.13	0.78
1:A:360:ARG:HD3	32:f:858:LYS:HB2	1.65	0.78
33:y:6:LYS:HZ2	33:y:12:THR:HB	1.47	0.78
29:c:192:LEU:HA	29:c:196:LEU:HB2	1.64	0.77
24:X:332:GLU:O	24:X:336:ILE:HG12	1.83	0.77
6:F:438:TYR:HE1	12:L:77:LEU:HD22	1.49	0.77
32:f:412:ALA:CB	32:f:819:TYR:CE2	2.67	0.77
33:x:63:LYS:H	33:x:63:LYS:HE3	1.48	0.77
1:A:360:ARG:CD	32:f:858:LYS:CD	2.52	0.76
33:x:60:ASN:CB	33:y:8:LEU:HD13	2.15	0.76
33:u:64:GLU:O	33:u:64:GLU:OE1	2.03	0.76
21:U:700:GLU:H	21:U:706:VAL:HG21	1.51	0.76
32:f:583:VAL:HG12	32:f:584:SER:H	1.49	0.76
7:g:113:MET:HE1	15:o:70:THR:HA	1.68	0.76
4:D:127:ASN:HB3	4:D:252:ARG:NH1	2.00	0.75
3:C:227:GLY:HA2	3:C:230:MET:HE2	1.69	0.75
32:f:412:ALA:HB1	32:f:819:TYR:CE2	2.22	0.74
33:x:57:SER:HB3	33:y:73:LEU:HD12	1.65	0.74
32:f:723:TYR:CD1	32:f:761:MET:SD	2.80	0.74
12:L:166:GLN:HA	12:L:169:ARG:HD3	1.69	0.74
33:x:62:GLN:HB3	33:y:9:THR:HA	1.69	0.74
33:x:59:TYR:C	33:x:60:ASN:OD1	2.30	0.74
21:U:34:PHE:O	21:U:37:GLU:HG2	1.88	0.74
32:f:862:ILE:HD11	32:f:879:ARG:CG	2.18	0.74
33:x:19:PRO:HB2	33:y:74:ARG:N	2.03	0.73
29:c:54:MET:HE1	33:u:74:ARG:C	2.13	0.73
24:X:297:ARG:HB2	24:X:337:ARG:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:343:LYS:HG3	32:f:773:LYS:HE2	1.70	0.73
2:B:49:LEU:HD21	32:f:673:ARG:HD3	1.71	0.73
2:B:71:TYR:OH	32:f:606:VAL:HA	1.88	0.73
18:R:139:MET:O	18:R:143:TYR:HB2	1.89	0.73
29:c:125:VAL:HG22	34:v:28:UNK:O	1.89	0.73
23:W:326:PHE:HE1	23:W:336:TRP:CA	2.01	0.73
32:f:343:LYS:HE3	32:f:773:LYS:HE2	1.71	0.73
33:y:8:LEU:HD22	33:y:70:VAL:HA	1.71	0.73
24:X:24:ILE:HG12	24:X:56:LEU:HD13	1.71	0.72
32:f:413:SER:N	32:f:819:TYR:OH	2.21	0.72
32:f:723:TYR:CB	32:f:761:MET:SD	2.78	0.72
20:t:50:MET:HE1	20:t:192:VAL:HB	1.71	0.72
1:A:253:GLY:HA2	1:A:256:MET:HE3	1.70	0.72
32:f:292:LYS:HD3	32:f:837:LEU:HD11	1.72	0.72
32:f:710:LEU:HB2	32:f:729:MET:HE2	1.71	0.72
33:x:1:MET:SD	33:y:76:GLY:O	2.47	0.72
1:A:360:ARG:CG	32:f:858:LYS:HD2	2.19	0.72
1:A:55:LEU:HD23	2:B:72:LEU:HB3	1.72	0.71
9:i:53:HIS:HD2	9:i:55:LEU:H	1.37	0.71
20:T:188:GLN:HG3	20:T:201:GLY:HA3	1.73	0.71
32:f:847:GLY:C	32:f:878:GLU:OE1	2.34	0.71
9:I:143:TYR:HB2	9:I:146:GLN:HE21	1.55	0.71
18:R:177:TYR:CE1	18:R:186:ARG:HG2	2.25	0.71
30:d:23:LEU:HG	30:d:27:LYS:HZ3	1.56	0.71
12:L:225:ASP:H	12:L:228:ASP:HB2	1.56	0.70
10:J:50:VAL:HB	10:J:54:GLN:HB2	1.72	0.70
10:j:68:ASN:HA	10:j:211:MET:HE1	1.74	0.70
18:R:177:TYR:HE1	18:R:186:ARG:HG2	1.57	0.70
32:f:343:LYS:O	32:f:382:ASN:ND2	2.24	0.70
2:B:71:TYR:OH	32:f:606:VAL:CA	2.40	0.70
21:U:398:ASN:HB2	29:c:174:PRO:HB3	1.73	0.70
24:X:74:ARG:HH22	24:X:116:TRP:HB2	1.56	0.70
27:a:286:ALA:HA	27:a:289:ARG:HE	1.57	0.70
29:c:257:LYS:HA	29:c:260:GLU:HG2	1.74	0.70
32:f:385:PHE:CE2	32:f:773:LYS:HE3	2.27	0.70
32:f:520:LEU:HD21	32:f:798:THR:HG23	1.73	0.70
33:y:73:LEU:O	33:y:74:ARG:CB	2.40	0.70
9:i:53:HIS:CD2	9:i:55:LEU:H	2.10	0.69
33:y:71:LEU:HD12	33:y:71:LEU:N	2.06	0.69
10:J:226:GLU:HA	10:J:229:VAL:HG12	1.75	0.69
32:f:102:HIS:HB3	32:f:105:LYS:HE3	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:297:ARG:CB	24:X:337:ARG:HG3	2.22	0.69
29:c:125:VAL:HG11	33:u:74:ARG:HD2	1.73	0.69
3:C:244:SER:H	3:C:289:ILE:HD13	1.57	0.69
33:x:60:ASN:CA	33:y:8:LEU:HD13	2.22	0.69
2:B:271:PHE:HD2	2:B:315:GLN:HG3	1.58	0.69
21:U:185:MET:HE1	21:U:194:ARG:HH11	1.57	0.69
32:f:855:GLN:NE2	32:f:861:THR:CG2	2.54	0.69
1:A:38:GLN:HB3	1:A:42:SER:HB3	1.75	0.68
10:j:156:TRP:CH2	11:k:59:MET:HE1	2.28	0.68
26:Z:212:LEU:HD11	27:a:349:MET:HE3	1.75	0.68
2:B:68:ILE:HA	32:f:670:MET:HE2	1.73	0.68
21:U:208:LEU:HD23	21:U:210:LYS:H	1.57	0.68
25:Y:238:GLU:HG3	25:Y:239:LYS:HG3	1.74	0.68
2:B:230:THR:HG21	2:B:353:PHE:HB3	1.75	0.68
32:f:723:TYR:CG	32:f:761:MET:CE	2.71	0.68
32:f:131:MET:HE1	32:f:161:HIS:HB3	1.76	0.68
33:x:60:ASN:OD1	33:x:60:ASN:N	2.27	0.68
4:D:163:MET:HG3	4:D:165:ALA:H	1.59	0.67
24:X:106:GLU:HB3	24:X:136:LEU:HD21	1.75	0.67
23:W:326:PHE:CE1	23:W:336:TRP:HA	2.24	0.67
33:x:20:SER:N	33:y:73:LEU:HD11	2.09	0.67
32:f:852:VAL:HG21	32:f:859:PRO:CB	2.25	0.67
1:A:231:ASN:HD21	32:f:865:PHE:HE2	1.40	0.67
4:D:99:ASN:HA	4:D:115:ILE:HG12	1.76	0.67
32:f:585:GLU:H	32:f:585:GLU:CD	2.03	0.67
32:f:585:GLU:CB	32:f:586:PRO:HD2	2.23	0.67
21:U:373:ASN:HD22	21:U:385:PHE:HB3	1.59	0.67
25:Y:15:PRO:HD2	25:Y:146:ARG:HB3	1.77	0.67
33:x:38:PRO:C	33:x:40:GLN:H	2.04	0.66
23:W:172:LEU:HA	23:W:175:MET:HE3	1.77	0.66
32:f:412:ALA:HB3	32:f:819:TYR:CE2	2.30	0.66
3:C:352:PRO:HD2	3:C:391:MET:HE3	1.78	0.66
29:c:54:MET:CE	33:u:75:GLY:N	2.57	0.66
1:A:323:ARG:HH11	2:B:294:ARG:HE	1.43	0.66
20:t:96:MET:HE1	20:t:106:LEU:HB2	1.78	0.66
33:u:42:ARG:NH1	33:u:72:ARG:CG	2.59	0.66
26:Z:263:ALA:HB1	29:c:288:VAL:HG13	1.77	0.66
33:x:20:SER:CB	33:y:73:LEU:HD21	2.26	0.66
3:C:243:PRO:HB3	3:C:288:ASN:HB2	1.75	0.66
30:d:24:GLY:HA2	30:d:27:LYS:HE2	1.78	0.66
33:x:60:ASN:CB	33:y:8:LEU:CB	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLU:HB3	1:A:406:GLU:HG2	1.79	0.65
12:L:93:LEU:HD21	19:S:70:ALA:HB1	1.78	0.65
32:f:318:THR:HA	32:f:321:MET:SD	2.36	0.65
3:C:74:GLY:HA2	3:C:89:VAL:O	1.96	0.65
22:V:32:ALA:HB2	22:V:40:PHE:HB2	1.77	0.65
4:D:248:ARG:HG2	4:D:295:GLN:HE22	1.62	0.65
2:B:287:ILE:HD13	2:B:329:MET:HE2	1.79	0.65
32:f:253:LEU:HB2	32:f:268:LEU:HD22	1.79	0.65
33:y:51:GLU:HB2	33:y:54:ARG:HD3	1.78	0.65
2:B:82:GLN:HG2	32:f:681:TYR:CD2	2.31	0.64
17:Q:25:ILE:HG22	17:Q:26:VAL:HG13	1.79	0.64
32:f:704:LEU:HD23	32:f:707:LEU:HD21	1.78	0.64
1:A:101:ILE:HA	1:A:113:ILE:HG12	1.77	0.64
5:E:182:LEU:HD22	37:E:401:ADP:H2'	1.80	0.64
23:W:382:VAL:HG11	24:X:341:PRO:HB3	1.80	0.64
33:y:42:ARG:CZ	33:y:72:ARG:HA	2.27	0.64
32:f:855:GLN:HE22	32:f:861:THR:HG21	1.60	0.64
21:U:530:GLU:CD	33:y:64:GLU:HB3	2.22	0.64
26:Z:29:VAL:O	33:y:48:LYS:NZ	2.22	0.64
32:f:560:LEU:HD11	32:f:801:VAL:HG11	1.79	0.64
2:B:68:ILE:O	2:B:72:LEU:HD23	1.97	0.64
22:V:402:LYS:HE2	22:V:404:TYR:HE1	1.63	0.64
2:B:51:LEU:HD13	2:B:51:LEU:N	2.13	0.64
19:S:169:ASP:HA	19:S:172:MET:HE3	1.79	0.64
13:m:204:VAL:HG13	13:m:205:LYS:HG2	1.79	0.64
5:E:171:LEU:HA	5:E:277:MET:HB2	1.79	0.64
22:V:402:LYS:HB2	22:V:404:TYR:HE1	1.63	0.64
29:c:86:ALA:HB2	33:u:73:LEU:HB3	1.80	0.64
32:f:416:MET:HE1	32:f:819:TYR:HE1	1.63	0.63
9:I:197:LEU:HA	9:I:200:THR:HG22	1.81	0.63
32:f:886:GLU:HG3	32:f:887:PHE:CD2	2.32	0.63
11:k:77:ALA:HB3	11:k:142:LEU:HB2	1.80	0.63
25:Y:221:THR:O	25:Y:225:TYR:CD2	2.52	0.63
28:b:157:VAL:HG21	28:b:170:LEU:HB2	1.80	0.63
11:k:236:GLU:HA	11:k:239:LYS:HE3	1.80	0.63
1:A:171:ASP:OD1	32:f:865:PHE:HE1	1.79	0.63
19:s:4:PRO:HB2	20:t:100:ARG:HH21	1.64	0.63
10:J:36:ARG:HA	10:J:41:VAL:HG12	1.80	0.63
22:V:29:LEU:HD23	22:V:41:VAL:HG12	1.80	0.63
32:f:662:MET:HE1	32:f:781:TYR:HE1	1.62	0.63
4:D:86:PRO:HA	5:E:80:VAL:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.80	0.63
23:W:369:LEU:HD13	23:W:373:GLU:HB3	1.80	0.63
28:b:24:THR:HG22	28:b:26:LEU:H	1.63	0.63
33:x:63:LYS:HE2	33:y:76:GLY:C	2.23	0.63
32:f:550:LEU:HD11	32:f:585:GLU:HG2	1.80	0.63
4:D:92:PHE:CE2	4:D:125:LYS:HD2	2.34	0.62
33:x:19:PRO:CG	33:y:74:ARG:HA	2.27	0.62
14:N:139:VAL:HG23	14:N:155:PHE:HZ	1.64	0.62
33:x:60:ASN:HD22	33:y:8:LEU:HB3	1.62	0.62
11:K:36:THR:HA	11:K:171:GLY:HA3	1.80	0.62
14:N:147:MET:HE3	14:N:151:GLU:HB3	1.81	0.62
32:f:549:GLU:HG3	32:f:587:PHE:CG	2.34	0.62
7:g:18:PRO:O	7:g:19:GLU:HB2	1.99	0.62
16:p:158:MET:HE1	16:p:162:HIS:HB2	1.79	0.62
20:t:27:LEU:HD11	20:t:34:ALA:HB1	1.81	0.62
15:O:50:ALA:HB2	16:P:129:CYS:HB2	1.81	0.62
33:x:19:PRO:HG2	33:y:74:ARG:CA	2.28	0.62
3:C:20:LEU:HD12	3:C:21:ARG:HG3	1.81	0.62
3:C:44:ARG:HG3	22:V:443:PHE:HE2	1.65	0.62
4:D:125:LYS:HG3	4:D:125:LYS:O	2.00	0.62
25:Y:210:SER:HB3	25:Y:213:LEU:HD23	1.81	0.62
20:t:27:LEU:HD22	20:t:184:TYR:HB2	1.80	0.62
10:J:208:LEU:HD22	10:J:220:LEU:HG	1.81	0.62
33:u:23:ILE:HB	33:u:52:ASP:HA	1.81	0.62
19:S:27:THR:HB	19:S:40:SER:H	1.65	0.62
23:W:348:ILE:HD11	23:W:367:LEU:HD11	1.81	0.62
32:f:557:TRP:HA	32:f:560:LEU:HD12	1.81	0.62
21:U:685:GLN:HB2	21:U:726:ALA:HA	1.82	0.62
28:b:35:ILE:HD12	28:b:184:ILE:HD13	1.80	0.62
2:B:223:ILE:HG13	2:B:347:ILE:HG21	1.82	0.62
1:A:38:GLN:HG3	1:A:42:SER:HB3	1.81	0.62
11:K:52:LYS:HG2	11:K:66:LYS:HZ1	1.64	0.62
21:U:90:VAL:HG11	21:U:140:ARG:HG3	1.81	0.62
26:Z:208:ILE:HG23	27:a:353:LEU:HD21	1.80	0.62
17:q:25:ILE:HG22	17:q:26:VAL:HG13	1.82	0.62
4:D:45:LYS:HG2	21:U:187:LEU:HD13	1.82	0.61
21:U:327:LYS:HE2	21:U:332:GLU:HB2	1.82	0.61
25:Y:361:SER:O	25:Y:365:GLN:NE2	2.33	0.61
33:y:6:LYS:HG3	33:y:66:THR:CG2	2.29	0.61
2:B:71:TYR:OH	32:f:606:VAL:HB	1.99	0.61
19:S:37:THR:HA	20:T:151:ARG:HH22	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:412:ALA:CB	32:f:819:TYR:CZ	2.83	0.61
11:k:36:THR:HA	11:k:171:GLY:HA3	1.82	0.61
23:W:112:THR:HA	23:W:115:MET:HE3	1.81	0.61
27:a:193:GLN:HB3	27:a:225:LEU:HD13	1.83	0.61
29:c:96:LEU:HD12	33:u:8:LEU:HD22	1.80	0.61
23:W:12:ARG:HH22	23:W:28:VAL:HG12	1.64	0.61
11:K:235:GLU:HA	11:K:238:ILE:HG22	1.83	0.61
13:M:35:THR:HA	13:M:166:GLY:HA3	1.83	0.61
16:p:50:TYR:HD2	16:p:190:ILE:HD11	1.65	0.61
32:f:862:ILE:HD13	32:f:879:ARG:HB3	1.76	0.61
1:A:411:GLU:OE1	1:A:415:LYS:NZ	2.32	0.61
20:T:25:ASP:OD1	20:T:41:ARG:NH2	2.33	0.61
21:U:798:PRO:O	21:U:880:ASN:ND2	2.34	0.61
32:f:343:LYS:HG3	32:f:773:LYS:CE	2.30	0.61
33:y:6:LYS:HZ3	33:y:12:THR:HB	1.64	0.61
25:Y:297:ARG:HA	25:Y:300:ARG:HD2	1.83	0.60
29:c:195:GLY:O	29:c:198:ARG:HB2	2.00	0.60
29:c:196:LEU:C	29:c:198:ARG:H	2.08	0.60
32:f:289:VAL:HA	32:f:292:LYS:HG2	1.83	0.60
1:A:309:PHE:H	6:F:238:ARG:HH21	1.49	0.60
2:B:373:THR:HB	2:B:413:LYS:HE3	1.83	0.60
4:D:320:ALA:O	4:D:326:ARG:NH1	2.34	0.60
4:D:92:PHE:HE2	4:D:125:LYS:HD2	1.64	0.60
6:F:304:ARG:O	6:F:308:ARG:NH1	2.34	0.60
13:M:80:LEU:H	13:M:133:CYS:HB3	1.67	0.60
11:k:73:HIS:ND1	11:k:146:VAL:O	2.34	0.60
6:F:438:TYR:CE1	12:L:77:LEU:HD22	2.35	0.60
28:b:25:ARG:NH1	28:b:114:GLY:O	2.34	0.60
19:s:8:ASN:ND2	19:s:31:GLU:OE2	2.34	0.60
28:b:26:LEU:HD11	28:b:80:PRO:HG3	1.83	0.60
15:o:206:LYS:HD3	16:p:161:ASP:HB3	1.82	0.60
33:x:19:PRO:C	33:y:73:LEU:CD1	2.73	0.60
21:U:808:PRO:HD3	21:U:874:ASN:HA	1.83	0.60
16:p:35:VAL:HG12	16:p:36:THR:HG23	1.83	0.60
20:T:44:ARG:NH2	20:T:47:ASN:OD1	2.34	0.60
22:V:297:GLN:HB2	22:V:300:LEU:HB3	1.83	0.60
32:f:566:HIS:HB3	32:f:569:LYS:HB2	1.83	0.60
21:U:802:TYR:HB2	21:U:878:LEU:HB2	1.84	0.60
2:B:68:ILE:HG22	2:B:72:LEU:HD23	1.82	0.60
2:B:229:GLY:HA2	37:B:501:ADP:H5'1	1.84	0.60
12:L:176:MET:HE1	13:M:56:LYS:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:166:ARG:NH2	14:n:140:ASP:OD2	2.34	0.60
32:f:688:ARG:HG2	32:f:720:GLU:HB2	1.83	0.60
7:G:86:ASP:OD1	13:M:120:HIS:NE2	2.33	0.60
32:f:412:ALA:HB3	32:f:819:TYR:OH	2.02	0.60
14:n:44:CYS:HB2	14:n:99:ILE:HB	1.83	0.60
33:x:63:LYS:HE2	33:y:76:GLY:O	2.01	0.60
1:A:72:LEU:HD11	2:B:103:ARG:HH22	1.67	0.59
5:E:161:ARG:NH2	23:W:124:GLU:OE2	2.35	0.59
14:N:4:MET:HE1	14:N:156:THR:HA	1.82	0.59
21:U:500:ASN:OD1	21:U:503:GLN:NE2	2.35	0.59
23:W:337:LYS:HA	23:W:340:LYS:HZ3	1.67	0.59
25:Y:13:LYS:HD3	25:Y:16:ASP:HB2	1.84	0.59
11:k:56:SER:HB3	11:k:59:MET:HE3	1.83	0.59
33:x:19:PRO:CG	33:y:74:ARG:C	2.74	0.59
33:y:6:LYS:HG3	33:y:66:THR:HG21	1.83	0.59
33:y:45:PHE:CG	33:y:46:ALA:N	2.70	0.59
2:B:82:GLN:CG	32:f:681:TYR:CD1	2.85	0.59
24:X:82:LYS:HD2	24:X:82:LYS:C	2.23	0.59
29:c:30:GLN:HB3	29:c:66:THR:HG22	1.84	0.59
33:y:8:LEU:HD23	33:y:69:LEU:O	2.02	0.59
10:J:38:ARG:HE	10:J:182:GLU:HA	1.67	0.59
22:V:292:ARG:HB3	22:V:296:ARG:HH21	1.66	0.59
14:n:110:GLN:OE1	14:n:122:ARG:NH1	2.35	0.59
7:G:41:ALA:HB3	7:G:166:THR:HB	1.84	0.59
18:R:39:PRO:HA	18:R:184:TRP:HE1	1.67	0.59
16:p:65:GLN:OE1	17:q:86:ARG:NH2	2.36	0.59
3:C:44:ARG:HB2	22:V:442:ARG:HH12	1.67	0.59
23:W:337:LYS:HD3	23:W:340:LYS:HZ3	1.68	0.59
24:X:53:LEU:HD12	24:X:56:LEU:HD11	1.85	0.59
32:f:345:PRO:HG3	32:f:378:ASN:HB2	1.82	0.59
3:C:232:ARG:HH12	3:C:275:GLU:HB3	1.66	0.59
15:O:143:ARG:NH1	15:O:145:ASP:O	2.36	0.59
32:f:574:GLU:HA	32:f:577:LEU:HD12	1.84	0.59
1:A:355:PHE:O	1:A:359:ALA:HB3	2.03	0.59
2:B:314:ASN:O	2:B:322:ARG:NH2	2.36	0.59
4:D:133:HIS:HB3	4:D:137:ASN:H	1.68	0.59
4:D:249:ASP:OD1	4:D:252:ARG:NH2	2.36	0.59
23:W:325:VAL:HA	23:W:335:ARG:HH11	1.68	0.59
32:f:822:VAL:HA	32:f:825:MET:HE2	1.84	0.59
7:g:196:GLU:OE2	7:g:245:ARG:NH2	2.36	0.59
8:h:159:LYS:HE3	9:i:57:ASP:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:161:ALA:HB3	10:j:53:LEU:HD21	1.84	0.59
15:O:190:THR:HG22	15:O:192:PRO:HD3	1.85	0.59
21:U:346:ASN:ND2	21:U:380:THR:OG1	2.35	0.59
22:V:439:LYS:NZ	30:d:257:VAL:O	2.36	0.59
23:W:157:GLU:HA	23:W:167:ARG:HD3	1.85	0.59
28:b:179:LEU:HD23	28:b:181:ASP:H	1.68	0.59
10:j:110:TYR:CZ	10:j:114:LEU:HD21	2.37	0.59
18:R:167:ASP:C	16:p:34:MET:HE1	2.28	0.58
21:U:443:LEU:HA	21:U:446:LEU:HD13	1.85	0.58
9:i:115:CYS:SG	10:j:81:ARG:NH2	2.76	0.58
2:B:402:ALA:HA	2:B:405:MET:HE3	1.84	0.58
6:F:85:THR:HG22	6:F:87:PRO:HD2	1.85	0.58
6:F:436:GLN:O	6:F:437:TYR:C	2.46	0.58
21:U:403:THR:HG23	21:U:777:HIS:HE2	1.67	0.58
22:V:402:LYS:HB2	22:V:404:TYR:CE1	2.39	0.58
29:c:270:LEU:HA	29:c:273:LYS:HG2	1.84	0.58
10:j:158:ALA:HB3	11:k:58:LEU:HD21	1.84	0.58
1:A:125:LEU:HA	1:A:149:ILE:HB	1.85	0.58
1:A:237:PHE:HD1	1:A:271:LEU:HD23	1.69	0.58
24:X:407:MET:HE3	26:Z:266:ILE:HD12	1.85	0.58
30:d:82:TYR:HA	30:d:86:LYS:HE3	1.84	0.58
32:f:94:LYS:HA	32:f:97:LYS:HD3	1.84	0.58
23:W:156:VAL:HG12	23:W:167:ARG:HG3	1.85	0.58
28:b:51:LEU:HD11	28:b:61:LEU:HB2	1.84	0.58
5:E:83:CYS:HB2	5:E:89:LYS:HE2	1.84	0.58
22:V:443:PHE:HB2	22:V:444:PRO:HD3	1.85	0.58
32:f:343:LYS:CG	32:f:773:LYS:HE2	2.32	0.58
32:f:723:TYR:CD2	32:f:761:MET:HE1	2.39	0.58
3:C:183:PRO:O	3:C:290:LYS:NZ	2.35	0.58
4:D:408:LYS:HG2	4:D:409:LYS:HD3	1.84	0.58
5:E:265:ASP:OD2	5:E:291:ARG:NH2	2.37	0.58
15:O:126:THR:HB	15:O:131:SER:HB2	1.86	0.58
25:Y:49:ASN:OD1	25:Y:77:ASN:ND2	2.37	0.58
9:i:52:ILE:O	9:i:53:HIS:C	2.47	0.58
15:o:78:THR:HG22	15:o:82:MET:HE2	1.85	0.58
18:r:160:ILE:HD13	18:r:174:VAL:HG23	1.85	0.58
2:B:82:GLN:HG2	32:f:681:TYR:CD1	2.38	0.58
4:D:378:ILE:HG23	4:D:402:ALA:HB1	1.85	0.58
13:M:108:LEU:HD12	13:M:111:LEU:HD23	1.85	0.58
32:f:606:VAL:O	32:f:610:GLN:HG2	2.03	0.58
9:i:197:LEU:O	9:i:201:MET:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:203:LEU:HD21	4:D:330:LYS:HD3	1.86	0.58
15:O:198:ARG:NH1	16:P:155:GLU:OE2	2.37	0.58
25:Y:374:ASP:HA	25:Y:377:LEU:HD12	1.86	0.58
2:B:49:LEU:O	2:B:51:LEU:HD22	2.02	0.57
27:a:252:LYS:HA	27:a:255:TRP:HE3	1.69	0.57
32:f:409:SER:O	32:f:819:TYR:OH	2.22	0.57
7:g:202:LEU:HA	7:g:205:VAL:HG12	1.85	0.57
12:l:39:LYS:HD2	12:l:142:PRO:HB2	1.85	0.57
33:y:23:ILE:HG12	33:y:54:ARG:O	2.04	0.57
21:U:483:LEU:HD11	21:U:781:LEU:HD11	1.85	0.57
24:X:70:LEU:HD22	24:X:109:LEU:HG	1.85	0.57
24:X:332:GLU:O	24:X:336:ILE:CG1	2.51	0.57
30:d:201:ASN:HB3	30:d:204:LYS:HB3	1.87	0.57
33:x:57:SER:HB3	33:y:73:LEU:HD13	1.84	0.57
2:B:53:THR:HB	2:B:54:PRO:HD2	1.86	0.57
4:D:235:PHE:HB3	4:D:246:MET:HE3	1.86	0.57
33:u:4:PHE:CD2	33:u:64:GLU:HG2	2.32	0.57
4:D:145:PRO:HB2	4:D:256:GLU:HG3	1.86	0.57
4:D:229:ARG:NH2	5:E:262:ASN:OD1	2.38	0.57
22:V:124:ASN:O	22:V:126:LYS:NZ	2.37	0.57
9:i:84:ASN:O	9:i:88:ASN:ND2	2.36	0.57
18:r:33:LYS:HG2	18:r:45:MET:HE3	1.86	0.57
33:x:20:SER:HB3	33:y:73:LEU:HD21	1.87	0.57
2:B:120:HIS:HA	2:B:134:SER:HA	1.87	0.57
37:E:401:ADP:O1B	6:F:344:ARG:NH1	2.38	0.57
21:U:218:GLN:NE2	21:U:752:THR:O	2.36	0.57
22:V:60:LEU:HD11	22:V:118:VAL:HG22	1.85	0.57
2:B:183:THR:HG22	2:B:184:TYR:H	1.68	0.57
16:P:62:THR:HG23	17:Q:86:ARG:HH12	1.68	0.57
21:U:697:GLN:NE2	21:U:744:VAL:O	2.38	0.57
22:V:268:ALA:HB1	22:V:271:PHE:HB3	1.85	0.57
25:Y:367:GLN:O	25:Y:371:LYS:NZ	2.37	0.57
30:d:86:LYS:HD3	30:d:89:LEU:HD22	1.87	0.57
11:K:41:GLN:NE2	11:K:151:PRO:O	2.37	0.57
15:O:140:ASP:OD2	20:t:171:ARG:NH2	2.38	0.57
18:R:27:ALA:O	16:p:177:ARG:NH1	2.38	0.57
27:a:279:GLU:HG2	27:a:339:ARG:NH2	2.20	0.57
28:b:90:ILE:HD11	28:b:127:LEU:HD13	1.86	0.57
32:f:590:PHE:CD1	32:f:594:LEU:HD23	2.40	0.57
32:f:666:ILE:O	32:f:669:GLU:HG3	2.05	0.57
10:j:189:LYS:HA	10:j:232:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:y:71:LEU:N	33:y:71:LEU:CD1	2.68	0.57
4:D:163:MET:HE3	4:D:164:TYR:HB2	1.87	0.57
5:E:246:GLY:O	5:E:251:ARG:NH1	2.38	0.57
23:W:337:LYS:HD3	23:W:340:LYS:NZ	2.20	0.57
8:h:118:MET:HE1	8:h:149:SER:OG	2.05	0.57
11:k:203:LYS:NZ	11:k:241:ILE:OXT	2.35	0.57
13:M:117:MET:HA	13:M:117:MET:HE3	1.86	0.57
4:D:200:ARG:NH1	4:D:303:VAL:O	2.33	0.56
5:E:109:ARG:NH2	6:F:100:ASP:OD1	2.38	0.56
9:I:38:LEU:HD12	9:I:160:LYS:HA	1.85	0.56
15:O:164:PHE:O	19:s:38:ARG:NH2	2.37	0.56
23:W:155:GLN:NE2	23:W:157:GLU:OE1	2.38	0.56
32:f:412:ALA:HB3	32:f:819:TYR:CZ	2.40	0.56
3:C:88:LYS:HB2	3:C:94:LYS:NZ	2.20	0.56
7:G:165:ALA:HB3	8:H:56:LEU:HD22	1.87	0.56
32:f:339:ILE:C	32:f:341:GLU:H	2.13	0.56
32:f:852:VAL:HG22	32:f:852:VAL:O	2.05	0.56
4:D:234:GLU:O	4:D:237:GLN:NE2	2.38	0.56
5:E:344:ARG:NH1	37:E:401:ADP:O3'	2.38	0.56
6:F:367:GLN:O	6:F:371:ARG:NH1	2.39	0.56
11:K:210:LEU:HG	11:K:238:ILE:HD11	1.88	0.56
22:V:23:LYS:HE2	22:V:96:PRO:HB3	1.87	0.56
22:V:211:TYR:HE2	30:d:120:GLU:HG2	1.70	0.56
13:m:34:SER:OG	13:m:65:ARG:NH1	2.35	0.56
18:r:127:SER:HB3	18:r:136:TYR:CE1	2.41	0.56
19:s:21:ALA:HB3	19:s:198:VAL:HB	1.87	0.56
21:U:530:GLU:HA	21:U:533:VAL:HG12	1.88	0.56
29:c:54:MET:HE1	33:u:74:ARG:CA	2.35	0.56
15:o:215:LYS:HB3	16:p:197:THR:HB	1.87	0.56
6:F:266:LYS:HD2	6:F:269:ARG:HH12	1.70	0.56
20:t:25:ASP:HA	20:t:187:PHE:HA	1.87	0.56
33:u:1:MET:N	33:u:17:VAL:O	2.36	0.56
4:D:99:ASN:ND2	4:D:115:ILE:O	2.39	0.56
10:J:148:ASP:OD1	10:J:152:THR:N	2.36	0.56
21:U:757:MET:HE3	21:U:758:PRO:HD3	1.87	0.56
23:W:163:GLU:HB3	23:W:166:GLU:HB2	1.86	0.56
23:W:434:GLU:HA	23:W:437:ILE:HD12	1.86	0.56
25:Y:101:ARG:HH21	25:Y:132:VAL:HB	1.71	0.56
32:f:317:LEU:HG	32:f:321:MET:HE1	1.87	0.56
32:f:550:LEU:CD2	32:f:586:PRO:HB2	2.33	0.56
3:C:49:ARG:NH1	21:U:639:LEU:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:231:VAL:HG11	5:E:216:ARG:HH21	1.70	0.56
5:E:102:MET:HG2	5:E:103:THR:HG23	1.87	0.56
20:T:152:GLU:OE1	20:T:156:LYS:NZ	2.38	0.56
24:X:205:LYS:NZ	24:X:243:ASP:OD2	2.39	0.56
32:f:847:GLY:CA	32:f:878:GLU:OE1	2.53	0.56
33:y:8:LEU:HD21	33:y:70:VAL:HA	1.85	0.56
1:A:423:PHE:HD2	1:A:426:THR:H	1.54	0.56
3:C:62:GLU:HG2	3:C:66:LEU:HD13	1.88	0.56
3:C:321:ASN:H	3:C:324:ALA:HB3	1.70	0.56
16:P:35:VAL:HG12	16:P:36:THR:HG23	1.87	0.56
1:A:81:ALA:HB2	32:f:712:LYS:HZ3	1.70	0.56
7:G:73:THR:OG1	7:G:74:GLU:OE1	2.24	0.56
21:U:155:LEU:O	21:U:158:ARG:NH1	2.39	0.56
26:Z:26:ILE:HD11	26:Z:35:VAL:HG22	1.88	0.56
33:x:19:PRO:O	33:y:73:LEU:CD1	2.51	0.56
5:E:235:ILE:O	5:E:239:GLY:N	2.32	0.56
14:N:57:ASP:OD2	15:O:84:LYS:NZ	2.39	0.56
21:U:580:ARG:NH2	21:U:768:GLN:OE1	2.39	0.56
29:c:115:HIS:HB3	29:c:118:PHE:HB2	1.88	0.56
12:L:196:ARG:NH1	12:L:237:GLU:O	2.40	0.55
24:X:297:ARG:CD	24:X:337:ARG:HG3	2.36	0.55
11:k:121:LEU:HD23	11:k:160:GLY:HA3	1.88	0.55
1:A:319:MET:HE3	1:A:320:ALA:N	2.21	0.55
16:P:58:THR:O	17:Q:85:ARG:NH2	2.39	0.55
19:S:36:HIS:O	20:T:151:ARG:NH2	2.39	0.55
22:V:274:THR:HA	22:V:277:LYS:HD2	1.88	0.55
27:a:135:ILE:HG12	27:a:158:LEU:HD13	1.88	0.55
17:q:1:MET:SD	17:q:2:GLU:N	2.79	0.55
4:D:121:ARG:HB3	29:c:275:VAL:HA	1.87	0.55
21:U:334:ALA:O	21:U:338:HIS:ND1	2.40	0.55
25:Y:12:PRO:O	25:Y:146:ARG:NH1	2.40	0.55
33:y:18:GLU:H	33:y:21:ASP:CG	2.14	0.55
2:B:357:ASP:OD1	10:J:200:GLN:NE2	2.39	0.55
3:C:237:MET:HB2	3:C:241:HIS:CE1	2.42	0.55
3:C:270:GLN:HA	3:C:273:MET:HG2	1.88	0.55
21:U:70:HIS:O	22:V:183:ARG:NH2	2.39	0.55
22:V:363:ARG:NH2	25:Y:348:ASP:OD2	2.40	0.55
27:a:321:LYS:HB2	27:a:335:TRP:HB3	1.87	0.55
30:d:171:LEU:HD22	30:d:175:ARG:HH12	1.72	0.55
6:F:107:ASP:HB2	26:Z:85:VAL:HA	1.89	0.55
6:F:175:MET:HE3	6:F:249:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:243:GLY:HA2	27:a:275:LEU:HG	1.88	0.55
7:g:20:GLY:HA3	8:h:28:ALA:CB	2.32	0.55
6:F:194:GLN:HA	6:F:352:ILE:HD11	1.88	0.55
17:Q:144:ASP:OD2	18:r:166:ARG:NH2	2.40	0.55
12:l:164:ARG:NH1	12:l:198:THR:O	2.40	0.55
5:E:4:PRO:HG2	5:E:8:ALA:H	1.71	0.55
22:V:249:TYR:O	22:V:253:ARG:HB2	2.07	0.55
25:Y:347:ILE:HG13	25:Y:354:VAL:HG12	1.89	0.55
8:h:203:MET:HA	8:h:207:ASN:HD21	1.70	0.55
12:l:73:SER:HB3	12:l:133:LEU:HB2	1.88	0.55
15:O:30:ASN:OD1	15:O:187:ARG:NH2	2.37	0.55
24:X:173:GLU:HA	24:X:176:THR:HG22	1.89	0.55
29:c:31:VAL:HG23	29:c:203:ILE:HD13	1.89	0.55
32:f:414:LEU:HD21	32:f:428:GLN:HE22	1.70	0.55
4:D:278:GLN:HE22	4:D:283:ARG:HD3	1.72	0.55
18:R:192:VAL:HG11	16:p:205:ASP:HB3	1.88	0.55
20:T:28:GLY:HA3	20:T:39:ILE:HD11	1.88	0.55
25:Y:300:ARG:NH1	25:Y:333:GLU:OE2	2.40	0.55
11:k:97:GLN:HG3	18:r:61:ARG:HG2	1.87	0.55
33:x:63:LYS:CE	33:y:76:GLY:O	2.54	0.55
32:f:855:GLN:NE2	32:f:861:THR:HG21	2.20	0.55
16:P:14:MET:HG3	16:P:163:LEU:HD11	1.87	0.54
21:U:14:GLU:O	21:U:20:LYS:NZ	2.40	0.54
32:f:405:HIS:CE1	32:f:813:LYS:HD2	2.42	0.54
16:p:67:LEU:HD11	16:p:90:MET:SD	2.48	0.54
33:y:8:LEU:HD23	33:y:8:LEU:H	1.72	0.54
3:C:53:ASN:HD21	21:U:643:SER:HA	1.71	0.54
6:F:94:ILE:HD12	6:F:123:VAL:HG12	1.89	0.54
20:T:9:THR:O	20:T:41:ARG:NH1	2.39	0.54
29:c:125:VAL:CG1	33:u:74:ARG:HD2	2.36	0.54
32:f:479:LEU:HD21	32:f:816:TYR:CZ	2.42	0.54
33:x:23:ILE:HG12	33:x:54:ARG:O	2.07	0.54
33:x:60:ASN:CG	33:y:8:LEU:HD13	2.32	0.54
28:b:61:LEU:HD23	28:b:74:LYS:HD2	1.89	0.54
12:L:164:ARG:HB3	12:L:198:THR:HG23	1.88	0.54
27:a:216:LEU:HA	27:a:219:HIS:HB2	1.89	0.54
12:l:196:ARG:NH1	12:l:237:GLU:O	2.41	0.54
2:B:107:MET:HB2	3:C:96:VAL:HB	1.88	0.54
3:C:134:LEU:HD13	3:C:230:MET:HG2	1.90	0.54
24:X:306:LEU:HD12	24:X:313:LEU:HD13	1.89	0.54
9:i:72:MET:HE2	9:i:110:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:62:GLN:H	33:x:62:GLN:CD	2.15	0.54
1:A:367:ASP:HB2	1:A:406:GLU:HG3	1.89	0.54
13:M:125:TYR:HB2	13:M:128:VAL:HG22	1.90	0.54
21:U:35:TRP:CZ3	21:U:71:LEU:HA	2.43	0.54
29:c:54:MET:HE1	33:u:74:ARG:HA	1.90	0.54
9:i:196:VAL:HG23	9:i:199:LYS:HE3	1.90	0.54
10:j:31:THR:OG1	10:j:163:ARG:O	2.25	0.54
1:A:319:MET:HE3	1:A:320:ALA:H	1.72	0.54
3:C:83:LYS:HG2	3:C:105:ILE:HD11	1.89	0.54
