



## Full wwPDB EM Validation Report ⓘ

Apr 28, 2025 – 05:50 PM EDT

PDB ID : 9NKI / pdb\_00009nki  
EMDB ID : EMD-49509  
Title : Structure of substrate engaged MIDN-bound human 26S proteasome, EB  
MIDN\_UBL state (Composite map)  
Authors : Peddada, N.; Beutler, B.  
Deposited on : 2025-02-28  
Resolution : 2.94 Å(reported)  
Based on initial model : 6mse

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

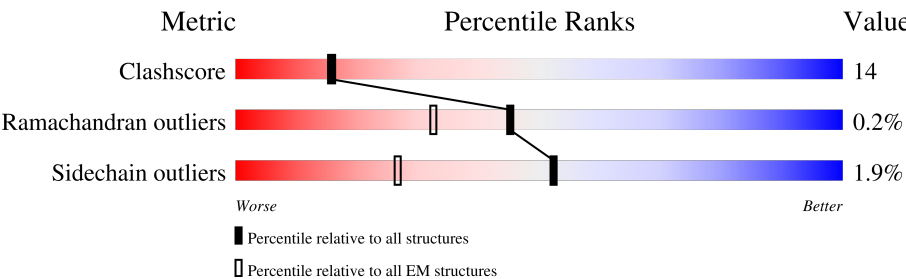
EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

# 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 2.94 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	433	
2	B	440	
3	C	406	
4	D	418	
5	E	403	
6	F	439	
7	G	246	
7	g	246	

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Mol	Chain	Length	Quality of chain
8	H	234	
8	h	234	
9	I	261	
9	i	261	
10	J	248	
10	j	248	
11	K	241	
11	k	241	
12	L	263	
12	l	263	
13	M	255	
13	m	255	
14	N	239	
14	n	239	
15	O	277	
15	o	277	
16	P	205	
16	p	205	
17	Q	201	
17	q	201	
18	R	263	
18	r	263	
19	S	241	
19	s	241	
20	T	264	

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Mol	Chain	Length	Quality of chain
20	t	264	
21	V	534	
22	W	456	
23	X	422	
24	Y	389	
25	Z	324	
26	a	376	
27	b	377	
28	d	350	
29	e	70	
30	v	12	
31	z	468	
32	U	953	
33	c	310	
34	f	908	

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 200583 atoms, of which 97961 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	390	Total	C	H	N	O	S	0	0
			6166	1928	3106	537	578	17		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	393	Total	C	H	N	O	S	0	0
			6129	1936	3053	524	601	15		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	389	Total	C	H	N	O	S	0	0
			6264	1932	3193	550	571	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	380	Total	C	H	N	O	S	0	0
			6114	1923	3075	524	579	13		

- Molecule 5 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	389	Total	C	H	N	O	S	0	0
			6248	1947	3150	552	582	17		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	415	Total	C	H	N	O	S	0	0
			6569	2038	3318	561	634	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	G	240	Total	C	H	N	O	S	0	0
			3394	1106	1656	304	316	12		
7	g	240	Total	C	H	N	O	S	0	0
			3445	1124	1687	306	316	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	H	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		
8	h	229	Total	C	H	N	O	S	0	0
			3252	1080	1590	288	288	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	I	247	Total	C	H	N	O	S	0	0
			3543	1150	1741	322	320	10		
9	i	247	Total	C	H	N	O	S	0	0
			3503	1143	1717	320	313	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
10	J	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		
10	j	232	Total	C	H	N	O	S	0	0
			3151	1038	1518	306	284	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	233	Total	C	H	N	O	S	0	0
			3264	1062	1597	287	307	11		
11	k	233	Total	C	H	N	O	S	0	0
			3249	1056	1589	287	306	11		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	9	TYR	ASP	conflict	UNP P28066

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Chain	Residue	Modelled	Actual	Comment	Reference
k	9	TYR	ASP	conflict	UNP P28066

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

Mol	Chain	Residues	Atoms						AltConf	Trace
12	L	233	Total	C	H	N	O	S	0	0
			3359	1090	1649	318	293	9		
12	l	233	Total	C	H	N	O	S	0	0
			3352	1089	1645	315	293	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
13	M	239	Total	C	H	N	O	S	0	0
			3440	1131	1680	308	311	10		
13	m	239	Total	C	H	N	O	S	0	0
			3444	1131	1683	308	312	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
14	N	202	Total	C	H	N	O	S	0	0
			2891	928	1422	257	272	12		
14	n	202	Total	C	H	N	O	S	0	0
			2881	926	1416	256	271	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
15	O	220	Total	C	H	N	O	S	0	0
			3139	1005	1559	272	294	9		
15	o	220	Total	C	H	N	O	S	0	0
			3131	1003	1555	272	292	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	P	204	Total	C	H	N	O	S	0	0
			3096	992	1550	262	273	19		
16	p	204	Total	C	H	N	O	S	0	0
			3081	989	1543	263	268	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
17	Q	196	Total	C	H	N	O	S	0	0
			2986	974	1477	259	268	8		
17	q	196	Total	C	H	N	O	S	0	0
			2981	973	1475	259	266	8		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	200	Total	C	H	N	O	S	0	0
			2953	957	1449	271	267	9		
18	r	200	Total	C	H	N	O	S	0	0
			2938	954	1438	270	267	9		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
19	S	212	Total	C	H	N	O	S	0	0
			3163	1016	1579	279	279	10		
19	s	212	Total	C	H	N	O	S	0	0
			3168	1017	1581	279	281	10		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
20	T	212	Total	C	H	N	O	S	0	0
			3102	1003	1526	280	282	11		
20	t	212	Total	C	H	N	O	S	0	0
			3079	998	1511	279	280	11		

- Molecule 21 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	V	442	Total	C	H	N	O	S	0	0
			7256	2293	3658	642	650	13		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	440	Total	C	N	O	S	0	0
			3588	2272	612	681	23		



- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	X	384	Total	C	H	N	O	S	0	0
			6174	1935	3134	513	580	12		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	Y	380	Total	C	H	N	O	S	0	0
			6260	1995	3133	535	580	17		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	286	Total	C	H	N	O	S	0	0
			4593	1457	2312	392	427	5		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
26	a	373	Total	C	H	N	O	S	0	0
			6007	1911	3012	510	559	15		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	b	191	Total	C	H	N	O	S	0	0
			2963	910	1505	261	279	8		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	d	270	Total	C	H	N	O	S	0	0
			4414	1417	2221	360	407	9		

- Molecule 29 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	e	48	Total	C	H	N	O		0	0
			725	249	316	63	97			

- Molecule 30 is a protein called Unknown density-substrate density.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	v	12	Total	C	N	O	0	0
			60	36	12	12		

- Molecule 31 is a protein called Midnolin.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	z	81	Total	C	H	N	O	S	0	0
			1257	383	645	111	116	2		

- Molecule 32 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	U	818	Total	C	H	N	O	S	0	0
			12773	4046	6402	1085	1196	44		

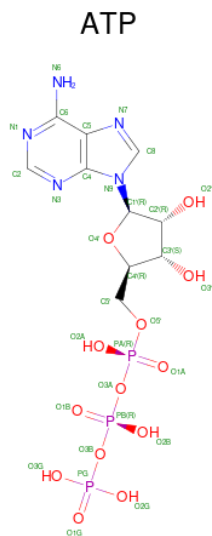
- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	c	283	Total	C	H	N	O	S	0	0
			4473	1412	2241	385	418	17		

- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	f	836	Total	C	H	N	O	S	0	0
			12946	4084	6486	1097	1234	45		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
35	A	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
35	B	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
35	D	1	Total 43	C 10	H 12	N 5	O 13	P 3	0
35	F	1	Total 43	C 10	H 12	N 5	O 13	P 3	0

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

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

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

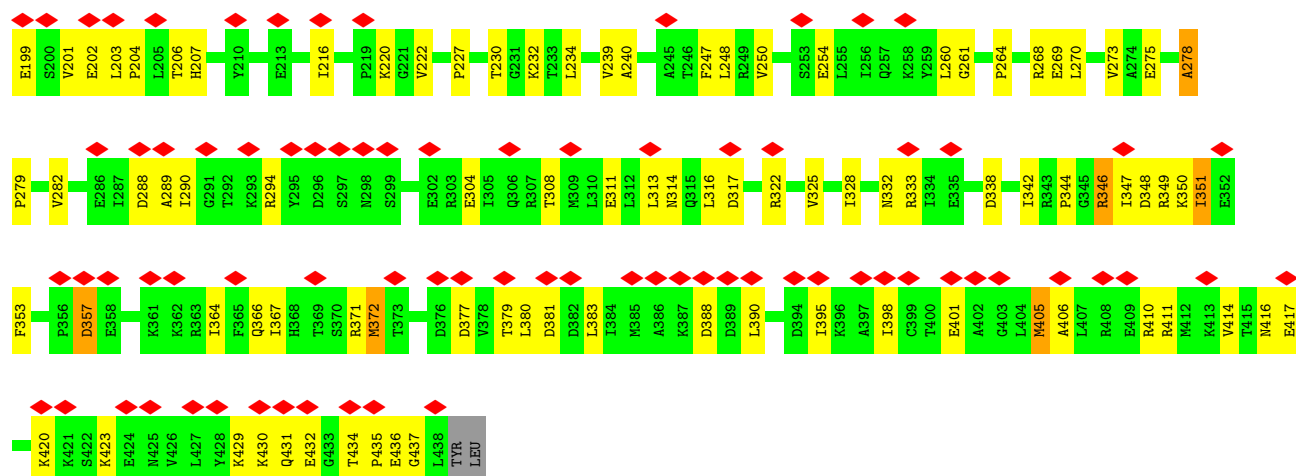


Mol	Chain	Residues	Atoms						AltConf
37	E	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

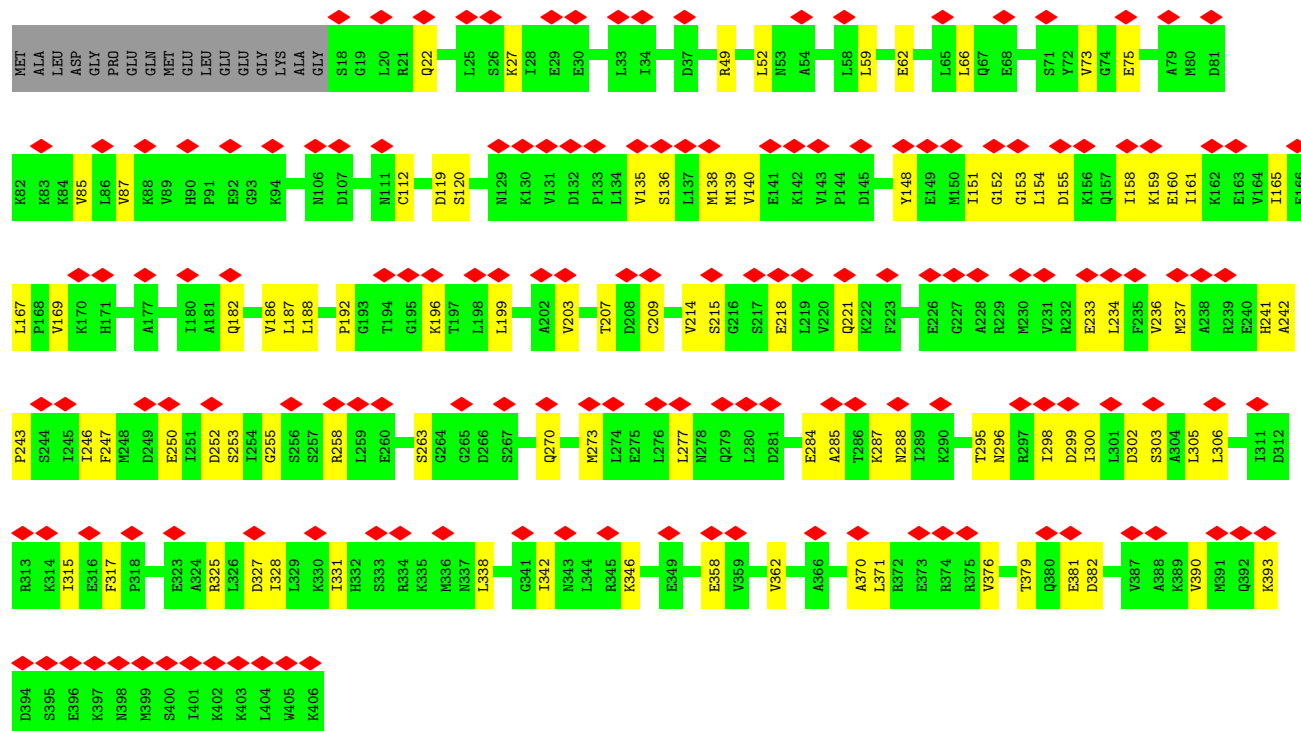
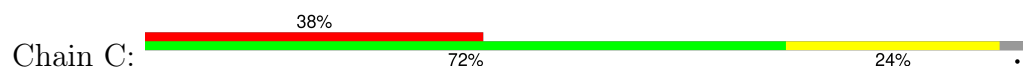
- Molecule 38 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

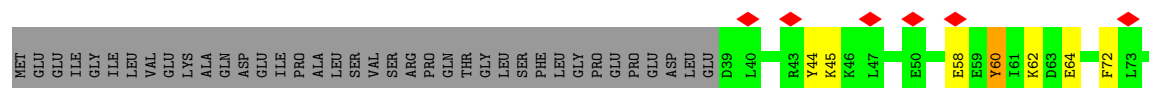


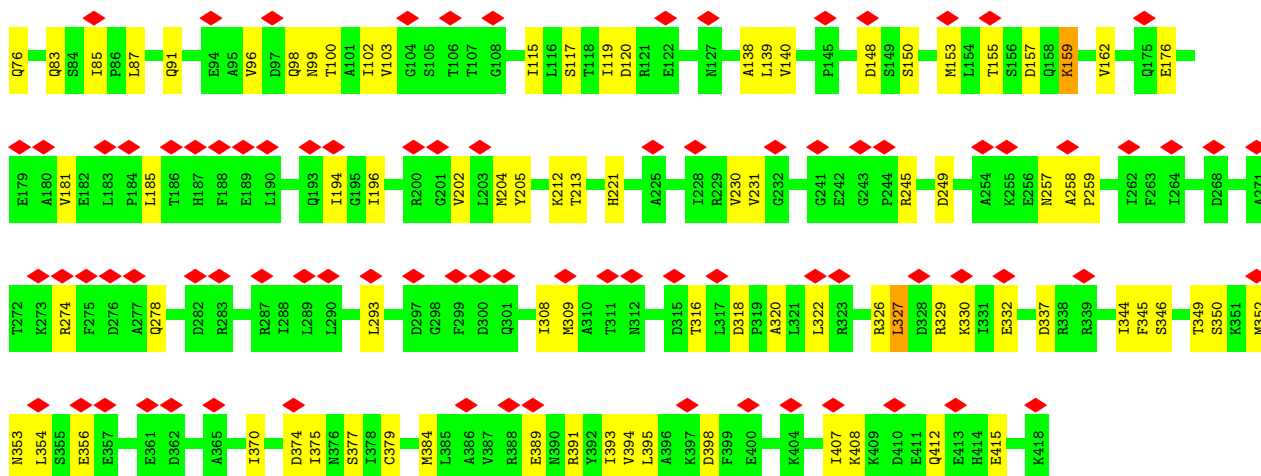


• Molecule 3: 26S protease regulatory subunit 8

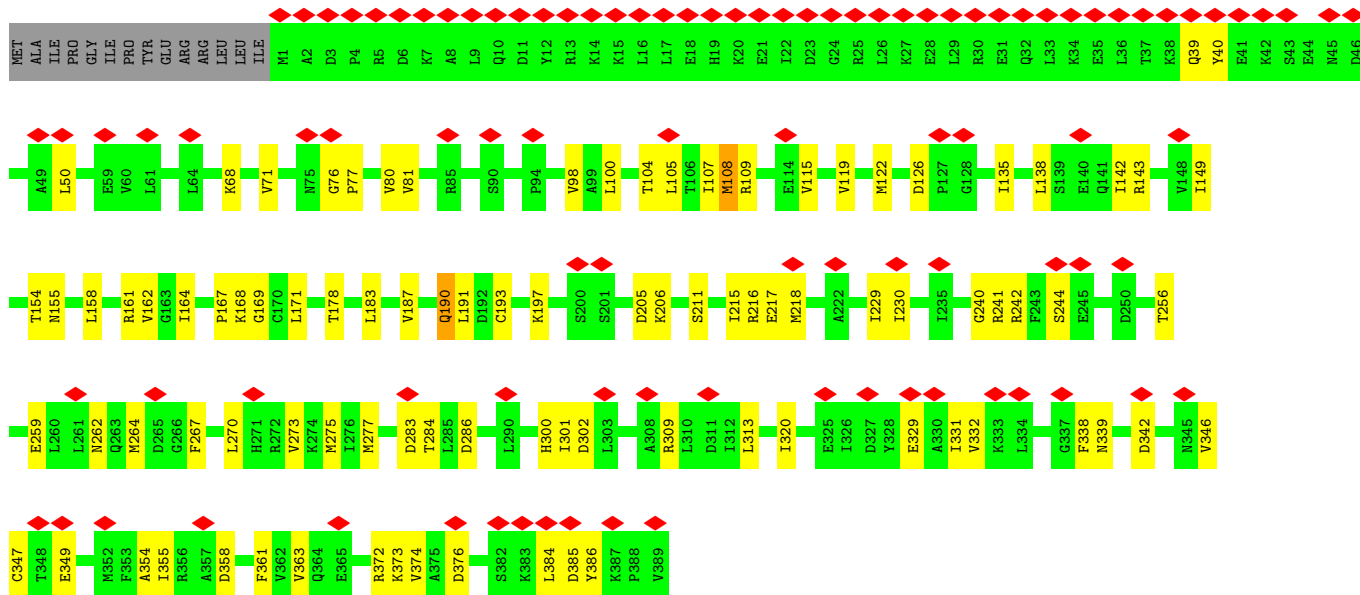


• Molecule 4: 26S proteasome regulatory subunit 6B

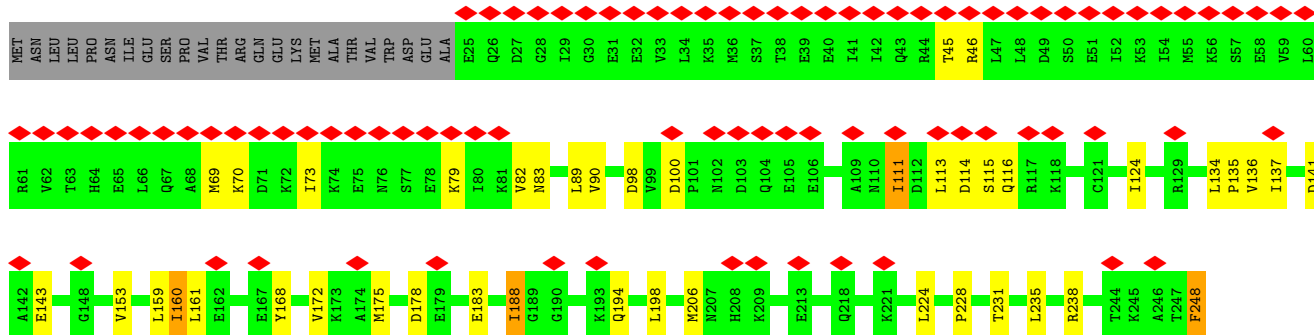


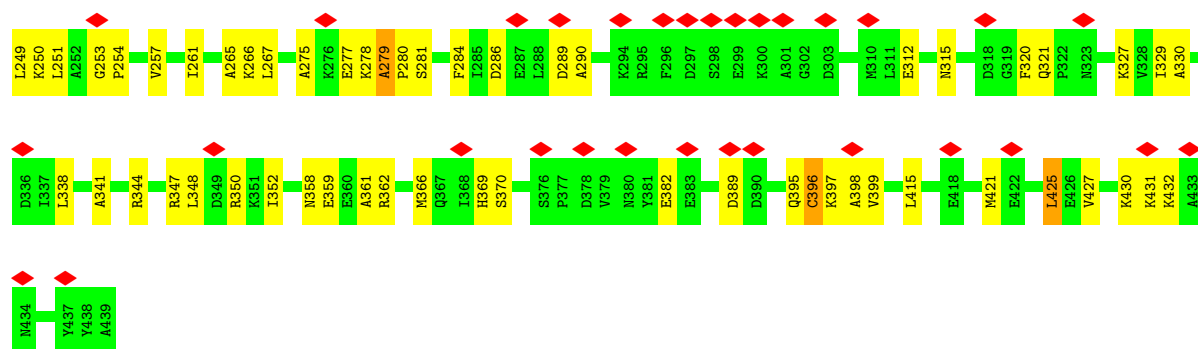


• Molecule 5: 26S proteasome regulatory subunit 10B

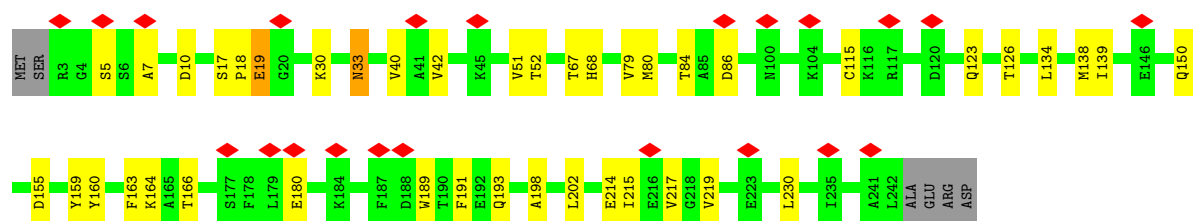
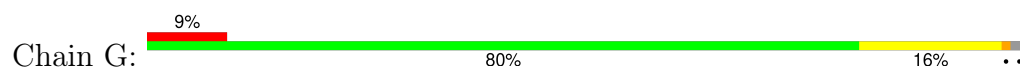


