



Full wwPDB EM Validation Report ⓘ

Jun 29, 2025 – 01:06 am BST

PDB ID : 7QXP / pdb_00007qxp
EMDB ID : EMD-14202
Title : Proteasome-ZFAND5 Complex Z+B state
Authors : Zhu, Y.; Lu, Y.
Deposited on : 2022-01-26
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

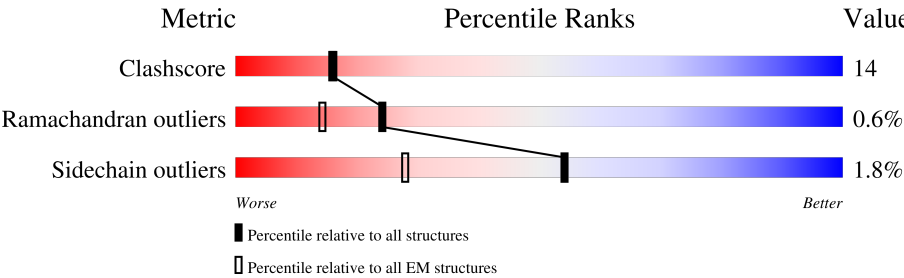
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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.





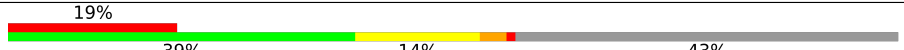
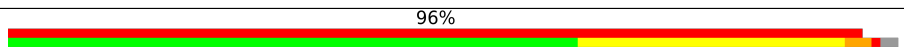

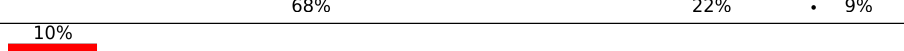
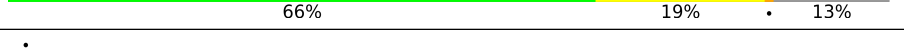





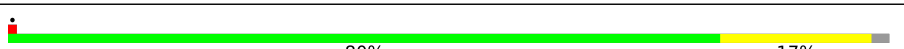


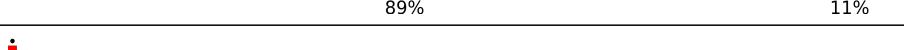








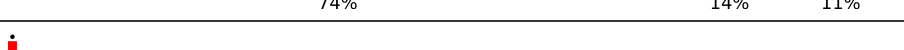
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	U	953	<div> <div>10%</div> <div>60%</div> <div>24%</div> <div>15%</div> </div>
2	V	533	<div> <div>22%</div> <div>56%</div> <div>33%</div> <div>5%</div> </div>
3	W	456	<div> <div>14%</div> <div>60%</div> <div>36%</div> <div>.</div> </div>
4	X	422	<div> <div>12%</div> <div>72%</div> <div>18%</div> <div>10%</div> </div>
5	Y	389	<div> <div>.</div> <div>65%</div> <div>30%</div> <div>..</div> </div>
6	Z	324	<div> <div>6%</div> <div>57%</div> <div>27%</div> <div>12%</div> </div>
7	a	376	<div> <div>12%</div> <div>69%</div> <div>30%</div> <div>..</div> </div>
8	b	377	<div> <div>11%</div> <div>34%</div> <div>16%</div> <div>49%</div> </div>














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Mol	Chain	Length	Quality of chain
9	c	309	
10	d	349	
11	e	70	
12	f	908	
13	A	433	
14	B	440	
15	C	398	
16	D	418	
17	E	403	
18	F	439	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	
24	l	268	
25	M	254	
25	m	254	
26	N	238	

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Mol	Chain	Length	Quality of chain
26	n	238	 68%12%20%
27	O	276	 68%12%20%
27	o	276	 68%11%20%
28	P	204	 87%13%
28	p	204	 86%14%
29	Q	201	 81%18%.
29	q	201	 80%19%.
30	R	262	 65%12%23%
30	r	262	 66%11%23%
31	S	240	 77%12%11%
31	s	240	 77%12%11%
32	T	263	 70%12%18%
32	t	263	 72%10%18%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 103732 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	812	Total	C	N	O	S	0	0
			6334	4023	1078	1189	44		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	508	Total	C	N	O	S	0	0
			3994	2530	712	738	14		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A	394	Total	C	N	O	S	0	0
			3096	1951	543	584	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	B	384	Total	C	N	O	S	0	0
			3018	1901	515	587	15		

- Molecule 15 is a protein called Isoform 2 of 26S proteasome regulatory subunit 8.

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

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

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

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

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

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

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

- Molecule 19 is a protein called Proteasome subunit alpha type-6.

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

- Molecule 20 is a protein called Proteasome subunit alpha type-2.

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

- Molecule 21 is a protein called Proteasome subunit alpha type-4.

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

- Molecule 22 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	J	239	Total	C	N	O	S	0	0
			1713	1062	311	335	5		
22	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 23 is a protein called Proteasome subunit alpha type-5.

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

- Molecule 24 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

- Molecule 25 is a protein called Proteasome subunit alpha type-3.

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

- Molecule 26 is a protein called Proteasome subunit beta type-6.

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

- Molecule 27 is a protein called Proteasome subunit beta type-7.

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

- Molecule 28 is a protein called Proteasome subunit beta type-3.

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

- Molecule 29 is a protein called Proteasome subunit beta type-2.

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

- Molecule 30 is a protein called Proteasome subunit beta type-5.

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

- Molecule 31 is a protein called Proteasome subunit beta type-1.

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
31	s	213	Total	C	N	O	S	0	0
			1644	1039	282	313	10		

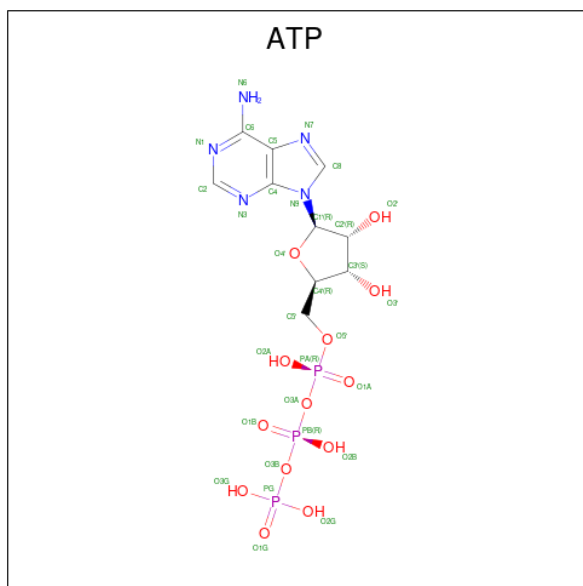
- Molecule 32 is a protein called Proteasome subunit beta type-4.

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

- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



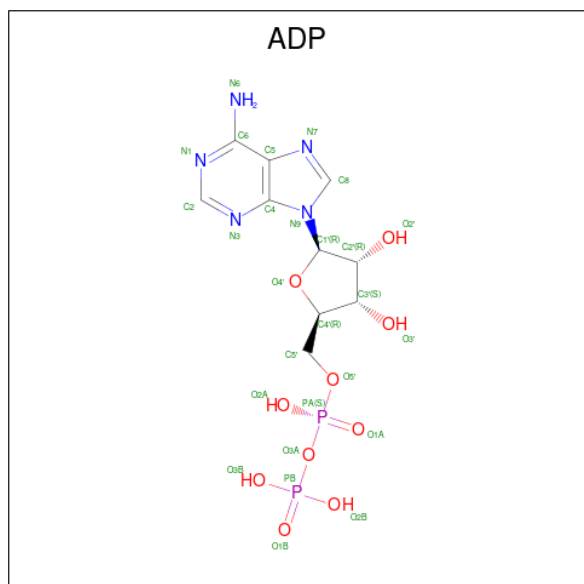
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Mol	Chain	Residues	Atoms					AltConf
34	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

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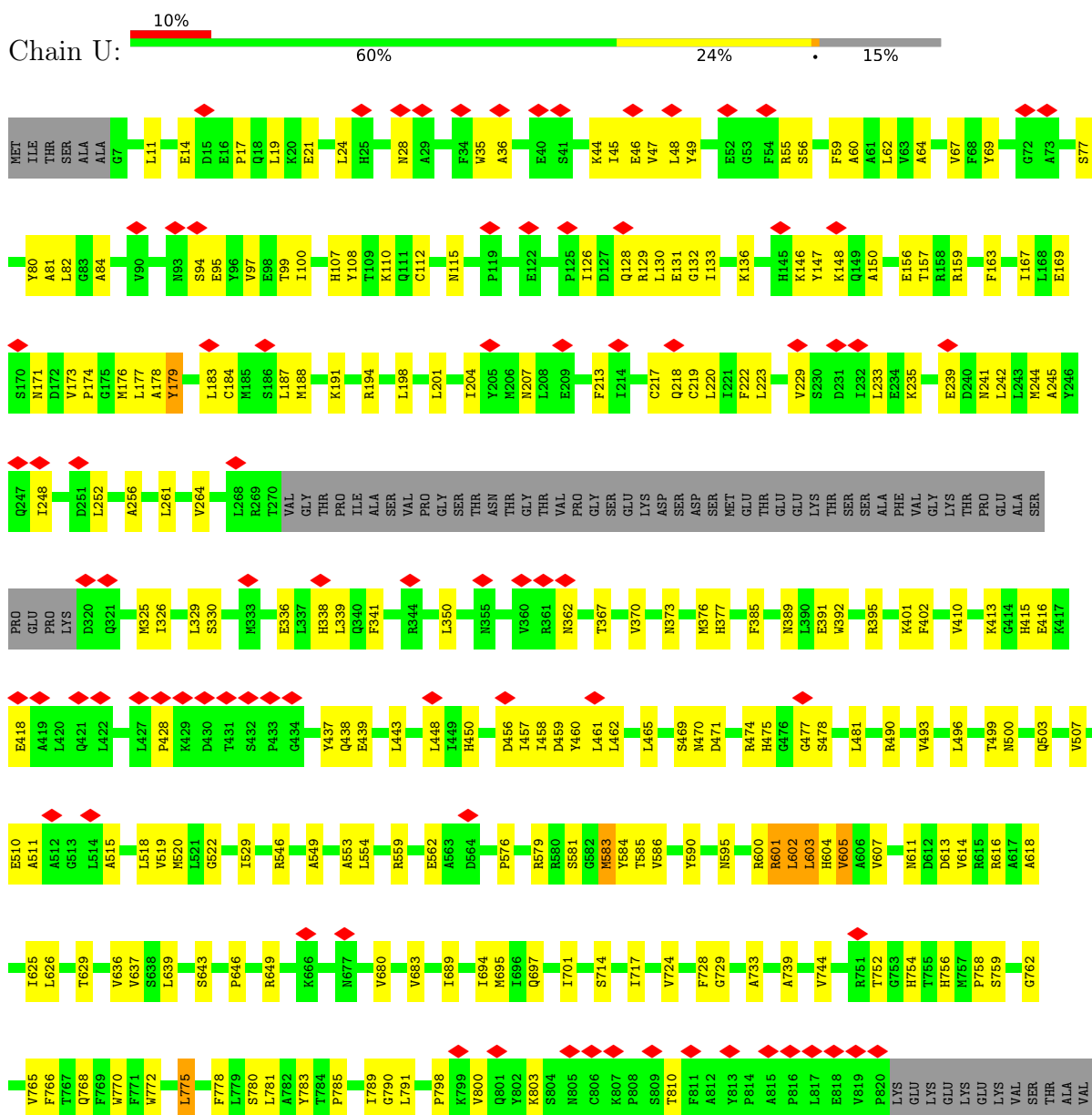
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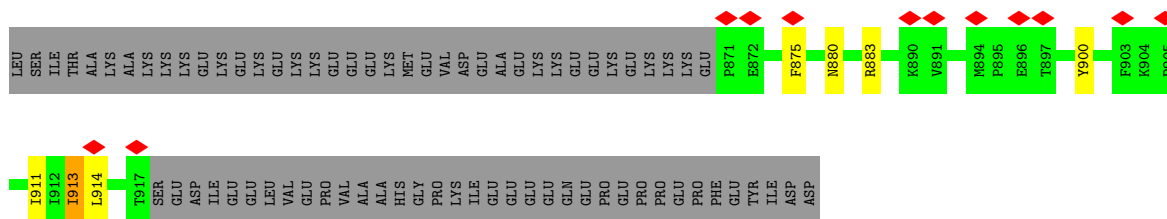
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	F	1	27	10	5	10	2	0

3 Residue-property plots

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

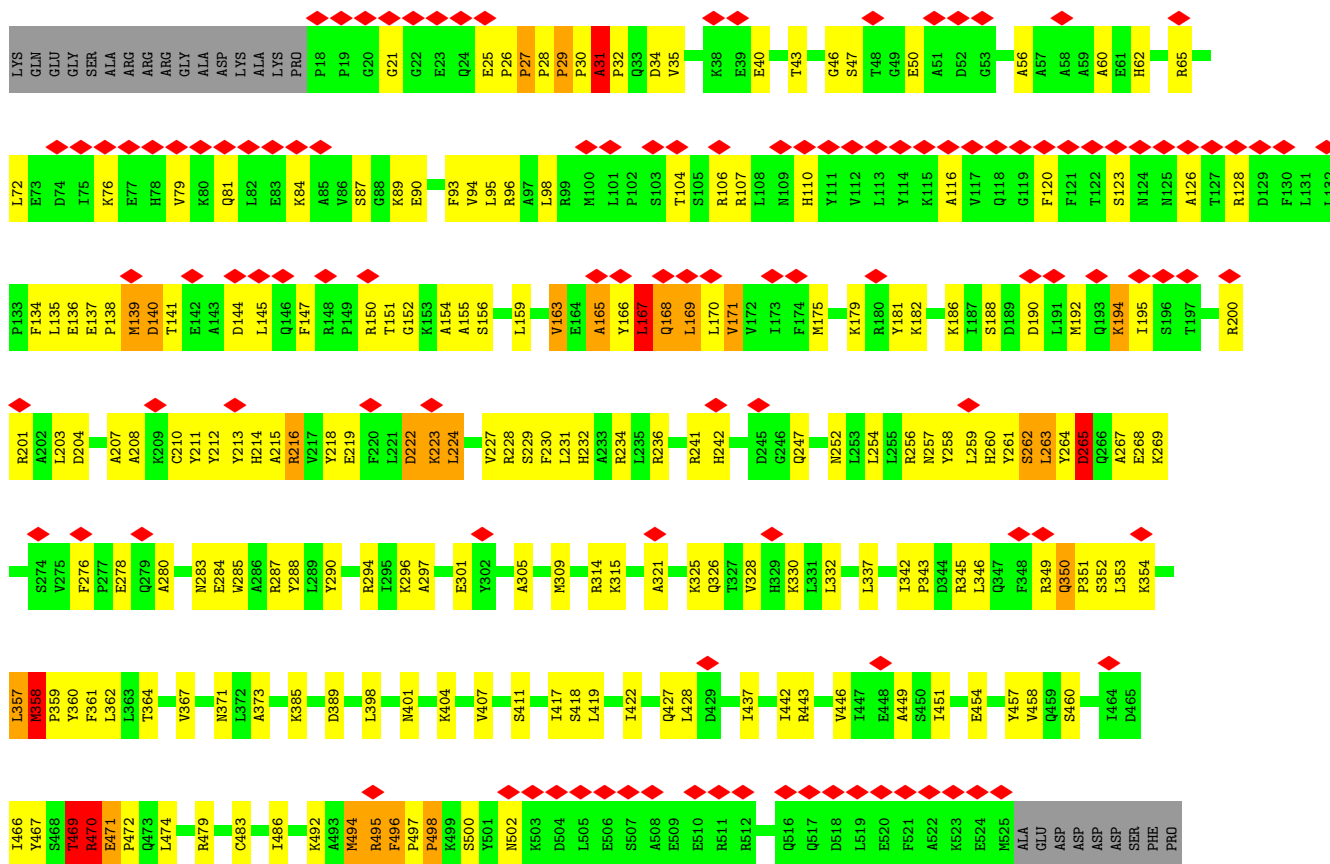
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1





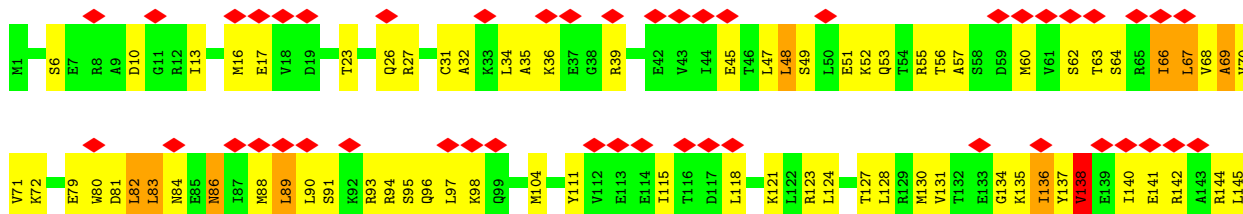
• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

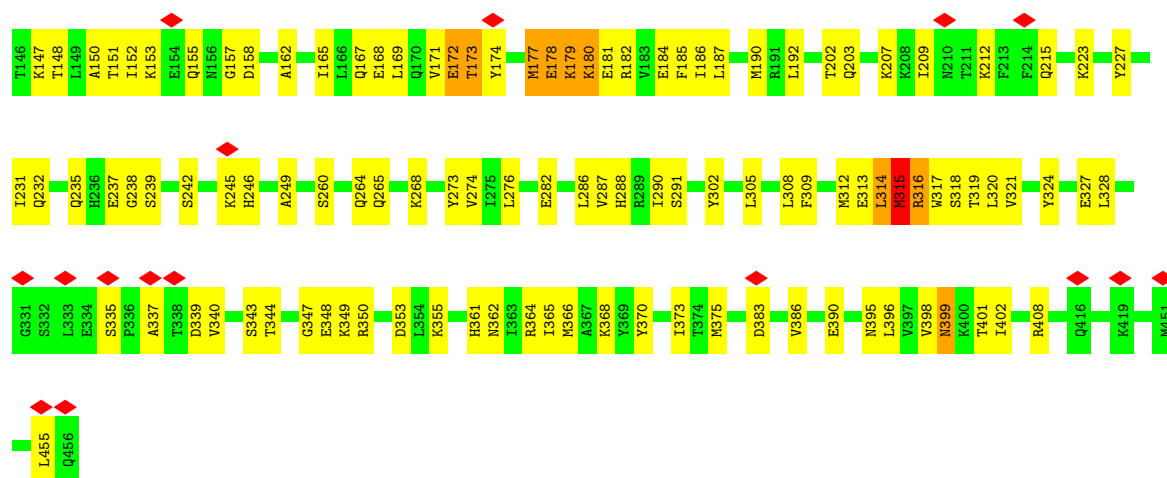
Chain V: 22% 56% 33% 5%



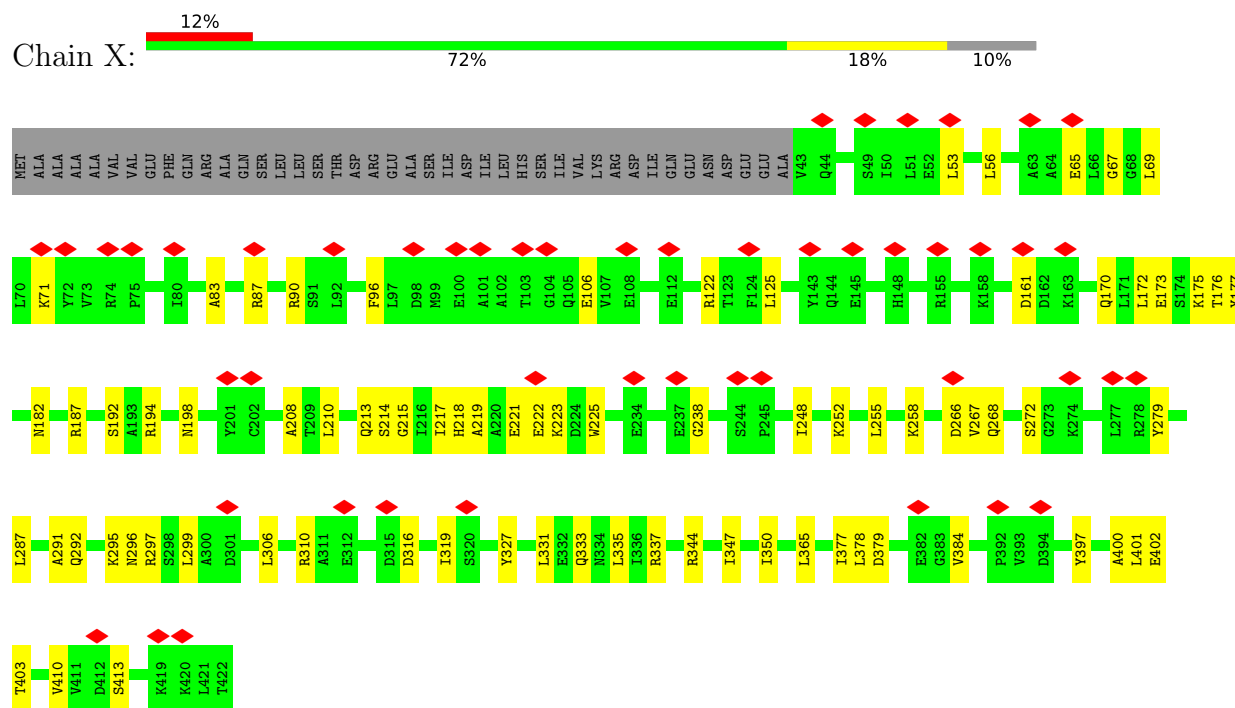
• Molecule 3: 26S proteasome non-ATPase regulatory subunit 12

Chain W: 14% 60% 36%

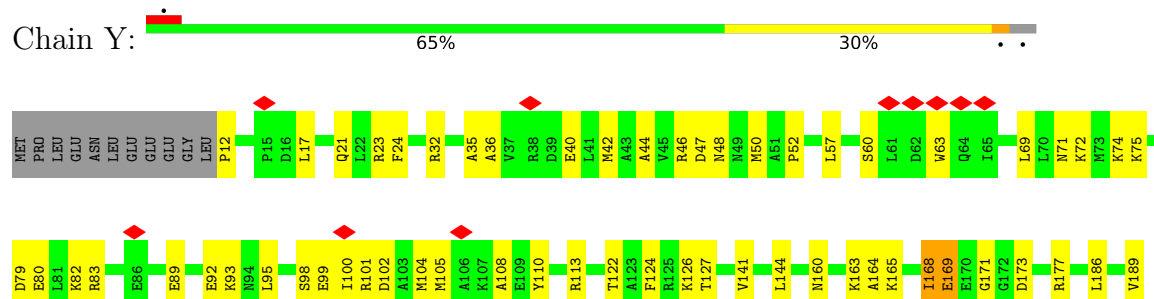


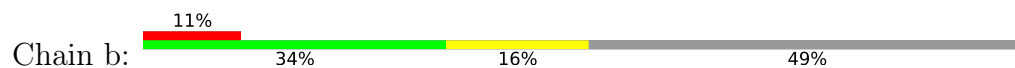


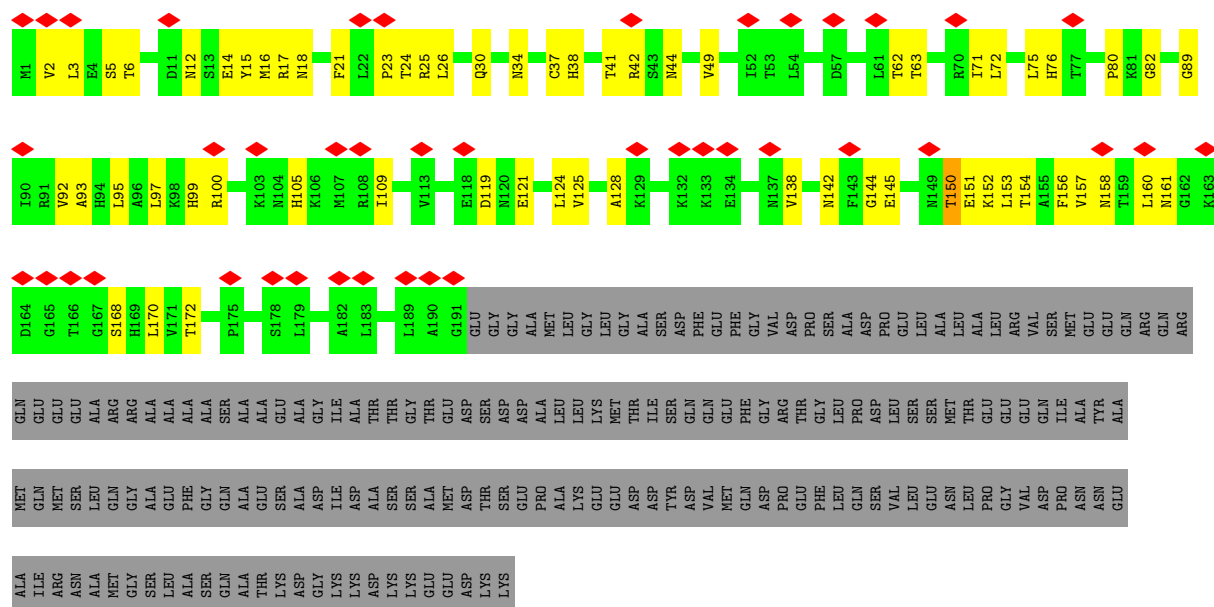
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11



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

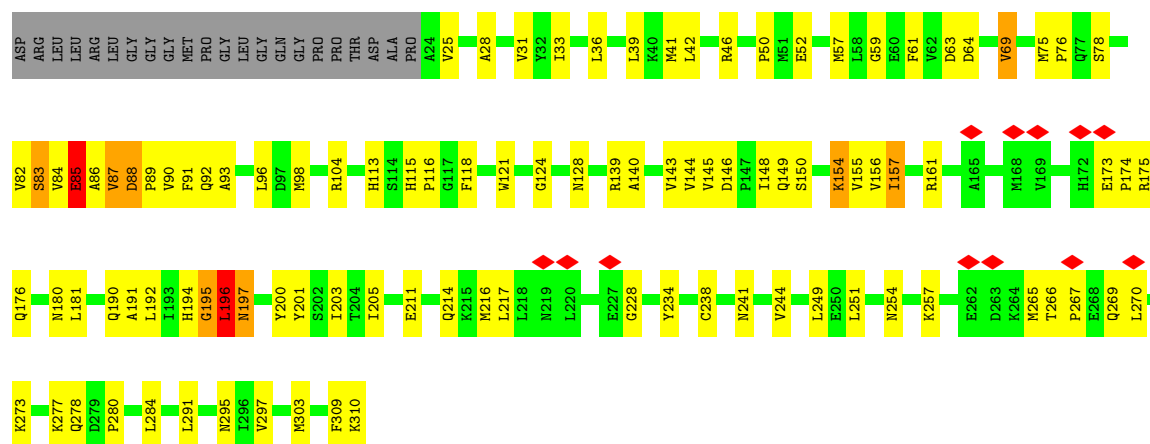






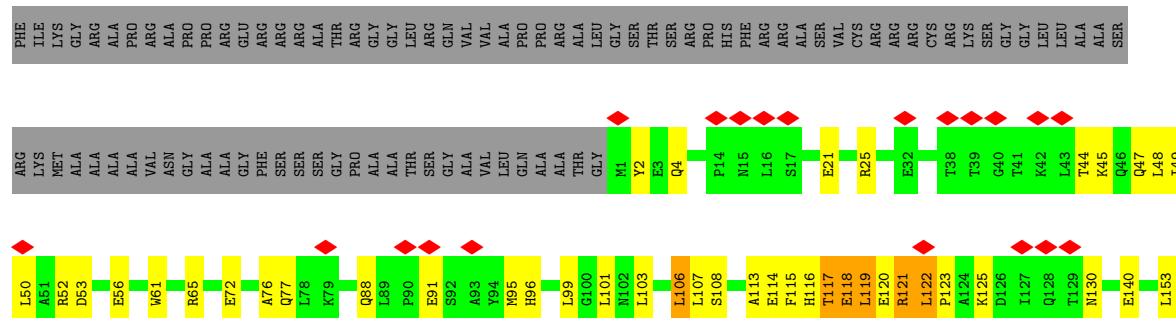
• Molecule 9: 26S proteasome non-ATPase regulatory subunit 14

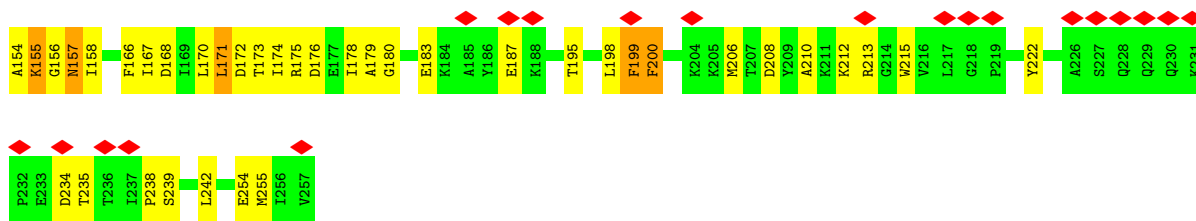
Chain c: 60% 30% 7%



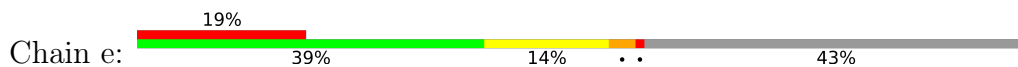
• Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 11% 50% 20% 26%

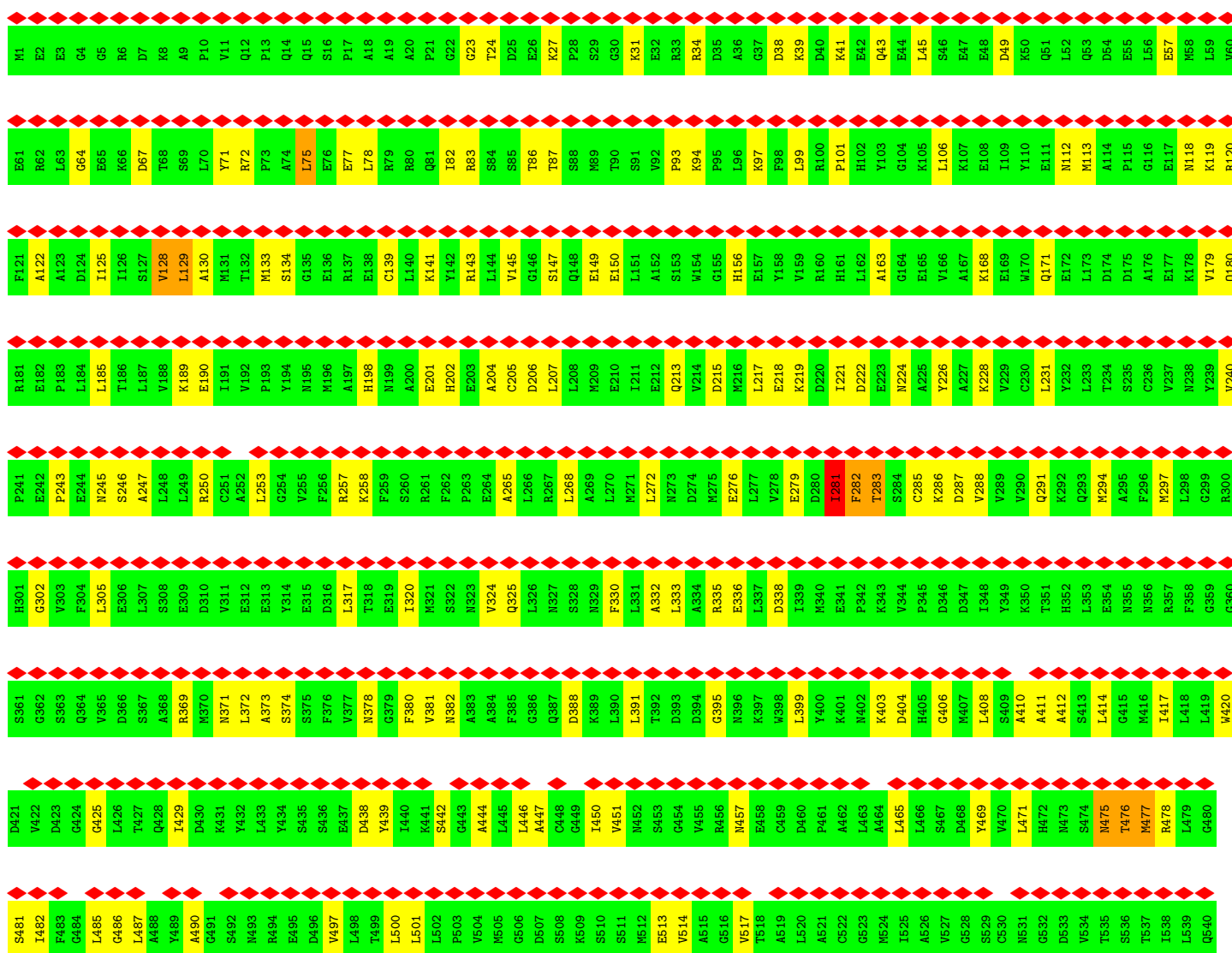


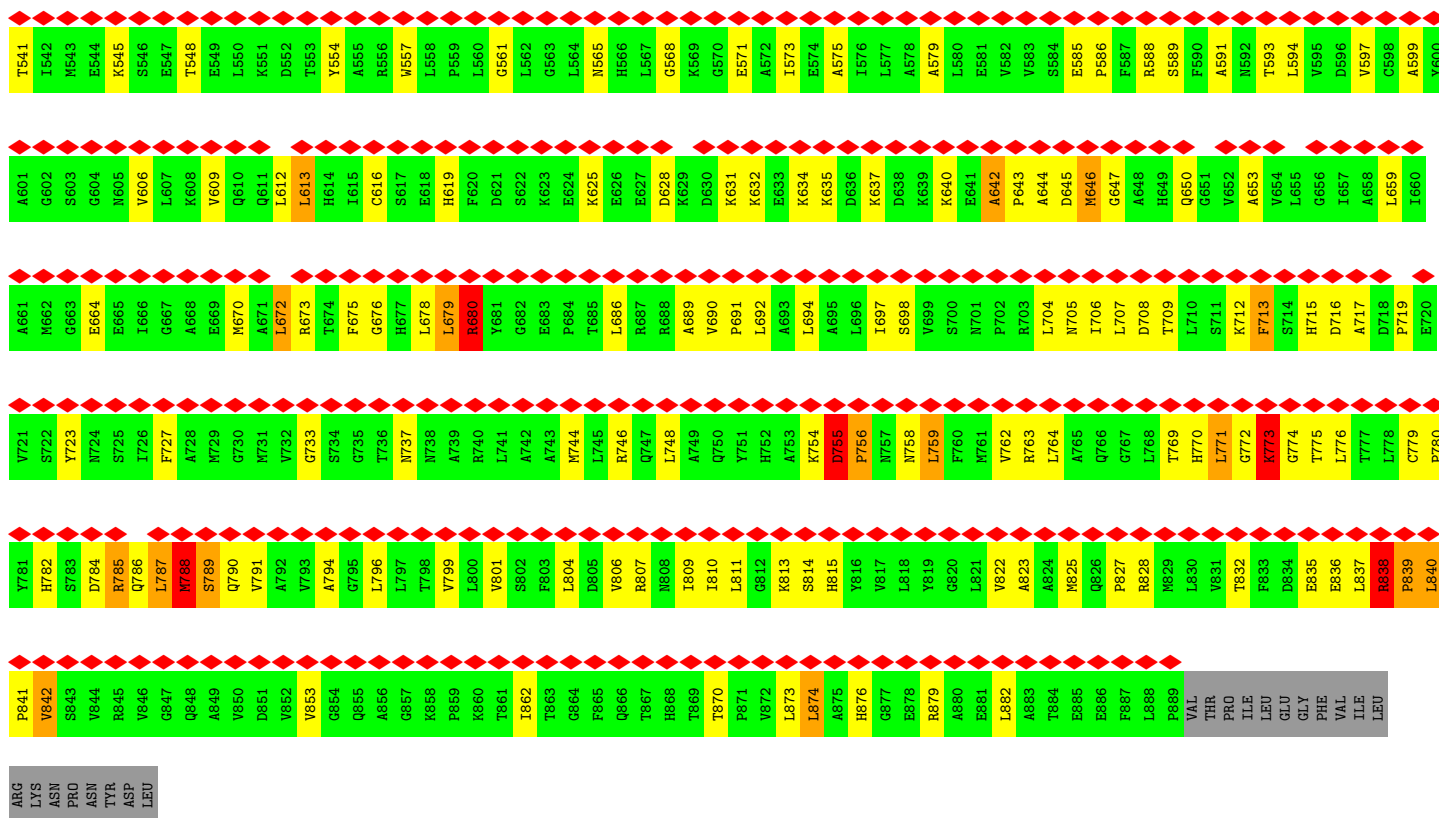


• Molecule 11: 26S proteasome complex subunit SEM1



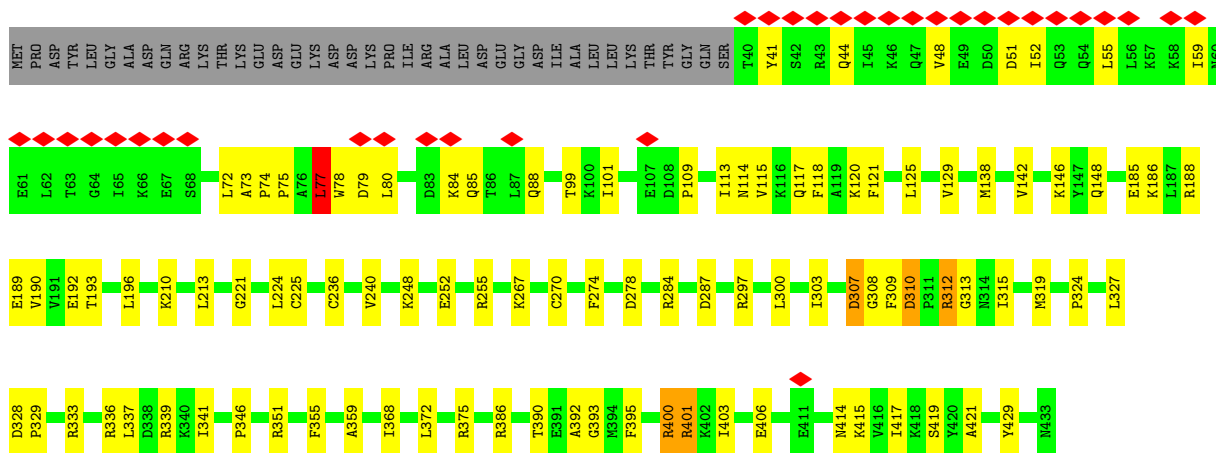
• Molecule 12: 26S proteasome non-ATPase regulatory subunit 2





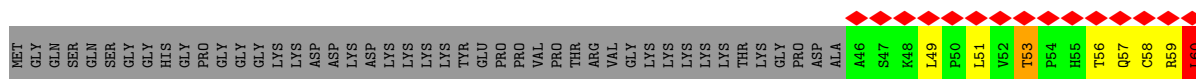
• Molecule 13: 26S protease regulatory subunit 7

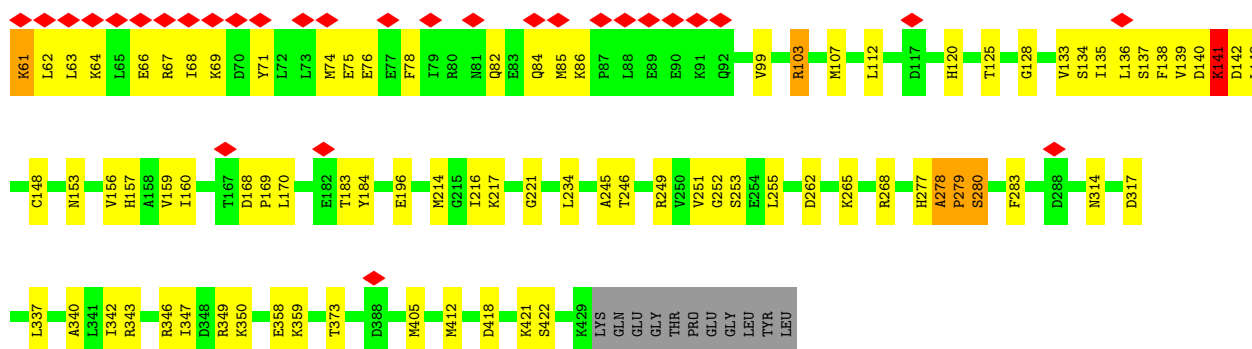
Chain A:



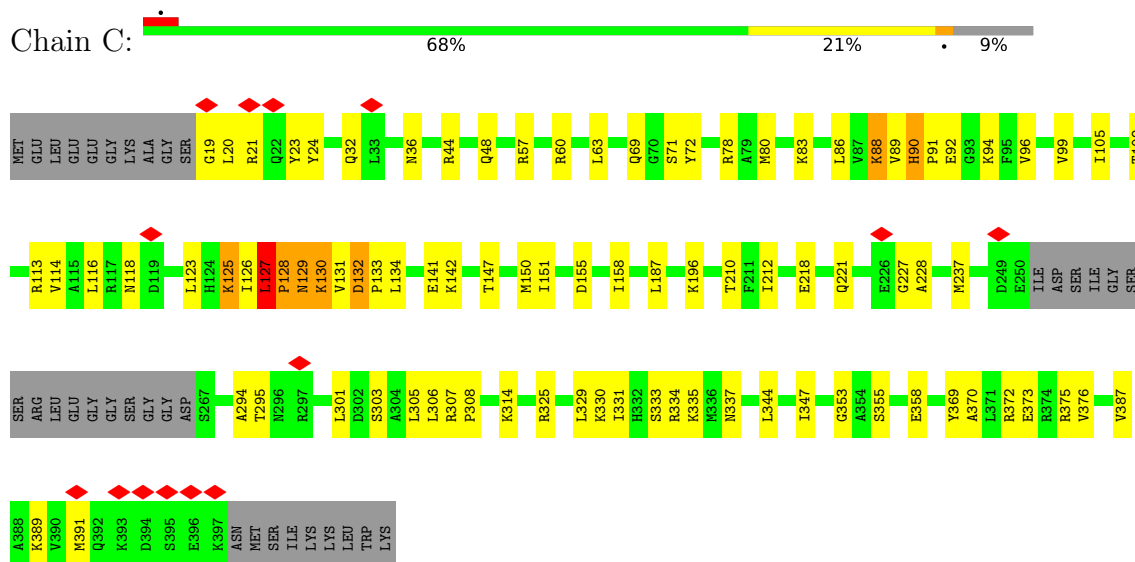
• Molecule 14: 26S protease regulatory subunit 4

Chain B:

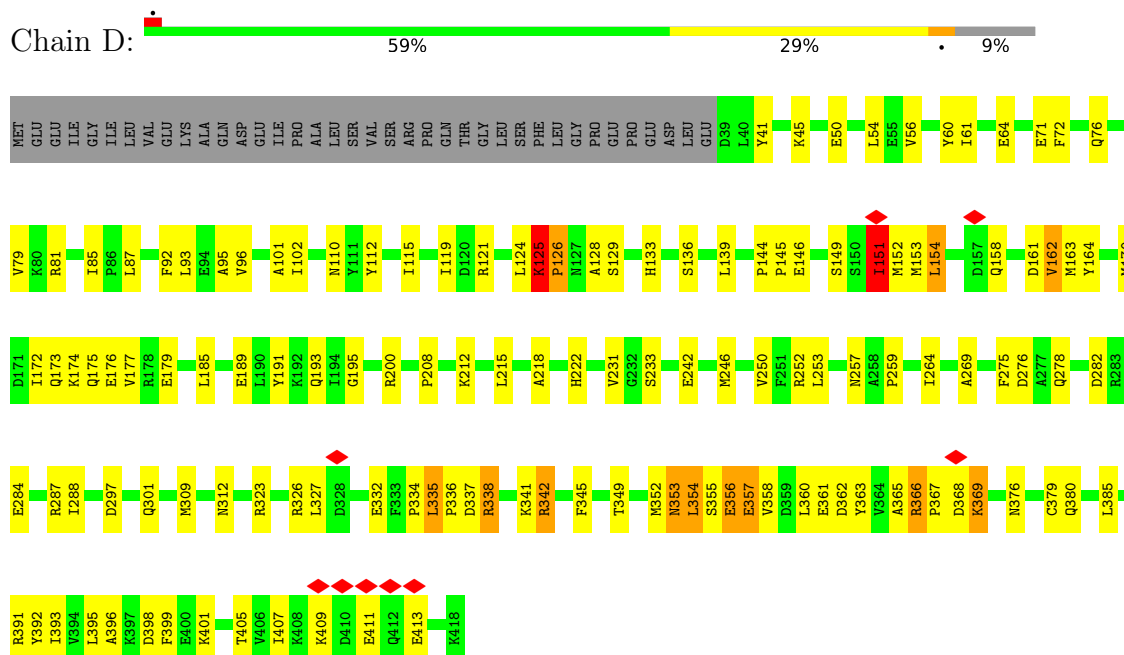




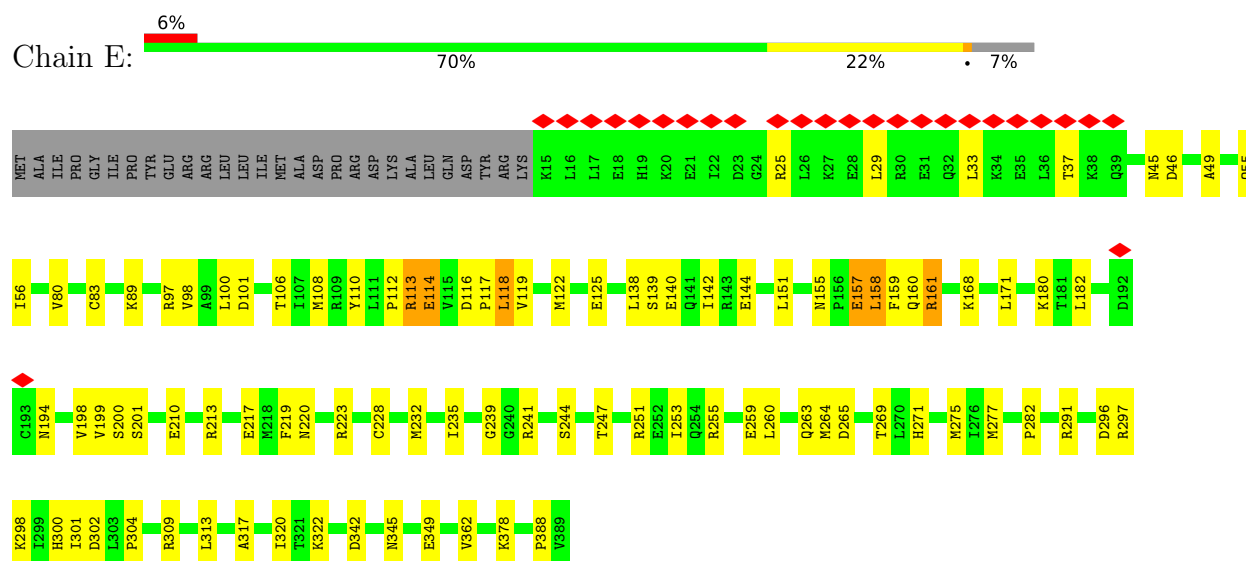
- Molecule 15: Isoform 2 of 26S proteasome regulatory subunit 8



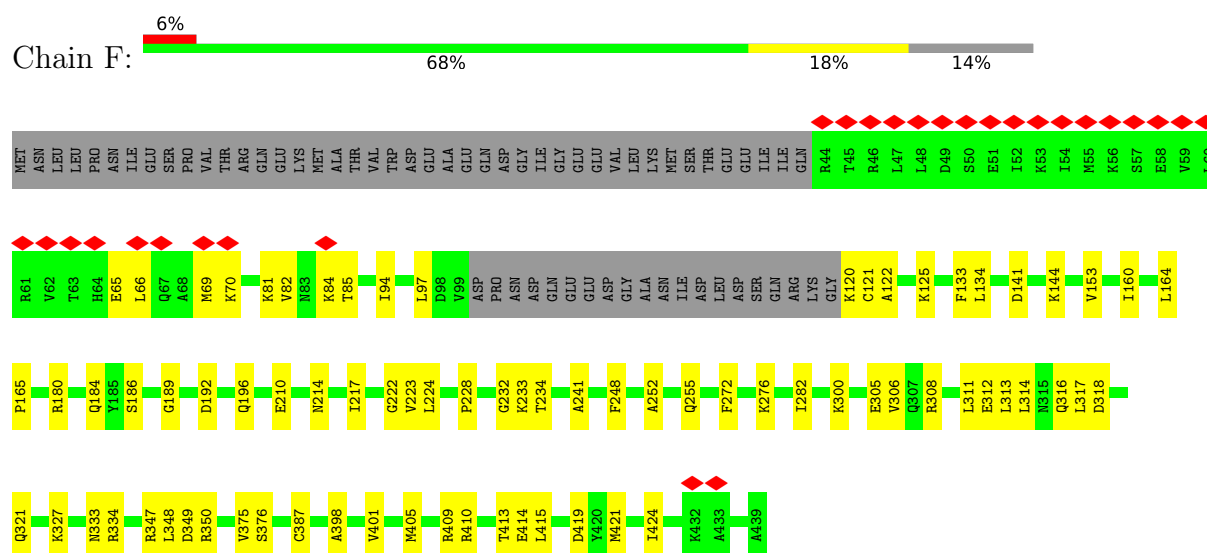
- Molecule 16: 26S protease regulatory subunit 6B