3:C:300:ILE:HG13	3:C:301:LEU:HD22	1.90	0.54
7:G:6:SER:OG	7:G:11:ARG:NH1	2.36	0.54
21:U:678:ASP:O	21:U:684:ARG:NH1	2.35	0.54
24:X:172:LEU:HD12	24:X:175:LYS:HD3	1.90	0.54
11:k:107:MET:HE3	11:k:112:VAL:HG22	1.90	0.54
3:C:248:MET:HE1	3:C:251:ILE:HD11	1.90	0.54
6:F:43:GLN:HA	6:F:46:ARG:HG2	1.89	0.54
33:x:18:GLU:N	33:x:21:ASP:OD2	2.41	0.54
6:F:111:ILE:HG12	6:F:113:LEU:H	1.71	0.54
12:L:41:LYS:HG3	12:L:42:THR:HG23	1.89	0.54
22:V:402:LYS:HE2	22:V:404:TYR:CE1	2.43	0.54
11:k:32:LYS:NZ	11:k:174:SER:OG	2.40	0.54
15:o:215:LYS:NZ	15:o:217:THR:OG1	2.41	0.54
20:T:26:MET:HG3	20:T:38:ASN:HA	1.90	0.54
22:V:426:ARG:HG3	25:Y:377:LEU:HD11	1.89	0.54
24:X:297:ARG:HD2	24:X:337:ARG:CG	2.38	0.54
10:j:42:VAL:HG22	10:j:210:VAL:HG12	1.90	0.54
33:x:19:PRO:CG	33:y:74:ARG:CA	2.85	0.54
33:x:57:SER:HB3	33:y:73:LEU:HA	1.89	0.54
33:y:36:ILE:O	33:y:41:GLN:NE2	2.41	0.54
2:B:122:ILE:HD11	2:B:130:GLU:HB3	1.90	0.53
3:C:44:ARG:HG3	22:V:443:PHE:CE2	2.44	0.53
5:E:208:ILE:HG12	34:v:9:UNK:O	2.08	0.53
7:G:137:CYS:SG	7:G:138:MET:N	2.82	0.53
23:W:386:THR:HG23	23:W:387:ILE:HD12	1.90	0.53
24:X:365:LEU:HA	24:X:368:MET:HE3	1.89	0.53
25:Y:71:ASN:HA	25:Y:74:LYS:HG2	1.89	0.53
31:e:29:ASP:OD1	31:e:32:ASN:ND2	2.41	0.53
32:f:559:PRO:HG2	32:f:594:LEU:HD21	1.91	0.53
32:f:602:GLY:HA3	32:f:788:MET:HE1	1.90	0.53
7:g:10:ASP:O	7:g:24:GLN:NE2	2.41	0.53
17:q:29:LYS:NZ	17:q:31:ASP:OD1	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:HB2	2:B:310:LEU:HD21	1.91	0.53
23:W:152:GLN:OE1	23:W:186:ARG:NH1	2.41	0.53
25:Y:349:LYS:O	25:Y:351:ASN:N	2.41	0.53
32:f:405:HIS:CE1	32:f:813:LYS:HB3	2.43	0.53
1:A:333:ARG:NH1	35:F:501:ATP:O5'	2.41	0.53
4:D:155:THR:OG1	4:D:158:GLN:OE1	2.24	0.53
22:V:284:LEU:HD21	22:V:311:THR:HG23	1.90	0.53
25:Y:101:ARG:NH1	25:Y:102:ASP:OD1	2.40	0.53
33:u:44:ILE:HB	33:u:68:HIS:HB2	1.91	0.53
3:C:262:GLY:HA2	3:C:270:GLN:HE22	1.73	0.53
6:F:235:LEU:HD21	35:F:501:ATP:H2'	1.90	0.53
8:H:119:GLN:NE2	9:I:82:ASP:OD1	2.41	0.53
13:M:213:LEU:HG	13:M:227:VAL:HG21	1.90	0.53
13:M:229:LYS:HA	13:M:232:ARG:HG2	1.91	0.53
14:N:165:GLU:OE2	20:t:37:ARG:NH1	2.41	0.53
22:V:363:ARG:HH21	25:Y:351:ASN:CG	2.16	0.53
28:b:20:ASP:OD1	28:b:20:ASP:N	2.40	0.53
9:I:119:GLN:NE2	10:J:79:ASP:OD1	2.40	0.53
13:M:67:PHE:HB2	13:M:75:MET:HB3	1.91	0.53
26:Z:70:LEU:HD11	26:Z:108:ILE:HG23	1.89	0.53
26:Z:212:LEU:HD21	27:a:349:MET:HG3	1.89	0.53
18:r:35:ILE:N	18:r:43:GLY:O	2.42	0.53
2:B:248:LEU:HD12	2:B:282:VAL:HG12	1.90	0.53
23:W:417:LEU:HA	23:W:421:MET:CE	2.39	0.53
32:f:662:MET:CE	32:f:781:TYR:HE1	2.21	0.53
25:Y:26:LEU:HD13	25:Y:63:TRP:HH2	1.73	0.53
32:f:695:ALA:C	32:f:731:MET:HE1	2.34	0.53
9:i:54:LYS:HG3	9:i:55:LEU:HD12	1.89	0.53
14:n:40:ARG:HG2	14:n:103:TRP:HE3	1.73	0.53
16:p:44:PRO:O	16:p:68:LYS:NZ	2.42	0.53
19:s:27:THR:HB	19:s:40:SER:H	1.74	0.53
3:C:233:GLU:HA	3:C:236:VAL:HB	1.89	0.53
5:E:75:ASN:HD22	6:F:130:GLN:HG2	1.74	0.53
6:F:363:ALA:HA	6:F:366:MET:HE3	1.90	0.53
10:J:11:SER:OG	10:J:15:HIS:N	2.40	0.53
22:V:45:LEU:HD23	22:V:48:LEU:HD13	1.91	0.53
32:f:778:LEU:HD13	32:f:821:LEU:HD11	1.91	0.53
11:k:186:HIS:H	11:k:189:MET:HE1	1.73	0.53
8:H:196:LYS:HE2	8:H:203:MET:HE2	1.91	0.53
17:Q:4:LEU:HD11	17:Q:45:LEU:HB3	1.91	0.53
16:p:53:LEU:HG	16:p:107:PRO:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:41:GLN:HG2	33:x:69:LEU:HD11	1.91	0.53
5:E:84:ARG:NH1	6:F:114:ASP:OD2	2.42	0.53
5:E:136:GLY:O	37:E:401:ADP:N6	2.41	0.53
21:U:383:ASP:HB3	21:U:386:LEU:HB3	1.90	0.53
22:V:55:LEU:HD23	22:V:121:PHE:HB2	1.90	0.53
24:X:211:ASP:HB2	24:X:235:ALA:HB2	1.91	0.53
24:X:255:LEU:HD22	24:X:267:VAL:HG22	1.90	0.53
27:a:15:GLY:O	27:a:18:GLN:NE2	2.38	0.53
32:f:563:GLY:HA2	32:f:595:VAL:HG13	1.91	0.53
9:i:122:THR:HB	9:i:129:PRO:HB3	1.89	0.53
12:l:152:ASN:HD21	13:m:81:LEU:HD12	1.74	0.53
17:q:35:MET:HG3	17:q:45:LEU:HG	1.91	0.53
1:A:114:ASN:HA	1:A:120:LYS:HA	1.92	0.52
5:E:352:MET:HE3	6:F:200:GLU:HB3	1.92	0.52
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.92	0.52
16:P:66:ARG:HG3	16:P:94:LEU:HD11	1.90	0.52
23:W:404:LYS:HE2	23:W:408:ASN:HB3	1.90	0.52
26:Z:139:ILE:O	26:Z:156:GLU:N	2.35	0.52
32:f:505:MET:HG3	32:f:518:THR:HG23	1.90	0.52
16:p:62:THR:HG23	17:q:86:ARG:HH12	1.74	0.52
6:F:314:LEU:HD21	6:F:342:LEU:HA	1.90	0.52
6:F:341:ALA:O	6:F:347:ARG:NH1	2.42	0.52
8:H:135:LEU:HG	8:H:163:MET:HE3	1.90	0.52
23:W:131:THR:HG21	23:W:154:LEU:HD21	1.91	0.52
31:e:44:GLU:O	31:e:48:HIS:ND1	2.42	0.52
9:i:53:HIS:CD2	9:i:54:LYS:H	2.27	0.52
9:i:136:TYR:HB2	9:i:148:TYR:HB2	1.90	0.52
33:x:63:LYS:NZ	33:y:76:GLY:O	2.34	0.52
2:B:78:PHE:CE2	32:f:613:LEU:HD13	2.44	0.52
2:B:150:VAL:HA	2:B:162:VAL:HA	1.91	0.52
25:Y:235:ASP:O	25:Y:239:LYS:NZ	2.41	0.52
25:Y:360:ASP:OD2	25:Y:363:ASN:ND2	2.40	0.52
20:t:109:THR:HG23	20:t:126:ASP:HA	1.92	0.52
33:y:71:LEU:O	33:y:72:ARG:C	2.52	0.52
25:Y:240:VAL:HG23	25:Y:241:ILE:HG13	1.90	0.52
27:a:61:GLU:HG3	27:a:79:ILE:HD13	1.92	0.52
28:b:9:CYS:HB3	28:b:111:ALA:HA	1.90	0.52
12:l:122:ARG:NH1	13:m:127:ALA:O	2.38	0.52
16:p:71:LEU:HD11	16:p:82:ILE:HG21	1.91	0.52
5:E:147:GLU:HA	5:E:151:LEU:HD12	1.90	0.52
20:T:9:THR:HG22	20:T:10:SER:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:35:HIS:NE2	28:b:14:GLU:O	2.42	0.52
32:f:344:VAL:HG22	32:f:347:ASP:HB3	1.91	0.52
32:f:412:ALA:C	32:f:819:TYR:OH	2.52	0.52
19:s:16:ALA:HB2	19:s:121:VAL:HG23	1.91	0.52
2:B:171:VAL:HG13	2:B:175:LYS:HD2	1.90	0.52
21:U:62:LEU:HD11	21:U:87:LEU:HB3	1.91	0.52
21:U:541:HIS:HB2	21:U:544:ILE:HG22	1.92	0.52
23:W:325:VAL:HG13	23:W:335:ARG:HD3	1.92	0.52
32:f:339:ILE:O	32:f:341:GLU:N	2.42	0.52
32:f:402:ASN:HB2	32:f:407:MET:HB2	1.91	0.52
13:m:77:VAL:HG11	13:m:84:ALA:HB1	1.92	0.52
16:p:7:ASN:ND2	16:p:29:GLY:O	2.39	0.52
2:B:78:PHE:CZ	32:f:613:LEU:HB3	2.45	0.52
5:E:127:PRO:HD2	6:F:320:PHE:HE1	1.74	0.52
5:E:265:ASP:HB2	5:E:294:ARG:HG2	1.92	0.52
5:E:372:ARG:HD3	13:M:170:GLN:HB3	1.90	0.52
16:P:83:LYS:HD3	16:P:85:TYR:H	1.74	0.52
21:U:581:SER:O	21:U:585:THR:OG1	2.24	0.52
32:f:747:GLN:HA	32:f:750:GLN:OE1	2.08	0.52
8:h:42:ASN:ND2	8:h:183:GLU:OE2	2.43	0.52
18:r:190:ASP:OD1	18:r:191:ASN:N	2.43	0.52
1:A:265:ARG:NH1	1:A:311:PRO:O	2.39	0.52
24:X:12:ALA:HB2	24:X:26:ILE:HG21	1.91	0.52
27:a:249:GLN:HA	27:a:252:LYS:HB2	1.91	0.52
32:f:852:VAL:HA	32:f:861:THR:HG21	1.91	0.52
3:C:57:ARG:NH2	21:U:643:SER:O	2.43	0.52
6:F:294:LYS:NZ	6:F:336:ASP:O	2.42	0.52
10:J:2:SER:OG	10:J:3:TYR:N	2.41	0.52
18:R:166:ARG:NH1	16:p:34:MET:O	2.42	0.52
21:U:530:GLU:OE1	33:y:64:GLU:HB3	2.10	0.52
10:j:110:TYR:O	10:j:114:LEU:HD23	2.10	0.52
2:B:197:ILE:HG13	2:B:235:LEU:HD21	1.91	0.52
3:C:164:VAL:HG13	3:C:165:ILE:HG13	1.91	0.52
4:D:269:ALA:O	5:E:255:ARG:NE	2.43	0.52
16:P:193:ASP:N	16:P:193:ASP:OD1	2.41	0.52
1:A:114:ASN:HB3	1:A:120:LYS:HG2	1.92	0.51
9:I:175:LEU:O	9:I:179:TYR:HB2	2.09	0.51
21:U:564:ASP:OD1	21:U:564:ASP:N	2.41	0.51
24:X:237:GLU:HA	24:X:240:ASP:HB2	1.92	0.51
30:d:234:ASP:OD1	30:d:235:THR:N	2.44	0.51
32:f:723:TYR:HD1	32:f:761:MET:SD	2.32	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:92:GLN:HA	17:q:62:LYS:HE3	1.91	0.51
10:J:31:THR:OG1	10:J:163:ARG:O	2.24	0.51
11:K:77:ALA:HB3	11:K:142:LEU:HB2	1.93	0.51
21:U:30:VAL:HA	21:U:33:ASP:HB2	1.92	0.51
21:U:133:ILE:HG22	21:U:136:LYS:HE2	1.91	0.51
23:W:151:LEU:HD22	23:W:177:LEU:HD12	1.91	0.51
23:W:225:TYR:HA	23:W:228:ILE:HD12	1.91	0.51
24:X:333:GLN:HA	24:X:336:ILE:CG1	2.41	0.51
25:Y:191:ILE:HD12	31:e:23:VAL:HG11	1.92	0.51
10:j:146:GLN:NE2	10:j:147:THR:O	2.43	0.51
11:k:50:VAL:HG21	11:k:66:LYS:HB2	1.93	0.51
11:k:91:LYS:HG2	11:k:119:LEU:HD13	1.91	0.51
33:x:6:LYS:O	33:x:68:HIS:HA	2.10	0.51
17:Q:8:GLN:HA	17:Q:13:VAL:HA	1.92	0.51
18:R:133:VAL:HG21	17:q:137:PHE:HB3	1.92	0.51
32:f:470:VAL:HG13	32:f:471:LEU:HG	1.93	0.51
16:p:15:LYS:NZ	16:p:134:ASP:OD1	2.36	0.51
33:x:60:ASN:HB3	33:y:8:LEU:HD12	1.73	0.51
2:B:264:PRO:HG3	2:B:311:GLU:HG2	1.92	0.51
4:D:160:PRO:HG3	4:D:220:ALA:HB3	1.91	0.51
6:F:359:GLU:HG2	6:F:360:GLU:HG3	1.92	0.51
17:Q:104:LEU:HB3	17:Q:116:TYR:HB2	1.91	0.51
12:l:14:SER:HB2	12:l:18:ARG:H	1.75	0.51
13:m:108:LEU:HD22	13:m:139:SER:HB3	1.91	0.51
7:G:138:MET:HB2	7:G:154:CYS:HB3	1.93	0.51
8:H:34:PRO:HG3	8:H:165:LYS:HB3	1.93	0.51
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.75	0.51
19:S:38:ARG:NH2	15:o:164:PHE:O	2.43	0.51
21:U:574:LYS:HD2	29:c:214:GLN:HG2	1.92	0.51
32:f:348:ILE:O	32:f:352:HIS:N	2.43	0.51
32:f:707:LEU:O	32:f:729:MET:HE1	2.10	0.51
14:n:160:LEU:HD23	14:n:174:ILE:HG23	1.92	0.51
33:x:19:PRO:HG3	33:y:74:ARG:C	2.35	0.51
4:D:163:MET:HG3	4:D:165:ALA:N	2.26	0.51
12:L:134:ILE:HB	12:L:145:PHE:HB2	1.91	0.51
14:N:44:CYS:HB2	14:N:99:ILE:HB	1.92	0.51
32:f:862:ILE:CG1	32:f:879:ARG:HD2	2.41	0.51
10:j:196:LEU:HA	10:j:199:VAL:HG12	1.91	0.51
13:m:211:LEU:O	13:m:232:ARG:NH2	2.43	0.51
16:p:87:LEU:HD12	16:p:90:MET:SD	2.50	0.51
33:x:62:GLN:HB2	33:x:63:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:CYS:HB2	1:A:139:ARG:NH1	2.26	0.51
1:A:386:ARG:NH1	35:A:501:ATP:O3'	2.43	0.51
3:C:246:ILE:HB	3:C:291:VAL:HG12	1.92	0.51
5:E:329:GLU:HA	5:E:332:VAL:HG12	1.92	0.51
33:x:19:PRO:HB2	33:y:74:ARG:CA	2.40	0.51
33:x:73:LEU:HD23	33:x:73:LEU:N	2.18	0.51
13:M:19:ARG:NH2	13:M:24:GLU:OE1	2.42	0.51
21:U:62:LEU:HD12	21:U:84:ALA:HB1	1.92	0.51
21:U:616:ARG:HB2	21:U:647:HIS:HB3	1.92	0.51
21:U:623:GLY:HA3	21:U:658:ILE:HG13	1.92	0.51
22:V:97:ARG:NH1	22:V:104:THR:O	2.44	0.51
30:d:183:GLU:HG3	30:d:213:ARG:HH21	1.74	0.51
32:f:585:GLU:O	32:f:587:PHE:N	2.44	0.51
11:k:85:ALA:HB2	11:k:139:VAL:HG11	1.93	0.51
16:p:12:MET:HG3	16:p:171:MET:HE2	1.93	0.51
33:u:39:ASP:O	33:u:42:ARG:NH1	2.44	0.51
5:E:375:ALA:O	5:E:379:LYS:NZ	2.40	0.51
6:F:65:GLU:O	6:F:69:MET:HG3	2.11	0.51
6:F:137:ILE:HD13	6:F:142:ALA:HB2	1.93	0.51
8:H:177:ARG:NH1	24:X:162:ASP:OD1	2.44	0.51
19:S:119:GLY:O	19:S:132:ARG:NH2	2.44	0.51
21:U:366:HIS:NE2	21:U:392:TRP:O	2.43	0.51
29:c:43:LYS:O	29:c:46:ARG:NH1	2.44	0.51
29:c:68:ARG:HH12	29:c:208:ARG:HB2	1.76	0.51
33:x:42:ARG:NH1	33:x:72:ARG:HG3	2.25	0.51
7:G:123:GLN:O	7:G:126:THR:OG1	2.25	0.51
16:P:62:THR:OG1	17:Q:85:ARG:NH2	2.41	0.51
24:X:332:GLU:O	24:X:336:ILE:HG23	2.11	0.51
27:a:156:TYR:HE2	27:a:196:ARG:HH21	1.59	0.51
4:D:56:VAL:HG21	21:U:599:ILE:HG23	1.93	0.50
4:D:318:ASP:OD1	4:D:318:ASP:N	2.42	0.50
11:K:111:SER:HA	11:K:114:GLN:HG3	1.92	0.50
15:O:81:ARG:HD2	15:O:84:LYS:HE3	1.94	0.50
21:U:422:LEU:HD21	21:U:446:LEU:HD11	1.93	0.50
27:a:77:VAL:HA	27:a:80:ILE:HG22	1.93	0.50
32:f:849:ALA:HB1	32:f:879:ARG:HH21	1.76	0.50
10:j:7:ILE:HG13	10:j:8:THR:HG23	1.92	0.50
4:D:202:VAL:HG23	4:D:329:ARG:HB2	1.91	0.50
5:E:237:ALA:O	6:F:308:ARG:NE	2.44	0.50
11:K:215:ILE:HD11	11:K:234:LEU:HD21	1.92	0.50
21:U:265:ILE:HA	21:U:268:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:592:GLY:HA3	21:U:628:ARG:HH21	1.75	0.50
29:c:57:MET:HA	29:c:72:VAL:HA	1.92	0.50
16:p:50:TYR:CD2	16:p:190:ILE:HD11	2.46	0.50
1:A:38:GLN:CB	1:A:42:SER:HB3	2.40	0.50
2:B:49:LEU:CD2	32:f:673:ARG:HD3	2.41	0.50
4:D:191:TYR:HA	4:D:196:ILE:HD12	1.93	0.50
9:I:13:SER:OG	9:I:17:ARG:N	2.39	0.50
13:M:77:VAL:HG23	13:M:135:PHE:HB3	1.92	0.50
13:M:134:SER:HB2	13:M:153:PRO:HD3	1.93	0.50
23:W:159:TYR:O	23:W:167:ARG:NH2	2.42	0.50
12:l:171:TYR:HD1	12:l:174:ARG:HH21	1.58	0.50
1:A:66:LYS:HZ3	1:A:71:GLY:H	1.57	0.50
9:I:118:LYS:HD2	9:I:152:PRO:HA	1.93	0.50
21:U:362:ASN:OD1	21:U:363:SER:N	2.44	0.50
24:X:82:LYS:HE3	24:X:122:ARG:CZ	2.41	0.50
2:B:411:ARG:NH2	2:B:418:ASP:OD1	2.42	0.50
5:E:247:THR:HG23	5:E:250:ASP:H	1.75	0.50
32:f:385:PHE:HZ	32:f:773:LYS:HD2	1.76	0.50
32:f:707:LEU:HD13	32:f:744:MET:HE1	1.93	0.50
32:f:862:ILE:HG12	32:f:879:ARG:HD2	1.94	0.50
20:t:56:ASP:HB2	20:t:107:TRP:HB3	1.94	0.50
7:G:66:VAL:HA	13:M:158:TYR:HE1	1.76	0.50
10:J:120:GLN:NE2	11:K:135:ARG:O	2.43	0.50
12:L:204:ASP:OD1	12:L:239:ARG:NH2	2.44	0.50
17:Q:31:ASP:N	17:Q:31:ASP:OD1	2.45	0.50
22:V:344:ARG:HH21	30:d:116:HIS:HD2	1.59	0.50
18:r:38:ASN:OD1	18:r:41:LEU:N	2.44	0.50
19:s:99:ARG:HD3	19:s:102:PHE:HD2	1.76	0.50
2:B:124:SER:HA	2:B:130:GLU:HG3	1.93	0.50
8:H:14:SER:HG	8:H:18:LYS:H	1.58	0.50
15:O:1:THR:N	15:O:168:GLY:O	2.45	0.50
22:V:359:LEU:O	25:Y:346:LYS:NZ	2.42	0.50
29:c:32:TYR:HB3	29:c:68:ARG:NH1	2.25	0.50
29:c:213:GLU:HA	29:c:216:MET:HG3	1.94	0.50
30:d:114:GLU:HA	30:d:117:THR:HG22	1.94	0.50
32:f:343:LYS:HZ2	32:f:773:LYS:HG2	1.76	0.50
32:f:600:TYR:O	32:f:660:ILE:HG12	2.12	0.50
7:g:21:ARG:CG	7:g:21:ARG:NH1	2.38	0.50
3:C:117:ARG:HG2	3:C:124:HIS:CE1	2.47	0.50
9:I:25:MET:HE1	9:I:152:PRO:HD2	1.93	0.50
13:M:181:MET:N	13:M:181:MET:SD	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:13:LEU:HD11	19:S:149:LEU:HD11	1.94	0.50
32:f:819:TYR:O	32:f:822:VAL:HG13	2.12	0.50
3:C:88:LYS:HB2	3:C:94:LYS:HZ3	1.77	0.50
4:D:297:ASP:OD1	4:D:326:ARG:NE	2.45	0.50
5:E:380:LEU:HD13	6:F:335:VAL:HG11	1.94	0.50
18:R:179:VAL:HG22	18:R:184:TRP:HB3	1.93	0.50
21:U:894:MET:HE1	21:U:906:LEU:HB3	1.94	0.50
11:k:44:GLU:O	11:k:221:GLN:NE2	2.45	0.50
2:B:269:GLU:OE2	2:B:272:ARG:NH1	2.45	0.49
19:S:125:ASP:OD1	19:S:129:SER:N	2.45	0.49
21:U:78:LEU:HD11	21:U:104:CYS:HB2	1.93	0.49
32:f:512:MET:HE1	32:f:554:TYR:HD2	1.77	0.49
7:g:80:MET:SD	7:g:138:MET:HG2	2.52	0.49
19:s:99:ARG:NE	19:s:104:TYR:OH	2.45	0.49
3:C:139:MET:HG3	3:C:214:VAL:HG22	1.94	0.49
5:E:159:PHE:CG	5:E:166:PRO:HG3	2.47	0.49
24:X:297:ARG:HD2	24:X:337:ARG:HG3	1.95	0.49
27:a:90:PRO:HA	27:a:93:ALA:HB3	1.93	0.49
7:g:145:GLU:OE2	15:o:75:ARG:NH2	2.42	0.49
12:l:65:HIS:NE2	12:l:67:ASP:O	2.45	0.49
12:l:104:PRO:HB2	12:l:107:ARG:HD2	1.92	0.49
33:u:63:LYS:CE	33:u:64:GLU:HB2	2.20	0.49
1:A:52:ILE:HD11	2:B:68:ILE:HG22	1.94	0.49
2:B:82:GLN:HG3	32:f:681:TYR:CD1	2.47	0.49
16:P:65:GLN:HA	16:P:68:LYS:HE2	1.94	0.49
23:W:59:CYS:HB3	23:W:68:LEU:HB2	1.93	0.49
24:X:255:LEU:HD12	24:X:287:LEU:HD13	1.92	0.49
28:b:22:LEU:HB2	28:b:23:PRO:CD	2.32	0.49
28:b:180:ALA:HA	28:b:183:LEU:HB2	1.94	0.49
33:y:55:THR:OG1	33:y:57:SER:OG	2.28	0.49
1:A:97:ARG:NH1	2:B:130:GLU:O	2.46	0.49
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.45	0.49
1:A:376:LEU:HB3	1:A:417:ILE:HD11	1.93	0.49
4:D:292:LEU:O	4:D:296:MET:HG3	2.12	0.49
7:G:90:GLN:HE21	7:G:134:LEU:HD23	1.78	0.49
12:L:42:THR:HB	12:L:217:LYS:NZ	2.28	0.49
14:N:160:LEU:O	14:N:164:MET:HG2	2.12	0.49
32:f:494:ARG:NH2	32:f:496:ASP:OD2	2.45	0.49
32:f:723:TYR:HB3	32:f:761:MET:SD	2.48	0.49
16:p:178:ASP:HB3	16:p:181:SER:HB2	1.94	0.49
12:L:44:ALA:HB2	12:L:142:PRO:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:27:LEU:HD11	20:T:34:ALA:HB1	1.94	0.49
25:Y:238:GLU:HA	25:Y:242:LYS:HB2	1.94	0.49
26:Z:71:ASP:HB3	26:Z:74:TYR:HB3	1.93	0.49
26:Z:170:VAL:HA	29:c:152:LYS:HD3	1.94	0.49
32:f:385:PHE:CE2	32:f:773:LYS:CE	2.93	0.49
32:f:616:CYS:SG	32:f:653:ALA:HB3	2.53	0.49
7:g:38:THR:O	7:g:52:THR:OG1	2.28	0.49
7:g:58:ASP:N	7:g:58:ASP:OD1	2.44	0.49
7:g:86:ASP:OD1	13:m:120:HIS:NE2	2.36	0.49
19:s:13:LEU:HD13	19:s:145:LEU:HD21	1.95	0.49
33:y:1:MET:N	33:y:17:VAL:O	2.40	0.49
8:H:185:GLU:HG3	24:X:122:ARG:HH21	1.78	0.49
10:J:92:GLN:HB3	17:Q:62:LYS:HG3	1.94	0.49
15:O:14:LEU:HB2	15:O:176:CYS:HB3	1.94	0.49
21:U:2:ILE:HD12	30:d:36:LEU:HD11	1.93	0.49
21:U:163:PHE:O	21:U:166:THR:OG1	2.30	0.49
27:a:70:ARG:HH21	28:b:80:PRO:HD2	1.77	0.49
30:d:155:LYS:HD3	30:d:167:ILE:HD12	1.93	0.49
32:f:382:ASN:HA	32:f:385:PHE:HD2	1.77	0.49
32:f:408:LEU:HD12	32:f:439:TYR:HA	1.95	0.49
32:f:493:ASN:OD1	32:f:529:SER:OG	2.30	0.49
32:f:723:TYR:CG	32:f:761:MET:SD	3.05	0.49
16:p:189:ILE:HB	16:p:196:THR:HB	1.94	0.49
1:A:99:THR:OG1	1:A:114:ASN:O	2.31	0.49
2:B:53:THR:HG21	2:B:61:LYS:HG3	1.94	0.49
32:f:82:ILE:HD11	32:f:125:ILE:HG12	1.94	0.49
33:x:20:SER:O	33:x:21:ASP:C	2.55	0.49
1:A:223:THR:OG1	35:A:501:ATP:O2B	2.31	0.49
5:E:60:VAL:HG22	5:E:71:VAL:HG12	1.94	0.49
17:Q:20:VAL:H	17:Q:34:LYS:HZ3	1.59	0.49
24:X:258:LYS:HD3	24:X:266:ASP:HB3	1.95	0.49
25:Y:68:ASP:N	25:Y:68:ASP:OD1	2.46	0.49
30:d:27:LYS:O	30:d:31:LEU:HB2	2.12	0.49
32:f:343:LYS:CE	32:f:773:LYS:HE2	2.40	0.49
32:f:688:ARG:HG2	32:f:720:GLU:CB	2.42	0.49
11:k:16:SER:OG	11:k:18:GLU:OE1	2.31	0.49
12:l:64:LEU:HB2	12:l:72:ILE:HD11	1.93	0.49
12:l:66:VAL:HG11	12:l:88:MET:HE1	1.95	0.49
16:p:149:MET:HE1	16:p:170:ALA:HA	1.94	0.49
33:u:42:ARG:CZ	33:u:72:ARG:HG2	2.42	0.49
33:x:63:LYS:H	33:x:63:LYS:HE2	1.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HB2	2:B:148:CYS:H	1.78	0.49
7:G:128:ASN:HB3	7:G:130:GLU:HG2	1.95	0.49
9:I:155:ASN:OD1	10:J:77:THR:OG1	2.30	0.49
14:N:147:MET:HE3	14:N:151:GLU:CB	2.43	0.49
28:b:22:LEU:CB	28:b:23:PRO:HD3	2.28	0.49
32:f:341:GLU:HG3	32:f:343:LYS:HG2	1.94	0.49
32:f:852:VAL:HG21	32:f:859:PRO:CA	2.43	0.49
13:m:230:ASP:OD1	13:m:230:ASP:N	2.46	0.49
2:B:71:TYR:N	2:B:71:TYR:CD1	2.80	0.49
3:C:145:ASP:OD1	3:C:201:ARG:NH2	2.45	0.49
3:C:244:SER:O	3:C:289:ILE:HA	2.12	0.49
3:C:258:ARG:NH1	3:C:302:ASP:OD2	2.46	0.49
21:U:16:GLU:HB2	21:U:20:LYS:HB2	1.95	0.49
25:Y:202:LEU:HD11	25:Y:239:LYS:HD2	1.95	0.49
25:Y:271:PHE:HZ	25:Y:299:MET:HE2	1.78	0.49
11:k:20:ARG:NH2	11:k:25:GLU:OE2	2.38	0.49
24:X:21:GLU:HA	24:X:24:ILE:HD12	1.95	0.48
29:c:89:PRO:HG2	33:u:44:ILE:HD11	1.94	0.48
32:f:333:LEU:HD22	32:f:829:MET:SD	2.53	0.48
32:f:860:LYS:O	32:f:860:LYS:NZ	2.45	0.48
20:t:50:MET:N	20:t:50:MET:SD	2.86	0.48
4:D:151:ILE:HG21	4:D:250:VAL:HG22	1.95	0.48
6:F:265:ALA:HA	6:F:312:GLU:HG2	1.94	0.48
14:N:84:LYS:HD2	14:N:120:MET:HB2	1.95	0.48
25:Y:127:THR:O	25:Y:131:THR:N	2.46	0.48
25:Y:193:ASP:OD2	25:Y:196:GLN:NE2	2.45	0.48
32:f:368:ALA:HB1	32:f:402:ASN:HA	1.95	0.48
16:p:15:LYS:HE3	16:p:121:ILE:HG12	1.93	0.48
1:A:38:GLN:OE1	2:B:57:GLN:NE2	2.46	0.48
17:Q:52:ASP:OD1	18:R:88:TYR:OH	2.28	0.48
21:U:495:ASP:OD1	21:U:498:LYS:NZ	2.41	0.48
21:U:699:THR:OG1	21:U:810:THR:O	2.30	0.48
32:f:193:PRO:HA	32:f:196:MET:HG3	1.95	0.48
32:f:297:MET:O	32:f:300:ARG:NH1	2.46	0.48
32:f:556:ARG:NH2	32:f:648:ALA:HB2	2.27	0.48
32:f:590:PHE:CE1	32:f:594:LEU:HD23	2.49	0.48
16:p:158:MET:HE1	16:p:162:HIS:CB	2.42	0.48
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.39	0.48
24:X:70:LEU:HD12	24:X:92:LEU:HD22	1.96	0.48
8:h:93:LEU:HD13	8:h:113:ARG:HB3	1.96	0.48
9:i:47:ALA:HB3	9:i:212:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:208:LEU:O	10:j:220:LEU:HB2	2.14	0.48
32:f:389:LYS:HB2	32:f:392:THR:HB	1.96	0.48
4:D:351:LYS:NZ	5:E:163:GLY:O	2.45	0.48
23:W:356:THR:HG22	23:W:357:ARG:HG3	1.94	0.48
24:X:150:GLY:HA2	24:X:154:LEU:HB2	1.95	0.48
32:f:710:LEU:CB	32:f:729:MET:HE2	2.41	0.48
13:m:66:LEU:HD23	13:m:76:ALA:HB2	1.95	0.48
1:A:88:GLN:HG3	32:f:751:TYR:HE1	1.79	0.48
2:B:151:LEU:N	2:B:161:GLY:O	2.40	0.48
10:J:67:ASP:OD1	10:J:67:ASP:N	2.46	0.48
23:W:359:THR:HG22	23:W:397:ILE:HG13	1.95	0.48
24:X:134:VAL:HG11	24:X:149:LEU:HD12	1.96	0.48
26:Z:179:ILE:HD13	29:c:218:LEU:HD12	1.94	0.48
32:f:140:LEU:HD23	32:f:165:GLU:HB3	1.94	0.48
11:k:203:LYS:HA	11:k:210:LEU:HD11	1.95	0.48
33:x:7:THR:C	33:x:9:THR:H	2.21	0.48
3:C:113:ARG:NH2	3:C:128:PRO:O	2.38	0.48
5:E:169:GLY:HA3	5:E:275:MET:SD	2.54	0.48
8:H:3:GLU:HG2	8:H:4:ARG:HG2	1.94	0.48
21:U:889:LEU:HD13	21:U:892:LEU:HD21	1.95	0.48
25:Y:364:TRP:NE1	25:Y:368:GLU:OE2	2.47	0.48
26:Z:136:GLU:OE2	26:Z:157:HIS:ND1	2.42	0.48
28:b:16:MET:HE3	28:b:25:ARG:HB3	1.96	0.48
7:g:138:MET:HE1	7:g:140:LEU:HG	1.96	0.48
10:j:46:GLU:O	10:j:61:LYS:NZ	2.45	0.48
10:j:109:ARG:NH2	18:r:70:ASN:OD1	2.46	0.48
14:n:115:PRO:HG2	14:n:119:MET:HE2	1.96	0.48
33:y:72:ARG:CZ	33:y:73:LEU:HB2	2.44	0.48
21:U:7:GLY:H	30:d:80:CYS:HB2	1.79	0.48
21:U:542:GLU:O	21:U:546:ARG:N	2.44	0.48
21:U:740:GLY:HA3	21:U:744:VAL:HG22	1.96	0.48
22:V:424:HIS:ND1	30:d:249:TYR:OH	2.42	0.48
24:X:1:MET:HE2	24:X:35:ILE:HD12	1.96	0.48
24:X:141:LYS:HD2	24:X:141:LYS:HA	1.72	0.48
26:Z:69:PHE:HE2	28:b:95:LEU:HB3	1.78	0.48
32:f:369:ARG:HH12	32:f:760:PHE:HD1	1.60	0.48
7:g:155:ASP:OD1	7:g:159:TYR:N	2.44	0.48
10:j:11:SER:OG	10:j:15:HIS:N	2.47	0.48
14:n:189:LEU:HD22	14:n:193:GLN:HB3	1.95	0.48
1:A:140:VAL:HG12	1:A:152:PRO:HA	1.96	0.48
2:B:51:LEU:N	2:B:51:LEU:CD1	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:MET:HG3	2:B:78:PHE:CE2	2.49	0.48
2:B:284:ILE:HG23	2:B:287:ILE:HD11	1.96	0.48
3:C:270:GLN:HA	3:C:273:MET:HE3	1.94	0.48
19:S:11:THR:HG21	19:S:141:ALA:HB3	1.96	0.48
22:V:408:LYS:NZ	22:V:409:GLU:O	2.47	0.48
23:W:417:LEU:HA	23:W:421:MET:HE2	1.94	0.48
32:f:53:GLN:HA	32:f:56:LEU:HD12	1.95	0.48
32:f:783:SER:HA	32:f:895:GLU:OE2	2.14	0.48
32:f:852:VAL:HG21	32:f:859:PRO:HA	1.96	0.48
18:r:97:MET:H	18:r:116:SER:HB3	1.79	0.48
1:A:258:ARG:HH12	6:F:255:GLN:HG2	1.79	0.47
2:B:67:ARG:CD	32:f:606:VAL:HG11	2.44	0.47
4:D:83:GLN:O	4:D:87:LEU:HD21	2.14	0.47
9:I:74:CYS:HB2	9:I:134:LEU:HD11	1.95	0.47
11:K:141:LEU:H	11:K:156:MET:HB2	1.79	0.47
20:T:20:VAL:HG11	20:T:122:LEU:HD13	1.96	0.47
23:W:91:GLN:NE2	23:W:92:GLN:OE1	2.46	0.47
27:a:100:THR:HG22	27:a:103:LYS:HE2	1.95	0.47
30:d:78:LEU:HD13	30:d:98:LEU:HD21	1.96	0.47
10:j:221:ASN:CG	10:j:224:GLU:HG2	2.39	0.47
4:D:95:ALA:HA	4:D:101:ALA:HA	1.96	0.47
7:G:23:TYR:HB3	7:G:27:TYR:HE2	1.80	0.47
13:M:15:SER:HB3	13:M:19:ARG:H	1.79	0.47
13:M:214:SER:HA	13:M:227:VAL:HG23	1.96	0.47
18:R:130:SER:OG	18:R:167:ASP:OD2	2.24	0.47
20:T:126:ASP:OD1	20:T:130:VAL:N	2.46	0.47
21:U:500:ASN:O	21:U:503:GLN:NE2	2.45	0.47
24:X:222:GLU:HG3	24:X:225:TRP:HZ2	1.79	0.47
32:f:686:LEU:O	32:f:690:VAL:HG23	2.14	0.47
13:m:37:ILE:HD11	13:m:193:VAL:HG13	1.95	0.47
4:D:39:ASP:OD2	4:D:43:ARG:NH2	2.48	0.47
8:H:106:PRO:HB2	8:H:109:GLN:HG2	1.95	0.47
9:I:219:GLU:OE1	9:I:220:ASN:ND2	2.43	0.47
13:M:39:ILE:HD12	13:M:193:VAL:HG12	1.97	0.47
22:V:158:TYR:OH	22:V:181:ARG:NE	2.47	0.47
23:W:393:ARG:HH11	24:X:349:HIS:CD2	2.32	0.47
24:X:190:LEU:O	24:X:194:ARG:HG2	2.14	0.47
24:X:297:ARG:O	24:X:334:ASN:ND2	2.47	0.47
29:c:198:ARG:O	29:c:199:HIS:HB2	2.15	0.47
29:c:283:HIS:HA	29:c:286:GLU:HG2	1.96	0.47
32:f:151:LEU:HB3	32:f:159:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:107:TRP:HA	20:t:127:MET:HE1	1.96	0.47
33:u:42:ARG:CZ	33:u:72:ARG:CG	2.92	0.47
3:C:145:ASP:OD1	3:C:145:ASP:N	2.45	0.47