• Molecule 6: 26S proteasome regulatory subunit 6A

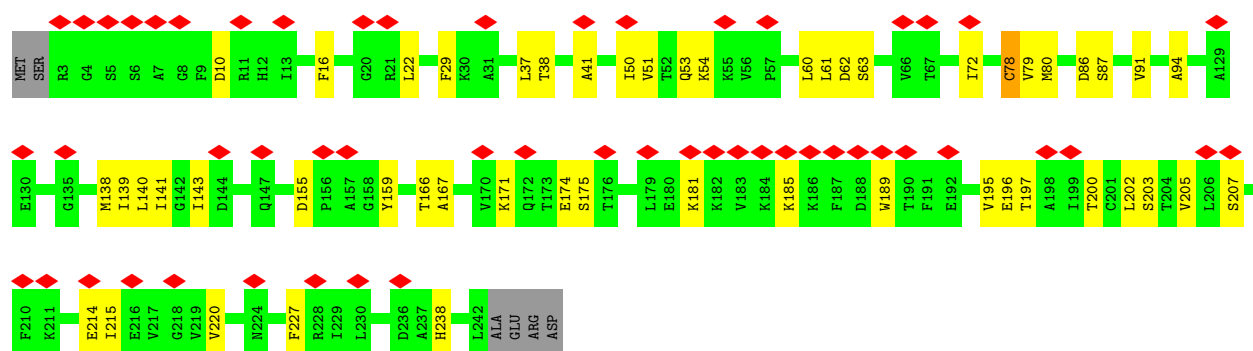
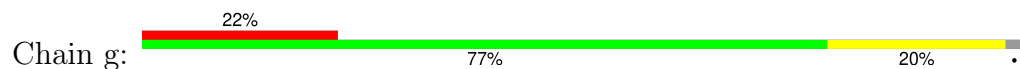




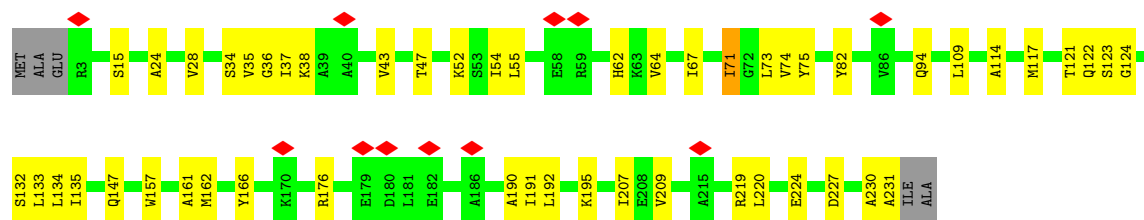
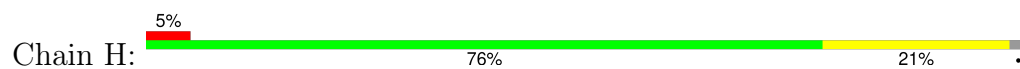
• Molecule 7: Proteasome subunit alpha type-6



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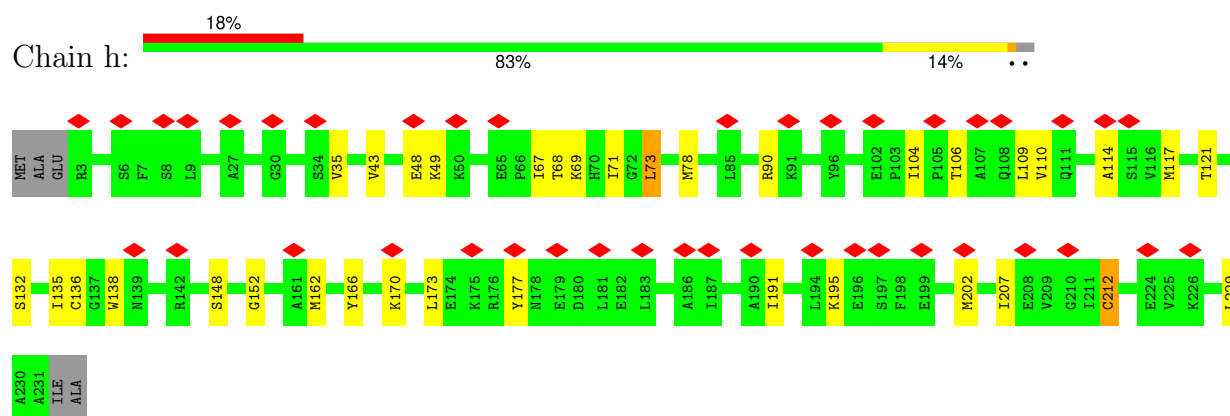


• Molecule 8: Proteasome subunit alpha type-2

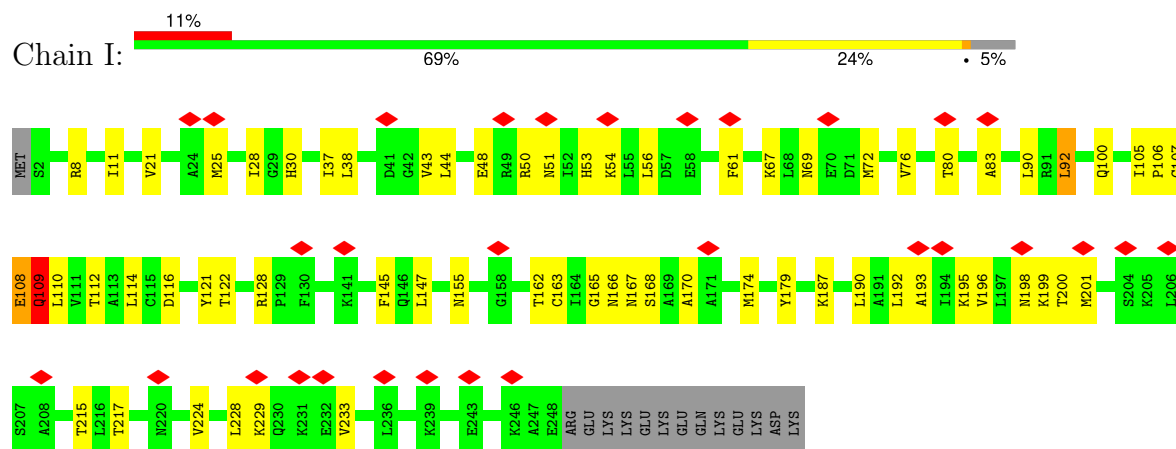


• Molecule 8: Proteasome subunit alpha type-2

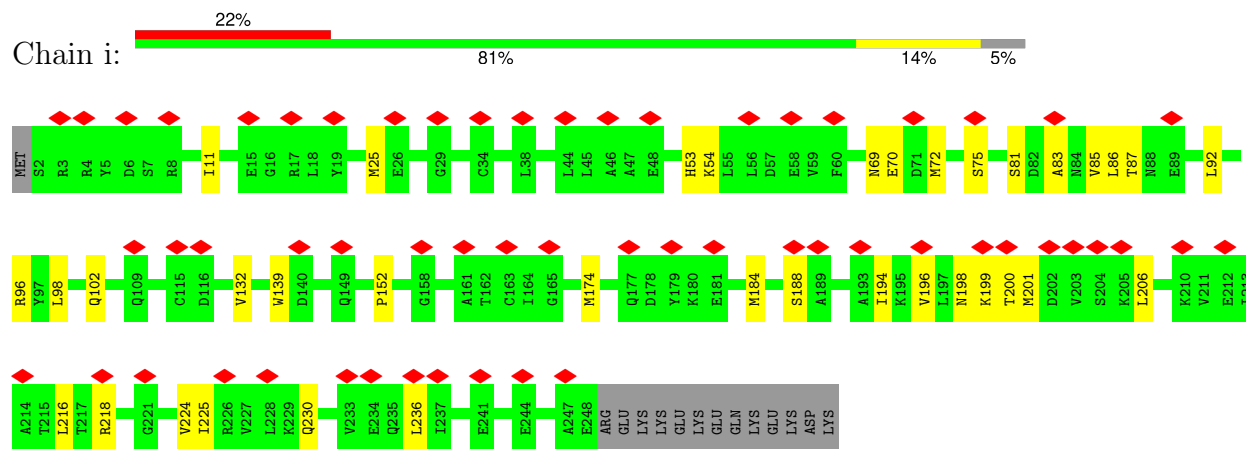




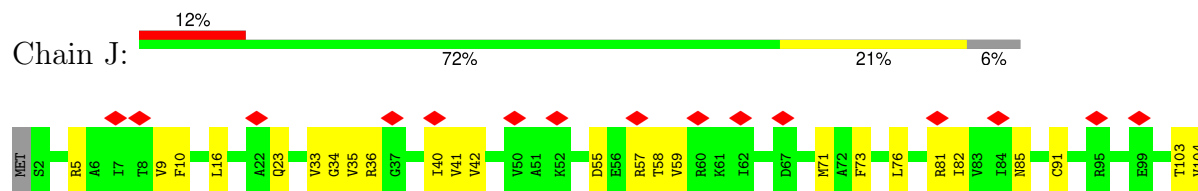
• Molecule 9: Proteasome subunit alpha type-4

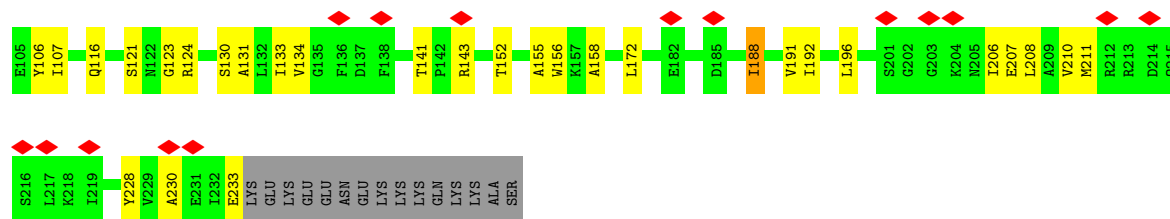


• Molecule 9: Proteasome subunit alpha type-4

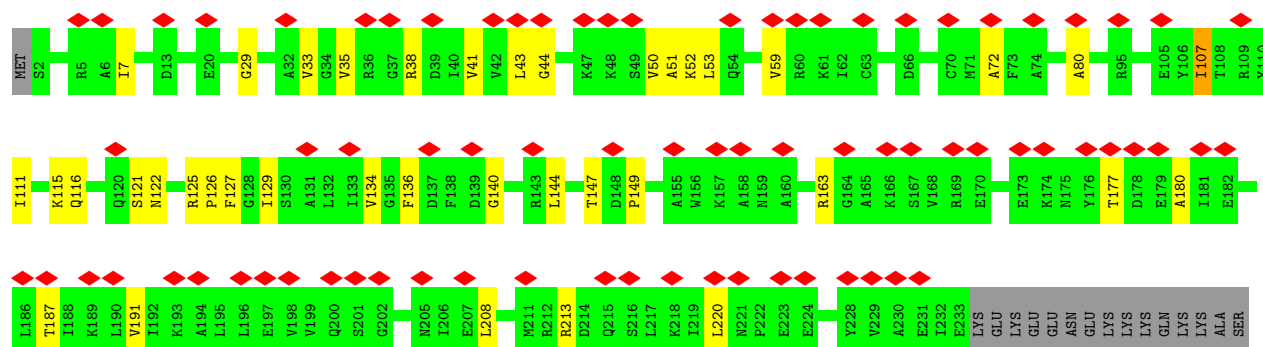
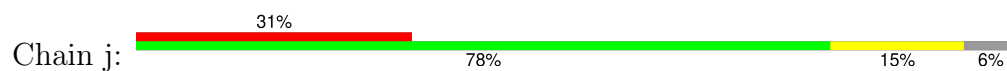


• Molecule 10: Proteasome subunit alpha type-7

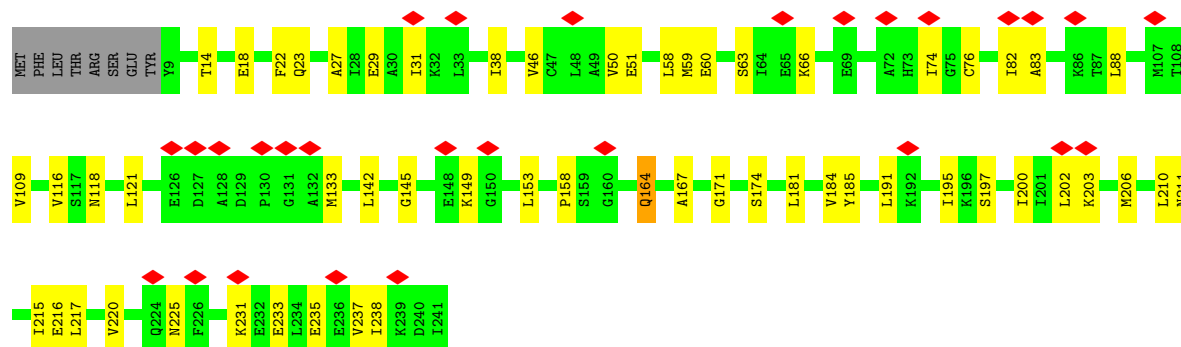
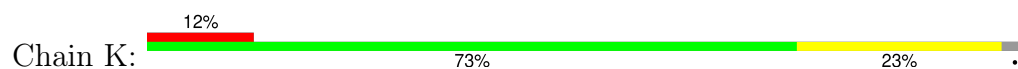




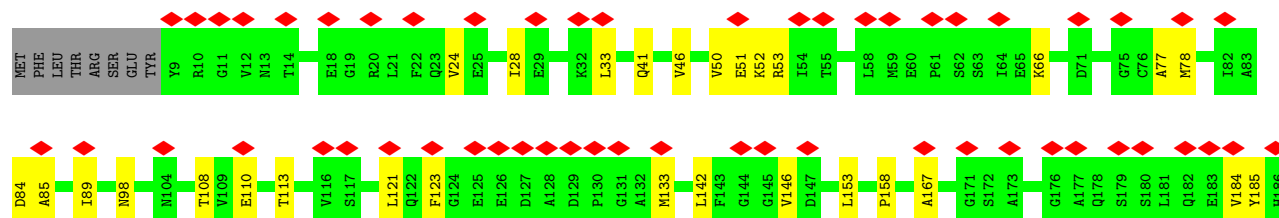
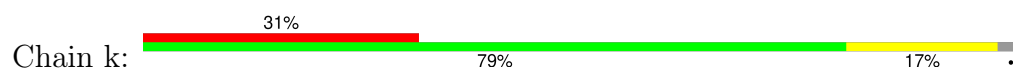
• Molecule 10: Proteasome subunit alpha type-7

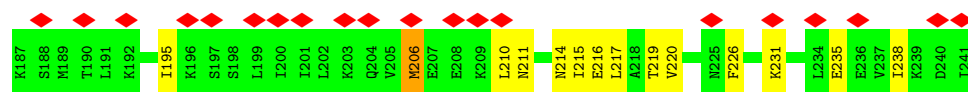


• Molecule 11: Proteasome subunit alpha type-5

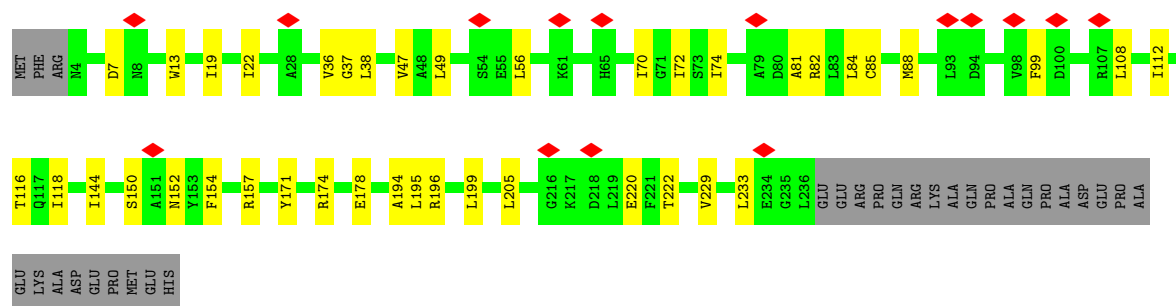
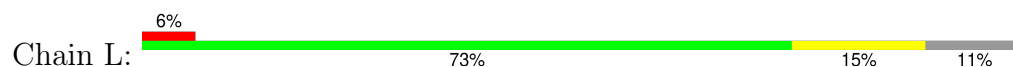


• Molecule 11: Proteasome subunit alpha type-5

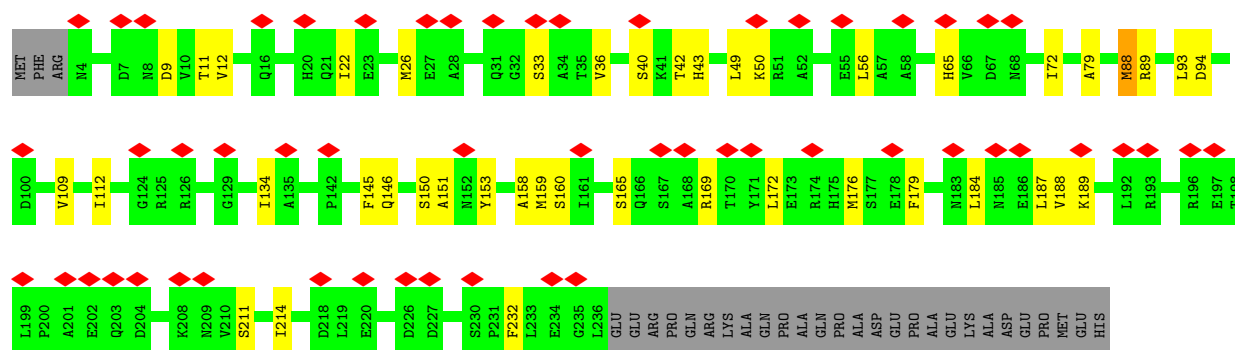




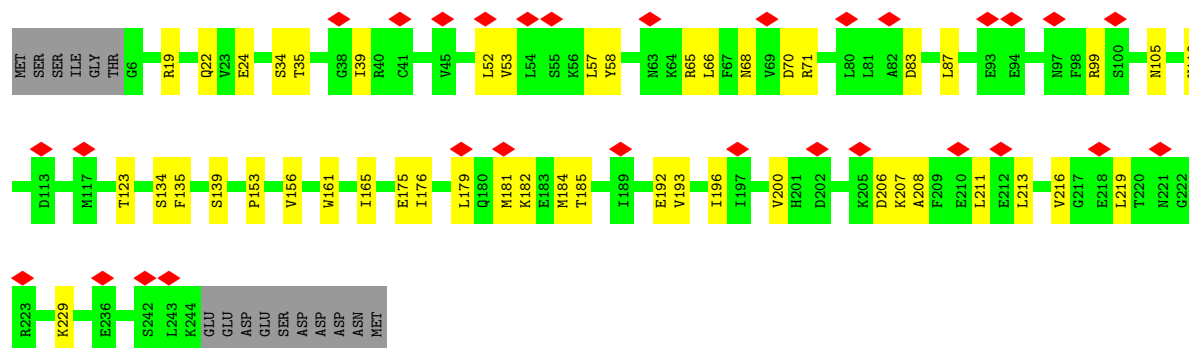
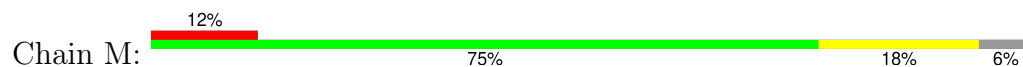
• Molecule 12: Proteasome subunit alpha type-1



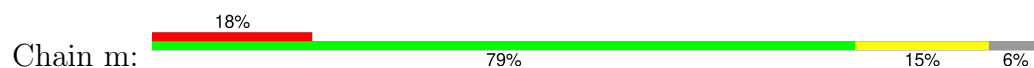
• Molecule 12: Proteasome subunit alpha type-1