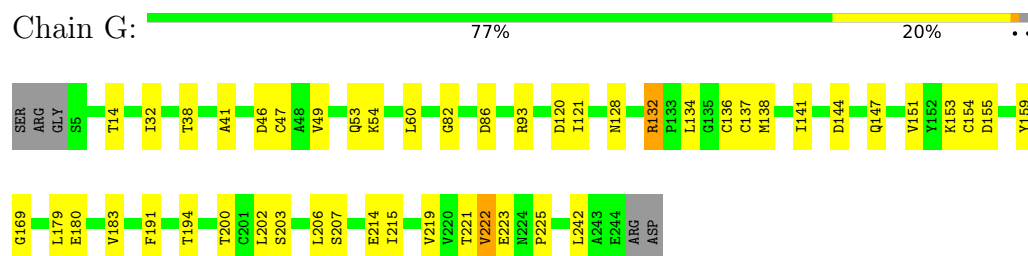
- Molecule 17: 26S proteasome regulatory subunit 10B



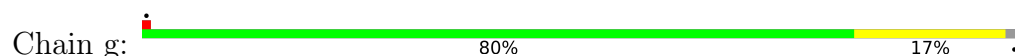
- Molecule 18: 26S protease regulatory subunit 6A

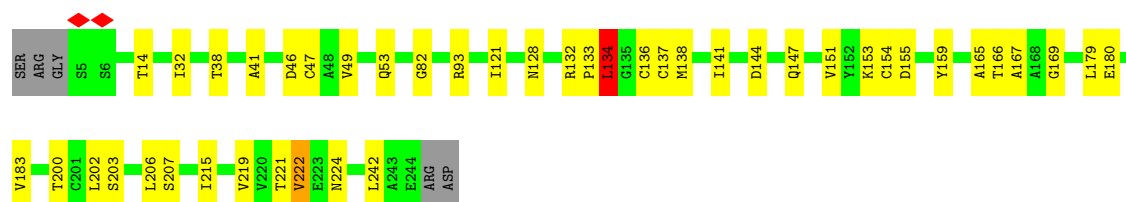


- Molecule 19: Proteasome subunit alpha type-6



- Molecule 19: Proteasome subunit alpha type-6





- Molecule 20: Proteasome subunit alpha type-2

Chain H: 88% 12%



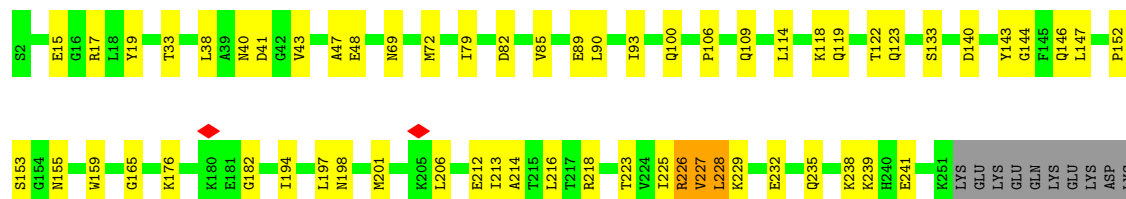
- Molecule 20: Proteasome subunit alpha type-2

Chain h: 89% 11%



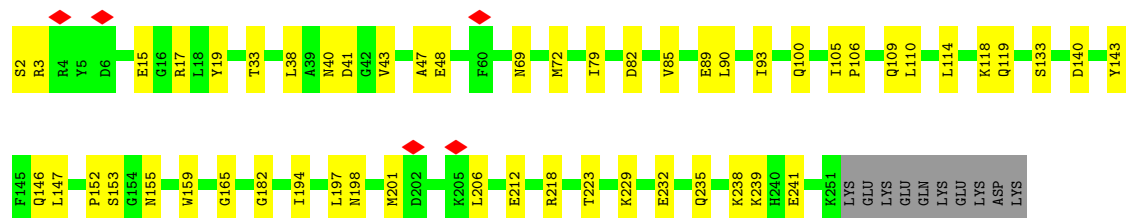
- Molecule 21: Proteasome subunit alpha type-4

Chain I: 73% 22%



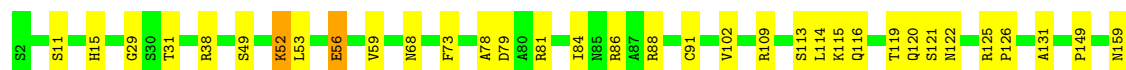
- Molecule 21: Proteasome subunit alpha type-4

Chain i: 75% 21%



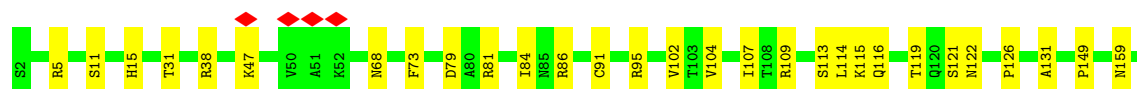
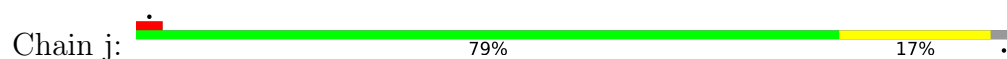
- Molecule 22: Proteasome subunit alpha type-7

Chain J: 79% 17%

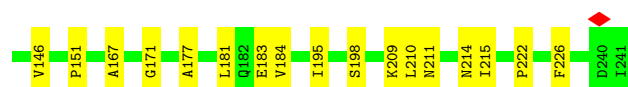
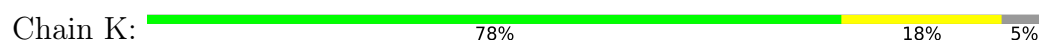




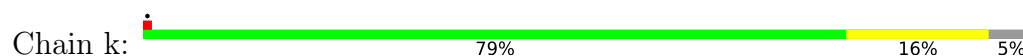
- Molecule 22: Proteasome subunit alpha type-7



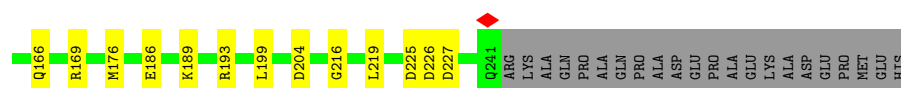
- Molecule 23: Proteasome subunit alpha type-5



- Molecule 23: Proteasome subunit alpha type-5

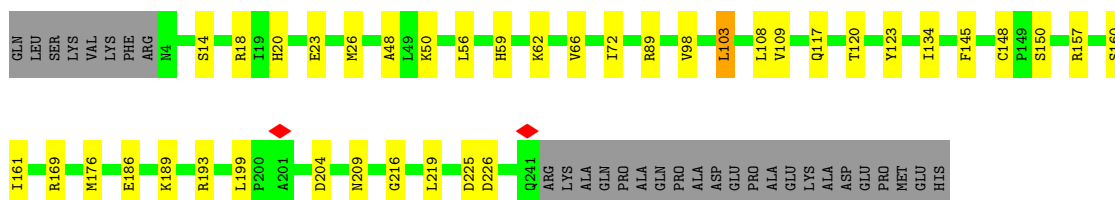


- Molecule 24: Isoform Long of Proteasome subunit alpha type-1

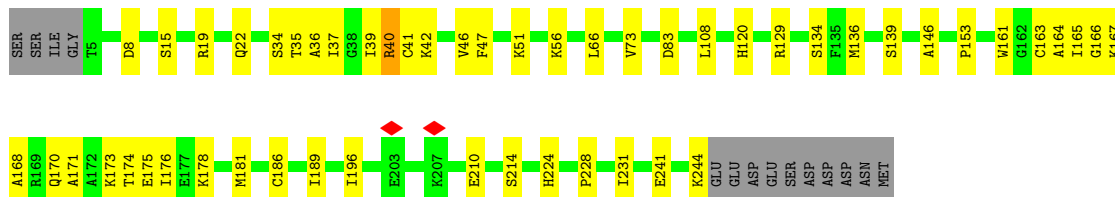


- Molecule 24: Isoform Long of Proteasome subunit alpha type-1

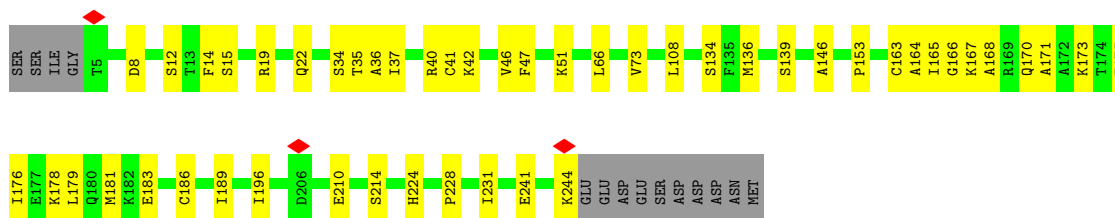
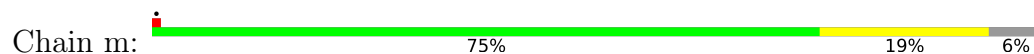




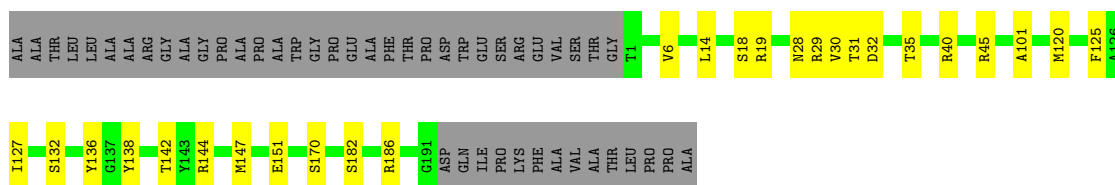
• Molecule 25: Proteasome subunit alpha type-3



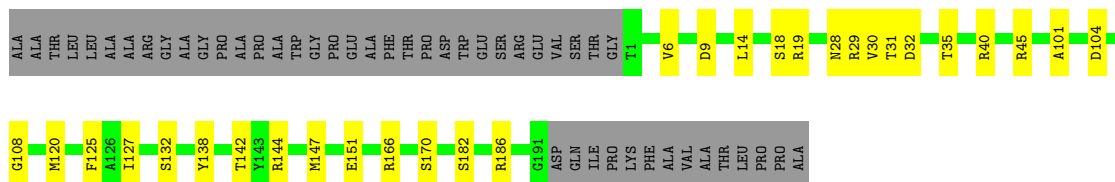
• Molecule 25: Proteasome subunit alpha type-3



• Molecule 26: Proteasome subunit beta type-6

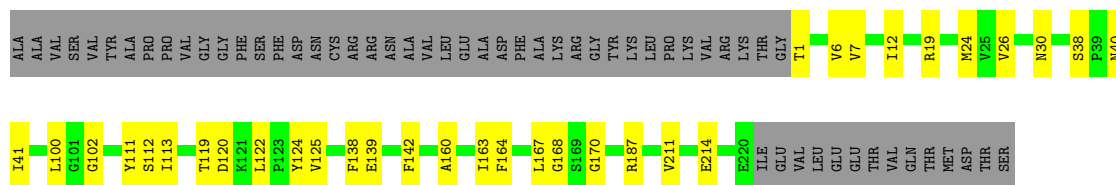


• Molecule 26: Proteasome subunit beta type-6



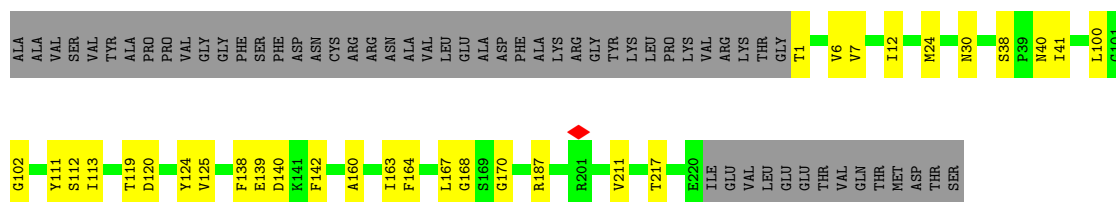
• Molecule 27: Proteasome subunit beta type-7

Chain O:  68% 12% 20%




- Molecule 27: Proteasome subunit beta type-7

Chain o:  68% 11% 20%




- Molecule 28: Proteasome subunit beta type-3

Chain P:  87% 13%




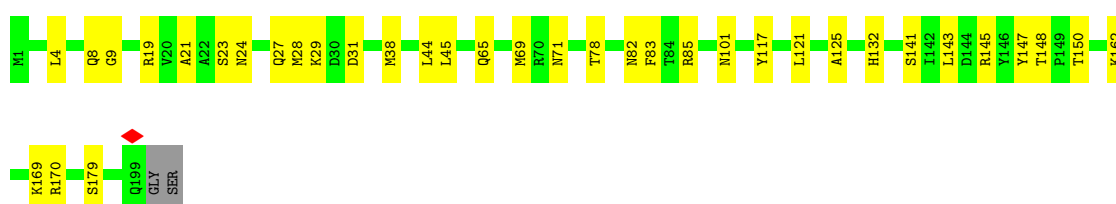
- Molecule 28: Proteasome subunit beta type-3

Chain p:  86% 14%




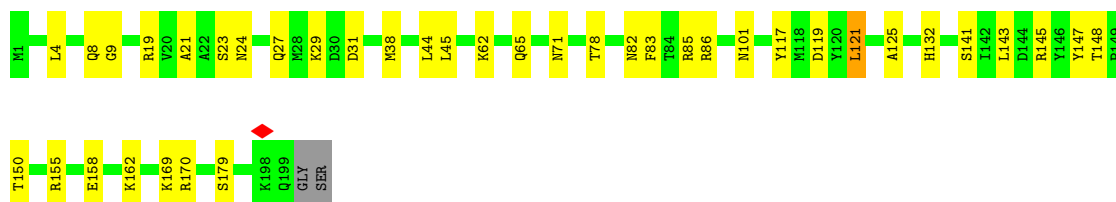
- Molecule 29: Proteasome subunit beta type-2

Chain Q:  81% 18%

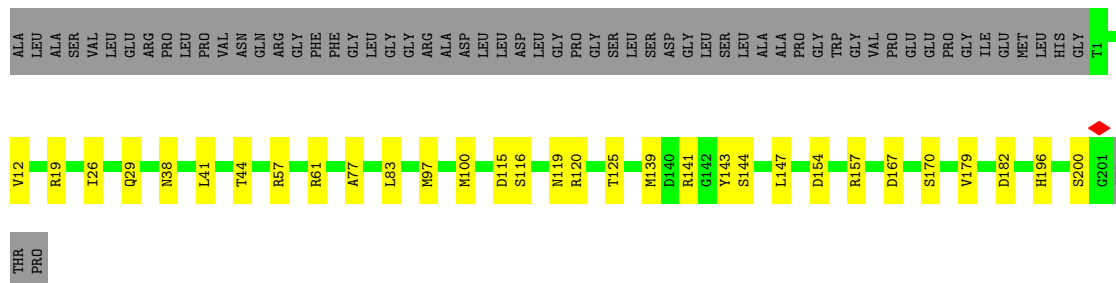


- Molecule 29: Proteasome subunit beta type-2

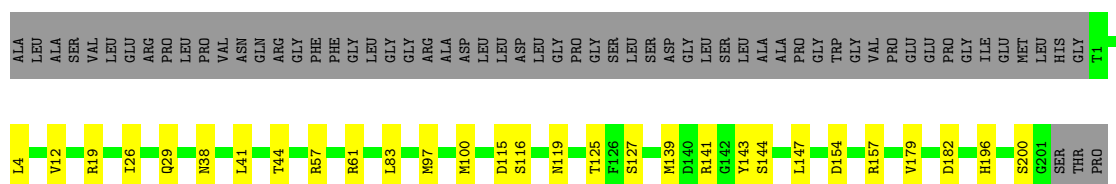
Chain q:  80% 19%



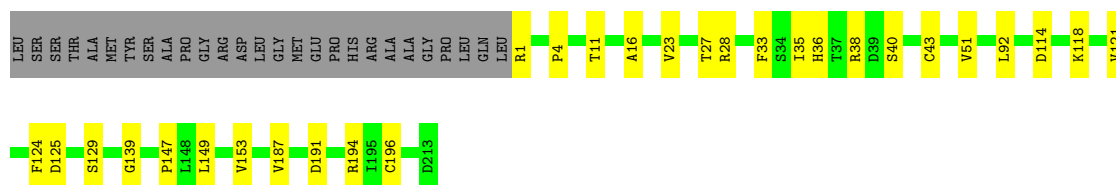
• Molecule 30: Proteasome subunit beta type-5



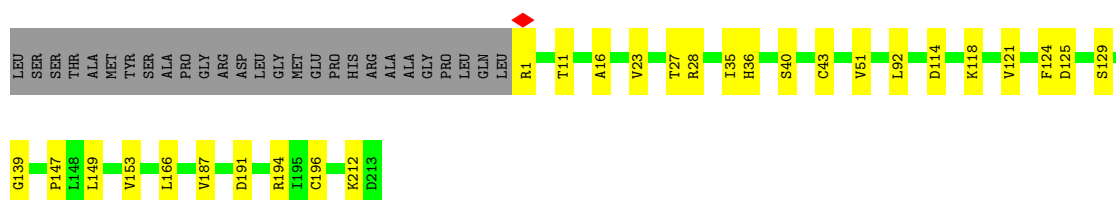
• Molecule 30: Proteasome subunit beta type-5



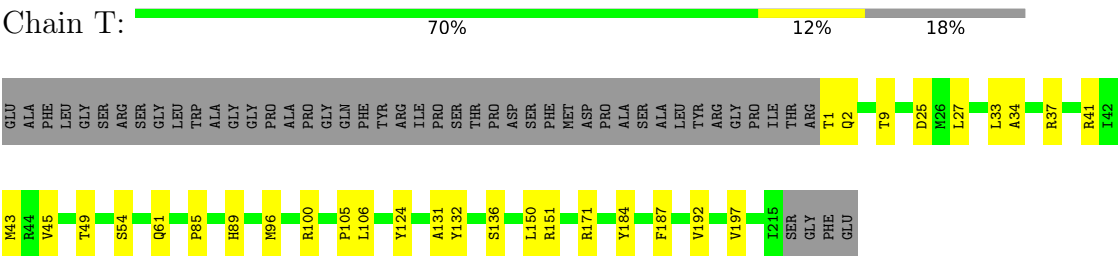
• Molecule 31: Proteasome subunit beta type-1



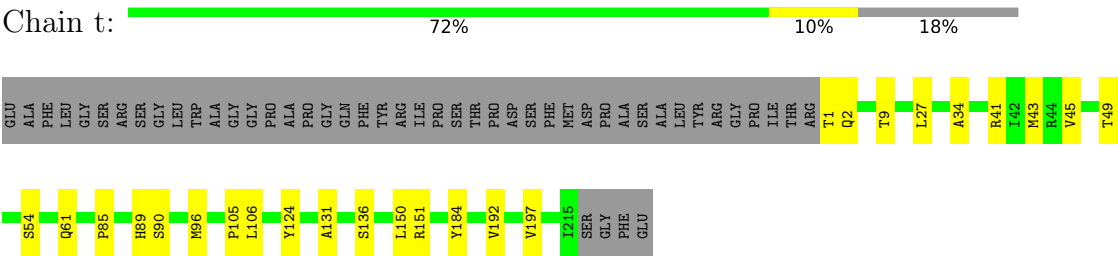
• Molecule 31: Proteasome subunit beta type-1



● Molecule 32: Proteasome subunit beta type-4



● Molecule 32: Proteasome subunit beta type-4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90097	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 ($e^-/\text{\AA}^2$)	46.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.0354	Depositor
Map size (Å)	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.27	0/6449	0.61	0/8729
2	V	0.32	0/4072	0.79	13/5510 (0.2%)
3	W	0.31	0/3751	0.75	4/5042 (0.1%)
4	X	0.24	0/3053	0.56	0/4115
5	Y	0.31	0/3173	0.65	1/4273 (0.0%)
6	Z	0.32	0/2324	0.72	4/3150 (0.1%)
7	a	0.27	0/3053	0.64	0/4133
8	b	0.25	0/1478	0.66	0/2001
9	c	0.30	0/2302	0.73	2/3110 (0.1%)
10	d	0.28	0/2162	0.72	1/2919 (0.0%)
11	e	0.32	0/338	0.81	1/450 (0.2%)
12	f	0.28	0/6980	0.77	12/9433 (0.1%)
13	A	0.30	0/3148	0.65	3/4250 (0.1%)
14	B	0.30	0/3061	0.63	2/4129 (0.0%)
15	C	0.29	0/2902	0.70	4/3904 (0.1%)
16	D	0.33	0/3089	0.66	1/4168 (0.0%)
17	E	0.30	0/2904	0.62	4/3924 (0.1%)
18	F	0.30	0/2896	0.58	0/3912
19	G	0.27	0/1859	0.49	0/2523
19	g	0.26	0/1859	0.48	0/2523
20	H	0.27	0/1743	0.49	0/2372
20	h	0.27	0/1743	0.49	0/2372
21	I	0.29	0/1942	0.55	0/2628
21	i	0.29	0/1942	0.54	0/2628
22	J	0.27	0/1737	0.55	0/2369
22	j	0.27	0/1728	0.54	0/2358
23	K	0.27	0/1747	0.50	0/2364
23	k	0.27	0/1747	0.50	0/2364
24	L	0.29	0/1885	0.59	1/2552 (0.0%)
24	l	0.29	0/1885	0.59	2/2552 (0.1%)
25	M	0.28	0/1891	0.53	0/2552
25	m	0.28	0/1891	0.52	0/2552

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	N	0.27	0/1454	0.44	0/1967
26	n	0.27	0/1454	0.44	0/1967
27	O	0.28	0/1670	0.48	0/2265
27	o	0.28	0/1670	0.48	0/2265
28	P	0.29	0/1620	0.47	0/2184
28	p	0.29	0/1620	0.47	0/2184
29	Q	0.31	0/1603	0.52	0/2174
29	q	0.32	0/1603	0.54	0/2174
30	R	0.30	0/1579	0.44	0/2134
30	r	0.30	0/1579	0.44	0/2134
31	S	0.30	0/1671	0.48	0/2253
31	s	0.30	0/1674	0.48	0/2257
32	T	0.30	0/1700	0.50	0/2305
32	t	0.30	0/1700	0.50	0/2305
All	All	0.29	0/105331	0.61	55/142429 (0.0%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	C	127	LEU	CA-C-N	11.97	134.81	119.84
15	C	127	LEU	C-N-CA	11.97	134.81	119.84
6	Z	250	TYR	N-CA-C	-11.10	99.19	111.07
2	V	496	PHE	CA-C-N	8.50	129.13	120.38
2	V	496	PHE	C-N-CA	8.50	129.13	120.38
12	f	679	LEU	N-CA-C	8.46	122.26	109.41
14	B	60	LEU	N-CA-C	-7.52	103.16	111.36
6	Z	245	PHE	N-CA-C	-7.48	102.28	111.33
17	E	116	ASP	CA-C-N	7.21	128.85	119.84
17	E	116	ASP	C-N-CA	7.21	128.85	119.84
12	f	477	MET	N-CA-C	-7.08	104.72	113.15
12	f	679	LEU	CA-C-N	6.61	134.16	121.54
12	f	679	LEU	C-N-CA	6.61	134.16	121.54
13	A	310	ASP	CA-C-N	6.48	126.45	119.78
13	A	310	ASP	C-N-CA	6.48	126.45	119.78
12	f	475	ASN	N-CA-C	6.39	124.41	110.80
2	V	469	THR	N-CA-C	-6.30	98.91	108.67
11	e	58	ALA	N-CA-C	6.22	118.49	109.71
13	A	401	ARG	N-CA-C	6.22	117.90	110.19
3	W	27	ARG	N-CA-C	-6.06	106.86	114.56
2	V	29	PRO	CA-C-N	6.02	126.46	119.47
2	V	29	PRO	C-N-CA	6.02	126.46	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	d	154	ALA	N-CA-C	-5.94	104.80	111.28
12	f	755	ASP	CA-C-N	5.93	127.26	119.84
12	f	755	ASP	C-N-CA	5.93	127.26	119.84
9	c	195	GLY	O-C-N	5.92	129.36	122.73
12	f	713	PHE	N-CA-C	-5.89	104.77	111.07
14	B	53	THR	N-CA-C	5.75	122.51	109.81
3	W	316	ARG	CB-CA-C	-5.69	110.00	116.54
5	Y	288	PHE	N-CA-C	-5.68	98.69	110.80
2	V	31	ALA	CA-C-N	5.46	126.66	119.84
2	V	31	ALA	C-N-CA	5.46	126.66	119.84
2	V	222	ASP	N-CA-C	5.44	117.04	109.31
6	Z	249	PHE	O-C-N	5.36	127.81	122.03
6	Z	143	GLU	N-CA-C	5.30	117.12	110.24
24	l	225	ASP	CA-C-N	5.28	131.63	121.54
24	l	225	ASP	C-N-CA	5.28	131.63	121.54
9	c	85	GLU	CB-CA-C	-5.25	110.50	116.54
2	V	165	ALA	CA-C-N	5.21	131.50	121.54
2	V	165	ALA	C-N-CA	5.21	131.50	121.54
15	C	132	ASP	CA-C-N	5.21	126.35	119.84
15	C	132	ASP	C-N-CA	5.21	126.35	119.84
16	D	369	LYS	N-CA-C	5.21	121.89	110.80
12	f	773	LYS	N-CA-C	5.20	117.52	111.02
12	f	874	LEU	N-CA-C	5.16	121.80	110.80
2	V	27	PRO	N-CA-C	5.12	116.95	110.70
3	W	399	ASN	CA-C-N	5.12	129.60	122.08
3	W	399	ASN	C-N-CA	5.12	129.60	122.08
24	L	225	ASP	N-CA-C	5.10	117.74	109.06
2	V	502	ASN	CA-C-N	-5.09	115.82	123.00
2	V	502	ASN	C-N-CA	-5.09	115.82	123.00
17	E	241	ARG	CA-C-N	5.04	131.96	122.84
17	E	241	ARG	C-N-CA	5.04	131.96	122.84
12	f	619	HIS	CA-C-N	5.03	131.14	121.54
12	f	619	HIS	C-N-CA	5.03	131.14	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6334	0	6366	202	0
2	V	3994	0	3960	347	0
3	W	3703	0	3822	237	0
4	X	3009	0	3113	49	0
5	Y	3115	0	3120	122	0
6	Z	2281	0	2312	144	0
7	a	2995	0	3012	106	0
8	b	1458	0	1505	55	0
9	c	2260	0	2276	107	0
10	d	2116	0	2146	92	0
11	e	334	0	294	12	0
12	f	6866	0	6865	394	0
13	A	3096	0	3139	101	0
14	B	3018	0	3082	115	0
15	C	2864	0	2971	95	0
16	D	3039	0	3075	155	0
17	E	2860	0	2827	95	0
18	F	2858	0	2852	57	0
19	G	1826	0	1796	36	0
19	g	1826	0	1796	33	0
20	H	1708	0	1594	17	0
20	h	1708	0	1594	13	0
21	I	1912	0	1851	67	0
21	i	1912	0	1851	36	0
22	J	1713	0	1537	34	0
22	j	1704	0	1517	26	0
23	K	1722	0	1673	25	0
23	k	1722	0	1673	22	0
24	L	1850	0	1822	25	0
24	l	1850	0	1822	23	0
25	M	1856	0	1814	44	0
25	m	1856	0	1816	39	0
26	N	1430	0	1398	17	0
26	n	1430	0	1398	18	0
27	O	1643	0	1644	22	0
27	o	1643	0	1644	21	0
28	P	1591	0	1609	21	0
28	p	1591	0	1609	21	0
29	Q	1570	0	1547	27	0
29	q	1570	0	1547	29	0
30	R	1548	0	1499	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	r	1548	0	1499	20	0
31	S	1641	0	1618	20	0
31	s	1644	0	1627	19	0
32	T	1667	0	1628	23	0
32	t	1667	0	1628	19	0
33	c	1	0	0	0	0
34	A	31	0	12	1	0
34	B	31	0	12	1	0
34	D	31	0	12	1	0
34	E	31	0	12	4	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	D	1	0	0	0	0
35	E	1	0	0	0	0
35	F	1	0	0	0	0
36	C	27	0	12	0	0
36	F	27	0	12	2	0
All	All	103732	0	102860	2926	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 14.