6:F:108:GLY:H	29:c:77:GLN:H	1.62	0.47
15:O:63:LEU:HD11	15:O:79:ALA:HB2	1.97	0.47
21:U:695:MET:HE2	21:U:706:VAL:HA	1.96	0.47
23:W:186:ARG:HA	23:W:189:ILE:HG12	1.96	0.47
23:W:299:LEU:HB3	23:W:301:ARG:HH21	1.79	0.47
30:d:131:VAL:HA	30:d:134:LYS:HB3	1.96	0.47
30:d:215:TRP:HE3	30:d:222:TYR:HB3	1.79	0.47
32:f:504:VAL:HG13	32:f:518:THR:HG21	1.96	0.47
32:f:741:LEU:HA	32:f:744:MET:HE3	1.97	0.47
7:g:205:VAL:HG13	7:g:206:LEU:HD12	1.95	0.47
12:l:139:ASP:N	12:l:139:ASP:OD1	2.47	0.47
33:x:60:ASN:ND2	33:y:8:LEU:HB3	2.28	0.47
3:C:182:GLN:HG3	3:C:286:THR:HB	1.97	0.47
4:D:127:ASN:O	4:D:252:ARG:NH1	2.47	0.47
7:G:173:THR:OG1	7:G:174:GLU:OE1	2.32	0.47
8:H:223:PRO:HA	8:H:226:VAL:HB	1.97	0.47
10:J:72:ALA:HB3	10:J:132:LEU:HB2	1.97	0.47
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.47	0.47
21:U:59:PHE:HA	21:U:62:LEU:HD13	1.96	0.47
23:W:441:GLN:HB2	26:Z:103:LYS:HE2	1.97	0.47
32:f:556:ARG:HD3	32:f:590:PHE:CZ	2.49	0.47
32:f:662:MET:HE1	32:f:781:TYR:CE1	2.47	0.47
9:i:190:LEU:HD13	9:i:236:LEU:HD11	1.95	0.47
10:j:120:GLN:HB2	11:k:133:MET:SD	2.54	0.47
12:l:43:HIS:CE1	12:l:184:LEU:HD21	2.49	0.47
4:D:60:TYR:CD1	21:U:603:LEU:HB3	2.50	0.47
12:L:7:ASP:O	12:L:21:GLN:NE2	2.34	0.47
21:U:701:ILE:HD12	21:U:810:THR:HG21	1.97	0.47
31:e:16:ASP:OD1	31:e:16:ASP:N	2.48	0.47
32:f:339:ILE:C	32:f:341:GLU:N	2.71	0.47
19:s:60:ASP:OD1	20:t:97:TYR:OH	2.24	0.47
33:x:57:SER:HG	33:y:73:LEU:HA	1.76	0.47
1:A:231:ASN:ND2	32:f:865:PHE:CE2	2.83	0.47
3:C:80:MET:HE1	3:C:86:LEU:HB2	1.95	0.47
3:C:90:HIS:CE1	4:D:110:ASN:HB2	2.50	0.47
4:D:229:ARG:HE	5:E:267:PHE:HD2	1.62	0.47
5:E:3:ASP:OD1	5:E:3:ASP:N	2.47	0.47
6:F:413:THR:OG1	6:F:414:GLU:OE1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:30:ASP:OD1	17:Q:30:ASP:N	2.42	0.47
21:U:26:LYS:NZ	30:d:34:ASN:OD1	2.33	0.47
21:U:173:VAL:HA	21:U:176:MET:HB2	1.96	0.47
21:U:519:VAL:HG23	21:U:520:MET:SD	2.54	0.47
21:U:768:GLN:HB2	21:U:775:LEU:HD22	1.95	0.47
24:X:333:GLN:O	24:X:336:ILE:HG13	2.14	0.47
24:X:397:TYR:HE1	26:Z:258:VAL:HG11	1.80	0.47
26:Z:144:VAL:HG22	26:Z:151:THR:HA	1.96	0.47
29:c:107:MET:HE1	33:u:9:THR:O	2.15	0.47
30:d:236:THR:O	30:d:239:SER:OG	2.28	0.47
32:f:586:PRO:O	32:f:587:PHE:C	2.57	0.47
7:g:50:ILE:HG21	7:g:79:VAL:HB	1.97	0.47
20:t:184:TYR:HE2	20:t:186:ARG:HD3	1.80	0.47
1:A:297:ARG:HH22	6:F:306:VAL:HG21	1.79	0.47
3:C:347:ILE:HG23	3:C:387:VAL:HG21	1.95	0.47
4:D:57:GLN:O	4:D:61:ILE:HG12	2.15	0.47
12:L:49:LEU:HB3	12:L:195:LEU:HD21	1.96	0.47
19:S:184:GLU:HA	19:S:211:ARG:HH11	1.80	0.47
20:T:25:ASP:HA	20:T:187:PHE:HA	1.97	0.47
24:X:333:GLN:O	24:X:337:ARG:HB2	2.15	0.47
32:f:749:ALA:HB2	32:f:762:VAL:HG11	1.97	0.47
1:A:255:ARG:HA	1:A:258:ARG:HG2	1.96	0.47
1:A:362:MET:HE1	2:B:216:ILE:HD11	1.97	0.47
2:B:383:LEU:HD22	2:B:423:LYS:HD2	1.95	0.47
6:F:98:ASP:HB3	6:F:120:LYS:HD2	1.96	0.47
7:G:113:MET:HE3	7:G:113:MET:HB3	1.82	0.47
15:O:54:MET:HG2	16:P:96:TYR:CZ	2.50	0.47
17:Q:18:ASP:OD1	17:Q:18:ASP:N	2.46	0.47
21:U:415:HIS:O	21:U:450:HIS:NE2	2.48	0.47
28:b:124:LEU:HD21	28:b:152:LYS:HB3	1.97	0.47
16:p:87:LEU:HA	16:p:90:MET:HG3	1.97	0.47
4:D:341:LYS:NZ	4:D:367:PRO:O	2.42	0.47
5:E:200:SER:OG	5:E:233:ASP:O	2.25	0.47
15:O:42:TYR:HE2	15:O:183:LEU:HD11	1.80	0.47
16:P:38:ASP:OD1	16:P:38:ASP:N	2.48	0.47
23:W:431:ILE:HB	26:Z:226:ILE:HD11	1.95	0.47
26:Z:262:LEU:O	26:Z:266:ILE:HG12	2.14	0.47
32:f:849:ALA:HB1	32:f:879:ARG:NH2	2.30	0.47
16:p:47:ASP:OD1	16:p:47:ASP:N	2.44	0.47
33:x:38:PRO:O	33:x:40:GLN:N	2.48	0.47
1:A:238:ILE:HB	1:A:272:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:232:GLY:HA3	5:E:258:MET:HE1	1.97	0.46
25:Y:223:THR:HA	25:Y:226:VAL:CG1	2.45	0.46
32:f:72:ARG:NH2	32:f:113:MET:SD	2.86	0.46
32:f:535:THR:HA	32:f:538:ILE:HG22	1.97	0.46
17:q:168:GLN:NE2	17:q:175:LEU:O	2.48	0.46
12:L:4:ASN:OD1	12:L:5:GLN:NE2	2.48	0.46
13:M:34:SER:OG	13:M:65:ARG:NH1	2.43	0.46
18:R:154:ASP:OD1	18:R:157:ARG:NH2	2.42	0.46
21:U:109:THR:OG1	21:U:156:GLU:O	2.33	0.46
21:U:759:SER:HA	21:U:782:ALA:HA	1.98	0.46
22:V:61:TYR:HD1	22:V:82:LEU:HD11	1.81	0.46
22:V:66:GLY:HA2	22:V:95:ARG:HD3	1.97	0.46
22:V:78:LEU:HD11	22:V:134:ILE:HD12	1.97	0.46
22:V:302:ARG:HH11	31:e:12:TRP:HB2	1.80	0.46
32:f:83:ARG:HH21	32:f:153:SER:HB2	1.80	0.46
32:f:285:CYS:O	32:f:291:GLN:NE2	2.46	0.46
10:j:156:TRP:CZ2	11:k:59:MET:HE1	2.50	0.46
3:C:234:LEU:HA	3:C:237:MET:SD	2.54	0.46
10:J:170:GLU:HA	10:J:173:GLU:HG3	1.96	0.46
16:P:51:ILE:HG22	16:P:109:ILE:HG12	1.97	0.46
22:V:142:ILE:HG12	22:V:150:LEU:HD21	1.98	0.46
25:Y:50:MET:O	25:Y:54:TYR:N	2.47	0.46
26:Z:70:LEU:HD12	26:Z:111:LEU:HD22	1.97	0.46
9:i:180:LYS:HB2	9:i:184:MET:HE3	1.97	0.46
7:G:80:MET:HE1	7:G:138:MET:HE1	1.98	0.46
11:K:212:ALA:HA	11:K:234:LEU:HD22	1.97	0.46
18:R:1:THR:HA	18:R:33:LYS:HZ3	1.80	0.46
27:a:87:MET:SD	27:a:88:THR:N	2.89	0.46
28:b:126:LYS:HA	28:b:129:LYS:HG2	1.98	0.46
29:c:196:LEU:O	29:c:198:ARG:N	2.48	0.46
30:d:106:LEU:HD21	30:d:114:GLU:HB2	1.97	0.46
32:f:343:LYS:HA	32:f:347:ASP:OD2	2.16	0.46
32:f:385:PHE:CZ	32:f:773:LYS:HD2	2.50	0.46
12:l:117:GLN:O	12:l:120:THR:OG1	2.29	0.46
19:s:125:ASP:OD1	19:s:129:SER:N	2.48	0.46
2:B:427:LEU:O	2:B:431:GLN:HB2	2.15	0.46
3:C:332:HIS:CD2	3:C:360:LYS:HD2	2.50	0.46
4:D:199:PRO:HB3	4:D:328:ASP:HB2	1.98	0.46
10:J:57:ARG:O	10:J:60:ARG:NH1	2.48	0.46
10:J:119:THR:HG22	10:J:126:PRO:HB3	1.98	0.46
12:L:157:ARG:NH1	13:M:56:LYS:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:151:ASN:OD1	19:S:158:MET:HE2	2.15	0.46
23:W:90:VAL:HG21	23:W:123:VAL:HG12	1.98	0.46
23:W:404:LYS:NZ	23:W:412:ASP:OD2	2.39	0.46
24:X:171:LEU:HD11	24:X:210:LEU:HA	1.98	0.46
17:q:7:ILE:HB	17:q:14:LEU:HB3	1.97	0.46
14:N:14:LEU:HB2	14:N:177:ALA:HB3	1.96	0.46
22:V:408:LYS:HD2	22:V:408:LYS:HA	1.78	0.46
25:Y:162:GLU:HA	25:Y:165:LYS:HG2	1.98	0.46
27:a:100:THR:HA	27:a:103:LYS:HG2	1.98	0.46
32:f:349:TYR:CD1	32:f:350:LYS:HG2	2.51	0.46
13:m:68:ASN:OD1	13:m:224:HIS:ND1	2.37	0.46
13:m:117:MET:O	13:m:117:MET:HE3	2.16	0.46
2:B:233:THR:N	37:B:501:ADP:O1A	2.39	0.46
4:D:267:ILE:HD13	4:D:309:MET:HG3	1.98	0.46
21:U:214:ILE:HD12	21:U:904:LYS:HZ3	1.80	0.46
32:f:845:ARG:O	32:f:880:ALA:HA	2.16	0.46
7:g:46:ASP:N	7:g:46:ASP:OD1	2.48	0.46
9:i:40:ASN:OD1	9:i:182:GLY:O	2.34	0.46
10:j:155:ALA:HB3	11:k:63:SER:HB2	1.96	0.46
18:r:115:ASP:OD1	18:r:119:ASN:N	2.48	0.46
19:s:148:LEU:HD23	19:s:178:VAL:HG12	1.96	0.46
2:B:116:ILE:HG22	2:B:117:ASP:H	1.81	0.46
3:C:44:ARG:HB2	22:V:442:ARG:NH1	2.29	0.46
3:C:57:ARG:HH22	21:U:649:ARG:HD3	1.81	0.46
24:X:296:ASN:O	24:X:337:ARG:NH1	2.48	0.46
25:Y:288:PHE:HA	25:Y:291:HIS:HD2	1.81	0.46
32:f:416:MET:SD	32:f:416:MET:N	2.89	0.46
32:f:594:LEU:HD12	32:f:595:VAL:N	2.31	0.46
16:p:45:MET:HE3	16:p:51:ILE:CG2	2.46	0.46
33:x:63:LYS:HE2	33:x:63:LYS:HB3	1.54	0.46
33:y:6:LYS:CG	33:y:66:THR:HG23	2.31	0.46
14:N:70:LEU:HB3	14:N:72:GLU:HG3	1.98	0.46
16:P:124:LEU:HG	16:P:130:PRO:HA	1.98	0.46
22:V:192:ASP:N	22:V:192:ASP:OD1	2.47	0.46
23:W:168:VAL:HG11	23:W:207:LEU:HD21	1.98	0.46
24:X:307:THR:HA	24:X:310:ARG:HE	1.81	0.46
26:Z:226:ILE:HG22	26:Z:230:LEU:HB2	1.98	0.46
29:c:196:LEU:C	29:c:198:ARG:N	2.73	0.46
32:f:202:HIS:CE1	32:f:203:GLU:HG3	2.51	0.46
32:f:382:ASN:HA	32:f:385:PHE:CD2	2.51	0.46
32:f:803:PHE:CD2	32:f:810:ILE:HG13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ARG:HD3	32:f:858:LYS:CB	2.40	0.46
4:D:171:ASP:OD1	4:D:171:ASP:N	2.47	0.46
6:F:169:ASP:HB3	6:F:172:VAL:HG23	1.97	0.46
10:J:38:ARG:NE	10:J:182:GLU:HA	2.30	0.46
16:P:14:MET:HE1	16:P:136:PHE:HB3	1.98	0.46
22:V:172:ASP:N	22:V:172:ASP:OD1	2.47	0.46
22:V:342:ILE:HA	22:V:345:LEU:HD12	1.98	0.46
27:a:25:LEU:HD22	27:a:44:PHE:HE2	1.81	0.46
32:f:534:VAL:HG23	32:f:565:ASN:ND2	2.31	0.46
16:p:191:GLU:CD	16:p:192:LYS:H	2.23	0.46
33:x:62:GLN:OE1	33:x:62:GLN:N	2.32	0.46
2:B:150:VAL:HG12	2:B:162:VAL:HG23	1.97	0.45
4:D:85:ILE:HB	4:D:86:PRO:CD	2.47	0.45
13:M:8:ASP:O	13:M:22:GLN:NE2	2.40	0.45
21:U:713:TYR:HB3	21:U:734:GLN:HE21	1.81	0.45
22:V:66:GLY:O	22:V:69:THR:OG1	2.31	0.45
25:Y:142:PHE:HE2	25:Y:176:ARG:HD2	1.82	0.45
26:Z:265:LEU:O	26:Z:268:SER:OG	2.28	0.45
29:c:88:ASP:N	29:c:88:ASP:OD1	2.48	0.45
32:f:294:MET:HA	32:f:297:MET:HG3	1.98	0.45
32:f:517:VAL:HG22	32:f:557:TRP:HZ3	1.81	0.45
10:j:73:PHE:HE2	10:j:77:THR:HG22	1.81	0.45
14:n:167:ASP:HB3	14:n:170:SER:HB2	1.99	0.45
1:A:82:ALA:HB3	2:B:98:LYS:HE2	1.97	0.45
6:F:348:LEU:O	6:F:351:LYS:NZ	2.49	0.45
10:J:39:ASP:OD1	10:J:39:ASP:N	2.49	0.45
18:R:196:HIS:CE1	16:p:204:MET:HG3	2.50	0.45
21:U:579:ARG:O	21:U:583:MET:HG2	2.17	0.45
26:Z:148:GLY:HA3	27:a:181:GLY:HA3	1.97	0.45
29:c:178:THR:O	29:c:183:HIS:ND1	2.49	0.45
32:f:553:THR:HA	32:f:556:ARG:HE	1.80	0.45
19:s:99:ARG:HG2	19:s:102:PHE:HB3	1.98	0.45
33:x:25:ASN:O	33:x:28:ALA:HB3	2.17	0.45
3:C:378:VAL:HG12	3:C:383:PHE:CE1	2.52	0.45
9:I:137:ILE:HD12	9:I:216:LEU:HD23	1.98	0.45
10:J:71:MET:HG2	10:J:84:ILE:HD12	1.98	0.45
11:K:121:LEU:HD12	12:L:79:ALA:HB3	1.98	0.45
14:N:141:ALA:HB2	14:n:162:LEU:HD11	1.98	0.45
24:X:335:LEU:C	24:X:337:ARG:H	2.25	0.45
29:c:279:ASP:OD1	29:c:279:ASP:N	2.48	0.45
30:d:5:LEU:HD11	30:d:50:LEU:HD23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:j:154:HIS:HB2	10:j:156:TRP:HE1	1.81	0.45
11:k:141:LEU:H	11:k:156:MET:HB3	1.81	0.45
11:k:221:GLN:HB3	11:k:224:GLN:HG2	1.98	0.45
33:x:19:PRO:HG3	33:y:75:GLY:N	2.31	0.45
16:P:130:PRO:C	16:P:131:MET:HE2	2.42	0.45
21:U:351:MET:HE3	21:U:355:ASN:HB3	1.98	0.45
21:U:695:MET:SD	21:U:698:GLN:HB2	2.56	0.45
24:X:316:ASP:HB3	24:X:319:ILE:HG23	1.98	0.45
32:f:343:LYS:HZ2	32:f:773:LYS:CG	2.29	0.45
12:l:65:HIS:NE2	12:l:220:GLU:OE2	2.49	0.45
12:l:172:LEU:O	12:l:176:MET:HG3	2.15	0.45
15:o:112:SER:HB3	15:o:125:VAL:HG11	1.98	0.45
33:x:55:THR:OG1	33:y:73:LEU:HD13	2.17	0.45
1:A:276:GLU:OE2	2:B:314:ASN:ND2	2.50	0.45
1:A:360:ARG:CG	32:f:858:LYS:CD	2.90	0.45
6:F:106:GLU:HG2	26:Z:87:ALA:H	1.81	0.45
6:F:438:TYR:O	6:F:439:ALA:HB3	2.16	0.45
7:G:89:SER:HB3	13:M:117:MET:HE2	1.97	0.45
19:S:141:ALA:HA	19:S:144:MET:HE2	1.99	0.45
21:U:100:ILE:HA	21:U:103:LYS:HE3	1.97	0.45
27:a:312:MET:HE3	27:a:312:MET:HB3	1.88	0.45
27:a:373:ASP:N	27:a:373:ASP:OD1	2.49	0.45
32:f:352:HIS:CD2	32:f:353:LEU:H	2.34	0.45
32:f:416:MET:HE1	32:f:819:TYR:CE1	2.49	0.45
12:l:200:PRO:HD2	12:l:203:GLN:HG3	1.98	0.45
13:m:228:PRO:HD2	13:m:231:ILE:HD12	1.99	0.45
4:D:121:ARG:HA	4:D:124:LEU:HD23	1.98	0.45
5:E:290:LEU:HD23	5:E:295:LEU:HD13	1.98	0.45
7:G:245:ARG:HD3	23:W:37:LYS:HZ2	1.81	0.45
21:U:148:LYS:HA	21:U:151:ILE:HG22	1.99	0.45
26:Z:124:ILE:HG22	26:Z:135:THR:HG22	1.99	0.45
26:Z:140:SER:HA	26:Z:155:PHE:HA	1.99	0.45
26:Z:140:SER:HB2	26:Z:155:PHE:HD1	1.81	0.45
28:b:97:LEU:HB3	28:b:107:MET:HE1	1.98	0.45
32:f:646:MET:O	32:f:649:HIS:HB3	2.16	0.45
17:q:11:ASP:N	17:q:11:ASP:OD1	2.46	0.45
20:t:7:THR:OG1	20:t:29:SER:OG	2.27	0.45
33:y:17:VAL:HG21	33:y:56:LEU:CD1	2.47	0.45
3:C:182:GLN:NE2	3:C:286:THR:HB	2.32	0.45
16:P:70:ARG:HD2	16:P:94:LEU:HD12	1.98	0.45
21:U:719:ASP:HB3	21:U:722:ASP:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:364:ILE:HD12	22:V:369:ILE:HB	1.99	0.45
23:W:257:LEU:HD23	23:W:257:LEU:HA	1.86	0.45
23:W:390:LYS:HA	24:X:342:PHE:HA	1.98	0.45
26:Z:6:VAL:HG23	26:Z:48:LEU:HD23	1.99	0.45
26:Z:39:LEU:H	26:Z:94:TRP:HA	1.81	0.45
27:a:321:LYS:O	27:a:334:THR:OG1	2.27	0.45
28:b:94:HIS:NE2	28:b:134:GLU:OE2	2.49	0.45
32:f:371:ASN:OD1	32:f:398:TRP:NE1	2.45	0.45
32:f:385:PHE:CZ	32:f:773:LYS:CD	2.99	0.45
32:f:429:ILE:HG23	32:f:444:ALA:HB1	1.99	0.45
15:o:17:ASP:OD1	15:o:17:ASP:N	2.46	0.45
20:t:9:THR:O	20:t:54:SER:OG	2.28	0.45
1:A:83:ASP:O	1:A:86:THR:OG1	2.30	0.45
1:A:209:PRO:HD3	6:F:405:MET:HE1	1.99	0.45
3:C:196:LYS:HA	3:C:317:PHE:HE2	1.82	0.45
13:M:55:SER:OG	13:M:56:LYS:N	2.49	0.45
22:V:165:TYR:HD2	22:V:174:VAL:HG22	1.82	0.45
23:W:189:ILE:HA	23:W:192:LYS:HE2	1.99	0.45
25:Y:247:LEU:HD23	25:Y:250:LEU:HD21	1.98	0.45
27:a:163:TYR:CG	27:a:172:TYR:HB2	2.52	0.45
28:b:51:LEU:HD23	28:b:71:ILE:HG23	1.99	0.45
29:c:242:GLU:OE2	29:c:246:LYS:NZ	2.46	0.45
32:f:449:GLY:HA2	32:f:488:ALA:HB2	1.99	0.45
33:y:50:LEU:CD2	33:y:59:TYR:CD2	3.00	0.45
1:A:327:LEU:HD12	1:A:331:LEU:HD11	1.98	0.45
5:E:64:LEU:HD12	5:E:68:LYS:HG2	1.99	0.45
6:F:233:LYS:NZ	35:F:501:ATP:O1B	2.42	0.45
15:O:19:ARG:NH2	19:s:213:ASP:OD2	2.45	0.45
20:T:184:TYR:HE2	20:T:186:ARG:HD3	1.82	0.45
24:X:420:LYS:HA	24:X:420:LYS:HD3	1.82	0.45
27:a:34:TRP:HD1	28:b:18:ASN:HA	1.81	0.45
29:c:163:ILE:HD12	29:c:163:ILE:HA	1.91	0.45
32:f:556:ARG:HB3	32:f:590:PHE:CE1	2.52	0.45
16:p:53:LEU:HB3	16:p:60:VAL:HG22	1.98	0.45
1:A:98:CYS:HB2	1:A:139:ARG:HH12	1.82	0.45
4:D:50:GLU:HA	4:D:53:PHE:HB3	1.98	0.45
6:F:98:ASP:OD1	6:F:98:ASP:N	2.50	0.45
8:H:74:LEU:HD12	8:H:87:VAL:HG22	1.98	0.45
16:P:135:ASP:OD1	16:P:135:ASP:N	2.49	0.45
32:f:557:TRP:HD1	32:f:560:LEU:HD12	1.82	0.45
7:g:221:THR:HB	7:g:224:ASN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:140:ASP:OD1	9:i:144:GLY:N	2.50	0.45
1:A:112:ILE:HG12	1:A:122:VAL:HG22	1.99	0.44
4:D:393:ILE:HD12	23:W:119:GLY:HA2	1.98	0.44
10:J:90:GLU:HG3	10:J:110:TYR:CZ	2.51	0.44
13:M:68:ASN:OD1	13:M:224:HIS:ND1	2.44	0.44
21:U:254:GLU:OE2	21:U:751:ARG:NH1	2.50	0.44
24:X:87:ARG:HG3	24:X:90:ARG:NH2	2.32	0.44
25:Y:105:MET:HE3	25:Y:136:HIS:CD2	2.52	0.44
26:Z:165:GLU:HB3	26:Z:168:GLU:HG2	1.98	0.44
7:g:88:ARG:HE	7:g:88:ARG:HB3	1.57	0.44
8:h:204:THR:OG1	8:h:206:ASP:OD1	2.32	0.44
2:B:170:LEU:HA	2:B:173:VAL:HB	1.99	0.44
4:D:296:MET:HA	4:D:299:PHE:CZ	2.52	0.44
6:F:93:VAL:HG12	6:F:149:ASP:H	1.82	0.44
16:P:203:ARG:HH11	16:P:204:MET:H	1.65	0.44
22:V:48:LEU:HD11	22:V:116:LEU:HD11	1.99	0.44
24:X:97:LEU:HB2	24:X:132:ARG:NH2	2.32	0.44
32:f:79:ARG:HB2	32:f:125:ILE:HD11	1.98	0.44
32:f:267:ARG:NH1	32:f:893:ILE:HD12	2.33	0.44
12:l:66:VAL:O	19:s:77:HIS:HE1	2.00	0.44
16:p:45:MET:HE3	16:p:51:ILE:HB	2.00	0.44
1:A:38:GLN:CG	1:A:42:SER:HB3	2.45	0.44
2:B:440:LEU:HG	10:J:61:LYS:HD2	1.99	0.44
5:E:286:ASP:HB3	5:E:289:LEU:HG	1.99	0.44
8:H:79:MET:HG2	8:H:82:ASP:OD2	2.17	0.44
9:I:37:ILE:HD12	9:I:193:ALA:HB2	1.99	0.44
11:K:78:MET:HE1	11:K:82:ILE:HA	1.98	0.44
15:O:163:ILE:HG12	15:O:170:GLY:HA2	1.98	0.44
16:P:189:ILE:HB	16:P:196:THR:HB	1.99	0.44
20:T:15:LYS:HD2	20:T:120:SER:HB2	1.99	0.44
25:Y:314:LEU:O	25:Y:354:VAL:N	2.49	0.44
2:B:234:LEU:HD11	37:B:501:ADP:H2'	1.99	0.44
3:C:232:ARG:NH2	3:C:275:GLU:O	2.50	0.44
3:C:285:ALA:O	3:C:287:LYS:N	2.50	0.44
5:E:36:LEU:HA	5:E:39:GLN:CD	2.42	0.44
6:F:289:ASP:OD1	6:F:289:ASP:N	2.49	0.44
10:J:65:LEU:C	17:Q:69:MET:HE2	2.42	0.44
10:J:89:VAL:HG22	17:Q:66:LEU:HD21	1.98	0.44
15:O:21:THR:HG22	15:O:26:VAL:HG22	2.00	0.44
20:T:173:MET:HE1	20:T:187:PHE:CE2	2.53	0.44
23:W:159:TYR:HB3	23:W:162:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:440:LEU:H	23:W:440:LEU:HG	1.61	0.44
27:a:34:TRP:HZ3	27:a:64:ILE:HG23	1.83	0.44
30:d:23:LEU:HA	30:d:26:LEU:HD12	2.00	0.44
32:f:65:GLU:O	32:f:67:ASP:N	2.51	0.44
32:f:339:ILE:HG13	32:f:773:LYS:CD	2.38	0.44
18:r:39:PRO:HA	18:r:184:TRP:HE1	1.82	0.44
33:y:67:LEU:N	33:y:67:LEU:HD12	2.33	0.44
3:C:280:LEU:HD23	3:C:310:ARG:HB3	2.00	0.44
5:E:225:HIS:HB2	5:E:228:CYS:SG	2.57	0.44
7:G:244:GLU:O	23:W:37:LYS:NZ	2.46	0.44
14:N:167:ASP:HB3	14:N:170:SER:HB2	1.99	0.44
21:U:194:ARG:O	21:U:198:LEU:HB2	2.17	0.44
23:W:350:ILE:HA	23:W:353:LYS:HD2	2.00	0.44
29:c:100:LYS:HG2	29:c:105:PRO:HA	1.98	0.44
32:f:343:LYS:NZ	32:f:773:LYS:HD3	2.33	0.44
8:h:29:VAL:HG21	8:h:151:PRO:HG2	1.99	0.44
9:i:133:SER:HB3	9:i:164:ILE:HD13	1.99	0.44
10:j:140:GLY:HA3	10:j:213:ARG:HE	1.82	0.44
2:B:153:ASN:O	2:B:157:HIS:ND1	2.50	0.44
6:F:380:ASN:HB3	6:F:383:GLU:HB2	1.98	0.44
23:W:110:ILE:HG21	23:W:134:LEU:HD13	2.00	0.44
24:X:82:LYS:HE3	24:X:122:ARG:NH2	2.33	0.44
24:X:268:GLN:HA	24:X:271:VAL:HG22	1.99	0.44
24:X:333:GLN:HA	24:X:336:ILE:HG12	1.99	0.44
25:Y:221:THR:O	25:Y:225:TYR:CE2	2.70	0.44
26:Z:82:PHE:HA	26:Z:85:VAL:HG12	1.99	0.44
27:a:217:LEU:O	27:a:218:MET:HE2	2.17	0.44
27:a:290:GLN:HG2	27:a:330:ARG:HD3	1.98	0.44
32:f:412:ALA:CB	32:f:819:TYR:OH	2.66	0.44
7:g:51:VAL:HG12	7:g:217:VAL:HG22	2.00	0.44
10:j:211:MET:HB2	10:j:217:LEU:HD13	2.00	0.44
3:C:369:TYR:HD1	3:C:372:ARG:HE	1.66	0.44
18:R:10:HIS:O	18:R:178:HIS:NE2	2.44	0.44
27:a:78:GLU:O	27:a:81:LEU:HG	2.18	0.44
12:l:7:ASP:OD1	12:l:21:GLN:NE2	2.51	0.44
12:l:88:MET:HE2	12:l:88:MET:HB2	1.74	0.44
19:s:6:VAL:HG12	19:s:57:PHE:HE1	1.82	0.44
19:s:48:ASP:OD1	19:s:48:ASP:N	2.50	0.44
5:E:69:PHE:HZ	5:E:89:LYS:HD3	1.82	0.44
11:K:203:LYS:HB2	11:K:210:LEU:HD22	1.99	0.44
13:M:76:ALA:O	13:M:136:MET:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:99:ARG:NH2	13:M:105:ASN:OD1	2.36	0.44
14:N:20:THR:HB	14:N:28:ASN:HB3	1.99	0.44
16:P:121:ILE:HD12	16:P:137:VAL:HG22	2.00	0.44
19:S:19:ASP:N	19:S:19:ASP:OD1	2.51	0.44
20:T:50:MET:HE3	20:T:192:VAL:HB	1.99	0.44
21:U:770:TRP:O	29:c:178:THR:OG1	2.35	0.44
23:W:172:LEU:HD23	23:W:175:MET:HE3	1.99	0.44
25:Y:51:ALA:HA	25:Y:54:TYR:HB3	1.98	0.44
25:Y:112:CYS:HB3	25:Y:124:PHE:HE2	1.83	0.44
25:Y:224:VAL:HG21	25:Y:256:VAL:HG13	1.99	0.44
32:f:662:MET:HB2	32:f:662:MET:HE2	1.76	0.44
32:f:858:LYS:HA	32:f:859:PRO:HD3	1.68	0.44
10:j:8:THR:HG21	11:k:134:SER:HB3	2.00	0.44
13:m:8:ASP:N	13:m:8:ASP:OD1	2.51	0.44
15:o:46:ALA:HB3	15:o:97:ALA:HB3	1.98	0.44
2:B:103:ARG:HB2	2:B:160:ILE:HD13	2.00	0.44
3:C:249:ASP:N	3:C:249:ASP:OD1	2.50	0.44
5:E:102:MET:SD	5:E:102:MET:N	2.85	0.44
6:F:235:LEU:HD11	35:F:501:ATP:C4	2.53	0.44
6:F:384:LEU:O	6:F:388:THR:OG1	2.27	0.44
11:K:161:THR:HG23	12:L:78:THR:HG21	2.00	0.44
16:P:11:VAL:HG23	16:P:24:ALA:HB2	1.99	0.44
21:U:167:ILE:HB	21:U:177:LEU:HD11	2.00	0.44
23:W:417:LEU:HD11	29:c:305:ASP:HB3	1.99	0.44
32:f:352:HIS:CG	32:f:353:LEU:N	2.85	0.44
32:f:557:TRP:CD1	32:f:560:LEU:HD12	2.52	0.44
7:g:57:PRO:HD2	7:g:61:LEU:HD12	2.00	0.44
8:h:51:LYS:HB3	8:h:207:ASN:HB2	2.00	0.44
20:t:97:TYR:HA	20:t:100:ARG:HG2	2.00	0.44
4:D:303:VAL:HG12	4:D:305:VAL:HG23	1.99	0.43
5:E:109:ARG:HH11	5:E:111:LEU:HD23	1.83	0.43
6:F:217:ILE:HG13	6:F:218:GLN:H	1.83	0.43
17:Q:137:PHE:HB3	18:r:133:VAL:HG21	1.99	0.43
21:U:398:ASN:CB	29:c:174:PRO:HB3	2.47	0.43
25:Y:11:LEU:HG	25:Y:179:ARG:HH11	1.83	0.43
29:c:29:GLU:OE2	29:c:139:ARG:NH2	2.51	0.43
9:i:42:GLY:HA3	9:i:186:LEU:HD21	2.00	0.43
10:j:185:ASP:OD1	10:j:185:ASP:N	2.49	0.43
16:p:124:LEU:HD23	16:p:128:GLY:HA2	1.99	0.43
19:s:38:ARG:HG3	20:t:151:ARG:HH22	1.83	0.43
2:B:343:ARG:HH21	2:B:346:ARG:HH21	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:44:ARG:HD3	22:V:442:ARG:NH2	2.33	0.43
5:E:254:GLN:HA	5:E:257:LEU:HG	1.99	0.43
13:M:230:ASP:OD1	13:M:230:ASP:N	2.49	0.43
16:P:149:MET:HE3	19:s:147:PRO:HB2	2.00	0.43
21:U:557:TYR:HB2	21:U:588:MET:HE1	2.00	0.43
24:X:343:SER:HA	24:X:387:ILE:HB	1.99	0.43
27:a:35:HIS:CD2	28:b:15:TYR:HA	2.54	0.43
30:d:55:LEU:HB2	30:d:78:LEU:HD21	2.00	0.43
32:f:586:PRO:O	32:f:589:SER:N	2.47	0.43
32:f:862:ILE:HD11	32:f:879:ARG:HD2	2.00	0.43
13:m:150:MET:HE3	13:m:151:ILE:N	2.33	0.43
14:n:115:PRO:HG3	20:t:36:PHE:HZ	1.83	0.43
16:p:38:ASP:N	16:p:38:ASP:OD1	2.50	0.43
33:y:8:LEU:CD2	33:y:69:LEU:O	2.65	0.43
33:y:45:PHE:O	33:y:46:ALA:C	2.61	0.43
3:C:258:ARG:HG3	3:C:259:LEU:H	1.83	0.43
3:C:338:LEU:O	25:Y:207:THR:OG1	2.28	0.43
5:E:69:PHE:HD2	5:E:82:GLY:HA2	1.82	0.43
8:H:67:PRO:HA	8:H:73:GLY:HA2	1.99	0.43
12:L:50:LYS:HB3	12:L:59:HIS:HB3	2.00	0.43
17:Q:38:MET:CG	17:Q:44:LEU:HD23	2.48	0.43
22:V:344:ARG:HH21	30:d:116:HIS:CD2	2.35	0.43
23:W:325:VAL:CG1	23:W:335:ARG:HD3	2.49	0.43
26:Z:74:TYR:CD2	26:Z:78:MET:HE1	2.53	0.43
28:b:4:GLU:HA	28:b:106:LYS:H	1.83	0.43
29:c:130:GLN:NE2	29:c:134:GLU:OE2	2.45	0.43
32:f:550:LEU:HD11	32:f:585:GLU:CG	2.48	0.43
32:f:851:ASP:O	32:f:855:GLN:NE2	2.51	0.43
7:g:18:PRO:O	7:g:19:GLU:CB	2.65	0.43
33:y:70:VAL:C	33:y:71:LEU:HD12	2.42	0.43
2:B:438:LEU:HB2	9:I:155:ASN:HD22	1.84	0.43
8:H:175:GLU:HG2	9:I:54:LYS:HE2	2.01	0.43
21:U:198:LEU:HD21	21:U:219:CYS:HB2	2.01	0.43
21:U:360:VAL:HG21	21:U:392:TRP:HZ2	1.83	0.43
27:a:106:SER:OG	27:a:107:SER:N	2.51	0.43
27:a:273:GLN:HB3	27:a:310:LEU:HD11	2.00	0.43
32:f:502:LEU:HA	32:f:505:MET:HE1	2.00	0.43
32:f:590:PHE:CD2	32:f:648:ALA:HB1	2.54	0.43
32:f:830:LEU:HD12	32:f:896:GLY:O	2.19	0.43
33:y:18:GLU:O	33:y:21:ASP:N	2.49	0.43
1:A:189:GLU:O	1:A:193:THR:OG1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:SER:OG	3:C:205:HIS:HB3	2.18	0.43
5:E:172:LEU:HD12	5:E:301:ILE:HD11	2.00	0.43
5:E:251:ARG:O	5:E:255:ARG:HG2	2.18	0.43
6:F:97:LEU:O	6:F:121:CYS:N	2.41	0.43
7:G:13:ILE:HG13	7:G:15:ILE:HG12	1.99	0.43
15:O:32:SER:HB2	15:O:187:ARG:HH12	1.83	0.43
21:U:234:GLU:O	21:U:238:LYS:HG2	2.18	0.43
24:X:347:ILE:HA	24:X:350:ILE:HG22	1.99	0.43
28:b:140:ILE:HB	28:b:170:LEU:HD12	2.00	0.43
29:c:192:LEU:CA	29:c:196:LEU:HB2	2.41	0.43
32:f:343:LYS:HD2	32:f:773:LYS:HG2	2.00	0.43
32:f:894:LEU:HA	32:f:898:VAL:HG21	2.01	0.43
16:p:14:MET:HB3	16:p:21:ALA:HB3	2.00	0.43
17:q:38:MET:HE3	17:q:44:LEU:HB3	2.00	0.43
34:v:25:LYS:O	34:v:27:UNK:N	2.51	0.43
1:A:34:LYS:NZ	1:A:43:ARG:HH11	2.16	0.43
4:D:380:GLN:HG2	5:E:164:ILE:HG23	2.00	0.43
6:F:367:GLN:HG2	6:F:371:ARG:HH12	1.84	0.43
10:J:4:ASP:HA	10:J:122:ASN:HB3	1.99	0.43
16:P:138:VAL:HG11	16:P:146:MET:HB3	1.99	0.43
21:U:124:LYS:HB2	21:U:124:LYS:HE2	1.76	0.43
21:U:803:LYS:O	21:U:893:THR:N	2.40	0.43
21:U:886:PRO:HA	21:U:889:LEU:HD23	2.00	0.43
26:Z:120:VAL:HG22	26:Z:139:ILE:HD13	2.01	0.43
26:Z:206:LEU:HD23	26:Z:209:ARG:HD3	2.00	0.43
32:f:240:VAL:O	32:f:245:ASN:ND2	2.40	0.43
32:f:523:GLY:HA3	32:f:561:GLY:HA2	2.00	0.43
32:f:585:GLU:CD	32:f:585:GLU:N	2.75	0.43
7:g:38:THR:HG21	7:g:206:LEU:HD11	2.01	0.43
10:j:110:TYR:CE1	10:j:114:LEU:HD21	2.54	0.43
11:k:235:GLU:HA	11:k:238:ILE:HB	2.00	0.43
33:u:37:PRO:HA	33:u:38:PRO:HD3	1.92	0.43
1:A:155:PRO:HG2	1:A:157:ILE:HD11	2.01	0.43
4:D:391:ARG:HG2	4:D:393:ILE:H	1.82	0.43
5:E:36:LEU:HD11	6:F:73:ILE:HG21	1.99	0.43
13:M:171:ALA:HA	13:M:174:THR:HG22	2.01	0.43
17:Q:53:THR:HG22	17:Q:100:VAL:HG12	2.00	0.43
23:W:391:VAL:HA	23:W:398:ILE:HG22	1.99	0.43