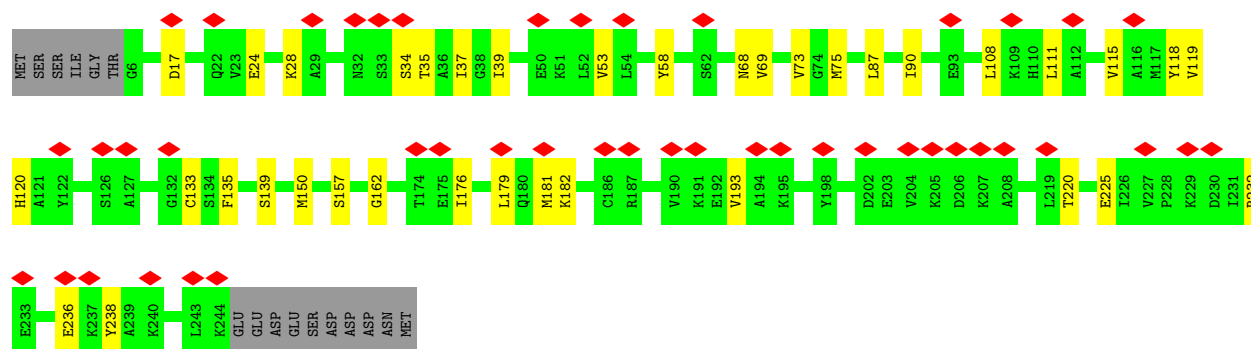


• Molecule 13: Proteasome subunit alpha type-3

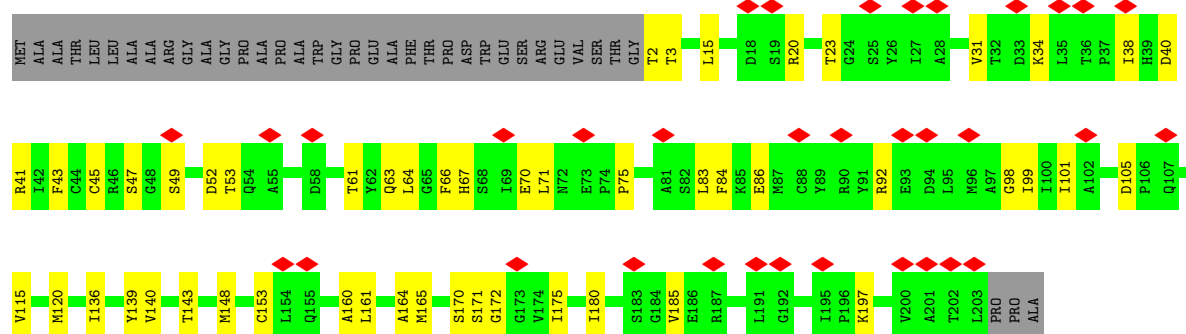


• Molecule 13: Proteasome subunit alpha type-3

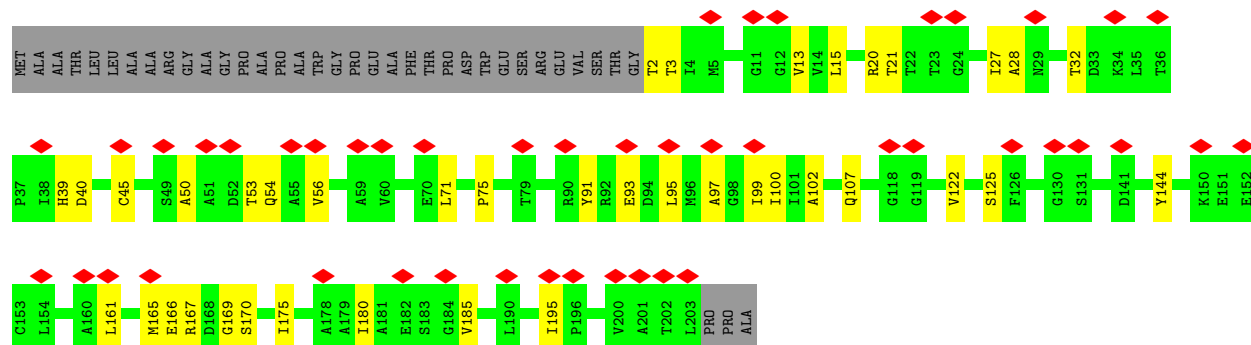




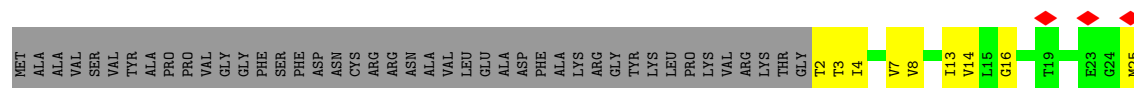
• Molecule 14: Proteasome subunit beta type-6

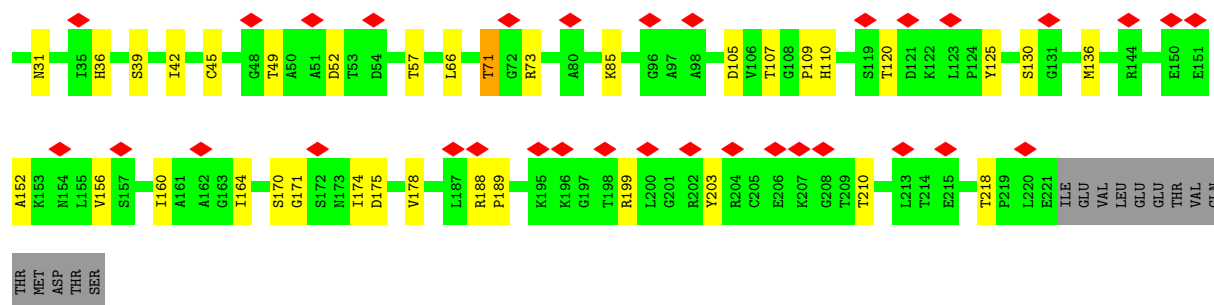


• Molecule 14: Proteasome subunit beta type-6

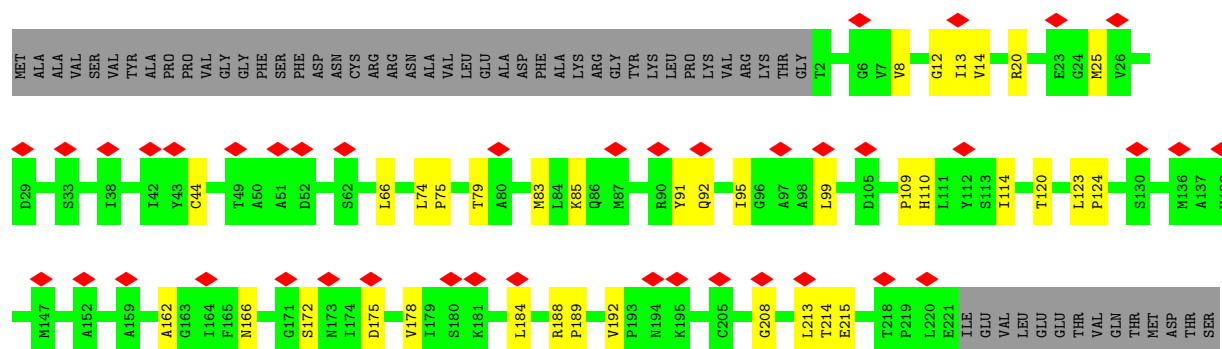


• Molecule 15: Proteasome subunit beta type-7

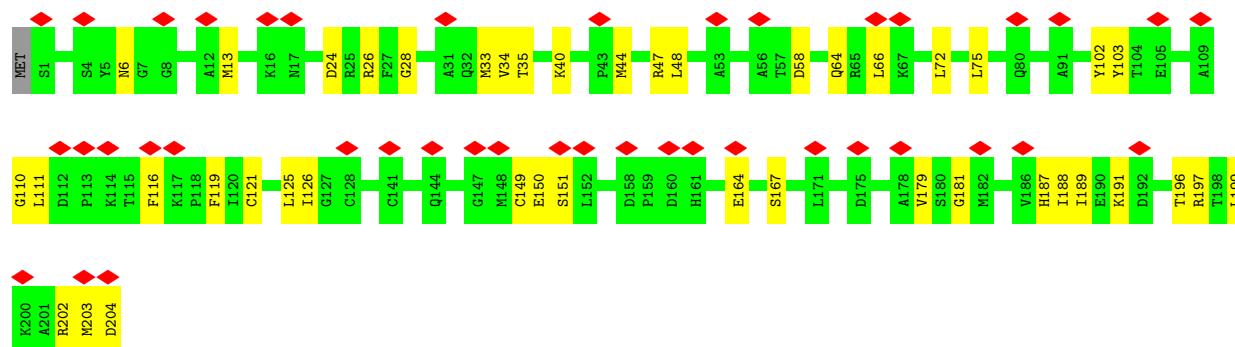
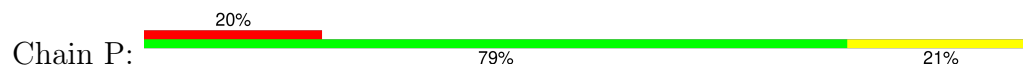




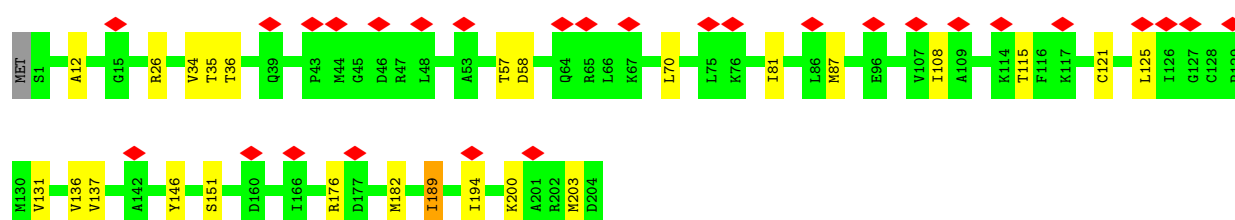
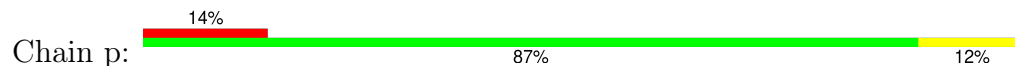
• Molecule 15: Proteasome subunit beta type-7



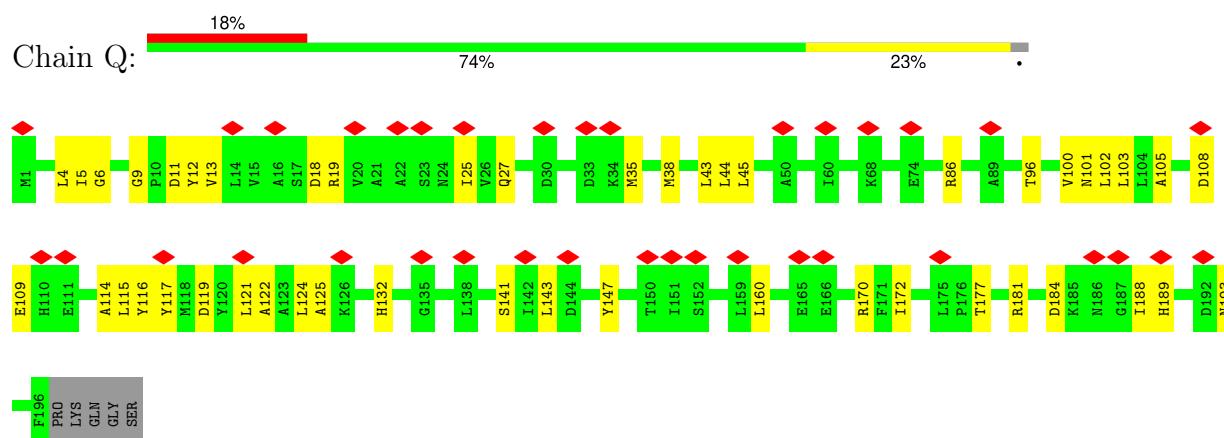
• Molecule 16: Proteasome subunit beta type-3



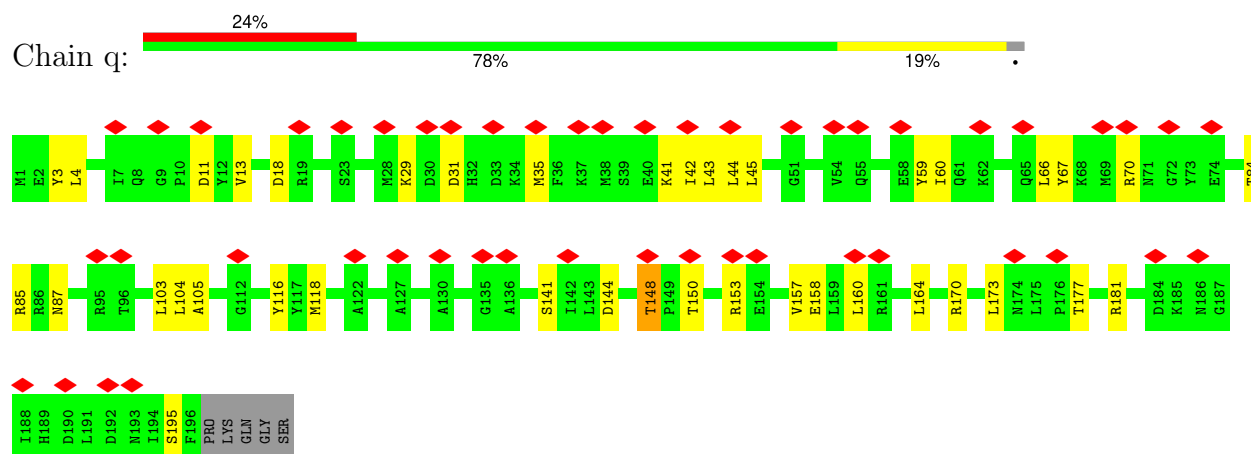
• Molecule 16: Proteasome subunit beta type-3



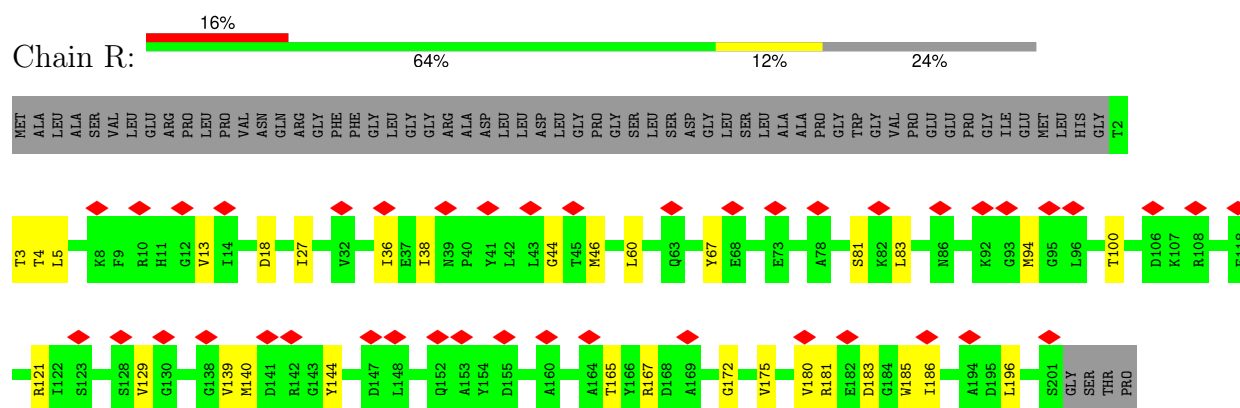
- Molecule 17: Proteasome subunit beta type-2



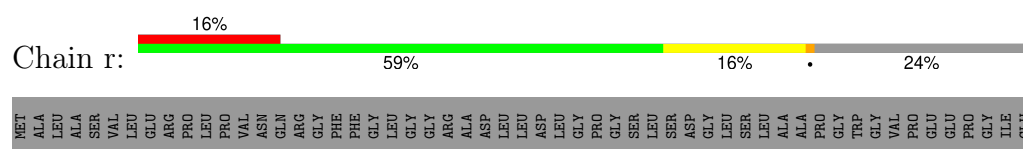
- Molecule 17: Proteasome subunit beta type-2

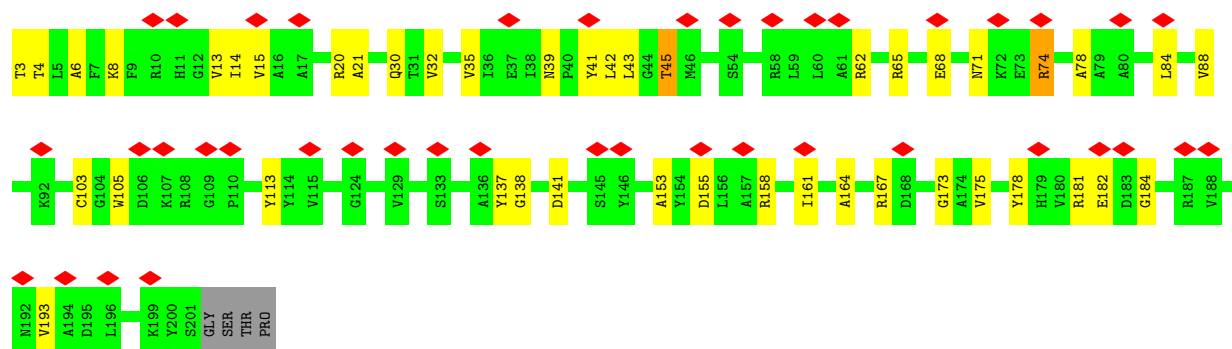


- Molecule 18: Proteasome subunit beta type-5

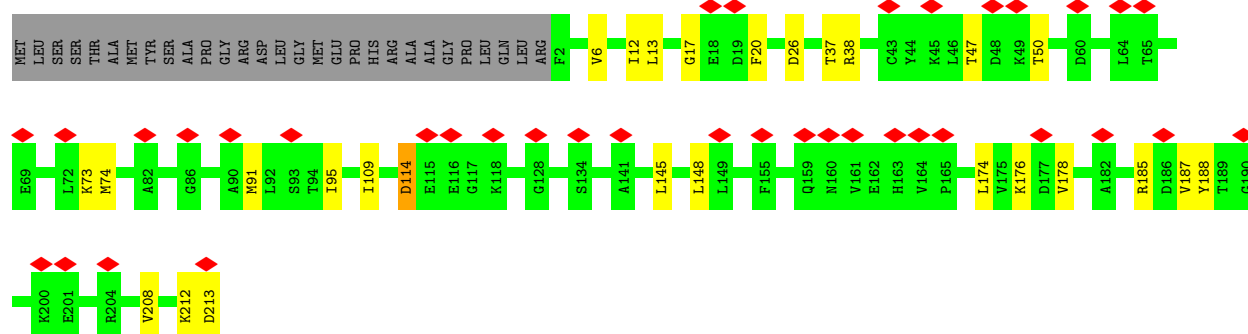


- Molecule 18: Proteasome subunit beta type-5

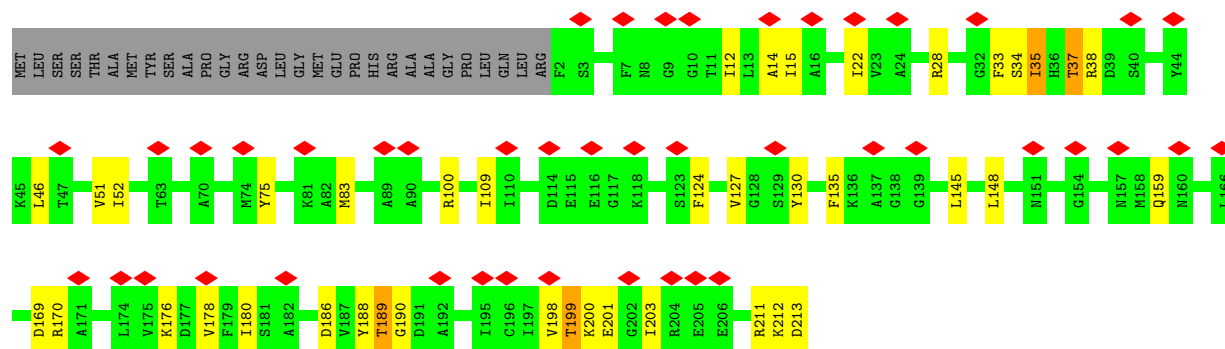




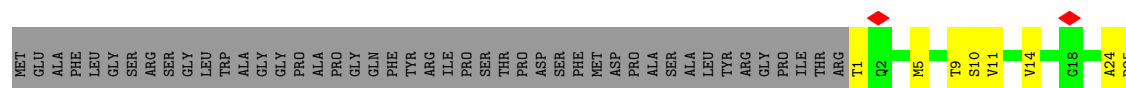
• Molecule 19: Proteasome subunit beta type-1