All (2926) 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)
12:f:297:MET:HB2	12:f:770:HIS:CE1	1.34	1.58
1:U:167:ILE:HG22	1:U:177:LEU:CD2	1.29	1.56
12:f:764:LEU:CD2	12:f:774:GLY:HA3	1.35	1.55
2:V:497:PRO:HG3	6:Z:278:ASN:CG	1.23	1.52
12:f:838:ARG:HB3	12:f:839:PRO:CD	1.33	1.52
3:W:83:LEU:HD11	3:W:91:SER:CB	1.37	1.51
25:m:41:CYS:SG	25:m:189:ILE:HG13	1.47	1.51
25:M:41:CYS:SG	25:M:189:ILE:HG13	1.50	1.50
2:V:94:VAL:CG2	2:V:137:GLU:HG2	1.42	1.48
2:V:94:VAL:HG22	2:V:137:GLU:CG	1.44	1.45
3:W:83:LEU:CD1	3:W:91:SER:HB2	1.47	1.44
12:f:670:MET:HG2	12:f:673:ARG:NH1	1.26	1.43
12:f:764:LEU:HD11	12:f:774:GLY:N	1.18	1.43
2:V:135:LEU:HG	2:V:181:TYR:CE2	1.52	1.42
12:f:258:LYS:HG2	12:f:770:HIS:NE2	1.11	1.41
2:V:497:PRO:CG	6:Z:278:ASN:ND2	1.81	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:155:ASN:CG	17:E:158:LEU:CD1	1.91	1.41
17:E:155:ASN:CG	17:E:158:LEU:HD11	0.99	1.41
2:V:497:PRO:CG	6:Z:278:ASN:CG	1.95	1.40
3:W:142:ARG:HH12	3:W:185:PHE:CB	1.34	1.40
12:f:838:ARG:CB	12:f:839:PRO:HD2	1.44	1.40
1:U:603:LEU:CD2	16:D:60:TYR:CD1	2.05	1.39
2:V:94:VAL:HG21	2:V:137:GLU:CD	1.44	1.39
2:V:497:PRO:HG3	6:Z:278:ASN:ND2	1.31	1.39
3:W:142:ARG:NH1	3:W:185:PHE:HB2	1.38	1.39
9:c:196:LEU:HD22	9:c:197:ASN:N	1.32	1.38
15:C:90:HIS:CD2	15:C:91:PRO:HD3	1.56	1.38
12:f:297:MET:CB	12:f:770:HIS:CE1	2.07	1.38
1:U:179:TYR:CE2	1:U:183:LEU:HD11	1.57	1.37
12:f:258:LYS:CG	12:f:770:HIS:NE2	1.87	1.35
9:c:196:LEU:CD2	9:c:197:ASN:H	1.39	1.35
2:V:497:PRO:CG	6:Z:278:ASN:OD1	1.71	1.34
12:f:764:LEU:HD21	12:f:774:GLY:CA	1.57	1.34
12:f:764:LEU:CD1	12:f:774:GLY:H	1.40	1.34
1:U:603:LEU:HD23	16:D:60:TYR:CD1	1.61	1.34
1:U:167:ILE:CG2	1:U:177:LEU:HD22	1.58	1.31
2:V:497:PRO:CG	6:Z:278:ASN:HD21	1.37	1.31
3:W:141:GLU:HG3	3:W:172:GLU:OE1	1.27	1.30
2:V:497:PRO:CD	6:Z:278:ASN:HD21	1.43	1.30
7:a:5:PRO:HA	7:a:8:LEU:CD2	1.62	1.30
2:V:94:VAL:CG2	2:V:137:GLU:CG	2.01	1.29
21:I:216:LEU:CD1	21:I:225:ILE:HD11	1.62	1.29
3:W:137:TYR:CE1	16:D:392:TYR:HD2	1.50	1.27
5:Y:168:ILE:HG22	5:Y:177:ARG:NH1	1.48	1.27
21:I:214:ALA:HB2	21:I:227:VAL:CG2	1.64	1.27
2:V:497:PRO:HG3	6:Z:278:ASN:OD1	1.27	1.26
15:C:90:HIS:CG	15:C:91:PRO:HD3	1.70	1.26
6:Z:252:LYS:HG2	9:c:234:TYR:OH	1.17	1.25
15:C:114:VAL:C	15:C:127:LEU:HD11	1.63	1.23
3:W:141:GLU:HG3	3:W:172:GLU:CD	1.64	1.23
14:B:168:ASP:OD2	14:B:169:PRO:HD2	1.31	1.23
16:D:354:LEU:HD12	16:D:399:PHE:CZ	1.74	1.22
2:V:171:VAL:HG13	2:V:175:MET:CE	1.68	1.22
3:W:35:ALA:O	3:W:86:ASN:ND2	1.71	1.22
12:f:258:LYS:HG2	12:f:770:HIS:CE1	1.73	1.21
17:E:155:ASN:OD1	17:E:158:LEU:HD11	1.36	1.21
10:d:107:LEU:HD21	10:d:140:GLU:OE1	1.36	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:764:LEU:CD1	12:f:774:GLY:N	1.98	1.20
25:M:41:CYS:SG	25:M:189:ILE:CG1	2.27	1.20
9:c:194:HIS:O	9:c:196:LEU:HD12	1.38	1.19
12:f:690:VAL:HB	12:f:713:PHE:CE1	1.75	1.19
1:U:179:TYR:CE2	1:U:183:LEU:CD1	2.25	1.19
3:W:141:GLU:OE1	3:W:172:GLU:HG2	1.40	1.19
12:f:764:LEU:HD11	12:f:774:GLY:CA	1.74	1.18
2:V:165:ALA:HB3	2:V:167:LEU:CD2	1.72	1.17
2:V:350:GLN:HB3	2:V:351:PRO:CD	1.73	1.17
25:m:41:CYS:SG	25:m:189:ILE:CG1	2.30	1.17
1:U:167:ILE:CG2	1:U:177:LEU:CD2	2.19	1.16
14:B:278:ALA:HB1	14:B:279:PRO:CD	1.74	1.16
12:f:643:PRO:HB2	14:B:67:ARG:NH1	1.58	1.16
16:D:125:LYS:HB3	16:D:126:PRO:HD3	1.26	1.16
2:V:31:ALA:HB3	2:V:32:PRO:CD	1.74	1.15
2:V:358:MET:HA	2:V:358:MET:HE3	1.28	1.15
3:W:142:ARG:NH1	3:W:185:PHE:CB	1.98	1.15
2:V:497:PRO:HA	6:Z:282:ASN:ND2	1.60	1.15
1:U:603:LEU:HD21	16:D:60:TYR:CD1	1.82	1.14
2:V:258:TYR:CE2	2:V:265:ASP:OD2	2.00	1.13
2:V:135:LEU:CG	2:V:181:TYR:CE2	2.30	1.13
1:U:603:LEU:CD2	16:D:60:TYR:CE1	2.31	1.13
12:f:646:MET:O	14:B:67:ARG:CD	1.96	1.13
2:V:262:SER:OG	10:d:121:ARG:NH2	1.79	1.13
2:V:94:VAL:CG2	2:V:137:GLU:CD	2.18	1.13
2:V:135:LEU:HD11	2:V:181:TYR:CD2	1.84	1.12
3:W:137:TYR:CE1	16:D:392:TYR:CD2	2.35	1.13
3:W:142:ARG:NH1	3:W:185:PHE:CG	2.14	1.12
14:B:103:ARG:NH1	14:B:160:ILE:HG22	1.63	1.12
2:V:31:ALA:CB	2:V:32:PRO:HD2	1.79	1.12
12:f:835:GLU:HA	12:f:840:LEU:HD21	1.15	1.12
2:V:128:ARG:NH1	2:V:169:LEU:HD12	1.62	1.12
7:a:5:PRO:O	7:a:8:LEU:HG	1.49	1.12
5:Y:168:ILE:HG22	5:Y:177:ARG:CZ	1.80	1.11
10:d:107:LEU:HD11	10:d:140:GLU:HB2	1.17	1.11
12:f:670:MET:HE2	12:f:673:ARG:HD2	1.13	1.11
16:D:125:LYS:CB	16:D:126:PRO:HD3	1.80	1.11
6:Z:252:LYS:CG	9:c:234:TYR:OH	1.98	1.11
12:f:680:ARG:HD2	12:f:715:HIS:CE1	1.83	1.11
12:f:471:LEU:HD22	12:f:477:MET:HG3	1.14	1.11
2:V:171:VAL:HG13	2:V:175:MET:HE3	1.21	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:350:GLN:CB	2:V:351:PRO:CD	2.30	1.10
17:E:155:ASN:OD1	17:E:158:LEU:CD1	1.94	1.10
17:E:155:ASN:ND2	17:E:158:LEU:HD11	1.64	1.10
21:I:213:ILE:CG2	21:I:228:LEU:HD11	1.81	1.10
21:I:216:LEU:HD12	21:I:225:ILE:HD11	1.19	1.10
3:W:83:LEU:HD11	3:W:91:SER:HB3	1.23	1.10
3:W:83:LEU:HD22	3:W:95:SER:HB3	1.13	1.10
3:W:315:MET:HE1	3:W:320:LEU:HB2	1.10	1.10
19:G:46:ASP:O	19:G:222:VAL:HG23	1.52	1.10
2:V:94:VAL:HG21	2:V:137:GLU:OE2	1.48	1.09
3:W:142:ARG:NH2	3:W:182:ARG:HA	1.65	1.09
3:W:141:GLU:CG	3:W:172:GLU:CD	2.25	1.09
10:d:114:GLU:HA	10:d:117:THR:CG2	1.82	1.09
12:f:785:ARG:NH2	12:f:791:VAL:HG12	1.66	1.09
2:V:171:VAL:CG1	2:V:175:MET:HE3	1.81	1.08
2:V:258:TYR:CE1	2:V:263:LEU:HD23	1.86	1.08
3:W:141:GLU:CD	3:W:172:GLU:HG2	1.76	1.08
3:W:97:LEU:HD21	3:W:138:VAL:HG21	1.34	1.08
3:W:141:GLU:CD	3:W:172:GLU:CD	2.20	1.08
3:W:83:LEU:CD2	3:W:95:SER:HB3	1.82	1.08
1:U:167:ILE:HG22	1:U:177:LEU:HD21	1.35	1.08
1:U:179:TYR:HE2	1:U:183:LEU:CD1	1.61	1.07
7:a:5:PRO:HA	7:a:8:LEU:HD21	1.20	1.07
16:D:125:LYS:CB	16:D:126:PRO:CD	2.32	1.07
5:Y:165:LYS:HA	5:Y:168:ILE:HD13	1.35	1.07
16:D:338:ARG:HH11	16:D:365:ALA:HA	1.11	1.07
21:I:214:ALA:HB2	21:I:227:VAL:HG22	1.11	1.07
12:f:218:GLU:O	12:f:222:ASP:HB2	1.53	1.07
12:f:690:VAL:HB	12:f:713:PHE:HE1	0.91	1.07
25:m:41:CYS:SG	25:m:189:ILE:HG21	1.95	1.07
21:I:216:LEU:HD12	21:I:225:ILE:CD1	1.86	1.06
3:W:141:GLU:CD	3:W:172:GLU:CG	2.28	1.06
17:E:158:LEU:H	17:E:158:LEU:HD12	1.18	1.06
12:f:764:LEU:CD2	12:f:774:GLY:CA	2.22	1.05
16:D:354:LEU:HD12	16:D:399:PHE:CE2	1.91	1.05
2:V:166:TYR:OH	2:V:216:ARG:HD2	1.53	1.05
12:f:380:PHE:HB3	12:f:755:ASP:HB3	1.34	1.05
12:f:692:LEU:HD13	13:A:77:LEU:CD2	1.84	1.05
10:d:103:LEU:HD13	10:d:118:GLU:OE2	1.55	1.04
12:f:838:ARG:HD3	12:f:839:PRO:HD3	1.36	1.04
16:D:125:LYS:HB2	16:D:126:PRO:CD	1.86	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:691:PRO:HD3	12:f:713:PHE:CZ	1.92	1.04
3:W:142:ARG:CZ	3:W:185:PHE:HB2	1.87	1.04
3:W:137:TYR:HB3	3:W:144:ARG:CZ	1.88	1.04
3:W:142:ARG:HH21	3:W:182:ARG:HA	0.98	1.04
12:f:764:LEU:HD21	12:f:774:GLY:C	1.83	1.04
13:A:78:TRP:CD1	14:B:138:PHE:HA	1.91	1.04
12:f:692:LEU:HB3	13:A:77:LEU:CD2	1.87	1.03
1:U:584:TYR:OH	1:U:768:GLN:NE2	1.91	1.03
2:V:166:TYR:OH	2:V:216:ARG:CD	2.06	1.03
2:V:497:PRO:CB	6:Z:278:ASN:OD1	2.06	1.03
12:f:222:ASP:OD1	14:B:60:LEU:CD1	2.06	1.03
2:V:494:MET:HB2	6:Z:275:LEU:HD23	1.40	1.03
2:V:350:GLN:CB	2:V:351:PRO:HD3	1.86	1.03
16:D:342:ARG:HH22	16:D:361:GLU:HG2	1.23	1.02
12:f:670:MET:CG	12:f:673:ARG:NH1	2.22	1.02
12:f:764:LEU:HD21	12:f:774:GLY:HA3	1.06	1.02
21:I:213:ILE:HG22	21:I:228:LEU:HD11	1.41	1.02
15:C:90:HIS:CD2	15:C:91:PRO:CD	2.43	1.02
16:D:337:ASP:O	16:D:341:LYS:HB2	1.60	1.02
2:V:497:PRO:HB2	2:V:498:PRO:HD3	1.41	1.02
3:W:173:THR:HG22	3:W:177:MET:SD	2.00	1.02
7:a:7:PHE:CE2	7:a:63:PHE:CE2	2.48	1.02
10:d:115:PHE:O	10:d:119:LEU:CD2	2.07	1.02
17:E:113:ARG:HH12	17:E:220:ASN:HB3	1.23	1.01
3:W:142:ARG:HH22	3:W:185:PHE:HB3	1.24	1.01
3:W:315:MET:CE	3:W:320:LEU:HB2	1.89	1.01
9:c:78:SER:HB2	9:c:85:GLU:HG3	1.41	1.01
1:U:167:ILE:HG22	1:U:177:LEU:HD22	1.04	1.00
2:V:31:ALA:CB	2:V:32:PRO:CD	2.33	1.00
2:V:135:LEU:CD1	2:V:181:TYR:CD2	2.43	1.00
14:B:103:ARG:NH1	14:B:160:ILE:CG2	2.24	1.00
15:C:114:VAL:CA	15:C:127:LEU:HD11	1.89	1.00
2:V:212:TYR:O	2:V:216:ARG:HG3	1.60	1.00
2:V:171:VAL:CG1	2:V:175:MET:CE	2.39	1.00
12:f:258:LYS:CB	12:f:770:HIS:NE2	2.23	1.00
9:c:143:VAL:HG13	9:c:157:ILE:HD11	1.40	1.00
12:f:785:ARG:HH21	12:f:791:VAL:HG12	1.22	1.00
10:d:155:LYS:NZ	10:d:167:ILE:HD12	1.77	0.99
12:f:764:LEU:HD22	12:f:774:GLY:HA3	1.42	0.99
15:C:132:ASP:OD1	15:C:133:PRO:HD2	1.62	0.99
1:U:603:LEU:HD21	16:D:60:TYR:CE1	1.92	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:764:LEU:CD1	12:f:774:GLY:CA	2.38	0.99
5:Y:168:ILE:CG2	5:Y:177:ARG:CZ	2.40	0.99
15:C:127:LEU:H	15:C:127:LEU:HD12	1.26	0.98
12:f:692:LEU:HD13	13:A:77:LEU:HD21	1.43	0.98
2:V:350:GLN:HB3	2:V:351:PRO:HD3	1.00	0.98
12:f:690:VAL:CB	12:f:713:PHE:HE1	1.76	0.98
3:W:317:TRP:CZ3	3:W:355:LYS:HD3	1.98	0.98
12:f:122:ALA:HB2	12:f:129:LEU:CD1	1.94	0.98
1:U:167:ILE:CB	1:U:177:LEU:HD22	1.93	0.98
7:a:7:PHE:CD2	7:a:63:PHE:CE2	2.51	0.98
3:W:83:LEU:HD11	3:W:91:SER:HB2	1.03	0.97
2:V:497:PRO:HA	6:Z:282:ASN:HD21	0.82	0.97
7:a:7:PHE:CD2	7:a:63:PHE:HE2	1.82	0.97
12:f:258:LYS:HB3	12:f:770:HIS:CD2	1.99	0.97
12:f:835:GLU:HA	12:f:840:LEU:CD2	1.94	0.97
17:E:155:ASN:O	17:E:158:LEU:HD13	1.64	0.97
3:W:137:TYR:HE1	16:D:392:TYR:HD2	1.02	0.97
12:f:222:ASP:OD1	14:B:60:LEU:HD12	1.62	0.97
16:D:355:SER:OG	16:D:395:LEU:HD13	1.64	0.97
10:d:113:ALA:O	10:d:117:THR:HG22	1.65	0.97
1:U:179:TYR:HE2	1:U:183:LEU:HD11	0.83	0.96
3:W:97:LEU:HD21	3:W:138:VAL:CG2	1.94	0.96
12:f:404:ASP:C	12:f:439:TYR:CD1	2.37	0.96
3:W:141:GLU:CG	3:W:172:GLU:CG	2.43	0.96
1:U:603:LEU:HD23	16:D:60:TYR:CE1	1.98	0.96
12:f:680:ARG:CD	12:f:715:HIS:CE1	2.50	0.95
10:d:103:LEU:HD13	10:d:118:GLU:CD	1.89	0.95
12:f:650:GLN:HG3	14:B:68:ILE:HG13	1.46	0.95
10:d:115:PHE:O	10:d:119:LEU:HD21	1.66	0.95
2:V:497:PRO:CA	6:Z:282:ASN:HD21	1.78	0.95
12:f:643:PRO:HB2	14:B:67:ARG:HH12	1.26	0.95
12:f:692:LEU:HB3	13:A:77:LEU:HD21	1.49	0.95
15:C:127:LEU:CB	15:C:128:PRO:HD2	1.94	0.95
12:f:690:VAL:HG11	12:f:713:PHE:CD1	2.01	0.95
12:f:381:VAL:HG23	12:f:755:ASP:O	1.66	0.94
14:B:103:ARG:HH11	14:B:160:ILE:CG2	1.77	0.94
3:W:97:LEU:CD2	3:W:138:VAL:HG21	1.97	0.94
7:a:93:ALA:O	7:a:97:LEU:HB2	1.68	0.94
12:f:712:LYS:HE2	12:f:712:LYS:HA	1.50	0.94
13:A:78:TRP:HB3	14:B:137:SER:O	1.67	0.94
12:f:838:ARG:CD	12:f:839:PRO:HD3	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:88:ASP:OD2	9:c:91:PHE:HB2	1.68	0.94
12:f:670:MET:HG2	12:f:673:ARG:HH12	1.23	0.94
17:E:151:LEU:CD1	17:E:159:PHE:HE2	1.81	0.94
2:V:46:GLY:O	2:V:50:GLU:HB2	1.68	0.94
2:V:494:MET:CB	6:Z:275:LEU:HD23	1.97	0.94
5:Y:164:ALA:O	5:Y:168:ILE:CD1	2.16	0.94
3:W:52:LYS:HE2	3:W:82:LEU:HD21	1.50	0.93
12:f:670:MET:HG2	12:f:673:ARG:HH11	1.25	0.93
14:B:278:ALA:HB1	14:B:279:PRO:HD2	1.46	0.93
2:V:135:LEU:HD11	2:V:181:TYR:HD2	1.29	0.93
2:V:31:ALA:HB3	2:V:32:PRO:HD2	0.94	0.93
3:W:141:GLU:CG	3:W:172:GLU:OE1	2.13	0.93
12:f:646:MET:HE1	14:B:49:LEU:HG	1.50	0.92
12:f:646:MET:O	14:B:67:ARG:NE	2.01	0.92
14:B:103:ARG:NH1	14:B:138:PHE:HE2	1.66	0.92
17:E:97:ARG:NH1	17:E:114:GLU:HG3	1.84	0.92
3:W:83:LEU:CD1	3:W:91:SER:CB	2.20	0.92
14:B:278:ALA:HB1	14:B:279:PRO:HD3	1.51	0.92
12:f:673:ARG:NH2	12:f:785:ARG:O	2.02	0.91
19:g:46:ASP:O	19:g:222:VAL:HG23	1.70	0.91
12:f:279:GLU:O	12:f:281:ILE:HD12	1.71	0.91
2:V:497:PRO:HG2	6:Z:278:ASN:CG	1.96	0.91
9:c:196:LEU:CD2	9:c:197:ASN:HB2	2.00	0.91
1:U:457:ILE:O	1:U:461:LEU:HB2	1.71	0.91
2:V:25:GLU:O	2:V:28:PRO:HD2	1.71	0.91
3:W:344:THR:O	3:W:348:GLU:HB2	1.71	0.91
12:f:646:MET:O	14:B:67:ARG:HD3	1.70	0.91
12:f:785:ARG:NH2	12:f:791:VAL:CG1	2.33	0.91
2:V:497:PRO:HD3	6:Z:278:ASN:HD21	1.36	0.91
1:U:603:LEU:HD23	16:D:60:TYR:HD1	1.28	0.91
12:f:838:ARG:HD3	12:f:839:PRO:CD	2.01	0.91
5:Y:165:LYS:CA	5:Y:168:ILE:HD13	2.01	0.90
9:c:196:LEU:HD22	9:c:197:ASN:CA	1.99	0.90
3:W:84:ASN:ND2	3:W:89:LEU:HD12	1.86	0.90
2:V:214:HIS:O	2:V:218:TYR:HB3	1.71	0.90
6:Z:252:LYS:HE2	6:Z:252:LYS:HA	1.52	0.90
7:a:64:ILE:O	7:a:68:GLU:HB2	1.70	0.90
12:f:690:VAL:CB	12:f:713:PHE:CE1	2.51	0.90
12:f:690:VAL:CG1	12:f:713:PHE:CD1	2.54	0.90
2:V:135:LEU:CD1	2:V:181:TYR:HD2	1.79	0.90
21:I:214:ALA:CB	21:I:227:VAL:HG22	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:M:41:CYS:SG	25:M:189:ILE:CD1	2.59	0.90
12:f:764:LEU:CG	12:f:774:GLY:HA3	2.02	0.90
2:V:258:TYR:CZ	2:V:263:LEU:HD23	2.07	0.90
2:V:358:MET:HA	2:V:358:MET:CE	2.01	0.90
17:E:151:LEU:HD12	17:E:159:PHE:CE2	2.06	0.89
14:B:278:ALA:CB	14:B:279:PRO:CD	2.48	0.89
16:D:354:LEU:CD1	16:D:399:PHE:CE2	2.56	0.89
2:V:165:ALA:HB3	2:V:167:LEU:HD23	1.54	0.89
3:W:84:ASN:CG	3:W:89:LEU:HD12	1.97	0.89
9:c:78:SER:CB	9:c:85:GLU:HG3	2.02	0.89
12:f:222:ASP:CG	14:B:60:LEU:HD13	1.97	0.89
12:f:404:ASP:O	12:f:439:TYR:CD1	2.25	0.89
12:f:838:ARG:CB	12:f:839:PRO:CD	2.19	0.89
25:m:46:VAL:CG2	25:m:186:CYS:SG	2.61	0.89
1:U:167:ILE:HA	1:U:177:LEU:CD1	2.02	0.89
2:V:165:ALA:HB3	2:V:167:LEU:HD22	1.55	0.89
12:f:609:VAL:HG13	12:f:612:LEU:HD23	1.55	0.89
2:V:212:TYR:O	2:V:216:ARG:CG	2.21	0.88
13:A:312:ARG:HG3	13:A:312:ARG:HH11	1.37	0.88
25:M:46:VAL:CG2	25:M:186:CYS:SG	2.61	0.88
2:V:265:ASP:O	2:V:269:LYS:HG3	1.72	0.88
3:W:81:ASP:HA	3:W:84:ASN:HB2	1.53	0.88
3:W:137:TYR:HB3	3:W:144:ARG:NH2	1.88	0.88
7:a:5:PRO:O	7:a:8:LEU:CG	2.22	0.88
12:f:773:LYS:HD2	12:f:776:LEU:HD13	1.56	0.87
2:V:135:LEU:HG	2:V:181:TYR:HE2	0.87	0.87
7:a:186:LYS:HA	7:a:186:LYS:CE	2.04	0.87
9:c:191:ALA:O	9:c:196:LEU:HB3	1.73	0.87
21:I:216:LEU:HD11	21:I:225:ILE:HD11	1.55	0.87
1:U:325:MET:O	1:U:329:LEU:HB2	1.75	0.87
12:f:755:ASP:CG	12:f:756:PRO:HD3	2.00	0.87
3:W:308:LEU:HB3	3:W:314:LEU:HD11	1.57	0.87
12:f:690:VAL:HG11	12:f:713:PHE:HD1	1.36	0.87
25:M:214:SER:HG	25:M:224:HIS:HE2	1.20	0.87
6:Z:252:LYS:HG2	9:c:234:TYR:HH	1.35	0.86
15:C:88:LYS:HB2	15:C:94:LYS:HG2	1.57	0.86
16:D:368:ASP:OD2	16:D:409:LYS:HE3	1.75	0.86
10:d:171:LEU:O	10:d:175:ARG:HG2	1.75	0.86
3:W:142:ARG:HH21	3:W:182:ARG:CA	1.87	0.86
12:f:41:LYS:O	12:f:45:LEU:HB2	1.74	0.86
31:s:23:VAL:HB	31:s:196:CYS:SG	2.14	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:180:LYS:HD3	3:W:180:LYS:N	1.87	0.86
12:f:692:LEU:CD1	13:A:77:LEU:HD21	2.06	0.86
25:m:41:CYS:SG	25:m:189:ILE:CG2	2.63	0.86
3:W:124:LEU:O	3:W:128:LEU:HB2	1.75	0.86
10:d:155:LYS:C	10:d:155:LYS:HD3	2.01	0.86
12:f:764:LEU:HD21	12:f:774:GLY:O	1.75	0.86
2:V:29:PRO:HB2	2:V:30:PRO:HD3	1.56	0.86
12:f:395:GLY:O	12:f:399:LEU:HB2	1.73	0.86
17:E:114:GLU:OE1	17:E:114:GLU:N	2.09	0.86
31:S:23:VAL:HB	31:S:196:CYS:SG	2.14	0.86
3:W:83:LEU:HD22	3:W:95:SER:CB	2.02	0.86
10:d:155:LYS:NZ	10:d:167:ILE:CD1	2.38	0.86
12:f:704:LEU:O	12:f:708:ASP:HB2	1.76	0.86
21:I:214:ALA:CB	21:I:227:VAL:CG2	2.53	0.85
6:Z:247:LYS:O	6:Z:251:LEU:CB	2.24	0.85
16:D:342:ARG:NH2	16:D:361:GLU:HG2	1.90	0.85
12:f:279:GLU:O	12:f:281:ILE:CD1	2.24	0.85
14:B:62:LEU:O	14:B:66:GLU:HB2	1.76	0.85
15:C:114:VAL:CA	15:C:127:LEU:CD1	2.54	0.85
16:D:342:ARG:HH22	16:D:361:GLU:CG	1.89	0.85
21:I:214:ALA:HB2	21:I:227:VAL:HG23	1.58	0.85
2:V:258:TYR:CD2	2:V:265:ASP:OD2	2.29	0.85
12:f:281:ILE:HD12	12:f:281:ILE:H	1.42	0.85
2:V:494:MET:CG	6:Z:275:LEU:HD23	2.06	0.85
2:V:188:SER:O	2:V:192:MET:HB2	1.76	0.85
7:a:5:PRO:CA	7:a:8:LEU:HD21	2.04	0.85
2:V:497:PRO:CD	6:Z:278:ASN:ND2	2.28	0.85
3:W:315:MET:HE1	3:W:320:LEU:CB	2.01	0.84
2:V:496:PHE:N	2:V:497:PRO:HD2	1.90	0.84
5:Y:330:ILE:O	5:Y:334:LEU:HG	1.76	0.84
5:Y:336:ARG:HH21	5:Y:336:ARG:HG2	1.42	0.84
7:a:5:PRO:C	7:a:8:LEU:HG	2.03	0.84
3:W:141:GLU:HG3	3:W:172:GLU:CG	2.05	0.84
4:X:306:LEU:O	4:X:310:ARG:HB2	1.78	0.84
12:f:145:VAL:O	12:f:149:GLU:HB3	1.77	0.84
2:V:171:VAL:O	2:V:175:MET:SD	2.35	0.84
16:D:338:ARG:NH1	16:D:365:ALA:HA	1.92	0.84
1:U:184:CYS:O	1:U:188:MET:HB2	1.77	0.84
9:c:52:GLU:HB3	9:c:83:SER:O	1.78	0.84
12:f:471:LEU:HD22	12:f:477:MET:CG	2.04	0.83
12:f:680:ARG:NE	12:f:715:HIS:CE1	2.45	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:m:214:SER:HG	25:m:224:HIS:HE2	1.21	0.83
2:V:494:MET:HE3	2:V:494:MET:C	2.03	0.83
12:f:764:LEU:CD1	12:f:774:GLY:HA3	2.06	0.83
2:V:258:TYR:CE1	2:V:263:LEU:CD2	2.60	0.83
2:V:135:LEU:CG	2:V:181:TYR:CD2	2.62	0.83
12:f:780:PRO:O	12:f:784:ASP:HB2	1.79	0.83
2:V:497:PRO:HB3	6:Z:278:ASN:OD1	1.77	0.83
12:f:222:ASP:OD1	14:B:60:LEU:HD13	1.77	0.83
14:B:56:THR:O	14:B:61:LYS:NZ	2.12	0.83
12:f:646:MET:SD	14:B:49:LEU:HD11	2.19	0.82
16:D:125:LYS:HB2	16:D:126:PRO:HD2	1.58	0.82
17:E:155:ASN:CB	17:E:158:LEU:HD11	2.07	0.82
12:f:288:VAL:HG11	12:f:873:LEU:HD22	1.59	0.82
12:f:122:ALA:CB	12:f:129:LEU:HD12	2.10	0.82
17:E:97:ARG:HH12	17:E:114:GLU:HG3	1.37	0.82
3:W:52:LYS:CE	3:W:82:LEU:HD21	2.09	0.82
3:W:231:ILE:O	3:W:235:GLN:HB2	1.80	0.82
12:f:250:ARG:NH1	12:f:281:ILE:HG12	1.95	0.82
12:f:680:ARG:HD2	12:f:715:HIS:HE1	1.43	0.82
3:W:142:ARG:CZ	3:W:185:PHE:CB	2.52	0.82
16:D:376:ASN:O	16:D:380:GLN:HB2	1.79	0.82
3:W:142:ARG:NH2	3:W:185:PHE:HB3	1.93	0.82
15:C:127:LEU:HB3	15:C:128:PRO:HD2	1.59	0.81
19:g:47:CYS:HB3	19:g:221:THR:HG22	1.62	0.81
7:a:5:PRO:HA	7:a:8:LEU:CG	2.09	0.81
21:I:216:LEU:CD1	21:I:225:ILE:CD1	2.51	0.81
19:g:133:PRO:HG2	25:m:14:PHE:HE2	1.43	0.81
12:f:690:VAL:CG1	12:f:713:PHE:CE1	2.63	0.81
16:D:368:ASP:OD2	16:D:409:LYS:CE	2.27	0.81
12:f:764:LEU:HD12	12:f:771:LEU:HD12	1.63	0.81
14:B:74:MET:O	14:B:78:PHE:HB2	1.80	0.81
9:c:78:SER:HB2	9:c:85:GLU:CG	2.11	0.81
11:e:48:VAL:O	11:e:52:PHE:HB3	1.81	0.81
12:f:755:ASP:OD1	12:f:755:ASP:N	2.12	0.81
1:U:167:ILE:HG22	1:U:177:LEU:HD23	1.61	0.81
12:f:643:PRO:CB	14:B:67:ARG:HH12	1.93	0.81
10:d:114:GLU:HA	10:d:117:THR:HG22	1.62	0.81
16:D:354:LEU:HD12	16:D:399:PHE:HZ	1.36	0.81
17:E:151:LEU:CD1	17:E:159:PHE:CE2	2.63	0.81
2:V:135:LEU:HG	2:V:181:TYR:CD2	2.14	0.80
2:V:466:ILE:HA	2:V:469:THR:OG1	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:178:GLU:HG2	3:W:182:ARG:HB2	1.62	0.80
6:Z:244:GLU:O	6:Z:248:ALA:N	2.12	0.80
12:f:609:VAL:HA	12:f:612:LEU:HB3	1.63	0.80
2:V:470:ARG:HB2	6:Z:250:TYR:CD1	2.17	0.80
3:W:142:ARG:NH1	3:W:185:PHE:CD1	2.47	0.80
9:c:192:LEU:HD12	9:c:196:LEU:HG	1.63	0.80
12:f:692:LEU:CB	13:A:77:LEU:HD21	2.12	0.80
11:e:57:ARG:CZ	11:e:57:ARG:HB2	2.10	0.80
9:c:88:ASP:OD2	9:c:91:PHE:CB	2.30	0.80
12:f:297:MET:CG	12:f:770:HIS:CE1	2.65	0.80
2:V:140:ASP:OD1	2:V:140:ASP:N	2.15	0.79
3:W:315:MET:O	3:W:319:THR:OG1	2.00	0.79
12:f:642:ALA:H	12:f:643:PRO:HD3	1.47	0.79
12:f:643:PRO:HB2	14:B:67:ARG:CZ	2.12	0.79
14:B:246:THR:OG1	14:B:280:SER:HB3	1.82	0.79
15:C:125:LYS:NZ	16:D:112:TYR:OH	2.16	0.79
1:U:602:LEU:O	1:U:602:LEU:HD22	1.81	0.79
3:W:134:GLY:HA2	3:W:137:TYR:CE2	2.18	0.79
16:D:338:ARG:HH11	16:D:365:ALA:CA	1.92	0.79
6:Z:252:LYS:HA	6:Z:252:LYS:CE	2.11	0.79
12:f:297:MET:CB	12:f:770:HIS:HE1	1.63	0.79
13:A:308:GLY:HA2	18:F:234:THR:HG21	1.64	0.79
1:U:171:ASN:ND2	1:U:176:MET:HE2	1.98	0.79
10:d:155:LYS:CE	10:d:167:ILE:HD12	2.12	0.79
17:E:155:ASN:OD1	17:E:158:LEU:HD12	1.83	0.79
19:G:132:ARG:HG2	19:G:132:ARG:HH21	1.48	0.79
8:b:150:THR:CB	8:b:153:LEU:HB2	2.12	0.78
2:V:497:PRO:HG2	6:Z:278:ASN:ND2	1.91	0.78
21:I:213:ILE:HB	21:I:228:LEU:CD1	2.13	0.78
2:V:94:VAL:HG22	2:V:137:GLU:CB	2.12	0.78
12:f:122:ALA:HB2	12:f:129:LEU:HD12	1.65	0.78
17:E:158:LEU:CD1	17:E:158:LEU:H	1.96	0.78
2:V:165:ALA:CB	2:V:167:LEU:CD2	2.59	0.78
3:W:178:GLU:HA	3:W:179:LYS:HZ2	1.46	0.78
11:e:56:LEU:HD21	11:e:59:GLU:HB3	1.65	0.78
3:W:83:LEU:O	3:W:83:LEU:HD12	1.84	0.78
3:W:173:THR:CG2	3:W:177:MET:SD	2.72	0.78
2:V:358:MET:HB2	2:V:359:PRO:HD3	1.66	0.78
3:W:64:SER:O	3:W:66:ILE:HG22	1.84	0.78
12:f:442:SER:O	12:f:446:LEU:HB2	1.84	0.78
14:B:56:THR:O	14:B:61:LYS:CE	2.32	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:258:LYS:CB	12:f:770:HIS:CD2	2.65	0.77
22:J:56:GLU:N	22:J:56:GLU:OE1	2.18	0.77
9:c:280:PRO:O	9:c:284:LEU:HB2	1.84	0.77
12:f:646:MET:HE1	14:B:49:LEU:CG	2.15	0.77
12:f:692:LEU:HB3	13:A:77:LEU:HD22	1.66	0.77
1:U:171:ASN:HD22	1:U:176:MET:CE	1.98	0.77
9:c:196:LEU:CD2	9:c:197:ASN:N	2.16	0.77
12:f:680:ARG:O	12:f:763:ARG:NH2	2.17	0.77
2:V:21:GLY:O	2:V:25:GLU:HB2	1.84	0.77
3:W:82:LEU:O	3:W:82:LEU:HD12	1.85	0.77
2:V:135:LEU:CD2	2:V:181:TYR:CE2	2.67	0.77
9:c:196:LEU:CG	9:c:197:ASN:H	1.97	0.77
16:D:133:HIS:HD2	16:D:136:SER:H	1.32	0.77
19:g:47:CYS:CB	19:g:221:THR:HG22	2.15	0.77
12:f:712:LYS:O	12:f:715:HIS:CB	2.33	0.77
19:G:46:ASP:O	19:G:222:VAL:CG2	2.32	0.77
9:c:196:LEU:HD22	9:c:197:ASN:H	0.65	0.77
6:Z:247:LYS:O	6:Z:251:LEU:HB2	1.85	0.76
3:W:69:ALA:HA	3:W:72:LYS:HE3	1.66	0.76
12:f:404:ASP:C	12:f:439:TYR:HD1	1.94	0.76
12:f:213:GLN:O	12:f:217:LEU:HB2	1.86	0.76
12:f:692:LEU:CG	13:A:77:LEU:HD21	2.15	0.76
1:U:167:ILE:HA	1:U:177:LEU:HD11	1.67	0.76
2:V:494:MET:HG3	6:Z:275:LEU:HA	1.68	0.76
12:f:672:LEU:O	12:f:672:LEU:HD22	1.86	0.76
5:Y:319:MET:O	5:Y:323:PHE:HB3	1.86	0.76
3:W:135:LYS:HB2	3:W:144:ARG:HH21	1.50	0.76
3:W:142:ARG:NH2	3:W:185:PHE:CB	2.49	0.76
15:C:89:VAL:HG12	15:C:91:PRO:HD2	1.67	0.76
5:Y:334:LEU:N	5:Y:334:LEU:HD23	2.01	0.75
7:a:367:VAL:O	7:a:371:ALA:HB3	1.85	0.75
12:f:67:ASP:O	12:f:71:TYR:HB2	1.86	0.75
3:W:83:LEU:HD12	3:W:91:SER:HB2	1.65	0.75
12:f:297:MET:HB3	12:f:770:HIS:CE1	2.21	0.75
12:f:438:ASP:HA	12:f:477:MET:HE2	1.67	0.75
16:D:357:GLU:OE1	16:D:357:GLU:N	2.15	0.75
2:V:29:PRO:HD2	2:V:30:PRO:HD2	1.68	0.75
3:W:179:LYS:H	3:W:179:LYS:HD2	1.52	0.75
10:d:107:LEU:CD1	10:d:140:GLU:HB2	2.07	0.75
16:D:253:LEU:O	16:D:257:ASN:HB2	1.87	0.75
12:f:297:MET:HA	12:f:772:GLY:HA2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:128:ARG:HH12	2:V:169:LEU:HD12	1.50	0.75
10:d:155:LYS:HZ1	10:d:167:ILE:CD1	1.99	0.75
17:E:155:ASN:CB	17:E:158:LEU:CD1	2.63	0.75
17:E:157:GLU:OE1	17:E:157:GLU:HA	1.85	0.75
2:V:26:PRO:O	2:V:30:PRO:HG2	1.87	0.75
14:B:278:ALA:CB	14:B:279:PRO:HD2	2.15	0.74
19:G:203:SER:O	19:G:207:SER:HA	1.88	0.74
12:f:691:PRO:HD3	12:f:713:PHE:HZ	1.50	0.74
12:f:692:LEU:HD13	13:A:77:LEU:HD23	1.67	0.74
1:U:171:ASN:ND2	1:U:176:MET:CE	2.49	0.74
9:c:143:VAL:HG13	9:c:157:ILE:CD1	2.17	0.74
10:d:114:GLU:HA	10:d:117:THR:HG21	1.69	0.74
12:f:637:LYS:HE2	12:f:673:ARG:HB2	1.69	0.74
12:f:712:LYS:HE2	12:f:712:LYS:CA	2.16	0.74
12:f:642:ALA:O	12:f:769:THR:OG1	2.05	0.74
16:D:355:SER:OG	16:D:395:LEU:HA	1.87	0.74
19:g:203:SER:O	19:g:207:SER:HA	1.88	0.74
14:B:103:ARG:HH11	14:B:138:PHE:HE2	1.34	0.73
2:V:497:PRO:HB2	2:V:498:PRO:CD	2.18	0.73
9:c:194:HIS:O	9:c:196:LEU:CD1	2.28	0.73
12:f:646:MET:HE1	14:B:49:LEU:CD1	2.18	0.73
13:A:307:ASP:OD1	13:A:336:ARG:NE	2.21	0.73
3:W:137:TYR:HE1	16:D:392:TYR:CD2	1.90	0.73
12:f:680:ARG:CZ	12:f:715:HIS:CE1	2.71	0.73
13:A:417:ILE:O	13:A:421:ALA:HB2	1.88	0.73
16:D:337:ASP:O	16:D:341:LYS:CB	2.36	0.73
2:V:137:GLU:N	2:V:138:PRO:HD2	2.03	0.73
5:Y:336:ARG:HG2	5:Y:336:ARG:NH2	1.99	0.73
2:V:29:PRO:CB	2:V:30:PRO:HD3	2.18	0.73
2:V:128:ARG:HH11	2:V:169:LEU:HD12	1.50	0.73
8:b:150:THR:HB	8:b:153:LEU:HB2	1.69	0.73
15:C:114:VAL:N	15:C:127:LEU:CD1	2.52	0.73
5:Y:21:GLN:HG3	5:Y:286:TRP:CE3	2.24	0.72
9:c:196:LEU:HD22	9:c:197:ASN:CB	2.19	0.72
12:f:646:MET:O	14:B:67:ARG:CG	2.36	0.72
16:D:50:GLU:O	16:D:54:LEU:HB2	1.89	0.72
12:f:680:ARG:CG	12:f:716:ASP:HA	2.19	0.72
12:f:712:LYS:HA	12:f:712:LYS:CE	2.13	0.72
2:V:353:LEU:HA	2:V:357:LEU:HD22	1.72	0.72
12:f:258:LYS:HG2	12:f:770:HIS:CD2	2.19	0.72
12:f:835:GLU:CA	12:f:840:LEU:HD21	2.09	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:94:VAL:HG21	2:V:137:GLU:CG	1.89	0.72
10:d:115:PHE:O	10:d:119:LEU:HD23	1.89	0.72
14:B:135:ILE:HG22	14:B:139:VAL:HG11	1.71	0.72
25:M:47:PHE:HB2	25:M:214:SER:HB3	1.71	0.72
2:V:135:LEU:C	2:V:137:GLU:OE1	2.32	0.72
2:V:350:GLN:HB2	2:V:351:PRO:CD	2.19	0.72
7:a:5:PRO:O	7:a:8:LEU:CD1	2.37	0.72
12:f:609:VAL:HG12	12:f:613:LEU:CD1	2.19	0.72
17:E:113:ARG:NH1	17:E:220:ASN:HB3	2.03	0.72
19:G:132:ARG:HG2	19:G:132:ARG:NH2	2.01	0.72
1:U:229:VAL:O	1:U:233:LEU:HB2	1.90	0.72
12:f:122:ALA:HB2	12:f:129:LEU:HD11	1.70	0.72
14:B:103:ARG:HH11	14:B:160:ILE:HG23	1.54	0.72
21:I:143:TYR:HB2	21:I:146:GLN:HE21	1.55	0.72
25:m:47:PHE:HB2	25:m:214:SER:HB3	1.71	0.72
17:E:151:LEU:HD12	17:E:159:PHE:HE2	1.48	0.72
2:V:227:VAL:O	2:V:231:LEU:HB2	1.90	0.71
2:V:72:LEU:O	2:V:76:LYS:HB2	1.89	0.71
12:f:486:GLY:O	12:f:490:ALA:HB2	1.90	0.71
7:a:186:LYS:HA	7:a:186:LYS:HE3	1.70	0.71
12:f:297:MET:HB2	12:f:770:HIS:HE1	0.70	0.71
12:f:471:LEU:CD2	12:f:477:MET:HG3	2.09	0.71
2:V:151:THR:O	2:V:155:ALA:HB2	1.89	0.71
19:G:134:LEU:H	19:G:134:LEU:HD12	1.54	0.71
22:J:53:LEU:HD12	22:J:53:LEU:O	1.90	0.71
7:a:7:PHE:CE2	7:a:63:PHE:HE2	1.99	0.71
13:A:236:CYS:HB2	13:A:270:CYS:SG	2.30	0.71
21:i:143:TYR:HB2	21:i:146:GLN:HE21	1.55	0.71
3:W:395:ASN:O	3:W:399:ASN:HB2	1.90	0.71
9:c:157:ILE:C	9:c:157:ILE:HD12	2.16	0.71
12:f:642:ALA:N	12:f:643:PRO:HD3	2.04	0.71
2:V:128:ARG:NH1	2:V:169:LEU:CD1	2.49	0.71
2:V:165:ALA:CB	2:V:167:LEU:HD23	2.21	0.71
9:c:267:PRO:HA	9:c:270:LEU:HB2	1.73	0.71
10:d:103:LEU:CD1	10:d:118:GLU:OE2	2.35	0.71
12:f:281:ILE:HD12	12:f:281:ILE:N	2.05	0.71
10:d:107:LEU:CD2	10:d:140:GLU:OE1	2.29	0.70
9:c:85:GLU:HA	9:c:85:GLU:OE2	1.90	0.70
8:b:150:THR:OG1	8:b:153:LEU:HB2	1.91	0.70
21:I:213:ILE:CB	21:I:228:LEU:HD11	2.22	0.70
9:c:78:SER:H	9:c:85:GLU:HG3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:151:ILE:HD13	16:D:151:ILE:N	2.05	0.70
2:V:257:ASN:HA	2:V:260:HIS:HB3	1.73	0.70
2:V:471:GLU:H	2:V:472:PRO:HD2	1.55	0.70
14:B:168:ASP:OD2	14:B:169:PRO:CD	2.25	0.70
3:W:82:LEU:HD12	3:W:82:LEU:C	2.16	0.70
6:Z:248:ALA:O	6:Z:252:LYS:N	2.23	0.70
7:a:7:PHE:CD2	7:a:63:PHE:CD2	2.79	0.70
28:p:2:SER:N	28:p:5:SER:HG	1.89	0.70
2:V:171:VAL:O	2:V:175:MET:CG	2.39	0.70
12:f:692:LEU:CD1	13:A:77:LEU:CD2	2.63	0.70
13:A:312:ARG:NH1	13:A:315:ILE:O	2.25	0.70
17:E:151:LEU:HD13	17:E:159:PHE:HE2	1.53	0.70
2:V:26:PRO:O	2:V:30:PRO:CG	2.40	0.70
12:f:380:PHE:HB3	12:f:755:ASP:CB	2.19	0.70
17:E:97:ARG:HH12	17:E:114:GLU:CG	2.05	0.70
2:V:150:ARG:O	2:V:154:ALA:HB3	1.91	0.69
7:a:188:LEU:HB3	7:a:189:PRO:CD	2.22	0.69
10:d:172:ASP:O	10:d:175:ARG:N	2.24	0.69
2:V:494:MET:HG3	6:Z:275:LEU:HD23	1.72	0.69
9:c:157:ILE:HD12	9:c:157:ILE:O	1.91	0.69
3:W:17:GLU:HG3	3:W:62:SER:HB2	1.74	0.69
3:W:317:TRP:CE3	3:W:355:LYS:HD3	2.26	0.69
12:f:335:ARG:HB3	12:f:853:VAL:HG21	1.75	0.69
12:f:755:ASP:CB	12:f:756:PRO:HD3	2.21	0.69
2:V:219:GLU:CG	2:V:257:ASN:HD21	2.05	0.69
3:W:282:GLU:O	3:W:286:LEU:HB2	1.91	0.69
16:D:353:ASN:ND2	16:D:392:TYR:O	2.26	0.69
1:U:496:LEU:O	1:U:500:ASN:HB2	1.90	0.69
14:B:135:ILE:CG2	14:B:139:VAL:HG11	2.22	0.69
16:D:342:ARG:NH2	16:D:361:GLU:CG	2.53	0.69
2:V:26:PRO:O	2:V:30:PRO:CD	2.41	0.69
5:Y:122:THR:O	5:Y:126:LYS:HB2	1.92	0.69
19:g:134:LEU:H	19:g:134:LEU:CD1	2.05	0.69
2:V:166:TYR:OH	2:V:216:ARG:HD3	1.90	0.69
2:V:470:ARG:HG3	2:V:470:ARG:HH21	1.57	0.69
24:L:14:SER:HB3	24:L:18:ARG:H	1.58	0.69
10:d:208:ASP:O	10:d:212:LYS:HB2	1.93	0.69
1:U:171:ASN:HD22	1:U:176:MET:HE3	1.57	0.68
12:f:288:VAL:CG1	12:f:873:LEU:HD22	2.22	0.68
16:D:354:LEU:CD1	16:D:399:PHE:CZ	2.66	0.68
10:d:21:GLU:O	10:d:25:ARG:HB2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:107:LEU:HD11	10:d:140:GLU:CB	2.11	0.68
24:l:14:SER:HB3	24:l:18:ARG:H	1.58	0.68
5:Y:168:ILE:N	5:Y:168:ILE:HD12	2.08	0.68
12:f:712:LYS:O	12:f:715:HIS:HB3	1.93	0.68
14:B:99:VAL:O	14:B:103:ARG:HG2	1.93	0.68
15:C:114:VAL:O	15:C:127:LEU:HD11	1.94	0.68
22:J:52:LYS:HD3	22:J:52:LYS:N	2.07	0.68
2:V:171:VAL:HG13	2:V:175:MET:SD	2.33	0.68
4:X:175:LYS:HG2	4:X:213:GLN:HE22	1.58	0.68
5:Y:168:ILE:HG21	5:Y:177:ARG:CZ	2.24	0.68
7:a:321:LYS:HB2	7:a:335:TRP:HB3	1.75	0.68
8:b:38:HIS:O	8:b:42:ARG:HB2	1.93	0.68
15:C:90:HIS:CG	15:C:91:PRO:CD	2.64	0.68
15:C:113:ARG:HB3	15:C:127:LEU:HD13	1.74	0.68
13:A:307:ASP:OD1	13:A:336:ARG:CG	2.40	0.68
3:W:52:LYS:HE2	3:W:82:LEU:CD2	2.20	0.68
3:W:141:GLU:OE2	3:W:172:GLU:CD	2.36	0.68
14:B:103:ARG:HH12	14:B:160:ILE:HG22	1.56	0.68
1:U:583:MET:HA	1:U:583:MET:HE3	1.75	0.68
1:U:601:ARG:HH11	1:U:601:ARG:HG3	1.58	0.68
3:W:178:GLU:H	3:W:178:GLU:CD	2.02	0.68
10:d:107:LEU:HD21	10:d:140:GLU:CD	2.17	0.68
12:f:670:MET:HE2	12:f:673:ARG:CD	2.07	0.68
12:f:764:LEU:HD11	12:f:774:GLY:H	0.65	0.68
1:U:167:ILE:HA	1:U:177:LEU:HD13	1.76	0.67
2:V:470:ARG:CB	6:Z:250:TYR:CD1	2.77	0.67
12:f:838:ARG:CD	12:f:839:PRO:CD	2.66	0.67
21:i:2:SER:N	24:l:123:TYR:HH	1.92	0.67
12:f:759:LEU:HG	12:f:806:VAL:CG1	2.24	0.67
25:m:41:CYS:SG	25:m:189:ILE:CB	2.81	0.67
3:W:142:ARG:HH22	3:W:185:PHE:CB	2.02	0.67
16:D:353:ASN:HD22	16:D:393:ILE:HA	1.57	0.67
25:m:46:VAL:HG23	25:m:186:CYS:SG	2.34	0.67
1:U:458:ILE:O	1:U:462:LEU:HB2	1.95	0.67
5:Y:233:ARG:N	5:Y:234:PRO:HD2	2.08	0.67
10:d:155:LYS:HE2	10:d:167:ILE:HD12	1.74	0.67
2:V:350:GLN:HB2	2:V:351:PRO:HD2	1.76	0.67
12:f:642:ALA:N	12:f:643:PRO:CD	2.58	0.67
1:U:77:SER:O	1:U:81:ALA:HB2	1.94	0.67
12:f:609:VAL:HG12	12:f:613:LEU:HD12	1.75	0.67
2:V:29:PRO:CD	2:V:30:PRO:HD2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:176:LYS:HB3	22:J:53:LEU:HD21	1.75	0.67
7:a:188:LEU:HB3	7:a:189:PRO:HD2	1.76	0.67
2:V:354:LYS:CA	2:V:357:LEU:HD21	2.25	0.66
12:f:692:LEU:CB	13:A:77:LEU:CD2	2.67	0.66
19:G:134:LEU:H	19:G:134:LEU:CD1	2.08	0.66
26:n:120:MET:H	32:t:61:GLN:HE22	1.40	0.66
6:Z:247:LYS:O	6:Z:251:LEU:HB3	1.95	0.66
17:E:158:LEU:HD12	17:E:158:LEU:N	2.01	0.66
18:F:312:GLU:O	18:F:316:GLN:HB3	1.95	0.66
19:G:134:LEU:HD12	19:G:134:LEU:N	2.10	0.66
25:m:41:CYS:HG	25:m:189:ILE:HG21	1.60	0.66
2:V:27:PRO:HA	2:V:30:PRO:HG2	1.77	0.66
2:V:137:GLU:N	2:V:138:PRO:CD	2.58	0.66
12:f:297:MET:HG3	12:f:770:HIS:CE1	2.30	0.66
13:A:312:ARG:HG3	13:A:312:ARG:NH1	2.09	0.66
25:M:46:VAL:HG23	25:M:186:CYS:SG	2.34	0.66
9:c:196:LEU:O	9:c:200:TYR:O	2.14	0.66
12:f:680:ARG:HG3	12:f:716:ASP:HA	1.78	0.66
17:E:155:ASN:O	17:E:158:LEU:CD1	2.42	0.66
2:V:354:LYS:N	2:V:357:LEU:HD21	2.10	0.66
5:Y:104:MET:O	5:Y:108:ALA:HB3	1.95	0.66
5:Y:377:LEU:O	5:Y:381:GLN:HB2	1.95	0.66
9:c:88:ASP:OD1	9:c:90:VAL:HB	1.94	0.66
12:f:258:LYS:CG	12:f:770:HIS:CD2	2.76	0.66
3:W:312:MET:HE2	7:a:312:MET:HB3	1.77	0.66
9:c:195:GLY:C	9:c:196:LEU:HD13	2.21	0.66
2:V:466:ILE:O	2:V:469:THR:OG1	2.14	0.66
7:a:7:PHE:CE2	7:a:63:PHE:CD2	2.84	0.66
7:a:297:ALA:O	7:a:301:LYS:HA	1.94	0.66
10:d:116:HIS:HA	10:d:119:LEU:HD23	1.77	0.66
2:V:171:VAL:O	2:V:175:MET:HG3	1.95	0.66
2:V:470:ARG:CB	6:Z:250:TYR:CE1	2.78	0.66
12:f:404:ASP:OD2	12:f:439:TYR:OH	2.09	0.66
12:f:764:LEU:HD12	12:f:771:LEU:CD1	2.25	0.66
16:D:363:TYR:HA	16:D:366:ARG:HD3	1.76	0.66
6:Z:10:VAL:HG13	6:Z:163:GLY:HA3	1.76	0.65
9:c:196:LEU:HD22	9:c:197:ASN:HB2	1.70	0.65
14:B:57:GLN:HA	14:B:61:LYS:NZ	2.11	0.65
3:W:137:TYR:CB	3:W:144:ARG:NH1	2.59	0.65
2:V:321:ALA:HA	2:V:325:LYS:HB3	1.77	0.65
2:V:471:GLU:HG3	2:V:472:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:287:LEU:O	5:Y:287:LEU:HD22	1.96	0.65
7:a:341:LEU:HB2	7:a:345:GLN:HE21	1.62	0.65
8:b:34:ASN:O	8:b:38:HIS:ND1	2.29	0.65
16:D:96:VAL:HG23	16:D:102:ILE:HD11	1.76	0.65
21:I:214:ALA:CB	21:I:227:VAL:HG23	2.23	0.65
3:W:67:LEU:O	3:W:67:LEU:HD13	1.97	0.65
30:R:19:ARG:NH2	28:p:205:ASP:OD2	2.30	0.65
16:D:407:ILE:HD12	16:D:409:LYS:HZ3	1.61	0.65
1:U:179:TYR:CE2	1:U:183:LEU:HD12	2.31	0.65
2:V:163:VAL:HG22	2:V:175:MET:HG2	1.79	0.65
3:W:315:MET:CE	3:W:320:LEU:N	2.60	0.65
4:X:331:LEU:O	4:X:335:LEU:HB2	1.97	0.65
12:f:679:LEU:HD21	12:f:686:LEU:HD11	1.76	0.65
10:d:195:THR:O	10:d:200:PHE:CE1	2.50	0.65
17:E:155:ASN:ND2	17:E:158:LEU:HD21	2.11	0.65
2:V:25:GLU:O	2:V:28:PRO:CD	2.45	0.65
3:W:67:LEU:C	3:W:67:LEU:HD22	2.21	0.65
5:Y:304:TYR:O	5:Y:308:LEU:HB2	1.96	0.65
14:B:153:ASN:HD22	14:B:156:VAL:HG22	1.61	0.65
5:Y:276:ALA:O	5:Y:280:GLN:HB2	1.96	0.65
6:Z:153:LYS:H	6:Z:153:LYS:HE3	1.62	0.65
8:b:150:THR:HB	8:b:153:LEU:HD22	1.78	0.65
16:D:149:SER:OG	16:D:250:VAL:HG22	1.97	0.65
2:V:326:GLN:HE21	2:V:352:SER:HB3	1.62	0.65
10:d:155:LYS:HZ3	10:d:167:ILE:HD12	1.58	0.65
5:Y:164:ALA:O	5:Y:168:ILE:HD12	1.96	0.64
12:f:222:ASP:CG	14:B:60:LEU:CD1	2.65	0.64
12:f:276:GLU:O	12:f:286:LYS:NZ	2.30	0.64
12:f:643:PRO:CB	14:B:67:ARG:NH1	2.46	0.64
15:C:132:ASP:OD1	15:C:133:PRO:CD	2.43	0.64
25:M:41:CYS:SG	25:M:189:ILE:HD12	2.37	0.64
2:V:265:ASP:HA	2:V:268:GLU:HB3	1.79	0.64
2:V:345:ARG:NH1	2:V:357:LEU:HB3	2.12	0.64
2:V:350:GLN:CB	2:V:351:PRO:HD2	2.27	0.64
6:Z:142:GLU:OE1	6:Z:142:GLU:N	2.25	0.64
6:Z:248:ALA:HA	6:Z:251:LEU:HB3	1.79	0.64
10:d:114:GLU:CA	10:d:117:THR:HG22	2.28	0.64
2:V:346:LEU:HA	2:V:353:LEU:HD12	1.79	0.64
3:W:315:MET:N	3:W:315:MET:SD	2.70	0.64
10:d:119:LEU:HD22	10:d:119:LEU:N	2.12	0.64
12:f:680:ARG:HD2	12:f:715:HIS:ND1	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:759:LEU:CD2	12:f:806:VAL:HG11	2.27	0.64
13:A:210:LYS:NZ	13:A:313:GLY:O	2.30	0.64
5:Y:23:ARG:HH22	5:Y:52:PRO:HB2	1.62	0.64
9:c:192:LEU:HA	9:c:196:LEU:HG	1.79	0.64
14:B:418:ASP:O	14:B:422:SER:HB2	1.96	0.64
1:U:402:PHE:HB2	1:U:437:TYR:HB3	1.80	0.64
3:W:83:LEU:HD13	3:W:91:SER:HB2	1.72	0.64
12:f:691:PRO:CD	12:f:713:PHE:CZ	2.76	0.64
13:A:210:LYS:CB	13:A:312:ARG:HH22	2.10	0.64
13:A:307:ASP:OD1	13:A:336:ARG:HG2	1.96	0.64
15:C:90:HIS:CE1	16:D:110:ASN:OD1	2.51	0.64
20:H:119:GLN:NE2	21:I:82:ASP:OD1	2.31	0.64
3:W:67:LEU:O	3:W:67:LEU:HD22	1.97	0.64
5:Y:168:ILE:O	5:Y:177:ARG:NH1	2.31	0.64
8:b:100:ARG:HH12	8:b:105:HIS:HB2	1.61	0.64
12:f:297:MET:HG3	12:f:770:HIS:NE2	2.12	0.64
12:f:712:LYS:O	12:f:715:HIS:HB2	1.98	0.64
12:f:723:TYR:O	12:f:727:PHE:HB3	1.98	0.64
15:C:63:LEU:HD12	16:D:79:VAL:HA	1.79	0.64
3:W:49:SER:O	3:W:53:GLN:HB2	1.98	0.64
6:Z:25:ARG:HH11	9:c:104:ARG:H	1.45	0.64
9:c:150:SER:HA	9:c:154:LYS:O	1.97	0.64
12:f:755:ASP:OD1	12:f:756:PRO:HD3	1.97	0.64
18:F:252:ALA:HB3	18:F:255:GLN:HB2	1.80	0.64
23:K:167:ALA:H	24:L:56:LEU:HD13	1.63	0.64
2:V:27:PRO:N	2:V:28:PRO:CD	2.61	0.63
2:V:94:VAL:HG22	2:V:137:GLU:HG2	0.69	0.63
2:V:495:ARG:HB2	15:C:44:ARG:NH1	2.13	0.63
3:W:141:GLU:OE2	3:W:172:GLU:OE2	2.16	0.63
3:W:315:MET:CE	3:W:320:LEU:CB	2.69	0.63
6:Z:172:VAL:HG13	9:c:217:LEU:HD21	1.79	0.63
10:d:156:GLY:H	10:d:158:ILE:HD12	1.62	0.63
15:C:114:VAL:N	15:C:127:LEU:HD11	2.13	0.63
1:U:167:ILE:HB	1:U:177:LEU:HD22	1.80	0.63
2:V:354:LYS:C	2:V:357:LEU:HD21	2.24	0.63
2:V:466:ILE:C	2:V:469:THR:OG1	2.41	0.63
3:W:316:ARG:HG2	3:W:383:ASP:OD2	1.98	0.63
8:b:25:ARG:NH2	8:b:145:GLU:OE1	2.31	0.63
12:f:646:MET:O	14:B:67:ARG:HG2	1.97	0.63
15:C:127:LEU:HD12	15:C:127:LEU:N	2.05	0.63
17:E:151:LEU:HD12	17:E:159:PHE:CZ	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:29:ARG:NH1	27:O:139:GLU:OE2	2.31	0.63
5:Y:287:LEU:O	5:Y:287:LEU:HD13	1.97	0.63
25:M:41:CYS:SG	25:M:189:ILE:HG21	2.39	0.63
2:V:116:ALA:O	2:V:120:PHE:HB2	1.98	0.63
2:V:204:ASP:O	2:V:208:ALA:HB2	1.98	0.63
6:Z:243:GLN:OE1	6:Z:243:GLN:HA	1.99	0.63
12:f:198:HIS:O	12:f:202:HIS:HB2	1.98	0.63
12:f:288:VAL:HG11	12:f:873:LEU:CD2	2.27	0.63
21:I:85:VAL:O	21:I:89:GLU:HB2	1.98	0.63
8:b:26:LEU:O	8:b:30:GLN:HB2	1.99	0.63
12:f:646:MET:HG3	14:B:64:LYS:HD3	1.81	0.63
21:i:85:VAL:O	21:i:89:GLU:HB2	1.98	0.63
1:U:80:TYR:O	1:U:84:ALA:HB2	1.98	0.63
1:U:376:MET:HA	1:U:739:ALA:HA	1.81	0.63
2:V:290:TYR:OH	2:V:294:ARG:NH2	2.31	0.63
2:V:296:LYS:HE2	2:V:305:ALA:HB2	1.79	0.63
3:W:137:TYR:HB3	3:W:144:ARG:NH1	2.12	0.63
3:W:167:GLN:HG3	3:W:168:GLU:HG3	1.80	0.63
7:a:227:ASN:O	7:a:231:GLN:NE2	2.32	0.63
12:f:762:VAL:HA	12:f:807:ARG:HH11	1.63	0.63
14:B:245:ALA:HB1	14:B:279:PRO:O	1.99	0.63
5:Y:287:LEU:HD22	5:Y:287:LEU:C	2.24	0.63
7:a:129:GLN:HG3	7:a:130:VAL:HG23	1.81	0.63
12:f:759:LEU:HG	12:f:806:VAL:HG11	1.81	0.63
19:g:133:PRO:HG2	25:m:14:PHE:CE2	2.31	0.63
1:U:126:ILE:HG23	1:U:130:LEU:HB3	1.80	0.63
5:Y:21:GLN:CG	5:Y:286:TRP:CE3	2.81	0.63
16:D:354:LEU:CD1	16:D:399:PHE:HE2	2.09	0.63
2:V:470:ARG:HB3	6:Z:250:TYR:CE1	2.34	0.62
3:W:96:GLN:HE22	3:W:138:VAL:HG22	1.63	0.62
10:d:107:LEU:O	10:d:107:LEU:HD23	1.99	0.62
12:f:39:LYS:O	12:f:43:GLN:HB2	1.99	0.62
16:D:242:GLU:O	16:D:246:MET:HB2	1.99	0.62
6:Z:153:LYS:HE3	6:Z:153:LYS:N	2.14	0.62
15:C:125:LYS:NZ	16:D:112:TYR:CZ	2.66	0.62
1:U:252:LEU:O	1:U:256:ALA:HB3	1.99	0.62
2:V:166:TYR:HE1	2:V:216:ARG:HB2	1.64	0.62
5:Y:50:MET:HE2	5:Y:74:LYS:HB3	1.80	0.62
6:Z:248:ALA:O	6:Z:252:LYS:HB2	1.98	0.62
10:d:2:TYR:O	10:d:25:ARG:NH2	2.32	0.62
15:C:114:VAL:HA	15:C:127:LEU:CD1	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:559:ARG:HB3	1:U:562:GLU:HB2	1.81	0.62
2:V:223:LYS:HG2	2:V:223:LYS:O	1.98	0.62
9:c:82:VAL:O	9:c:82:VAL:HG12	2.00	0.62
12:f:708:ASP:OD1	12:f:785:ARG:CG	2.48	0.62
28:p:58:THR:O	29:q:85:ARG:NH2	2.33	0.62
12:f:122:ALA:HB1	12:f:129:LEU:HD12	1.82	0.62
18:F:232:GLY:HA2	36:F:501:ADP:H5'2	1.80	0.62
1:U:602:LEU:HD22	1:U:602:LEU:C	2.22	0.62
2:V:257:ASN:O	2:V:261:TYR:N	2.33	0.62
5:Y:285:ASP:O	5:Y:289:ALA:HB2	1.99	0.62
8:b:15:TYR:O	8:b:25:ARG:NH1	2.32	0.62
13:A:307:ASP:CG	13:A:336:ARG:NE	2.41	0.62
2:V:257:ASN:O	2:V:261:TYR:CD1	2.52	0.62
19:g:134:LEU:H	19:g:134:LEU:HD12	1.64	0.62
27:o:163:ILE:HG12	27:o:170:GLY:HA2	1.82	0.62
13:A:41:TYR:HB2	13:A:44:GLN:HB3	1.82	0.62
16:D:352:MET:HE1	16:D:379:CYS:HB3	1.82	0.62
3:W:96:GLN:HE22	3:W:138:VAL:CG2	2.12	0.62
3:W:137:TYR:CB	3:W:144:ARG:CZ	2.74	0.62
16:D:87:LEU:HB3	17:E:80:VAL:HB	1.81	0.62
16:D:335:LEU:HD12	16:D:336:PRO:CD	2.30	0.62
19:g:132:ARG:HB2	25:m:12:SER:HA	1.80	0.62
2:V:134:PHE:C	2:V:137:GLU:OE2	2.42	0.62
3:W:141:GLU:CG	3:W:172:GLU:HG3	2.28	0.62
6:Z:109:ASN:ND2	6:Z:140:SER:OG	2.33	0.62
16:D:368:ASP:HB3	16:D:409:LYS:NZ	2.14	0.62
1:U:701:ILE:HG21	1:U:810:THR:HA	1.81	0.61
2:V:328:VAL:O	2:V:332:LEU:HB2	2.00	0.61
2:V:470:ARG:HH21	2:V:470:ARG:CG	2.13	0.61
12:f:240:VAL:HA	12:f:257:ARG:HH21	1.64	0.61
13:A:101:ILE:HD12	13:A:138:MET:HB3	1.82	0.61
14:B:63:LEU:O	14:B:67:ARG:HB2	2.00	0.61
25:M:108:LEU:HD21	25:M:139:SER:HB3	1.81	0.61
28:P:2:SER:N	28:P:5:SER:HG	1.97	0.61
25:M:46:VAL:HG21	25:M:186:CYS:SG	2.41	0.61
26:n:35:THR:OG1	26:n:45:ARG:NH2	2.33	0.61
14:B:139:VAL:O	14:B:139:VAL:HG22	2.00	0.61
32:T:27:LEU:HD11	32:T:34:ALA:HB1	1.82	0.61
25:m:108:LEU:HD21	25:m:139:SER:HB3	1.81	0.61
32:t:27:LEU:HD11	32:t:34:ALA:HB1	1.82	0.61
2:V:497:PRO:CB	2:V:498:PRO:HD3	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:368:ASP:OD2	16:D:409:LYS:HE2	1.99	0.61
23:K:100:TRP:O	30:R:57:ARG:NH2	2.34	0.61
1:U:82:LEU:O	1:U:129:ARG:NH2	2.33	0.61
3:W:315:MET:O	3:W:315:MET:HE2	2.00	0.61
12:f:404:ASP:O	12:f:439:TYR:HD1	1.78	0.61
13:A:210:LYS:HB2	13:A:312:ARG:NH2	2.15	0.61
2:V:467:TYR:CD2	6:Z:251:LEU:HD12	2.36	0.61
3:W:180:LYS:O	3:W:184:GLU:HG3	2.01	0.61
5:Y:42:MET:SD	5:Y:46:ARG:NH2	2.74	0.61
6:Z:144:VAL:HG23	6:Z:150:PRO:HB3	1.83	0.61
15:C:88:LYS:HB2	15:C:94:LYS:CG	2.30	0.61
16:D:368:ASP:HB3	16:D:409:LYS:HZ2	1.65	0.61
2:V:29:PRO:CD	2:V:30:PRO:CD	2.79	0.61
2:V:494:MET:HE3	2:V:494:MET:O	2.00	0.61
3:W:401:THR:HG23	3:W:402:ILE:HD12	1.83	0.61
10:d:114:GLU:CA	10:d:117:THR:CG2	2.70	0.61
12:f:380:PHE:O	12:f:755:ASP:HB2	2.00	0.61
16:D:163:MET:HA	16:D:222:HIS:HE1	1.66	0.61
5:Y:40:GLU:O	5:Y:44:ALA:HB2	2.01	0.61
6:Z:250:TYR:OH	10:d:234:ASP:O	2.18	0.61
12:f:125:ILE:HG21	12:f:129:LEU:HB2	1.83	0.61
12:f:672:LEU:HD12	12:f:709:THR:HB	1.81	0.61
12:f:691:PRO:HD3	12:f:713:PHE:CE1	2.36	0.61
13:A:355:PHE:O	13:A:359:ALA:HB3	1.99	0.61
5:Y:271:PHE:O	5:Y:275:LEU:HB2	2.01	0.61
10:d:103:LEU:HB2	10:d:118:GLU:OE2	2.00	0.61
12:f:476:THR:C	12:f:478:ARG:H	2.08	0.61
12:f:586:PRO:HA	12:f:589:SER:HB2	1.83	0.61
15:C:88:LYS:CB	15:C:94:LYS:HG2	2.30	0.61
16:D:358:VAL:HG22	16:D:396:ALA:HB2	1.83	0.61
30:R:125:THR:OG1	29:q:170:ARG:NH2	2.33	0.61
2:V:27:PRO:C	2:V:30:PRO:HD2	2.26	0.60
3:W:302:TYR:HA	3:W:305:LEU:HB2	1.83	0.60
10:d:4:GLN:HB3	10:d:25:ARG:HE	1.65	0.60
12:f:201:GLU:O	12:f:205:CYS:HB2	2.01	0.60
16:D:115:ILE:HA	16:D:139:LEU:HB2	1.82	0.60
26:N:35:THR:OG1	26:N:45:ARG:NH2	2.33	0.60
1:U:465:LEU:HD11	1:U:477:GLY:HA3	1.82	0.60
1:U:694:ILE:HG23	1:U:695:MET:HG3	1.82	0.60
2:V:418:SER:HA	2:V:457:TYR:HA	1.82	0.60
12:f:222:ASP:OD2	14:B:60:LEU:HD13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:478:ARG:HG3	12:f:514:VAL:HG11	1.84	0.60
19:G:132:ARG:HH21	19:G:132:ARG:CG	2.14	0.60
25:m:46:VAL:HG21	25:m:186:CYS:SG	2.40	0.60
2:V:258:TYR:CZ	2:V:265:ASP:OD2	2.53	0.60
2:V:466:ILE:CA	2:V:469:THR:OG1	2.49	0.60
12:f:49:ASP:OD1	12:f:128:VAL:HG21	2.02	0.60
17:E:342:ASP:OD2	17:E:378:LYS:NZ	2.34	0.60
19:G:137:CYS:SG	19:G:138:MET:N	2.74	0.60
2:V:219:GLU:HG3	2:V:257:ASN:HD21	1.65	0.60
7:a:132:LYS:O	7:a:136:GLU:HB2	2.00	0.60
12:f:129:LEU:C	12:f:129:LEU:HD22	2.26	0.60
12:f:764:LEU:HD13	12:f:774:GLY:N	2.10	0.60
16:D:208:PRO:HB2	17:E:291:ARG:HD3	1.83	0.60
16:D:335:LEU:HD12	16:D:336:PRO:HD2	1.83	0.60
17:E:97:ARG:HH22	17:E:114:GLU:HB3	1.65	0.60
12:f:250:ARG:NH1	12:f:285:CYS:SG	2.73	0.60
12:f:838:ARG:HH11	12:f:838:ARG:CG	2.14	0.60
9:c:115:HIS:HB3	9:c:118:PHE:HB2	1.83	0.60
12:f:771:LEU:HD21	12:f:773:LYS:NZ	2.17	0.60
14:B:358:GLU:HG3	22:J:200:GLN:HE22	1.66	0.60
15:C:113:ARG:C	15:C:127:LEU:CD1	2.74	0.60
21:I:213:ILE:HB	21:I:228:LEU:HD12	1.83	0.60
2:V:29:PRO:HD2	2:V:30:PRO:CD	2.31	0.60
2:V:171:VAL:CG1	2:V:175:MET:HE1	2.28	0.60
2:V:219:GLU:HG3	2:V:256:ARG:HH12	1.65	0.60
2:V:496:PHE:N	2:V:497:PRO:CD	2.65	0.60
5:Y:164:ALA:C	5:Y:168:ILE:CD1	2.74	0.60
6:Z:279:LYS:HA	6:Z:279:LYS:CE	2.29	0.60
12:f:612:LEU:HD12	12:f:612:LEU:O	2.00	0.60
13:A:51:ASP:O	13:A:55:LEU:HB2	2.02	0.60
17:E:247:THR:O	17:E:251:ARG:NH2	2.34	0.60
27:O:163:ILE:HG12	27:O:170:GLY:HA2	1.82	0.60
2:V:79:VAL:HG13	2:V:81:GLN:H	1.66	0.60
2:V:141:THR:O	2:V:141:THR:HG22	2.02	0.60
2:V:492:LYS:O	15:C:44:ARG:NH1	2.35	0.60
4:X:214:SER:O	4:X:218:HIS:ND1	2.35	0.60
5:Y:24:PHE:CD2	5:Y:286:TRP:HB2	2.36	0.60
6:Z:142:GLU:H	6:Z:142:GLU:CD	2.09	0.60
6:Z:256:GLN:NE2	9:c:295:ASN:O	2.34	0.60
6:Z:283:ARG:C	6:Z:285:ALA:H	2.09	0.60
8:b:150:THR:OG1	8:b:150:THR:O	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:425:GLY:HA3	12:f:451:VAL:HG11	1.84	0.60
1:U:62:LEU:HD12	1:U:84:ALA:HB1	1.84	0.59
2:V:171:VAL:HG13	2:V:171:VAL:O	2.01	0.59
5:Y:21:GLN:CD	5:Y:286:TRP:CE3	2.80	0.59
28:P:62:THR:OG1	29:Q:85:ARG:NH2	2.34	0.59
23:k:177:ALA:O	23:k:181:LEU:HB2	2.02	0.59
1:U:601:ARG:HH11	1:U:601:ARG:CG	2.14	0.59
2:V:497:PRO:CA	6:Z:282:ASN:ND2	2.50	0.59
12:f:213:GLN:NE2	12:f:246:SER:OG	2.35	0.59
1:U:173:VAL:O	1:U:173:VAL:HG12	2.02	0.59
2:V:470:ARG:HB2	6:Z:250:TYR:HD1	1.67	0.59
12:f:465:LEU:O	12:f:481:SER:OG	2.20	0.59
15:C:83:LYS:HD2	15:C:105:ILE:HD11	1.84	0.59
16:D:119:ILE:O	16:D:121:ARG:NH1	2.34	0.59
1:U:242:LEU:HA	1:U:245:ALA:HB3	1.85	0.59
3:W:343:SER:O	3:W:347:GLY:HA3	2.02	0.59
7:a:5:PRO:HA	7:a:8:LEU:HG	1.84	0.59
7:a:255:TRP:O	7:a:258:GLN:NE2	2.35	0.59
12:f:282:PHE:N	12:f:282:PHE:HD1	1.99	0.59
1:U:46:GLU:HA	1:U:49:TYR:HB3	1.85	0.59
6:Z:246:VAL:HG12	6:Z:250:TYR:CD2	2.37	0.59
7:a:19:PRO:HA	7:a:22:TRP:HD1	1.68	0.59
8:b:151:GLU:OE1	8:b:152:LYS:NZ	2.36	0.59
9:c:92:GLN:O	9:c:96:LEU:HB2	2.02	0.59
17:E:83:CYS:HB2	17:E:89:LYS:HE2	1.84	0.59
19:G:202:LEU:O	19:G:206:LEU:HB2	2.03	0.59
23:K:177:ALA:O	23:K:181:LEU:HB2	2.02	0.59
30:R:141:ARG:NH2	29:q:162:LYS:O	2.35	0.59
26:n:18:SER:HB2	26:n:31:THR:H	1.67	0.59
2:V:232:HIS:O	2:V:236:ARG:HB2	2.03	0.59
7:a:342:ASP:OD1	7:a:345:GLN:NE2	2.36	0.59
34:E:401:ATP:O3G	18:F:347:ARG:NH2	2.34	0.59
2:V:32:PRO:HA	2:V:35:VAL:HG22	1.83	0.59
3:W:52:LYS:HD3	3:W:55:ARG:HD3	1.84	0.59
3:W:178:GLU:HB2	3:W:182:ARG:H	1.68	0.59
9:c:59:GLY:HA3	9:c:69:VAL:HA	1.84	0.59
12:f:258:LYS:HB3	12:f:770:HIS:HD2	1.60	0.59
12:f:755:ASP:N	12:f:756:PRO:CD	2.66	0.59
19:G:120:ASP:OD1	20:H:84:ARG:NH1	2.36	0.59
1:U:217:CYS:HB2	1:U:248:ILE:HD12	1.85	0.59
7:a:112:ILE:HB	7:a:151:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:575:ALA:O	12:f:579:ALA:HB3	2.03	0.59
13:A:252:GLU:OE2	13:A:255:ARG:NH1	2.35	0.59
7:a:201:GLY:O	7:a:205:LEU:HB2	2.01	0.59
21:I:216:LEU:HG	21:I:225:ILE:HG13	1.85	0.59
31:S:4:PRO:O	32:T:100:ARG:NH2	2.36	0.59
28:p:62:THR:OG1	29:q:85:ARG:NH2	2.35	0.59
3:W:56:THR:O	3:W:60:MET:HB2	2.03	0.59
3:W:84:ASN:ND2	3:W:89:LEU:O	2.36	0.59
3:W:315:MET:HE3	3:W:320:LEU:N	2.18	0.59
25:M:40:ARG:HG3	25:M:40:ARG:O	2.02	0.59
1:U:218:GLN:NE2	1:U:752:THR:O	2.36	0.58
6:Z:237:LEU:HD21	9:c:310:LYS:HD3	1.84	0.58
1:U:584:TYR:HH	1:U:768:GLN:NE2	1.99	0.58
6:Z:109:ASN:HD22	6:Z:155:PHE:HE1	1.50	0.58
8:b:124:LEU:O	8:b:128:ALA:HB2	2.02	0.58
8:b:142:ASN:HD22	8:b:172:THR:HA	1.67	0.58
15:C:151:ILE:HG21	15:C:158:ILE:HD11	1.85	0.58
17:E:182:LEU:HD22	34:E:401:ATP:H2'	1.84	0.58
24:L:26:MET:HE1	24:L:148:CYS:HB2	1.86	0.58
24:l:26:MET:HE1	24:l:148:CYS:HB2	1.86	0.58
16:D:284:GLU:OE1	16:D:287:ARG:NH1	2.36	0.58
29:Q:19:ARG:HH21	29:Q:31:ASP:HB2	1.68	0.58
19:g:202:LEU:O	19:g:206:LEU:HB2	2.03	0.58
29:q:143:LEU:O	29:q:147:TYR:HB2	2.04	0.58
2:V:352:SER:O	2:V:357:LEU:HD23	2.02	0.58
5:Y:301:ILE:HG13	5:Y:343:LEU:HD12	1.84	0.58
6:Z:9:VAL:HA	6:Z:48:LEU:HB3	1.84	0.58
9:c:88:ASP:CG	9:c:91:PHE:H	2.11	0.58
14:B:196:GLU:OE2	14:B:349:ARG:NH1	2.32	0.58
1:U:456:ASP:O	1:U:460:TYR:HB3	2.03	0.58
2:V:29:PRO:N	2:V:30:PRO:CD	2.66	0.58
5:Y:101:ARG:HE	5:Y:127:THR:HA	1.68	0.58
6:Z:184:VAL:HG13	6:Z:188:SER:HB3	1.86	0.58
12:f:568:GLY:H	12:f:599:ALA:HA	1.67	0.58
21:I:216:LEU:HG	21:I:225:ILE:CG1	2.33	0.58
19:g:134:LEU:HD12	19:g:134:LEU:N	2.18	0.58
1:U:219:CYS:SG	1:U:220:LEU:N	2.77	0.58
15:C:196:LYS:NZ	15:C:295:THR:O	2.37	0.58
24:L:117:GLN:NE2	25:M:83:ASP:OD1	2.36	0.58
29:Q:143:LEU:O	29:Q:147:TYR:HB2	2.03	0.58
2:V:89:LYS:HD2	2:V:93:PHE:HE2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:144:ASP:H	2:V:150:ARG:HH22	1.50	0.58
3:W:212:LYS:O	3:W:223:LYS:NZ	2.37	0.58
6:Z:123:ILE:HB	6:Z:136:GLU:HB3	1.86	0.58
10:d:155:LYS:HZ3	10:d:167:ILE:CD1	2.13	0.58
12:f:378:ASN:O	12:f:382:ASN:ND2	2.36	0.58
12:f:646:MET:CE	14:B:49:LEU:HG	2.27	0.58
12:f:790:GLN:HG2	12:f:794:ALA:HB3	1.85	0.58
29:q:78:THR:O	29:q:82:ASN:HB2	2.03	0.58
2:V:297:ALA:HA	2:V:301:GLU:HG2	1.86	0.58
3:W:174:TYR:HB2	17:E:161:ARG:NH1	2.19	0.58
12:f:180:GLN:O	12:f:219:LYS:NZ	2.37	0.58
12:f:282:PHE:N	12:f:282:PHE:CD1	2.72	0.58
12:f:764:LEU:CG	12:f:774:GLY:CA	2.71	0.58
15:C:113:ARG:HH21	15:C:128:PRO:HB2	1.68	0.58
18:F:376:SER:HB3	18:F:414:GLU:HG3	1.86	0.58
27:O:41:ILE:HG12	27:O:102:GLY:HA3	1.86	0.58
29:q:19:ARG:HH21	29:q:31:ASP:HB2	1.68	0.58
1:U:169:GLU:HG3	1:U:171:ASN:H	1.69	0.57
1:U:499:THR:O	1:U:503:GLN:NE2	2.37	0.57
12:f:670:MET:CG	12:f:673:ARG:HH12	2.02	0.57
17:E:144:GLU:OE2	17:E:297:ARG:NH1	2.37	0.57
26:N:18:SER:HB2	26:N:31:THR:H	1.67	0.57
25:m:168:ALA:HB1	25:m:171:ALA:HB3	1.86	0.57
2:V:371:ASN:OD1	2:V:427:GLN:NE2	2.37	0.57
12:f:609:VAL:O	12:f:613:LEU:HD12	2.04	0.57
17:E:244:SER:H	18:F:300:LYS:HA	1.69	0.57
2:V:62:HIS:HA	2:V:65:ARG:HB3	1.85	0.57
2:V:135:LEU:CG	2:V:181:TYR:HE2	1.80	0.57
4:X:255:LEU:HB2	4:X:287:LEU:HD13	1.86	0.57
5:Y:192:ARG:NH2	5:Y:290:PRO:O	2.37	0.57
7:a:33:LEU:HA	8:b:18:ASN:HD22	1.68	0.57
29:q:8:GLN:NE2	29:q:9:GLY:O	2.37	0.57
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.36	0.57
2:V:404:LYS:HD2	2:V:446:VAL:HG21	1.87	0.57
3:W:178:GLU:HB3	3:W:180:LYS:HZ3	1.69	0.57
7:a:186:LYS:HA	7:a:186:LYS:NZ	2.19	0.57
14:B:107:MET:HB2	15:C:96:VAL:HB	1.85	0.57
16:D:355:SER:CB	16:D:395:LEU:HD13	2.34	0.57
2:V:265:ASP:HA	2:V:268:GLU:CB	2.33	0.57
3:W:128:LEU:HD13	3:W:131:VAL:HG21	1.86	0.57
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:238:PRO:O	10:d:242:LEU:HB2	2.04	0.57
12:f:637:LYS:CE	12:f:673:ARG:HB2	2.33	0.57
21:i:218:ARG:NH1	21:i:223:THR:OG1	2.38	0.57
25:m:175:GLU:HA	25:m:178:LYS:HD3	1.86	0.57
1:U:167:ILE:CB	1:U:177:LEU:CD2	2.73	0.57
1:U:639:LEU:HD21	16:D:61:ILE:HD11	1.87	0.57
2:V:28:PRO:HB2	2:V:29:PRO:HD3	1.87	0.57
3:W:179:LYS:H	3:W:179:LYS:CD	2.16	0.57
16:D:162:VAL:O	16:D:162:VAL:HG12	2.03	0.57
18:F:313:LEU:O	18:F:317:LEU:HB2	2.04	0.57
21:I:229:LYS:N	21:I:232:GLU:OE2	2.38	0.57
25:M:168:ALA:HB1	25:M:171:ALA:HB3	1.86	0.57
2:V:212:TYR:O	2:V:216:ARG:HG2	2.04	0.57
13:A:210:LYS:HB2	13:A:312:ARG:HH22	1.69	0.57
13:A:297:ARG:HH22	18:F:306:VAL:HG21	1.68	0.57
29:Q:8:GLN:NE2	29:Q:9:GLY:O	2.37	0.57
29:Q:78:THR:O	29:Q:82:ASN:HB2	2.03	0.57
5:Y:288:PHE:CD1	5:Y:291:HIS:CE1	2.92	0.57
9:c:89:PRO:O	9:c:93:ALA:HB2	2.04	0.57
27:O:1:THR:N	27:O:168:GLY:O	2.38	0.57
29:Q:169:LYS:O	29:q:27:GLN:NE2	2.32	0.57
3:W:48:LEU:HA	3:W:51:GLU:HB2	1.86	0.57
6:Z:232:ASP:O	6:Z:236:LEU:HB2	2.05	0.57
16:D:368:ASP:HB3	16:D:409:LYS:HE3	1.87	0.57
31:S:28:ARG:NH2	31:S:191:ASP:OD1	2.38	0.57
27:o:138:PHE:O	27:o:142:PHE:HB2	2.05	0.57
7:a:115:LYS:HD3	7:a:118:ILE:HD12	1.86	0.57
10:d:48:LEU:O	10:d:52:ARG:CB	2.53	0.57
13:A:339:ARG:NH2	18:F:405:MET:SD	2.78	0.57
3:W:142:ARG:NH2	3:W:182:ARG:CA	2.54	0.56
3:W:169:LEU:O	3:W:182:ARG:NH1	2.37	0.56
12:f:733:GLY:O	12:f:746:ARG:NH1	2.37	0.56
12:f:870:THR:OG1	12:f:874:LEU:HD12	2.05	0.56
14:B:58:CYS:SG	14:B:59:ARG:N	2.77	0.56
16:D:129:SER:OG	16:D:252:ARG:NH1	2.37	0.56
27:O:138:PHE:O	27:O:142:PHE:HB2	2.05	0.56
2:V:27:PRO:N	2:V:28:PRO:HD3	2.20	0.56
3:W:90:LEU:HD22	3:W:93:ARG:NH1	2.20	0.56
3:W:268:LYS:NZ	3:W:302:TYR:OH	2.36	0.56
12:f:487:LEU:HD11	12:f:804:LEU:HD12	1.86	0.56
12:f:709:THR:O	12:f:713:PHE:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:F:228:PRO:O	18:F:233:LYS:NZ	2.39	0.56
18:F:311:LEU:HD23	18:F:314:LEU:HD12	1.87	0.56
2:V:29:PRO:N	2:V:30:PRO:HD2	2.21	0.56
3:W:96:GLN:NE2	3:W:135:LYS:O	2.38	0.56
6:Z:73:ASP:OD1	6:Z:77:ASN:ND2	2.38	0.56
6:Z:135:THR:HG21	6:Z:162:ILE:HD11	1.86	0.56
7:a:70:ARG:HH21	8:b:17:ARG:HG2	1.69	0.56
9:c:140:ALA:O	9:c:161:ARG:NE	2.38	0.56
10:d:200:PHE:N	10:d:200:PHE:CD1	2.73	0.56
12:f:99:LEU:HG	12:f:101:PRO:HD2	1.86	0.56
12:f:139:CYS:O	12:f:143:ARG:NH1	2.38	0.56
12:f:279:GLU:O	12:f:281:ILE:HD11	2.02	0.56
12:f:541:THR:O	12:f:545:LYS:HB3	2.06	0.56
12:f:650:GLN:HG3	14:B:68:ILE:CG1	2.28	0.56
18:F:141:ASP:OD1	18:F:144:LYS:NZ	2.35	0.56
18:F:318:ASP:HB3	18:F:347:ARG:HG2	1.86	0.56
21:I:218:ARG:NH1	21:I:223:THR:OG1	2.38	0.56
23:K:209:LYS:O	23:K:214:ASN:ND2	2.38	0.56
25:M:175:GLU:HA	25:M:178:LYS:HD3	1.86	0.56
25:M:241:GLU:O	25:M:244:LYS:NZ	2.37	0.56
19:g:137:CYS:SG	19:g:138:MET:N	2.74	0.56
23:k:50:VAL:HG11	23:k:66:LYS:HB2	1.88	0.56
27:o:1:THR:N	27:o:168:GLY:O	2.38	0.56
27:o:41:ILE:HG12	27:o:102:GLY:HA3	1.86	0.56
7:a:7:PHE:HD2	7:a:63:PHE:CD2	2.22	0.56
7:a:8:LEU:HD12	7:a:9:GLN:HG2	1.87	0.56
8:b:2:VAL:O	8:b:44:ASN:ND2	2.38	0.56
8:b:72:LEU:O	8:b:76:HIS:ND1	2.36	0.56
12:f:712:LYS:HD3	12:f:715:HIS:HB2	1.88	0.56
15:C:90:HIS:CD2	15:C:90:HIS:H	2.21	0.56
1:U:636:VAL:HG23	1:U:637:VAL:HG23	1.88	0.56
12:f:634:LYS:HD2	12:f:637:LYS:HD2	1.88	0.56
23:k:209:LYS:O	23:k:214:ASN:ND2	2.38	0.56
7:a:5:PRO:CA	7:a:8:LEU:HG	2.36	0.56
9:c:196:LEU:HD23	9:c:197:ASN:HB2	1.85	0.56
12:f:836:GLU:OE1	12:f:840:LEU:HD23	2.05	0.56
21:I:119:GLN:NE2	22:J:79:ASP:OD1	2.38	0.56
32:T:192:VAL:HG12	32:T:197:VAL:HG22	1.87	0.56
2:V:210:CYS:O	2:V:214:HIS:HB2	2.05	0.56
2:V:284:GLU:O	2:V:288:TYR:HB2	2.06	0.56
7:a:172:TYR:O	7:a:176:ALA:HB2	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:150:THR:HB	8:b:153:LEU:CB	2.35	0.56
8:b:150:THR:HG21	8:b:172:THR:HG22	1.87	0.56
11:e:56:LEU:HD12	11:e:56:LEU:O	2.05	0.56
31:S:114:ASP:OD1	31:S:118:LYS:N	2.37	0.56
2:V:210:CYS:O	2:V:214:HIS:CB	2.54	0.56
7:a:153:SER:O	7:a:157:ASP:HB2	2.06	0.56
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.88	0.56
12:f:125:ILE:CG2	12:f:129:LEU:HB2	2.35	0.56
13:A:78:TRP:HB3	14:B:137:SER:C	2.30	0.56
13:A:248:LYS:NZ	16:D:278:GLN:OE1	2.38	0.56
23:K:50:VAL:HG11	23:K:66:LYS:HB2	1.88	0.56
28:P:149:MET:HE3	31:s:147:PRO:HB2	1.87	0.56
1:U:219:CYS:O	1:U:223:LEU:HB2	2.06	0.56
2:V:203:LEU:O	2:V:207:ALA:CB	2.53	0.56
2:V:247:GLN:NE2	2:V:276:PHE:O	2.38	0.56
3:W:141:GLU:HG3	3:W:172:GLU:HG3	1.85	0.56
10:d:125:LYS:HB3	10:d:130:ASN:HD22	1.71	0.56
13:A:210:LYS:CB	13:A:312:ARG:NH2	2.69	0.56
2:V:283:ASN:ND2	11:e:3:GLU:OE2	2.37	0.56
12:f:150:GLU:O	12:f:156:HIS:ND1	2.39	0.56
14:B:251:VAL:HG12	14:B:253:SER:H	1.71	0.56
17:E:55:GLN:HB2	18:F:133:PHE:HB3	1.88	0.56
23:k:183:GLU:HG3	23:k:184:VAL:HG13	1.88	0.56
32:t:192:VAL:HG12	32:t:197:VAL:HG22	1.88	0.56
1:U:35:TRP:HE1	1:U:67:VAL:HA	1.71	0.55
1:U:471:ASP:HA	1:U:474:ARG:HB2	1.88	0.55
1:U:900:TYR:HB3	1:U:914:LEU:HG	1.86	0.55
2:V:227:VAL:HA	2:V:230:PHE:HB3	1.87	0.55
2:V:470:ARG:HD2	2:V:470:ARG:C	2.31	0.55
12:f:57:GLU:HG2	12:f:93:PRO:HB3	1.88	0.55
25:m:66:LEU:HD21	25:m:214:SER:HB2	1.87	0.55
2:V:87:SER:HB3	2:V:126:ALA:H	1.71	0.55
3:W:344:THR:O	3:W:348:GLU:CB	2.50	0.55
6:Z:252:LYS:HG2	9:c:234:TYR:CZ	2.31	0.55
14:B:337:LEU:HD11	14:B:342:ILE:HD11	1.89	0.55
23:K:183:GLU:HG3	23:K:184:VAL:HG13	1.88	0.55
25:m:241:GLU:O	25:m:244:LYS:NZ	2.37	0.55
28:p:2:SER:OG	28:p:3:ILE:N	2.39	0.55
1:U:132:GLY:O	1:U:136:LYS:HB2	2.06	0.55
15:C:114:VAL:HA	15:C:127:LEU:HD12	1.88	0.55
21:I:225:ILE:O	21:I:225:ILE:HG22	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S:23:VAL:O	31:S:196:CYS:SG	2.62	0.55
2:V:227:VAL:O	2:V:231:LEU:CB	2.54	0.55
2:V:398:LEU:HD13	2:V:401:ASN:HD22	1.70	0.55
7:a:324:ILE:HA	7:a:331:VAL:HG12	1.89	0.55
12:f:838:ARG:CG	12:f:839:PRO:CD	2.82	0.55
21:i:109:GLN:OE1	29:q:71:ASN:ND2	2.38	0.55
1:U:241:ASN:HD22	1:U:244:MET:HE3	1.71	0.55
1:U:600:ARG:HE	16:D:56:VAL:HG22	1.71	0.55
2:V:262:SER:HG	10:d:121:ARG:HH21	1.50	0.55
3:W:17:GLU:HG2	3:W:63:THR:HG23	1.88	0.55
5:Y:191:ILE:HD11	11:e:40:GLU:HB3	1.88	0.55
12:f:39:LYS:HD2	12:f:120:ARG:HH22	1.71	0.55
15:C:141:GLU:O	16:D:323:ARG:NH1	2.38	0.55
16:D:164:TYR:O	16:D:174:LYS:NZ	2.40	0.55
31:s:114:ASP:OD1	31:s:118:LYS:N	2.37	0.55
3:W:375:MET:HE2	3:W:386:VAL:HB	1.89	0.55
6:Z:224:HIS:CD2	6:Z:224:HIS:N	2.75	0.55
16:D:345:PHE:HB3	16:D:360:LEU:HD23	1.88	0.55
29:Q:38:MET:O	29:Q:65:GLN:NE2	2.40	0.55
31:s:28:ARG:NH2	31:s:191:ASP:OD1	2.38	0.55
1:U:416:GLU:OE1	1:U:450:HIS:NE2	2.38	0.55
2:V:165:ALA:CB	2:V:167:LEU:HD22	2.28	0.55
3:W:142:ARG:HD3	3:W:145:LEU:HB2	1.89	0.55
6:Z:246:VAL:CG1	6:Z:250:TYR:CE2	2.89	0.55
7:a:360:VAL:O	7:a:364:GLU:HB2	2.07	0.55
9:c:31:VAL:HB	9:c:205:ILE:HG22	1.88	0.55
28:P:58:THR:O	29:Q:85:ARG:NH2	2.39	0.55
20:h:4:ARG:NH1	20:h:5:GLY:O	2.40	0.55
22:j:38:ARG:HH12	22:j:182:GLU:HA	1.72	0.55
1:U:601:ARG:NH1	1:U:601:ARG:HB2	2.21	0.55
2:V:29:PRO:CB	2:V:30:PRO:CD	2.84	0.55
2:V:494:MET:HG3	6:Z:275:LEU:CD2	2.35	0.55
3:W:315:MET:HE3	3:W:320:LEU:CA	2.36	0.55
7:a:8:LEU:CD2	7:a:29:TYR:OH	2.54	0.55
12:f:253:LEU:HD11	12:f:272:LEU:HB3	1.89	0.55
14:B:136:LEU:O	14:B:139:VAL:HG12	2.07	0.55
17:E:199:VAL:HG23	17:E:201:SER:H	1.71	0.55
18:F:94:ILE:HD11	18:F:125:LYS:HB2	1.89	0.55
22:J:38:ARG:HH12	22:J:182:GLU:HA	1.72	0.55
23:K:36:THR:HA	23:K:171:GLY:HA3	1.89	0.55
25:M:41:CYS:SG	25:M:189:ILE:CG2	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:179:TYR:CD2	1:U:179:TYR:C	2.85	0.55
1:U:583:MET:HE2	1:U:605:VAL:HG11	1.89	0.55
10:d:183:GLU:HA	10:d:215:TRP:HE1	1.72	0.55
12:f:281:ILE:CD1	12:f:281:ILE:H	2.07	0.55
25:M:66:LEU:HD21	25:M:214:SER:HB2	1.87	0.55
1:U:171:ASN:ND2	1:U:176:MET:HE3	2.20	0.55
1:U:603:LEU:HD21	16:D:60:TYR:CG	2.35	0.55
6:Z:98:GLY:HA3	6:Z:123:ILE:HG23	1.89	0.55
6:Z:249:PHE:HZ	9:c:303:MET:HG2	1.72	0.55
12:f:680:ARG:HG2	12:f:716:ASP:HA	1.87	0.55
12:f:796:LEU:HA	12:f:799:VAL:HG12	1.89	0.55
13:A:85:GLN:HA	13:A:88:GLN:HB3	1.89	0.55
16:D:368:ASP:HB3	16:D:409:LYS:CE	2.37	0.55
18:F:272:PHE:HD2	18:F:316:GLN:HG3	1.72	0.55
1:U:798:PRO:O	1:U:880:ASN:ND2	2.40	0.54
2:V:494:MET:CG	6:Z:275:LEU:CD2	2.83	0.54
6:Z:235:ASN:HD21	7:a:335:TRP:HA	1.71	0.54
6:Z:279:LYS:CE	6:Z:279:LYS:CA	2.86	0.54
12:f:403:LYS:O	12:f:406:GLY:N	2.40	0.54
12:f:616:CYS:SG	12:f:632:LYS:NZ	2.72	0.54
15:C:60:ARG:NH2	16:D:71:GLU:OE2	2.40	0.54
16:D:115:ILE:HG22	16:D:139:LEU:HD12	1.89	0.54
20:H:4:ARG:NH1	20:H:5:GLY:O	2.40	0.54
3:W:390:GLU:HG3	3:W:408:ARG:HH21	1.72	0.54
9:c:78:SER:N	9:c:85:GLU:HG3	2.20	0.54
16:D:172:ILE:O	16:D:176:GLU:HB2	2.06	0.54
17:E:194:ASN:HB3	17:E:228:CYS:HA	1.89	0.54
21:I:176:LYS:HB3	22:J:53:LEU:CD2	2.37	0.54
29:Q:117:TYR:HB3	29:Q:125:ALA:HB3	1.88	0.54
29:Q:141:SER:O	29:Q:145:ARG:HB2	2.07	0.54
1:U:477:GLY:O	1:U:481:LEU:HB2	2.08	0.54
3:W:315:MET:CE	3:W:320:LEU:CA	2.85	0.54
14:B:221:GLY:HA3	14:B:347:ILE:HA	1.89	0.54
31:S:147:PRO:HB2	28:p:149:MET:HE3	1.89	0.54
2:V:56:ALA:O	2:V:60:ALA:HB2	2.08	0.54
2:V:265:ASP:HB2	2:V:269:LYS:NZ	2.22	0.54
4:X:299:LEU:HD21	4:X:331:LEU:HA	1.87	0.54
10:d:45:LYS:HZ1	10:d:88:GLN:HA	1.72	0.54
12:f:218:GLU:HA	12:f:221:ILE:HG22	1.89	0.54
12:f:646:MET:C	14:B:67:ARG:HE	2.14	0.54
15:C:221:GLN:HE22	15:C:228:ALA:HB3	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:194:ILE:O	21:I:198:ASN:HB2	2.07	0.54
30:R:139:MET:O	30:R:143:TYR:HB2	2.08	0.54
30:r:139:MET:O	30:r:143:TYR:HB2	2.08	0.54
1:U:604:HIS:C	1:U:604:HIS:CD2	2.85	0.54
2:V:216:ARG:HH22	11:e:5:LYS:HB3	1.73	0.54
4:X:172:LEU:HD12	4:X:175:LYS:HD3	1.89	0.54
12:f:93:PRO:HB2	12:f:97:LYS:HG3	1.90	0.54
12:f:591:ALA:HA	12:f:594:LEU:HD23	1.90	0.54
16:D:391:ARG:NH2	16:D:398:ASP:OD2	2.40	0.54
18:F:224:LEU:HB2	18:F:348:LEU:HD23	1.89	0.54
21:I:123:GLN:HG3	22:J:125:ARG:HE	1.73	0.54
19:g:32:ILE:HA	19:g:82:GLY:HA2	1.90	0.54
21:i:194:ILE:O	21:i:198:ASN:HB2	2.07	0.54
29:q:117:TYR:HB3	29:q:125:ALA:HB3	1.88	0.54
1:U:646:PRO:HA	1:U:649:ARG:HB2	1.88	0.54
3:W:203:GLN:O	3:W:207:LYS:HB2	2.08	0.54
14:B:60:LEU:O	14:B:64:LYS:HB2	2.07	0.54
17:E:198:VAL:HG12	17:E:200:SER:H	1.72	0.54
23:K:76:CYS:SG	23:K:77:ALA:N	2.81	0.54
19:g:47:CYS:HB2	19:g:221:THR:HG22	1.88	0.54
1:U:133:ILE:HA	1:U:136:LYS:HB3	1.90	0.54
1:U:179:TYR:CZ	1:U:183:LEU:HD11	2.29	0.54
2:V:135:LEU:HD21	2:V:181:TYR:CE2	2.42	0.54
12:f:119:LYS:HA	12:f:122:ALA:HB3	1.88	0.54
12:f:129:LEU:HD22	12:f:129:LEU:O	2.07	0.54
12:f:838:ARG:CG	12:f:839:PRO:HD2	2.31	0.54
13:A:236:CYS:SG	13:A:267:LYS:NZ	2.75	0.54
17:E:313:LEU:O	17:E:317:ALA:HB2	2.06	0.54
29:q:38:MET:O	29:q:65:GLN:NE2	2.40	0.54
3:W:288:HIS:HA	3:W:291:SER:HB3	1.90	0.54
5:Y:101:ARG:NH2	5:Y:126:LYS:O	2.40	0.54
6:Z:246:VAL:CG1	6:Z:250:TYR:HE2	2.21	0.54
8:b:24:THR:HG22	8:b:26:LEU:H	1.72	0.54
12:f:171:GLN:HE21	12:f:179:VAL:HG13	1.73	0.54
13:A:189:GLU:OE2	18:F:409:ARG:NH2	2.41	0.54
16:D:392:TYR:HD1	17:E:161:ARG:HG2	1.73	0.54
30:R:196:HIS:O	30:R:200:SER:CB	2.55	0.54
23:k:36:THR:HA	23:k:171:GLY:HA3	1.89	0.54
1:U:413:LYS:HD2	1:U:780:SER:HB2	1.90	0.54
7:a:292:THR:HG23	7:a:295:GLU:H	1.73	0.54
10:d:48:LEU:O	10:d:52:ARG:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:E:180:LYS:NZ	34:E:401:ATP:O2G	2.40	0.54
32:T:9:THR:O	32:T:41:ARG:NH2	2.41	0.54
26:n:40:ARG:NH2	26:n:182:SER:O	2.41	0.54
29:q:141:SER:O	29:q:145:ARG:HB2	2.07	0.54
30:r:196:HIS:O	30:r:200:SER:CB	2.55	0.54
5:Y:69:LEU:HA	5:Y:72:LYS:HE3	1.90	0.54
5:Y:262:SER:OG	5:Y:267:ARG:O	2.26	0.54
13:A:346:PRO:O	13:A:351:ARG:NH1	2.41	0.54
14:B:112:LEU:HD12	14:B:148:CYS:HB3	1.90	0.54
18:F:210:GLU:O	18:F:214:ASN:HB2	2.08	0.54
19:G:141:ILE:HG22	19:G:151:VAL:HG22	1.89	0.54
19:g:141:ILE:HG22	19:g:151:VAL:HG22	1.89	0.54
27:o:30:ASN:OD1	27:o:187:ARG:NH2	2.41	0.54
2:V:134:PHE:HA	2:V:137:GLU:OE2	2.08	0.53
2:V:166:TYR:CE1	2:V:216:ARG:HB2	2.43	0.53
2:V:358:MET:CB	2:V:359:PRO:HD3	2.36	0.53
10:d:168:ASP:HA	10:d:171:LEU:HB2	1.89	0.53
12:f:548:THR:HG21	12:f:554:TYR:HE2	1.72	0.53
12:f:680:ARG:O	12:f:763:ARG:CZ	2.56	0.53
19:G:32:ILE:HA	19:G:82:GLY:HA2	1.90	0.53
21:I:198:ASN:HA	21:I:206:LEU:HD21	1.91	0.53
22:j:86:ARG:HE	22:j:114:LEU:HD11	1.73	0.53
31:s:23:VAL:O	31:s:196:CYS:SG	2.62	0.53
32:t:27:LEU:HD22	32:t:184:TYR:HB2	1.90	0.53
2:V:136:GLU:O	2:V:136:GLU:HG2	2.07	0.53
2:V:467:TYR:OH	6:Z:255:ASP:OD1	2.26	0.53
9:c:265:MET:HE3	9:c:266:THR:HG22	1.91	0.53
12:f:94:LYS:HA	12:f:97:LYS:HB2	1.90	0.53
13:A:190:VAL:HG21	13:A:339:ARG:HG3	1.89	0.53
13:A:400:ARG:HG2	13:A:400:ARG:HH11	1.72	0.53
15:C:69:GLN:HG3	15:C:118:ASN:HD21	1.72	0.53
26:N:40:ARG:NH2	26:N:182:SER:O	2.41	0.53
1:U:252:LEU:O	1:U:256:ALA:CB	2.57	0.53
3:W:88:MET:C	3:W:90:LEU:H	2.17	0.53
7:a:58:LYS:O	7:a:62:ASN:HB2	2.08	0.53
12:f:305:LEU:HB2	12:f:317:LEU:HD22	1.91	0.53
12:f:646:MET:CE	14:B:49:LEU:CD1	2.85	0.53
18:F:153:VAL:HG22	18:F:160:ILE:HG22	1.90	0.53
1:U:590:TYR:HD1	1:U:595:ASN:HD22	1.56	0.53
2:V:84:LYS:HG2	2:V:123:SER:HB2	1.90	0.53
5:Y:71:ASN:O	5:Y:75:LYS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:141:VAL:HG13	5:Y:160:ASN:HB2	1.91	0.53
12:f:291:GLN:HE22	12:f:324:VAL:HG11	1.73	0.53
18:F:313:LEU:O	18:F:317:LEU:CB	2.56	0.53
21:I:213:ILE:CB	21:I:228:LEU:CD1	2.79	0.53
23:k:76:CYS:SG	23:k:77:ALA:N	2.81	0.53
1:U:235:LYS:O	1:U:239:GLU:HB2	2.09	0.53
1:U:714:SER:HA	1:U:717:ILE:HG22	1.90	0.53
2:V:94:VAL:CG2	2:V:137:GLU:CB	2.78	0.53
4:X:65:GLU:O	4:X:69:LEU:HB2	2.08	0.53
14:B:103:ARG:NH1	14:B:138:PHE:CE2	2.59	0.53
16:D:338:ARG:NH1	16:D:365:ALA:O	2.41	0.53
22:J:38:ARG:NH1	22:J:181:ILE:O	2.42	0.53
2:V:265:ASP:CA	2:V:268:GLU:HB3	2.38	0.53
2:V:470:ARG:HD2	2:V:470:ARG:O	2.09	0.53
5:Y:334:LEU:HD23	5:Y:334:LEU:H	1.74	0.53
9:c:41:MET:HE3	9:c:145:VAL:HB	1.90	0.53
13:A:400:ARG:HG2	13:A:400:ARG:NH1	2.22	0.53
16:D:368:ASP:CB	16:D:409:LYS:NZ	2.72	0.53
19:G:155:ASP:OD1	19:G:159:TYR:N	2.41	0.53
32:t:9:THR:O	32:t:41:ARG:NH2	2.41	0.53
2:V:259:LEU:HD11	2:V:294:ARG:HD2	1.91	0.53
3:W:79:GLU:HA	3:W:82:LEU:HD23	1.89	0.53
9:c:78:SER:HB2	9:c:85:GLU:CD	2.33	0.53
25:M:15:SER:OG	25:M:19:ARG:N	2.41	0.53
2:V:471:GLU:H	2:V:472:PRO:CD	2.22	0.53
10:d:21:GLU:O	10:d:25:ARG:CB	2.56	0.53
12:f:708:ASP:OD1	12:f:785:ARG:HG3	2.08	0.53
14:B:373:THR:OG1	14:B:412:MET:O	2.27	0.53
16:D:212:LYS:NZ	34:D:501:ATP:O1G	2.42	0.53
23:K:48:LEU:HD21	23:K:77:ALA:HB2	1.91	0.53
32:T:27:LEU:HD22	32:T:184:TYR:HB2	1.90	0.53
23:k:100:TRP:O	30:r:57:ARG:NH2	2.42	0.53
30:r:196:HIS:O	30:r:200:SER:OG	2.26	0.53
2:V:43:THR:O	2:V:47:SER:OG	2.24	0.53
3:W:90:LEU:CD2	3:W:93:ARG:NH1	2.72	0.53
5:Y:336:ARG:HH21	5:Y:336:ARG:CG	2.14	0.53
27:O:30:ASN:OD1	27:O:187:ARG:NH2	2.41	0.53
21:i:118:LYS:HD3	21:i:152:PRO:HA	1.91	0.53
1:U:326:ILE:O	1:U:330:SER:OG	2.26	0.53
3:W:274:VAL:HG21	3:W:290:ILE:HD13	1.90	0.53
12:f:838:ARG:HG2	12:f:838:ARG:NH1	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B:49:LEU:HD13	14:B:51:LEU:H	1.71	0.53
15:C:78:ARG:HH12	15:C:80:MET:HE3	1.73	0.53
16:D:363:TYR:HE2	16:D:399:PHE:HB3	1.74	0.53
24:L:50:LYS:HB3	24:L:59:HIS:HB3	1.90	0.53
21:i:3:ARG:HB2	22:j:5:ARG:HH12	1.72	0.53
1:U:475:HIS:NE2	1:U:507:VAL:O	2.38	0.52
2:V:29:PRO:HB2	2:V:30:PRO:CD	2.34	0.52
3:W:309:PHE:HE1	3:W:314:LEU:HD22	1.75	0.52
12:f:67:ASP:O	12:f:71:TYR:CB	2.56	0.52
14:B:57:GLN:HA	14:B:61:LYS:HZ3	1.74	0.52
15:C:373:GLU:HG3	15:C:375:ARG:HG3	1.91	0.52
24:l:50:LYS:HB3	24:l:59:HIS:HB3	1.90	0.52
2:V:171:VAL:HG11	2:V:175:MET:CE	2.33	0.52
2:V:228:ARG:O	2:V:232:HIS:ND1	2.42	0.52
2:V:353:LEU:C	2:V:357:LEU:CD2	2.82	0.52
2:V:449:ALA:HB3	2:V:460:SER:HA	1.91	0.52
3:W:142:ARG:HG3	3:W:142:ARG:O	2.09	0.52
5:Y:169:GLU:O	5:Y:171:GLY:O	2.27	0.52
7:a:159:SER:OG	7:a:175:ASP:OD2	2.27	0.52
10:d:195:THR:O	10:d:200:PHE:CZ	2.62	0.52
19:G:144:ASP:HB3	19:G:147:GLN:HB2	1.91	0.52
26:N:32:ASP:OD1	26:N:186:ARG:NH2	2.43	0.52
21:i:40:ASN:ND2	21:i:182:GLY:O	2.40	0.52
26:n:32:ASP:OD1	26:n:186:ARG:NH2	2.43	0.52
2:V:195:ILE:HD11	2:V:241:ARG:HH21	1.74	0.52
6:Z:15:VAL:HA	6:Z:18:SER:HB3	1.90	0.52
12:f:373:ALA:HB2	12:f:744:MET:HA	1.92	0.52
14:B:262:ASP:OD1	14:B:265:LYS:NZ	2.42	0.52
15:C:329:LEU:O	15:C:333:SER:CB	2.57	0.52
16:D:233:SER:OG	17:E:259:GLU:OE1	2.27	0.52
21:I:176:LYS:CB	22:J:53:LEU:CD2	2.87	0.52
22:j:38:ARG:NH1	22:j:181:ILE:O	2.42	0.52
31:s:1:ARG:HH21	32:t:2:GLN:HE22	1.57	0.52
1:U:126:ILE:HG22	1:U:128:GLN:H	1.75	0.52
2:V:151:THR:O	2:V:155:ALA:CB	2.56	0.52
6:Z:153:LYS:N	6:Z:153:LYS:CE	2.73	0.52
30:R:196:HIS:O	30:R:200:SER:OG	2.26	0.52
19:g:134:LEU:CD1	19:g:134:LEU:N	2.73	0.52
1:U:522:GLY:O	1:U:559:ARG:NH2	2.42	0.52
6:Z:180:LYS:NZ	6:Z:182:THR:OG1	2.42	0.52
12:f:813:LYS:HD3	12:f:815:HIS:HE1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:411:GLU:HG2	16:D:413:GLU:H	1.74	0.52
17:E:114:GLU:H	17:E:114:GLU:CD	2.14	0.52
17:E:119:VAL:O	17:E:122:MET:N	2.36	0.52
19:G:223:GLU:O	19:G:225:PRO:HD3	2.09	0.52
22:J:31:THR:HA	22:J:162:GLY:HA3	1.92	0.52
3:W:231:ILE:O	3:W:235:GLN:CB	2.55	0.52
6:Z:252:LYS:HD3	6:Z:252:LYS:C	2.34	0.52
12:f:168:LYS:HD3	12:f:204:ALA:HB1	1.92	0.52
12:f:650:GLN:HA	12:f:653:ALA:HB3	1.92	0.52
12:f:670:MET:CE	12:f:673:ARG:HD2	2.09	0.52
13:A:78:TRP:CD1	14:B:138:PHE:CA	2.80	0.52
13:A:210:LYS:HB3	13:A:312:ARG:HH22	1.75	0.52
16:D:208:PRO:HD3	16:D:312:ASN:HD21	1.74	0.52
19:g:144:ASP:HB3	19:g:147:GLN:HB2	1.91	0.52
21:i:198:ASN:HA	21:i:206:LEU:HD21	1.91	0.52
3:W:260:SER:O	3:W:264:GLN:N	2.43	0.52
12:f:49:ASP:OD1	12:f:128:VAL:CG2	2.58	0.52
12:f:814:SER:HA	12:f:882:LEU:HD12	1.91	0.52
16:D:338:ARG:NH1	16:D:365:ALA:C	2.67	0.52
21:I:118:LYS:HD3	21:I:152:PRO:HA	1.91	0.52
22:J:11:SER:OG	22:J:15:HIS:N	2.43	0.52
31:S:35:ILE:HB	32:T:151:ARG:HH12	1.73	0.52
1:U:179:TYR:CE2	1:U:183:LEU:CG	2.91	0.52
1:U:187:LEU:HD13	16:D:45:LYS:HE2	1.91	0.52
7:a:5:PRO:HA	7:a:8:LEU:HD23	1.78	0.52
12:f:198:HIS:O	12:f:202:HIS:CB	2.58	0.52
12:f:369:ARG:HA	12:f:372:LEU:HD13	1.92	0.52
12:f:690:VAL:HG12	12:f:713:PHE:CD1	2.40	0.52
14:B:405:MET:HE2	14:B:421:LYS:HD2	1.91	0.52
16:D:125:LYS:CB	16:D:125:LYS:NZ	2.73	0.52
17:E:232:MET:HB3	17:E:277:MET:HG2	1.92	0.52
21:i:33:THR:HA	21:i:165:GLY:HA2	1.92	0.52
23:k:48:LEU:HD21	23:k:77:ALA:HB2	1.91	0.52
2:V:106:ARG:O	2:V:110:HIS:ND1	2.39	0.52
2:V:128:ARG:HH11	2:V:169:LEU:CD1	2.18	0.52
5:Y:99:GLU:HA	5:Y:102:ASP:HB3	1.91	0.52
15:C:132:ASP:OD1	15:C:237:MET:HE1	2.10	0.52
21:i:133:SER:HB2	21:i:152:PRO:HD3	1.92	0.52
5:Y:104:MET:O	5:Y:108:ALA:CB	2.57	0.51
5:Y:164:ALA:O	5:Y:168:ILE:HD13	2.07	0.51
6:Z:187:LEU:HD23	10:d:254:GLU:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:189:PRO:HB2	7:a:192:GLU:H	1.75	0.51
12:f:680:ARG:CZ	12:f:715:HIS:NE2	2.73	0.51
15:C:72:TYR:N	15:C:116:LEU:O	2.41	0.51
16:D:152:MET:HE3	16:D:154:LEU:HD13	1.93	0.51
17:E:140:GLU:O	17:E:144:GLU:HB2	2.09	0.51
22:J:86:ARG:HE	22:J:114:LEU:HD11	1.73	0.51
28:P:126:LEU:HD12	28:P:127:ILE:HG23	1.92	0.51
1:U:389:ASN:HD21	1:U:392:TRP:HE3	1.58	0.51
1:U:625:ILE:HG13	1:U:626:LEU:HG	1.91	0.51
3:W:265:GLN:OE1	3:W:335:SER:OG	2.26	0.51
4:X:173:GLU:HA	4:X:176:THR:HG22	1.92	0.51
7:a:255:TRP:HB3	7:a:261:LEU:HD11	1.92	0.51
19:G:200:THR:HA	19:G:203:SER:HB2	1.92	0.51
21:I:33:THR:HA	21:I:165:GLY:HA2	1.92	0.51
22:J:52:LYS:N	22:J:52:LYS:CD	2.73	0.51
31:S:51:VAL:HG11	31:S:196:CYS:SG	2.51	0.51
1:U:496:LEU:HA	1:U:499:THR:HG22	1.91	0.51
2:V:194:LYS:HG3	2:V:200:ARG:HE	1.74	0.51
3:W:179:LYS:CD	3:W:179:LYS:N	2.73	0.51
6:Z:138:TYR:HA	6:Z:157:HIS:HA	1.92	0.51
6:Z:193:ASN:OD1	9:c:228:GLY:N	2.37	0.51
6:Z:209:ARG:HD3	7:a:353:LEU:HD12	1.93	0.51
7:a:28:LEU:HB3	7:a:33:LEU:HD11	1.93	0.51
17:E:265:ASP:OD2	17:E:291:ARG:NH1	2.43	0.51
21:I:40:ASN:ND2	21:I:182:GLY:O	2.40	0.51
28:p:126:LEU:HD12	28:p:127:ILE:HG23	1.93	0.51
2:V:137:GLU:N	2:V:137:GLU:OE1	2.44	0.51
2:V:156:SER:HA	2:V:159:LEU:HB2	1.93	0.51
4:X:198:ASN:HD21	15:C:389:LYS:HB2	1.75	0.51
6:Z:222:ILE:O	6:Z:223:ASN:OD1	2.29	0.51
7:a:7:PHE:HE2	7:a:63:PHE:CE2	2.22	0.51
1:U:191:LYS:HD2	1:U:194:ARG:HH11	1.75	0.51
1:U:772:TRP:HB3	1:U:775:LEU:HB2	1.93	0.51
2:V:40:GLU:HA	2:V:43:THR:HB	1.91	0.51
2:V:211:TYR:O	2:V:215:ALA:HB2	2.10	0.51
3:W:137:TYR:CZ	16:D:392:TYR:CD2	2.96	0.51
9:c:89:PRO:O	9:c:93:ALA:CB	2.59	0.51
12:f:571:GLU:HG3	12:f:573:ILE:H	1.75	0.51