25:Y:194:PHE:CE2	25:Y:295:TYR:HE2	2.37	0.43
25:Y:197:ALA:HA	25:Y:200:LEU:HB2	2.00	0.43
28:b:52:ILE:HD13	28:b:60:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:511:SER:HB3	32:f:514:VAL:HG12	2.01	0.43
33:x:54:ARG:H	33:x:54:ARG:HG2	1.46	0.43
33:y:4:PHE:O	33:y:67:LEU:HD12	2.19	0.43
1:A:413:VAL:HA	1:A:416:VAL:HG22	2.01	0.43
2:B:170:LEU:O	2:B:174:MET:HG2	2.19	0.43
5:E:252:GLU:HA	5:E:255:ARG:HG2	2.01	0.43
6:F:100:ASP:OD1	6:F:100:ASP:N	2.51	0.43
6:F:311:LEU:HD23	6:F:311:LEU:HA	1.91	0.43
12:L:112:ILE:HA	12:L:112:ILE:HD13	1.69	0.43
12:L:154:PHE:HD1	13:M:63:ASN:HD21	1.67	0.43
16:P:34:MET:SD	16:P:35:VAL:N	2.91	0.43
21:U:628:ARG:NH1	21:U:749:GLN:OE1	2.52	0.43
21:U:664:GLY:N	21:U:698:GLN:HE22	2.17	0.43
27:a:286:ALA:HA	27:a:289:ARG:NE	2.28	0.43
32:f:862:ILE:HD11	32:f:879:ARG:CD	2.48	0.43
9:i:22:GLU:HA	9:i:25:MET:HG2	2.01	0.43
33:y:38:PRO:O	33:y:39:ASP:C	2.61	0.43
1:A:330:ALA:O	1:A:336:ARG:NH1	2.39	0.43
1:A:360:ARG:HG2	32:f:858:LYS:CD	2.49	0.43
5:E:23:ASP:OD2	5:E:27:LYS:NZ	2.52	0.43
15:O:206:LYS:HD2	16:P:161:ASP:HB3	2.01	0.43
20:T:209:TRP:HB2	14:n:190:LEU:HD13	2.01	0.43
21:U:542:GLU:OE2	29:c:208:ARG:NH1	2.49	0.43
22:V:292:ARG:HD2	22:V:296:ARG:HH21	1.83	0.43
22:V:441:MET:HE3	22:V:441:MET:HB3	1.90	0.43
23:W:54:ALA:HA	23:W:57:LYS:HG2	2.01	0.43
23:W:188:GLN:HG3	23:W:192:LYS:NZ	2.33	0.43
29:c:296:ILE:HG22	29:c:300:LEU:HD23	2.01	0.43
32:f:46:SER:HB3	32:f:49:ASP:HB2	2.00	0.43
32:f:803:PHE:HZ	32:f:818:LEU:HD11	1.83	0.43
11:k:133:MET:HG3	11:k:135:ARG:H	1.83	0.43
1:A:301:GLU:HB2	6:F:254:PRO:HG2	2.01	0.43
1:A:362:MET:HB3	1:A:364:VAL:HG13	2.00	0.43
2:B:82:GLN:CG	32:f:681:TYR:CG	2.88	0.43
2:B:288:ASP:OD1	2:B:288:ASP:N	2.50	0.43
21:U:325:MET:HA	21:U:328:ILE:HG12	2.01	0.43
21:U:376:MET:HE3	21:U:735:GLY:HA2	2.01	0.43
25:Y:184:GLN:OE1	25:Y:187:TYR:HD2	2.02	0.43
32:f:408:LEU:HB2	32:f:439:TYR:HB3	2.01	0.43
32:f:416:MET:HE2	32:f:416:MET:HB2	1.42	0.43
2:B:232:LYS:NZ	2:B:331:THR:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:10:ASP:HA	7:G:15:ILE:HG13	2.01	0.42
21:U:603:LEU:HD21	21:U:622:LEU:HD21	1.99	0.42
22:V:353:GLY:HA2	22:V:356:MET:SD	2.59	0.42
24:X:407:MET:HA	24:X:410:VAL:HG22	2.01	0.42
29:c:177:THR:HG23	29:c:179:SER:H	1.84	0.42
29:c:202:SER:OG	29:c:203:ILE:N	2.51	0.42
32:f:96:LEU:HD12	32:f:129:LEU:HD13	2.01	0.42
16:p:90:MET:HE2	16:p:90:MET:HB2	1.82	0.42
1:A:355:PHE:O	1:A:359:ALA:CB	2.66	0.42
5:E:365:GLU:HA	5:E:368:MET:HE2	2.01	0.42
9:I:38:LEU:HD21	9:I:147:LEU:HB2	2.00	0.42
10:J:90:GLU:HG3	10:J:110:TYR:CE2	2.54	0.42
14:N:14:LEU:HD21	14:N:101:ALA:HB3	2.01	0.42
21:U:261:LEU:HA	21:U:264:VAL:HG12	2.01	0.42
22:V:258:ASN:OD1	22:V:261:ARG:NH1	2.52	0.42
23:W:270:ASP:HB3	23:W:274:ARG:HH22	1.84	0.42
24:X:97:LEU:HB2	24:X:132:ARG:HH21	1.84	0.42
25:Y:387:ILE:HD12	25:Y:387:ILE:HA	1.91	0.42
27:a:278:MET:O	27:a:339:ARG:NH2	2.51	0.42
30:d:3:GLU:HB2	30:d:25:ARG:HD3	2.00	0.42
11:k:203:LYS:HE3	11:k:203:LYS:HB2	1.88	0.42
17:q:18:ASP:N	17:q:18:ASP:OD1	2.47	0.42
18:r:139:MET:O	18:r:143:TYR:CB	2.67	0.42
33:x:42:ARG:HB3	33:x:70:VAL:HB	2.01	0.42
3:C:237:MET:HB2	3:C:241:HIS:ND1	2.33	0.42
6:F:373:MET:SD	6:F:373:MET:N	2.91	0.42
13:M:134:SER:OG	13:M:151:ILE:O	2.31	0.42
15:O:11:GLY:HA2	15:O:108:PRO:HB3	2.01	0.42
21:U:469:SER:OG	21:U:470:ASN:N	2.52	0.42
32:f:600:TYR:CE2	32:f:608:LYS:HE3	2.55	0.42
12:l:159:MET:HB2	12:l:159:MET:HE3	1.89	0.42
12:l:175:HIS:ND1	12:l:178:GLU:OE2	2.39	0.42
17:q:22:ALA:HA	17:q:27:GLN:HA	2.01	0.42
33:u:42:ARG:NH2	33:u:72:ARG:HG2	2.34	0.42
4:D:121:ARG:O	4:D:124:LEU:HB2	2.19	0.42
6:F:111:ILE:HB	29:c:51:MET:HE3	2.01	0.42
6:F:123:VAL:HG22	6:F:133:PHE:HD1	1.84	0.42
7:G:106:GLY:HA3	15:O:81:ARG:HG3	2.00	0.42
11:K:52:LYS:HD2	11:K:214:ASN:HA	2.00	0.42
14:N:3:ILE:O	14:N:128:GLY:N	2.52	0.42
22:V:120:ILE:HA	22:V:123:MET:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:304:LEU:O	22:V:308:PHE:N	2.38	0.42
26:Z:208:ILE:HD11	26:Z:230:LEU:HD11	2.00	0.42
29:c:75:MET:HE2	33:u:73:LEU:HD23	2.01	0.42
32:f:501:LEU:HD23	32:f:501:LEU:HA	1.87	0.42
10:j:67:ASP:OD1	10:j:67:ASP:N	2.49	0.42
13:m:65:ARG:HH21	13:m:78:ALA:HA	1.83	0.42
20:t:26:MET:N	20:t:26:MET:SD	2.92	0.42
33:x:42:ARG:HD3	33:x:44:ILE:HD11	2.01	0.42
1:A:55:LEU:CD2	2:B:72:LEU:HB3	2.46	0.42
1:A:135:GLU:N	1:A:138:MET:SD	2.93	0.42
1:A:158:ASP:O	1:A:162:THR:HG23	2.18	0.42
2:B:156:VAL:HG23	2:B:158:ALA:H	1.84	0.42
7:G:26:GLU:OE1	7:G:30:LYS:NZ	2.53	0.42
9:I:30:HIS:HA	9:I:166:ASN:HD21	1.85	0.42
16:P:91:VAL:HG21	16:P:109:ILE:HD11	2.01	0.42
17:Q:165:GLU:OE2	18:r:141:ARG:NH1	2.52	0.42
18:R:42:LEU:HB2	18:R:102:CYS:HB3	2.00	0.42
18:R:182:ASP:N	18:R:182:ASP:OD1	2.50	0.42
20:T:50:MET:HE2	20:T:197:VAL:HG13	2.01	0.42
23:W:421:MET:HE2	23:W:421:MET:HB2	1.84	0.42
26:Z:225:GLN:HG3	26:Z:226:ILE:HG13	2.00	0.42
27:a:39:LEU:HD23	27:a:42:LEU:HD12	2.01	0.42
27:a:74:LEU:HD22	27:a:113:LEU:HD21	2.01	0.42
30:d:10:ASN:OD1	30:d:11:ARG:N	2.53	0.42
32:f:850:VAL:HG21	32:f:863:THR:HG23	2.00	0.42
10:j:222:PRO:HA	10:j:225:ILE:HD12	2.02	0.42
33:y:50:LEU:HD23	33:y:59:TYR:CE2	2.54	0.42
1:A:336:ARG:HH22	35:F:501:ATP:PG	2.42	0.42
7:G:217:VAL:HB	7:G:230:LEU:HB2	2.01	0.42
23:W:175:MET:HB2	23:W:187:THR:HG23	2.01	0.42
24:X:394:ASP:OD1	24:X:394:ASP:N	2.45	0.42
25:Y:379:ARG:HD2	25:Y:379:ARG:HA	1.87	0.42
32:f:109:ILE:HD13	32:f:109:ILE:HA	1.94	0.42
32:f:682:GLY:HA3	32:f:686:LEU:HD23	2.01	0.42
8:h:148:GLN:OE1	8:h:158:TRP:NE1	2.49	0.42
10:j:173:GLU:OE2	11:k:56:SER:OG	2.37	0.42
15:o:1:THR:N	15:o:168:GLY:O	2.42	0.42
15:o:63:LEU:HD21	15:o:74:PRO:HG3	2.01	0.42
33:y:32:ASP:OD1	33:y:32:ASP:C	2.62	0.42
4:D:319:PRO:HA	4:D:322:LEU:HD12	2.02	0.42
8:H:203:MET:HA	8:H:207:ASN:HD21	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:65:LEU:HB2	10:J:69:VAL:HG23	2.02	0.42
12:L:19:ILE:HB	12:L:22:ILE:HB	2.00	0.42
12:L:69:HIS:NE2	12:L:102:PRO:HB3	2.35	0.42
21:U:18:GLN:C	21:U:18:GLN:CD	2.86	0.42
28:b:100:ARG:HH11	28:b:105:HIS:HB2	1.85	0.42
32:f:266:LEU:HD12	32:f:266:LEU:HA	1.86	0.42
8:h:115:ALA:HA	8:h:118:MET:HE3	2.00	0.42
13:m:72:HIS:CE1	13:m:105:ASN:HB3	2.54	0.42
16:p:159:ASP:OD1	16:p:159:ASP:N	2.49	0.42
17:q:183:ILE:HG12	17:q:188:ILE:HG12	2.00	0.42
18:r:139:MET:O	18:r:143:TYR:HB3	2.19	0.42
2:B:73:LEU:O	2:B:76:GLU:HG3	2.19	0.42
2:B:241:ASN:C	2:B:241:ASN:HD22	2.28	0.42
3:C:130:LYS:HG3	3:C:131:VAL:H	1.84	0.42
11:K:35:SER:O	11:K:79:SER:OG	2.35	0.42
11:K:72:ALA:O	11:K:226:PHE:N	2.49	0.42
20:T:8:GLY:O	20:T:54:SER:OG	2.30	0.42
20:T:96:MET:HE1	20:T:106:LEU:HD12	2.02	0.42
21:U:124:LYS:HD3	21:U:125:PRO:HD2	2.02	0.42
22:V:125:SER:HB3	22:V:127:ARG:HE	1.84	0.42
23:W:12:ARG:HE	23:W:31:THR:HG21	1.84	0.42
23:W:346:HIS:CE1	23:W:350:ILE:HD13	2.55	0.42
23:W:378:LEU:HD22	23:W:391:VAL:HG11	2.02	0.42
26:Z:65:ASP:N	26:Z:65:ASP:OD1	2.51	0.42
26:Z:200:GLY:O	26:Z:204:LYS:HG2	2.19	0.42
12:l:215:VAL:HB	12:l:221:PHE:HD1	1.85	0.42
33:x:38:PRO:C	33:x:40:GLN:N	2.66	0.42
1:A:97:ARG:HH12	2:B:129:SER:HB2	1.85	0.42
5:E:19:HIS:CE1	6:F:48:LEU:HD22	2.55	0.42
7:G:112:ASP:OD1	7:G:112:ASP:N	2.51	0.42
8:H:229:TYR:HE1	24:X:83:ALA:HB2	1.85	0.42
17:Q:38:MET:HG3	17:Q:44:LEU:HD23	2.01	0.42
21:U:443:LEU:HD11	21:U:464:GLN:NE2	2.35	0.42
27:a:342:ASP:N	27:a:342:ASP:OD1	2.51	0.42
29:c:31:VAL:HB	29:c:205:ILE:HG13	2.01	0.42
29:c:233:ASP:O	29:c:237:HIS:HB2	2.19	0.42
29:c:257:LYS:HA	29:c:260:GLU:CG	2.45	0.42
32:f:274:ASP:N	32:f:274:ASP:OD1	2.52	0.42
11:k:103:TYR:HE1	19:s:91:MET:SD	2.42	0.42
15:o:143:ARG:O	15:o:146:MET:HE3	2.19	0.42
17:q:31:ASP:OD1	17:q:31:ASP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:q:43:LEU:HB2	17:q:183:ILE:HD11	2.01	0.42
33:x:9:THR:C	33:x:11:LYS:H	2.27	0.42
33:x:36:ILE:HD12	33:x:69:LEU:HD21	2.01	0.42
1:A:48:VAL:HG11	2:B:65:LEU:HB3	2.02	0.42
1:A:103:ASN:HA	1:A:136:GLU:HG2	2.02	0.42
1:A:333:ARG:HH21	1:A:336:ARG:NH2	2.17	0.42
4:D:67:ASN:HD22	21:U:607:VAL:HG12	1.85	0.42
5:E:312:ILE:HG21	5:E:340:GLY:HA2	2.02	0.42
7:G:80:MET:SD	7:G:87:SER:HB3	2.60	0.42
7:G:155:ASP:OD1	7:G:159:TYR:N	2.49	0.42
12:L:9:ASP:OD2	12:L:11:THR:OG1	2.36	0.42
20:T:70:MET:HE1	20:T:91:TRP:CZ2	2.55	0.42
21:U:229:VAL:HA	21:U:232:ILE:HG12	2.02	0.42
21:U:712:LEU:HG	21:U:715:LYS:HE3	2.02	0.42
25:Y:326:GLY:HA2	31:e:48:HIS:CE1	2.55	0.42
26:Z:198:LEU:HD22	29:c:229:LEU:HD21	2.00	0.42
26:Z:202:ASN:ND2	27:a:361:LYS:HD3	2.35	0.42
28:b:134:GLU:HG2	28:b:136:VAL:HG23	2.01	0.42
29:c:131:GLN:HA	29:c:134:GLU:HB2	2.02	0.42
32:f:249:LEU:HB3	32:f:268:LEU:HD21	2.02	0.42
32:f:418:LEU:HD13	32:f:425:GLY:HA2	2.02	0.42
32:f:486:GLY:HA2	32:f:525:ILE:HD11	2.02	0.42
32:f:553:THR:HG22	32:f:556:ARG:HH21	1.84	0.42
32:f:585:GLU:HB2	32:f:586:PRO:CD	2.31	0.42
12:l:66:VAL:HB	12:l:70:ILE:O	2.20	0.42
13:m:244:LYS:HE3	13:m:244:LYS:HB2	1.87	0.42
33:x:51:GLU:HB2	33:x:54:ARG:NE	2.34	0.42
7:G:141:ILE:HD12	7:G:220:VAL:HG12	2.02	0.41
10:J:209:ALA:HB1	10:J:217:LEU:HD11	2.02	0.41
14:N:127:ILE:HD11	14:N:136:TYR:CD1	2.54	0.41
23:W:172:LEU:HD13	23:W:210:LYS:HE2	2.01	0.41
25:Y:241:ILE:HG12	25:Y:261:PHE:HE1	1.86	0.41
27:a:279:GLU:HG2	27:a:339:ARG:HH22	1.82	0.41
32:f:159:VAL:HG11	32:f:195:ASN:HD21	1.85	0.41
32:f:679:LEU:HG	32:f:690:VAL:HG11	2.02	0.41
15:o:187:ARG:HA	15:o:188:PRO:HA	1.90	0.41
1:A:277:ILE:HG22	1:A:280:ILE:HD12	2.02	0.41
3:C:71:SER:O	4:D:112:TYR:N	2.53	0.41
4:D:83:GLN:C	4:D:85:ILE:H	2.28	0.41
14:N:17:ASP:HB3	14:N:164:MET:CE	2.44	0.41
17:Q:83:PHE:O	17:Q:87:ASN:ND2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:34:ALA:O	14:n:166:ARG:NH1	2.53	0.41
25:Y:263:LEU:HB2	25:Y:271:PHE:CE1	2.55	0.41
28:b:25:ARG:NH2	28:b:145:GLU:OE1	2.53	0.41
29:c:192:LEU:HB2	29:c:196:LEU:HG	2.02	0.41
8:h:9:SER:OG	8:h:10:LEU:N	2.53	0.41
9:i:213:ILE:HD12	9:i:233:VAL:HG22	2.02	0.41
12:l:155:ASP:HB2	13:m:62:SER:HB2	2.02	0.41
16:p:34:MET:HB2	16:p:34:MET:HE2	1.80	0.41
20:t:136:SER:OG	20:t:147:GLN:OE1	2.31	0.41
33:y:6:LYS:CD	33:y:12:THR:HB	2.50	0.41
1:A:133:ASP:O	1:A:138:MET:HE1	2.20	0.41
4:D:81:ARG:HH21	29:c:149:GLN:HB3	1.83	0.41
5:E:253:ILE:HG13	6:F:308:ARG:HH22	1.85	0.41
7:G:123:GLN:NE2	8:H:82:ASP:OD1	2.54	0.41
18:R:11:GLY:HA2	18:R:104:TRP:HZ3	1.85	0.41
27:a:27:GLU:O	27:a:30:THR:OG1	2.25	0.41
32:f:270:LEU:HD22	32:f:301:HIS:CE1	2.56	0.41
11:k:228:MET:N	11:k:228:MET:SD	2.93	0.41
7:G:72:ILE:HD13	7:G:76:ILE:HG22	2.02	0.41
10:J:146:GLN:NE2	10:J:147:THR:O	2.54	0.41
17:Q:173:LEU:HD23	17:q:173:LEU:HD23	2.02	0.41
18:R:58:LEU:O	18:R:61:ARG:HG3	2.20	0.41
18:R:168:ALA:HB2	16:p:34:MET:SD	2.60	0.41
22:V:70:SER:H	22:V:97:ARG:NH2	2.17	0.41
22:V:178:LEU:HG	22:V:197:LEU:HD22	2.03	0.41
22:V:441:MET:HB2	26:Z:278:ASN:HD22	1.84	0.41
24:X:216:ILE:HD13	24:X:216:ILE:HA	1.96	0.41
24:X:258:LYS:HE2	24:X:258:LYS:HB2	1.89	0.41
30:d:81:TYR:CE2	30:d:86:LYS:HE2	2.55	0.41
32:f:573:ILE:HD12	32:f:573:ILE:HA	1.86	0.41
7:g:84:THR:HA	7:g:87:SER:HB2	2.02	0.41
10:j:220:LEU:HD22	10:j:220:LEU:HA	1.77	0.41
16:p:67:LEU:HD12	16:p:67:LEU:HA	1.63	0.41
19:s:52:ILE:HG13	19:s:110:ILE:HG12	2.01	0.41
1:A:395:PHE:CD1	1:A:398:ARG:HD2	2.55	0.41
2:B:76:GLU:HA	2:B:79:ILE:HG22	2.01	0.41
3:C:31:LEU:HB3	4:D:47:LEU:HB3	2.02	0.41
4:D:64:GLU:O	4:D:68:LEU:HG	2.20	0.41
5:E:116:ASP:O	5:E:118:LEU:N	2.54	0.41
5:E:145:LEU:HA	5:E:148:VAL:HG12	2.03	0.41
9:I:15:GLU:N	9:I:15:GLU:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:139:MET:O	18:R:143:TYR:CB	2.62	0.41
20:T:105:PRO:HB2	20:T:127:MET:HE3	2.02	0.41
21:U:233:LEU:HA	21:U:236:LEU:HD12	2.01	0.41
22:V:28:GLN:HB3	22:V:40:PHE:HB3	2.01	0.41
32:f:348:ILE:O	32:f:349:TYR:C	2.63	0.41
32:f:658:ALA:HB2	32:f:693:ALA:HB1	2.03	0.41
32:f:851:ASP:OD1	32:f:853:VAL:HG12	2.21	0.41
2:B:74:MET:HG2	32:f:610:GLN:OE1	2.21	0.41
3:C:182:GLN:CD	3:C:286:THR:HB	2.45	0.41
3:C:252:ASP:N	3:C:252:ASP:OD1	2.53	0.41
4:D:125:LYS:N	4:D:126:PRO:HD3	2.36	0.41
4:D:173:GLN:HE22	4:D:334:PRO:HD2	1.86	0.41
4:D:233:SER:OG	5:E:258:MET:SD	2.73	0.41
6:F:35:LYS:HD3	6:F:39:GLU:HB2	2.02	0.41
18:R:161:TYR:OH	18:R:196:HIS:ND1	2.42	0.41
21:U:194:ARG:HH12	21:U:222:PHE:HB3	1.86	0.41
23:W:291:LEU:O	23:W:295:THR:HG23	2.20	0.41
27:a:190:VAL:HA	27:a:193:GLN:HB2	2.01	0.41
30:d:188:LYS:HD2	30:d:221:ASN:HD21	1.85	0.41
32:f:131:MET:HE3	32:f:158:TYR:HA	2.02	0.41
12:l:107:ARG:HE	20:t:77:LEU:HD23	1.85	0.41
15:o:209:THR:OG1	16:p:169:GLN:NE2	2.37	0.41
33:x:57:SER:OG	33:y:73:LEU:CA	2.52	0.41
2:B:78:PHE:HE2	32:f:613:LEU:HD13	1.84	0.41
10:J:57:ARG:HG3	10:J:60:ARG:HH12	1.86	0.41
19:S:12:ILE:HG13	19:S:109:ILE:HD12	2.03	0.41
21:U:461:LEU:HB2	21:U:481:LEU:HD13	2.02	0.41
25:Y:113:ARG:HD2	25:Y:113:ARG:HA	1.84	0.41
28:b:107:MET:HA	28:b:107:MET:HE3	2.02	0.41
32:f:72:ARG:NH1	32:f:118:ASN:HB3	2.36	0.41
32:f:120:ARG:NH1	32:f:145:VAL:O	2.54	0.41
7:g:110:PRO:HG2	7:g:113:MET:HB2	2.03	0.41
13:m:99:ARG:NH2	13:m:105:ASN:OD1	2.48	0.41
20:t:43:MET:HE3	20:t:43:MET:HB3	1.62	0.41
4:D:230:VAL:HB	4:D:264:ILE:HG13	2.03	0.41
7:G:177:SER:HA	7:G:180:GLU:HG2	2.02	0.41
12:L:88:MET:HA	12:L:88:MET:HE2	2.03	0.41
13:M:163:CYS:SG	13:M:164:ALA:N	2.94	0.41
21:U:119:PRO:HA	21:U:123:LYS:HD3	2.03	0.41
22:V:111:GLU:O	22:V:115:GLN:HG2	2.21	0.41
24:X:80:ILE:HB	24:X:81:SER:H	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:72:HIS:NE2	28:b:61:LEU:O	2.53	0.41
32:f:743:ALA:HA	32:f:746:ARG:NE	2.36	0.41
32:f:778:LEU:HD11	32:f:821:LEU:HD21	2.01	0.41
10:j:219:ILE:HD12	10:j:219:ILE:HA	1.82	0.41
11:k:189:MET:N	11:k:189:MET:SD	2.94	0.41
17:q:39:SER:OG	17:q:40:GLU:N	2.51	0.41
33:u:40:GLN:HA	33:u:72:ARG:HB2	2.02	0.41
33:y:22:THR:O	33:y:23:ILE:C	2.64	0.41
1:A:56:LEU:HD12	2:B:72:LEU:CD1	2.51	0.41
1:A:210:LYS:HB3	1:A:312:ARG:HH12	1.86	0.41
1:A:327:LEU:HD11	1:A:332:MET:HE3	2.03	0.41
1:A:382:GLY:HA3	35:A:501:ATP:C4	2.56	0.41
2:B:112:LEU:N	2:B:148:CYS:O	2.45	0.41
2:B:151:LEU:HD12	2:B:161:GLY:HA3	2.03	0.41
3:C:144:PRO:HB2	3:C:205:HIS:HB2	2.02	0.41
6:F:178:ASP:OD1	6:F:178:ASP:N	2.50	0.41
12:L:88:MET:CE	12:L:112:ILE:HD11	2.51	0.41
14:N:160:LEU:HD23	14:N:160:LEU:HA	1.93	0.41
17:Q:66:LEU:HG	17:Q:70:ARG:HD3	2.03	0.41
20:T:67:LEU:HA	20:T:70:MET:HG2	2.02	0.41
21:U:16:GLU:HA	21:U:17:PRO:HD3	1.87	0.41
21:U:27:LEU:HA	21:U:30:VAL:HG22	2.02	0.41
21:U:90:VAL:HG23	21:U:136:LYS:HE3	2.02	0.41
22:V:122:MET:HE2	22:V:130:GLU:HB2	2.03	0.41
23:W:216:ILE:HD13	23:W:232:TYR:CE1	2.56	0.41
23:W:232:TYR:CE2	23:W:254:SER:HB3	2.56	0.41
23:W:315:LYS:HA	23:W:315:LYS:HD3	1.96	0.41
24:X:44:GLN:HA	24:X:47:GLU:OE1	2.21	0.41
24:X:297:ARG:HB2	24:X:337:ARG:CG	2.47	0.41
26:Z:226:ILE:HG21	26:Z:226:ILE:HD13	1.81	0.41
27:a:115:LYS:HD3	27:a:118:ILE:HD12	2.02	0.41
27:a:168:ASN:ND2	27:a:171:SER:OG	2.51	0.41
30:d:190:LEU:HD22	30:d:192:THR:HG22	2.01	0.41
32:f:343:LYS:HZ1	32:f:773:LYS:HD3	1.86	0.41
32:f:371:ASN:HD21	32:f:398:TRP:CD1	2.39	0.41
32:f:405:HIS:ND1	32:f:813:LYS:HD2	2.36	0.41
32:f:692:LEU:O	32:f:695:ALA:HB3	2.21	0.41
32:f:847:GLY:HA2	32:f:878:GLU:OE1	2.20	0.41
17:q:85:ARG:HB2	17:q:118:MET:HE1	2.03	0.41
20:t:184:TYR:HE2	20:t:186:ARG:HH11	1.68	0.41
33:y:54:ARG:H	33:y:54:ARG:HG2	1.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:LYS:HA	1:A:422:LYS:HD3	1.82	0.41
2:B:283:PHE:HD1	2:B:328:ILE:HG23	1.86	0.41
2:B:401:GLU:HG3	2:B:405:MET:HE2	2.02	0.41
5:E:33:LEU:O	5:E:37:THR:OG1	2.31	0.41
5:E:379:LYS:HA	5:E:379:LYS:HD3	1.93	0.41
8:H:45:VAL:HG23	8:H:212:ILE:HG22	2.03	0.41
12:L:209:ASN:OD1	12:L:209:ASN:N	2.52	0.41
15:O:205:GLU:O	15:O:208:THR:OG1	2.25	0.41
19:S:89:ALA:HA	19:S:124:PHE:HZ	1.86	0.41
21:U:556:MET:SD	21:U:556:MET:O	2.79	0.41
27:a:123:LEU:HD13	27:a:161:LYS:HG2	2.03	0.41
28:b:176:GLY:HA2	28:b:177:PRO:HD3	1.93	0.41
30:d:245:GLN:O	30:d:248:GLU:HG3	2.21	0.41
32:f:163:ALA:HB1	32:f:207:LEU:HD21	2.01	0.41
32:f:564:LEU:HA	32:f:564:LEU:HD12	1.85	0.41
33:y:18:GLU:C	33:y:20:SER:N	2.78	0.41
2:B:67:ARG:CD	32:f:606:VAL:CG1	2.99	0.40
2:B:71:TYR:C	2:B:73:LEU:N	2.74	0.40
8:H:157:ALA:HB1	9:I:57:ASP:HB3	2.03	0.40
9:I:176:LYS:NZ	10:J:52:LYS:HE2	2.36	0.40
21:U:248:ILE:HD12	21:U:248:ILE:HA	1.96	0.40
21:U:611:ASN:HB3	21:U:614:VAL:HG22	2.02	0.40
23:W:253:LYS:NZ	23:W:320:SER:O	2.52	0.40
24:X:299:LEU:O	24:X:302:PHE:N	2.53	0.40
25:Y:155:ASP:N	25:Y:155:ASP:OD1	2.51	0.40
26:Z:106:ILE:HD11	26:Z:153:LYS:HG2	2.02	0.40
26:Z:212:LEU:HA	26:Z:215:VAL:HG12	2.03	0.40
32:f:369:ARG:NH2	32:f:370:MET:HA	2.36	0.40
32:f:412:ALA:HB1	32:f:819:TYR:CZ	2.52	0.40
10:j:199:VAL:HG11	10:j:206:ILE:HD11	2.03	0.40
12:l:176:MET:HE1	13:m:56:LYS:O	2.20	0.40
20:t:69:GLN:HA	20:t:72:ILE:HG22	2.02	0.40
33:y:18:GLU:O	33:y:20:SER:N	2.54	0.40
1:A:142:VAL:HG22	1:A:149:ILE:HA	2.03	0.40
3:C:90:HIS:HB3	3:C:91:PRO:HD2	1.81	0.40
4:D:231:VAL:HB	4:D:234:GLU:HB3	2.03	0.40
10:J:127:PHE:HB3	10:J:129:ILE:HG12	2.02	0.40
17:Q:17:SER:OG	17:Q:35:MET:SD	2.78	0.40
18:R:83:LEU:HA	18:R:86:MET:HG2	2.03	0.40
18:R:197:GLU:O	18:R:200:SER:OG	2.31	0.40
19:S:176:LYS:HE2	19:S:208:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:14:GLU:HB3	30:d:73:ARG:HH11	1.86	0.40
21:U:632:GLN:O	21:U:635:SER:OG	2.38	0.40
21:U:879:ASP:OD1	21:U:879:ASP:N	2.54	0.40
24:X:318:ILE:HD12	24:X:318:ILE:HG23	1.90	0.40
25:Y:142:PHE:HB3	25:Y:146:ARG:HH21	1.86	0.40
25:Y:275:LEU:HD23	25:Y:296:VAL:HG23	2.03	0.40
29:c:60:GLU:HA	29:c:107:MET:HB3	2.03	0.40
32:f:803:PHE:CE2	32:f:810:ILE:HG13	2.57	0.40
11:k:117:SER:HB2	12:l:82:ARG:HH12	1.86	0.40
16:p:45:MET:HE3	16:p:51:ILE:CB	2.51	0.40
20:t:210:ASP:N	20:t:210:ASP:OD1	2.54	0.40
33:x:19:PRO:CB	33:y:74:ARG:CA	2.99	0.40
2:B:266:LEU:O	2:B:270:LEU:HG	2.22	0.40
5:E:59:GLU:O	5:E:72:LYS:N	2.44	0.40
5:E:205:ASP:OD1	5:E:205:ASP:N	2.54	0.40
5:E:237:ALA:HB1	6:F:308:ARG:HG3	2.03	0.40
10:J:230:ALA:HA	10:J:233:GLU:OE1	2.21	0.40
12:L:71:GLY:HA3	12:L:221:PHE:CE1	2.56	0.40
12:L:103:LEU:HD23	12:L:108:LEU:HD13	2.04	0.40
14:N:166:ARG:HA	14:N:166:ARG:HD3	1.92	0.40
22:V:175:ARG:HH22	22:V:208:TYR:HB2	1.86	0.40
22:V:438:VAL:HA	22:V:441:MET:HE1	2.02	0.40
26:Z:170:VAL:HG22	29:c:152:LYS:HA	2.04	0.40
27:a:371:ALA:O	27:a:375:LEU:HB2	2.22	0.40
32:f:292:LYS:HG3	32:f:899:ILE:CD1	2.51	0.40
10:j:116:GLN:HA	10:j:119:THR:HG22	2.03	0.40
17:q:3:TYR:H	17:q:18:ASP:CG	2.28	0.40
20:t:112:ILE:HD13	20:t:112:ILE:HA	1.99	0.40
6:F:80:ILE:HD13	6:F:80:ILE:HA	1.96	0.40
14:N:30:VAL:HG11	20:t:211:ILE:HG23	2.03	0.40
14:N:68:ILE:HD12	14:N:68:ILE:HA	1.95	0.40
20:T:20:VAL:HG23	20:T:120:SER:HB3	2.04	0.40
21:U:804:SER:HA	21:U:892:LEU:HA	2.03	0.40
24:X:335:LEU:HA	24:X:338:VAL:HG22	2.03	0.40
26:Z:118:ASN:OD1	26:Z:118:ASN:N	2.53	0.40
27:a:212:ASN:OD1	27:a:213:PHE:N	2.55	0.40
32:f:142:TYR:HA	32:f:145:VAL:HB	2.03	0.40
32:f:566:HIS:CD2	32:f:569:LYS:HE3	2.57	0.40
7:g:153:LYS:HD3	7:g:163:PHE:HE2	1.86	0.40
13:m:197:ILE:HA	13:m:200:VAL:HG22	2.03	0.40
33:x:63:LYS:HE2	33:x:63:LYS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:121:CYS:SG	6:F:122:ALA:N	2.94	0.40
14:N:39:ASP:OD1	14:N:39:ASP:N	2.55	0.40
18:R:17:ASP:OD1	18:R:17:ASP:N	2.55	0.40
19:S:213:ASP:OD2	15:o:19:ARG:NH2	2.50	0.40
20:T:1:THR:N	20:T:105:PRO:O	2.39	0.40
21:U:692:ALA:HB2	21:U:733:ALA:HB1	2.02	0.40
23:W:88:LYS:HA	23:W:88:LYS:HD3	1.74	0.40
23:W:230:LYS:HE3	23:W:271:LEU:HD11	2.03	0.40
26:Z:205:LEU:HA	26:Z:208:ILE:HG22	2.02	0.40
30:d:105:PHE:HD1	30:d:166:PHE:HE1	1.70	0.40
32:f:705:ASN:OD1	32:f:705:ASN:N	2.52	0.40
7:g:133:PRO:HD2	13:m:14:PHE:HE2	1.85	0.40
20:t:122:LEU:HG	20:t:137:LEU:HD12	2.03	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	404/433 (93%)	358 (89%)	44 (11%)	2 (0%)	24	63
2	B	395/440 (90%)	347 (88%)	46 (12%)	2 (0%)	24	63
3	C	379/398 (95%)	331 (87%)	44 (12%)	4 (1%)	11	45
4	D	378/418 (90%)	330 (87%)	43 (11%)	5 (1%)	9	41
5	E	387/403 (96%)	353 (91%)	34 (9%)	0	100	100
6	F	413/439 (94%)	376 (91%)	36 (9%)	1 (0%)	43	78
7	G	242/246 (98%)	233 (96%)	9 (4%)	0	100	100
7	g	238/246 (97%)	223 (94%)	14 (6%)	1 (0%)	30	67
8	H	230/234 (98%)	220 (96%)	10 (4%)	0	100	100
8	h	230/234 (98%)	220 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	249/261 (95%)	242 (97%)	7 (3%)	0	100	100
9	i	246/261 (94%)	235 (96%)	10 (4%)	1 (0%)	30	67
10	J	237/248 (96%)	224 (94%)	13 (6%)	0	100	100
10	j	237/248 (96%)	225 (95%)	12 (5%)	0	100	100
11	K	232/241 (96%)	218 (94%)	14 (6%)	0	100	100
11	k	236/241 (98%)	226 (96%)	10 (4%)	0	100	100
12	L	236/263 (90%)	229 (97%)	7 (3%)	0	100	100
12	l	238/263 (90%)	226 (95%)	12 (5%)	0	100	100
13	M	238/255 (93%)	235 (99%)	3 (1%)	0	100	100
13	m	240/255 (94%)	233 (97%)	7 (3%)	0	100	100
14	N	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
14	n	200/239 (84%)	193 (96%)	7 (4%)	0	100	100
15	O	218/277 (79%)	214 (98%)	4 (2%)	0	100	100
15	o	218/277 (79%)	211 (97%)	7 (3%)	0	100	100
16	P	202/205 (98%)	193 (96%)	9 (4%)	0	100	100
16	p	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
17	Q	197/201 (98%)	192 (98%)	5 (2%)	0	100	100
17	q	197/201 (98%)	193 (98%)	4 (2%)	0	100	100
18	R	199/263 (76%)	192 (96%)	7 (4%)	0	100	100
18	r	199/263 (76%)	193 (97%)	6 (3%)	0	100	100
19	S	211/241 (88%)	204 (97%)	7 (3%)	0	100	100
19	s	211/241 (88%)	206 (98%)	5 (2%)	0	100	100
20	T	214/264 (81%)	205 (96%)	9 (4%)	0	100	100
20	t	214/264 (81%)	205 (96%)	9 (4%)	0	100	100
21	U	812/953 (85%)	765 (94%)	47 (6%)	0	100	100
22	V	442/534 (83%)	432 (98%)	9 (2%)	1 (0%)	43	78
23	W	439/456 (96%)	430 (98%)	9 (2%)	0	100	100
24	X	420/422 (100%)	399 (95%)	19 (4%)	2 (0%)	24	63
25	Y	387/389 (100%)	358 (92%)	28 (7%)	1 (0%)	36	72
26	Z	284/324 (88%)	252 (89%)	32 (11%)	0	100	100
27	a	371/376 (99%)	341 (92%)	29 (8%)	1 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	b	189/377 (50%)	172 (91%)	16 (8%)	1 (0%)	24	63
29	c	285/310 (92%)	261 (92%)	23 (8%)	1 (0%)	30	67
30	d	255/350 (73%)	219 (86%)	36 (14%)	0	100	100
31	e	48/70 (69%)	42 (88%)	6 (12%)	0	100	100
32	f	840/908 (92%)	777 (92%)	56 (7%)	7 (1%)	16	53
33	u	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
33	x	74/76 (97%)	59 (80%)	12 (16%)	3 (4%)	2	18
33	y	74/76 (97%)	56 (76%)	16 (22%)	2 (3%)	4	25
34	v	1/28 (4%)	1 (100%)	0	0	100	100
All	All	13562/15132 (90%)	12707 (94%)	820 (6%)	35 (0%)	37	72