• Molecule 19: Proteasome subunit beta type-1

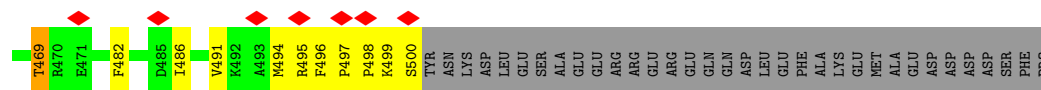


• Molecule 20: Proteasome subunit beta type-4

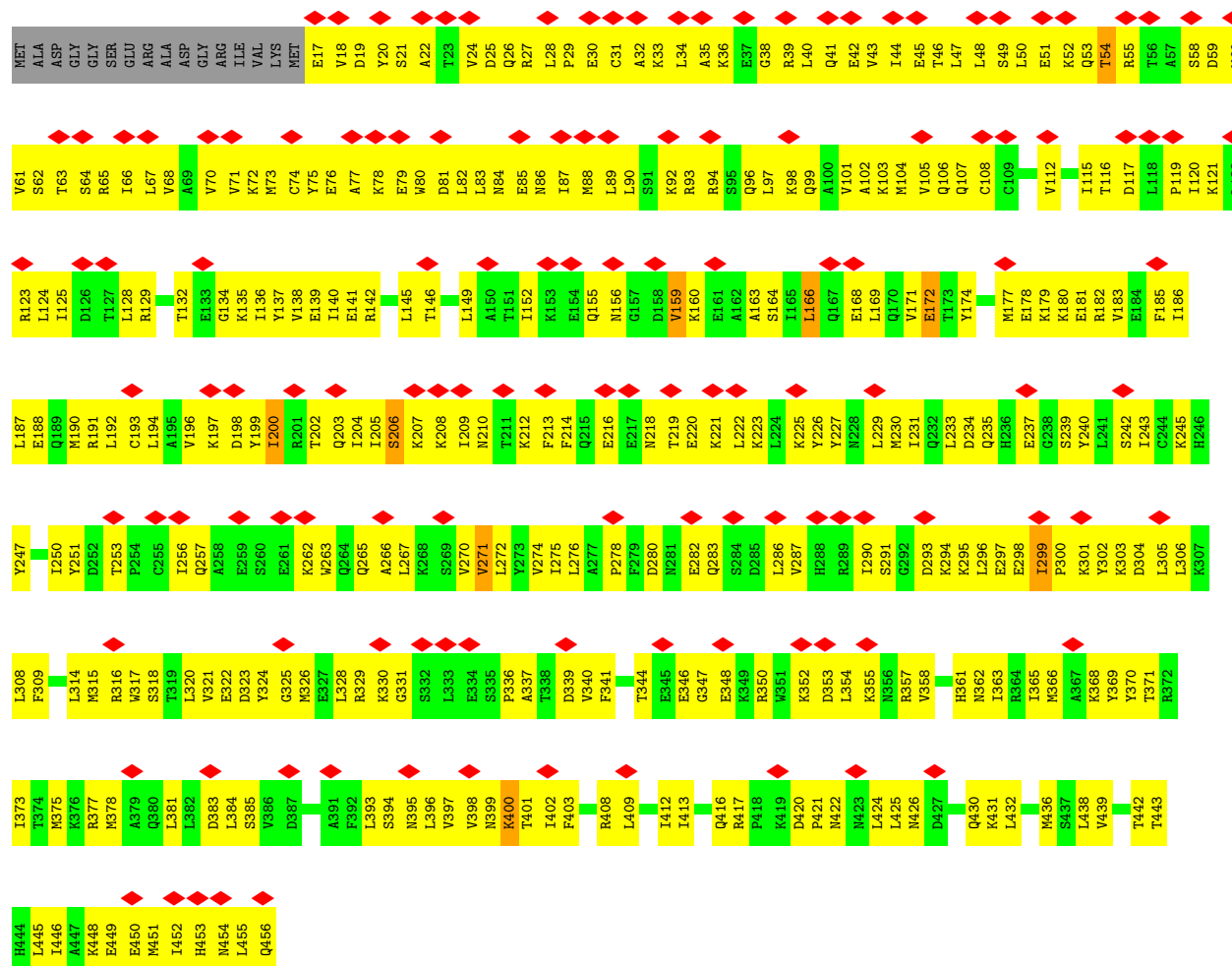




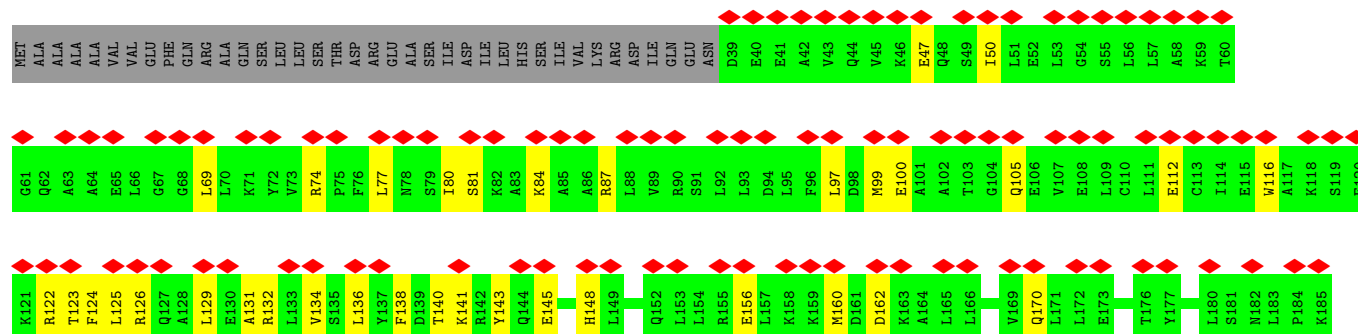




• Molecule 22: 26S proteasome non-ATPase regulatory subunit 12

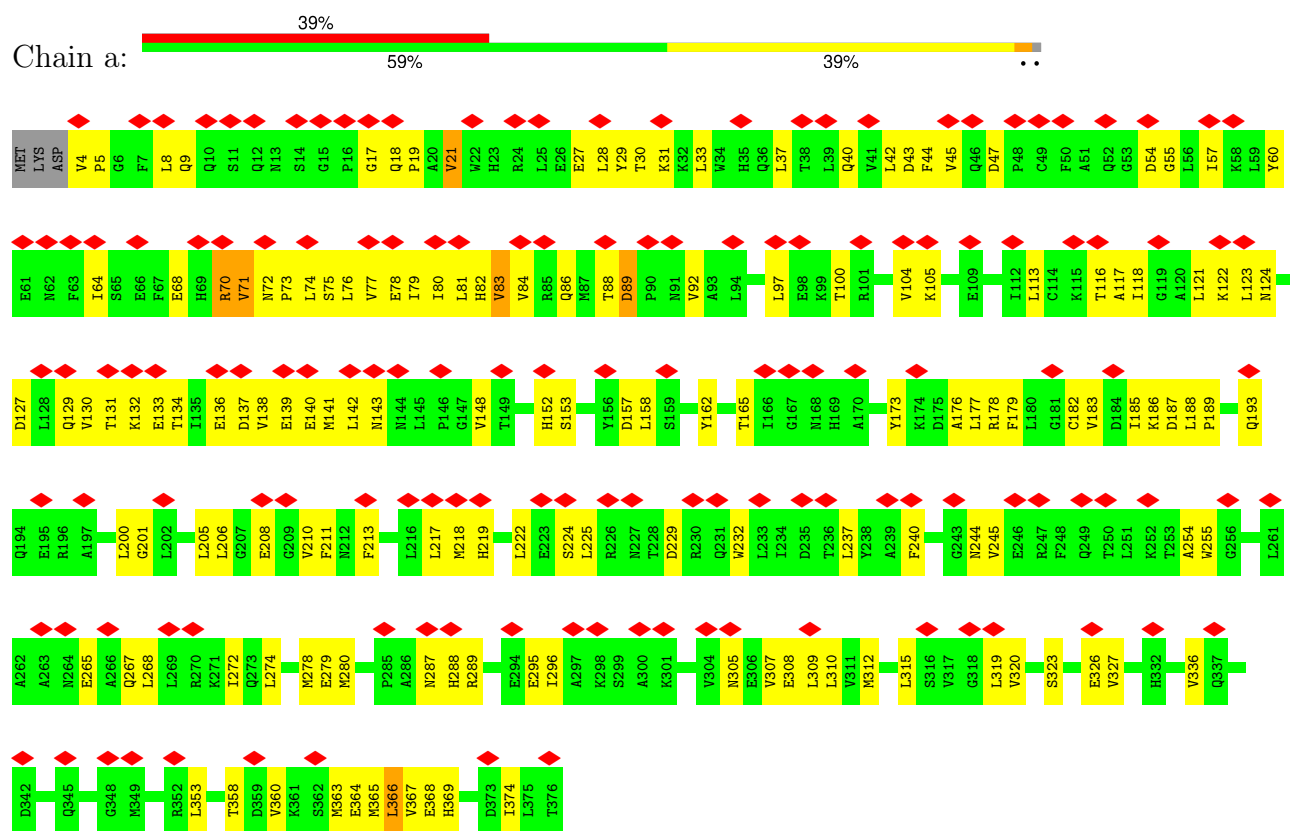


• Molecule 23: 26S proteasome non-ATPase regulatory subunit 11

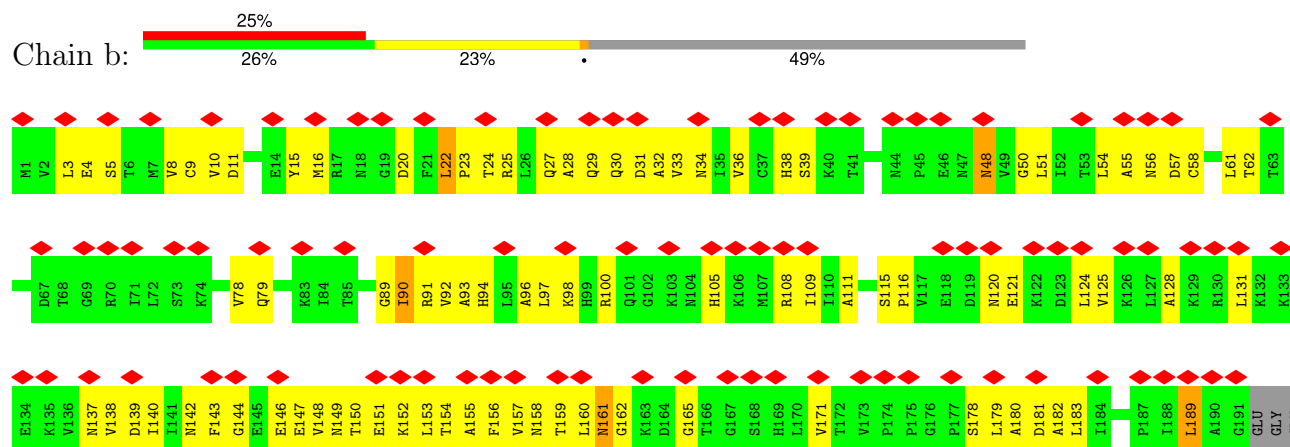




- Molecule 26: 26S proteasome non-ATPase regulatory subunit 13



- Molecule 27: 26S proteasome non-ATPase regulatory subunit 4

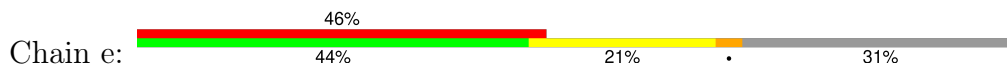


[illegible]

- Molecule 28: 26S proteasome non-ATPase regulatory subunit 8

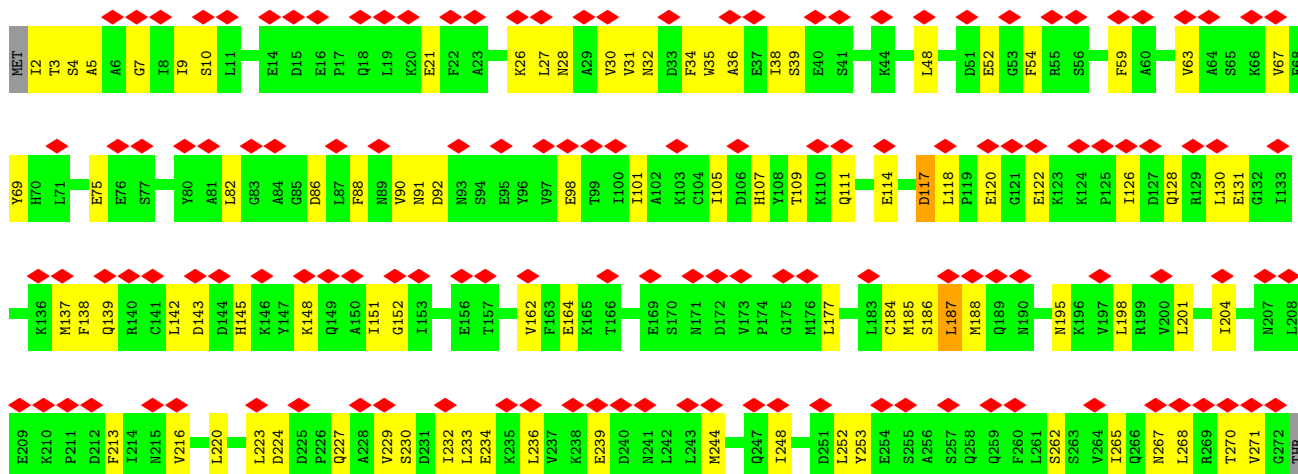
[illegible]

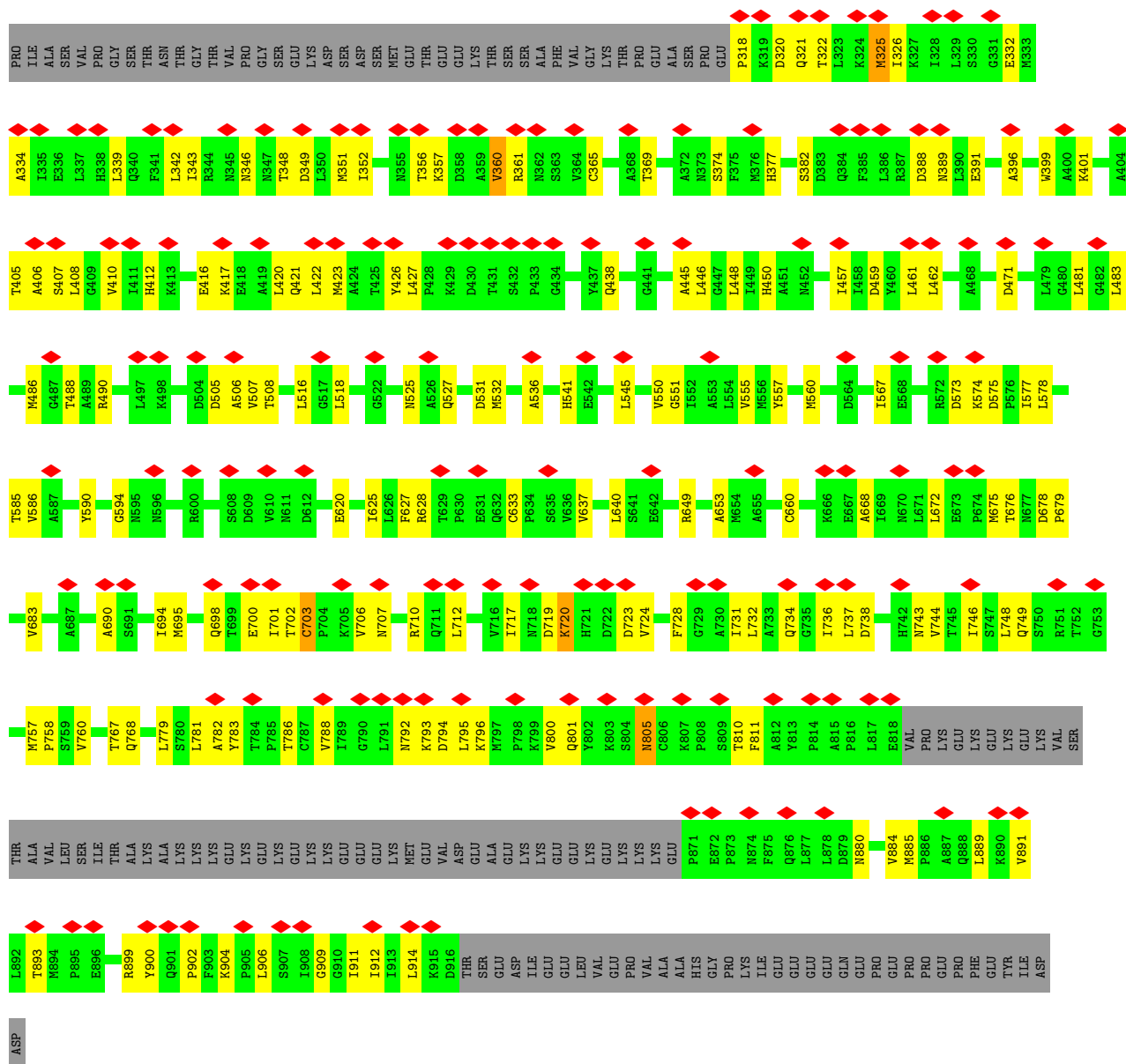
- Molecule 29: 26S proteasome complex subunit SEM1

[illegible]

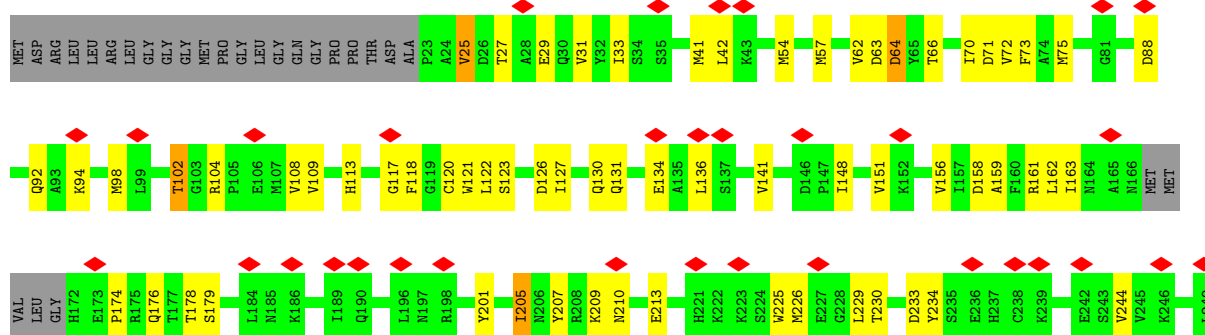
- Molecule 30: Unknown density-substrate density

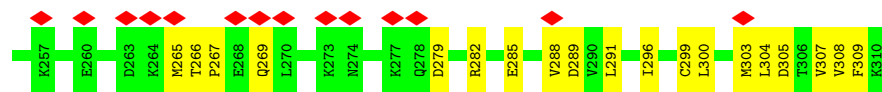




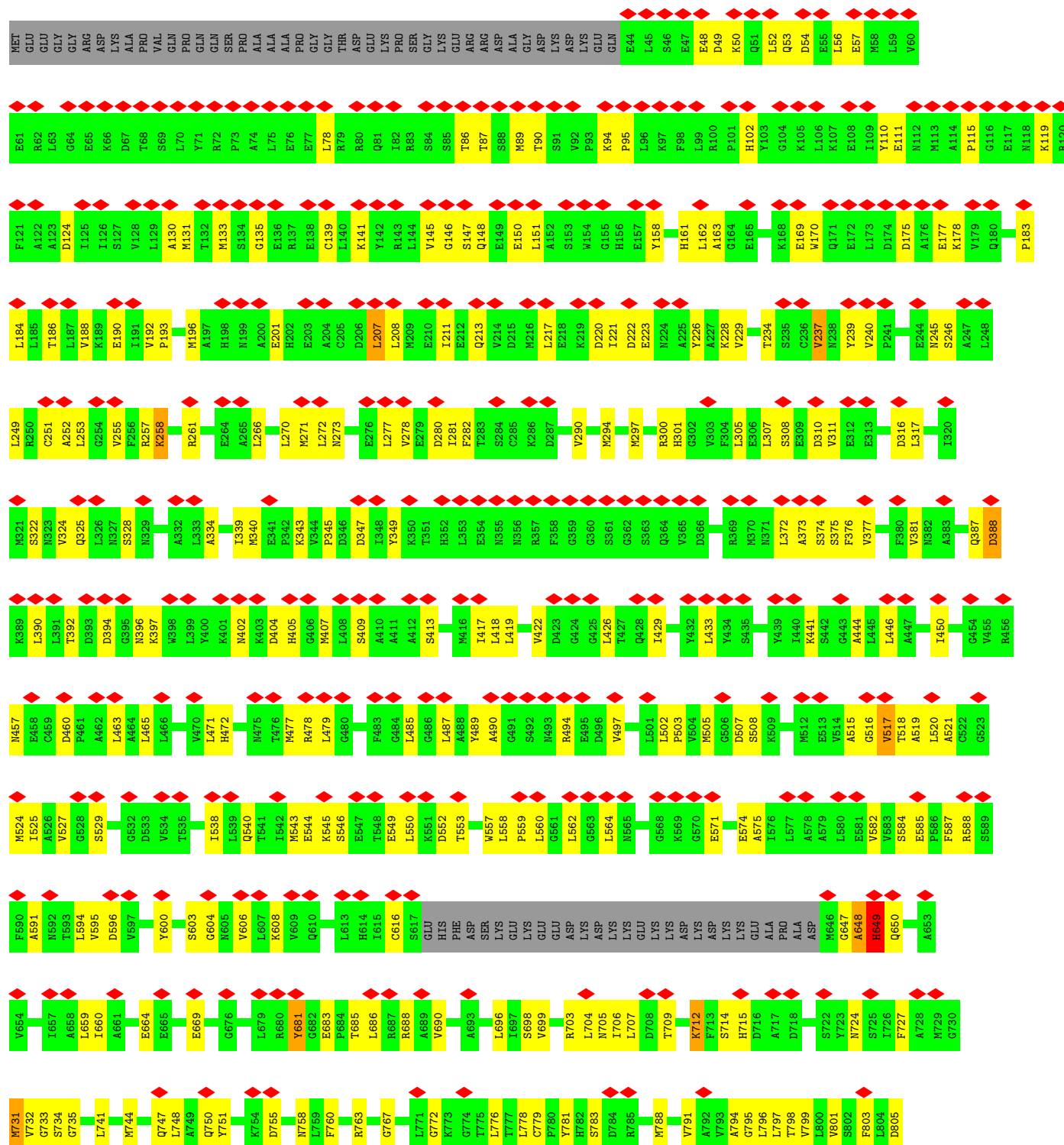
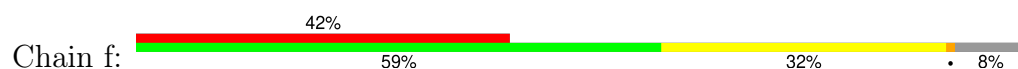


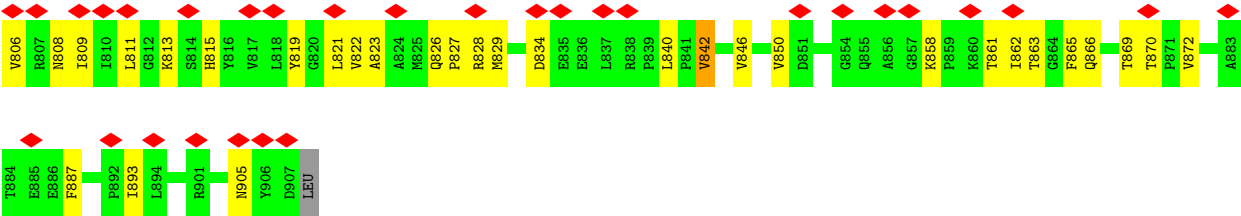
- Molecule 33: 26S proteasome non-ATPase regulatory subunit 14





• Molecule 34: 26S proteasome non-ATPase regulatory subunit 2







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	94665	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	105000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.227	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.031	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	518.322, 518.322, 518.322	wwPDB
Map dimensions	602, 602, 602	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86100006, 0.86100006, 0.86100006	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.34	0/3110	0.48	1/4196 (0.0%)
2	B	0.31	0/3120	0.48	0/4210
3	C	0.27	0/3112	0.42	0/4182
4	D	0.34	0/3089	0.48	0/4168
5	E	0.34	0/3146	0.43	0/4233
6	F	0.34	0/3292	0.47	2/4435 (0.0%)
7	G	0.34	0/1767	0.43	0/2398
7	g	0.31	0/1790	0.44	0/2429
8	H	0.33	0/1701	0.44	0/2318
8	h	0.29	0/1701	0.39	0/2318
9	I	0.43	1/1831 (0.1%)	0.71	5/2487 (0.2%)
9	i	0.29	0/1815	0.38	0/2466
10	J	0.29	0/1657	0.45	0/2261
10	j	0.28	0/1657	0.44	0/2261
11	K	0.31	0/1694	0.47	0/2301
11	k	0.29	0/1686	0.42	0/2290
12	L	0.34	0/1744	0.44	0/2371
12	l	0.30	0/1741	0.41	0/2367
13	M	0.33	0/1795	0.43	0/2434
13	m	0.29	0/1796	0.41	0/2435
14	N	0.31	0/1495	0.43	0/2026
14	n	0.30	0/1491	0.42	0/2021
15	O	0.30	0/1607	0.43	0/2185
15	o	0.31	0/1603	0.45	0/2180
16	P	0.31	0/1575	0.44	0/2128
16	p	0.32	0/1567	0.44	0/2118
17	Q	0.31	0/1541	0.44	0/2092
17	q	0.33	0/1538	0.44	0/2088
18	R	0.31	0/1535	0.43	0/2080
18	r	0.35	0/1531	0.45	0/2076
19	S	0.30	0/1614	0.41	0/2178
19	s	0.30	0/1617	0.44	0/2182