14:B:74:MET:O	14:B:78:PHE:CB	2.56	0.51
14:B:82:GLN:HG2	14:B:86:LYS:HG3	1.93	0.51
17:E:300:HIS:NE2	17:E:302:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:47:ALA:HB3	21:I:212:GLU:HB2	1.92	0.51
32:T:49:THR:HB	32:T:85:PRO:HG3	1.92	0.51
32:T:136:SER:HB2	32:T:150:LEU:HD13	1.93	0.51
2:V:349:ARG:HA	2:V:353:LEU:HB2	1.92	0.51
2:V:352:SER:O	2:V:357:LEU:CD2	2.59	0.51
3:W:180:LYS:HD3	3:W:180:LYS:H	1.73	0.51
3:W:187:LEU:HA	3:W:190:MET:HE3	1.93	0.51
9:c:174:PRO:HB2	9:c:175:ARG:HG3	1.93	0.51
10:d:155:LYS:HG3	10:d:171:LEU:HD21	1.91	0.51
12:f:625:LYS:HB2	12:f:628:ASP:HB3	1.91	0.51
15:C:19:GLY:O	15:C:23:TYR:HB3	2.10	0.51
15:C:113:ARG:C	15:C:127:LEU:HD13	2.36	0.51
17:E:155:ASN:CB	17:E:158:LEU:HD13	2.40	0.51
20:H:71:HIS:HA	20:H:218:PHE:H	1.76	0.51
19:g:165:ALA:HB1	19:g:179:LEU:HD13	1.93	0.51
2:V:139:MET:SD	2:V:139:MET:C	2.94	0.51
7:a:269:LEU:HD12	7:a:272:ILE:HD11	1.92	0.51
10:d:119:LEU:CD2	10:d:119:LEU:N	2.73	0.51
12:f:469:TYR:OH	12:f:478:ARG:NH1	2.43	0.51
15:C:130:LYS:HE2	15:C:131:VAL:HG12	1.92	0.51
16:D:332:GLU:HG3	16:D:334:PRO:HD3	1.91	0.51
17:E:220:ASN:OD1	17:E:223:ARG:NH2	2.44	0.51
24:L:117:GLN:O	24:L:120:THR:OG1	2.27	0.51
3:W:49:SER:O	3:W:53:GLN:CB	2.58	0.51
3:W:137:TYR:HB2	3:W:144:ARG:NH1	2.25	0.51
7:a:197:ALA:HB2	7:a:222:LEU:HD22	1.92	0.51
10:d:44:THR:O	10:d:47:GLN:NE2	2.44	0.51
10:d:156:GLY:H	10:d:158:ILE:CD1	2.24	0.51
10:d:200:PHE:HD1	10:d:200:PHE:H	1.59	0.51
12:f:697:ILE:HG12	12:f:737:ASN:HD21	1.75	0.51
18:F:282:ILE:HG22	18:F:327:LYS:HB2	1.93	0.51
21:I:133:SER:HB2	21:I:152:PRO:HD3	1.92	0.51
19:g:46:ASP:O	19:g:222:VAL:CG2	2.53	0.51
32:t:49:THR:HB	32:t:85:PRO:HG3	1.92	0.51
1:U:36:ALA:HB1	2:V:268:GLU:HG3	1.91	0.51
6:Z:12:HIS:ND1	6:Z:50:VAL:O	2.32	0.51
12:f:228:LYS:HB3	12:f:231:LEU:HD13	1.92	0.51
13:A:75:PRO:HA	13:A:78:TRP:CZ2	2.46	0.51
17:E:304:PRO:O	17:E:309:ARG:NH1	2.44	0.51
19:g:200:THR:HA	19:g:203:SER:HB2	1.92	0.51
31:s:51:VAL:HG11	31:s:196:CYS:SG	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:317:TRP:CE3	3:W:355:LYS:CD	2.94	0.51
5:Y:160:ASN:HA	5:Y:163:LYS:HB2	1.92	0.51
7:a:132:LYS:O	7:a:136:GLU:CB	2.59	0.51
12:f:545:LYS:HE3	12:f:588:ARG:HA	1.92	0.51
12:f:764:LEU:CD2	12:f:774:GLY:O	2.56	0.51
15:C:370:ALA:HB1	15:C:375:ARG:HB2	1.93	0.51
16:D:264:ILE:HB	16:D:309:MET:HG2	1.92	0.51
23:K:20:ARG:HG2	23:K:21:LEU:H	1.76	0.51
21:i:47:ALA:HB3	21:i:212:GLU:HB2	1.92	0.51
21:i:106:PRO:HD2	21:i:109:GLN:HE21	1.76	0.51
25:m:34:SER:HA	25:m:167:LYS:HE3	1.93	0.51
1:U:163:PHE:HE2	1:U:201:LEU:HD11	1.76	0.50
6:Z:121:LEU:HD11	6:Z:138:TYR:HD2	1.76	0.50
7:a:43:ASP:HA	7:a:46:GLN:HG2	1.91	0.50
12:f:23:GLY:HA2	12:f:27:LYS:HD3	1.92	0.50
16:D:358:VAL:O	16:D:358:VAL:HG12	2.11	0.50
1:U:44:LYS:HD3	1:U:47:VAL:HG21	1.92	0.50
20:h:71:HIS:HA	20:h:218:PHE:H	1.76	0.50
22:j:31:THR:HA	22:j:162:GLY:HA3	1.92	0.50
1:U:77:SER:O	1:U:81:ALA:CB	2.60	0.50
1:U:415:HIS:CD2	1:U:418:GLU:H	2.30	0.50
2:V:325:LYS:HA	2:V:328:VAL:HG12	1.93	0.50
3:W:141:GLU:CB	3:W:172:GLU:HG3	2.42	0.50
3:W:180:LYS:CE	3:W:181:GLU:HG3	2.42	0.50
5:Y:234:PRO:O	5:Y:237:ARG:HG3	2.11	0.50
5:Y:334:LEU:N	5:Y:334:LEU:CD2	2.73	0.50
10:d:156:GLY:C	10:d:158:ILE:H	2.18	0.50
10:d:198:LEU:HB2	10:d:200:PHE:CE1	2.47	0.50
10:d:234:ASP:OD1	10:d:234:ASP:N	2.44	0.50
12:f:226:TYR:OH	14:B:63:LEU:O	2.29	0.50
12:f:680:ARG:CD	12:f:715:HIS:ND1	2.72	0.50
12:f:835:GLU:CA	12:f:840:LEU:CD2	2.77	0.50
12:f:838:ARG:CG	12:f:838:ARG:NH1	2.73	0.50
15:C:301:LEU:HD13	15:C:305:LEU:HD23	1.93	0.50
19:G:165:ALA:HB1	19:G:179:LEU:HD13	1.93	0.50
25:M:8:ASP:O	25:M:22:GLN:NE2	2.44	0.50
1:U:213:PHE:HE2	1:U:244:MET:HB2	1.76	0.50
1:U:428:PRO:HA	1:U:439:GLU:HB2	1.94	0.50
1:U:643:SER:O	15:C:57:ARG:NH1	2.42	0.50
3:W:32:ALA:HA	3:W:35:ALA:HB3	1.94	0.50
6:Z:68:TRP:HE1	6:Z:111:LEU:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:5:PRO:CA	7:a:8:LEU:CG	2.87	0.50
12:f:759:LEU:CG	12:f:806:VAL:HG11	2.41	0.50
13:A:312:ARG:HD3	13:A:312:ARG:H	1.76	0.50
16:D:357:GLU:H	16:D:357:GLU:CD	2.16	0.50
17:E:25:ARG:O	17:E:29:LEU:CB	2.60	0.50
19:g:41:ALA:HB3	19:g:166:THR:HB	1.94	0.50
2:V:330:LYS:NZ	2:V:389:ASP:OD2	2.43	0.50
2:V:454:GLU:N	10:d:187:GLU:OE2	2.44	0.50
9:c:33:ILE:HG23	9:c:69:VAL:HG13	1.93	0.50
16:D:353:ASN:OD1	16:D:353:ASN:N	2.43	0.50
18:F:398:ALA:HA	18:F:401:VAL:HG12	1.93	0.50
25:m:15:SER:OG	25:m:19:ARG:N	2.41	0.50
2:V:90:GLU:O	2:V:94:VAL:HG12	2.11	0.50
2:V:159:LEU:HG	2:V:182:LYS:HD3	1.93	0.50
2:V:166:TYR:HH	2:V:216:ARG:HD2	1.71	0.50
2:V:467:TYR:HD2	6:Z:251:LEU:HD12	1.74	0.50
7:a:189:PRO:C	7:a:191:SER:N	2.69	0.50
10:d:91:GLU:OE1	10:d:96:HIS:NE2	2.44	0.50
12:f:24:THR:HG23	12:f:31:LYS:HG3	1.94	0.50
12:f:371:ASN:HA	12:f:374:SER:HB2	1.94	0.50
12:f:723:TYR:O	12:f:727:PHE:CB	2.58	0.50
16:D:189:GLU:O	16:D:193:GLN:HB2	2.11	0.50
27:O:7:VAL:HG22	27:O:12:ILE:HG12	1.94	0.50
22:j:31:THR:OG1	22:j:163:ARG:O	2.30	0.50
1:U:17:PRO:O	1:U:55:ARG:NH1	2.37	0.50
1:U:475:HIS:HD2	1:U:511:ALA:HB2	1.77	0.50
2:V:466:ILE:HG13	2:V:471:GLU:OE2	2.11	0.50
2:V:471:GLU:O	2:V:474:LEU:N	2.43	0.50
3:W:48:LEU:HD12	3:W:52:LYS:HG2	1.92	0.50
4:X:402:GLU:HB2	9:c:249:LEU:HD11	1.94	0.50
10:d:101:LEU:HG	10:d:166:PHE:HE2	1.77	0.50
12:f:646:MET:SD	14:B:49:LEU:CD1	2.98	0.50
12:f:698:SER:HB3	13:A:80:LEU:HD13	1.93	0.50
13:A:324:PRO:HA	13:A:327:LEU:HD13	1.93	0.50
14:B:249:ARG:HG3	14:B:283:PHE:HD2	1.77	0.50
16:D:353:ASN:ND2	16:D:393:ILE:HA	2.25	0.50
16:D:362:ASP:O	16:D:366:ARG:HD2	2.12	0.50
21:I:100:GLN:HE21	29:Q:83:PHE:HE1	1.60	0.50
22:J:31:THR:OG1	22:J:163:ARG:O	2.30	0.50
23:K:97:GLN:HB3	30:R:61:ARG:HG3	1.94	0.50
19:g:155:ASP:OD1	19:g:159:TYR:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:11:SER:OG	22:j:15:HIS:N	2.43	0.50
24:l:157:ARG:HD2	24:l:176:MET:HE3	1.94	0.50
1:U:157:THR:HG23	1:U:159:ARG:H	1.77	0.50
1:U:607:VAL:HG13	16:D:64:GLU:OE2	2.11	0.50
5:Y:241:ILE:HG23	5:Y:242:LYS:HG2	1.92	0.50
15:C:90:HIS:CD2	15:C:90:HIS:N	2.80	0.50
20:H:100:VAL:HG13	28:P:93:ASN:HD22	1.77	0.50
25:M:35:THR:HA	25:M:166:GLY:HA3	1.93	0.50
25:M:174:THR:O	25:M:178:LYS:NZ	2.42	0.50
21:i:90:LEU:HA	21:i:93:ILE:HD12	1.94	0.50
1:U:229:VAL:O	1:U:233:LEU:CB	2.59	0.50
3:W:158:ASP:O	3:W:162:ALA:CB	2.60	0.50
3:W:287:VAL:O	3:W:291:SER:HB2	2.12	0.50
3:W:287:VAL:O	3:W:291:SER:CB	2.60	0.50
10:d:103:LEU:HD13	10:d:118:GLU:OE1	2.10	0.50
12:f:828:ARG:HH22	12:f:842:VAL:HG23	1.77	0.50
15:C:147:THR:HG22	15:C:150:MET:HE3	1.92	0.50
28:P:2:SER:N	28:P:5:SER:OG	2.45	0.50
23:k:20:ARG:HG2	23:k:21:LEU:H	1.76	0.50
25:m:35:THR:HA	25:m:166:GLY:HA3	1.93	0.50
25:m:134:SER:HB2	25:m:153:PRO:HD3	1.94	0.50
32:t:1:THR:N	32:t:105:PRO:O	2.43	0.50
1:U:171:ASN:HD21	1:U:176:MET:HE2	1.74	0.49
1:U:350:LEU:HA	1:U:385:PHE:HE1	1.77	0.49
1:U:643:SER:O	1:U:649:ARG:NH1	2.42	0.49
12:f:609:VAL:HG12	12:f:613:LEU:HD11	1.91	0.49
12:f:764:LEU:CD2	12:f:774:GLY:C	2.72	0.49
13:A:307:ASP:CG	13:A:336:ARG:HE	2.19	0.49
16:D:162:VAL:HG12	16:D:218:ALA:HA	1.94	0.49
25:M:34:SER:HA	25:M:167:LYS:HE3	1.93	0.49
27:O:24:MET:HE3	31:s:187:VAL:HG21	1.94	0.49
1:U:341:PHE:HZ	1:U:883:ARG:HB3	1.76	0.49
1:U:770:TRP:HA	9:c:180:ASN:HB3	1.93	0.49
2:V:212:TYR:OH	2:V:287:ARG:NH2	2.45	0.49
2:V:407:VAL:O	2:V:411:SER:OG	2.30	0.49
5:Y:335:SER:C	5:Y:337:PHE:H	2.19	0.49
6:Z:283:ARG:C	6:Z:285:ALA:N	2.69	0.49
12:f:302:GLY:HA2	12:f:317:LEU:HD11	1.94	0.49
12:f:332:ALA:HA	12:f:336:GLU:HB2	1.93	0.49
12:f:764:LEU:HD11	12:f:774:GLY:C	2.36	0.49
19:G:41:ALA:HB3	19:G:166:THR:HB	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:73:PHE:HA	22:j:131:ALA:HA	1.94	0.49
25:m:40:ARG:NH2	25:m:146:ALA:O	2.45	0.49
25:m:41:CYS:SG	25:m:189:ILE:CD1	2.97	0.49
32:t:43:MET:HE3	32:t:45:VAL:HG22	1.94	0.49
32:t:136:SER:HB2	32:t:150:LEU:HD13	1.93	0.49
2:V:330:LYS:O	2:V:360:TYR:OH	2.23	0.49
5:Y:95:LEU:HD11	5:Y:98:SER:HA	1.94	0.49
5:Y:215:ASP:O	5:Y:218:THR:OG1	2.30	0.49
8:b:124:LEU:HD13	8:b:156:PHE:HB2	1.93	0.49
12:f:593:THR:O	12:f:635:LYS:NZ	2.43	0.49
13:A:77:LEU:CD1	13:A:77:LEU:C	2.86	0.49
18:F:97:LEU:N	18:F:121:CYS:O	2.44	0.49
19:G:14:THR:OG1	19:G:128:ASN:O	2.30	0.49
19:G:138:MET:HB3	19:G:154:CYS:HB3	1.93	0.49
20:H:150:ASP:OD1	20:H:154:ALA:N	2.45	0.49
21:i:15:GLU:OE2	21:i:17:ARG:NE	2.45	0.49
25:m:8:ASP:O	25:m:22:GLN:NE2	2.44	0.49
1:U:132:GLY:O	1:U:136:LYS:CB	2.60	0.49
6:Z:142:GLU:HB2	6:Z:153:LYS:HE2	1.95	0.49
12:f:215:ASP:HA	12:f:218:GLU:HG3	1.93	0.49
13:A:73:ALA:HB3	13:A:78:TRP:HE1	1.77	0.49
17:E:118:LEU:CD1	17:E:118:LEU:C	2.86	0.49
24:L:48:ALA:HB1	24:L:62:LYS:HE3	1.94	0.49
32:T:171:ARG:NH2	27:o:140:ASP:OD2	2.45	0.49
26:n:127:ILE:HG12	26:n:132:SER:HB2	1.95	0.49
5:Y:23:ARG:NH1	5:Y:52:PRO:O	2.44	0.49
5:Y:336:ARG:O	5:Y:336:ARG:HG3	2.10	0.49
7:a:100:THR:HA	7:a:103:LYS:HG2	1.95	0.49
12:f:221:ILE:HA	12:f:224:ASN:HB2	1.93	0.49
12:f:283:THR:O	12:f:287:ASP:HB2	2.13	0.49
12:f:670:MET:CG	12:f:673:ARG:HH11	2.08	0.49
12:f:775:THR:O	12:f:779:CYS:HB2	2.12	0.49
15:C:337:ASN:ND2	15:C:376:VAL:O	2.46	0.49
16:D:162:VAL:CG1	16:D:218:ALA:HB2	2.42	0.49
17:E:33:LEU:O	17:E:37:THR:CB	2.60	0.49
18:F:272:PHE:O	18:F:276:LYS:HB2	2.13	0.49
25:M:134:SER:HB2	25:M:153:PRO:HD3	1.94	0.49
31:S:187:VAL:HG21	27:o:24:MET:HE3	1.94	0.49
21:i:153:SER:OG	21:i:155:ASN:OD1	2.31	0.49
3:W:57:ALA:HA	3:W:60:MET:HB3	1.94	0.49
4:X:379:ASP:HB3	4:X:384:VAL:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:101:ARG:O	5:Y:105:MET:HB3	2.12	0.49
9:c:28:ALA:HA	9:c:181:LEU:HD22	1.95	0.49
10:d:47:GLN:HG2	10:d:48:LEU:HG	1.94	0.49
21:I:90:LEU:HA	21:I:93:ILE:HD12	1.94	0.49
21:I:140:ASP:OD1	21:I:144:GLY:N	2.45	0.49
24:l:20:HIS:HA	24:l:23:GLU:HB2	1.94	0.49
27:o:7:VAL:HG22	27:o:12:ILE:HG12	1.93	0.49
27:o:100:LEU:HB3	27:o:111:TYR:HB2	1.95	0.49
27:o:113:ILE:HG12	27:o:119:THR:HG22	1.95	0.49
30:r:196:HIS:O	30:r:200:SER:HB3	2.13	0.49
1:U:477:GLY:O	1:U:481:LEU:CB	2.61	0.49
2:V:353:LEU:CA	2:V:357:LEU:HD22	2.41	0.49
3:W:312:MET:HG3	3:W:313:GLU:H	1.77	0.49
9:c:273:LYS:O	9:c:277:LYS:NZ	2.45	0.49
12:f:429:ILE:HG23	12:f:444:ALA:HB1	1.93	0.49
12:f:759:LEU:HG	12:f:806:VAL:HG12	1.94	0.49
13:A:312:ARG:HB2	13:A:315:ILE:HD12	1.95	0.49
15:C:344:LEU:HD23	15:C:347:ILE:HD12	1.94	0.49
21:I:106:PRO:HD2	21:I:109:GLN:HE21	1.76	0.49
22:J:116:GLN:O	22:J:119:THR:OG1	2.30	0.49
24:L:20:HIS:HA	24:L:23:GLU:HB2	1.94	0.49
24:L:216:GLY:HA3	24:L:219:LEU:HB3	1.95	0.49
3:W:118:LEU:HA	3:W:121:LYS:HZ3	1.78	0.49
5:Y:21:GLN:HG3	5:Y:286:TRP:CD2	2.48	0.49
7:a:187:ASP:O	7:a:188:LEU:HG	2.13	0.49
9:c:146:ASP:OD2	9:c:149:GLN:NE2	2.45	0.49
21:I:197:LEU:O	21:I:201:MET:CB	2.61	0.49
21:I:214:ALA:HA	21:I:227:VAL:HA	1.95	0.49
21:I:226:ARG:HD2	21:I:226:ARG:O	2.11	0.49
22:j:200:GLN:OE1	22:j:200:GLN:HA	2.12	0.49
1:U:261:LEU:HA	1:U:264:VAL:HG12	1.94	0.49
1:U:410:VAL:HG23	1:U:448:LEU:HD13	1.93	0.49
2:V:28:PRO:CB	2:V:29:PRO:HD3	2.43	0.49
3:W:6:SER:O	3:W:10:ASP:HB2	2.12	0.49
5:Y:168:ILE:CD1	5:Y:168:ILE:N	2.73	0.49
13:A:221:GLY:O	13:A:225:CYS:HB2	2.12	0.49
17:E:253:ILE:HG21	18:F:308:ARG:HH21	1.76	0.49
28:P:191:GLU:OE2	28:P:194:LYS:NZ	2.37	0.49
29:Q:27:GLN:NE2	29:q:169:LYS:O	2.42	0.49
19:g:14:THR:OG1	19:g:128:ASN:O	2.30	0.49
19:g:138:MET:HB3	19:g:154:CYS:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:150:ASP:OD1	20:h:154:ALA:N	2.45	0.49
1:U:112:CYS:HA	1:U:115:ASN:HB2	1.95	0.49
2:V:126:ALA:HB2	2:V:134:PHE:HE2	1.76	0.49
2:V:201:ARG:HH21	2:V:242:HIS:HB3	1.77	0.49
12:f:106:LEU:HB2	12:f:141:LYS:HD2	1.94	0.49
31:S:27:THR:HB	31:S:40:SER:H	1.78	0.49
1:U:198:LEU:HD23	1:U:223:LEU:HD13	1.95	0.48
3:W:141:GLU:HB3	3:W:172:GLU:HG3	1.95	0.48
5:Y:48:ASN:ND2	5:Y:110:TYR:OH	2.35	0.48
5:Y:168:ILE:HG22	5:Y:168:ILE:O	2.12	0.48
6:Z:246:VAL:HG12	6:Z:250:TYR:HD2	1.77	0.48
7:a:14:SER:H	7:a:19:PRO:HG3	1.77	0.48
9:c:211:GLU:HA	9:c:214:GLN:HB2	1.94	0.48
12:f:585:GLU:HG3	12:f:588:ARG:HE	1.77	0.48
13:A:372:LEU:HD23	13:A:375:ARG:HH21	1.78	0.48
16:D:401:LYS:O	16:D:405:THR:OG1	2.29	0.48
21:I:226:ARG:C	21:I:226:ARG:CD	2.85	0.48
22:J:119:THR:HG22	22:J:126:PRO:HB3	1.95	0.48
24:L:157:ARG:HD2	24:L:176:MET:HE3	1.94	0.48
19:g:93:ARG:HH21	19:g:121:ILE:HD13	1.78	0.48
19:g:202:LEU:HB2	19:g:206:LEU:HD13	1.95	0.48
24:l:48:ALA:HB1	24:l:62:LYS:HE3	1.94	0.48
2:V:470:ARG:C	2:V:470:ARG:CD	2.85	0.48
4:X:161:ASP:HB2	20:H:177:ARG:HA	1.95	0.48
4:X:177:TYR:O	4:X:182:ASN:N	2.42	0.48
4:X:221:GLU:O	4:X:223:LYS:NZ	2.37	0.48
5:Y:190:ALA:HA	5:Y:287:LEU:HD21	1.95	0.48
6:Z:279:LYS:HA	6:Z:279:LYS:HD3	1.71	0.48
9:c:254:ASN:OD1	9:c:278:GLN:NE2	2.46	0.48
12:f:708:ASP:OD1	12:f:785:ARG:HG2	2.13	0.48
13:A:113:ILE:HG22	13:A:121:PHE:H	1.78	0.48
13:A:309:PHE:CZ	18:F:248:PHE:CZ	3.01	0.48
14:B:183:THR:OG1	14:B:184:TYR:N	2.46	0.48
15:C:187:LEU:HB3	15:C:314:LYS:HG2	1.95	0.48
16:D:95:ALA:HA	16:D:101:ALA:HA	1.94	0.48
16:D:242:GLU:O	16:D:246:MET:CB	2.60	0.48
18:F:97:LEU:HB2	18:F:121:CYS:HB2	1.95	0.48
19:G:93:ARG:HH21	19:G:121:ILE:HD13	1.78	0.48
27:O:113:ILE:HG12	27:O:119:THR:HG22	1.95	0.48
29:Q:38:MET:HE1	29:Q:44:LEU:HB2	1.96	0.48
21:i:140:ASP:OD1	21:i:144:GLY:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:60:GLU:OE1	23:k:63:SER:N	2.46	0.48
7:a:239:ALA:HA	7:a:242:SER:HB3	1.95	0.48
12:f:414:LEU:HD23	12:f:417:ILE:HD12	1.96	0.48
12:f:482:ILE:HD11	12:f:517:VAL:HG23	1.95	0.48
12:f:646:MET:HB2	14:B:67:ARG:HD3	1.95	0.48
12:f:673:ARG:NH2	12:f:786:GLN:HA	2.29	0.48
16:D:345:PHE:O	16:D:349:THR:OG1	2.28	0.48
19:G:202:LEU:HB2	19:G:206:LEU:HD13	1.95	0.48
3:W:245:LYS:O	3:W:249:ALA:CB	2.62	0.48
8:b:14:GLU:O	8:b:17:ARG:NE	2.39	0.48
18:F:375:VAL:HG22	18:F:415:LEU:HD12	1.96	0.48
27:O:100:LEU:HB3	27:O:111:TYR:HB2	1.95	0.48
29:q:38:MET:HE1	29:q:44:LEU:HB2	1.96	0.48
2:V:107:ARG:NH2	2:V:141:THR:CG2	2.77	0.48
2:V:264:TYR:CZ	2:V:267:ALA:HB3	2.48	0.48
3:W:31:CYS:O	3:W:35:ALA:CB	2.62	0.48
3:W:111:TYR:HB3	3:W:115:ILE:HG22	1.94	0.48
5:Y:279:GLU:HB2	5:Y:296:VAL:HG21	1.94	0.48
6:Z:238:PRO:HG2	9:c:309:PHE:HB3	1.94	0.48
7:a:264:ASN:HB3	7:a:267:GLN:HE21	1.79	0.48
14:B:133:VAL:HG11	14:B:157:HIS:HB2	1.95	0.48
21:I:15:GLU:OE2	21:I:17:ARG:NE	2.45	0.48
22:J:73:PHE:HA	22:J:131:ALA:HA	1.94	0.48
30:R:196:HIS:O	30:R:200:SER:HB3	2.13	0.48
32:T:43:MET:HE3	32:T:45:VAL:HG22	1.94	0.48
2:V:145:LEU:HA	2:V:151:THR:HG21	1.96	0.48
3:W:104:MET:HB3	3:W:123:ARG:HH22	1.78	0.48
3:W:150:ALA:HA	3:W:153:LYS:HB2	1.95	0.48
5:Y:36:ALA:O	5:Y:40:GLU:CB	2.62	0.48
8:b:119:ASP:HB3	8:b:152:LYS:HE3	1.95	0.48
12:f:686:LEU:HA	12:f:689:ALA:HB3	1.96	0.48
15:C:329:LEU:O	15:C:333:SER:HB3	2.13	0.48
18:F:387:CYS:HB3	24:L:166:GLN:HG2	1.95	0.48
23:K:210:LEU:HD11	23:K:215:ILE:HG12	1.96	0.48
21:i:197:LEU:O	21:i:201:MET:CB	2.61	0.48
27:o:38:SER:OG	27:o:40:ASN:OD1	2.27	0.48
1:U:469:SER:OG	1:U:470:ASN:N	2.47	0.48
2:V:165:ALA:C	2:V:167:LEU:H	2.22	0.48
2:V:190:ASP:OD1	2:V:234:ARG:NH1	2.40	0.48
2:V:224:LEU:HD22	2:V:227:VAL:HB	1.96	0.48
3:W:97:LEU:CD2	3:W:138:VAL:CG2	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:227:TYR:O	3:W:246:HIS:NE2	2.35	0.48
6:Z:66:SER:OG	6:Z:103:LYS:NZ	2.47	0.48
9:c:192:LEU:HD12	9:c:196:LEU:CG	2.39	0.48
10:d:118:GLU:O	10:d:118:GLU:HG2	2.12	0.48
13:A:59:ILE:HG21	14:B:76:GLU:HG3	1.96	0.48
15:C:329:LEU:O	15:C:333:SER:OG	2.29	0.48
21:I:153:SER:OG	21:I:155:ASN:OD1	2.31	0.48
31:S:11:THR:HA	31:S:139:GLY:HA3	1.96	0.48
28:p:2:SER:N	28:p:5:SER:OG	2.45	0.48
31:s:27:THR:HB	31:s:40:SER:H	1.78	0.48
2:V:179:LYS:HA	2:V:182:LYS:HE3	1.96	0.48
2:V:211:TYR:O	2:V:215:ALA:CB	2.62	0.48
2:V:224:LEU:HG	2:V:257:ASN:ND2	2.29	0.48
2:V:314:ARG:NH2	5:Y:381:GLN:HE21	2.12	0.48
2:V:358:MET:O	2:V:362:LEU:HB2	2.14	0.48
3:W:135:LYS:O	3:W:138:VAL:HG23	2.13	0.48
3:W:245:LYS:O	3:W:249:ALA:HB2	2.14	0.48
5:Y:165:LYS:HA	5:Y:168:ILE:CD1	2.25	0.48
6:Z:153:LYS:HE3	6:Z:153:LYS:HB2	1.57	0.48
10:d:72:GLU:O	10:d:76:ALA:CB	2.62	0.48
12:f:811:LEU:HD21	12:f:862:ILE:HD13	1.95	0.48
23:K:60:GLU:OE1	23:K:63:SER:N	2.46	0.48
1:U:601:ARG:HB2	1:U:601:ARG:CZ	2.43	0.48
2:V:204:ASP:O	2:V:208:ALA:CB	2.62	0.48
6:Z:17:LEU:HD22	9:c:36:LEU:HB3	1.95	0.48
7:a:57:ILE:HG13	7:a:61:GLU:HG2	1.96	0.48
7:a:189:PRO:C	7:a:191:SER:H	2.22	0.48
8:b:16:MET:HA	8:b:25:ARG:HH11	1.79	0.48
8:b:150:THR:CG2	8:b:172:THR:HG22	2.44	0.48
15:C:71:SER:HB3	16:D:112:TYR:HB3	1.96	0.48
18:F:413:THR:OG1	18:F:414:GLU:OE1	2.32	0.48
27:O:6:VAL:HG23	27:O:124:TYR:HB3	1.96	0.48
31:S:1:ARG:HH21	32:T:2:GLN:HE22	1.61	0.48
2:V:107:ARG:NH2	2:V:141:THR:HG22	2.29	0.48
3:W:90:LEU:CD2	3:W:93:ARG:CZ	2.92	0.48
3:W:373:ILE:HA	7:a:326:GLU:HB3	1.95	0.48
6:Z:69:PHE:HE2	8:b:95:LEU:HB3	1.78	0.48
6:Z:244:GLU:O	6:Z:247:LYS:N	2.47	0.48
12:f:294:MET:HB2	12:f:320:ILE:HG22	1.96	0.48
13:A:125:LEU:HD23	13:A:129:VAL:HG23	1.96	0.48
25:M:181:MET:N	25:M:181:MET:SD	2.83	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:127:ILE:HG12	26:N:132:SER:HB2	1.95	0.48
32:T:37:ARG:HH21	26:n:166:ARG:HH22	1.62	0.48
22:j:47:LYS:HA	22:j:200:GLN:HG3	1.95	0.48
23:k:99:HIS:HB2	23:k:107:MET:HE3	1.96	0.48
24:l:189:LYS:HZ2	24:l:193:ARG:HH12	1.60	0.48
29:q:19:ARG:HB3	29:q:31:ASP:HA	1.96	0.48
32:t:96:MET:HE1	32:t:106:LEU:HD12	1.96	0.48
1:U:21:GLU:HA	1:U:24:LEU:HG	1.94	0.47
1:U:780:SER:HA	1:U:783:TYR:HD2	1.78	0.47
8:b:161:ASN:HB3	8:b:168:SER:HB2	1.96	0.47
9:c:64:ASP:OD1	9:c:139:ARG:NH2	2.47	0.47
12:f:64:GLY:HA2	12:f:67:ASP:HB3	1.96	0.47
12:f:476:THR:C	12:f:478:ARG:N	2.70	0.47
12:f:497:VAL:HA	12:f:500:LEU:HB2	1.95	0.47
12:f:680:ARG:HG2	12:f:717:ALA:H	1.79	0.47
20:H:34:PRO:HA	20:H:164:GLY:HA3	1.96	0.47
23:k:210:LEU:HD11	23:k:215:ILE:HG12	1.96	0.47
1:U:204:ILE:HD12	1:U:207:ASN:HB2	1.96	0.47
2:V:203:LEU:O	2:V:207:ALA:HB2	2.14	0.47
6:Z:56:VAL:HG11	6:Z:70:LEU:HD22	1.96	0.47
6:Z:58:PHE:HE1	6:Z:68:TRP:HB2	1.79	0.47
12:f:873:LEU:CD1	12:f:876:HIS:O	2.62	0.47
13:A:113:ILE:HD11	13:A:142:VAL:HG21	1.94	0.47
13:A:189:GLU:O	13:A:193:THR:OG1	2.33	0.47
25:M:51:LYS:HB3	25:M:210:GLU:HB3	1.96	0.47
28:P:36:THR:OG1	28:P:38:ASP:OD1	2.31	0.47
20:h:34:PRO:HA	20:h:164:GLY:HA3	1.96	0.47
2:V:353:LEU:C	2:V:357:LEU:HD22	2.39	0.47
3:W:69:ALA:O	3:W:71:VAL:N	2.47	0.47
6:Z:282:ASN:O	6:Z:286:GLU:HG2	2.14	0.47
10:d:206:MET:O	10:d:210:ALA:CB	2.62	0.47
13:A:78:TRP:O	13:A:80:LEU:N	2.48	0.47
18:F:97:LEU:O	18:F:120:LYS:N	2.47	0.47
22:j:119:THR:HG22	22:j:126:PRO:HB3	1.95	0.47
24:l:160:SER:O	24:l:169:ARG:NH2	2.48	0.47
31:s:125:ASP:OD1	31:s:129:SER:N	2.47	0.47
2:V:167:LEU:O	2:V:169:LEU:N	2.47	0.47
2:V:219:GLU:OE2	2:V:257:ASN:ND2	2.48	0.47
2:V:257:ASN:O	2:V:261:TYR:HD1	1.97	0.47
2:V:326:GLN:HE21	2:V:352:SER:CB	2.25	0.47
5:Y:12:PRO:HD3	5:Y:110:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:83:ARG:HD3	12:f:113:MET:HG2	1.96	0.47
13:A:84:LYS:O	13:A:88:GLN:CB	2.62	0.47
15:C:99:VAL:HA	15:C:123:LEU:HB3	1.97	0.47
16:D:50:GLU:O	16:D:54:LEU:CB	2.60	0.47
17:E:46:ASP:HA	17:E:49:ALA:HB3	1.97	0.47
24:L:121:GLN:HG3	25:M:129:ARG:HG2	1.96	0.47
30:R:44:THR:HG21	30:R:100:MET:HE3	1.97	0.47
24:l:216:GLY:HA3	24:l:219:LEU:HB3	1.95	0.47
3:W:239:SER:HB3	3:W:242:SER:HB3	1.97	0.47
12:f:676:GLY:O	12:f:782:HIS:NE2	2.48	0.47
16:D:357:GLU:N	16:D:357:GLU:CD	2.73	0.47
17:E:235:ILE:O	17:E:239:GLY:N	2.40	0.47
23:K:84:ASP:OD1	23:K:84:ASP:N	2.48	0.47
31:S:125:ASP:OD1	31:S:129:SER:N	2.47	0.47
21:i:229:LYS:N	21:i:232:GLU:OE2	2.47	0.47
24:l:117:GLN:O	24:l:120:THR:OG1	2.27	0.47
25:m:51:LYS:HB3	25:m:210:GLU:HB3	1.96	0.47
1:U:515:ALA:HA	1:U:518:LEU:HB2	1.96	0.47
2:V:224:LEU:HG	2:V:257:ASN:HD22	1.79	0.47
3:W:135:LYS:C	3:W:137:TYR:H	2.21	0.47
7:a:172:TYR:O	7:a:176:ALA:CB	2.62	0.47
8:b:21:PHE:HD2	8:b:25:ARG:HG2	1.78	0.47
12:f:78:LEU:HA	12:f:82:ILE:HD11	1.96	0.47
12:f:213:GLN:O	12:f:217:LEU:CB	2.62	0.47
14:B:135:ILE:HA	14:B:159:VAL:HB	1.96	0.47
16:D:146:GLU:O	16:D:252:ARG:NH2	2.38	0.47
16:D:170:MET:HG2	16:D:173:GLN:HB2	1.96	0.47
28:P:58:THR:OG1	29:Q:121:LEU:O	2.24	0.47
20:h:14:SER:OG	20:h:18:LYS:N	2.46	0.47
25:m:181:MET:SD	25:m:181:MET:N	2.83	0.47
2:V:228:ARG:NH1	2:V:254:LEU:O	2.46	0.47
3:W:152:ILE:HD11	3:W:165:ILE:HB	1.96	0.47
3:W:396:LEU:HD13	3:W:402:ILE:HD13	1.96	0.47
5:Y:89:GLU:O	5:Y:93:LYS:HB2	2.15	0.47
7:a:277:LEU:HD21	7:a:296:ILE:HG23	1.96	0.47
9:c:269:GLN:O	9:c:273:LYS:CB	2.63	0.47
10:d:212:LYS:HD2	10:d:213:ARG:HG2	1.97	0.47
13:A:236:CYS:SG	13:A:267:LYS:HG2	2.55	0.47
14:B:84:GLN:HG3	14:B:85:MET:HG3	1.95	0.47
17:E:322:LYS:HA	17:E:362:VAL:H	1.80	0.47
18:F:312:GLU:O	18:F:316:GLN:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:185:GLU:HA	20:H:188:ILE:HD12	1.97	0.47
22:J:56:GLU:O	22:J:59:VAL:HG12	2.14	0.47
22:J:81:ARG:HA	22:J:84:ILE:HD12	1.97	0.47
23:K:99:HIS:HB2	23:K:107:MET:HE3	1.96	0.47
24:L:160:SER:O	24:L:169:ARG:NH2	2.48	0.47
24:L:186:GLU:HA	24:L:189:LYS:HG2	1.97	0.47
30:R:12:VAL:HB	30:R:179:VAL:HB	1.97	0.47
32:T:96:MET:HE1	32:T:106:LEU:HD12	1.96	0.47
31:s:11:THR:HA	31:s:139:GLY:HA3	1.96	0.47
2:V:31:ALA:CB	2:V:32:PRO:HD3	2.36	0.47
2:V:280:ALA:HB3	2:V:285:TRP:HB2	1.96	0.47
3:W:142:ARG:NH1	3:W:145:LEU:HD13	2.29	0.47
5:Y:40:GLU:O	5:Y:44:ALA:CB	2.63	0.47
5:Y:197:ALA:HB3	5:Y:226:VAL:HG21	1.95	0.47
5:Y:204:THR:O	5:Y:216:TYR:OH	2.32	0.47
15:C:130:LYS:HD2	15:C:130:LYS:HA	1.44	0.47
19:G:47:CYS:HB3	19:G:221:THR:HG23	1.97	0.47
21:I:109:GLN:OE1	29:Q:71:ASN:ND2	2.48	0.47
25:M:73:VAL:HA	25:M:139:SER:HB2	1.97	0.47
1:U:583:MET:HA	1:U:583:MET:CE	2.39	0.47
2:V:31:ALA:HB1	2:V:32:PRO:CD	2.35	0.47
2:V:443:ARG:NH1	10:d:180:GLY:O	2.48	0.47
3:W:34:LEU:HA	3:W:39:ARG:HB2	1.97	0.47
3:W:80:TRP:HB2	3:W:130:MET:HE2	1.97	0.47
3:W:158:ASP:O	3:W:162:ALA:HB3	2.15	0.47
3:W:349:LYS:O	3:W:353:ASP:HB2	2.15	0.47
6:Z:14:LEU:HG	9:c:39:LEU:HB3	1.97	0.47
7:a:32:LYS:O	8:b:18:ASN:ND2	2.47	0.47
12:f:411:ALA:HB1	12:f:444:ALA:HB2	1.96	0.47
13:A:312:ARG:HB2	13:A:315:ILE:HB	1.96	0.47
16:D:354:LEU:HD11	16:D:399:PHE:CE2	2.47	0.47
17:E:113:ARG:HH22	17:E:220:ASN:CG	2.22	0.47
29:Q:19:ARG:HH11	29:Q:179:SER:HB3	1.79	0.47
20:h:100:VAL:HG13	28:p:93:ASN:HD22	1.80	0.47
26:n:138:TYR:O	26:n:142:THR:OG1	2.30	0.47
29:q:141:SER:O	29:q:145:ARG:CB	2.63	0.47
1:U:762:GLY:O	1:U:766:PHE:HB2	2.15	0.47
2:V:28:PRO:HD2	2:V:29:PRO:CD	2.45	0.47
2:V:186:LYS:NZ	2:V:211:TYR:OH	2.33	0.47
9:c:269:GLN:O	9:c:273:LYS:HB2	2.15	0.47
10:d:200:PHE:N	10:d:200:PHE:HD1	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:670:MET:HA	12:f:673:ARG:HH12	1.80	0.47
18:F:410:ARG:NH2	18:F:419:ASP:OD2	2.48	0.47
19:G:60:LEU:O	25:M:161:TRP:N	2.47	0.47
24:L:189:LYS:HZ2	24:L:193:ARG:HH12	1.63	0.47
21:i:17:ARG:HE	21:i:19:TYR:HE1	1.64	0.47
27:o:112:SER:HB3	27:o:125:VAL:HG11	1.97	0.47
4:X:291:ALA:O	4:X:295:LYS:HB2	2.15	0.46
5:Y:335:SER:C	5:Y:337:PHE:N	2.73	0.46
6:Z:246:VAL:HG12	6:Z:250:TYR:CE2	2.51	0.46
6:Z:283:ARG:O	6:Z:285:ALA:N	2.49	0.46
15:C:88:LYS:O	15:C:88:LYS:HD3	2.14	0.46
18:F:81:LYS:HG2	18:F:84:LYS:HE2	1.97	0.46
19:G:38:THR:HA	19:G:169:GLY:HA3	1.97	0.46
20:H:139:TRP:HA	20:H:144:PRO:HA	1.97	0.46
21:I:228:LEU:H	21:I:228:LEU:HG	1.45	0.46
22:J:56:GLU:N	22:J:56:GLU:CD	2.73	0.46
22:J:115:LYS:HD3	22:J:149:PRO:HA	1.97	0.46
29:Q:19:ARG:HB3	29:Q:31:ASP:HA	1.96	0.46
30:R:115:ASP:HB2	30:R:119:ASN:HB2	1.97	0.46
22:j:68:ASN:HA	22:j:211:MET:HE1	1.97	0.46
30:r:12:VAL:HB	30:r:179:VAL:HB	1.97	0.46
1:U:146:LYS:HE2	1:U:148:LYS:HB2	1.96	0.46
2:V:25:GLU:C	2:V:28:PRO:HD2	2.40	0.46
2:V:147:PHE:O	2:V:150:ARG:N	2.48	0.46
2:V:252:ASN:ND2	2:V:284:GLU:OE2	2.48	0.46
2:V:276:PHE:HD2	2:V:278:GLU:HG2	1.80	0.46
2:V:496:PHE:H	2:V:497:PRO:HD2	1.76	0.46
3:W:145:LEU:HA	3:W:148:THR:HG22	1.96	0.46
3:W:273:TYR:HA	3:W:276:LEU:HB2	1.97	0.46
7:a:153:SER:O	7:a:157:ASP:CB	2.63	0.46
9:c:149:GLN:HB3	16:D:81:ARG:HH11	1.80	0.46
9:c:280:PRO:O	9:c:284:LEU:CB	2.61	0.46
12:f:692:LEU:CB	13:A:77:LEU:HD22	2.41	0.46
17:E:219:PHE:HD2	17:E:263:GLN:HG3	1.80	0.46
18:F:82:VAL:O	18:F:85:THR:OG1	2.33	0.46
20:H:14:SER:OG	20:H:18:LYS:N	2.46	0.46
27:O:112:SER:HB3	27:O:125:VAL:HG11	1.97	0.46
24:l:186:GLU:HA	24:l:189:LYS:HG2	1.97	0.46
1:U:147:TYR:HA	1:U:150:ALA:HB3	1.95	0.46
2:V:342:ILE:HD12	2:V:343:PRO:HD2	1.98	0.46
3:W:215:GLN:HE21	3:W:223:LYS:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:57:LEU:HA	5:Y:60:SER:HB3	1.97	0.46
7:a:34:TRP:HZ3	7:a:64:ILE:HG23	1.80	0.46
12:f:788:MET:HB3	12:f:789:SER:H	1.50	0.46
18:F:122:ALA:HB3	18:F:134:LEU:HD11	1.97	0.46
22:j:81:ARG:HA	22:j:84:ILE:HD12	1.97	0.46
25:m:170:GLN:HA	25:m:173:LYS:HG2	1.97	0.46
27:o:6:VAL:HG23	27:o:124:TYR:HB3	1.96	0.46
29:q:4:LEU:HD22	29:q:45:LEU:HB3	1.97	0.46
29:q:19:ARG:HH11	29:q:179:SER:HB3	1.79	0.46
4:X:67:GLY:O	4:X:71:LYS:NZ	2.48	0.46
6:Z:22:HIS:HA	6:Z:25:ARG:HG2	1.97	0.46
7:a:19:PRO:HA	7:a:22:TRP:CD1	2.48	0.46
8:b:89:GLY:HA2	8:b:92:VAL:HG12	1.97	0.46
12:f:143:ARG:O	12:f:147:SER:OG	2.26	0.46
12:f:291:GLN:HB3	12:f:879:ARG:HH21	1.80	0.46
15:C:325:ARG:HD3	15:C:353:GLY:HA2	1.98	0.46
16:D:72:PHE:O	16:D:76:GLN:HB2	2.16	0.46
22:J:53:LEU:HD12	22:J:53:LEU:C	2.41	0.46
26:N:28:ASN:ND2	26:N:30:VAL:O	2.48	0.46
27:O:160:ALA:HA	27:O:163:ILE:HD12	1.97	0.46
24:l:98:VAL:O	32:t:90:SER:OG	2.31	0.46
1:U:167:ILE:CG2	1:U:177:LEU:HD21	2.20	0.46
2:V:470:ARG:CG	2:V:470:ARG:NH2	2.73	0.46
3:W:366:MET:O	3:W:370:TYR:HB2	2.15	0.46
5:Y:57:LEU:HD11	5:Y:63:TRP:HB2	1.98	0.46
5:Y:326:GLY:HA3	11:e:66:LYS:HD2	1.97	0.46
9:c:124:GLY:O	9:c:128:ASN:ND2	2.48	0.46
12:f:291:GLN:HE21	12:f:879:ARG:NH2	2.12	0.46
13:A:84:LYS:O	13:A:88:GLN:HB2	2.16	0.46
13:A:312:ARG:NH1	13:A:312:ARG:CG	2.73	0.46
28:P:124:LEU:HD23	28:P:128:GLY:HA2	1.97	0.46
32:T:89:HIS:NE2	32:T:124:TYR:O	2.47	0.46
25:m:42:LYS:HD2	25:m:183:GLU:HA	1.96	0.46
25:m:73:VAL:HA	25:m:139:SER:HB2	1.97	0.46
25:m:136:MET:HE3	25:m:163:CYS:HB3	1.98	0.46
1:U:401:LYS:HB3	1:U:438:GLN:HB2	1.97	0.46
2:V:470:ARG:HB2	6:Z:250:TYR:CE1	2.48	0.46
3:W:80:TRP:CG	3:W:130:MET:HE2	2.50	0.46
3:W:318:SER:HA	3:W:321:VAL:HG12	1.98	0.46
5:Y:17:LEU:HD22	5:Y:212:GLU:HB2	1.97	0.46
7:a:156:TYR:O	7:a:159:SER:OG	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:121:ARG:HB2	10:d:122:LEU:HD23	1.96	0.46
12:f:773:LYS:HD3	12:f:773:LYS:HA	1.66	0.46
14:B:99:VAL:HG12	14:B:103:ARG:HD3	1.97	0.46
16:D:200:ARG:HH22	16:D:301:GLN:H	1.63	0.46
16:D:338:ARG:NH1	16:D:365:ALA:CA	2.66	0.46
25:M:136:MET:HE3	25:M:163:CYS:HB3	1.98	0.46
29:Q:141:SER:O	29:Q:145:ARG:CB	2.63	0.46
20:h:222:THR:OG1	20:h:225:GLU:OE1	2.31	0.46
27:o:160:ALA:HA	27:o:163:ILE:HD12	1.97	0.46
28:p:124:LEU:HD23	28:p:128:GLY:HA2	1.97	0.46
2:V:201:ARG:HE	2:V:242:HIS:HB3	1.80	0.46
2:V:264:TYR:O	2:V:264:TYR:CG	2.69	0.46
2:V:353:LEU:C	2:V:357:LEU:HD21	2.41	0.46
8:b:121:GLU:HA	8:b:124:LEU:HG	1.98	0.46
14:B:103:ARG:HG2	14:B:103:ARG:H	1.49	0.46
16:D:269:ALA:O	17:E:255:ARG:NE	2.43	0.46
17:E:98:VAL:HG12	17:E:110:TYR:HA	1.97	0.46
17:E:244:SER:HB2	18:F:300:LYS:HG3	1.97	0.46
26:N:136:TYR:HE2	32:T:33:LEU:HD21	1.81	0.46
19:g:38:THR:HA	19:g:169:GLY:HA3	1.97	0.46
19:g:49:VAL:HG22	19:g:219:VAL:HG23	1.98	0.46
20:h:185:GLU:HA	20:h:188:ILE:HD12	1.97	0.46
22:j:115:LYS:HD3	22:j:149:PRO:HA	1.97	0.46
2:V:171:VAL:HG11	2:V:175:MET:HE3	1.87	0.46
2:V:326:GLN:HG2	2:V:352:SER:HB2	1.98	0.46
4:X:400:ALA:O	4:X:403:THR:OG1	2.32	0.46
5:Y:79:ASP:HA	5:Y:82:LYS:HE2	1.98	0.46
8:b:154:THR:O	8:b:158:ASN:HB2	2.15	0.46
19:G:49:VAL:HG22	19:G:219:VAL:HG23	1.98	0.46
28:P:2:SER:OG	28:P:3:ILE:N	2.39	0.46
22:j:116:GLN:O	22:j:119:THR:OG1	2.30	0.46
26:n:28:ASN:ND2	26:n:30:VAL:O	2.48	0.46
1:U:179:TYR:HE2	1:U:183:LEU:CG	2.24	0.46
2:V:497:PRO:CB	2:V:498:PRO:CD	2.87	0.46
6:Z:136:GLU:OE2	6:Z:157:HIS:ND1	2.48	0.46
12:f:72:ARG:HH21	12:f:112:ASN:HB3	1.80	0.46
12:f:823:ALA:HB1	12:f:825:MET:HG3	1.98	0.46
21:I:216:LEU:CG	21:I:225:ILE:CG1	2.94	0.46
25:M:41:CYS:HG	25:M:189:ILE:HD12	1.81	0.46
20:h:45:VAL:HG22	20:h:212:ILE:HG22	1.98	0.46
2:V:168:GLN:OE1	2:V:168:GLN:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:186:ILE:HD13	3:W:209:ILE:HD11	1.98	0.46
4:X:194:ARG:HD2	4:X:210:LEU:HD21	1.98	0.46
4:X:297:ARG:HH21	4:X:333:GLN:HE21	1.64	0.46
7:a:7:PHE:HE2	7:a:63:PHE:CD2	2.34	0.46
12:f:408:LEU:O	12:f:412:ALA:CB	2.64	0.46
12:f:664:GLU:HG3	14:B:86:LYS:HE3	1.98	0.46
13:A:224:LEU:HG	34:A:501:ATP:H2'	1.97	0.46
15:C:92:GLU:OE1	15:C:92:GLU:N	2.49	0.46
16:D:175:GLN:NE2	16:D:179:GLU:OE2	2.45	0.46
23:K:195:ILE:O	23:K:198:SER:OG	2.31	0.46
23:k:195:ILE:O	23:k:198:SER:OG	2.31	0.46
31:s:43:CYS:SG	31:s:194:ARG:HG3	2.56	0.46
1:U:601:ARG:CG	1:U:601:ARG:NH1	2.73	0.45
2:V:361:PHE:HA	2:V:364:THR:HG22	1.98	0.45
3:W:328:LEU:HB3	3:W:337:ALA:HB1	1.98	0.45
6:Z:253:THR:O	6:Z:256:GLN:N	2.49	0.45
7:a:33:LEU:HD13	7:a:36:GLN:HB2	1.98	0.45
7:a:201:GLY:O	7:a:205:LEU:CB	2.64	0.45
20:H:222:THR:OG1	20:H:225:GLU:OE1	2.31	0.45
25:M:228:PRO:HD2	25:M:231:ILE:HD12	1.97	0.45
31:S:38:ARG:NH2	27:o:164:PHE:O	2.49	0.45
32:T:1:THR:N	32:T:105:PRO:O	2.43	0.45
1:U:28:ASN:HB3	1:U:59:PHE:HZ	1.82	0.45
1:U:69:TYR:CZ	1:U:99:THR:HB	2.51	0.45
3:W:52:LYS:HE3	3:W:82:LEU:HD21	1.97	0.45
3:W:124:LEU:HA	3:W:127:THR:HG22	1.97	0.45
6:Z:25:ARG:HB2	9:c:104:ARG:HG2	1.99	0.45
7:a:156:TYR:HB3	7:a:179:PHE:HB2	1.98	0.45
7:a:170:ALA:HA	7:a:173:TYR:HB3	1.98	0.45
8:b:97:LEU:HA	8:b:100:ARG:HG3	1.98	0.45
12:f:82:ILE:O	12:f:86:THR:CB	2.64	0.45
12:f:163:ALA:HB1	12:f:185:LEU:HD11	1.97	0.45
12:f:771:LEU:CD2	12:f:773:LYS:NZ	2.80	0.45
14:B:66:GLU:HA	14:B:69:LYS:HB3	1.97	0.45
15:C:90:HIS:H	15:C:90:HIS:HD2	1.61	0.45
15:C:387:VAL:O	15:C:391:MET:HB2	2.17	0.45
21:I:17:ARG:HE	21:I:19:TYR:HE1	1.63	0.45
26:N:19:ARG:NH1	26:N:170:SER:O	2.50	0.45
28:P:107:PRO:HG2	28:P:124:LEU:HB2	1.98	0.45
20:h:139:TRP:HA	20:h:144:PRO:HA	1.97	0.45
21:i:119:GLN:NE2	22:j:79:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:72:ALA:O	23:k:226:PHE:N	2.46	0.45
28:p:36:THR:OG1	28:p:38:ASP:OD1	2.31	0.45
2:V:479:ARG:HH12	5:Y:370:ILE:HD11	1.81	0.45
3:W:136:ILE:HG22	3:W:140:ILE:HB	1.98	0.45
4:X:410:VAL:O	4:X:413:SER:OG	2.30	0.45
8:b:21:PHE:HE2	8:b:144:GLY:HA2	1.82	0.45
10:d:61:TRP:CZ3	10:d:65:ARG:HD2	2.52	0.45
12:f:243:PRO:HA	12:f:247:ALA:HB3	1.97	0.45
12:f:631:LYS:HD3	12:f:634:LYS:HB3	1.97	0.45
13:A:146:LYS:HD2	13:A:148:GLN:HG2	1.97	0.45
16:D:191:TYR:O	16:D:195:GLY:HA2	2.16	0.45
23:K:146:VAL:HG11	23:K:222:PRO:HA	1.98	0.45
24:L:157:ARG:NH2	25:M:56:LYS:O	2.49	0.45
31:S:33:PHE:HA	27:o:167:LEU:HD12	1.97	0.45
22:j:200:GLN:HB3	22:j:201:SER:H	1.65	0.45
26:n:19:ARG:NH1	26:n:170:SER:O	2.49	0.45
31:s:92:LEU:HD23	31:s:124:PHE:HE2	1.82	0.45
1:U:48:LEU:HD13	1:U:56:SER:HB3	1.99	0.45
1:U:338:HIS:CE1	1:U:785:PRO:HB3	2.51	0.45
1:U:729:GLY:O	1:U:733:ALA:HB2	2.16	0.45
2:V:265:ASP:HB2	2:V:269:LYS:HZ2	1.82	0.45
2:V:495:ARG:HG2	15:C:48:GLN:NE2	2.32	0.45
4:X:208:ALA:HB2	4:X:238:GLY:HA3	1.98	0.45
5:Y:243:GLY:O	5:Y:247:LEU:HB2	2.16	0.45
6:Z:116:CYS:O	6:Z:119:SER:OG	2.29	0.45
12:f:122:ALA:CB	12:f:129:LEU:CD1	2.70	0.45
12:f:606:VAL:HA	12:f:609:VAL:HG23	1.98	0.45
13:A:284:ARG:HH22	18:F:333:ASN:HD21	1.64	0.45
17:E:210:GLU:OE1	17:E:213:ARG:NE	2.35	0.45
17:E:345:ASN:O	17:E:349:GLU:HB2	2.16	0.45
18:F:305:GLU:HA	18:F:308:ARG:HH11	1.81	0.45
18:F:305:GLU:OE1	18:F:308:ARG:NH1	2.49	0.45
21:I:85:VAL:O	21:I:89:GLU:CB	2.65	0.45
1:U:456:ASP:O	1:U:460:TYR:CB	2.65	0.45
2:V:134:PHE:CA	2:V:137:GLU:OE2	2.65	0.45
3:W:32:ALA:O	3:W:36:LYS:N	2.39	0.45
3:W:178:GLU:CD	3:W:178:GLU:N	2.73	0.45
4:X:335:LEU:HD21	4:X:365:LEU:HD21	1.98	0.45
7:a:8:LEU:HD21	7:a:29:TYR:OH	2.17	0.45
8:b:62:THR:HG21	8:b:71:ILE:HA	1.99	0.45
12:f:442:SER:CB	12:f:476:THR:HB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:f:646:MET:HE1	14:B:49:LEU:HD12	1.98	0.45
17:E:56:ILE:HB	17:E:100:LEU:HB2	1.97	0.45
18:F:180:ARG:NH1	18:F:241:ALA:O	2.50	0.45
28:P:205:ASP:OD2	30:r:19:ARG:NH2	2.50	0.45
29:Q:4:LEU:HD22	29:Q:45:LEU:HB3	1.97	0.45
24:l:66:VAL:HA	24:l:89:ARG:HE	1.81	0.45
28:p:138:VAL:HG11	28:p:146:MET:HB3	1.99	0.45
30:r:44:THR:HG21	30:r:100:MET:HE3	1.97	0.45
1:U:576:PRO:HA	1:U:579:ARG:HE	1.82	0.45
2:V:98:LEU:HA	2:V:104:THR:HG22	1.98	0.45
2:V:150:ARG:O	2:V:154:ALA:CB	2.64	0.45
5:Y:47:ASP:OD2	5:Y:113:ARG:NH2	2.50	0.45
12:f:265:ALA:HB3	12:f:268:LEU:HB2	1.99	0.45
12:f:330:PHE:HA	12:f:333:LEU:HB2	1.97	0.45
14:B:343:ARG:HE	14:B:346:ARG:NH1	2.14	0.45
21:I:235:GLN:O	21:I:239:LYS:HB2	2.17	0.45
22:J:68:ASN:HA	22:J:211:MET:HE1	1.97	0.45
24:L:72:ILE:HG22	24:L:134:ILE:HG12	1.99	0.45
28:P:138:VAL:HG11	28:P:146:MET:HB3	1.99	0.45
31:S:43:CYS:SG	31:S:194:ARG:HG3	2.57	0.45
21:i:100:GLN:HE21	29:q:83:PHE:HE1	1.64	0.45
23:k:84:ASP:OD1	23:k:84:ASP:N	2.48	0.45
1:U:97:VAL:HA	1:U:100:ILE:HG12	1.99	0.45
3:W:172:GLU:CD	3:W:172:GLU:C	2.85	0.45
12:f:707:LEU:HD11	12:f:737:ASN:HD22	1.81	0.45
14:B:418:ASP:O	14:B:422:SER:CB	2.63	0.45
15:C:142:LYS:NZ	16:D:297:ASP:OD1	2.45	0.45
16:D:185:LEU:HD21	16:D:259:PRO:HB2	1.99	0.45
18:F:421:MET:HA	18:F:424:ILE:HD12	1.99	0.45
22:J:88:ARG:NH1	29:Q:69:MET:O	2.50	0.45
30:R:83:LEU:HD11	30:R:97:MET:HE1	1.99	0.45
31:s:149:LEU:O	31:s:153:VAL:HB	2.16	0.45
2:V:31:ALA:O	2:V:34:ASP:N	2.43	0.45
3:W:361:HIS:HA	3:W:364:ARG:HE	1.82	0.45
9:c:216:MET:HE3	9:c:216:MET:HB2	1.82	0.45
10:d:72:GLU:O	10:d:76:ALA:HB2	2.17	0.45
12:f:758:ASN:HB2	12:f:809:ILE:HG21	1.97	0.45
20:H:45:VAL:HG22	20:H:212:ILE:HG22	1.98	0.45
27:O:211:VAL:HG11	28:P:198:ARG:HD3	1.99	0.45
31:S:92:LEU:HD23	31:S:124:PHE:HE2	1.82	0.45
32:T:45:VAL:HB	32:T:49:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:97:GLN:HB3	30:r:61:ARG:HG3	1.99	0.45
30:r:115:ASP:HB2	30:r:119:ASN:HB2	1.97	0.45
1:U:107:HIS:HA	1:U:110:LYS:HG2	1.98	0.45
2:V:407:VAL:O	2:V:411:SER:CB	2.65	0.45
2:V:451:ILE:HG13	2:V:458:VAL:HG13	1.99	0.45
3:W:47:LEU:HD23	3:W:48:LEU:HD22	1.99	0.45
5:Y:101:ARG:HA	5:Y:104:MET:HG2	1.98	0.45
7:a:212:ASN:HD21	7:a:215:GLU:HB2	1.82	0.45
8:b:93:ALA:HB1	8:b:109:ILE:HD13	1.99	0.45
8:b:121:GLU:HB3	8:b:152:LYS:HG2	1.98	0.45
9:c:144:VAL:O	9:c:157:ILE:CD1	2.65	0.45
13:A:213:LEU:HD22	13:A:337:LEU:HD23	1.98	0.45
15:C:196:LYS:HD3	15:C:294:ALA:HB1	1.97	0.45
19:G:200:THR:HG23	19:G:242:LEU:HD11	1.99	0.45
22:J:120:GLN:O	23:K:134:SER:OG	2.32	0.45
24:L:103:LEU:HD12	24:L:108:LEU:HB2	1.99	0.45
25:M:170:GLN:HA	25:M:173:LYS:HG2	1.97	0.45
32:t:45:VAL:HB	32:t:49:THR:HG23	1.98	0.45
1:U:490:ARG:HB2	1:U:493:VAL:HG12	1.98	0.45
2:V:264:TYR:O	2:V:264:TYR:CD2	2.70	0.45
3:W:237:GLU:HG2	3:W:238:GLY:H	1.81	0.45
5:Y:104:MET:HB2	5:Y:108:ALA:HB2	1.99	0.45
13:A:192:GLU:HB2	13:A:196:LEU:HD13	1.99	0.45
13:A:368:ILE:HG22	13:A:406:GLU:HB2	1.98	0.45
17:E:217:GLU:HA	17:E:220:ASN:HB2	1.99	0.45
17:E:313:LEU:O	17:E:317:ALA:CB	2.65	0.45
23:k:146:VAL:HG11	23:k:222:PRO:HA	1.98	0.45
24:l:72:ILE:HG22	24:l:134:ILE:HG12	1.99	0.45
25:m:228:PRO:HD2	25:m:231:ILE:HD12	1.97	0.45
1:U:11:LEU:HD23	10:d:77:GLN:HE22	1.82	0.44
1:U:391:GLU:O	1:U:395:ARG:HB2	2.17	0.44
2:V:265:ASP:O	2:V:269:LYS:N	2.47	0.44
5:Y:124:PHE:HA	5:Y:127:THR:HG22	1.99	0.44
5:Y:247:LEU:HD12	5:Y:250:LEU:HD11	1.98	0.44
5:Y:261:PHE:O	5:Y:265:GLU:HB2	2.17	0.44
7:a:267:GLN:HA	7:a:270:ARG:HB3	1.99	0.44
12:f:575:ALA:O	12:f:579:ALA:CB	2.65	0.44
12:f:646:MET:HG3	14:B:64:LYS:CG	2.46	0.44
13:A:274:PHE:HB2	13:A:319:MET:HA	1.99	0.44
15:C:303:SER:HA	15:C:306:LEU:HB2	1.99	0.44
17:E:269:THR:O	17:E:271:HIS:ND1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:q:121:LEU:HD22	29:q:121:LEU:HA	1.75	0.44
32:t:41:ARG:HH21	32:t:54:SER:HA	1.82	0.44
32:t:89:HIS:NE2	32:t:124:TYR:O	2.47	0.44
1:U:336:GLU:HA	1:U:339:LEU:HB3	2.00	0.44
1:U:614:VAL:O	1:U:618:ALA:HB2	2.16	0.44
1:U:756:HIS:HD2	1:U:759:SER:HB2	1.82	0.44
3:W:52:LYS:HE2	3:W:79:GLU:HG2	1.99	0.44
4:X:53:LEU:HD23	4:X:56:LEU:HD12	1.99	0.44
4:X:292:GLN:NE2	4:X:296:ASN:OD1	2.43	0.44
6:Z:227:ILE:H	6:Z:227:ILE:HG13	1.68	0.44
7:a:258:GLN:HA	7:a:261:LEU:HD13	1.98	0.44
12:f:408:LEU:O	12:f:412:ALA:HB2	2.16	0.44
13:A:114:ASN:HA	13:A:120:LYS:HG3	1.99	0.44
13:A:393:GLY:HA2	14:B:214:MET:HE2	1.99	0.44
14:B:71:TYR:O	14:B:75:GLU:HB2	2.18	0.44
15:C:130:LYS:C	15:C:130:LYS:HE3	2.42	0.44
16:D:356:GLU:CD	16:D:356:GLU:C	2.85	0.44
22:J:226:GLU:O	22:J:230:ALA:HB2	2.17	0.44
23:K:69:GLU:HA	23:K:75:GLY:HA2	1.99	0.44
29:Q:170:ARG:NH2	30:r:125:THR:OG1	2.51	0.44
32:T:41:ARG:HH21	32:T:54:SER:HA	1.82	0.44
19:g:200:THR:HG23	19:g:242:LEU:HD11	1.99	0.44
21:i:41:ASP:OD1	21:i:41:ASP:N	2.50	0.44
21:i:79:ILE:HG22	21:i:82:ASP:H	1.82	0.44
22:j:193:LYS:O	22:j:197:GLU:CB	2.66	0.44
29:q:119:ASP:OD2	29:q:121:LEU:HB2	2.17	0.44
8:b:26:LEU:O	8:b:30:GLN:CB	2.65	0.44
12:f:130:ALA:HB1	12:f:133:MET:HE3	1.98	0.44
12:f:832:THR:O	14:B:53:THR:OG1	2.29	0.44
12:f:836:GLU:HB2	12:f:841:PRO:HD2	1.99	0.44
14:B:314:ASN:O	14:B:317:ASP:N	2.48	0.44
15:C:221:GLN:NE2	15:C:227:GLY:O	2.50	0.44
16:D:376:ASN:O	16:D:380:GLN:CB	2.58	0.44
26:N:144:ARG:NH2	26:N:151:GLU:OE1	2.50	0.44
29:Q:148:THR:HG22	29:Q:150:THR:H	1.83	0.44
28:p:191:GLU:OE2	28:p:194:LYS:NZ	2.37	0.44
3:W:174:TYR:HB2	17:E:161:ARG:HH12	1.81	0.44
3:W:282:GLU:O	3:W:286:LEU:CB	2.63	0.44
5:Y:366:TYR:O	5:Y:369:THR:OG1	2.29	0.44
6:Z:138:TYR:HB3	6:Z:155:PHE:HB3	2.00	0.44
7:a:374:ILE:HA	10:d:255:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:85:GLU:HB3	9:c:86:ALA:H	1.56	0.44
12:f:787:LEU:HB3	12:f:788:MET:H	1.59	0.44
16:D:151:ILE:HB	16:D:152:MET:H	1.65	0.44
16:D:352:MET:HE2	16:D:352:MET:HB3	1.85	0.44
17:E:114:GLU:N	17:E:114:GLU:CD	2.73	0.44
21:I:119:GLN:HG3	22:J:78:ALA:HB1	1.98	0.44
23:K:43:SER:HA	23:K:151:PRO:HG3	1.99	0.44
21:i:106:PRO:HB2	21:i:109:GLN:HG2	1.99	0.44
26:n:6:VAL:HG22	26:n:125:PHE:HB2	1.99	0.44
29:q:23:SER:OG	29:q:24:ASN:N	2.50	0.44
29:q:148:THR:HG22	29:q:150:THR:H	1.83	0.44
30:r:83:LEU:HD11	30:r:97:MET:HE1	1.99	0.44
1:U:458:ILE:O	1:U:462:LEU:CB	2.65	0.44
2:V:219:GLU:CD	2:V:257:ASN:HD21	2.26	0.44
4:X:258:LYS:HD3	4:X:266:ASP:HB2	1.98	0.44
5:Y:173:ASP:HA	15:C:334:ARG:HG3	2.00	0.44
8:b:124:LEU:O	8:b:128:ALA:CB	2.66	0.44
22:J:91:CYS:HB2	22:J:102:VAL:HG21	1.99	0.44
23:k:43:SER:HA	23:k:151:PRO:HG3	1.99	0.44
1:U:45:ILE:HG23	1:U:60:ALA:HB1	1.99	0.44
1:U:770:TRP:O	9:c:180:ASN:N	2.51	0.44
3:W:178:GLU:N	3:W:178:GLU:OE2	2.50	0.44
6:Z:279:LYS:HA	6:Z:279:LYS:NZ	2.33	0.44
10:d:116:HIS:CA	10:d:119:LEU:HD23	2.47	0.44
12:f:171:GLN:HG3	12:f:179:VAL:HG22	2.00	0.44
12:f:646:MET:HG3	14:B:64:LYS:CD	2.46	0.44
13:A:390:THR:HA	14:B:216:ILE:HD11	1.99	0.44
15:C:125:LYS:HB3	15:C:125:LYS:HE2	1.47	0.44
22:j:226:GLU:O	22:j:230:ALA:HB2	2.17	0.44
24:l:103:LEU:HD12	24:l:108:LEU:HB2	1.99	0.44
1:U:475:HIS:CD2	1:U:511:ALA:HB2	2.53	0.44
1:U:613:ASP:OD1	1:U:616:ARG:NH2	2.40	0.44
3:W:155:GLN:HG2	3:W:157:GLY:H	1.82	0.44
4:X:96:PHE:HE2	4:X:106:GLU:HA	1.83	0.44
5:Y:164:ALA:C	5:Y:168:ILE:HD13	2.43	0.44
6:Z:223:ASN:HB3	6:Z:227:ILE:HG12	1.99	0.44
10:d:49:ILE:HG23	10:d:50:LEU:HD12	2.00	0.44
12:f:690:VAL:O	12:f:694:LEU:HB2	2.17	0.44
13:A:300:LEU:HD23	13:A:303:ILE:HD12	1.99	0.44
18:F:222:GLY:O	18:F:349:ASP:N	2.45	0.44
24:L:66:VAL:HA	24:L:89:ARG:HE	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S:149:LEU:O	31:S:153:VAL:HB	2.17	0.44
21:i:38:LEU:HB3	21:i:43:VAL:HG23	2.00	0.44
24:l:148:CYS:SG	24:l:150:SER:OG	2.66	0.44
24:l:189:LYS:HG3	24:l:193:ARG:HH12	1.83	0.44
1:U:462:LEU:HG	1:U:496:LEU:HD21	2.00	0.44
1:U:603:LEU:CD2	16:D:60:TYR:CG	2.86	0.44
1:U:697:GLN:NE2	1:U:744:VAL:O	2.50	0.44
2:V:467:TYR:HH	4:X:397:TYR:HH	1.61	0.44
5:Y:325:VAL:HB	11:e:70:SER:HB2	2.00	0.44
6:Z:142:GLU:CD	6:Z:142:GLU:C	2.85	0.44
6:Z:250:TYR:OH	10:d:238:PRO:HG2	2.18	0.44
7:a:127:ASP:HB2	7:a:162:TYR:HE1	1.82	0.44
9:c:254:ASN:HD22	9:c:257:LYS:HB3	1.83	0.44
10:d:235:THR:O	10:d:239:SER:N	2.51	0.44
12:f:762:VAL:HG12	12:f:806:VAL:HA	1.99	0.44
14:B:342:ILE:HG22	14:B:350:LYS:HE3	1.99	0.44
16:D:149:SER:OG	16:D:250:VAL:CG2	2.64	0.44
21:I:119:GLN:O	21:I:122:THR:OG1	2.32	0.44
22:J:168:VAL:HG22	22:J:198:VAL:CB	2.47	0.44
26:N:6:VAL:HG22	26:N:125:PHE:HB2	1.99	0.44
22:j:47:LYS:HA	22:j:200:GLN:CG	2.48	0.44
22:j:91:CYS:HB2	22:j:102:VAL:HG21	1.99	0.44
23:k:69:GLU:HA	23:k:75:GLY:HA2	1.99	0.44
1:U:24:LEU:HB2	1:U:59:PHE:CD2	2.53	0.44
1:U:510:GLU:OE2	1:U:546:ARG:NH2	2.47	0.44
1:U:601:ARG:CZ	1:U:601:ARG:CB	2.95	0.44
2:V:163:VAL:HA	2:V:175:MET:HE2	1.99	0.44
2:V:166:TYR:O	2:V:171:VAL:HG11	2.17	0.44
3:W:67:LEU:C	3:W:67:LEU:CD2	2.91	0.44
3:W:90:LEU:HD12	3:W:90:LEU:N	2.32	0.44
3:W:90:LEU:HD23	3:W:93:ARG:CZ	2.48	0.44
7:a:7:PHE:O	7:a:7:PHE:CD1	2.70	0.44
9:c:238:CYS:HA	9:c:241:ASN:HD22	1.83	0.44
10:d:95:MET:O	10:d:99:LEU:HB2	2.18	0.44
12:f:185:LEU:O	12:f:189:LYS:HB3	2.18	0.44
20:H:227:LYS:O	20:H:231:ALA:HB2	2.18	0.44
21:I:79:ILE:HG22	21:I:82:ASP:H	1.82	0.44
21:i:235:GLN:O	21:i:239:LYS:HB2	2.17	0.44
26:n:144:ARG:NH2	26:n:151:GLU:OE1	2.50	0.44
28:p:107:PRO:HG2	28:p:124:LEU:HB2	1.98	0.44
1:U:474:ARG:O	1:U:478:SER:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:315:MET:HG2	3:W:319:THR:HG1	1.82	0.43
3:W:395:ASN:HA	3:W:398:VAL:HG22	1.99	0.43
6:Z:190:ARG:HH22	9:c:297:VAL:HA	1.82	0.43
6:Z:193:ASN:HD22	6:Z:197:GLY:HA3	1.83	0.43
7:a:48:PRO:HB2	7:a:51:ALA:HA	2.00	0.43
7:a:116:THR:O	7:a:120:ALA:HB2	2.18	0.43
9:c:88:ASP:OD2	9:c:91:PHE:N	2.51	0.43
12:f:513:GLU:HA	12:f:557:TRP:HZ3	1.83	0.43
12:f:744:MET:O	12:f:748:LEU:HB2	2.18	0.43
12:f:809:ILE:HG23	12:f:810:ILE:HG23	2.00	0.43
14:B:57:GLN:HA	14:B:61:LYS:HZ1	1.80	0.43
17:E:101:ASP:HB3	17:E:106:THR:H	1.83	0.43
19:G:86:ASP:OD1	25:M:120:HIS:NE2	2.38	0.43
27:O:138:PHE:O	27:O:142:PHE:CB	2.66	0.43
24:l:109:VAL:HG21	24:l:145:PHE:HD2	1.83	0.43
1:U:765:VAL:HG11	1:U:778:PHE:HD2	1.82	0.43
2:V:357:LEU:O	2:V:361:PHE:N	2.40	0.43
4:X:90:ARG:HH21	4:X:125:LEU:HA	1.83	0.43
5:Y:122:THR:O	5:Y:126:LYS:CB	2.64	0.43
5:Y:203:ASP:OD1	5:Y:203:ASP:N	2.51	0.43
6:Z:74:TYR:HE1	9:c:98:MET:HB3	1.82	0.43
15:C:129:ASN:OD1	15:C:129:ASN:N	2.51	0.43
16:D:154:LEU:N	16:D:158:GLN:HG3	2.32	0.43
21:I:38:LEU:HB3	21:I:43:VAL:HG23	2.00	0.43
21:I:226:ARG:HD2	21:I:226:ARG:C	2.43	0.43
24:L:109:VAL:HG21	24:L:145:PHE:HD2	1.83	0.43
29:Q:23:SER:OG	29:Q:24:ASN:N	2.50	0.43
30:R:38:ASN:HD22	30:R:41:LEU:HD12	1.84	0.43
1:U:126:ILE:HA	1:U:130:LEU:HD23	1.99	0.43
2:V:358:MET:N	2:V:358:MET:SD	2.91	0.43
5:Y:164:ALA:C	5:Y:168:ILE:HD11	2.44	0.43
8:b:3:LEU:HB3	8:b:105:HIS:HA	2.00	0.43
12:f:250:ARG:HH12	12:f:281:ILE:HG12	1.76	0.43
12:f:335:ARG:NH2	12:f:338:ASP:OD2	2.52	0.43
12:f:447:ALA:HA	12:f:450:ILE:HD12	1.99	0.43
13:A:429:TYR:HE2	14:B:340:ALA:HB2	1.83	0.43
14:B:56:THR:O	14:B:61:LYS:HE2	2.12	0.43
17:E:264:MET:HG2	17:E:275:MET:HE1	2.00	0.43
18:F:65:GLU:O	18:F:69:MET:CB	2.66	0.43
29:Q:101:ASN:HB3	29:Q:132:HIS:CD2	2.53	0.43
28:p:65:GLN:OE1	29:q:86:ARG:NH2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:14:GLU:HB2	1:U:19:LEU:HD23	1.99	0.43
3:W:162:ALA:HB1	3:W:192:LEU:HD13	2.00	0.43
4:X:255:LEU:HD22	4:X:267:VAL:HG13	2.01	0.43
5:Y:186:LEU:HA	5:Y:189:VAL:HG12	2.00	0.43
6:Z:106:ILE:HA	6:Z:155:PHE:HE2	1.82	0.43
12:f:597:VAL:HB	12:f:635:LYS:HZ1	1.83	0.43
12:f:762:VAL:CA	12:f:807:ARG:HH11	2.31	0.43
16:D:309:MET:HE1	16:D:327:LEU:HD21	1.99	0.43
16:D:385:LEU:HD23	16:D:398:ASP:HA	1.99	0.43
17:E:114:GLU:CD	17:E:114:GLU:C	2.85	0.43
21:I:33:THR:HB	21:I:48:GLU:HB3	2.01	0.43
24:L:189:LYS:HG3	24:L:193:ARG:HH12	1.83	0.43
1:U:220:LEU:HA	1:U:223:LEU:HB3	1.99	0.43
5:Y:233:ARG:N	5:Y:234:PRO:CD	2.79	0.43
9:c:196:LEU:CD1	9:c:196:LEU:N	2.82	0.43
10:d:171:LEU:HD22	10:d:171:LEU:HA	1.75	0.43
10:d:176:ASP:HA	10:d:179:ALA:HB3	2.00	0.43
10:d:199:PHE:HD1	10:d:199:PHE:HA	1.76	0.43
12:f:34:ARG:O	12:f:38:ASP:HB2	2.19	0.43
12:f:129:LEU:HD13	12:f:130:ALA:CB	2.48	0.43
28:P:88:MET:HG3	28:P:124:LEU:HD11	2.01	0.43
28:p:88:MET:HG3	28:p:124:LEU:HD11	2.01	0.43
31:s:16:ALA:HB2	31:s:121:VAL:HG23	2.00	0.43
2:V:290:TYR:HE1	2:V:309:MET:HE1	1.83	0.43
3:W:144:ARG:HA	3:W:147:LYS:HE3	1.99	0.43
3:W:362:ASN:HB3	3:W:366:MET:HE3	2.01	0.43
3:W:455:LEU:HD22	6:Z:103:LYS:HB2	2.01	0.43
4:X:215:GLY:O	4:X:219:ALA:CB	2.65	0.43
9:c:196:LEU:CD2	9:c:197:ASN:CB	2.78	0.43
12:f:485:LEU:HD22	12:f:501:LEU:HD11	2.00	0.43
16:D:368:ASP:CB	16:D:409:LYS:CE	2.96	0.43
19:G:180:GLU:HA	19:G:183:VAL:HG12	2.01	0.43
29:Q:162:LYS:O	30:r:141:ARG:NH2	2.51	0.43
30:r:144:SER:H	30:r:147:LEU:HD11	1.83	0.43
1:U:601:ARG:H	1:U:601:ARG:HG2	1.65	0.43
2:V:137:GLU:H	2:V:138:PRO:CD	2.32	0.43
3:W:316:ARG:N	3:W:316:ARG:HD2	2.34	0.43
5:Y:367:GLN:HE21	5:Y:371:LYS:HE2	1.83	0.43
6:Z:91:ILE:H	6:Z:91:ILE:HG13	1.64	0.43
6:Z:248:ALA:O	6:Z:252:LYS:CB	2.65	0.43
15:C:20:LEU:O	15:C:24:TYR:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:D:368:ASP:CG	16:D:409:LYS:CE	2.92	0.43
25:M:40:ARG:NH2	25:M:146:ALA:HB3	2.33	0.43
32:T:89:HIS:CE1	32:T:131:ALA:HB1	2.54	0.43
21:i:85:VAL:O	21:i:89:GLU:CB	2.65	0.43
27:o:138:PHE:O	27:o:142:PHE:CB	2.66	0.43
1:U:583:MET:O	1:U:586:VAL:HG12	2.18	0.43
2:V:137:GLU:H	2:V:138:PRO:HD2	1.82	0.43
2:V:483:CYS:HA	2:V:486:ILE:HG22	2.00	0.43
3:W:134:GLY:HA2	3:W:137:TYR:CD2	2.52	0.43
5:Y:164:ALA:O	5:Y:168:ILE:HD11	2.13	0.43
5:Y:297:ARG:HD3	11:e:48:VAL:HG22	1.99	0.43
6:Z:214:LYS:HA	6:Z:218:GLY:H	1.84	0.43
9:c:75:MET:SD	9:c:92:GLN:NE2	2.90	0.43
12:f:82:ILE:O	12:f:86:THR:HB	2.18	0.43
12:f:372:LEU:HD11	12:f:403:LYS:HE3	2.00	0.43
12:f:642:ALA:C	12:f:644:ALA:H	2.27	0.43
13:A:117:GLN:HE22	14:B:128:GLY:HA3	1.84	0.43
15:C:127:LEU:H	15:C:127:LEU:CD1	1.97	0.43
15:C:155:ASP:HA	15:C:158:ILE:HD12	2.00	0.43
18:F:189:GLY:H	36:F:501:ADP:HN62	1.66	0.43
30:R:144:SER:H	30:R:147:LEU:HD11	1.83	0.43
31:S:16:ALA:HB2	31:S:121:VAL:HG23	2.00	0.43
20:h:227:LYS:O	20:h:231:ALA:HB2	2.18	0.43
32:t:89:HIS:CE1	32:t:131:ALA:HB1	2.54	0.43
3:W:23:THR:HA	3:W:26:GLN:HB2	2.01	0.43
4:X:316:ASP:HB2	4:X:319:ILE:HG12	2.00	0.43
6:Z:73:ASP:H	8:b:63:THR:HG21	1.84	0.43
7:a:57:ILE:HD12	7:a:60:TYR:HB3	2.00	0.43
8:b:37:CYS:O	8:b:41:THR:CB	2.67	0.43
9:c:57:MET:HE2	9:c:69:VAL:HG21	1.99	0.43
9:c:196:LEU:HD13	9:c:196:LEU:N	2.33	0.43
10:d:172:ASP:C	10:d:174:ILE:N	2.77	0.43
13:A:346:PRO:HB2	13:A:351:ARG:HG3	2.01	0.43
15:C:92:GLU:N	15:C:92:GLU:CD	2.77	0.43
15:C:150:MET:HA	15:C:331:ILE:HG21	1.99	0.43
15:C:330:LYS:HE2	15:C:330:LYS:HB3	1.94	0.43
17:E:45:ASN:O	17:E:49:ALA:HB2	2.19	0.43
17:E:97:ARG:NH2	17:E:112:PRO:O	2.52	0.43
18:F:66:LEU:O	18:F:70:LYS:CB	2.67	0.43
21:I:90:LEU:HD13	21:I:114:LEU:HD22	2.01	0.43
20:h:9:SER:OG	20:h:123:GLN:O	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:l:50:LYS:N	24:l:209:ASN:O	2.44	0.43
2:V:165:ALA:C	2:V:167:LEU:HD23	2.44	0.43
2:V:497:PRO:HG2	6:Z:278:ASN:OD1	1.91	0.43
3:W:96:GLN:NE2	3:W:138:VAL:CG2	2.79	0.43
3:W:340:VAL:HA	3:W:350:ARG:HD2	2.00	0.43
4:X:252:LYS:HA	4:X:287:LEU:HD11	2.00	0.43
6:Z:109:ASN:O	6:Z:113:LYS:HB2	2.18	0.43
6:Z:252:LYS:HD3	6:Z:252:LYS:O	2.19	0.43
7:a:9:GLN:HE22	7:a:23:HIS:CE1	2.37	0.43
9:c:25:VAL:O	9:c:176:GLN:NE2	2.52	0.43
10:d:53:ASP:HA	10:d:56:GLU:HG3	2.01	0.43
11:e:5:LYS:HE2	11:e:5:LYS:HB2	1.83	0.43
15:C:90:HIS:HE1	16:D:110:ASN:OD1	2.01	0.43
16:D:335:LEU:HD12	16:D:336:PRO:HD3	1.99	0.43
16:D:363:TYR:CE2	16:D:399:PHE:HB3	2.52	0.43
26:n:14:LEU:HD11	26:n:101:ALA:HB3	2.01	0.43
29:q:101:ASN:HB3	29:q:132:HIS:CD2	2.54	0.43
1:U:126:ILE:HG21	1:U:131:GLU:HG2	2.01	0.42
1:U:611:ASN:HB3	1:U:614:VAL:HG12	2.01	0.42
3:W:96:GLN:HE21	3:W:135:LYS:N	2.17	0.42
4:X:170:GLN:NE2	4:X:192:SER:OG	2.46	0.42
9:c:75:MET:HE1	9:c:87:VAL:HA	2.01	0.42
13:A:287:ASP:N	13:A:287:ASP:OD1	2.52	0.42
14:B:57:GLN:CA	14:B:61:LYS:HZ1	2.31	0.42
14:B:120:HIS:HA	14:B:134:SER:HA	2.00	0.42
15:C:126:ILE:O	15:C:126:ILE:HG22	2.17	0.42
19:G:82:GLY:HA3	19:G:136:CYS:HA	2.01	0.42
21:I:106:PRO:HB2	21:I:109:GLN:HG2	1.99	0.42
22:J:29:GLY:O	22:J:163:ARG:N	2.45	0.42
30:R:26:ILE:HG21	30:R:29:GLN:HE21	1.84	0.42
21:i:90:LEU:HD13	21:i:114:LEU:HD22	2.01	0.42
26:n:144:ARG:H	26:n:147:MET:HE3	1.84	0.42
30:r:26:ILE:HG21	30:r:29:GLN:HE21	1.84	0.42
31:s:153:VAL:HG13	31:s:166:LEU:HD11	2.01	0.42
2:V:26:PRO:C	2:V:28:PRO:HD2	2.44	0.42
3:W:137:TYR:CZ	16:D:392:TYR:HD2	2.20	0.42
3:W:305:LEU:HD13	3:W:308:LEU:HD12	2.01	0.42
4:X:83:ALA:O	4:X:87:ARG:CB	2.68	0.42
4:X:222:GLU:HA	4:X:225:TRP:HE1	1.84	0.42
5:Y:288:PHE:HD1	5:Y:291:HIS:CE1	2.37	0.42
5:Y:297:ARG:HH22	11:e:51:ASP:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:14:LEU:O	6:Z:18:SER:HB2	2.18	0.42
6:Z:189:GLN:HA	6:Z:192:THR:HG22	2.00	0.42
16:D:297:ASP:OD2	16:D:326:ARG:NH2	2.52	0.42
18:F:184:GLN:HE22	18:F:186:SER:HB3	1.84	0.42
25:M:40:ARG:HE	25:M:40:ARG:HB2	1.77	0.42
28:P:135:ASP:OD1	28:P:135:ASP:N	2.45	0.42
29:Q:21:ALA:HB3	29:Q:29:LYS:HB3	2.01	0.42
30:R:154:ASP:OD1	30:R:157:ARG:NH1	2.52	0.42
1:U:376:MET:HG3	1:U:377:HIS:CD2	2.54	0.42
1:U:758:PRO:HB2	1:U:781:LEU:HB3	2.01	0.42
2:V:182:LYS:HE3	2:V:182:LYS:HB3	1.86	0.42
2:V:417:ILE:HD13	5:Y:349:LYS:HG3	2.02	0.42
3:W:232:GLN:HA	3:W:235:GLN:HB3	1.99	0.42
5:Y:32:ARG:HH22	5:Y:35:ALA:HB3	1.84	0.42
5:Y:344:HIS:CG	5:Y:359:PRO:HG3	2.54	0.42
7:a:78:GLU:O	7:a:82:HIS:ND1	2.49	0.42
12:f:771:LEU:HD12	12:f:771:LEU:C	2.44	0.42
13:A:73:ALA:HB1	13:A:74:PRO:HD2	2.01	0.42
14:B:252:GLY:HA2	14:B:255:LEU:HD23	2.00	0.42
17:E:125:GLU:O	18:F:321:GLN:NE2	2.52	0.42
17:E:251:ARG:HB3	17:E:255:ARG:HH12	1.85	0.42
27:O:38:SER:OG	27:O:40:ASN:OD1	2.27	0.42
31:S:36:HIS:HB3	32:T:132:TYR:CZ	2.55	0.42
1:U:367:THR:HA	1:U:370:VAL:HG22	2.01	0.42
1:U:459:ASP:HA	1:U:462:LEU:HB3	2.02	0.42
1:U:724:VAL:O	1:U:728:PHE:HB2	2.19	0.42
2:V:210:CYS:O	2:V:214:HIS:HB3	2.19	0.42
4:X:122:ARG:HH21	20:H:185:GLU:HG3	1.83	0.42
5:Y:80:GLU:HA	5:Y:83:ARG:HG2	2.01	0.42
5:Y:190:ALA:HA	5:Y:287:LEU:CD2	2.49	0.42
7:a:176:ALA:O	7:a:180:LEU:HB2	2.20	0.42
12:f:388:ASP:HB3	12:f:391:LEU:HB2	2.00	0.42
15:C:32:GLN:HG3	15:C:36:ASN:HD21	1.85	0.42
15:C:307:ARG:HA	15:C:308:PRO:HD3	1.92	0.42
16:D:357:GLU:CD	16:D:357:GLU:C	2.85	0.42
17:E:139:SER:HA	17:E:142:ILE:HD12	2.02	0.42
21:i:147:LEU:HD12	21:i:159:TRP:HB2	2.02	0.42
1:U:695:MET:HB2	1:U:695:MET:HE3	1.79	0.42
1:U:913:ILE:H	1:U:913:ILE:HG13	1.59	0.42
2:V:358:MET:HB2	2:V:359:PRO:CD	2.45	0.42
3:W:90:LEU:HB2	3:W:93:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:94:ARG:HG3	3:W:98:LYS:HD2	2.00	0.42
12:f:325:GLN:HE21	12:f:420:TRP:HE3	1.68	0.42
12:f:640:LYS:HG2	12:f:678:LEU:HD13	2.02	0.42
12:f:771:LEU:HD21	12:f:773:LYS:HZ3	1.84	0.42
13:A:48:VAL:HG12	14:B:69:LYS:HE2	2.01	0.42
13:A:186:LYS:HE3	13:A:341:ILE:HG13	2.01	0.42
16:D:144:PRO:HA	16:D:145:PRO:HD3	1.85	0.42
17:E:168:LYS:N	17:E:296:ASP:OD2	2.50	0.42
1:U:241:ASN:HB3	1:U:244:MET:HG2	2.01	0.42
1:U:800:VAL:HB	1:U:914:LEU:HD21	2.01	0.42
3:W:148:THR:O	3:W:151:THR:OG1	2.34	0.42
4:X:187:ARG:HH21	4:X:217:ILE:HG22	1.84	0.42
5:Y:36:ALA:O	5:Y:40:GLU:HB3	2.19	0.42
7:a:267:GLN:O	7:a:271:LYS:HB2	2.19	0.42
8:b:6:THR:HB	8:b:49:VAL:HG22	2.02	0.42
12:f:438:ASP:HA	12:f:477:MET:CE	2.44	0.42
12:f:442:SER:O	12:f:446:LEU:CB	2.61	0.42
16:D:368:ASP:CG	16:D:409:LYS:HE3	2.42	0.42
17:E:317:ALA:HA	17:E:320:ILE:HD12	2.00	0.42
20:H:9:SER:OG	20:H:123:GLN:O	2.30	0.42
21:I:47:ALA:O	21:I:212:GLU:N	2.52	0.42
23:K:121:LEU:HD21	24:L:126:ARG:HH12	1.85	0.42
23:K:211:ASN:OD1	23:K:214:ASN:N	2.52	0.42
24:L:148:CYS:SG	24:L:150:SER:OG	2.66	0.42
25:M:40:ARG:NH2	25:M:146:ALA:CB	2.77	0.42
24:l:204:ASP:OD1	24:l:204:ASP:N	2.53	0.42
31:s:35:ILE:HB	32:t:151:ARG:HH12	1.85	0.42
1:U:362:ASN:HB2	9:c:173:GLU:HB2	2.00	0.42
2:V:252:ASN:HD21	2:V:288:TYR:HB2	1.85	0.42
2:V:497:PRO:HD3	6:Z:278:ASN:ND2	2.15	0.42
3:W:64:SER:C	3:W:66:ILE:H	2.28	0.42
4:X:268:GLN:O	4:X:272:SER:OG	2.34	0.42
4:X:327:TYR:O	4:X:331:LEU:HB2	2.20	0.42
4:X:377:ILE:HG12	5:Y:312:ARG:HB3	2.01	0.42
5:Y:345:CYS:HA	5:Y:356:THR:HA	2.02	0.42
7:a:141:MET:N	7:a:141:MET:SD	2.93	0.42
8:b:5:SER:HB2	8:b:100:ARG:HD2	2.02	0.42
12:f:189:LYS:HG2	12:f:190:GLU:HG2	2.02	0.42
12:f:561:GLY:O	12:f:565:ASN:HB2	2.19	0.42
12:f:646:MET:CG	14:B:64:LYS:HD3	2.48	0.42
16:D:366:ARG:H	16:D:366:ARG:HG2	1.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:g:153:LYS:NZ	19:g:167:ALA:O	2.45	0.42
21:i:33:THR:HB	21:i:48:GLU:HB3	2.01	0.42
2:V:261:TYR:N	2:V:261:TYR:CD1	2.87	0.42
2:V:359:PRO:HG2	2:V:385:LYS:HG2	2.01	0.42
3:W:32:ALA:HB1	3:W:36:LYS:HB2	2.02	0.42
3:W:180:LYS:O	3:W:184:GLU:CG	2.68	0.42
5:Y:173:ASP:H	15:C:335:LYS:HA	1.85	0.42
6:Z:137:ALA:H	6:Z:157:HIS:CE1	2.37	0.42
6:Z:142:GLU:HB3	6:Z:153:LYS:HD3	2.02	0.42
10:d:153:LEU:O	10:d:157:ASN:HB2	2.19	0.42
12:f:75:LEU:HD13	12:f:77:GLU:HG3	2.00	0.42
12:f:690:VAL:HG12	12:f:713:PHE:CE1	2.51	0.42
26:N:28:ASN:HD21	27:O:122:LEU:HD21	1.84	0.42
26:N:138:TYR:O	26:N:142:THR:OG1	2.30	0.42
30:R:97:MET:O	30:R:116:SER:N	2.53	0.42
1:U:553:ALA:HA	1:U:585:THR:HG23	2.02	0.42
1:U:790:GLY:H	1:U:880:ASN:HB3	1.84	0.42
1:U:791:LEU:O	1:U:914:LEU:N	2.46	0.42
2:V:26:PRO:O	2:V:30:PRO:HD2	2.18	0.42
2:V:28:PRO:CD	2:V:29:PRO:CD	2.98	0.42
2:V:96:ARG:HA	2:V:107:ARG:HE	1.85	0.42
2:V:213:TYR:HA	2:V:216:ARG:HG3	2.02	0.42
3:W:190:MET:HB2	3:W:202:THR:HG23	2.02	0.42
8:b:30:GLN:HG3	8:b:75:LEU:HD13	2.02	0.42
9:c:118:PHE:HB3	9:c:121:TRP:CH2	2.54	0.42
9:c:148:ILE:HG21	16:D:85:ILE:HG22	2.02	0.42
12:f:218:GLU:O	12:f:222:ASP:CB	2.46	0.42
12:f:250:ARG:NH1	12:f:281:ILE:CG1	2.77	0.42
12:f:771:LEU:CD2	12:f:773:LYS:HZ3	2.33	0.42
12:f:785:ARG:CG	12:f:785:ARG:NH1	2.82	0.42
21:I:69:ASN:HD22	21:I:72:MET:HE3	1.85	0.42
24:L:204:ASP:OD1	24:L:204:ASP:N	2.53	0.42
22:j:200:GLN:HG3	22:j:205:ASN:HB3	2.01	0.42
2:V:228:ARG:HD3	2:V:228:ARG:HA	1.85	0.42
3:W:90:LEU:HD22	3:W:93:ARG:CZ	2.50	0.42
3:W:141:GLU:CB	3:W:172:GLU:CG	2.96	0.42
3:W:398:VAL:HG21	4:X:337:ARG:HH21	1.85	0.42
7:a:8:LEU:HD13	7:a:26:GLU:HB3	2.02	0.42
12:f:399:LEU:HD13	12:f:410:ALA:HB3	2.01	0.42
12:f:754:LYS:O	12:f:754:LYS:HG2	2.18	0.42
14:B:234:LEU:N	34:B:501:ATP:O1A	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:G:153:LYS:NZ	19:G:167:ALA:O	2.45	0.42
22:J:121:SER:OG	22:J:122:ASN:N	2.53	0.42
26:N:144:ARG:H	26:N:147:MET:HE3	1.84	0.42
30:r:154:ASP:OD1	30:r:157:ARG:NH1	2.52	0.42
7:a:194:GLN:HB3	7:a:225:LEU:HG	2.02	0.41
9:c:61:PHE:HZ	9:c:139:ARG:HD2	1.84	0.41
12:f:130:ALA:O	12:f:134:SER:N	2.48	0.41
13:A:115:VAL:HG21	13:A:118:PHE:HB2	2.01	0.41
16:D:92:PHE:HB3	16:D:128:ALA:HB3	2.01	0.41
16:D:177:VAL:HG11	16:D:215:LEU:HD21	2.01	0.41
17:E:155:ASN:HB3	17:E:158:LEU:HD13	2.02	0.41
17:E:171:LEU:HD21	17:E:298:LYS:HG2	2.02	0.41
27:O:120:ASP:OD1	27:O:120:ASP:N	2.53	0.41
21:i:15:GLU:HG3	21:i:17:ARG:HG2	2.02	0.41
2:V:419:LEU:HA	2:V:422:ILE:HG22	2.02	0.41
2:V:496:PHE:HD1	2:V:496:PHE:HA	1.77	0.41
5:Y:165:LYS:C	5:Y:168:ILE:HD13	2.44	0.41
6:Z:85:VAL:HA	9:c:76:PRO:HB3	2.02	0.41
9:c:78:SER:CA	9:c:85:GLU:HG3	2.50	0.41
9:c:244:VAL:HB	9:c:291:LEU:HD21	2.02	0.41
12:f:594:LEU:O	12:f:635:LYS:NZ	2.53	0.41
12:f:672:LEU:HD22	12:f:675:PHE:HB2	2.02	0.41
13:A:278:ASP:OD1	13:A:278:ASP:N	2.52	0.41
13:A:414:ASN:O	13:A:419:SER:N	2.52	0.41
14:B:245:ALA:CB	14:B:279:PRO:O	2.68	0.41
18:F:192:ASP:O	18:F:196:GLN:HB2	2.20	0.41
21:I:15:GLU:HG3	21:I:17:ARG:HG2	2.02	0.41
19:g:180:GLU:HA	19:g:183:VAL:HG12	2.01	0.41
22:j:104:VAL:HA	22:j:107:ILE:HG22	2.02	0.41
1:U:156:GLU:OE2	16:D:41:TYR:OH	2.36	0.41
1:U:373:ASN:HA	1:U:376:MET:HG2	2.01	0.41
1:U:789:ILE:HB	1:U:911:ILE:HA	2.02	0.41
2:V:95:LEU:O	2:V:96:ARG:NH1	2.44	0.41
3:W:84:ASN:HD22	3:W:84:ASN:HA	1.61	0.41
9:c:31:VAL:HG23	9:c:203:ILE:HG21	2.01	0.41
9:c:50:PRO:HB2	17:E:108:MET:HE1	2.02	0.41
12:f:185:LEU:O	12:f:189:LYS:CB	2.69	0.41
23:k:182:GLN:HG2	24:l:56:LEU:HD23	2.02	0.41
25:m:37:ILE:HD13	25:m:196:ILE:HD11	2.03	0.41
29:q:21:ALA:HB3	29:q:29:LYS:HB3	2.01	0.41
30:r:38:ASN:HD22	30:r:41:LEU:HD12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:377:LEU:O	5:Y:381:GLN:CB	2.65	0.41
7:a:106:SER:OG	7:a:107:SER:N	2.53	0.41
7:a:189:PRO:HB2	7:a:192:GLU:HB2	2.02	0.41
13:A:51:ASP:O	13:A:55:LEU:CB	2.67	0.41
13:A:99:THR:HG22	13:A:115:VAL:HG12	2.01	0.41
16:D:162:VAL:HG12	16:D:218:ALA:CA	2.50	0.41
16:D:163:MET:HA	16:D:222:HIS:CE1	2.51	0.41
17:E:180:LYS:NZ	34:E:401:ATP:O2B	2.51	0.41
17:E:253:ILE:HG13	18:F:308:ARG:HH22	1.85	0.41
19:G:191:PHE:O	19:G:194:THR:OG1	2.31	0.41
26:n:29:ARG:NH1	27:o:139:GLU:OE2	2.53	0.41
30:r:182:ASP:OD1	30:r:182:ASP:N	2.54	0.41
2:V:219:GLU:HG2	2:V:224:LEU:HB2	2.03	0.41
3:W:47:LEU:HB3	3:W:94:ARG:NH2	2.35	0.41
4:X:248:ILE:HD13	4:X:279:TYR:HB3	2.03	0.41
4:X:306:LEU:O	4:X:310:ARG:CB	2.59	0.41
9:c:190:GLN:O	9:c:194:HIS:ND1	2.41	0.41
15:C:369:TYR:HD1	15:C:372:ARG:HE	1.68	0.41
17:E:117:PRO:HD3	18:F:94:ILE:HG23	2.01	0.41
17:E:180:LYS:HG2	17:E:301:ILE:HD12	2.03	0.41
21:I:41:ASP:OD1	21:I:41:ASP:N	2.50	0.41
25:M:163:CYS:SG	25:M:164:ALA:N	2.94	0.41
27:O:164:PHE:HE1	31:s:212:LYS:HG3	1.85	0.41
19:g:82:GLY:HA3	19:g:136:CYS:HA	2.01	0.41
30:r:97:MET:O	30:r:116:SER:N	2.53	0.41
1:U:94:SER:OG	1:U:95:GLU:N	2.53	0.41
1:U:188:MET:HE3	1:U:194:ARG:HG3	2.03	0.41
1:U:680:VAL:HB	1:U:683:VAL:HG12	2.03	0.41
2:V:373:ALA:H	2:V:427:GLN:HE21	1.69	0.41
3:W:365:ILE:HG22	3:W:368:LYS:HD2	2.02	0.41
5:Y:144:LEU:HB3	5:Y:160:ASN:HD22	1.84	0.41
7:a:77:VAL:HA	7:a:80:ILE:HG22	2.02	0.41
9:c:197:ASN:HD22	9:c:197:ASN:HA	1.58	0.41
10:d:155:LYS:HD3	10:d:155:LYS:O	2.17	0.41
15:C:86:LEU:HD11	15:C:94:LYS:HD3	2.03	0.41
15:C:218:GLU:HB2	16:D:275:PHE:HD2	1.86	0.41
19:G:54:LYS:N	19:G:214:GLU:O	2.51	0.41
23:K:111:SER:HA	23:K:114:GLN:HG2	2.03	0.41
25:M:51:LYS:O	25:M:210:GLU:N	2.53	0.41
26:N:14:LEU:HD11	26:N:101:ALA:HB3	2.01	0.41
26:N:120:MET:H	32:T:61:GLN:HE22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:138:TYR:O	26:N:142:THR:CB	2.69	0.41
20:h:69:THR:HG22	20:h:72:ILE:HB	2.03	0.41
27:o:211:VAL:HG11	28:p:198:ARG:HD3	2.02	0.41
1:U:389:ASN:ND2	1:U:392:TRP:HB3	2.36	0.41
1:U:519:VAL:HG23	1:U:520:MET:HG2	2.02	0.41
1:U:791:LEU:HD22	1:U:911:ILE:HD11	2.02	0.41
6:Z:279:LYS:N	6:Z:279:LYS:HE2	2.35	0.41
7:a:116:THR:O	7:a:120:ALA:CB	2.68	0.41
12:f:719:PRO:HB3	12:f:754:LYS:HB2	2.02	0.41
13:A:240:VAL:HB	13:A:274:PHE:HD1	1.85	0.41
13:A:386:ARG:HD3	14:B:217:LYS:NZ	2.36	0.41
15:C:355:SER:OG	15:C:358:GLU:OE1	2.31	0.41
18:F:164:LEU:HA	18:F:165:PRO:HD3	1.90	0.41
25:M:37:ILE:HD13	25:M:196:ILE:HD11	2.03	0.41
25:M:173:LYS:HA	25:M:176:ILE:HD12	2.03	0.41
28:P:189:ILE:HG23	28:P:196:THR:HB	2.03	0.41
32:T:25:ASP:HA	32:T:187:PHE:HA	2.03	0.41
25:m:36:ALA:HB3	25:m:165:ILE:HG13	2.03	0.41
25:m:163:CYS:SG	25:m:164:ALA:N	2.94	0.41
28:p:135:ASP:OD1	28:p:135:ASP:N	2.45	0.41
1:U:45:ILE:HG21	1:U:64:ALA:HB2	2.02	0.41
1:U:222:PHE:HE1	1:U:754:HIS:HB2	1.85	0.41
2:V:337:LEU:HD22	2:V:367:VAL:HG11	2.01	0.41
2:V:358:MET:CB	2:V:359:PRO:CD	2.99	0.41
3:W:180:LYS:HE3	3:W:181:GLU:HG3	2.02	0.41
12:f:873:LEU:HD11	12:f:876:HIS:O	2.21	0.41
13:A:392:ALA:HA	13:A:395:PHE:HD2	1.86	0.41
15:C:127:LEU:HB2	15:C:128:PRO:HD2	1.93	0.41
16:D:153:MET:SD	16:D:153:MET:N	2.94	0.41
30:R:77:ALA:O	30:R:120:ARG:NH2	2.53	0.41
32:T:37:ARG:HE	26:n:166:ARG:HH12	1.68	0.41
25:m:173:LYS:HA	25:m:176:ILE:HD12	2.03	0.41
1:U:443:LEU:HD22	1:U:461:LEU:HG	2.03	0.41
2:V:152:GLY:HA3	2:V:203:LEU:HD21	2.03	0.41
2:V:194:LYS:HB2	2:V:200:ARG:HB2	2.02	0.41
2:V:229:SER:HA	2:V:232:HIS:HD1	1.86	0.41
3:W:66:ILE:O	3:W:66:ILE:HG13	2.21	0.41
3:W:97:LEU:HD21	3:W:138:VAL:CB	2.48	0.41
3:W:315:MET:O	3:W:315:MET:SD	2.78	0.41
3:W:339:ASP:OD2	3:W:350:ARG:NH1	2.54	0.41
5:Y:213:LEU:HD23	5:Y:213:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:387:ILE:HD13	6:Z:275:LEU:HD12	2.02	0.41
6:Z:83:LYS:NZ	6:Z:87:ALA:O	2.49	0.41
7:a:112:ILE:O	7:a:116:THR:OG1	2.32	0.41
8:b:14:GLU:HB3	8:b:82:GLY:H	1.86	0.41
9:c:42:LEU:O	9:c:46:ARG:HB2	2.21	0.41
9:c:161:ARG:HB3	9:c:201:TYR:CZ	2.56	0.41
12:f:39:LYS:O	12:f:43:GLN:CB	2.69	0.41
13:A:333:ARG:HE	13:A:336:ARG:HH22	1.68	0.41
14:B:246:THR:HG1	14:B:280:SER:HB3	1.79	0.41
15:C:19:GLY:O	15:C:23:TYR:CB	2.69	0.41
15:C:20:LEU:HD12	15:C:21:ARG:HE	1.85	0.41
16:D:189:GLU:O	16:D:193:GLN:CB	2.68	0.41
16:D:276:ASP:N	16:D:282:ASP:OD2	2.53	0.41
19:G:53:GLN:HA	19:G:215:ILE:HA	2.02	0.41
21:I:147:LEU:HD12	21:I:159:TRP:HB2	2.02	0.41
24:L:199:LEU:HD13	24:L:204:ASP:HA	2.03	0.41
27:O:167:LEU:HD23	27:O:167:LEU:HA	1.94	0.41
27:O:214:GLU:HA	28:P:198:ARG:HG2	2.03	0.41
28:P:28:PHE:HD2	28:P:35:VAL:HB	1.86	0.41
30:R:182:ASP:OD1	30:R:182:ASP:N	2.54	0.41
19:g:53:GLN:HA	19:g:215:ILE:HA	2.02	0.41
22:j:121:SER:OG	22:j:122:ASN:N	2.53	0.41
23:k:111:SER:HA	23:k:114:GLN:HG2	2.03	0.41
25:m:51:LYS:O	25:m:210:GLU:N	2.53	0.41
27:o:120:ASP:N	27:o:120:ASP:OD1	2.53	0.41
28:p:28:PHE:HD2	28:p:35:VAL:HB	1.86	0.41
3:W:13:ILE:HA	3:W:16:MET:HG2	2.03	0.41
4:X:397:TYR:O	4:X:401:LEU:HB2	2.21	0.41
6:Z:9:VAL:HG22	6:Z:160:SER:HA	2.02	0.41
12:f:691:PRO:HA	12:f:694:LEU:HB2	2.03	0.41
13:A:328:ASP:HA	13:A:329:PRO:HD3	1.96	0.41
14:B:141:LYS:H	14:B:141:LYS:HG3	1.57	0.41
17:E:217:GLU:HA	17:E:220:ASN:HD22	1.86	0.41
25:M:36:ALA:HB3	25:M:165:ILE:HG13	2.03	0.41
29:Q:23:SER:HB2	29:Q:28:MET:HG2	2.03	0.41
22:j:109:ARG:O	22:j:113:SER:HB3	2.21	0.41
25:m:179:LEU:HD13	25:m:179:LEU:HA	1.96	0.41
26:n:104:ASP:N	26:n:108:GLY:O	2.52	0.41
2:V:32:PRO:HG3	2:V:76:LYS:CE	2.51	0.40
2:V:285:TRP:HE1	2:V:315:LYS:NZ	2.18	0.40
2:V:494:MET:O	2:V:494:MET:SD	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:122:ARG:HD2	4:X:125:LEU:HB2	2.03	0.40
5:Y:92:GLU:HB3	5:Y:100:ILE:HD11	2.03	0.40
5:Y:312:ARG:HA	5:Y:356:THR:HG22	2.03	0.40
6:Z:34:ARG:HH12	6:Z:60:GLU:HG3	1.86	0.40
6:Z:69:PHE:HB2	8:b:99:HIS:CE1	2.56	0.40
7:a:93:ALA:O	7:a:97:LEU:CB	2.54	0.40
8:b:150:THR:HB	8:b:153:LEU:CD2	2.49	0.40
12:f:206:ASP:OD2	12:f:245:ASN:ND2	2.54	0.40
16:D:284:GLU:O	16:D:288:ILE:HG12	2.21	0.40
21:I:238:LYS:HA	21:I:241:GLU:HB2	2.03	0.40
22:J:109:ARG:O	22:J:113:SER:HB3	2.21	0.40
1:U:604:HIS:CD2	1:U:604:HIS:O	2.75	0.40
2:V:28:PRO:HD2	2:V:29:PRO:HD3	2.03	0.40
2:V:494:MET:HE2	2:V:494:MET:HB3	1.65	0.40
4:X:344:ARG:HH21	4:X:384:VAL:HG21	1.87	0.40
5:Y:337:PHE:HA	5:Y:340:ALA:HB3	2.04	0.40
6:Z:35:VAL:HB	6:Z:97:THR:HB	2.02	0.40
6:Z:137:ALA:O	6:Z:157:HIS:ND1	2.54	0.40
8:b:138:VAL:H	8:b:160:LEU:HD21	1.86	0.40
10:d:167:ILE:HA	10:d:170:LEU:HB3	2.03	0.40
12:f:705:ASN:OD1	12:f:706:ILE:N	2.54	0.40
12:f:801:VAL:HB	12:f:804:LEU:HD11	2.02	0.40
12:f:827:PRO:HA	12:f:862:ILE:HG13	2.03	0.40
12:f:873:LEU:HD12	12:f:876:HIS:O	2.22	0.40
13:A:185:GLU:OE1	13:A:188:ARG:NH2	2.55	0.40
13:A:415:LYS:O	13:A:419:SER:HB3	2.21	0.40
14:B:265:LYS:HA	14:B:268:ARG:HE	1.86	0.40
15:C:134:LEU:HD21	15:C:212:ILE:HG12	2.03	0.40
17:E:200:SER:HB2	17:E:232:MET:HE3	2.02	0.40
17:E:260:LEU:HG	17:E:264:MET:HE3	2.04	0.40
20:H:69:THR:HG22	20:H:72:ILE:HB	2.03	0.40
23:K:72:ALA:O	23:K:226:PHE:N	2.46	0.40
25:M:39:ILE:HD11	25:M:189:ILE:HG23	2.04	0.40
1:U:549:ALA:HB1	1:U:581:SER:HB2	2.04	0.40
2:V:345:ARG:HD2	2:V:361:PHE:HB2	2.03	0.40
2:V:428:LEU:HD21	2:V:437:ILE:HD13	2.04	0.40
3:W:324:TYR:HD1	3:W:327:GLU:HG2	1.86	0.40
8:b:37:CYS:O	8:b:41:THR:OG1	2.34	0.40
10:d:172:ASP:O	10:d:174:ILE:N	2.54	0.40
10:d:215:TRP:HB3	10:d:222:TYR:HB3	2.03	0.40
13:A:52:ILE:HA	13:A:55:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:R:167:ASP:HB3	30:R:170:SER:HB2	2.04	0.40
21:i:69:ASN:HD22	21:i:72:MET:HE3	1.85	0.40
22:j:95:ARG:HG2	29:q:62:LYS:HE3	2.03	0.40
23:k:12:VAL:HG12	23:k:23:GLN:HE22	1.86	0.40
27:o:217:THR:HB	28:p:195:ILE:HG22	2.02	0.40
28:p:189:ILE:HG23	28:p:196:THR:HB	2.03	0.40
1:U:474:ARG:O	1:U:478:SER:HB3	2.20	0.40
2:V:171:VAL:CG2	2:V:175:MET:HE3	2.52	0.40
2:V:470:ARG:HB3	6:Z:250:TYR:CD1	2.50	0.40
4:X:347:ILE:HA	4:X:350:ILE:HG22	2.03	0.40
4:X:378:LEU:HD23	5:Y:311:TYR:HE1	1.86	0.40
6:Z:142:GLU:HB2	6:Z:151:THR:HG22	2.03	0.40
8:b:95:LEU:O	8:b:99:HIS:ND1	2.39	0.40
12:f:83:ARG:O	12:f:87:THR:OG1	2.31	0.40
13:A:284:ARG:O	18:F:334:ARG:NH2	2.35	0.40
27:O:19:ARG:HH21	27:O:26:VAL:HG22	1.87	0.40
21:i:105:ILE:HD13	21:i:110:LEU:HD13	2.04	0.40
21:i:238:LYS:HA	21:i:241:GLU:HB2	2.04	0.40
24:l:199:LEU:HD13	24:l:204:ASP:HA	2.03	0.40
30:r:4:LEU:HA	30:r:127:SER:HA	2.03	0.40
32:t:41:ARG:HH11	32:t:41:ARG:HD3	1.78	0.40
1:U:803:LYS:HB2	1:U:875:PHE:HA	2.03	0.40
2:V:200:ARG:HD2	2:V:242:HIS:HB2	2.02	0.40
3:W:83:LEU:CD1	3:W:91:SER:HB3	2.17	0.40
3:W:180:LYS:HE2	3:W:181:GLU:HG3	2.03	0.40
5:Y:71:ASN:HA	5:Y:74:LYS:HG2	2.04	0.40
8:b:12:ASN:HB2	8:b:80:PRO:HA	2.04	0.40
8:b:125:VAL:HA	8:b:128:ALA:HB3	2.03	0.40
9:c:78:SER:H	9:c:85:GLU:CG	2.29	0.40
9:c:113:HIS:HE1	9:c:115:HIS:CD2	2.38	0.40
10:d:106:LEU:CD2	10:d:115:PHE:HA	2.52	0.40
12:f:204:ALA:HA	12:f:207:LEU:HG	2.04	0.40
12:f:785:ARG:CZ	12:f:791:VAL:CG1	2.97	0.40
17:E:282:PRO:HB2	17:E:388:PRO:HB3	2.02	0.40
18:F:81:LYS:HA	18:F:84:LYS:HE2	2.03	0.40
18:F:223:VAL:HG12	18:F:350:ARG:HB2	2.04	0.40
23:K:12:VAL:HG12	23:K:23:GLN:HE22	1.86	0.40
26:n:9:ASP:OD1	26:n:9:ASP:N	2.54	0.40
29:q:155:ARG:HA	29:q:158:GLU:HG2	2.03	0.40
31:s:36:HIS:O	32:t:151:ARG:NH2	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	806/953 (85%)	726 (90%)	78 (10%)	2 (0%)	44	73
2	V	506/533 (95%)	423 (84%)	71 (14%)	12 (2%)	5	30
3	W	454/456 (100%)	386 (85%)	61 (13%)	7 (2%)	8	39
4	X	378/422 (90%)	355 (94%)	23 (6%)	0	100	100
5	Y	376/389 (97%)	343 (91%)	31 (8%)	2 (0%)	25	59
6	Z	284/324 (88%)	241 (85%)	38 (13%)	5 (2%)	7	35
7	a	371/376 (99%)	324 (87%)	47 (13%)	0	100	100
8	b	189/377 (50%)	169 (89%)	19 (10%)	1 (0%)	25	59
9	c	285/309 (92%)	245 (86%)	35 (12%)	5 (2%)	7	35
10	d	255/349 (73%)	207 (81%)	45 (18%)	3 (1%)	11	43
11	e	36/70 (51%)	25 (69%)	9 (25%)	2 (6%)	1	15
12	f	887/908 (98%)	703 (79%)	171 (19%)	13 (2%)	8	39
13	A	392/433 (90%)	337 (86%)	51 (13%)	4 (1%)	13	46
14	B	382/440 (87%)	345 (90%)	33 (9%)	4 (1%)	13	46
15	C	359/398 (90%)	325 (90%)	32 (9%)	2 (1%)	22	55
16	D	378/418 (90%)	332 (88%)	38 (10%)	8 (2%)	5	33
17	E	373/403 (93%)	333 (89%)	40 (11%)	0	100	100
18	F	372/439 (85%)	340 (91%)	32 (9%)	0	100	100
19	G	238/245 (97%)	230 (97%)	8 (3%)	0	100	100
19	g	238/245 (97%)	228 (96%)	9 (4%)	1 (0%)	30	63
20	H	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
20	h	230/233 (99%)	220 (96%)	10 (4%)	0	100	100
21	I	248/260 (95%)	227 (92%)	21 (8%)	0	100	100
21	i	248/260 (95%)	228 (92%)	20 (8%)	0	100	100
22	J	237/247 (96%)	214 (90%)	21 (9%)	2 (1%)	16	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	j	237/247 (96%)	217 (92%)	18 (8%)	2 (1%)	16	51
23	K	224/240 (93%)	210 (94%)	14 (6%)	0	100	100
23	k	224/240 (93%)	210 (94%)	14 (6%)	0	100	100
24	L	236/268 (88%)	214 (91%)	20 (8%)	2 (1%)	16	51
24	l	236/268 (88%)	215 (91%)	20 (8%)	1 (0%)	30	63
25	M	238/254 (94%)	223 (94%)	15 (6%)	0	100	100
25	m	238/254 (94%)	224 (94%)	14 (6%)	0	100	100
26	N	189/238 (79%)	181 (96%)	8 (4%)	0	100	100
26	n	189/238 (79%)	180 (95%)	9 (5%)	0	100	100
27	O	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
27	o	218/276 (79%)	207 (95%)	11 (5%)	0	100	100
28	P	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
28	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	Q	197/201 (98%)	184 (93%)	13 (7%)	0	100	100
29	q	197/201 (98%)	184 (93%)	13 (7%)	0	100	100
30	R	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
30	r	199/262 (76%)	190 (96%)	9 (4%)	0	100	100
31	S	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
31	s	211/240 (88%)	205 (97%)	6 (3%)	0	100	100
32	T	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
32	t	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
All	All	13243/14859 (89%)	11962 (90%)	1203 (9%)	78 (1%)	24	55