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	90	HIS
3	C	288	ASN
4	D	85	ILE
4	D	300	ASP
6	F	437	TYR
28	b	23	PRO
32	f	66	LYS
32	f	586	PRO
3	C	89	VAL
27	a	214	GLY
32	f	340	MET
32	f	348	ILE
32	f	862	ILE
7	g	19	GLU
9	i	53	HIS
33	y	74	ARG
1	A	346	PRO
3	C	91	PRO
29	c	196	LEU
33	x	39	ASP
33	x	61	ILE
4	D	126	PRO
25	Y	350	VAL
32	f	338	ASP
33	y	35	GLY

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Mol	Chain	Res	Type
1	A	348	LEU
2	B	54	PRO
4	D	125	LYS
22	V	443	PHE
32	f	585	GLU
2	B	50	PRO
4	D	86	PRO
33	x	35	GLY
24	X	80	ILE
24	X	336	ILE

### 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	341/372 (92%)	339 (99%)	2 (1%)	78	81
2	B	345/385 (90%)	341 (99%)	4 (1%)	63	74
3	C	326/346 (94%)	321 (98%)	5 (2%)	57	71
4	D	333/366 (91%)	331 (99%)	2 (1%)	78	81
5	E	341/353 (97%)	341 (100%)	0	100	100
6	F	357/379 (94%)	356 (100%)	1 (0%)	86	84
7	G	205/210 (98%)	205 (100%)	0	100	100
7	g	202/210 (96%)	200 (99%)	2 (1%)	68	76
8	H	188/191 (98%)	187 (100%)	1 (0%)	81	82
8	h	187/191 (98%)	187 (100%)	0	100	100
9	I	207/221 (94%)	207 (100%)	0	100	100
9	i	202/221 (91%)	201 (100%)	1 (0%)	81	82
10	J	201/211 (95%)	198 (98%)	3 (2%)	57	71
10	j	197/211 (93%)	194 (98%)	3 (2%)	57	71
11	K	193/203 (95%)	193 (100%)	0	100	100
11	k	197/203 (97%)	197 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	202/224 (90%)	202 (100%)	0	100	100
12	l	202/224 (90%)	202 (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	696/816 (85%)	695 (100%)	1 (0%)	88	88
22	V	390/460 (85%)	390 (100%)	0	100	100
23	W	406/416 (98%)	405 (100%)	1 (0%)	87	86
24	X	362/362 (100%)	359 (99%)	3 (1%)	73	78
25	Y	344/344 (100%)	342 (99%)	2 (1%)	78	81
26	Z	257/295 (87%)	257 (100%)	0	100	100
27	a	333/336 (99%)	332 (100%)	1 (0%)	86	84
28	b	167/312 (54%)	167 (100%)	0	100	100
29	c	252/268 (94%)	250 (99%)	2 (1%)	73	78
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%)	700 (98%)	11 (2%)	57	71
33	u	68/68 (100%)	64 (94%)	4 (6%)	18	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	x	68/68 (100%)	59 (87%)	9 (13%)	4	16
33	y	68/68 (100%)	62 (91%)	6 (9%)	9	29
34	v	1/1 (100%)	0	1 (100%)	0	0
All	All	11594/12819 (90%)	11529 (99%)	65 (1%)	76	81