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
20	T	0.32	0/1606	0.46	0/2179
20	t	0.32	0/1598	0.47	0/2170
21	V	0.26	0/3668	0.47	2/4953 (0.0%)
22	W	0.26	0/3636	0.41	0/4891
23	X	0.24	0/3084	0.42	0/4157
24	Y	0.29	0/3185	0.45	0/4290
25	Z	0.35	0/2324	0.50	0/3150
26	a	0.30	0/3053	0.50	0/4133
27	b	0.24	0/1478	0.49	0/2001
28	d	0.22	0/2239	0.43	0/3025
29	e	0.19	0/420	0.37	0/572
31	z	0.27	0/620	0.42	0/836
32	U	0.31	0/6486	0.46	0/8777
33	c	0.34	0/2274	0.47	0/3072
34	f	0.32	1/6569 (0.0%)	0.55	6/8893 (0.1%)
All	All	0.31	2/104198 (0.0%)	0.46	16/141013 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	F	0	1
7	g	0	1
9	I	0	1
20	t	0	1
34	f	0	2
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	f	649	HIS	CG-CD2	6.31	1.42	1.35
9	I	109	GLN	N-CA	6.12	1.53	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	f	649	HIS	N-CA-CB	12.69	129.09	110.06
9	I	109	GLN	CB-CG-CD	-10.44	94.86	112.60
9	I	108	GLU	CA-C-N	-10.38	106.52	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	108	GLU	C-N-CA	-10.38	106.52	120.54
34	f	648	ALA	CA-C-N	-10.15	106.47	120.38
34	f	648	ALA	C-N-CA	-10.15	106.47	120.38
34	f	649	HIS	CB-CG-CD2	-9.25	119.18	131.20
34	f	649	HIS	ND1-CG-CD2	-8.87	97.23	106.10
9	I	109	GLN	CA-CB-CG	-8.46	97.17	114.10
21	V	494	MET	CA-C-N	8.43	134.65	122.77
21	V	494	MET	C-N-CA	8.43	134.65	122.77
6	F	396	CYS	N-CA-C	-8.34	103.70	114.04
34	f	649	HIS	CB-CA-C	-7.96	97.14	110.68
9	I	109	GLN	N-CA-CB	6.11	119.05	109.94
1	A	78	TRP	N-CA-C	-5.74	105.39	113.20
6	F	396	CYS	N-CA-CB	5.17	118.46	110.81

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	F	395	GLN	Peptide
9	I	109	GLN	Sidechain
34	f	647	GLY	Peptide
34	f	649	HIS	Sidechain
7	g	78	CYS	Peptide
20	t	109	THR	Peptide