All (78) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	167	LEU
2	V	168	GLN
2	V	350	GLN
3	W	70	VAL
3	W	315	MET
6	Z	150	PRO
6	Z	284	ASP
9	c	196	LEU
10	d	123	PRO

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Mol	Chain	Res	Type
11	e	57	ARG
12	f	281	ILE
12	f	475	ASN
12	f	645	ASP
12	f	646	MET
12	f	680	ARG
12	f	756	PRO
12	f	838	ARG
14	B	141	LYS
14	B	278	ALA
15	C	128	PRO
16	D	125	LYS
16	D	126	PRO
24	L	227	ASP
2	V	31	ALA
2	V	265	ASP
2	V	470	ARG
2	V	500	SER
13	A	79	ASP
14	B	140	ASP
16	D	369	LYS
22	J	198	VAL
24	L	226	ASP
1	U	174	PRO
1	U	178	ALA
2	V	139	MET
2	V	224	LEU
2	V	471	GLU
3	W	86	ASN
5	Y	288	PHE
6	Z	151	THR
6	Z	224	HIS
9	c	63	ASP
9	c	83	SER
11	e	59	GLU
16	D	154	LEU
16	D	161	ASP
22	J	49	SER
22	j	198	VAL
3	W	45	GLU
3	W	69	ALA
3	W	136	ILE