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	403	ILE
2	B	51	LEU
2	B	71	TYR
2	B	72	LEU
2	B	125	THR
3	C	88	LYS
3	C	89	VAL
3	C	210	THR
3	C	287	LYS
3	C	289	ILE
4	D	121	ARG
4	D	125	LYS
6	F	438	TYR
8	H	222	THR
10	J	38	ARG
10	J	219	ILE
10	J	220	LEU
21	U	18	GLN
23	W	440	LEU
24	X	82	LYS
24	X	336	ILE
24	X	337	ARG
25	Y	226	VAL
25	Y	351	ASN
27	a	215	GLU
29	c	196	LEU
29	c	198	ARG
32	f	66	LYS
32	f	338	ASP
32	f	339	ILE
32	f	341	GLU
32	f	348	ILE

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Mol	Chain	Res	Type
32	f	349	TYR
32	f	746	ARG
32	f	858	LYS
32	f	860	LYS
32	f	861	THR
32	f	862	ILE
7	g	19	GLU
7	g	21	ARG
9	i	52	ILE
10	j	219	ILE
10	j	220	LEU
10	j	221	ASN
33	u	63	LYS
33	u	72	ARG
33	u	73	LEU
33	u	74	ARG
34	v	25	LYS
33	x	20	SER
33	x	52	ASP
33	x	54	ARG
33	x	60	ASN
33	x	63	LYS
33	x	71	LEU
33	x	72	ARG
33	x	73	LEU
33	x	74	ARG
33	y	8	LEU
33	y	42	ARG
33	y	52	ASP
33	y	54	ARG
33	y	72	ARG
33	y	74	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (116) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
2	B	131	HIS
2	B	181	GLN
2	B	306	GLN
2	B	314	ASN
3	C	50	ASN

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Mol	Chain	Res	Type
3	C	53	ASN
3	C	64	GLN
3	C	69	GLN
3	C	221	GLN
3	C	270	GLN
4	D	67	ASN
4	D	98	GLN
4	D	127	ASN
4	D	187	HIS
4	D	257	ASN
4	D	278	GLN
4	D	294	ASN
4	D	295	GLN
4	D	353	ASN
5	E	10	GLN
5	E	45	ASN
5	E	226	GLN
6	F	92	ASN
6	F	104	GLN
6	F	116	GLN
6	F	214	ASN
7	G	24	GLN
7	G	75	ASN
7	G	90	GLN
8	H	88	HIS
9	I	146	GLN
9	I	166	ASN
10	J	215	GLN
11	K	41	GLN
11	K	204	GLN
12	L	5	GLN
12	L	60	GLN
12	L	190	HIS
13	M	63	ASN
14	N	7	GLN
14	N	77	HIS
15	O	91	GLN
17	Q	32	HIS
17	Q	63	ASN
17	Q	99	HIS
17	Q	168	GLN
18	R	119	ASN

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Mol	Chain	Res	Type
20	T	81	HIS
21	U	79	ASN
21	U	111	GLN
21	U	115	ASN
21	U	340	GLN
21	U	346	ASN
21	U	389	ASN
21	U	412	HIS
21	U	491	GLN
22	V	204	ASN
22	V	434	HIS
23	W	155	GLN
23	W	213	ASN
23	W	346	HIS
23	W	384	ASN
24	X	178	HIS
24	X	198	ASN
24	X	322	HIS
24	X	334	ASN
25	Y	367	GLN
25	Y	378	ASN
26	Z	77	ASN
26	Z	278	ASN
27	a	46	GLN
27	a	82	HIS
27	a	169	HIS
27	a	227	ASN
28	b	76	HIS
29	c	101	GLN
29	c	115	HIS
29	c	128	ASN
29	c	164	ASN
29	c	197	ASN
29	c	237	HIS
29	c	241	ASN
29	c	269	GLN
30	d	47	GLN
30	d	228	GLN
32	f	171	GLN
32	f	199	ASN
32	f	202	HIS
32	f	245	ASN

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Mol	Chain	Res	Type
32	f	273	ASN
32	f	301	HIS
32	f	323	ASN
32	f	382	ASN
32	f	402	ASN
32	f	428	GLN
32	f	614	HIS
32	f	752	HIS
32	f	782	HIS
32	f	815	HIS
32	f	855	GLN
7	g	68	HIS
7	g	90	GLN
7	g	238	HIS
8	h	140	ASN
9	i	53	HIS
9	i	102	GLN
9	i	166	ASN
10	j	15	HIS
10	j	215	GLN
11	k	122	GLN
12	l	21	GLN
17	q	101	ASN
17	q	110	HIS
33	u	49	GLN
33	y	68	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	ADP	B	501	-	27,29,29	1.37	4 (14%)	42,45,45	1.97	9 (21%)
35	ATP	F	501	36	29,33,33	0.30	0	44,52,52	0.50	1 (2%)
35	ATP	A	501	36	29,33,33	0.29	0	44,52,52	0.48	0
35	ATP	D	501	36	29,33,33	0.31	0	44,52,52	0.48	0
37	ADP	E	401	-	27,29,29	1.37	4 (14%)	42,45,45	2.03	11 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	B	501	-	-	3/16/32/32	0/3/3/3
35	ATP	F	501	36	-	2/22/38/38	0/3/3/3
35	ATP	A	501	36	-	1/22/38/38	0/3/3/3
35	ATP	D	501	36	-	7/22/38/38	0/3/3/3
37	ADP	E	401	-	-	2/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	B	501	ADP	C5-C4	4.56	1.47	1.39
37	E	401	ADP	C5-C4	4.54	1.47	1.39
37	E	401	ADP	C5-C6	2.70	1.48	1.41
37	B	501	ADP	C5-C6	2.56	1.48	1.41
37	B	501	ADP	C5-N7	-2.45	1.34	1.39
37	E	401	ADP	C8-N7	2.35	1.36	1.31
37	B	501	ADP	C8-N7	2.24	1.35	1.31
37	E	401	ADP	C5-N7	-2.20	1.34	1.39



All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	501	ADP	C5-C4-N3	-6.43	118.37	126.75
37	E	401	ADP	C5-C4-N3	-6.25	118.60	126.75
37	B	501	ADP	N3-C4-N9	5.09	135.47	127.08
37	E	401	ADP	N3-C4-N9	4.86	135.09	127.08
37	E	401	ADP	PA-O3A-PB	-4.43	117.61	132.83
37	E	401	ADP	C2-N3-C4	3.77	120.65	111.75
37	B	501	ADP	C2-N3-C4	3.74	120.58	111.75
37	B	501	ADP	PA-O3A-PB	-3.39	121.20	132.83
37	E	401	ADP	C4-C5-N7	-3.37	106.51	110.62
37	B	501	ADP	C4-C5-N7	-3.29	106.61	110.62
37	E	401	ADP	N3-C2-N1	-2.93	124.02	128.60
37	B	501	ADP	C5-N7-C8	2.86	107.58	103.51
37	B	501	ADP	N3-C2-N1	-2.83	124.17	128.60
37	E	401	ADP	C5-N7-C8	2.78	107.46	103.51
37	E	401	ADP	C4-N9-C8	2.60	108.55	105.73
37	B	501	ADP	C3'-C2'-C1'	2.58	106.33	101.43
37	B	501	ADP	C4-N9-C8	2.48	108.42	105.73
37	E	401	ADP	C3'-C2'-C1'	2.42	106.03	101.43
37	E	401	ADP	C6-C5-N7	2.10	135.93	132.02
35	F	501	ATP	PB-O3B-PG	2.08	139.98	132.83
37	E	401	ADP	N9-C8-N7	-2.01	111.17	113.91

There are no chirality outliers.