## 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	A	3060	3106	3107	93	0
2	B	3076	3053	3129	151	0
3	C	3071	3193	3193	73	0
4	D	3039	3075	3076	77	0
5	E	3098	3150	3174	79	0
6	F	3251	3318	3316	83	0
7	G	1738	1656	1656	26	0
7	g	1758	1687	1687	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1662	1590	1590	45	0
8	h	1662	1590	1590	24	0
9	I	1802	1741	1741	51	0
9	i	1786	1717	1717	29	0
10	J	1633	1518	1518	42	0
10	j	1633	1518	1518	28	0
11	K	1667	1597	1596	49	0
11	k	1660	1589	1589	31	0
12	L	1710	1649	1649	29	0
12	l	1707	1645	1645	31	0
13	M	1760	1680	1680	37	0
13	m	1761	1683	1683	24	0
14	N	1469	1422	1422	37	0
14	n	1465	1416	1416	24	0
15	O	1580	1559	1559	40	0
15	o	1576	1555	1555	31	0
16	P	1546	1550	1552	29	0
16	p	1538	1543	1545	19	0
17	Q	1509	1477	1477	37	0
17	q	1506	1475	1475	26	0
18	R	1504	1449	1449	20	0
18	r	1500	1438	1438	38	0
19	S	1584	1579	1579	18	0
19	s	1587	1581	1581	32	0
20	T	1576	1526	1528	21	0
20	t	1568	1511	1513	22	0
21	V	3598	3658	3658	116	0
22	W	3588	0	3704	483	0
23	X	3040	3134	3134	82	0
24	Y	3127	3133	3133	89	0
25	Z	2281	2312	2312	76	0
26	a	2995	3012	3012	159	0
27	b	1458	1505	1505	75	0
28	d	2193	2221	2221	80	0
29	e	409	316	316	17	0
30	v	60	0	14	0	0
31	z	612	645	645	17	0
32	U	6371	6402	6407	222	0
33	c	2232	2241	2242	73	0
34	f	6460	6486	6487	224	0
35	A	31	12	12	1	0
35	B	31	12	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	D	31	12	12	0	0
35	F	31	12	12	1	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	D	1	0	0	0	0
36	F	1	0	0	0	0
37	E	27	12	12	1	0
38	c	1	0	0	0	0
All	All	102622	97961	101793	2925	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 (2925) 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)
22:W:205:ILE:HA	22:W:208:LYS:HD2	1.24	1.13
22:W:205:ILE:HD12	22:W:208:LYS:HD3	1.23	1.13
32:U:446:LEU:HD21	32:U:457:ILE:HD12	1.36	1.07
22:W:79:GLU:HB3	22:W:82:LEU:HB2	1.34	1.04
25:Z:186:THR:OG1	25:Z:190:ARG:NH2	1.93	1.01
22:W:112:VAL:O	22:W:121:LYS:NZ	1.96	0.99
22:W:33:LYS:HA	22:W:36:LYS:HE2	1.44	0.98
37:E:401:ADP:O1B	6:F:344:ARG:NH1	1.97	0.97
22:W:194:LEU:HD21	22:W:202:THR:HG21	1.44	0.97
22:W:112:VAL:HG11	22:W:125:ILE:HD11	1.46	0.96
26:a:280:MET:HE1	26:a:296:ILE:HD13	1.47	0.95
22:W:146:THR:HG21	22:W:169:LEU:HD21	1.47	0.95
2:B:434:THR:HB	2:B:435:PRO:HD3	1.48	0.93
5:E:71:VAL:HG21	5:E:100:LEU:HD21	1.49	0.93
15:O:2:THR:N	15:O:170:SER:HG	1.66	0.93
16:P:6:ASN:ND2	16:P:28:GLY:O	2.02	0.93
4:D:274:ARG:NH1	5:E:244:SER:O	2.01	0.92
22:W:141:GLU:OE1	22:W:141:GLU:N	2.03	0.92
22:W:205:ILE:HA	22:W:208:LYS:CD	1.99	0.92
22:W:317:TRP:CD1	22:W:355:LYS:HE2	2.05	0.92
22:W:326:MET:HE2	22:W:326:MET:HA	1.51	0.90
22:W:212:LYS:HD2	22:W:212:LYS:O	1.71	0.90
32:U:267:ASN:O	32:U:270:THR:OG1	1.89	0.89
22:W:155:GLN:NE2	22:W:156:ASN:OD1	2.06	0.88
32:U:365:CYS:O	32:U:369:THR:HG23	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:145:ARG:NH2	28:d:183:PRO:O	2.06	0.88
34:f:388:ASP:OD1	34:f:392:THR:OG1	1.89	0.88
9:I:165:GLY:O	9:I:168:SER:OG	1.90	0.88
28:d:282:ILE:HG21	28:d:315:TYR:HA	1.56	0.88
22:W:182:ARG:O	22:W:186:ILE:HG13	1.73	0.87
32:U:36:ALA:O	32:U:39:SER:OG	1.91	0.87
10:J:36:ARG:NH1	11:K:60:GLU:OE1	2.08	0.87
32:U:700:GLU:OE2	32:U:707:ASN:ND2	2.09	0.86
22:W:132:THR:O	22:W:142:ARG:HD2	1.74	0.86
22:W:55:ARG:HD2	22:W:94:ARG:O	1.76	0.85
6:F:396:CYS:O	6:F:399:VAL:N	2.08	0.85
21:V:304:GLU:N	21:V:304:GLU:OE2	2.07	0.85
22:W:54:THR:HG22	22:W:59:ASP:HB3	1.58	0.85
34:f:396:ASN:OD1	34:f:397:LYS:NZ	2.10	0.85
8:H:230:ALA:HB1	23:X:87:ARG:CZ	2.07	0.85
15:o:208:GLY:O	19:s:159:GLN:NE2	2.10	0.84
22:W:98:LYS:HB2	22:W:137:TYR:CD2	2.11	0.84
24:Y:360:ASP:OD1	24:Y:361:SER:N	2.10	0.84
10:j:140:GLY:O	10:j:213:ARG:NH1	2.09	0.84
24:Y:30:GLU:N	24:Y:30:GLU:OE1	2.10	0.84
34:f:245:ASN:OD1	34:f:246:SER:N	2.11	0.84
18:r:35:VAL:CG1	18:r:43:LEU:HD13	2.07	0.84
24:Y:285:ASP:OD1	24:Y:286:TRP:N	2.11	0.84
34:f:226:TYR:OH	34:f:261:ARG:NH1	2.11	0.83
21:V:243:ASP:OD1	21:V:244:ALA:N	2.11	0.83
21:V:303:SER:OG	21:V:304:GLU:OE2	1.95	0.83
22:W:287:VAL:HG23	22:W:306:LEU:HD11	1.60	0.83
25:Z:186:THR:HG1	25:Z:190:ARG:NH2	1.75	0.83
10:J:40:ILE:HD11	10:J:210:VAL:HG13	1.60	0.83
29:e:20:GLU:OE1	29:e:20:GLU:N	2.12	0.83
3:C:62:GLU:OE1	4:D:117:SER:OG	1.95	0.83
4:D:346:SER:O	4:D:350:SER:OG	1.95	0.83
22:W:257:GLN:HA	22:W:263:TRP:HB3	1.61	0.83
9:i:184:MET:SD	9:i:188:SER:OG	2.36	0.83
22:W:214:PHE:HB3	22:W:223:LYS:HG3	1.60	0.82
23:X:407:MET:SD	25:Z:266:ILE:HD13	2.19	0.82
22:W:29:PRO:O	22:W:33:LYS:HG2	1.80	0.82
6:F:279:ALA:HB1	6:F:280:PRO:HD2	1.60	0.82
5:E:329:GLU:OE1	5:E:329:GLU:N	2.12	0.82
22:W:85:GLU:O	22:W:89:LEU:HD12	1.79	0.82
22:W:112:VAL:HG11	22:W:125:ILE:CD1	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:331:GLY:CA	22:W:337:ALA:HB2	2.10	0.81
34:f:472:HIS:O	34:f:478:ARG:NE	2.13	0.81
6:F:161:LEU:O	6:F:161:LEU:HD23	1.80	0.81
10:J:40:ILE:HD11	10:J:210:VAL:CG1	2.11	0.81
33:c:29:GLU:OE2	33:c:161:ARG:NH2	2.14	0.81
22:W:202:THR:HA	22:W:205:ILE:HG22	1.62	0.81
22:W:24:VAL:O	22:W:28:LEU:HG	1.80	0.81
26:a:296:ILE:HG21	26:a:307:VAL:HG13	1.61	0.81
9:I:109:GLN:HA	9:I:109:GLN:NE2	1.95	0.80
22:W:54:THR:HG21	22:W:62:SER:HB2	1.62	0.80
26:a:129:GLN:N	26:a:129:GLN:OE1	2.14	0.80
2:B:275:GLU:N	2:B:275:GLU:OE1	2.14	0.80
3:C:358:GLU:O	3:C:362:VAL:HG23	1.80	0.80
22:W:251:TYR:HB2	22:W:266:ALA:HB1	1.64	0.80
27:b:147:GLU:O	27:b:149:ASN:ND2	2.13	0.80
32:U:412:HIS:ND1	32:U:422:LEU:HD21	1.96	0.80
17:q:29:LYS:NZ	17:q:31:ASP:OD1	2.15	0.80
12:L:178:GLU:OE1	12:L:178:GLU:N	2.14	0.80
3:C:287:LYS:O	3:C:287:LYS:NZ	2.12	0.80
32:U:885:MET:HE2	32:U:885:MET:N	1.97	0.80
22:W:29:PRO:O	22:W:33:LYS:NZ	2.13	0.80
22:W:251:TYR:CE1	22:W:267:LEU:HG	2.16	0.80
32:U:805:ASN:OD1	32:U:893:THR:OG1	1.98	0.80
33:c:31:VAL:HG23	33:c:205:ILE:HD13	1.64	0.80
9:I:108:GLU:O	9:I:112:THR:HG22	1.80	0.79
32:U:795:LEU:O	32:U:796:LYS:NZ	2.10	0.79
1:A:73:ALA:O	1:A:78:TRP:NE1	2.15	0.79
2:B:429:LYS:O	2:B:430:LYS:HE2	1.82	0.79
22:W:210:ASN:OD1	22:W:212:LYS:N	2.15	0.79
25:Z:59:ASP:OD1	25:Z:60:GLU:N	2.16	0.79
26:a:141:MET:N	26:a:141:MET:SD	2.54	0.79
28:d:218:LYS:O	28:d:222:THR:OG1	1.99	0.79
34:f:316:ASP:OD1	34:f:317:LEU:N	2.14	0.79
26:a:121:LEU:O	26:a:124:ASN:ND2	2.15	0.79
28:d:267:ILE:O	28:d:271:ILE:HG23	1.83	0.79
3:C:258:ARG:O	3:C:270:GLN:NE2	2.16	0.79
4:D:115:ILE:HG12	4:D:139:LEU:HD22	1.64	0.79
21:V:404:LYS:HE2	21:V:404:LYS:HA	1.63	0.79
10:j:38:ARG:O	10:j:213:ARG:NH2	2.15	0.79
22:W:66:ILE:O	22:W:70:VAL:HG23	1.83	0.79
7:G:5:SER:N	7:G:19:GLU:OE2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:ASP:OD1	3:C:120:SER:N	2.15	0.78
24:Y:215:ASP:OD1	24:Y:216:TYR:N	2.16	0.78
4:D:407:ILE:HG23	4:D:407:ILE:O	1.83	0.78
28:d:335:LEU:HB3	33:c:303:MET:HE3	1.65	0.78
22:W:55:ARG:NH1	22:W:94:ARG:O	2.14	0.78
13:M:181:MET:HA	13:M:184:MET:HE3	1.66	0.78
3:C:284:GLU:OE1	3:C:284:GLU:N	2.17	0.78
6:F:382:GLU:OE1	6:F:382:GLU:N	2.17	0.78
21:V:232:HIS:CE1	21:V:254:LEU:HD21	2.19	0.78
22:W:171:VAL:HG11	22:W:186:ILE:HG12	1.65	0.78
20:t:46:ASN:OD1	20:t:49:THR:OG1	2.00	0.78
32:U:213:PHE:HB3	32:U:248:ILE:HD11	1.66	0.78
33:c:62:VAL:O	33:c:66:THR:OG1	2.00	0.78
32:U:483:LEU:HD23	32:U:486:MET:HE3	1.65	0.77
2:B:83:GLU:OE1	2:B:84:GLN:NE2	2.17	0.77
17:Q:103:LEU:HD22	17:Q:115:LEU:HD11	1.64	0.77
19:s:198:VAL:HG22	19:s:203:ILE:HD12	1.67	0.77
8:h:43:VAL:HG21	8:h:136:CYS:HB2	1.67	0.77
15:O:25:MET:HE3	19:S:187:VAL:HG21	1.65	0.77
22:W:265:GLN:NE2	22:W:336:PRO:HG2	1.99	0.77
22:W:214:PHE:HE1	22:W:222:LEU:HB2	1.49	0.76
21:V:131:LEU:HD12	21:V:171:VAL:HG21	1.66	0.76
27:b:36:VAL:O	27:b:39:SER:OG	2.02	0.76
10:J:211:MET:N	10:J:211:MET:SD	2.59	0.76
21:V:294:ARG:NH2	21:V:390:GLY:O	2.18	0.76
21:V:432:GLU:OE1	21:V:432:GLU:N	2.18	0.76
13:M:99:ARG:NH1	13:M:105:ASN:OD1	2.19	0.76
22:W:27:ARG:NH2	22:W:31:CYS:SG	2.58	0.76
27:b:25:ARG:NH1	27:b:144:GLY:O	2.18	0.76
33:c:158:ASP:OD1	33:c:159:ALA:N	2.18	0.76
34:f:544:GLU:OE1	34:f:545:LYS:NZ	2.19	0.76
22:W:205:ILE:HD12	22:W:208:LYS:CD	2.09	0.76
31:z:69:GLU:OE1	31:z:69:GLU:N	2.16	0.76
22:W:240:TYR:OH	22:W:353:ASP:OD2	2.03	0.76
21:V:443:ARG:NH2	21:V:444:ASP:OD1	2.18	0.76
22:W:237:GLU:OE1	22:W:237:GLU:N	2.19	0.76
34:f:507:ASP:OD1	34:f:508:SER:N	2.19	0.76
22:W:317:TRP:CE3	22:W:358:VAL:HG11	2.21	0.76
3:C:302:ASP:OD1	3:C:303:SER:N	2.19	0.75
34:f:479:LEU:HD22	34:f:517:VAL:HG21	1.67	0.75
22:W:192:LEU:O	22:W:196:VAL:HG13	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:171:GLY:N	11:K:174:SER:OG	2.19	0.75
12:l:65:HIS:O	12:l:89:ARG:NH1	2.20	0.75
32:U:320:ASP:OD1	32:U:321:GLN:N	2.20	0.75
7:G:193:GLN:OE1	7:G:193:GLN:N	2.18	0.75
4:D:318:ASP:OD1	4:D:320:ALA:N	2.18	0.75
22:W:64:SER:O	22:W:68:VAL:HG12	1.87	0.75
14:n:167:ARG:NH1	20:t:34:ALA:O	2.18	0.75
34:f:731:MET:O	34:f:734:SER:N	2.18	0.75
6:F:143:GLU:N	6:F:143:GLU:OE2	2.20	0.75
22:W:33:LYS:HA	22:W:36:LYS:CE	2.15	0.75
4:D:176:GLU:OE1	4:D:329:ARG:NH2	2.19	0.75
22:W:188:GLU:OE2	22:W:191:ARG:NH1	2.20	0.75
28:d:207:GLU:OE1	28:d:207:GLU:N	2.19	0.75
22:W:117:ASP:HB3	22:W:120:ILE:HB	1.68	0.74
27:b:5:SER:OG	27:b:48:ASN:OD1	2.02	0.74
16:p:189:ILE:HG22	16:p:194:ILE:CD1	2.17	0.74
15:O:199:ARG:NH1	16:P:151:SER:O	2.19	0.74
23:X:254:MET:SD	23:X:270:LEU:HD21	2.27	0.74
33:c:210:ASN:ND2	33:c:213:GLU:OE2	2.20	0.74
15:o:192:VAL:HG23	15:o:192:VAL:O	1.85	0.74
24:Y:41:LEU:O	24:Y:45:VAL:HG23	1.87	0.74
11:K:210:LEU:HD21	11:K:215:ILE:HD13	1.70	0.74
21:V:100:MET:N	21:V:100:MET:SD	2.60	0.74
22:W:187:LEU:HD23	22:W:225:LYS:HB3	1.70	0.74
22:W:377:ARG:NH2	26:a:308:GLU:OE1	2.21	0.74
34:f:520:LEU:HD22	34:f:560:LEU:HD22	1.67	0.74
22:W:101:VAL:O	22:W:105:VAL:HG23	1.86	0.74
34:f:688:ARG:O	34:f:724:ASN:ND2	2.21	0.73
34:f:791:VAL:HG12	34:f:823:ALA:HB1	1.70	0.73
10:J:188:ILE:HD11	10:J:210:VAL:HG21	1.69	0.73
20:T:5:MET:HA	20:T:5:MET:HE2	1.70	0.73
22:W:60:MET:HA	22:W:97:LEU:HD12	1.70	0.73
18:r:41:TYR:OH	18:r:182:GLU:O	2.05	0.73
11:K:133:MET:HE2	11:K:133:MET:HA	1.71	0.73
28:d:208:PHE:O	28:d:212:LEU:HD13	1.88	0.73
31:z:87:GLU:N	31:z:87:GLU:OE1	2.22	0.73
34:f:146:GLY:O	34:f:148:GLN:NE2	2.20	0.73
10:J:42:VAL:HG13	10:J:191:VAL:HG21	1.70	0.73
22:W:318:SER:O	22:W:322:GLU:HG2	1.87	0.73
22:W:331:GLY:HA3	22:W:337:ALA:HB2	1.70	0.73
18:r:35:VAL:HG13	18:r:43:LEU:HD13	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:159:LYS:NZ	4:D:221:HIS:O	2.22	0.73
24:Y:314:LEU:HD21	24:Y:318:TYR:HD1	1.53	0.73
22:W:135:LYS:HD3	22:W:137:TYR:OH	1.88	0.73
24:Y:314:LEU:HD22	24:Y:319:MET:HG3	1.70	0.73
25:Z:21:ASP:OD1	33:c:104:ARG:NH2	2.21	0.73
32:U:21:GLU:OE2	32:U:21:GLU:N	2.22	0.73
32:U:38:ILE:HD13	32:U:67:VAL:HG11	1.70	0.73
22:W:54:THR:CG2	22:W:59:ASP:HB3	2.19	0.72
33:c:71:ASP:OD1	33:c:72:VAL:N	2.21	0.72
1:A:102:ILE:HD11	1:A:114:ASN:HB2	1.72	0.72
14:N:63:GLN:NE2	14:N:83:LEU:HD22	2.05	0.72
32:U:550:VAL:HG21	32:U:768:GLN:OE1	1.90	0.72
15:O:7:VAL:HG23	15:O:125:TYR:HB3	1.70	0.72
31:z:107:MET:SD	31:z:108:SER:N	2.62	0.72
11:K:195:ILE:HG23	11:K:217:LEU:HD11	1.71	0.72
32:U:184:CYS:C	32:U:185:MET:HE2	2.14	0.72
18:R:167:ARG:NH1	17:q:144:ASP:OD1	2.23	0.72
21:V:482:PHE:CZ	21:V:486:ILE:HD11	2.24	0.72
2:B:112:LEU:HD22	2:B:144:LEU:CD2	2.20	0.72
26:a:217:LEU:HD11	26:a:237:LEU:HB3	1.70	0.72
34:f:727:PHE:CE2	34:f:803:PHE:CE2	2.78	0.72
22:W:400:LYS:O	22:W:400:LYS:HG2	1.89	0.72
16:p:189:ILE:HG22	16:p:194:ILE:HD12	1.70	0.72
32:U:213:PHE:HD2	32:U:236:LEU:HD11	1.55	0.72
15:O:4:ILE:HD12	15:O:45:CYS:HB2	1.72	0.72
22:W:369:TYR:CE2	26:a:312:MET:HE1	2.25	0.72
13:m:232:ARG:NH1	13:m:236:GLU:OE1	2.22	0.72
4:D:202:VAL:HB	4:D:308:ILE:HG22	1.72	0.71
22:W:128:LEU:O	22:W:132:THR:OG1	2.04	0.71
22:W:371:THR:HG23	26:a:323:SER:HB3	1.73	0.71
24:Y:183:TYR:CE1	24:Y:213:LEU:HD11	2.25	0.71
32:U:28:ASN:OD1	32:U:63:VAL:HG22	1.88	0.71
12:l:42:THR:O	12:l:43:HIS:ND1	2.23	0.71
2:B:317:ASP:O	2:B:346:ARG:NH1	2.23	0.71
22:W:32:ALA:HB3	22:W:33:LYS:NZ	2.05	0.71
13:M:206:ASP:OD1	13:M:207:LYS:N	2.23	0.71
22:W:308:LEU:O	22:W:315:MET:HE1	1.91	0.71
22:W:278:PRO:HG3	22:W:357:ARG:HH21	1.56	0.71
22:W:329:ARG:HG3	22:W:341:PHE:O	1.89	0.71
32:U:227:GLN:O	32:U:230:SER:OG	2.08	0.71
26:a:97:LEU:HD13	26:a:118:ILE:HG12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:360:VAL:O	32:U:361:ARG:NH1	2.23	0.71
32:U:388:ASP:OD1	32:U:389:ASN:N	2.22	0.71
3:C:151:ILE:HG22	3:C:151:ILE:O	1.91	0.71
16:p:70:LEU:HD11	16:p:81:ILE:HG21	1.72	0.71
31:z:75:HIS:O	31:z:78:THR:OG1	2.09	0.71
15:O:136:MET:HE3	20:T:179:ARG:NH2	2.06	0.71
22:W:93:ARG:HB2	22:W:96:GLN:HG2	1.73	0.71
23:X:256:LEU:HD22	23:X:319:ILE:HD13	1.73	0.71
32:U:107:HIS:NE2	32:U:111:GLN:OE1	2.24	0.71
6:F:248:PHE:O	6:F:249:LEU:HD12	1.91	0.70
25:Z:193:ASN:O	25:Z:195:VAL:N	2.24	0.70
34:f:546:SER:OG	34:f:549:GLU:OE2	2.08	0.70
22:W:33:LYS:HD3	22:W:36:LYS:NZ	2.05	0.70
32:U:505:ASP:OD1	32:U:506:ALA:N	2.23	0.70
2:B:410:ARG:NH2	3:C:167:LEU:HD11	2.07	0.70
22:W:112:VAL:HG22	22:W:124:LEU:CD2	2.21	0.70
22:W:451:MET:HE2	25:Z:102:HIS:O	1.92	0.70
23:X:312:GLU:OE1	23:X:312:GLU:N	2.23	0.70
5:E:211:SER:OG	5:E:256:THR:OG1	2.10	0.70
22:W:33:LYS:HD3	22:W:36:LYS:CE	2.20	0.70
24:Y:292:TYR:OH	24:Y:293:ARG:NH2	2.24	0.70
1:A:391:GLU:OE2	2:B:349:ARG:NH1	2.23	0.70
2:B:268:ARG:NH1	2:B:311:GLU:OE2	2.25	0.70
3:C:346:LYS:O	3:C:346:LYS:HD3	1.91	0.70
14:N:15:LEU:HD23	14:N:45:CYS:SG	2.31	0.70
22:W:63:THR:O	22:W:67:LEU:HD23	1.92	0.70
22:W:283:GLN:O	22:W:287:VAL:HG12	1.91	0.70
2:B:115:ILE:HG22	2:B:117:ASP:H	1.57	0.70
21:V:279:GLN:OE1	21:V:279:GLN:N	2.25	0.70
34:f:858:LYS:O	34:f:858:LYS:HD3	1.91	0.70
24:Y:308:LEU:O	24:Y:358:ARG:NH2	2.25	0.70
1:A:81:ALA:HB1	2:B:138:PHE:HB3	1.74	0.70
22:W:314:LEU:HD12	22:W:314:LEU:H	1.55	0.70
25:Z:193:ASN:OD1	25:Z:194:GLN:NE2	2.25	0.70
11:K:60:GLU:N	11:K:60:GLU:OE2	2.25	0.70
15:O:14:VAL:HG23	15:O:156:VAL:HG21	1.73	0.70
15:O:109:PRO:O	15:O:110:HIS:ND1	2.25	0.70
13:M:175:GLU:HB3	13:M:196:ILE:HD12	1.73	0.69
25:Z:52:ASN:OD1	25:Z:53:SER:N	2.25	0.69
22:W:438:LEU:O	22:W:442:THR:HG22	1.91	0.69
24:Y:357:ASN:O	24:Y:357:ASN:OD1	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:33:ILE:HD12	33:c:205:ILE:HD12	1.73	0.69
14:N:139:TYR:O	14:N:143:THR:HG22	1.92	0.69
22:W:346:GLU:OE2	22:W:350:ARG:NH2	2.24	0.69
16:P:47:ARG:NH1	16:P:191:LYS:O	2.25	0.69
21:V:162:GLU:OE1	21:V:162:GLU:N	2.23	0.69
22:W:200:ILE:H	22:W:200:ILE:HD12	1.56	0.69
22:W:206:SER:OG	22:W:230:MET:HE1	1.92	0.69
9:i:196:VAL:O	9:i:200:THR:OG1	2.06	0.69
34:f:683:GLU:OE1	34:f:683:GLU:N	2.26	0.69
6:F:168:TYR:OH	6:F:277:GLU:OE2	2.11	0.69
22:W:67:LEU:CD1	22:W:90:LEU:HD13	2.23	0.69
2:B:58:CYS:SG	2:B:59:ARG:N	2.65	0.69
23:X:256:LEU:HD22	23:X:319:ILE:CD1	2.23	0.69
24:Y:212:GLU:N	24:Y:212:GLU:OE1	2.26	0.69
27:b:181:ASP:OD1	27:b:182:ALA:N	2.25	0.69
18:r:3:THR:HG22	18:r:3:THR:O	1.92	0.69
8:H:220:LEU:HD23	8:H:224:GLU:HG2	1.75	0.69
22:W:19:ASP:OD1	22:W:21:SER:N	2.18	0.69
22:W:166:LEU:HD23	22:W:192:LEU:HD12	1.74	0.69
22:W:186:ILE:O	22:W:190:MET:HG3	1.93	0.69
22:W:331:GLY:HA2	22:W:337:ALA:HB2	1.74	0.69
22:W:369:TYR:HE2	26:a:312:MET:HE1	1.57	0.69
23:X:255:LEU:HD12	23:X:270:LEU:HD23	1.75	0.69
27:b:180:ALA:O	27:b:183:LEU:N	2.25	0.69
32:U:590:TYR:O	32:U:625:ILE:HD13	1.93	0.69
23:X:375:HIS:ND1	23:X:390:GLU:OE2	2.25	0.69
27:b:111:ALA:HB3	27:b:140:ILE:HD13	1.75	0.69
34:f:794:ALA:O	34:f:798:THR:HG23	1.93	0.69
22:W:22:ALA:HA	22:W:25:ASP:OD2	1.91	0.69
32:U:351:MET:HE2	32:U:351:MET:N	2.08	0.69
4:D:85:ILE:HD13	5:E:68:LYS:HD3	1.75	0.68
1:A:174:TYR:CD1	1:A:184:ILE:HD11	2.28	0.68
4:D:349:THR:HG22	4:D:379:CYS:SG	2.34	0.68
8:H:71:ILE:HD11	8:H:109:LEU:HD23	1.75	0.68
9:I:109:GLN:HA	9:I:109:GLN:HE21	1.55	0.68
15:O:8:VAL:HG22	15:O:13:ILE:HD13	1.75	0.68