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Mol	Chain	Res	Type
10	d	173	THR
12	f	118	ASN
12	f	647	GLY
12	f	789	SER
12	f	839	PRO
15	C	129	ASN
16	D	356	GLU
16	D	367	PRO
19	g	134	LEU
2	V	498	PRO
9	c	156	VAL
10	d	157	ASN
12	f	788	MET
13	A	109	PRO
13	A	310	ASP
24	l	226	ASP
2	V	358	MET
13	A	77	LEU
14	B	279	PRO
16	D	151	ILE
12	f	642	ALA
22	j	199	VAL
8	b	23	PRO
9	c	116	PRO
6	Z	99	PRO
3	W	138	VAL
5	Y	289	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	692/816 (85%)	680 (98%)	12 (2%)	56	75
2	V	415/459 (90%)	395 (95%)	20 (5%)	21	51
3	W	416/416 (100%)	399 (96%)	17 (4%)	26	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	X	327/362 (90%)	327 (100%)	0	100	100
5	Y	334/344 (97%)	326 (98%)	8 (2%)	44	67
6	Z	257/295 (87%)	241 (94%)	16 (6%)	15	44
7	a	333/336 (99%)	329 (99%)	4 (1%)	67	82
8	b	167/312 (54%)	166 (99%)	1 (1%)	84	92
9	c	252/267 (94%)	241 (96%)	11 (4%)	24	53
10	d	231/293 (79%)	218 (94%)	13 (6%)	17	47
11	e	38/63 (60%)	35 (92%)	3 (8%)	10	35
12	f	745/763 (98%)	721 (97%)	24 (3%)	34	61
13	A	337/372 (91%)	330 (98%)	7 (2%)	48	71
14	B	339/385 (88%)	328 (97%)	11 (3%)	34	61
15	C	314/346 (91%)	307 (98%)	7 (2%)	47	69
16	D	333/366 (91%)	320 (96%)	13 (4%)	27	57
17	E	298/353 (84%)	290 (97%)	8 (3%)	40	65
18	F	296/379 (78%)	295 (100%)	1 (0%)	91	96
19	G	193/209 (92%)	191 (99%)	2 (1%)	73	85
19	g	193/209 (92%)	190 (98%)	3 (2%)	58	76
20	H	164/190 (86%)	164 (100%)	0	100	100
20	h	164/190 (86%)	164 (100%)	0	100	100
21	I	193/220 (88%)	190 (98%)	3 (2%)	58	76
21	i	193/220 (88%)	193 (100%)	0	100	100
22	J	154/210 (73%)	150 (97%)	4 (3%)	41	65
22	j	152/210 (72%)	150 (99%)	2 (1%)	65	81
23	K	186/202 (92%)	186 (100%)	0	100	100
23	k	186/202 (92%)	186 (100%)	0	100	100
24	L	198/229 (86%)	196 (99%)	2 (1%)	73	85
24	l	198/229 (86%)	196 (99%)	2 (1%)	73	85
25	M	192/211 (91%)	190 (99%)	2 (1%)	73	85
25	m	192/211 (91%)	192 (100%)	0	100	100
26	N	148/180 (82%)	148 (100%)	0	100	100
26	n	148/180 (82%)	148 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	O	177/227 (78%)	177 (100%)	0	100	100
27	o	177/227 (78%)	177 (100%)	0	100	100
28	P	173/173 (100%)	173 (100%)	0	100	100
28	p	173/173 (100%)	173 (100%)	0	100	100
29	Q	164/171 (96%)	164 (100%)	0	100	100
29	q	164/171 (96%)	163 (99%)	1 (1%)	84	92
30	R	153/201 (76%)	153 (100%)	0	100	100
30	r	153/201 (76%)	153 (100%)	0	100	100
31	S	174/198 (88%)	174 (100%)	0	100	100
31	s	175/198 (88%)	175 (100%)	0	100	100
32	T	175/214 (82%)	175 (100%)	0	100	100
32	t	175/214 (82%)	175 (100%)	0	100	100
All	All	11011/12597 (87%)	10814 (98%)	197 (2%)	54	74