All (15) torsion outliers are listed below:

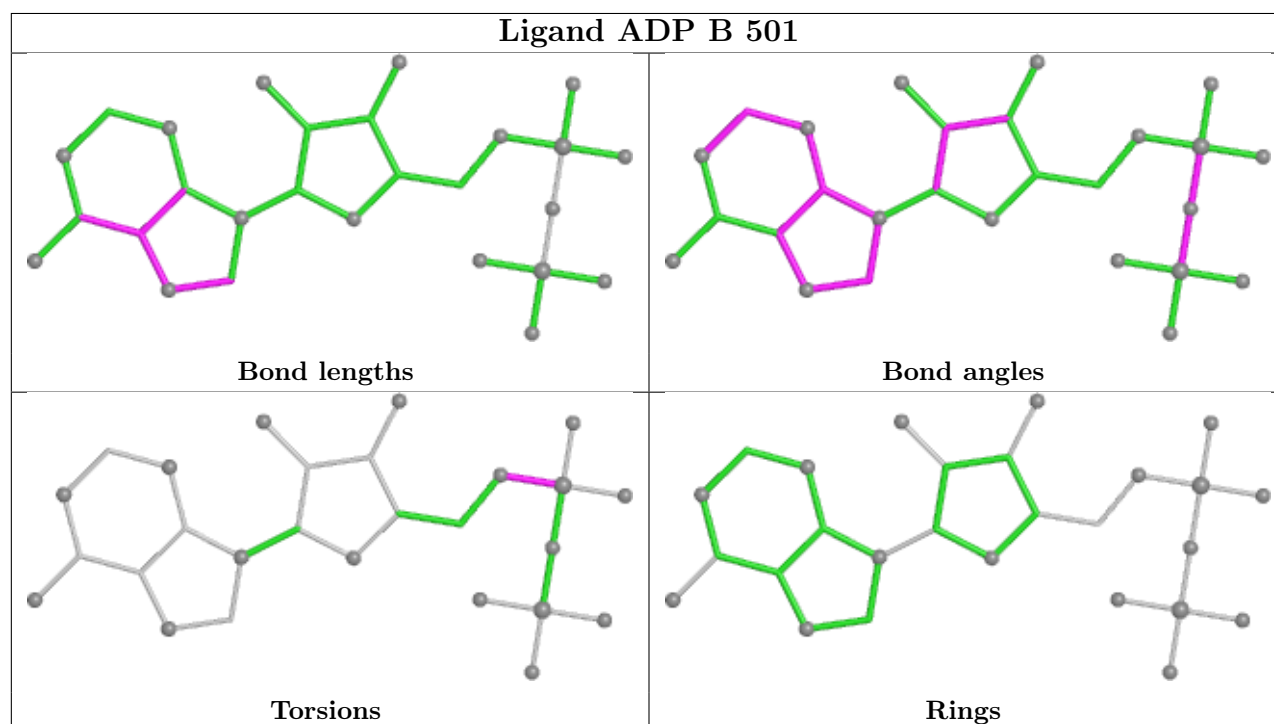
Mol	Chain	Res	Type	Atoms
35	D	501	ATP	C5'-O5'-PA-O3A
35	D	501	ATP	C4'-C5'-O5'-PA
35	D	501	ATP	C3'-C4'-C5'-O5'
35	F	501	ATP	C5'-O5'-PA-O3A
37	B	501	ADP	C5'-O5'-PA-O3A
37	E	401	ADP	O4'-C4'-C5'-O5'
37	E	401	ADP	C3'-C4'-C5'-O5'
35	D	501	ATP	O4'-C4'-C5'-O5'
35	D	501	ATP	C5'-O5'-PA-O1A
35	F	501	ATP	C5'-O5'-PA-O1A
37	B	501	ADP	C5'-O5'-PA-O1A
37	B	501	ADP	C5'-O5'-PA-O2A
35	A	501	ATP	PG-O3B-PB-O2B
35	D	501	ATP	PG-O3B-PB-O1B
35	D	501	ATP	PG-O3B-PB-O2B

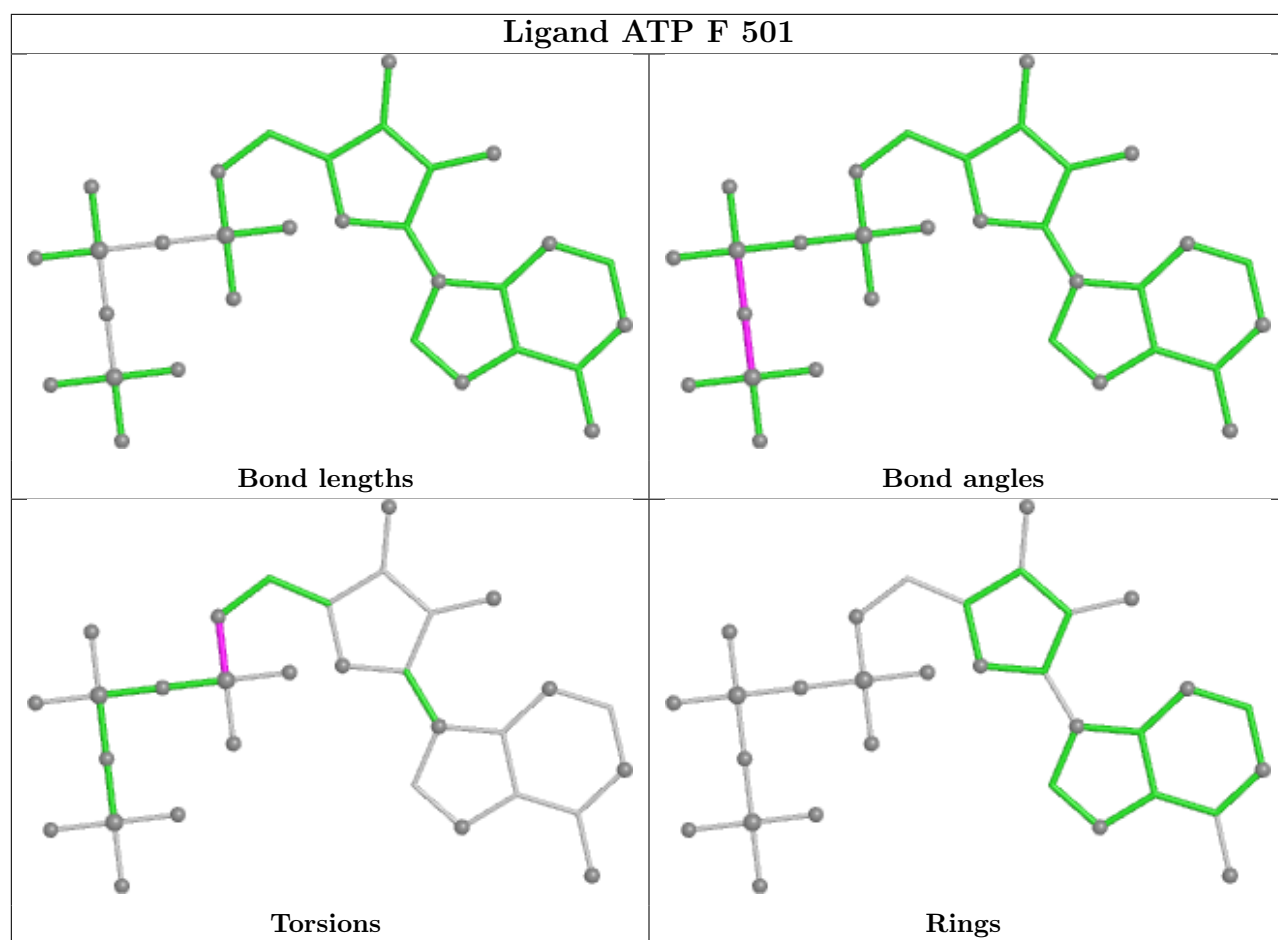
There are no ring outliers.

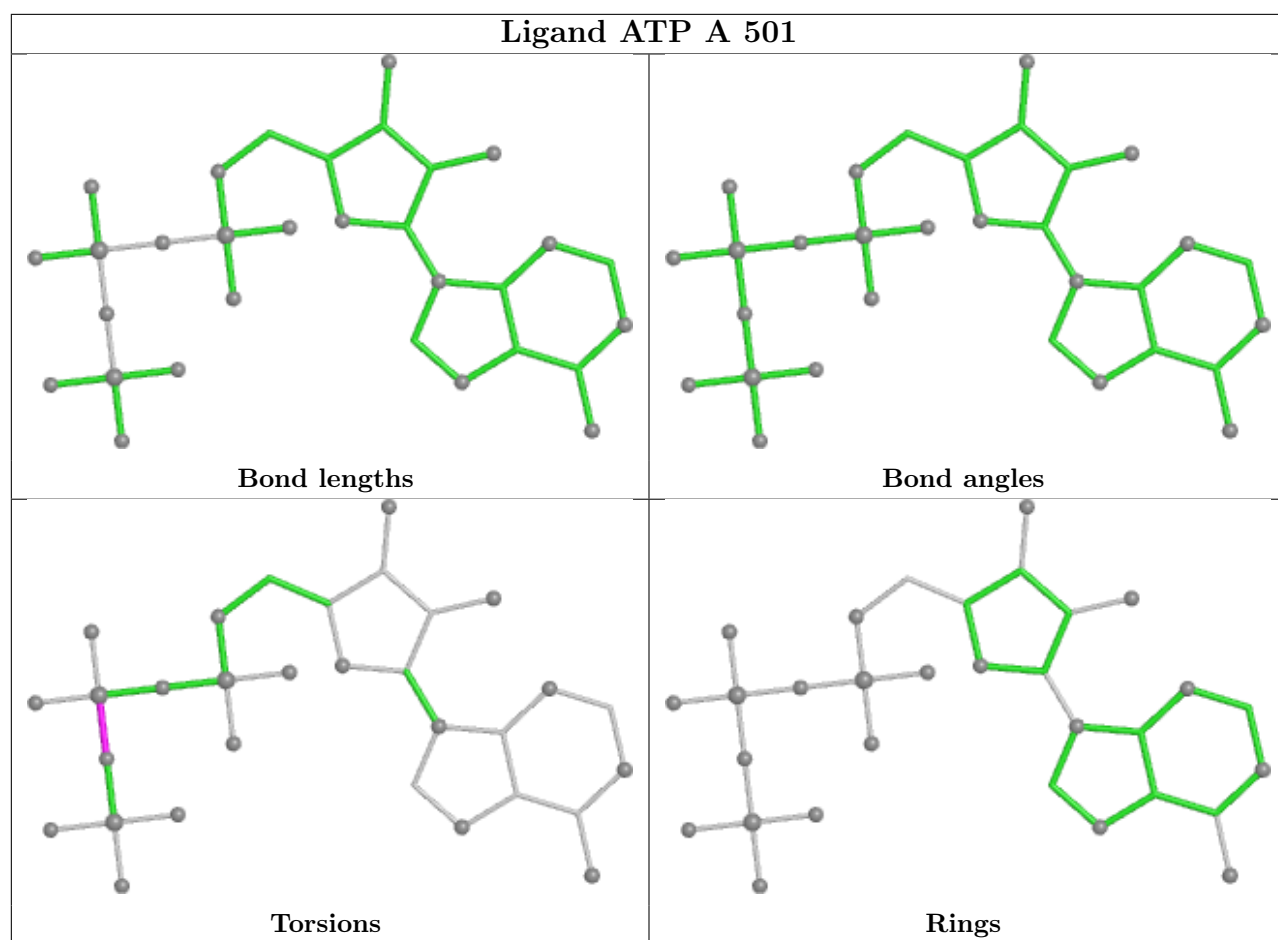
4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	B	501	ADP	3	0
35	F	501	ATP	5	0
35	A	501	ATP	3	0
37	E	401	ADP	4	0

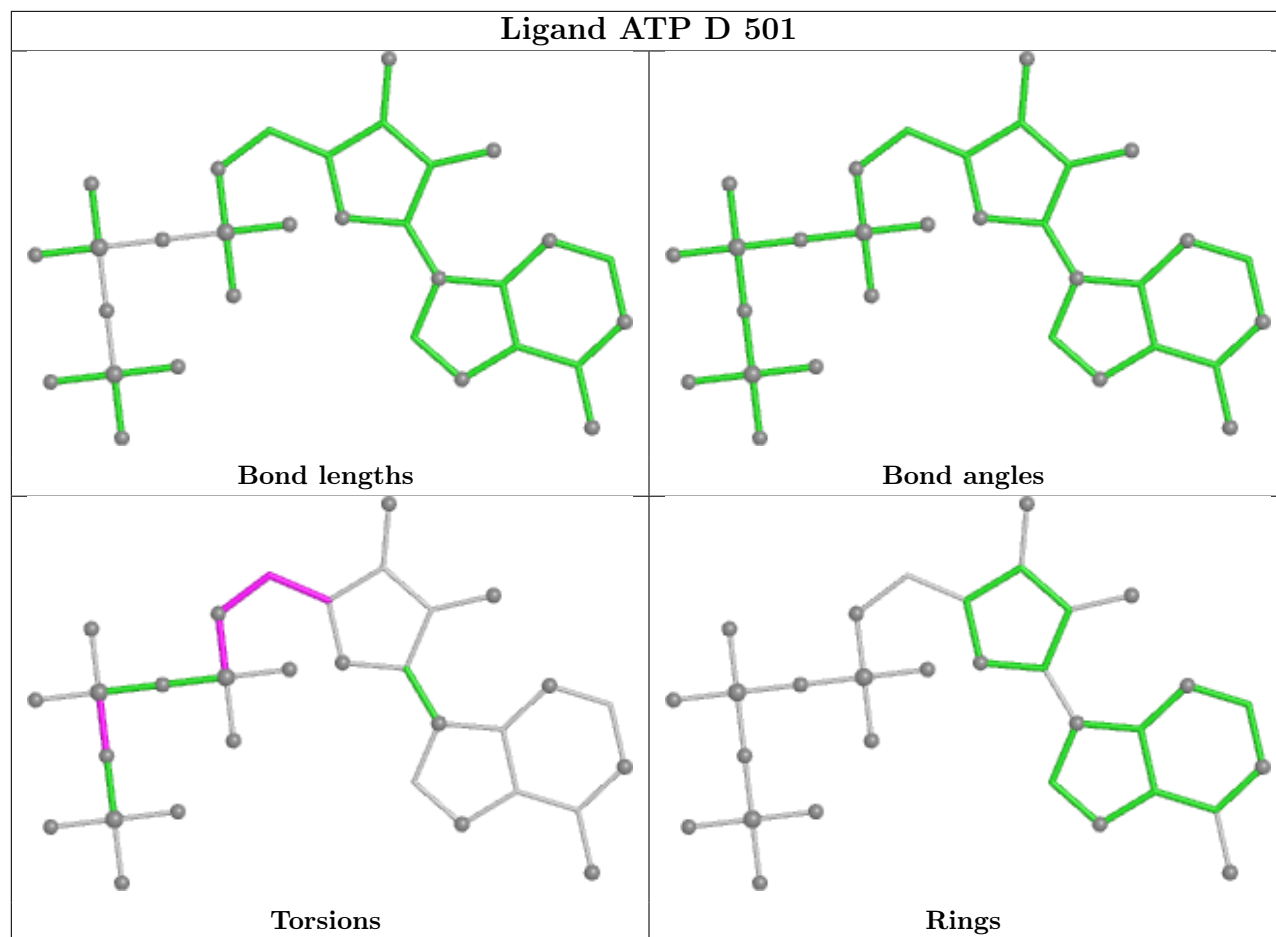
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



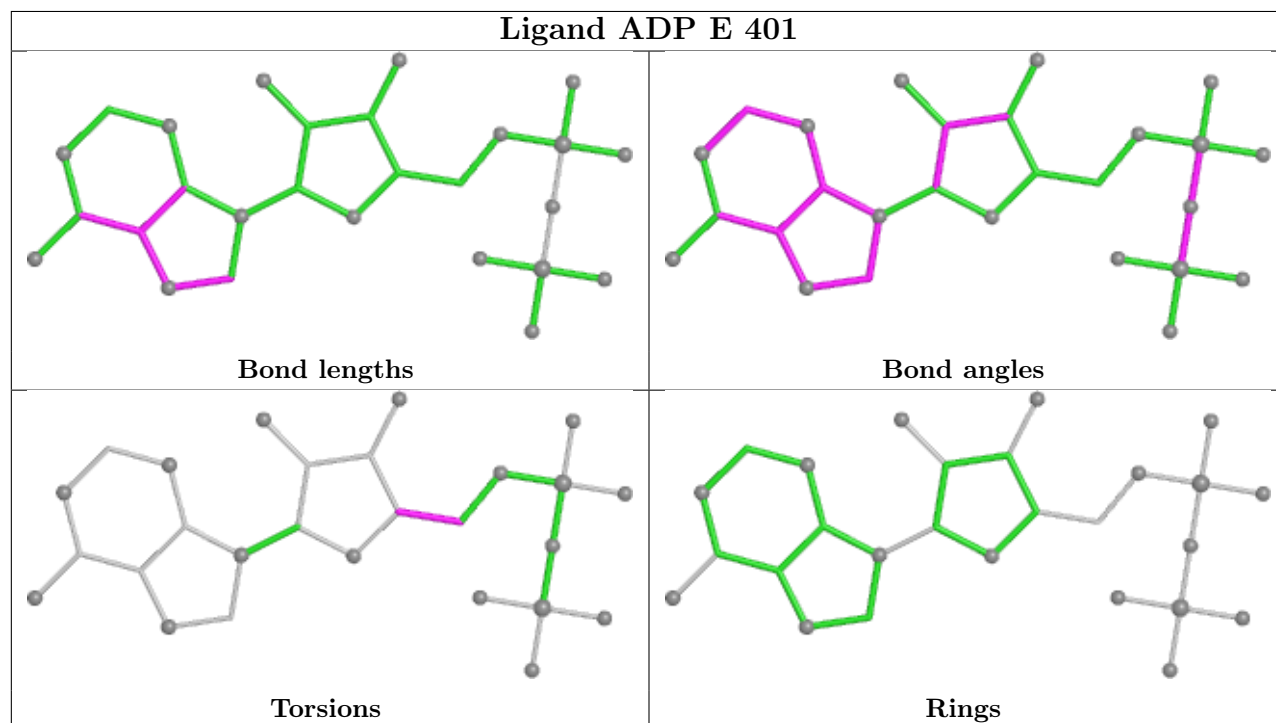




## Ligand ATP D 501



## Ligand ADP E 401



## 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.

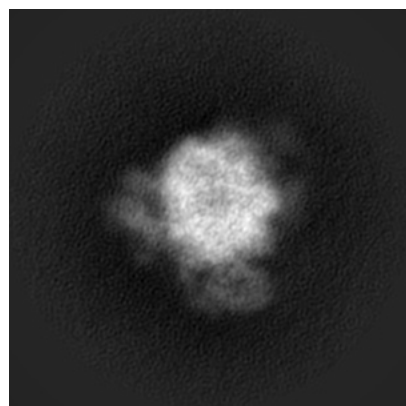
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-62068. 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](#)

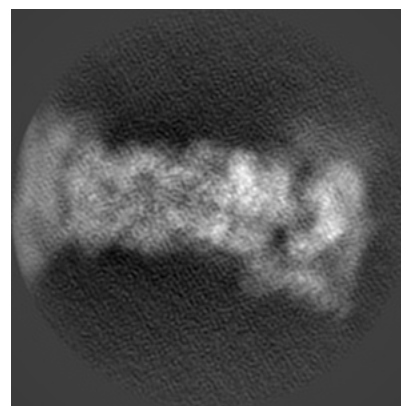
#### 6.1.1 Primary map



X

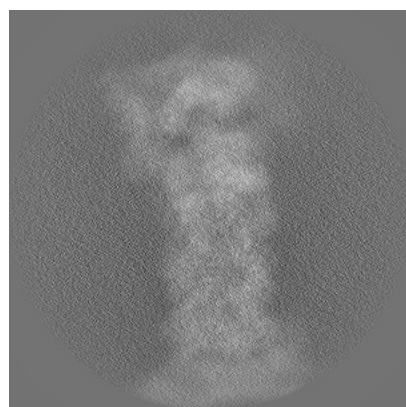


Y

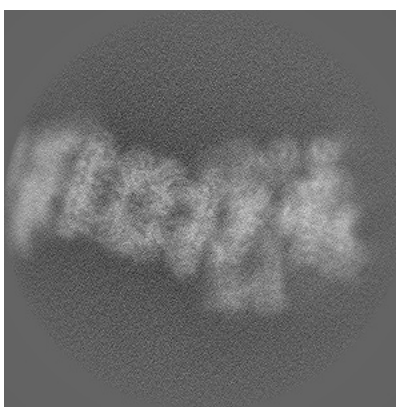


Z

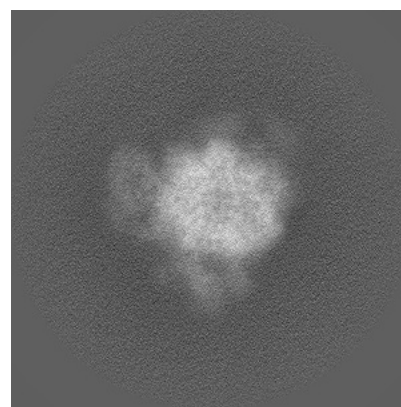
#### 6.1.2 Raw map



X



Y



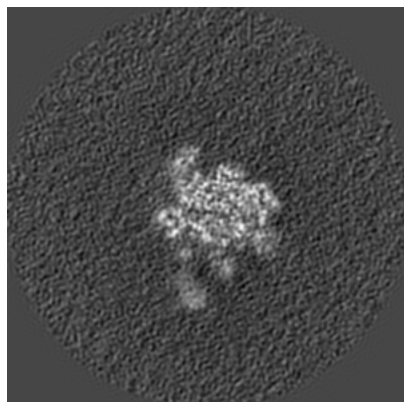
Z

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

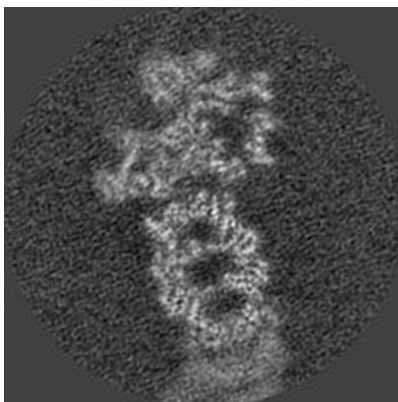


## 6.2 Central slices [i](#)

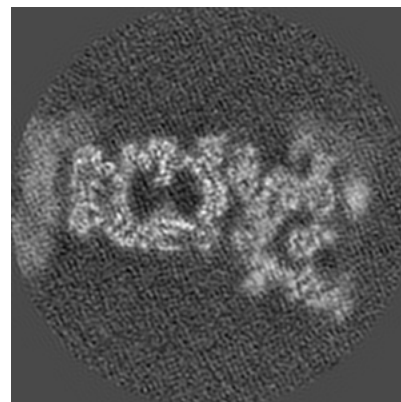
### 6.2.1 Primary map



X Index: 300

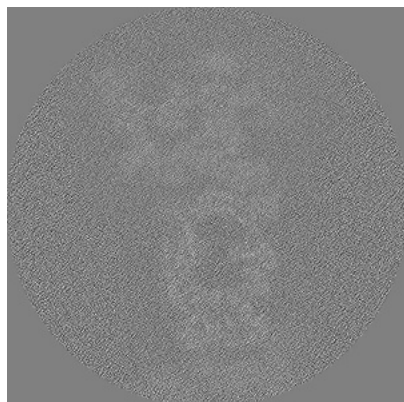


Y Index: 300

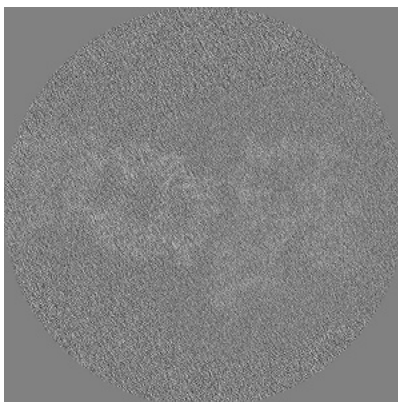


Z Index: 300

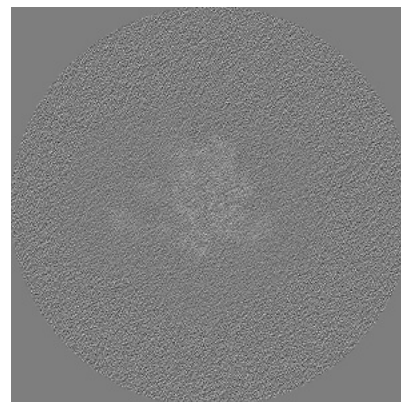
### 6.2.2 Raw map



X Index: 300



Y Index: 300



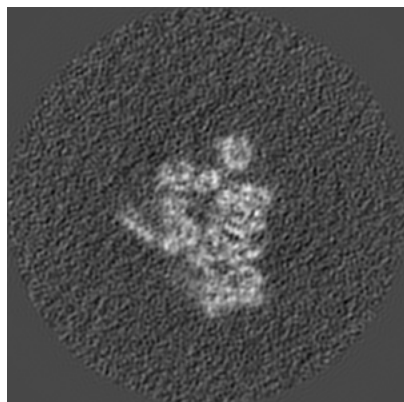
Z Index: 300

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

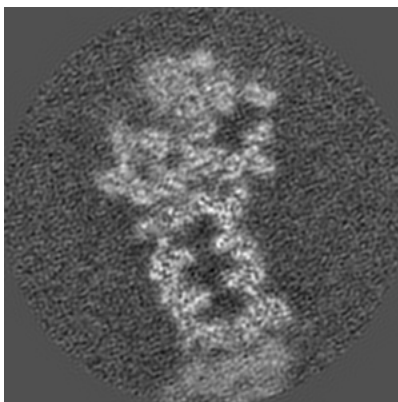


## 6.3 Largest variance slices [i](#)

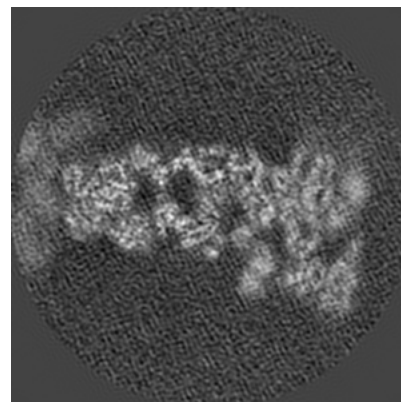
### 6.3.1 Primary map



X Index: 346

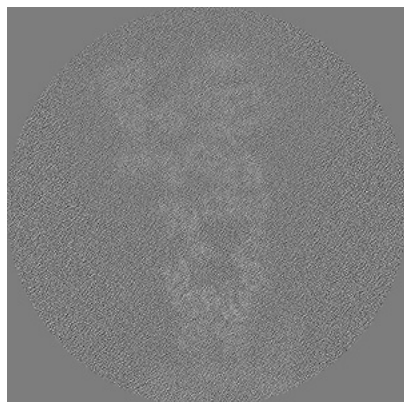


Y Index: 314

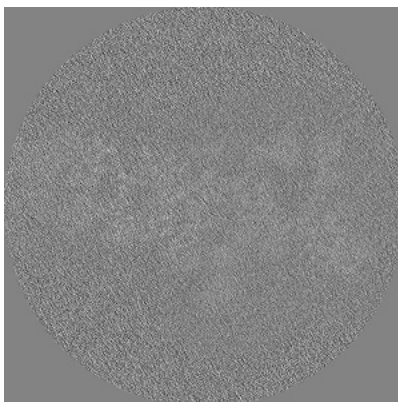


Z Index: 283

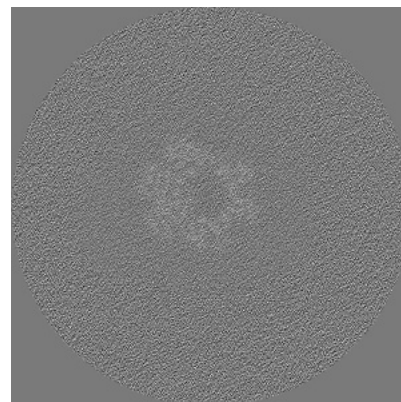
### 6.3.2 Raw map



X Index: 289



Y Index: 284

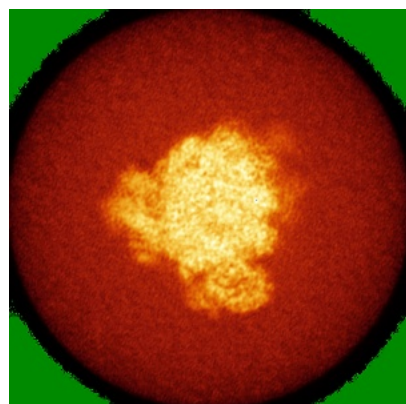


Z Index: 266

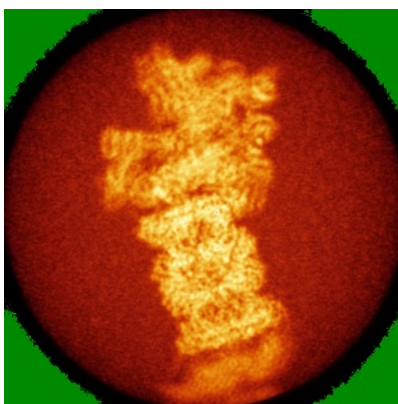
The images above show the largest variance slices of the map in three orthogonal directions.

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

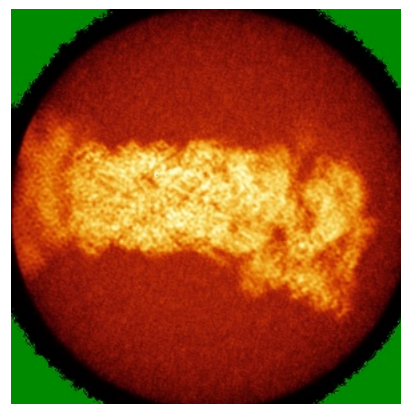
### 6.4.1 Primary map



X

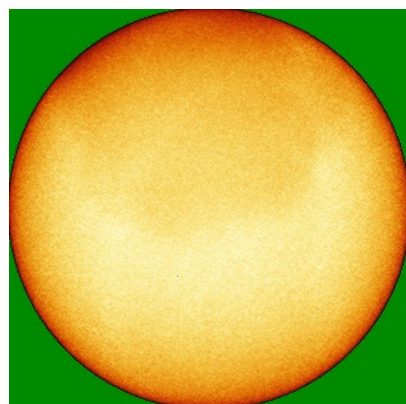


Y

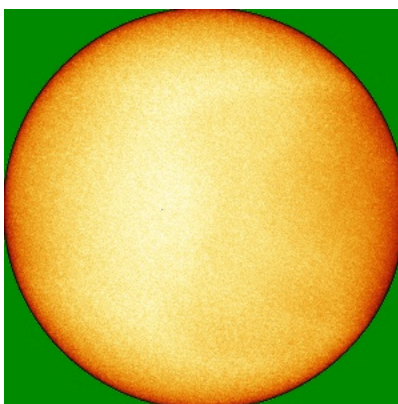


Z

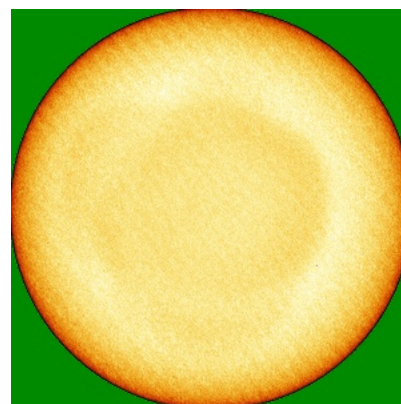
### 6.4.2 Raw map



X



Y

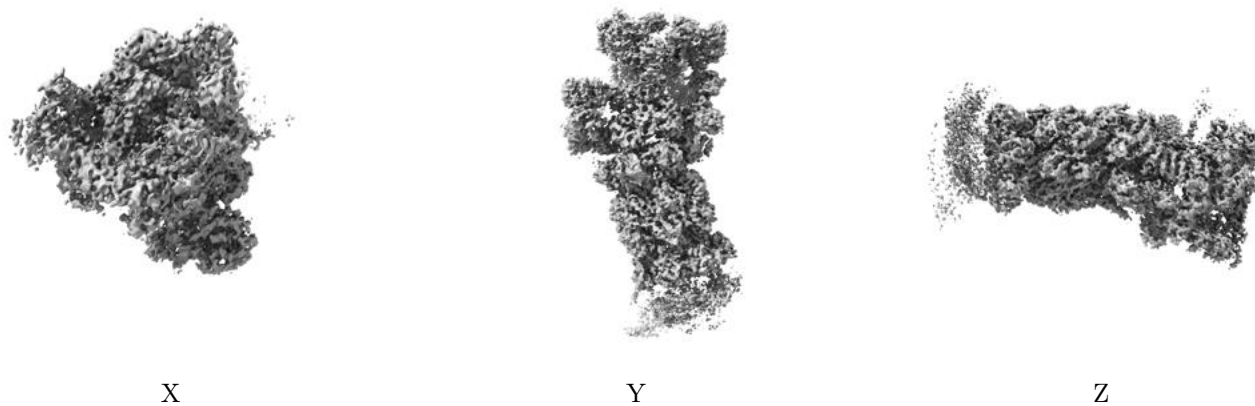


Z

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.