20:T:69:GLN:NE2	20:T:73:ASP:OD1	2.26	0.68
32:U:723:ASP:OD1	32:U:724:VAL:N	2.26	0.68
7:G:84:THR:HG21	13:M:156:VAL:HG23	1.74	0.68
22:W:344:THR:HG23	22:W:347:GLY:H	1.59	0.68
22:W:146:THR:CG2	22:W:169:LEU:HD11	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:ARG:HB3	2:B:160:ILE:HD12	1.76	0.68
12:l:88:MET:SD	12:l:112:ILE:HD11	2.33	0.68
1:A:78:TRP:C	1:A:81:ALA:HB3	2.19	0.68
22:W:348:GLU:O	22:W:352:LYS:HG2	1.93	0.68
22:W:194:LEU:HD12	22:W:229:LEU:HD12	1.76	0.68
32:U:906:LEU:O	32:U:909:GLY:N	2.27	0.68
3:C:49:ARG:NE	4:D:64:GLU:OE1	2.26	0.67
6:F:172:VAL:HG23	6:F:267:LEU:HD13	1.76	0.67
22:W:263:TRP:HZ3	22:W:267:LEU:HD12	1.59	0.67
3:C:152:GLY:N	3:C:327:ASP:OD2	2.26	0.67
1:A:345:LEU:H	1:A:345:LEU:HD12	1.59	0.67
2:B:435:PRO:HB2	9:I:155:ASN:HD22	1.59	0.67
5:E:309:ARG:NH1	5:E:332:VAL:O	2.28	0.67
22:W:41:GLN:O	22:W:45:GLU:HG2	1.94	0.67
22:W:226:TYR:HE1	22:W:230:MET:HE2	1.60	0.67
34:f:755:ASP:OD2	34:f:758:ASN:ND2	2.27	0.67
6:F:421:MET:O	6:F:425:LEU:HD22	1.95	0.67
2:B:278:ALA:HB1	2:B:279:PRO:CD	2.24	0.67
22:W:19:ASP:OD1	22:W:20:TYR:N	2.27	0.67
22:W:87:ILE:HA	22:W:104:MET:HE1	1.74	0.67
22:W:221:LYS:O	22:W:221:LYS:NZ	2.25	0.67
12:l:189:LYS:NZ	12:l:232:PHE:O	2.27	0.67
18:r:4:THR:HG21	18:r:45:THR:HB	1.76	0.67
12:L:88:MET:HE2	12:L:112:ILE:HD13	1.77	0.67
22:W:169:LEU:HD12	22:W:185:PHE:CE1	2.29	0.67
28:d:241:TYR:CE2	28:d:271:ILE:HG22	2.29	0.67
5:E:108:MET:HE2	6:F:111:ILE:CD1	2.25	0.67
9:I:37:ILE:HD12	9:I:44:LEU:HD11	1.77	0.67
26:a:40:GLN:HA	26:a:43:ASP:HB3	1.76	0.67
22:W:317:TRP:O	22:W:321:VAL:HG12	1.94	0.67
24:Y:204:THR:HG22	24:Y:204:THR:O	1.94	0.67
22:W:251:TYR:HE1	22:W:263:TRP:HE3	1.43	0.67
33:c:279:ASP:OD1	33:c:279:ASP:O	2.13	0.67
1:A:190:VAL:HG13	1:A:191:VAL:HG13	1.76	0.67
22:W:32:ALA:O	22:W:36:LYS:HG2	1.94	0.67
22:W:256:ILE:HD13	22:W:262:LYS:HB3	1.76	0.67
34:f:163:ALA:HB1	34:f:207:LEU:CD1	2.25	0.67
1:A:74:PRO:O	1:A:77:LEU:N	2.24	0.66
6:F:134:LEU:CD2	6:F:160:ILE:HG23	2.25	0.66
9:I:174:MET:HE1	9:I:195:LYS:HE2	1.77	0.66
26:a:71:VAL:O	26:a:71:VAL:HG12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:355:LYS:O	23:X:356:LEU:HD23	1.95	0.66
24:Y:201:PHE:HB3	24:Y:223:THR:HG23	1.77	0.66
29:e:51:ASP:O	29:e:54:ASN:N	2.24	0.66
5:E:168:LYS:HD2	5:E:275:MET:HE1	1.77	0.66
10:J:81:ARG:O	10:J:85:ASN:ND2	2.28	0.66
22:W:163:ALA:HB2	22:W:196:VAL:HG11	1.78	0.66
22:W:383:ASP:O	22:W:384:LEU:HD23	1.95	0.66
12:l:158:ALA:CB	12:l:172:LEU:HD22	2.26	0.66
32:U:678:ASP:OD2	32:U:683:VAL:HG11	1.94	0.66
15:O:2:THR:N	15:O:130:SER:HG	1.94	0.66
22:W:42:GLU:O	22:W:46:THR:HG22	1.94	0.66
27:b:140:ILE:HG21	27:b:153:LEU:HD21	1.76	0.66
10:J:116:GLN:HG3	11:K:83:ALA:HB1	1.76	0.66
22:W:280:ASP:OD1	22:W:282:GLU:N	2.28	0.66
22:W:361:HIS:O	22:W:365:ILE:HG22	1.96	0.66
34:f:177:GLU:OE1	34:f:177:GLU:N	2.29	0.66
1:A:400:ARG:NH1	34:f:89:MET:O	2.28	0.66
26:a:213:PHE:O	26:a:217:LEU:HD23	1.96	0.66
34:f:158:TYR:OH	34:f:162:LEU:HD22	1.95	0.66
22:W:139:GLU:OE2	22:W:174:TYR:HB3	1.96	0.66
32:U:396:ALA:O	32:U:401:LYS:NZ	2.29	0.66
7:G:51:VAL:HG22	7:G:217:VAL:HG13	1.78	0.66
17:Q:19:ARG:NH1	17:Q:193:ASN:OD1	2.28	0.66
22:W:193:CYS:O	22:W:196:VAL:HG22	1.94	0.66
22:W:214:PHE:CE1	22:W:222:LEU:HB2	2.31	0.66
6:F:228:PRO:O	6:F:231:THR:OG1	2.09	0.66
14:n:56:VAL:HG21	14:n:95:LEU:HD21	1.78	0.66
33:c:123:SER:OG	33:c:126:ASP:OD2	2.09	0.66
22:W:134:GLY:O	22:W:135:LYS:HG3	1.96	0.65
22:W:214:PHE:CB	22:W:223:LYS:HG3	2.26	0.65
24:Y:328:GLU:OE2	24:Y:332:GLN:NE2	2.29	0.65
15:o:25:MET:HE1	19:s:33:PHE:CE1	2.31	0.65
22:W:84:ASN:OD1	22:W:123:ARG:NH2	2.29	0.65
14:N:165:MET:HE1	14:N:175:ILE:CG1	2.26	0.65
22:W:164:SER:O	22:W:168:GLU:HG3	1.97	0.65
22:W:183:VAL:HG21	22:W:213:PHE:CE2	2.31	0.65
24:Y:111:LEU:HD13	24:Y:119:GLY:C	2.22	0.65
2:B:264:PRO:HD3	2:B:308:THR:HG22	1.77	0.65
22:W:43:VAL:O	22:W:47:LEU:HG	1.96	0.65
26:a:183:VAL:HG22	26:a:185:ILE:O	1.97	0.65
33:c:117:GLY:CA	33:c:148:ILE:HD11	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:388:ASP:OD1	34:f:388:ASP:N	2.26	0.65
34:f:450:ILE:HG23	34:f:822:VAL:HG21	1.78	0.65
8:H:71:ILE:CD1	8:H:109:LEU:HD23	2.26	0.65
23:X:221:GLU:N	23:X:221:GLU:OE1	2.29	0.65
15:o:109:PRO:O	15:o:110:HIS:ND1	2.28	0.65
32:U:3:THR:O	32:U:5:ALA:N	2.29	0.65
34:f:290:VAL:O	34:f:294:MET:HG3	1.96	0.65
34:f:485:LEU:HD23	34:f:485:LEU:C	2.20	0.65
2:B:436:GLU:OE1	2:B:436:GLU:HA	1.97	0.65
21:V:497:PRO:O	21:V:500:SER:N	2.29	0.65
22:W:314:LEU:CD2	22:W:381:LEU:HD21	2.27	0.65
23:X:398:GLU:OE2	24:Y:365:GLN:NE2	2.30	0.65
32:U:34:PHE:O	32:U:38:ILE:HG22	1.96	0.65
34:f:257:ARG:NH2	34:f:280:ASP:OD2	2.29	0.65
25:Z:19:VAL:HG22	25:Z:95:TYR:CE2	2.31	0.65
32:U:30:VAL:HG22	32:U:34:PHE:CD1	2.32	0.65
22:W:314:LEU:HD23	22:W:381:LEU:HD21	1.79	0.65
22:W:363:ILE:HG12	22:W:378:MET:HE3	1.79	0.65
23:X:317:PRO:O	23:X:321:THR:HG23	1.97	0.65
13:m:111:LEU:O	13:m:115:VAL:HG23	1.97	0.65
17:q:13:VAL:HG11	17:q:105:ALA:HB1	1.78	0.65
32:U:321:GLN:O	32:U:325:MET:HG3	1.97	0.65
9:I:108:GLU:O	9:I:109:GLN:C	2.34	0.65
22:W:73:MET:HE2	22:W:73:MET:N	2.12	0.65
34:f:388:ASP:OD2	34:f:417:ILE:HD13	1.96	0.65
4:D:91:GLN:OE1	4:D:245:ARG:NH1	2.30	0.65
9:I:76:VAL:HG11	9:I:83:ALA:HB2	1.79	0.65
10:j:51:ALA:O	10:j:53:LEU:N	2.29	0.65
12:l:33:SER:OG	12:l:49:LEU:O	2.11	0.65
5:E:216:ARG:NH1	5:E:259:GLU:OE2	2.29	0.64
7:G:164:LYS:NZ	8:H:54:ILE:O	2.30	0.64
26:a:131:THR:O	26:a:134:THR:OG1	2.12	0.64
7:g:181:LYS:O	7:g:185:LYS:NZ	2.27	0.64
7:g:203:SER:O	7:g:207:SER:N	2.29	0.64
33:c:117:GLY:HA3	33:c:148:ILE:HD11	1.79	0.64
34:f:222:ASP:OD1	34:f:223:GLU:N	2.31	0.64
34:f:699:VAL:HG13	34:f:731:MET:HE2	1.79	0.64
16:P:64:GLN:OE1	17:Q:86:ARG:NH2	2.30	0.64
4:D:391:ARG:NH2	4:D:398:ASP:OD2	2.30	0.64
21:V:94:VAL:O	21:V:97:ALA:N	2.29	0.64
8:h:43:VAL:HG22	8:h:212:CYS:SG	2.38	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:15:VAL:HG21	18:r:43:LEU:HD11	1.79	0.64
7:g:196:GLU:O	7:g:200:THR:HG22	1.97	0.64
15:O:8:VAL:HG22	15:O:13:ILE:CD1	2.27	0.64
18:R:27:ILE:O	16:p:176:ARG:NH1	2.30	0.64
22:W:99:GLN:OE1	22:W:99:GLN:N	2.26	0.64
22:W:381:LEU:HD23	22:W:381:LEU:O	1.97	0.64
27:b:31:ASP:HB3	27:b:179:LEU:HD21	1.78	0.64
34:f:253:LEU:HD21	34:f:281:ILE:HD11	1.80	0.64
34:f:659:LEU:HD11	34:f:797:LEU:CD2	2.28	0.64
2:B:153:ASN:OD1	2:B:154:HIS:N	2.30	0.64
21:V:115:LYS:NZ	21:V:144:ASP:OD2	2.24	0.64
14:n:3:THR:HG22	14:n:161:LEU:CD2	2.28	0.64
32:U:786:THR:OG1	32:U:884:VAL:O	2.16	0.64
1:A:80:LEU:HD13	1:A:85:GLN:OE1	1.98	0.64
8:H:230:ALA:HB1	23:X:87:ARG:NH2	2.12	0.64
21:V:245:ASP:OD1	21:V:246:GLY:N	2.30	0.64
28:d:233:GLU:OE1	28:d:233:GLU:HA	1.97	0.64
3:C:169:VAL:HG11	3:C:207:THR:OG1	1.98	0.64
10:j:116:GLN:NE2	11:k:84:ASP:OD1	2.31	0.64
16:P:44:MET:HE2	16:P:66:LEU:HG	1.80	0.64
16:P:58:ASP:OD2	16:P:103:TYR:N	2.30	0.64
22:W:317:TRP:NE1	22:W:355:LYS:HE2	2.12	0.64
28:d:271:ILE:HD11	28:d:291:LEU:HD13	1.80	0.64
32:U:541:HIS:ND1	33:c:63:ASP:OD2	2.30	0.64
32:U:653:ALA:HB2	32:U:675:MET:CE	2.28	0.64
2:B:278:ALA:HB1	2:B:279:PRO:HD2	1.77	0.64
2:B:357:ASP:OD1	2:B:357:ASP:N	2.25	0.64
34:f:543:MET:HE2	34:f:543:MET:O	1.98	0.64
22:W:226:TYR:CE1	22:W:230:MET:HE2	2.33	0.63
22:W:129:ARG:HH11	22:W:129:ARG:HG3	1.64	0.63
21:V:207:ALA:O	21:V:211:TYR:CD2	2.51	0.63
22:W:408:ARG:HH12	23:X:349:HIS:CG	2.17	0.63
32:U:471:ASP:OD2	32:U:507:VAL:HG12	1.98	0.63
22:W:112:VAL:HG22	22:W:124:LEU:HG	1.79	0.63
22:W:129:ARG:HH12	22:W:149:LEU:HD23	1.64	0.63
22:W:317:TRP:NE1	22:W:355:LYS:CE	2.61	0.63
32:U:185:MET:HE2	32:U:185:MET:N	2.14	0.63
32:U:351:MET:HE2	32:U:351:MET:H	1.63	0.63
32:U:710:ARG:NH2	32:U:737:LEU:HD22	2.13	0.63
28:d:282:ILE:HG23	28:d:283:LEU:N	2.13	0.63
2:B:234:LEU:HD12	2:B:234:LEU:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:d:116:LEU:HD21	28:d:150:ILE:CD1	2.29	0.63
11:k:78:MET:HE2	11:k:89:ILE:HD11	1.80	0.63
32:U:427:LEU:HD11	32:U:438:GLN:O	1.99	0.63
22:W:87:ILE:HG23	22:W:104:MET:HE1	1.81	0.63
27:b:16:MET:HA	27:b:16:MET:HE2	1.80	0.63
11:k:41:GLN:OE1	11:k:153:LEU:N	2.32	0.63
32:U:486:MET:HE2	32:U:518:LEU:HD22	1.80	0.63
34:f:184:LEU:O	34:f:188:VAL:HG13	1.99	0.63
2:B:199:GLU:OE1	2:B:349:ARG:NH2	2.31	0.63
3:C:139:MET:N	3:C:139:MET:SD	2.72	0.63
9:I:76:VAL:HG11	9:I:83:ALA:CB	2.29	0.63
22:W:39:ARG:O	22:W:43:VAL:HG22	1.99	0.63
18:r:65:ARG:NH1	18:r:68:GLU:OE1	2.32	0.63
2:B:406:ALA:CB	2:B:414:VAL:HG12	2.29	0.62
32:U:719:ASP:OD1	32:U:720:LYS:N	2.32	0.62
1:A:243:SER:OG	2:B:311:GLU:OE1	2.07	0.62
17:Q:35:MET:HE3	17:Q:45:LEU:HG	1.81	0.62
22:W:115:ILE:HD12	22:W:116:THR:H	1.64	0.62
27:b:30:GLN:OE1	27:b:31:ASP:N	2.31	0.62
23:X:105:GLN:OE1	23:X:105:GLN:N	2.33	0.62
32:U:471:ASP:OD1	32:U:508:THR:OG1	2.08	0.62
32:U:695:MET:O	32:U:695:MET:SD	2.57	0.62
2:B:406:ALA:HB2	2:B:414:VAL:HG12	1.80	0.62
5:E:98:VAL:CG2	5:E:107:ILE:HG23	2.29	0.62
7:G:79:VAL:HG12	7:G:139:ILE:HB	1.82	0.62
8:H:67:ILE:HD11	8:H:73:LEU:HD22	1.81	0.62
14:N:180:ILE:HG12	14:N:185:VAL:HG22	1.81	0.62
22:W:294:LYS:HE2	22:W:294:LYS:HA	1.81	0.62
26:a:224:SER:C	26:a:225:LEU:HD23	2.24	0.62
32:U:653:ALA:HB2	32:U:675:MET:HE3	1.80	0.62
12:L:38:LEU:O	12:L:144:ILE:HD11	1.99	0.62
22:W:108:CYS:O	22:W:112:VAL:HG23	1.99	0.62
16:p:108:ILE:HD12	16:p:121:CYS:SG	2.40	0.62
34:f:133:MET:SD	34:f:135:GLY:N	2.71	0.62
22:W:129:ARG:HA	22:W:132:THR:OG1	1.99	0.62
26:a:28:LEU:HD11	26:a:40:GLN:OE1	2.00	0.62
5:E:98:VAL:HG21	5:E:107:ILE:HG23	1.80	0.62
22:W:203:GLN:O	22:W:207:LYS:HD3	2.00	0.62
22:W:298:GLU:OE1	22:W:298:GLU:N	2.33	0.62
21:V:462:GLU:OE1	21:V:462:GLU:N	2.32	0.62
22:W:67:LEU:CD1	22:W:90:LEU:HD22	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:604:GLY:N	34:f:660:ILE:O	2.30	0.62
1:A:125:LEU:HD23	1:A:149:ILE:HD12	1.81	0.62
22:W:34:LEU:HB2	22:W:43:VAL:CG1	2.29	0.62
22:W:34:LEU:HD13	22:W:42:GLU:OE2	2.00	0.62
22:W:291:SER:HA	22:W:306:LEU:CD2	2.30	0.62
22:W:420:ASP:CG	22:W:421:PRO:HD2	2.25	0.62
32:U:516:LEU:HB3	32:U:532:MET:HE1	1.80	0.62
5:E:320:ILE:HD11	5:E:347:CYS:SG	2.40	0.62
22:W:272:LEU:HD13	22:W:340:VAL:HG11	1.82	0.62
28:d:190:GLN:O	28:d:256:TYR:OH	2.18	0.62
10:j:33:VAL:HG11	10:j:191:VAL:HG13	1.81	0.62
5:E:119:VAL:HG21	5:E:217:GLU:OE1	2.00	0.61
6:F:396:CYS:O	6:F:397:LYS:C	2.43	0.61
18:R:3:THR:N	18:R:18:ASP:OD2	2.29	0.61
22:W:276:LEU:HD22	22:W:353:ASP:HB3	1.81	0.61
9:i:86:LEU:HD12	9:i:132:VAL:HG11	1.82	0.61
32:U:213:PHE:HA	32:U:216:VAL:HG12	1.82	0.61
22:W:99:GLN:H	22:W:99:GLN:CD	2.06	0.61
24:Y:97:GLU:O	24:Y:99:GLU:N	2.33	0.61
25:Z:31:ASN:O	25:Z:31:ASN:ND2	2.33	0.61
5:E:122:MET:HE1	5:E:218:MET:HE2	1.81	0.61
22:W:31:CYS:O	22:W:43:VAL:HG11	2.00	0.61
23:X:255:LEU:HD23	23:X:287:LEU:HB3	1.83	0.61
25:Z:190:ARG:HD3	33:c:300:LEU:CD2	2.31	0.61
25:Z:205:LEU:HD12	26:a:353:LEU:HD22	1.82	0.61
33:c:88:ASP:O	33:c:88:ASP:OD1	2.18	0.61
19:S:148:LEU:HD23	19:S:178:VAL:HG12	1.82	0.61
22:W:32:ALA:HB3	22:W:33:LYS:HZ2	1.64	0.61
22:W:93:ARG:O	22:W:96:GLN:HB2	2.01	0.61
33:c:70:ILE:HG21	33:c:104:ARG:NH1	2.14	0.61
32:U:446:LEU:HD23	32:U:446:LEU:C	2.26	0.61
34:f:591:ALA:O	34:f:595:VAL:HG23	2.01	0.61
21:V:334:VAL:HG21	21:V:391:THR:HG21	1.81	0.61
25:Z:26:ILE:O	25:Z:30:GLY:N	2.30	0.61
26:a:54:ASP:OD1	26:a:55:GLY:N	2.34	0.61
26:a:176:ALA:HB3	26:a:200:LEU:HD21	1.82	0.61
28:d:282:ILE:HG23	28:d:283:LEU:H	1.65	0.61
15:o:20:ARG:NH2	19:s:213:ASP:OXT	2.34	0.61
32:U:649:ARG:NE	32:U:678:ASP:OD2	2.31	0.61
10:J:41:VAL:HG11	10:J:134:VAL:HB	1.83	0.61
14:N:47:SER:OG	14:N:98:GLY:O	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:125:LEU:HD12	16:P:126:ILE:HG23	1.82	0.61
21:V:491:VAL:HG11	28:d:350:VAL:HG13	1.83	0.61
22:W:115:ILE:HG12	22:W:120:ILE:CG2	2.31	0.61
22:W:239:SER:HB3	22:W:242:SER:OG	1.99	0.61
33:c:269:GLN:NE2	33:c:269:GLN:O	2.33	0.61
21:V:108:LEU:HD22	21:V:113:LEU:HD12	1.83	0.61
22:W:72:LYS:HZ3	22:W:73:MET:HE1	1.66	0.61
22:W:214:PHE:HD1	22:W:219:THR:HB	1.65	0.61
14:N:165:MET:HE1	14:N:175:ILE:HG12	1.82	0.61
22:W:47:LEU:HD13	22:W:70:VAL:HG22	1.81	0.61
24:Y:268:TYR:OH	24:Y:306:GLN:OE1	2.15	0.61
18:r:35:VAL:HG13	18:r:43:LEU:CD1	2.30	0.61
32:U:736:ILE:HD11	32:U:779:LEU:HD22	1.83	0.61
11:K:203:LYS:HB2	11:K:210:LEU:HD12	1.83	0.61
22:W:152:ILE:HA	22:W:155:GLN:OE1	2.00	0.61
16:p:36:THR:HG22	16:p:36:THR:O	2.00	0.61
32:U:805:ASN:OD1	32:U:805:ASN:N	2.34	0.61
23:X:222:GLU:OE1	23:X:222:GLU:N	2.32	0.60
32:U:356:THR:HG22	32:U:717:ILE:HD13	1.82	0.60
12:L:150:SER:O	12:L:152:ASN:N	2.34	0.60
22:W:250:ILE:O	22:W:253:THR:HG23	2.01	0.60
22:W:256:ILE:HD13	22:W:262:LYS:CD	2.31	0.60
23:X:205:LYS:HZ3	23:X:242:ILE:HD12	1.65	0.60
9:i:69:ASN:OD1	9:i:70:GLU:N	2.34	0.60
2:B:190:LEU:O	2:B:192:ASN:N	2.34	0.60
5:E:135:ILE:HG23	5:E:138:LEU:HD12	1.83	0.60
5:E:50:LEU:HD22	6:F:83:ASN:OD1	2.02	0.60
22:W:200:ILE:O	22:W:204:ILE:HG12	2.01	0.60
22:W:408:ARG:HG2	22:W:408:ARG:HH11	1.66	0.60
23:X:74:ARG:NH1	23:X:112:GLU:OE2	2.35	0.60
28:d:123:LEU:HD11	28:d:147:ILE:HG21	1.83	0.60
34:f:805:ASP:OD1	34:f:809:ILE:HD12	2.01	0.60
5:E:154:THR:HG1	5:E:155:ASN:CG	2.07	0.60
23:X:261:LEU:O	23:X:261:LEU:HD12	2.01	0.60
32:U:481:LEU:HD23	32:U:481:LEU:O	2.02	0.60
34:f:409:SER:OG	34:f:815:HIS:ND1	2.34	0.60
26:a:210:VAL:HG23	26:a:210:VAL:O	2.00	0.60
32:U:90:VAL:HG13	32:U:137:MET:HE1	1.83	0.60
34:f:520:LEU:CD2	34:f:560:LEU:HD22	2.30	0.60
32:U:567:ILE:HD12	32:U:586:VAL:HG23	1.84	0.60
12:L:88:MET:HE2	12:L:112:ILE:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:169:LEU:HD12	22:W:185:PHE:HE1	1.65	0.60
15:o:91:TYR:CG	15:o:95:ILE:HD12	2.36	0.60
32:U:82:LEU:HD21	32:U:130:LEU:HD12	1.82	0.60
4:D:148:ASP:OD1	4:D:150:SER:N	2.35	0.60
4:D:204:MET:O	4:D:212:LYS:NZ	2.35	0.60
13:M:181:MET:N	13:M:181:MET:SD	2.75	0.60
22:W:67:LEU:HD13	22:W:90:LEU:HD13	1.83	0.60
22:W:416:GLN:OE1	22:W:416:GLN:HA	2.01	0.60
23:X:285:GLU:C	23:X:285:GLU:OE1	2.45	0.60
23:X:390:GLU:OE1	23:X:390:GLU:N	2.35	0.60
12:l:158:ALA:HB1	12:l:172:LEU:HD13	1.84	0.60
18:r:3:THR:HG21	18:r:164:ALA:CB	2.32	0.60
34:f:538:ILE:HG21	34:f:562:LEU:HB2	1.83	0.60
1:A:67:GLU:OE1	1:A:67:GLU:N	2.35	0.60
1:A:349:GLU:CD	1:A:349:GLU:H	2.10	0.60
16:P:202:ARG:NE	16:P:204:ASP:OD2	2.26	0.60
22:W:102:ALA:HA	22:W:138:VAL:CG2	2.32	0.60
22:W:436:MET:HE3	33:c:309:PHE:HZ	1.66	0.60
23:X:382:GLU:OE1	23:X:382:GLU:N	2.35	0.60
19:s:28:ARG:NH2	19:s:212:LYS:O	2.31	0.60
2:B:270:LEU:HD21	2:B:282:VAL:HG11	1.83	0.59
14:n:180:ILE:HG12	14:n:185:VAL:HG23	1.84	0.59
1:A:241:ILE:HG13	2:B:314:ASN:ND2	2.17	0.59
21:V:131:LEU:CD1	21:V:171:VAL:HG21	2.31	0.59
27:b:161:ASN:O	27:b:165:GLY:N	2.32	0.59
18:r:181:ARG:N	18:r:184:GLY:O	2.35	0.59
1:A:111:TYR:CE1	1:A:125:LEU:HD21	2.38	0.59
22:W:67:LEU:HD11	22:W:90:LEU:HD22	1.83	0.59
22:W:72:LYS:HG2	22:W:73:MET:HE1	1.83	0.59
2:B:304:GLU:O	2:B:308:THR:HG23	2.02	0.59
13:M:65:ARG:C	13:M:66:LEU:HD12	2.28	0.59
21:V:108:LEU:HD22	21:V:113:LEU:CD1	2.31	0.59
22:W:108:CYS:SG	22:W:124:LEU:HD11	2.42	0.59
22:W:159:VAL:HG23	22:W:160:LYS:HD3	1.84	0.59
32:U:59:PHE:O	32:U:63:VAL:HG23	2.01	0.59
3:C:203:VAL:O	3:C:207:THR:HG22	2.03	0.59
21:V:185:GLN:NE2	21:V:189:ASP:OD2	2.34	0.59
22:W:291:SER:HA	22:W:306:LEU:HD21	1.83	0.59
27:b:34:ASN:OD1	27:b:38:HIS:NE2	2.34	0.59
34:f:869:THR:HG22	34:f:870:THR:H	1.67	0.59
2:B:70:ASP:CG	34:f:606:VAL:HG11	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:108:CYS:SG	22:W:128:LEU:HD21	2.42	0.59
22:W:409:LEU:C	22:W:409:LEU:HD23	2.27	0.59
7:g:37:LEU:CD2	7:g:53:GLN:HB2	2.33	0.59
34:f:485:LEU:HD21	34:f:497:VAL:CG1	2.32	0.59
22:W:166:LEU:CD2	22:W:192:LEU:HD12	2.32	0.59
24:Y:183:TYR:CD1	24:Y:213:LEU:HD11	2.36	0.59
22:W:256:ILE:CD1	22:W:262:LYS:HB3	2.33	0.59
11:k:98:ASN:OD1	18:r:62:ARG:NH1	2.36	0.59
32:U:391:GLU:OE1	32:U:391:GLU:N	2.36	0.59