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	179	TYR
1	U	529	ILE
1	U	554	LEU
1	U	583	MET
1	U	601	ARG
1	U	602	LEU
1	U	603	LEU
1	U	605	VAL
1	U	629	THR
1	U	689	ILE
1	U	775	LEU
1	U	913	ILE
2	V	140	ASP
2	V	163	VAL
2	V	167	LEU
2	V	169	LEU
2	V	170	LEU
2	V	171	VAL
2	V	194	LYS
2	V	216	ARG
2	V	222	ASP

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Mol	Chain	Res	Type
2	V	223	LYS
2	V	262	SER
2	V	263	LEU
2	V	265	ASP
2	V	357	LEU
2	V	358	MET
2	V	442	ILE
2	V	469	THR
2	V	470	ARG
2	V	494	MET
2	V	495	ARG
3	W	48	LEU
3	W	66	ILE
3	W	67	LEU
3	W	68	VAL
3	W	82	LEU
3	W	83	LEU
3	W	89	LEU
3	W	138	VAL
3	W	171	VAL
3	W	172	GLU
3	W	173	THR
3	W	177	MET
3	W	178	GLU
3	W	179	LYS
3	W	180	LYS
3	W	314	LEU
3	W	315	MET
5	Y	168	ILE
5	Y	169	GLU
5	Y	286	TRP
5	Y	287	LEU
5	Y	288	PHE
5	Y	296	VAL
5	Y	334	LEU
5	Y	336	ARG
6	Z	91	ILE
6	Z	142	GLU
6	Z	143	GLU
6	Z	144	VAL
6	Z	147	ASP
6	Z	149	THR

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Mol	Chain	Res	Type
6	Z	151	THR
6	Z	152	SER
6	Z	153	LYS
6	Z	193	ASN
6	Z	224	HIS
6	Z	243	GLN
6	Z	244	GLU
6	Z	252	LYS
6	Z	279	LYS
6	Z	283	ARG
7	a	8	LEU
7	a	165	THR
7	a	186	LYS
7	a	190	VAL
8	b	150	THR
9	c	69	VAL
9	c	84	VAL
9	c	85	GLU
9	c	87	VAL
9	c	88	ASP
9	c	154	LYS
9	c	155	VAL
9	c	157	ILE
9	c	196	LEU
9	c	197	ASN
9	c	251	LEU
10	d	106	LEU
10	d	108	SER
10	d	117	THR
10	d	118	GLU
10	d	119	LEU
10	d	120	GLU
10	d	121	ARG
10	d	122	LEU
10	d	155	LYS
10	d	171	LEU
10	d	178	ILE
10	d	199	PHE
10	d	200	PHE
11	e	53	SER
11	e	56	LEU
11	e	57	ARG

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Mol	Chain	Res	Type
12	f	75	LEU
12	f	128	VAL
12	f	129	LEU
12	f	281	ILE
12	f	282	PHE
12	f	283	THR
12	f	457	ASN
12	f	476	THR
12	f	613	LEU
12	f	659	LEU
12	f	672	LEU
12	f	680	ARG
12	f	755	ASP
12	f	759	LEU
12	f	771	LEU
12	f	773	LYS
12	f	785	ARG
12	f	787	LEU
12	f	788	MET
12	f	822	VAL
12	f	837	LEU
12	f	838	ARG
12	f	840	LEU
12	f	842	VAL
13	A	72	LEU
13	A	77	LEU
13	A	307	ASP
13	A	312	ARG
13	A	400	ARG
13	A	401	ARG
13	A	403	ILE
14	B	60	LEU
14	B	61	LYS
14	B	103	ARG
14	B	125	THR
14	B	141	LYS
14	B	142	ASP
14	B	143	LEU
14	B	170	LEU
14	B	277	HIS
14	B	280	SER
14	B	359	LYS

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Mol	Chain	Res	Type
15	C	88	LYS
15	C	90	HIS
15	C	109	THR
15	C	125	LYS
15	C	127	LEU
15	C	130	LYS
15	C	210	THR
16	D	93	LEU
16	D	124	LEU
16	D	125	LYS
16	D	151	ILE
16	D	162	VAL
16	D	231	VAL
16	D	335	LEU
16	D	338	ARG
16	D	342	ARG
16	D	353	ASN
16	D	354	LEU
16	D	357	GLU
16	D	366	ARG
17	E	113	ARG
17	E	114	GLU
17	E	118	LEU
17	E	138	LEU
17	E	157	GLU
17	E	158	LEU
17	E	160	GLN
17	E	161	ARG
18	F	217	ILE
19	G	132	ARG
19	G	222	VAL
21	I	226	ARG
21	I	227	VAL
21	I	228	LEU
22	J	52	LYS
22	J	56	GLU
22	J	159	ASN
22	J	201	SER
24	L	103	LEU
24	L	161	ILE
25	M	40	ARG
25	M	42	LYS

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Mol	Chain	Res	Type
19	g	134	LEU
19	g	222	VAL
19	g	224	ASN
22	j	159	ASN
22	j	201	SER
24	l	103	LEU
24	l	161	ILE
29	q	121	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (214) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	111	GLN
1	U	241	ASN
1	U	247	GLN
1	U	338	HIS
1	U	345	ASN
1	U	355	ASN
1	U	377	HIS
1	U	389	ASN
1	U	415	HIS
1	U	595	ASN
1	U	604	HIS
1	U	718	ASN
1	U	777	HIS
2	V	62	HIS
2	V	252	ASN
2	V	257	ASN
2	V	326	GLN
2	V	387	GLN
2	V	400	HIS
2	V	401	ASN
2	V	427	GLN
2	V	452	ASN
3	W	84	ASN
3	W	96	GLN
3	W	106	GLN
3	W	236	HIS
3	W	399	ASN
3	W	430	GLN
3	W	440	ASN
4	X	182	ASN

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Mol	Chain	Res	Type
4	X	213	GLN
4	X	333	GLN
4	X	380	GLN
5	Y	136	HIS
5	Y	273	GLN
5	Y	291	HIS
5	Y	363	ASN
5	Y	365	GLN
5	Y	367	GLN
6	Z	109	ASN
6	Z	174	HIS
6	Z	194	GLN
6	Z	202	ASN
6	Z	224	HIS
6	Z	225	GLN
6	Z	231	GLN
6	Z	273	HIS
6	Z	277	ASN
6	Z	282	ASN
7	a	12	GLN
7	a	18	GLN
7	a	23	HIS
7	a	35	HIS
7	a	164	GLN
7	a	212	ASN
7	a	231	GLN
7	a	249	GLN
7	a	258	GLN
7	a	290	GLN
7	a	337	GLN
7	a	345	GLN
7	a	370	GLN
8	b	105	HIS
9	c	30	GLN
9	c	44	HIS
9	c	101	GLN
9	c	113	HIS
9	c	130	GLN
9	c	149	GLN
9	c	164	ASN
9	c	166	ASN
9	c	197	ASN

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Mol	Chain	Res	Type
9	c	199	HIS
9	c	232	GLN
9	c	237	HIS
9	c	241	ASN
9	c	254	ASN
9	c	274	ASN
9	c	278	GLN
10	d	77	GLN
10	d	88	GLN
10	d	116	HIS
10	d	135	HIS
10	d	229	GLN
12	f	14	GLN
12	f	43	GLN
12	f	112	ASN
12	f	171	GLN
12	f	213	GLN
12	f	291	GLN
12	f	382	ASN
12	f	396	ASN
12	f	428	GLN
12	f	457	ASN
12	f	531	ASN
12	f	565	ASN
12	f	619	HIS
12	f	650	GLN
12	f	715	HIS
12	f	737	ASN
12	f	747	GLN
12	f	766	GLN
12	f	826	GLN
12	f	848	GLN
13	A	54	GLN
13	A	117	GLN
13	A	304	ASN
13	A	433	ASN
14	B	154	HIS
14	B	241	ASN
14	B	242	GLN
15	C	36	ASN
15	C	48	GLN
15	C	53	ASN

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Mol	Chain	Res	Type
15	C	64	GLN
15	C	90	HIS
15	C	221	GLN
15	C	241	HIS
15	C	337	ASN
15	C	380	GLN
16	D	49	GLN
16	D	67	ASN
16	D	98	GLN
16	D	133	HIS
16	D	173	GLN
16	D	222	HIS
16	D	257	ASN
16	D	312	ASN
16	D	380	GLN
16	D	390	ASN
16	D	412	GLN
17	E	75	ASN
17	E	323	HIS
18	F	83	ASN
18	F	184	GLN
18	F	196	GLN
18	F	208	HIS
18	F	369	HIS
18	F	380	ASN
19	G	12	HIS
19	G	68	HIS
19	G	92	GLN
19	G	128	ASN
20	H	21	GLN
20	H	63	HIS
20	H	169	ASN
21	I	84	ASN
21	I	100	GLN
21	I	102	GLN
21	I	146	GLN
22	J	116	GLN
22	J	159	ASN
23	K	23	GLN
23	K	41	GLN
23	K	98	ASN
23	K	118	ASN

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Mol	Chain	Res	Type
23	K	155	HIS
23	K	164	GLN
23	K	224	GLN
24	L	90	GLN
24	L	146	GLN
25	M	221	ASN
26	N	28	ASN
26	N	154	GLN
26	N	158	ASN
28	P	169	GLN
29	Q	8	GLN
29	Q	61	GLN
29	Q	82	ASN
31	S	131	GLN
32	T	2	GLN
32	T	61	GLN
32	T	213	HIS
19	g	33	ASN
19	g	68	HIS
19	g	92	GLN
19	g	128	ASN
20	h	63	HIS
20	h	102	GLN
20	h	109	GLN
20	h	169	ASN
21	i	20	GLN
21	i	53	HIS
21	i	84	ASN
21	i	100	GLN
21	i	102	GLN
21	i	146	GLN
21	i	220	ASN
22	j	54	GLN
22	j	122	ASN
22	j	159	ASN
22	j	205	ASN
23	k	23	GLN
23	k	41	GLN
23	k	98	ASN
23	k	118	ASN
23	k	164	GLN
23	k	224	GLN

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Mol	Chain	Res	Type
24	l	90	GLN
24	l	146	GLN
24	l	166	GLN
25	m	221	ASN
26	n	28	ASN
26	n	154	GLN
26	n	158	ASN
27	o	116	HIS
27	o	165	ASN
28	p	93	ASN
29	q	8	GLN
29	q	61	GLN
29	q	82	ASN
32	t	2	GLN
32	t	65	GLN
32	t	69	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	ATP	D	501	35	26,33,33	0.89	1 (3%)	31,52,52	1.72	5 (16%)
34	ATP	A	501	35	26,33,33	0.93	1 (3%)	31,52,52	1.66	5 (16%)
36	ADP	C	501	-	24,29,29	0.98	1 (4%)	29,45,45	1.54	4 (13%)
34	ATP	B	501	35	26,33,33	0.89	1 (3%)	31,52,52	1.73	5 (16%)
36	ADP	F	501	35	24,29,29	0.90	1 (4%)	29,45,45	1.48	5 (17%)
34	ATP	E	401	35	26,33,33	0.91	1 (3%)	31,52,52	1.68	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	ATP	D	501	35	-	2/18/38/38	0/3/3/3
34	ATP	A	501	35	-	0/18/38/38	0/3/3/3
36	ADP	C	501	-	-	3/12/32/32	0/3/3/3
34	ATP	B	501	35	-	0/18/38/38	0/3/3/3
36	ADP	F	501	35	-	4/12/32/32	0/3/3/3
34	ATP	E	401	35	-	6/18/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	C	501	ADP	C5-C4	2.45	1.47	1.40
34	E	401	ATP	C5-C4	2.29	1.47	1.40
34	A	501	ATP	C5-C4	2.28	1.47	1.40
36	F	501	ADP	C5-C4	2.24	1.46	1.40
34	D	501	ATP	C5-C4	2.21	1.46	1.40
34	B	501	ATP	C5-C4	2.19	1.46	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	501	ATP	PA-O3A-PB	-5.07	115.44	132.83
34	E	401	ATP	PA-O3A-PB	-4.79	116.39	132.83
34	D	501	ATP	PA-O3A-PB	-4.72	116.63	132.83
34	A	501	ATP	PB-O3B-PG	-4.25	118.24	132.83
36	F	501	ADP	PA-O3A-PB	-4.03	119.01	132.83
36	C	501	ADP	PA-O3A-PB	-3.82	119.73	132.83
34	D	501	ATP	PB-O3B-PG	-3.68	120.21	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	A	501	ATP	C3'-C2'-C1'	3.64	106.46	100.98
34	A	501	ATP	PA-O3A-PB	-3.57	120.59	132.83
34	E	401	ATP	PB-O3B-PG	-3.55	120.64	132.83
36	C	501	ADP	C3'-C2'-C1'	3.53	106.29	100.98
34	D	501	ATP	N3-C2-N1	-3.52	123.18	128.68
34	B	501	ATP	PB-O3B-PG	-3.41	121.13	132.83
34	B	501	ATP	N3-C2-N1	-3.39	123.38	128.68
34	B	501	ATP	C3'-C2'-C1'	3.26	105.88	100.98
34	E	401	ATP	C3'-C2'-C1'	3.13	105.69	100.98
34	E	401	ATP	N3-C2-N1	-3.11	123.82	128.68
36	F	501	ADP	C3'-C2'-C1'	3.08	105.62	100.98
34	D	501	ATP	C3'-C2'-C1'	3.06	105.59	100.98
36	C	501	ADP	N3-C2-N1	-3.06	123.90	128.68
34	A	501	ATP	C4-C5-N7	-2.91	106.36	109.40
36	F	501	ADP	N3-C2-N1	-2.81	124.29	128.68
34	A	501	ATP	N3-C2-N1	-2.79	124.32	128.68
36	F	501	ADP	C4-C5-N7	-2.58	106.71	109.40
34	B	501	ATP	C4-C5-N7	-2.54	106.76	109.40
34	E	401	ATP	C4-C5-N7	-2.47	106.82	109.40
36	C	501	ADP	C4-C5-N7	-2.40	106.89	109.40
34	D	501	ATP	C4-C5-N7	-2.33	106.97	109.40
36	F	501	ADP	O3B-PB-O2B	2.08	115.60	107.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