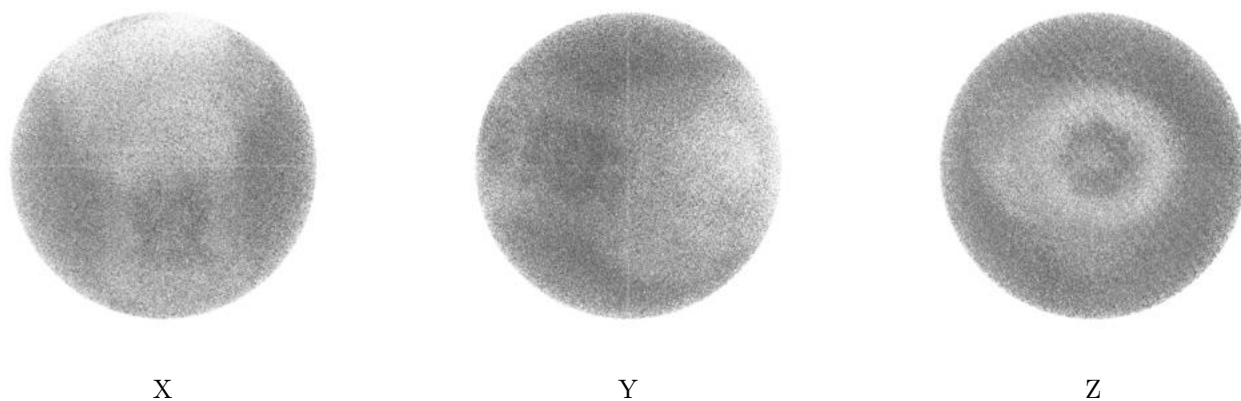
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00452. 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.

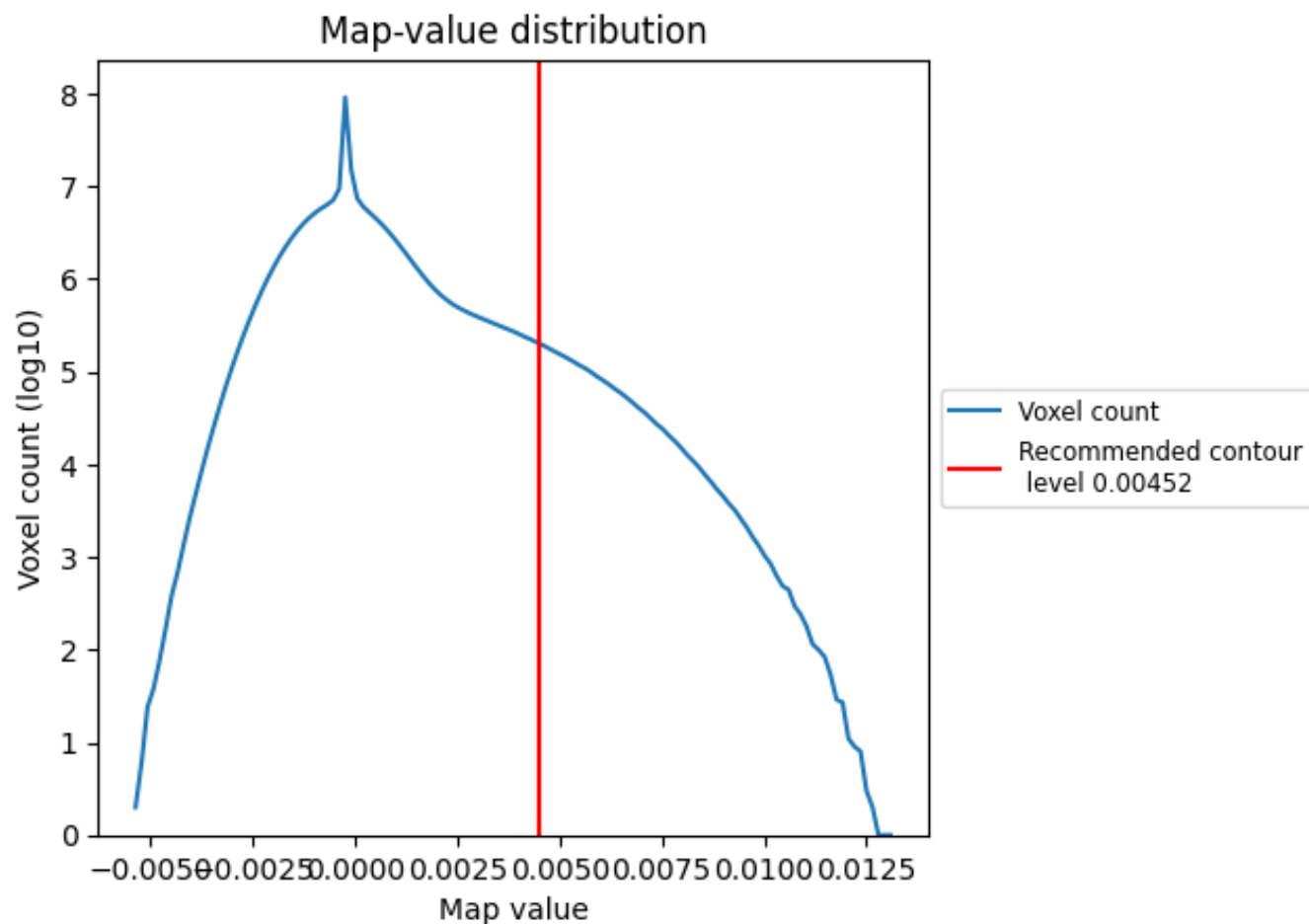
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

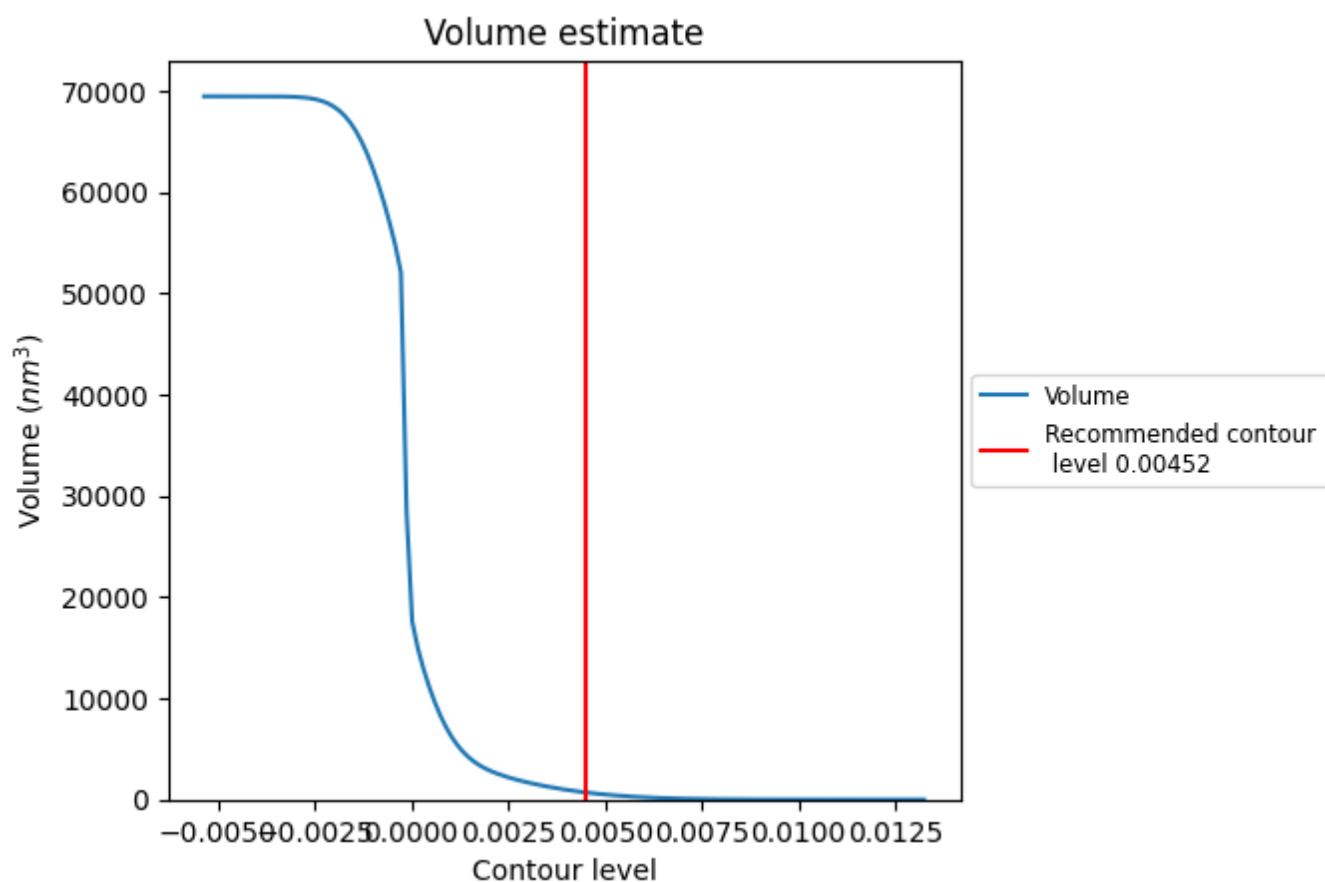
This section contains the results of statistical analysis of the map.

### 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.

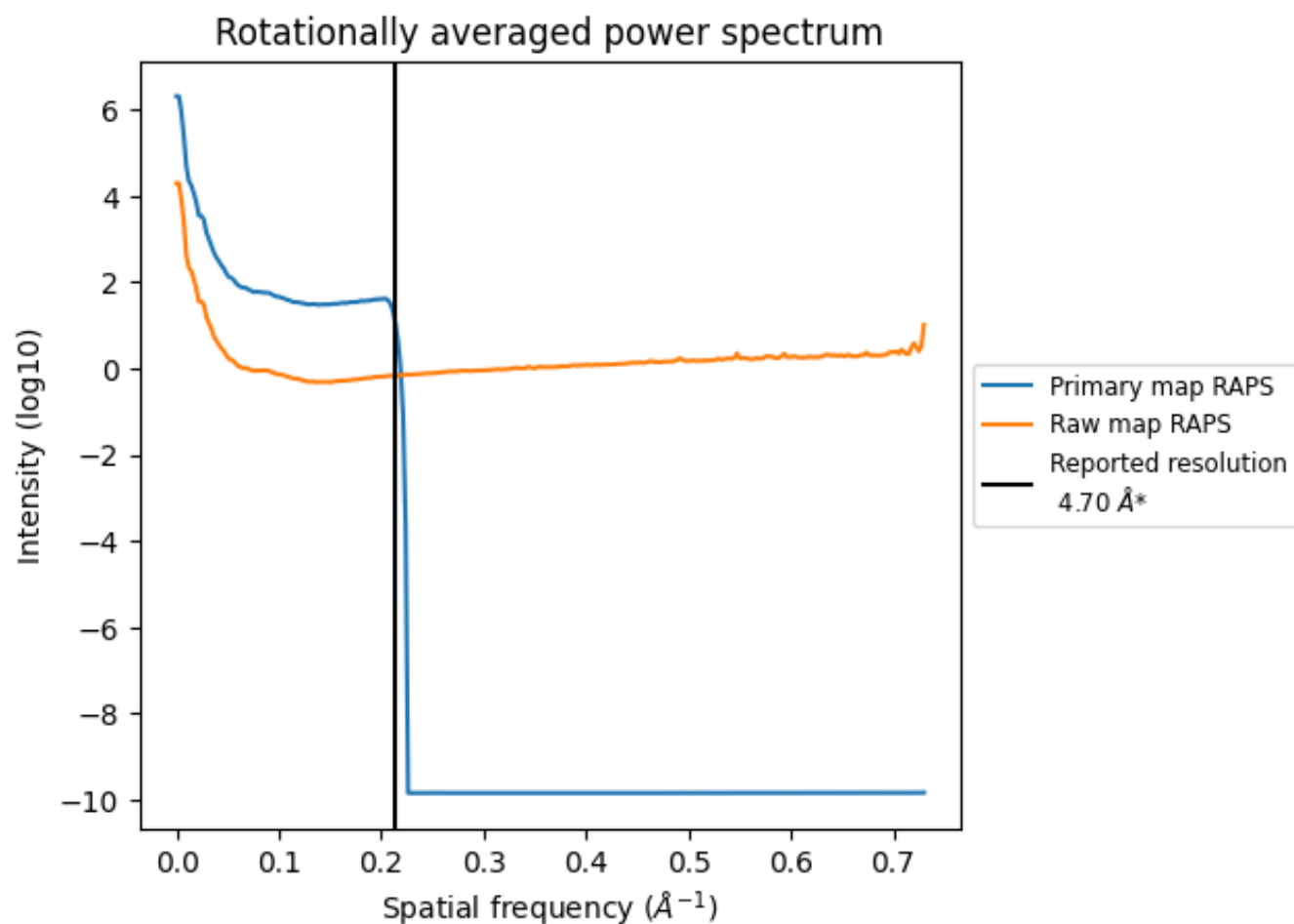
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 693 nm<sup>3</sup>; this corresponds to an approximate mass of 626 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 ⓘ



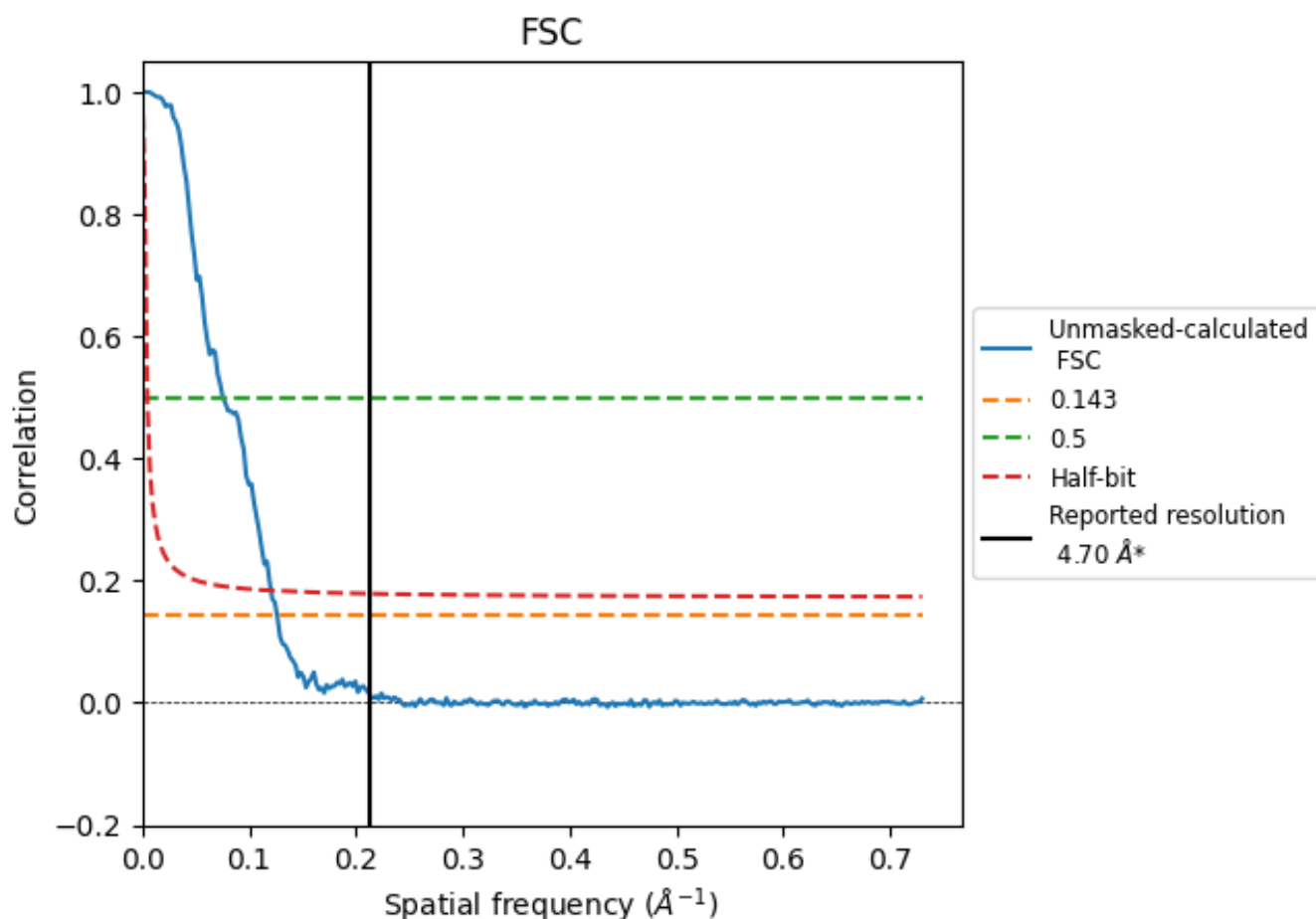
\*Reported resolution corresponds to spatial frequency of 0.213 Å<sup>-1</sup>



## 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 0.213  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.92	13.26	8.30

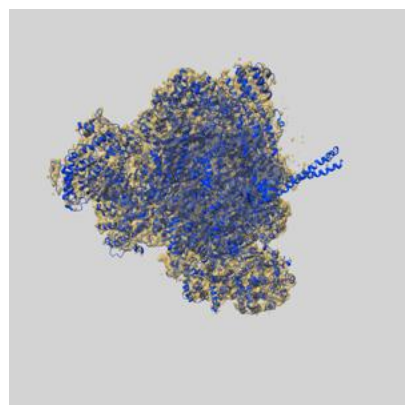
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.92 differs from the reported value 4.7 by more than 10 %



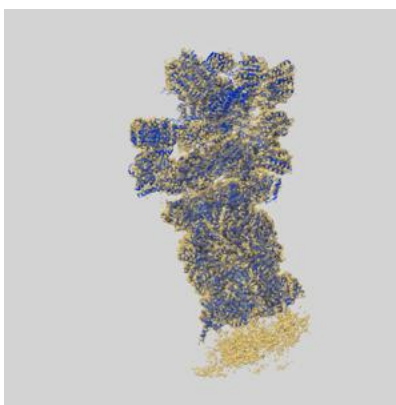
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-62068 and PDB model 9K4S. Per-residue inclusion information can be found in section [3](#) on page [13](#).

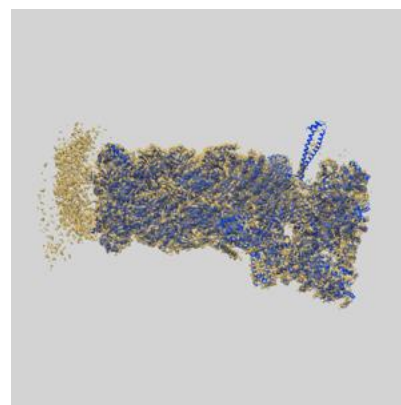
### 9.1 Map-model overlay [i](#)



X



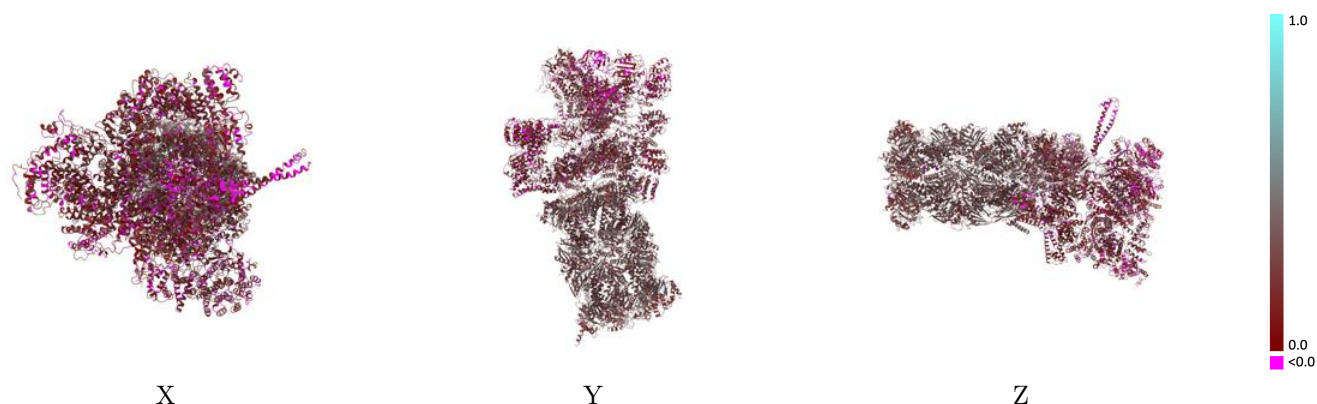
Y



Z

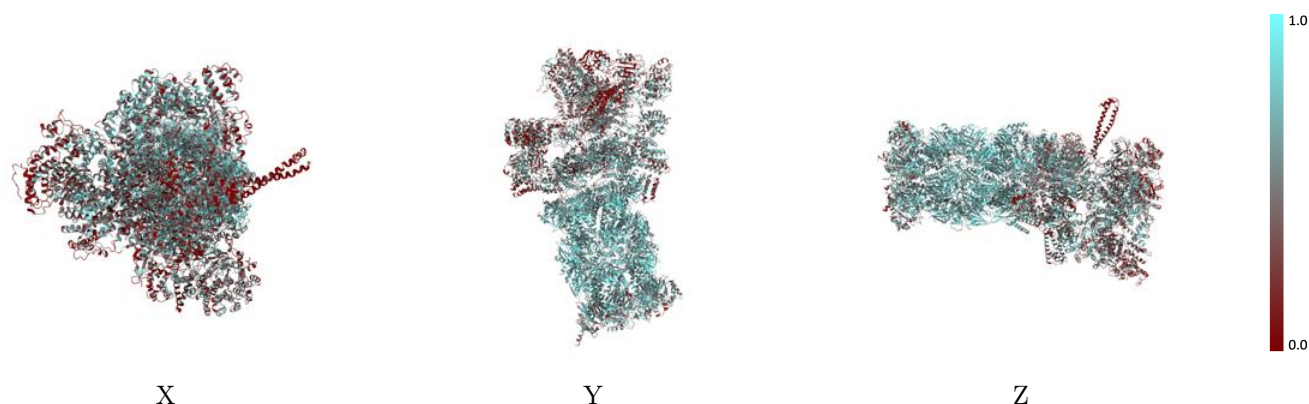
The images above show the 3D surface view of the map at the recommended contour level 0.00452 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



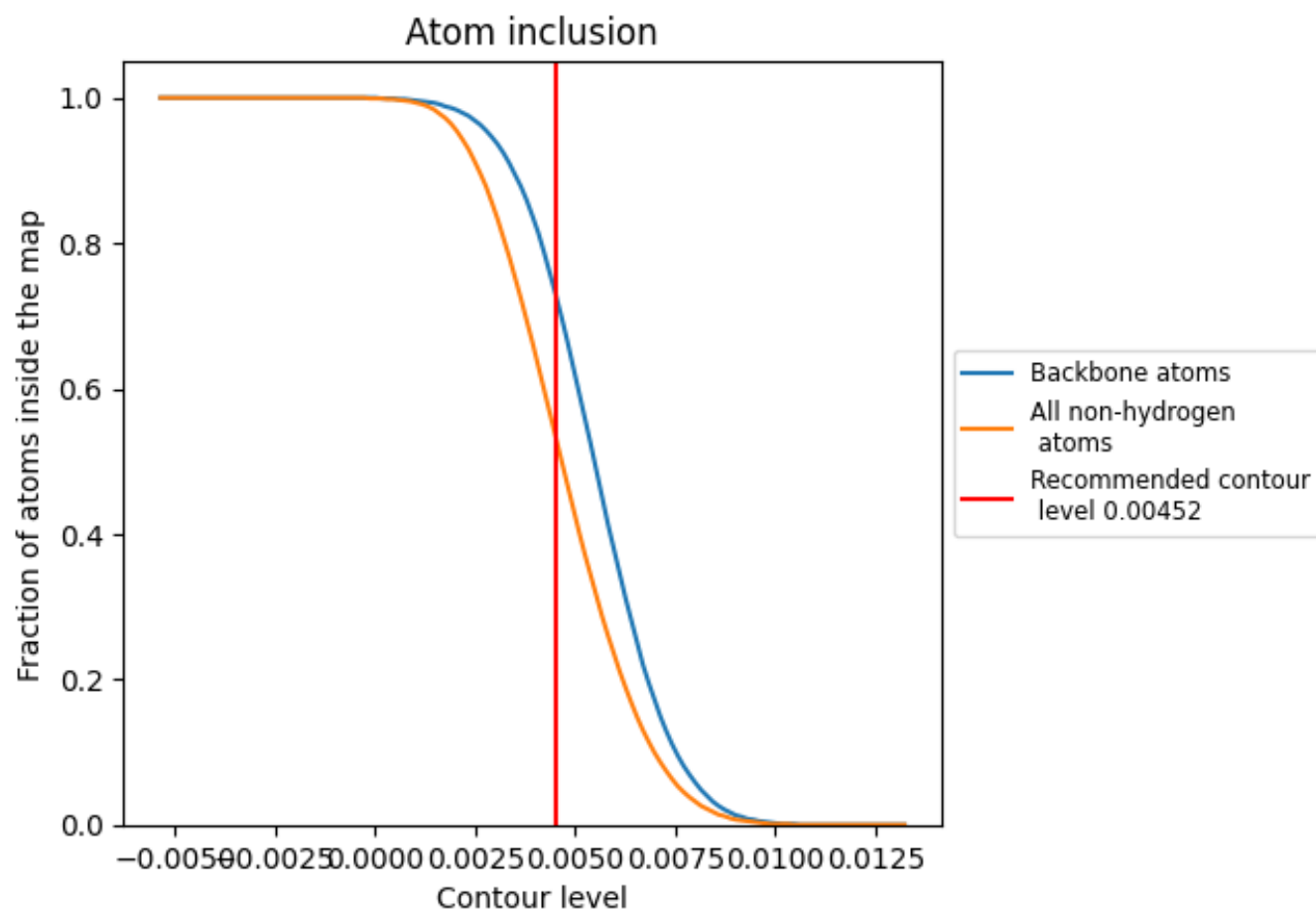
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00452).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 53% 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 (0.00452) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5330	 0.2440
A	 0.4780	 0.1980
B	 0.4620	 0.2000
C	 0.4160	 0.1560
D	 0.4740	 0.2130
E	 0.4990	 0.2240
F	 0.4550	 0.2030
G	 0.6850	 0.3160
H	 0.6870	 0.3220
I	 0.6880	 0.3040
J	 0.6370	 0.2810
K	 0.6430	 0.3120
L	 0.7120	 0.3230
M	 0.6930	 0.3140
N	 0.7070	 0.3190
O	 0.7240	 0.3390
P	 0.7270	 0.3340
Q	 0.7180	 0.3220
R	 0.7330	 0.3250
S	 0.6930	 0.3300
T	 0.7340	 0.3320
U	 0.4010	 0.1830
V	 0.4060	 0.1890
W	 0.5520	 0.2040
X	 0.4670	 0.2000
Y	 0.4960	 0.1810
Z	 0.4360	 0.1900
a	 0.4740	 0.1590
b	 0.3050	 0.1540
c	 0.4150	 0.1820
d	 0.2500	 0.1400
e	 0.3200	 0.1770
f	 0.3610	 0.1620
g	 0.5780	 0.3150
h	 0.5680	 0.3140



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
i	 0.5520	 0.3150
j	 0.4970	 0.2950
k	 0.5330	 0.3090
l	 0.6340	 0.3280
m	 0.5860	 0.3120
n	 0.6970	 0.3310
o	 0.7100	 0.3400
p	 0.7090	 0.3300
q	 0.6900	 0.3330
r	 0.6950	 0.3260
s	 0.6620	 0.3240
t	 0.7140	 0.3310
u	 0.3650	 0.1430
v	 0.2660	 0.1310
x	 0.2080	 0.0260
y	 0.1990	 0.0050