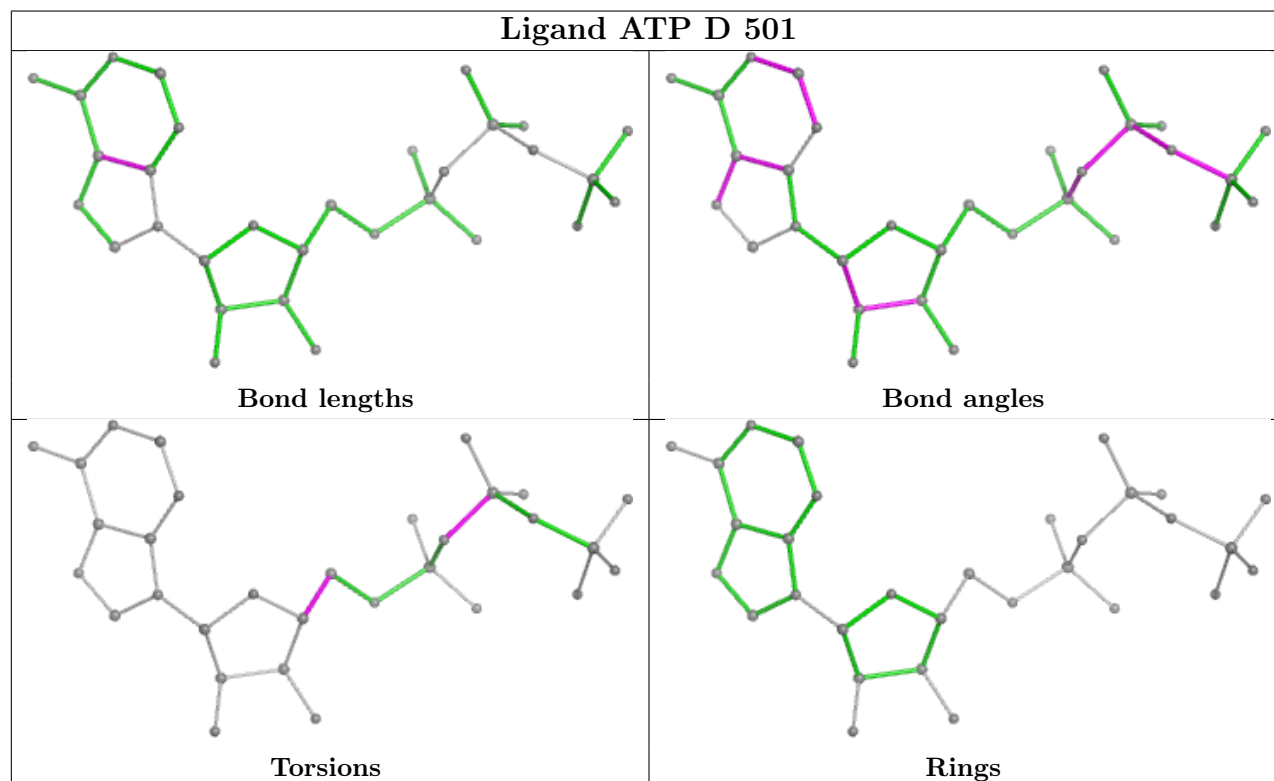
Mol	Chain	Res	Type	Atoms
34	E	401	ATP	PB-O3B-PG-O2G
34	E	401	ATP	C5'-O5'-PA-O2A
34	E	401	ATP	C5'-O5'-PA-O3A
34	E	401	ATP	O4'-C4'-C5'-O5'
36	C	501	ADP	C5'-O5'-PA-O1A
36	C	501	ADP	C5'-O5'-PA-O2A
36	F	501	ADP	C3'-C4'-C5'-O5'
34	E	401	ATP	C3'-C4'-C5'-O5'
36	F	501	ADP	O4'-C4'-C5'-O5'
36	C	501	ADP	C5'-O5'-PA-O3A
34	E	401	ATP	PB-O3B-PG-O1G
36	F	501	ADP	C5'-O5'-PA-O3A
34	D	501	ATP	PA-O3A-PB-O2B
36	F	501	ADP	C5'-O5'-PA-O2A
34	D	501	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

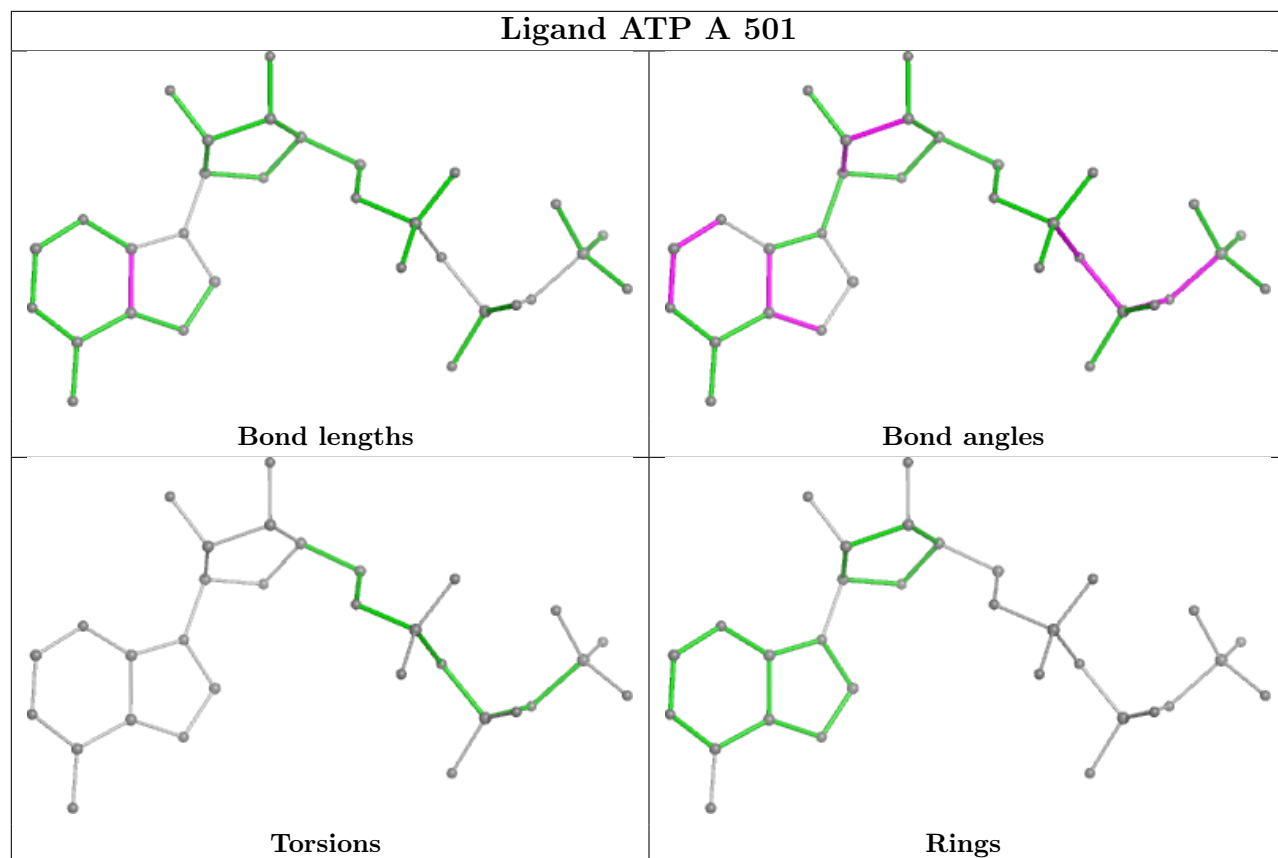
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	D	501	ATP	1	0
34	A	501	ATP	1	0
34	B	501	ATP	1	0
36	F	501	ADP	2	0
34	E	401	ATP	4	0

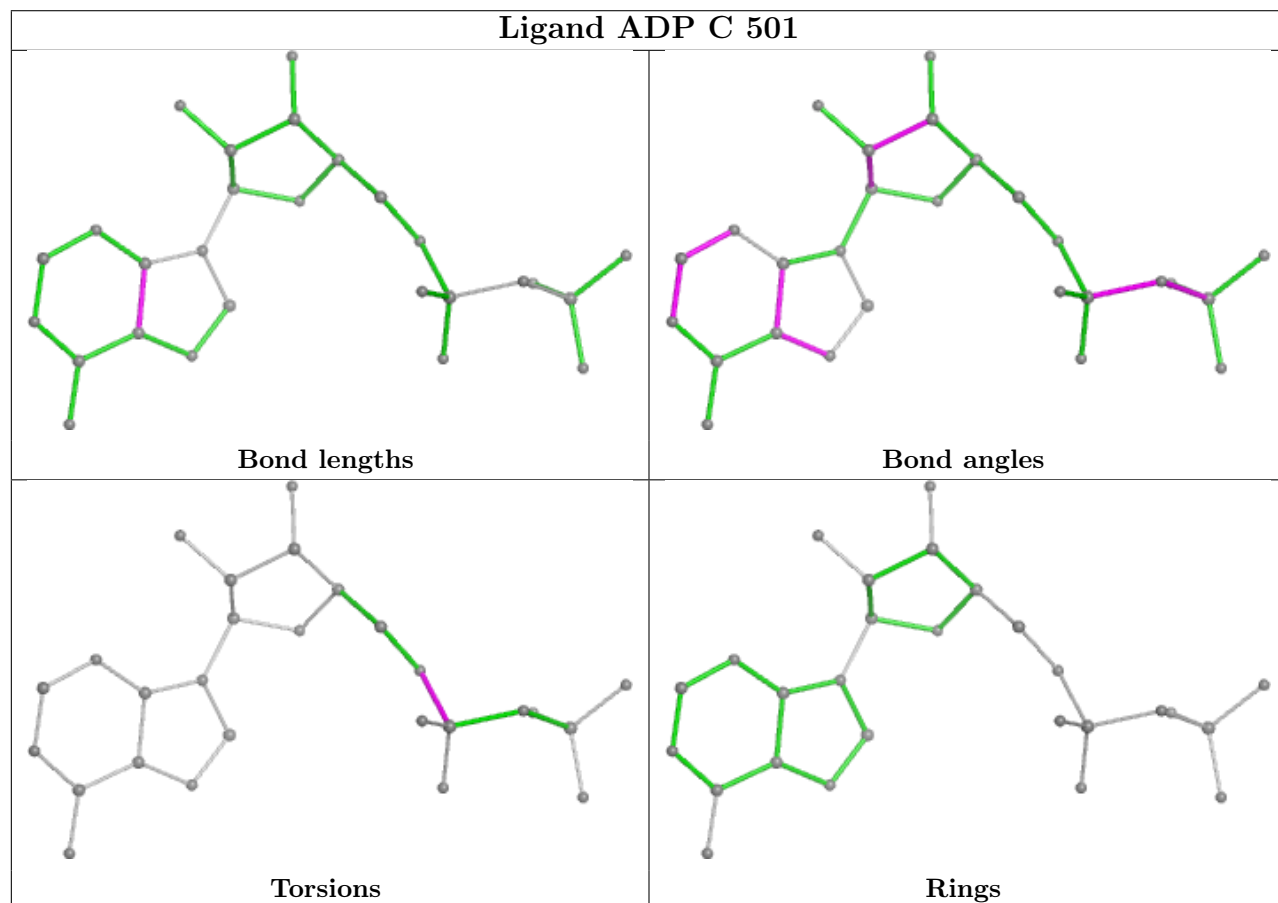
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

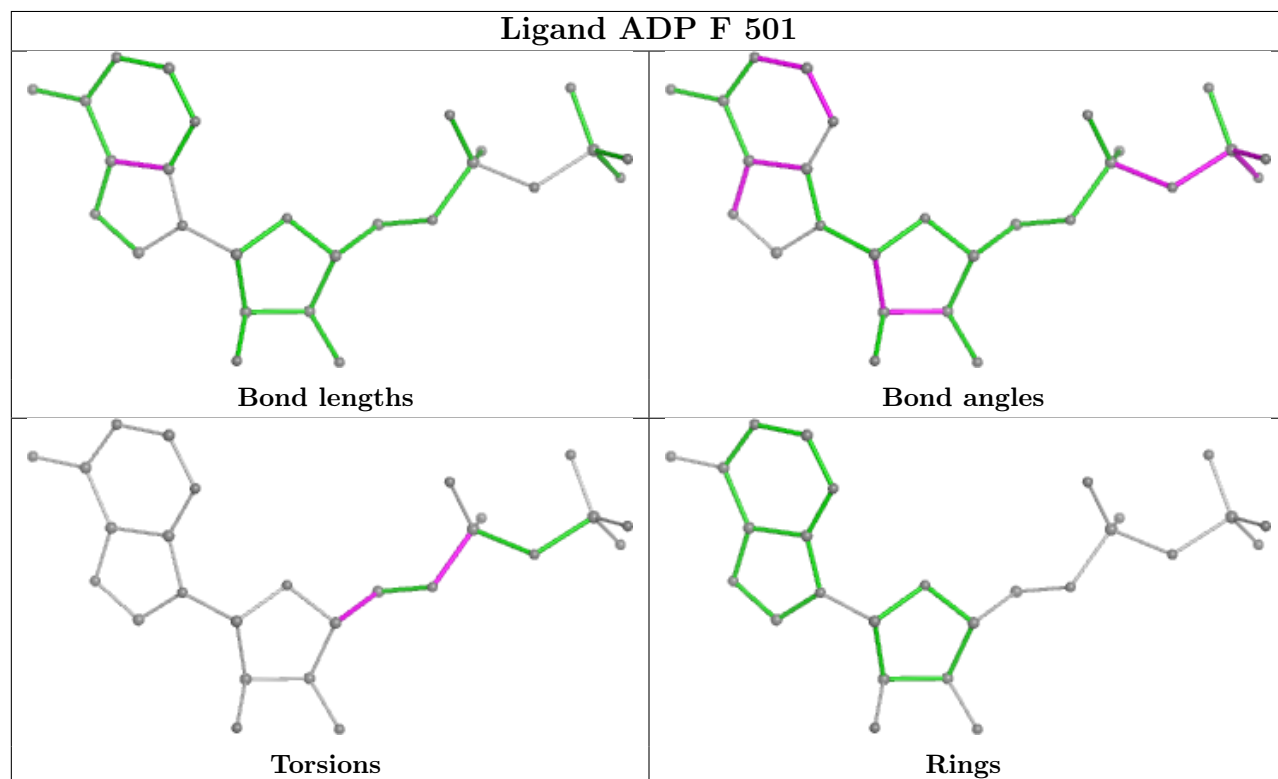
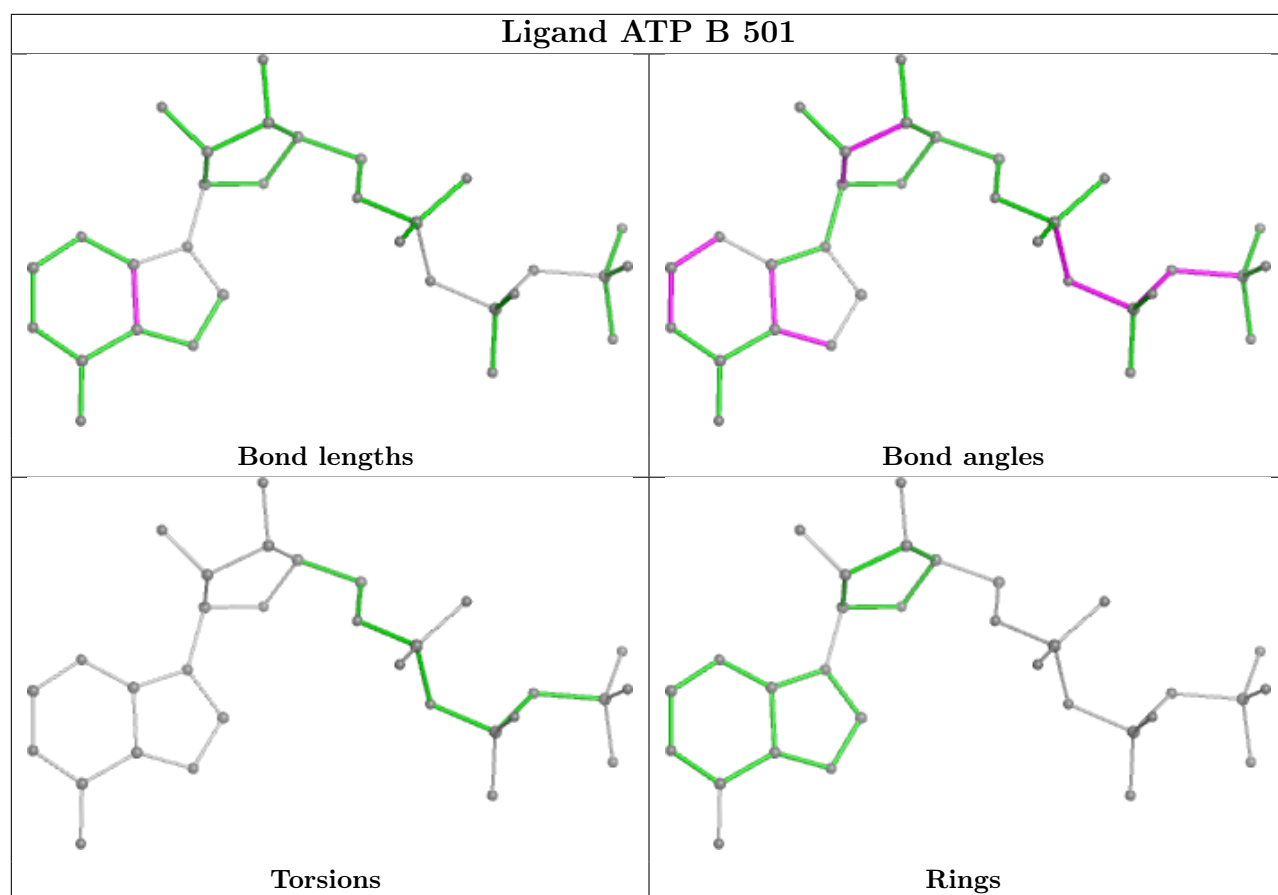


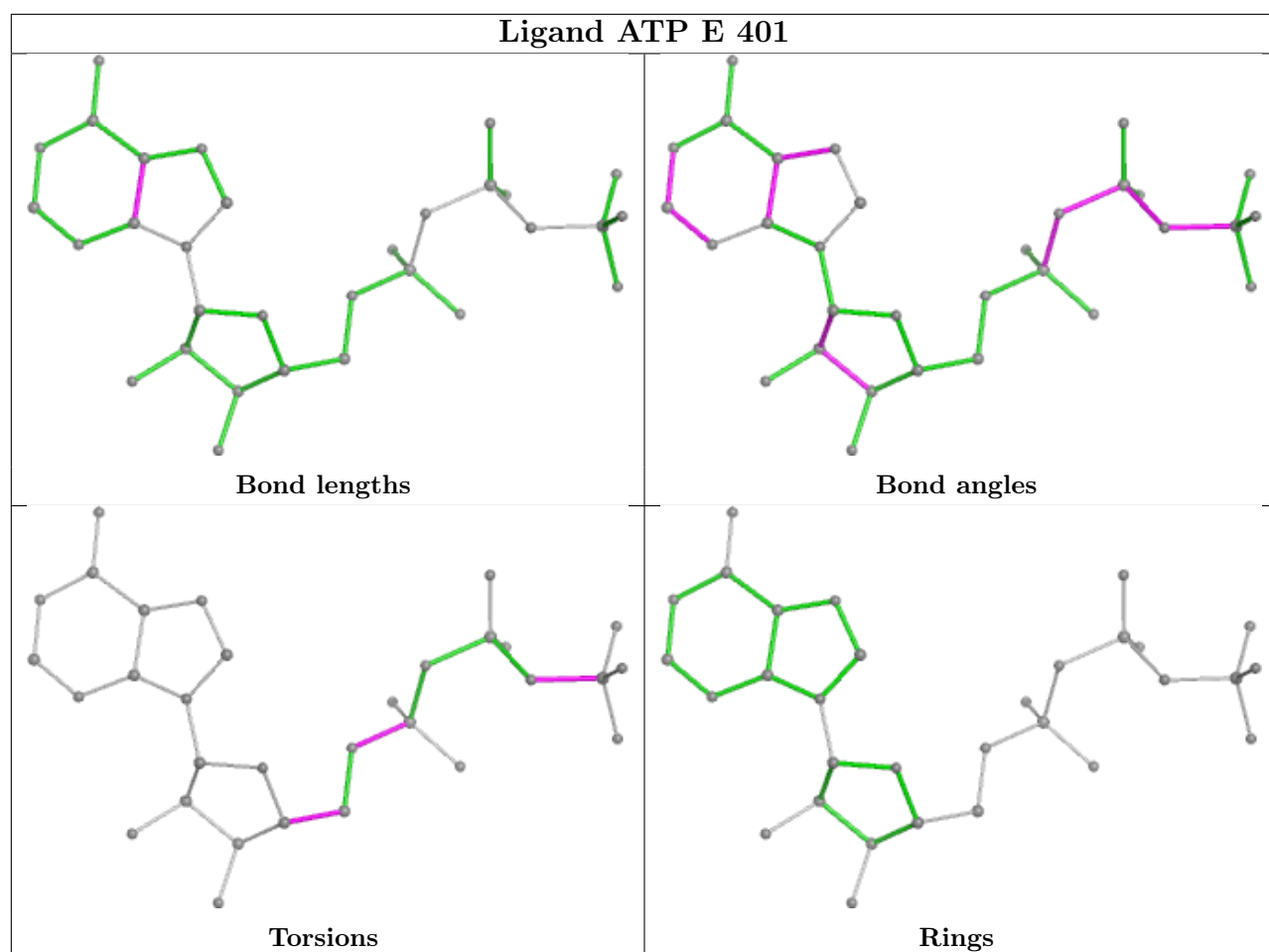
Ligand ATP A 501



Ligand ADP C 501







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

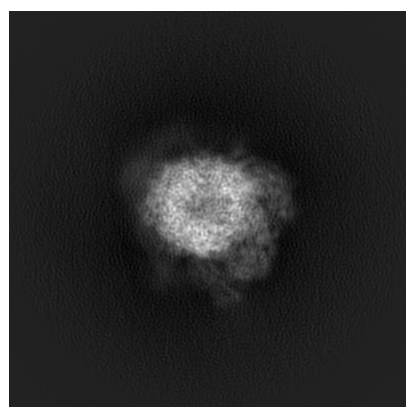
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14202. These allow visual inspection of the internal detail of the map and identification of artifacts.

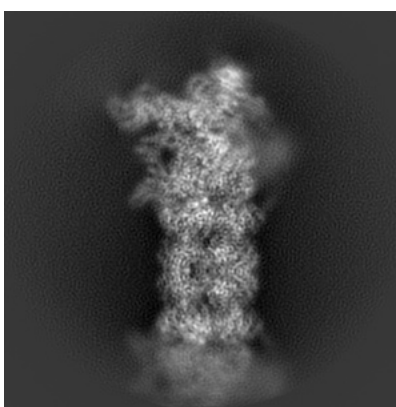
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

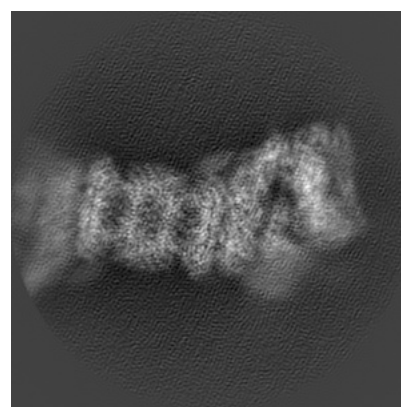
6.1.1 Primary map



X



Y

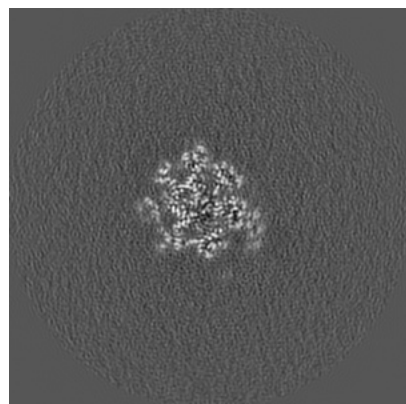


Z

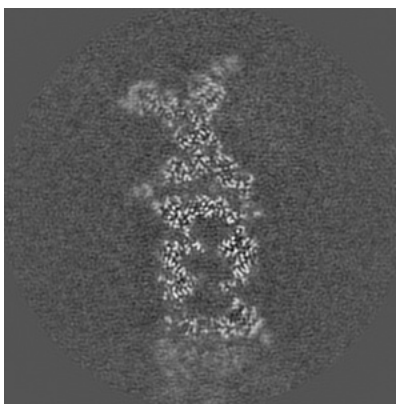
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

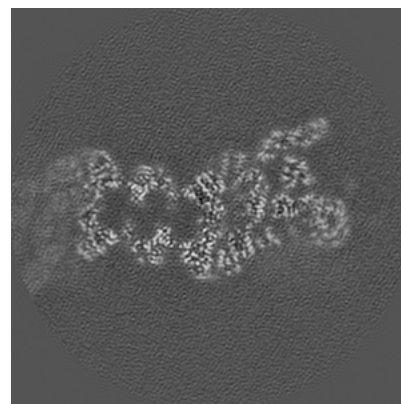
6.2.1 Primary map



X Index: 160



Y Index: 160

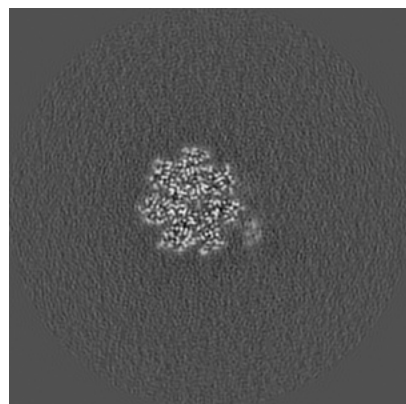


Z Index: 160

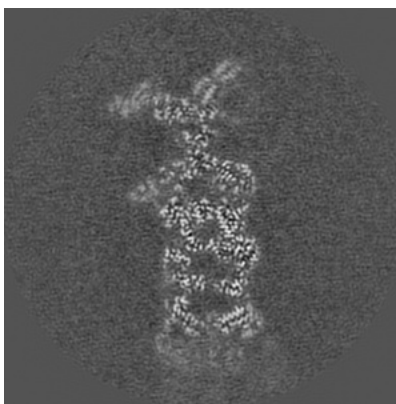
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

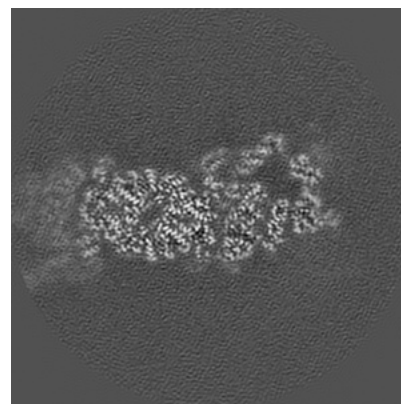
6.3.1 Primary map



X Index: 153



Y Index: 165

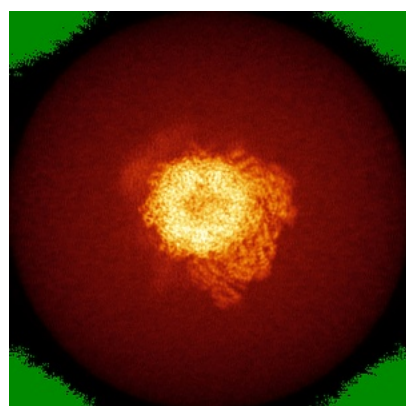


Z Index: 145

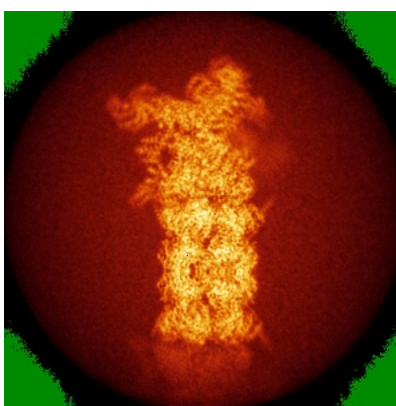
The images above show the largest variance slices of the map in three orthogonal directions.

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

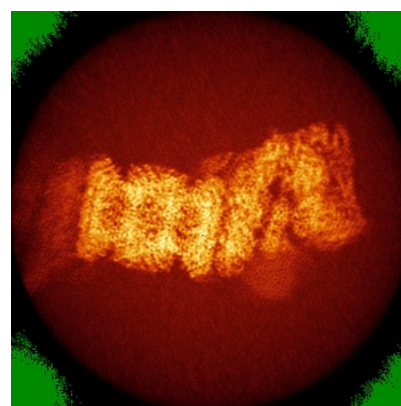
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

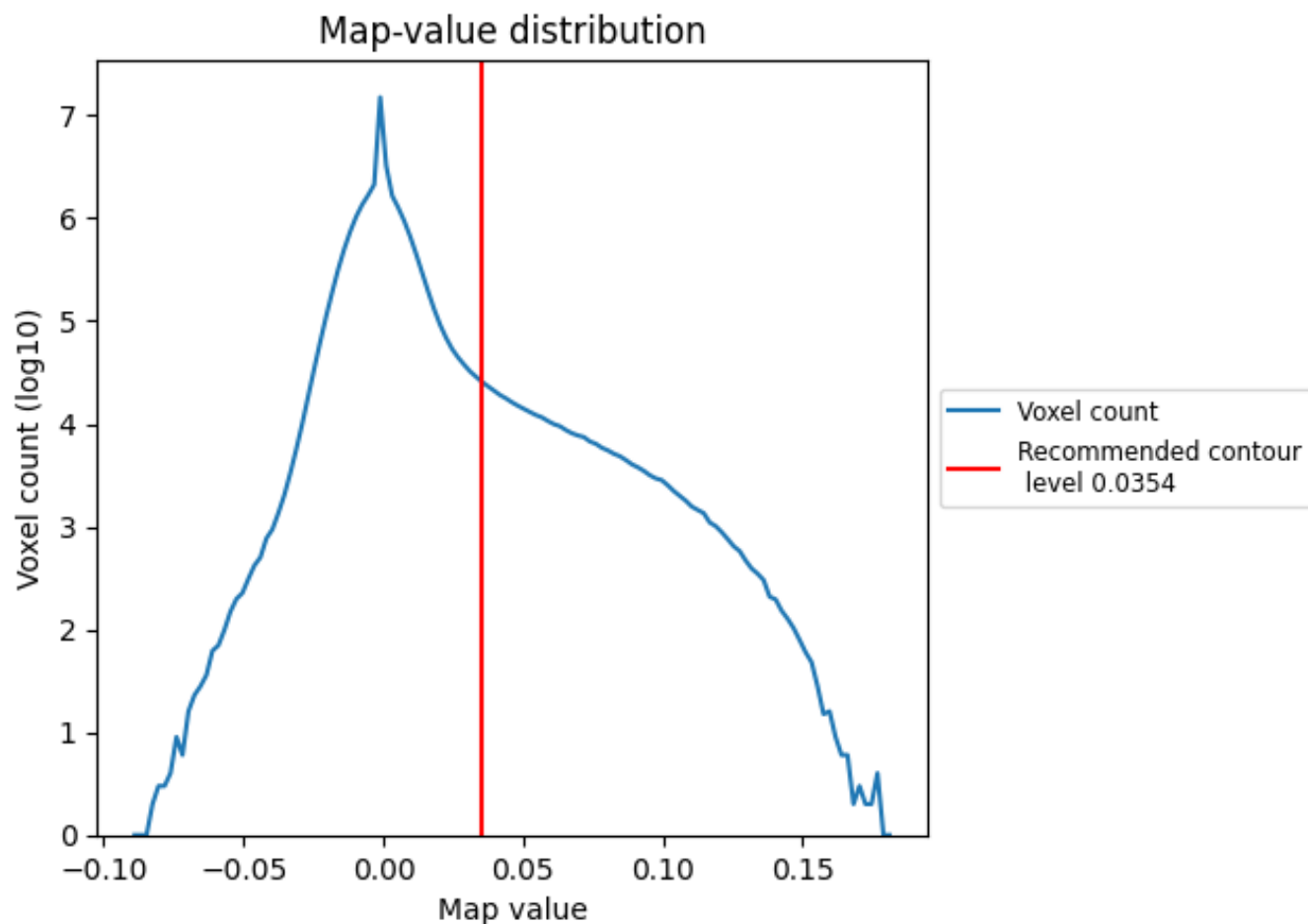
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

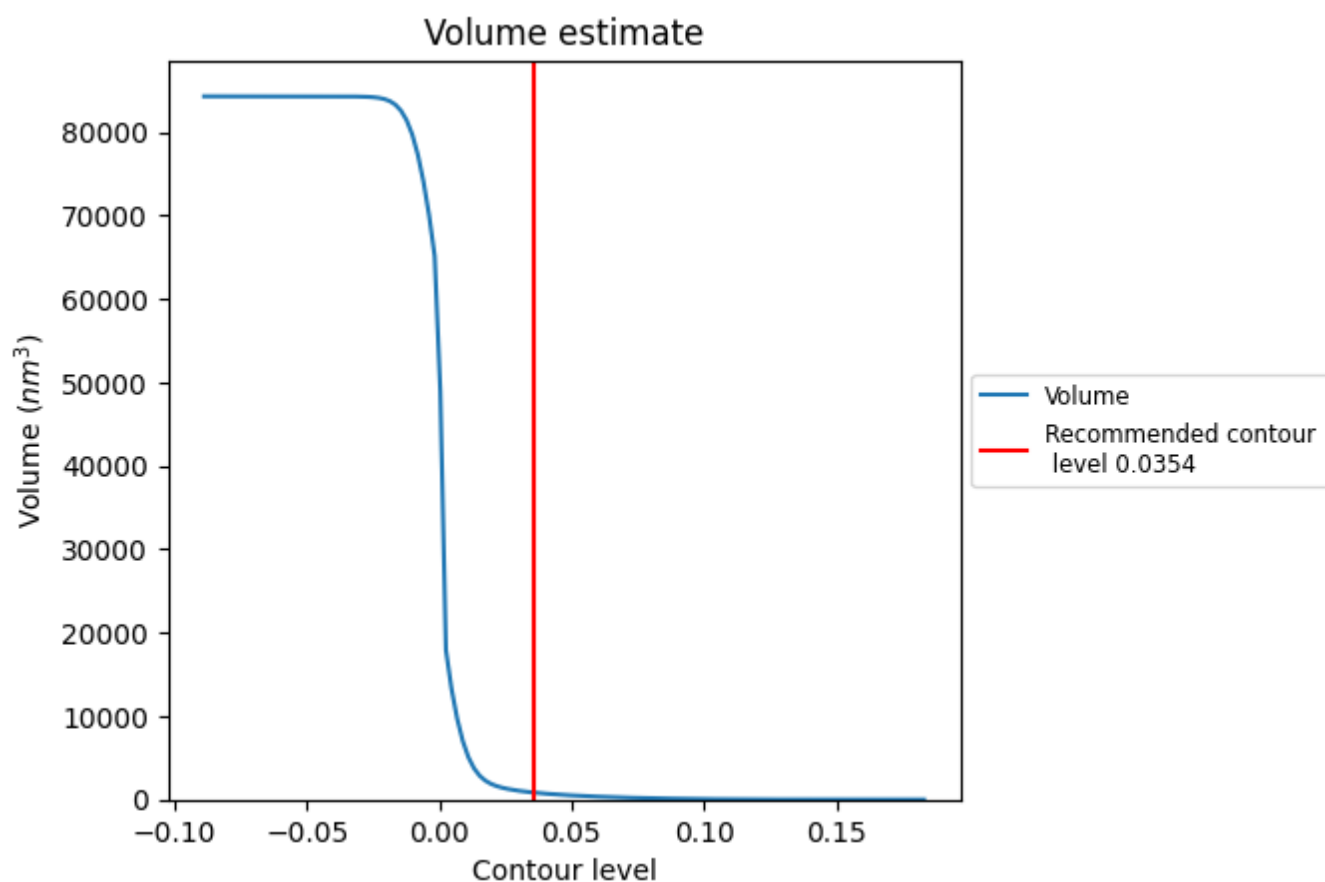
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

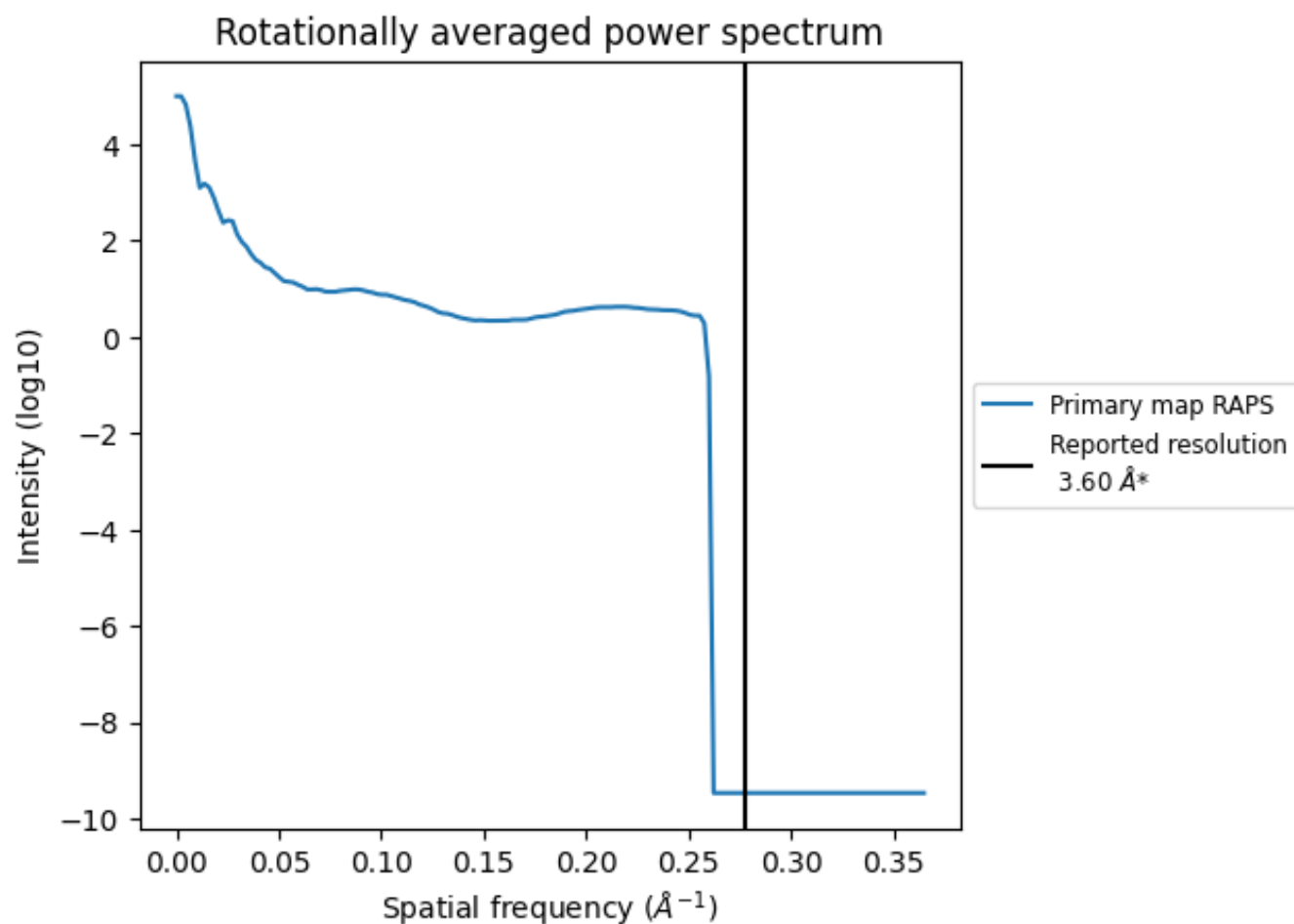
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 848 nm^3 ; this corresponds to an approximate mass of 766 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 0.278 Å⁻¹

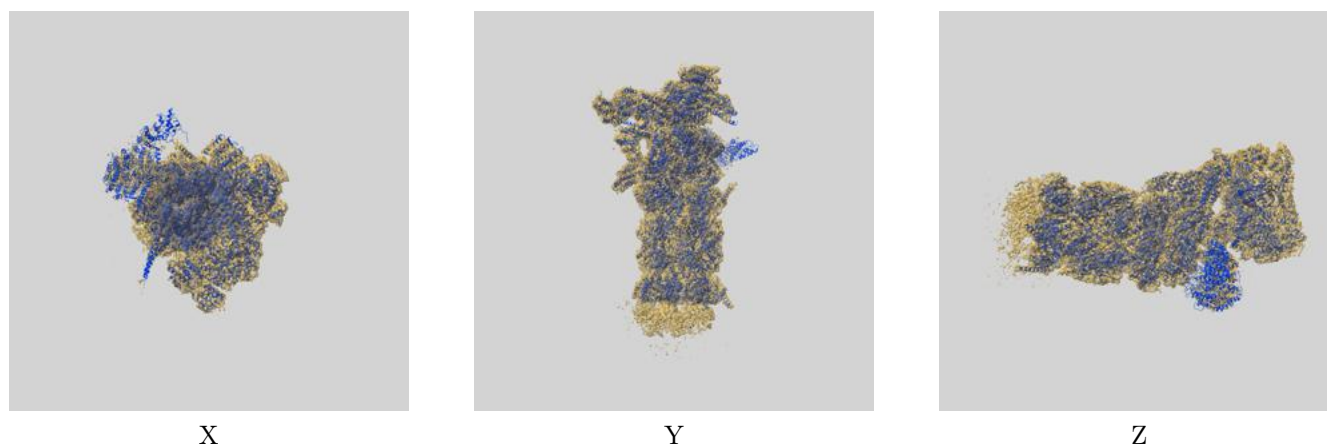
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

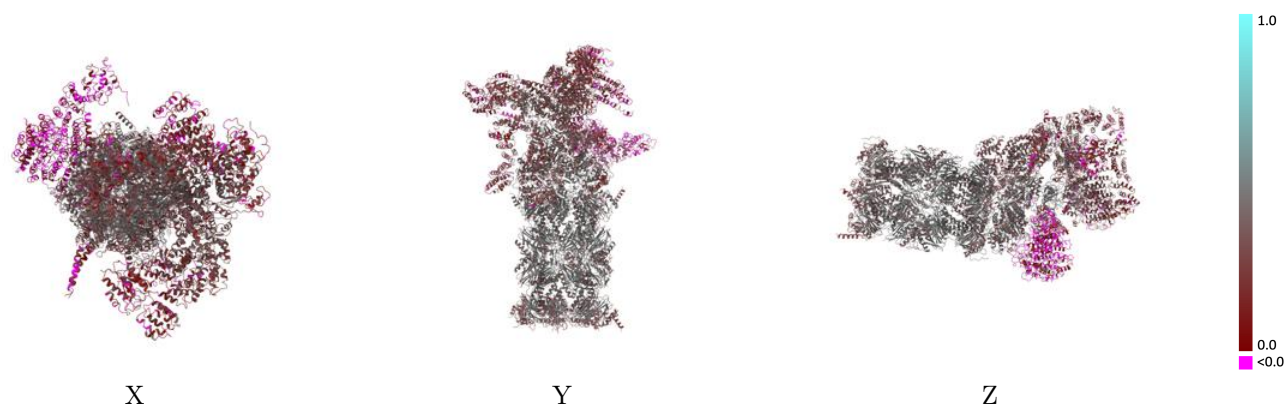
This section contains information regarding the fit between EMDB map EMD-14202 and PDB model 7QXP. Per-residue inclusion information can be found in section [3](#) on page [13](#).

9.1 Map-model overlay [i](#)



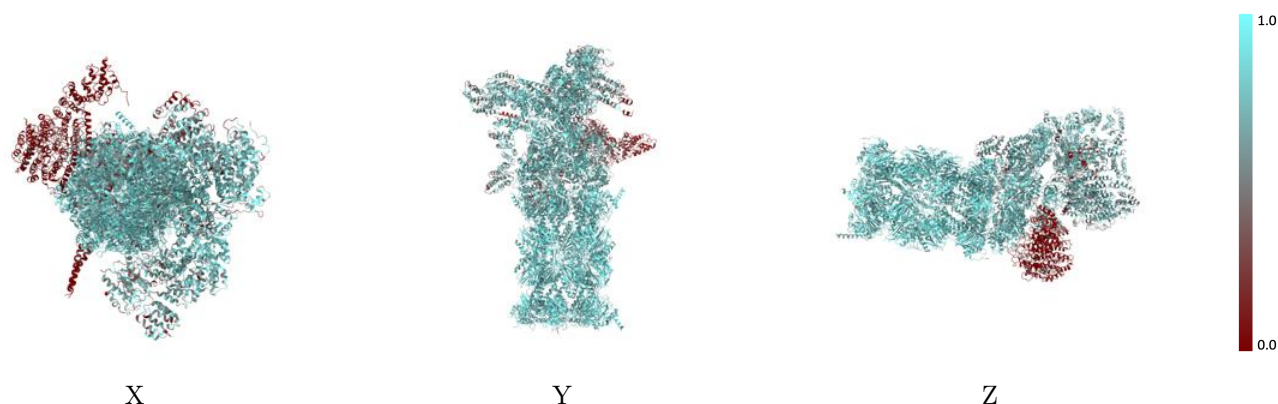
The images above show the 3D surface view of the map at the recommended contour level 0.0354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



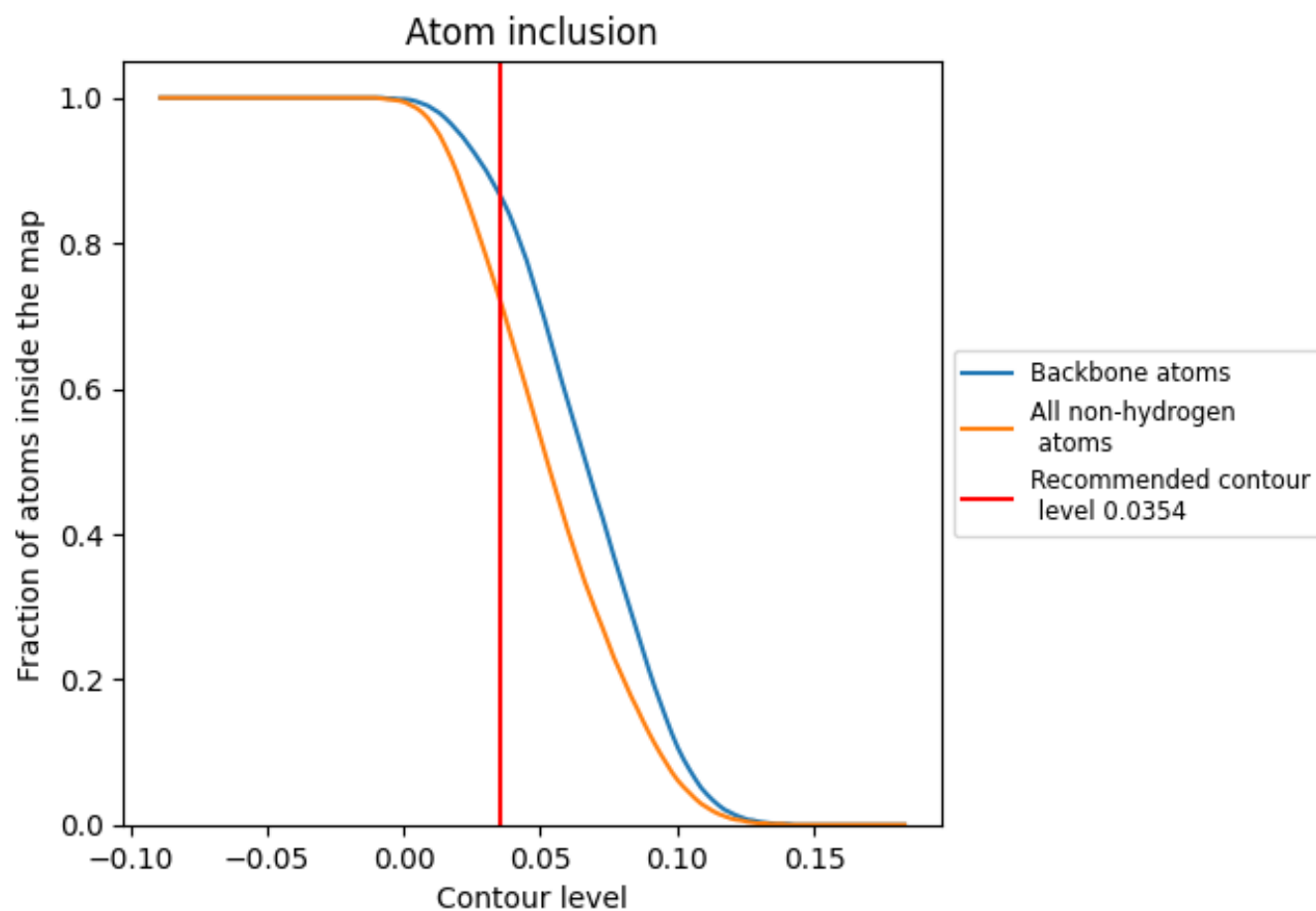
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0354).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 72% 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 (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7200	 0.3360
A	 0.7400	 0.3690
B	 0.6950	 0.3520
C	 0.7810	 0.3840
D	 0.7680	 0.3830
E	 0.7680	 0.3830
F	 0.7640	 0.3780
G	 0.8460	 0.4240
H	 0.8560	 0.4330
I	 0.8310	 0.3980
J	 0.8420	 0.4080
K	 0.8310	 0.4160
L	 0.8520	 0.4290
M	 0.8470	 0.4110
N	 0.8760	 0.4410
O	 0.8750	 0.4420
P	 0.8680	 0.4440
Q	 0.8680	 0.4440
R	 0.8870	 0.4430
S	 0.8800	 0.4520
T	 0.8840	 0.4510
U	 0.6620	 0.2410
V	 0.5890	 0.2020
W	 0.6460	 0.2270
X	 0.6430	 0.2950
Y	 0.7350	 0.2940
Z	 0.7110	 0.3130
a	 0.6620	 0.2350
b	 0.5760	 0.1840
c	 0.7380	 0.3490
d	 0.6500	 0.2010
e	 0.5060	 0.1250
f	 0.0420	 0.0340
g	 0.8180	 0.3970
h	 0.8390	 0.4130



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Chain	Atom inclusion	Q-score
i	 0.7770	 0.3720
j	 0.8010	 0.3710
k	 0.8030	 0.3970
l	 0.8170	 0.3940
m	 0.8040	 0.3930
n	 0.8550	 0.4330
o	 0.8740	 0.4440
p	 0.8640	 0.4520
q	 0.8620	 0.4330
r	 0.8880	 0.4410
s	 0.8650	 0.4390
t	 0.8710	 0.4410