5:E:119:VAL:HG21	5:E:217:GLU:CD	2.28	0.59
14:N:20:ARG:O	14:N:34:LYS:NZ	2.28	0.59
22:W:87:ILE:HG12	22:W:104:MET:CE	2.33	0.59
10:j:35:VAL:HG21	10:j:187:THR:HG22	1.85	0.59
32:U:695:MET:HE3	32:U:706:VAL:HG13	1.85	0.59
5:E:135:ILE:CG2	5:E:138:LEU:HD12	2.33	0.59
9:I:38:LEU:HD12	9:I:43:VAL:HG22	1.84	0.59
9:I:67:LYS:HB2	16:P:75:LEU:HD11	1.83	0.59
23:X:192:SER:O	23:X:195:THR:OG1	2.19	0.59
33:c:178:THR:O	33:c:179:SER:OG	2.18	0.59
27:b:94:HIS:ND1	27:b:97:LEU:HD11	2.17	0.58
20:t:9:THR:OG1	20:t:10:SER:N	2.36	0.58
32:U:75:GLU:HA	32:U:75:GLU:OE2	2.03	0.58
2:B:434:THR:HB	2:B:435:PRO:CD	2.28	0.58
4:D:87:LEU:HB2	5:E:80:VAL:HG12	1.85	0.58
22:W:72:LYS:HG2	22:W:73:MET:CE	2.32	0.58
22:W:231:ILE:HD13	22:W:247:TYR:CE2	2.38	0.58
23:X:192:SER:O	23:X:196:THR:HG23	2.03	0.58
28:d:248:LYS:HD2	28:d:251:ILE:HD11	1.84	0.58
5:E:98:VAL:HG13	5:E:100:LEU:CD1	2.34	0.58
12:L:72:ILE:HD11	12:L:85:CYS:SG	2.43	0.58
17:Q:124:LEU:HD23	17:Q:125:ALA:N	2.18	0.58
22:W:40:LEU:O	22:W:44:ILE:HG23	2.03	0.58
22:W:87:ILE:HG23	22:W:104:MET:CE	2.32	0.58
15:o:44:CYS:SG	15:o:99:LEU:HD22	2.43	0.58
34:f:582:VAL:HG22	34:f:582:VAL:O	2.03	0.58
2:B:145:GLU:OE1	2:B:145:GLU:N	2.36	0.58
22:W:117:ASP:OD1	22:W:119:PRO:HD2	2.03	0.58
34:f:585:GLU:OE1	34:f:585:GLU:N	2.36	0.58
22:W:205:ILE:O	22:W:208:LYS:HG3	2.02	0.58
23:X:308:ASP:OD1	23:X:309:TYR:N	2.36	0.58
26:a:4:VAL:HG11	26:a:29:TYR:CE2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:m:90:ILE:HD13	13:m:118:TYR:CE2	2.38	0.58
22:W:25:ASP:OD1	22:W:26:GLN:N	2.37	0.58
22:W:98:LYS:HD2	22:W:137:TYR:HB3	1.86	0.58
22:W:383:ASP:C	22:W:384:LEU:HD23	2.27	0.58
27:b:8:VAL:N	27:b:50:GLY:O	2.34	0.58
10:j:177:THR:O	10:j:180:ALA:N	2.36	0.58
14:n:20:ARG:NH1	14:n:169:GLY:O	2.35	0.58
33:c:285:GLU:O	33:c:288:VAL:HG12	2.03	0.58
34:f:893:ILE:HD12	34:f:893:ILE:N	2.19	0.58
2:B:136:LEU:HD12	2:B:160:ILE:HG22	1.84	0.58
22:W:178:GLU:O	22:W:182:ARG:HG3	2.03	0.58
22:W:375:MET:SD	22:W:413:ILE:HD11	2.44	0.58
23:X:131:ALA:O	23:X:134:VAL:HG12	2.04	0.58
1:A:204:LEU:HD23	1:A:206:ILE:HD11	1.85	0.58
3:C:85:VAL:HG23	3:C:87:VAL:HG13	1.85	0.58
14:N:2:THR:N	14:N:170:SER:HG	2.02	0.58
22:W:30:GLU:O	22:W:34:LEU:HG	2.04	0.58
22:W:44:ILE:O	22:W:48:LEU:HG	2.04	0.58
32:U:728:PHE:CE1	32:U:732:LEU:HD12	2.39	0.58
9:i:86:LEU:HD12	9:i:132:VAL:CG1	2.34	0.58
31:z:102:VAL:HG12	33:c:54:MET:SD	2.43	0.58
6:F:89:LEU:O	6:F:153:VAL:HG22	2.04	0.58
16:P:13:MET:HE2	16:P:149:CYS:SG	2.44	0.58
9:i:81:SER:O	9:i:85:VAL:HG23	2.04	0.58
32:U:186:SER:O	32:U:188:MET:N	2.34	0.58
21:V:344:ASP:OD1	21:V:344:ASP:N	2.36	0.57
25:Z:182:THR:HG22	25:Z:184:VAL:HG23	1.86	0.57
18:r:20:ARG:NH2	18:r:30:GLN:OE1	2.35	0.57
32:U:701:ILE:HD13	32:U:810:THR:CA	2.33	0.57
10:J:158:ALA:O	11:K:58:LEU:HD13	2.04	0.57
10:J:230:ALA:O	10:J:233:GLU:N	2.38	0.57
22:W:448:LYS:HZ3	22:W:448:LYS:HB2	1.69	0.57
4:D:356:GLU:OE1	4:D:356:GLU:N	2.37	0.57
5:E:149:ILE:HD12	5:E:229:ILE:HD13	1.87	0.57
26:a:97:LEU:HD12	26:a:121:LEU:HD11	1.86	0.57
5:E:40:TYR:HB2	6:F:69:MET:HE3	1.86	0.57
10:J:116:GLN:CG	11:K:83:ALA:HB1	2.34	0.57
27:b:3:LEU:HD23	27:b:105:HIS:CE1	2.39	0.57
6:F:235:LEU:HD22	35:F:501:ATP:H2'	1.86	0.57
13:M:53:VAL:O	13:M:53:VAL:HG23	2.05	0.57
21:V:345:ARG:NH2	29:e:46:ASP:OD2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:427:LEU:HD13	32:U:438:GLN:HG2	1.86	0.57
34:f:402:ASN:O	34:f:407:MET:HE2	2.05	0.57
1:A:81:ALA:HB1	2:B:138:PHE:CB	2.34	0.57
1:A:81:ALA:HB2	2:B:137:SER:HB2	1.86	0.57
5:E:98:VAL:HG13	5:E:100:LEU:HD12	1.87	0.57
11:K:121:LEU:O	11:K:121:LEU:HD23	2.04	0.57
21:V:230:PHE:CE1	21:V:234:ARG:HD2	2.39	0.57
22:W:39:ARG:HB3	22:W:42:GLU:HG2	1.86	0.57
34:f:163:ALA:HB1	34:f:207:LEU:HD12	1.86	0.57
34:f:169:GLU:OE1	34:f:184:LEU:HD11	2.03	0.57
34:f:735:GLY:O	34:f:828:ARG:NH1	2.37	0.57
2:B:222:VAL:CG2	2:B:328:ILE:HG23	2.34	0.57
15:O:210:THR:HG21	16:P:167:SER:OG	2.04	0.57
22:W:93:ARG:HB2	22:W:96:GLN:CG	2.35	0.57
24:Y:383:LEU:C	24:Y:383:LEU:HD23	2.30	0.57
32:U:792:ASN:ND2	32:U:794:ASP:OD1	2.37	0.57
34:f:252:ALA:O	34:f:255:VAL:HG22	2.05	0.57
21:V:168:GLN:O	21:V:172:VAL:HG13	2.04	0.57
29:e:59:GLU:O	29:e:63:HIS:N	2.33	0.57
11:k:28:ILE:HD13	11:k:158:PRO:HD2	1.86	0.57
19:s:169:ASP:OD1	19:s:170:ARG:N	2.38	0.57
34:f:840:LEU:HD21	34:f:887:PHE:CE2	2.39	0.57
2:B:317:ASP:HB3	2:B:346:ARG:HD3	1.87	0.57
5:E:108:MET:HE2	6:F:111:ILE:HD12	1.85	0.57
6:F:100:ASP:OD1	6:F:100:ASP:N	2.38	0.57
22:W:187:LEU:CD2	22:W:225:LYS:HB3	2.33	0.57
11:k:195:ILE:HD13	11:k:217:LEU:HD11	1.86	0.57
32:U:2:ILE:CG2	32:U:3:THR:HG23	2.34	0.57
32:U:117:ASP:O	32:U:118:LEU:HD12	2.04	0.57
1:A:113:ILE:HD11	1:A:123:VAL:HG21	1.86	0.57
21:V:166:TYR:O	21:V:170:LEU:HD12	2.05	0.57
22:W:72:LYS:HB3	22:W:73:MET:HE2	1.86	0.57
27:b:30:GLN:OE1	27:b:30:GLN:C	2.48	0.57
11:k:184:VAL:O	11:k:184:VAL:HG13	2.03	0.57
1:A:328:ASP:C	1:A:328:ASP:OD1	2.48	0.56
21:V:163:VAL:O	21:V:167:LEU:HG	2.05	0.56
23:X:371:ASP:OD1	24:Y:233:ARG:NH1	2.38	0.56
17:q:148:THR:HG22	17:q:150:THR:H	1.70	0.56
32:U:30:VAL:HG22	32:U:34:PHE:CE1	2.40	0.56
2:B:332:ASN:OD1	2:B:333:ARG:N	2.38	0.56
13:M:161:TRP:CH2	13:M:182:LYS:HD3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:125:SER:OG	14:n:144:TYR:OH	2.15	0.56
8:H:220:LEU:HG	8:H:224:GLU:CD	2.31	0.56
14:N:161:LEU:O	14:N:165:MET:SD	2.63	0.56
14:N:180:ILE:CG1	14:N:185:VAL:HG22	2.36	0.56
22:W:214:PHE:CD1	22:W:219:THR:HB	2.40	0.56
22:W:377:ARG:NE	26:a:308:GLU:OE1	2.38	0.56
22:W:449:GLU:HA	22:W:452:ILE:CG2	2.34	0.56
28:d:177:ASP:OD1	28:d:178:TYR:N	2.38	0.56
11:k:133:MET:N	11:k:133:MET:SD	2.78	0.56
17:q:35:MET:SD	17:q:181:ARG:HD2	2.46	0.56
32:U:676:THR:HG21	32:U:712:LEU:HD21	1.86	0.56
32:U:695:MET:O	32:U:695:MET:HE2	2.05	0.56
34:f:49:ASP:OD1	34:f:50:LYS:N	2.39	0.56
34:f:145:VAL:HG13	34:f:145:VAL:O	2.06	0.56
34:f:552:ASP:OD1	34:f:553:THR:N	2.37	0.56
1:A:386:ARG:NH2	2:B:348:ASP:OD2	2.37	0.56
5:E:119:VAL:HG21	5:E:217:GLU:OE2	2.06	0.56
22:W:35:ALA:HB2	22:W:43:VAL:HG21	1.88	0.56
22:W:108:CYS:SG	22:W:128:LEU:HD11	2.45	0.56
24:Y:354:VAL:O	24:Y:354:VAL:HG12	2.05	0.56
26:a:200:LEU:HD12	26:a:222:LEU:CD2	2.36	0.56
28:d:160:ASP:OD2	28:d:163:SER:OG	2.16	0.56
32:U:177:LEU:HD13	32:U:201:LEU:HD21	1.88	0.56
2:B:165:ASP:OD1	2:B:165:ASP:N	2.36	0.56
14:N:3:THR:HG22	14:N:171:SER:HB3	1.86	0.56
21:V:466:ILE:O	21:V:469:THR:OG1	2.22	0.56
23:X:346:GLN:N	23:X:346:GLN:OE1	2.38	0.56
26:a:86:GLN:O	26:a:88:THR:HG23	2.05	0.56
26:a:97:LEU:HD11	26:a:117:ALA:CB	2.35	0.56
26:a:287:ASN:OD1	26:a:288:HIS:N	2.38	0.56
26:a:363:MET:SD	26:a:366:LEU:HD13	2.46	0.56
32:U:318:PRO:O	32:U:322:THR:N	2.30	0.56
34:f:308:SER:OG	34:f:310:ASP:OD1	2.22	0.56
22:W:60:MET:N	22:W:60:MET:SD	2.79	0.56
22:W:87:ILE:HA	22:W:104:MET:CE	2.35	0.56
34:f:505:MET:HG2	34:f:518:THR:HB	1.87	0.56
22:W:112:VAL:HG22	22:W:124:LEU:CG	2.36	0.56
26:a:158:LEU:O	26:a:158:LEU:HD23	2.05	0.56
33:c:122:LEU:HD22	33:c:126:ASP:HB3	1.88	0.56
21:V:413:SER:HA	24:Y:338:ILE:HG21	1.88	0.56
22:W:213:PHE:O	22:W:216:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:z:43:TYR:OH	33:c:136:LEU:O	2.23	0.56
5:E:283:ASP:OD1	5:E:284:THR:HG23	2.06	0.56
14:N:92:ARG:NH2	20:t:56:ASP:OD2	2.38	0.56
22:W:202:THR:CA	22:W:205:ILE:HG22	2.34	0.56
26:a:122:LYS:CE	26:a:130:VAL:HG21	2.36	0.56
31:z:39:THR:HA	33:c:108:VAL:HG22	1.88	0.56
34:f:550:LEU:HB3	34:f:587:PHE:CD2	2.41	0.56
3:C:22:GLN:HB2	32:U:98:GLU:OE2	2.05	0.56
22:W:54:THR:O	22:W:58:SER:N	2.39	0.56
22:W:178:GLU:CD	22:W:179:LYS:H	2.14	0.56
27:b:150:THR:HG23	27:b:150:THR:O	2.05	0.56
32:U:744:VAL:HG21	32:U:783:TYR:HB3	1.88	0.56
34:f:659:LEU:HD11	34:f:797:LEU:HD23	1.88	0.56
10:J:40:ILE:HD11	10:J:210:VAL:HG11	1.88	0.55
17:Q:119:ASP:C	17:Q:119:ASP:OD1	2.49	0.55
22:W:177:MET:HE2	22:W:181:GLU:CB	2.37	0.55
22:W:251:TYR:HD1	22:W:266:ALA:HB3	1.71	0.55
22:W:301:LYS:NZ	22:W:323:ASP:OD1	2.38	0.55
15:o:74:LEU:HD23	15:o:75:PRO:HD2	1.88	0.55
16:p:36:THR:HG21	16:p:203:MET:HE1	1.88	0.55
20:t:50:MET:HE1	20:t:192:VAL:HG12	1.89	0.55
1:A:102:ILE:HD11	1:A:114:ASN:CB	2.37	0.55
2:B:227:PRO:O	2:B:230:THR:OG1	2.17	0.55
7:G:150:GLN:OE1	7:G:150:GLN:HA	2.06	0.55
14:N:66:PHE:CE2	14:N:70:GLU:OE1	2.59	0.55
22:W:117:ASP:OD2	22:W:119:PRO:HG2	2.05	0.55
1:A:81:ALA:HB1	2:B:138:PHE:CD2	2.41	0.55
15:O:210:THR:OG1	16:P:164:GLU:OE1	2.13	0.55
24:Y:241:ILE:HD11	24:Y:261:PHE:CE2	2.41	0.55
26:a:57:ILE:O	26:a:60:TYR:N	2.40	0.55
27:b:16:MET:HE2	27:b:16:MET:CA	2.37	0.55
1:A:190:VAL:HG11	1:A:212:VAL:CG1	2.36	0.55
22:W:17:GLU:HG2	22:W:18:VAL:HG13	1.88	0.55
22:W:136:ILE:HD13	22:W:139:GLU:OE1	2.06	0.55
22:W:366:MET:O	22:W:370:TYR:HB2	2.07	0.55
26:a:42:LEU:HD13	26:a:78:GLU:OE1	2.07	0.55
26:a:130:VAL:HG13	26:a:131:THR:N	2.21	0.55
26:a:217:LEU:HD21	26:a:237:LEU:HB3	1.87	0.55
27:b:9:CYS:HB3	27:b:54:LEU:HD11	1.89	0.55
9:i:216:LEU:HD12	9:i:225:ILE:HG12	1.88	0.55
10:j:208:LEU:HB3	10:j:220:LEU:HD12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:377:VAL:HG23	34:f:767:GLY:HA2	1.88	0.55
1:A:101:ILE:HG22	1:A:138:MET:O	2.05	0.55
2:B:273:VAL:HG13	2:B:273:VAL:O	2.07	0.55
3:C:382:ASP:C	3:C:382:ASP:OD1	2.50	0.55
6:F:266:LYS:HB2	6:F:266:LYS:NZ	2.22	0.55
22:W:452:ILE:O	22:W:456:GLN:NE2	2.40	0.55
2:B:294:ARG:NE	2:B:338:ASP:OD2	2.40	0.55
7:G:80:MET:HE3	7:G:138:MET:HG3	1.89	0.55
21:V:131:LEU:HD21	21:V:168:GLN:NE2	2.21	0.55
21:V:497:PRO:N	21:V:498:PRO:CD	2.69	0.55
22:W:344:THR:CG2	22:W:346:GLU:HG2	2.37	0.55
22:W:449:GLU:HA	22:W:452:ILE:HG22	1.88	0.55
23:X:99:MET:N	23:X:99:MET:HE2	2.22	0.55
25:Z:48:LEU:HD21	25:Z:92:VAL:CG1	2.36	0.55
1:A:203:ASN:OD1	1:A:204:LEU:N	2.39	0.55
19:S:13:LEU:HD13	19:S:145:LEU:CD1	2.37	0.55
22:W:183:VAL:O	22:W:187:LEU:HD13	2.06	0.55
26:a:97:LEU:HD11	26:a:117:ALA:HB1	1.89	0.55
8:h:48:GLU:HA	8:h:207:ILE:HG22	1.89	0.55
12:l:36:VAL:HG22	12:l:160:SER:HB3	1.87	0.55
15:o:8:VAL:HG22	15:o:13:ILE:CD1	2.36	0.55
15:o:25:MET:HE1	19:s:33:PHE:CD1	2.42	0.55
2:B:192:ASN:C	2:B:192:ASN:OD1	2.50	0.55
4:D:344:ILE:HG23	4:D:375:ILE:HG21	1.89	0.55
9:I:38:LEU:O	9:I:179:TYR:OH	2.24	0.55
11:K:184:VAL:HG23	11:K:185:TYR:N	2.21	0.55
23:X:122:ARG:O	23:X:123:THR:OG1	2.24	0.55
31:z:32:SER:N	31:z:92:ASP:OD1	2.40	0.55
34:f:479:LEU:HD22	34:f:517:VAL:CG2	2.36	0.55
11:K:210:LEU:HD23	11:K:211:ASN:N	2.22	0.55
22:W:141:GLU:O	22:W:145:LEU:HG	2.07	0.55
24:Y:155:ASP:OD1	24:Y:155:ASP:N	2.37	0.55
28:d:262:ILE:O	28:d:266:THR:OG1	2.25	0.55
34:f:485:LEU:HD23	34:f:485:LEU:O	2.06	0.55
2:B:101:ASP:C	2:B:101:ASP:OD1	2.51	0.55
22:W:26:GLN:O	22:W:29:PRO:HD2	2.07	0.55
26:a:240:PHE:HA	26:a:272:ILE:CD1	2.37	0.55
28:d:129:LEU:O	32:U:26:LYS:NZ	2.36	0.55
34:f:196:MET:HE1	34:f:221:ILE:HA	1.89	0.55
4:D:309:MET:SD	4:D:327:LEU:HD11	2.48	0.54
22:W:33:LYS:HD3	22:W:36:LYS:HZ3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:89:LEU:O	22:W:93:ARG:HG2	2.07	0.54
22:W:214:PHE:CG	22:W:223:LYS:HG3	2.42	0.54
22:W:296:LEU:HG	22:W:303:LYS:HB2	1.88	0.54
22:W:314:LEU:HD11	26:a:312:MET:HG2	1.88	0.54
22:W:432:LEU:HD22	33:c:309:PHE:CD2	2.42	0.54
23:X:145:GLU:O	23:X:148:HIS:ND1	2.32	0.54
24:Y:128:TYR:HB2	24:Y:140:ILE:HG21	1.89	0.54
24:Y:308:LEU:O	24:Y:308:LEU:HD23	2.07	0.54
18:r:39:ASN:OD1	18:r:42:LEU:N	2.40	0.54
34:f:53:GLN:NE2	34:f:54:ASP:OD1	2.38	0.54
34:f:277:LEU:O	34:f:281:ILE:HG12	2.06	0.54
3:C:209:CYS:HA	3:C:243:PRO:HB2	1.90	0.54
11:K:195:ILE:CG2	11:K:217:LEU:HD11	2.36	0.54
22:W:83:LEU:O	22:W:83:LEU:HD12	2.08	0.54
24:Y:143:TYR:O	24:Y:147:ILE:HG23	2.08	0.54
26:a:122:LYS:HE3	26:a:130:VAL:HG21	1.89	0.54
8:h:68:THR:OG1	8:h:69:LYS:N	2.40	0.54
9:i:216:LEU:HD12	9:i:225:ILE:CG1	2.37	0.54
16:p:151:SER:OG	19:s:148:LEU:HD21	2.07	0.54
32:U:2:ILE:HG23	32:U:3:THR:HG23	1.89	0.54
1:A:194:PRO:HB3	1:A:208:PRO:HG3	1.89	0.54
3:C:247:PHE:CD2	3:C:247:PHE:O	2.60	0.54
5:E:158:LEU:O	5:E:162:VAL:HG22	2.07	0.54
15:O:14:VAL:HG12	15:O:178:VAL:HG22	1.90	0.54
20:T:9:THR:OG1	20:T:10:SER:N	2.41	0.54
21:V:162:GLU:HG2	21:V:202:ALA:HB3	1.88	0.54
22:W:251:TYR:HE1	22:W:263:TRP:CE3	2.25	0.54
23:X:357:SER:OG	23:X:358:LYS:N	2.40	0.54
24:Y:237:ARG:HA	24:Y:241:ILE:HG22	1.89	0.54
25:Z:170:VAL:HG13	33:c:151:VAL:O	2.07	0.54
26:a:134:THR:O	26:a:138:VAL:HG12	2.08	0.54
10:j:80:ALA:HA	10:j:129:ILE:HD13	1.89	0.54
13:m:53:VAL:O	13:m:53:VAL:HG23	2.05	0.54
1:A:238:ILE:HD11	1:A:263:MET:HE1	1.90	0.54
22:W:245:LYS:HE3	22:W:286:LEU:HD11	1.88	0.54
25:Z:225:GLN:OE1	25:Z:225:GLN:N	2.41	0.54
11:k:146:VAL:HG13	11:k:220:VAL:HG12	1.87	0.54
34:f:497:VAL:HG11	34:f:525:ILE:HD13	1.89	0.54
1:A:319:MET:SD	1:A:337:LEU:HD11	2.47	0.54
3:C:255:GLY:HA3	3:C:273:MET:HE3	1.88	0.54
4:D:258:ALA:HB3	4:D:259:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:11:VAL:HG13	20:T:24:ALA:HB2	1.90	0.54
22:W:271:VAL:O	22:W:275:ILE:HG12	2.07	0.54
25:Z:263:ALA:HB1	33:c:288:VAL:HG23	1.90	0.54
26:a:173:TYR:CE1	26:a:177:LEU:HD11	2.42	0.54
29:e:42:ASN:ND2	29:e:45:ASP:OD1	2.38	0.54
13:m:75:MET:HE3	13:m:135:PHE:HB2	1.89	0.54
4:D:157:ASP:OD1	4:D:157:ASP:N	2.38	0.54
6:F:183:GLU:OE1	6:F:238:ARG:NH1	2.40	0.54
32:U:488:THR:O	32:U:490:ARG:N	2.40	0.54
34:f:560:LEU:HD12	34:f:801:VAL:HG11	1.88	0.54
1:A:238:ILE:CD1	1:A:263:MET:HE1	2.38	0.54
1:A:277:ILE:HG22	1:A:321:THR:HG22	1.88	0.54
4:D:318:ASP:OD1	4:D:320:ALA:HB3	2.07	0.54
6:F:137:ILE:HD12	6:F:137:ILE:H	1.72	0.54
9:I:198:ASN:OD1	9:I:198:ASN:C	2.50	0.54
21:V:321:ALA:HB1	21:V:324:PHE:HB3	1.90	0.54
23:X:332:GLU:OE1	23:X:368:MET:SD	2.66	0.54
25:Z:19:VAL:HG21	25:Z:124:ILE:HD12	1.90	0.54
32:U:701:ILE:HD13	32:U:810:THR:HA	1.88	0.54
32:U:786:THR:HG23	32:U:786:THR:O	2.07	0.54
34:f:441:LYS:HD3	34:f:477:MET:HE1	1.90	0.54
2:B:88:LEU:HD22	34:f:681:TYR:HD1	1.72	0.54
4:D:72:PHE:CZ	4:D:76:GLN:NE2	2.76	0.54
7:g:50:ILE:HD12	7:g:79:VAL:HG13	1.90	0.54
32:U:545:LEU:HB3	32:U:577:ILE:HG21	1.89	0.54
1:A:262:GLU:OE1	1:A:262:GLU:HA	2.08	0.54
2:B:112:LEU:HD22	2:B:144:LEU:HD22	1.89	0.54
4:D:153:MET:HE1	5:E:267:PHE:CE2	2.42	0.54
5:E:264:MET:HE1	5:E:277:MET:CE	2.38	0.54
21:V:313:LEU:HD21	21:V:329:HIS:NE2	2.23	0.54
23:X:376:GLY:O	23:X:377:ILE:HG23	2.08	0.54
26:a:188:LEU:HD11	26:a:193:GLN:HB3	1.89	0.54
20:t:70:MET:HE1	20:t:91:TRP:CE2	2.41	0.54
34:f:806:VAL:HG22	34:f:811:LEU:HD23	1.90	0.54
5:E:205:ASP:OD1	5:E:206:LYS:N	2.38	0.54
6:F:137:ILE:HG22	6:F:160:ILE:HD11	1.88	0.54
8:H:75:TYR:HB3	8:H:82:TYR:CD1	2.43	0.54
17:Q:96:THR:O	17:Q:96:THR:OG1	2.20	0.54
27:b:158:ASN:O	27:b:162:GLY:N	2.41	0.54
28:d:206:ALA:O	28:d:210:THR:HG23	2.08	0.54
20:t:91:TRP:CE3	20:t:92:LEU:HD12	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:249:ASP:C	4:D:249:ASP:OD1	2.50	0.53
11:K:171:GLY:O	11:K:174:SER:OG	2.24	0.53
21:V:199:ASN:OD1	21:V:241:ARG:NH1	2.41	0.53
22:W:181:GLU:OE2	22:W:181:GLU:N	2.30	0.53
26:a:8:LEU:HD21	26:a:60:TYR:CE2	2.43	0.53
19:s:46:LEU:HD13	19:s:52:ILE:HG22	1.90	0.53
32:U:746:ILE:HG23	32:U:782:ALA:HB1	1.89	0.53
32:U:800:VAL:HG22	32:U:801:GLN:N	2.22	0.53
33:c:31:VAL:HG23	33:c:205:ILE:CD1	2.37	0.53
2:B:380:LEU:HD23	2:B:380:LEU:H	1.73	0.53
21:V:254:LEU:HD23	21:V:270:LEU:CD2	2.39	0.53
21:V:357:LEU:O	21:V:360:TYR:N	2.40	0.53
22:W:98:LYS:HB2	22:W:137:TYR:CG	2.44	0.53
27:b:142:ASN:OD1	27:b:142:ASN:O	2.26	0.53
8:h:202:MET:HE3	8:h:229:LEU:HD21	1.89	0.53
18:r:21:ALA:HB2	18:r:32:VAL:HG21	1.91	0.53
32:U:148:LYS:O	32:U:151:ILE:HG22	2.07	0.53
3:C:75:GLU:OE1	3:C:112:CYS:N	2.41	0.53
4:D:389:GLU:OE1	4:D:391:ARG:NH1	2.40	0.53
14:N:43:PHE:CD1	14:N:180:ILE:HD11	2.44	0.53
16:P:48:LEU:HD12	16:P:110:GLY:HA3	1.89	0.53
21:V:234:ARG:NH2	21:V:237:THR:HG21	2.23	0.53
22:W:291:SER:CA	22:W:306:LEU:HD21	2.37	0.53
22:W:426:ASN:ND2	33:c:233:ASP:OD1	2.36	0.53
23:X:265:GLU:OE1	23:X:265:GLU:N	2.34	0.53
25:Z:101:LEU:HD12	25:Z:105:ASP:OD2	2.08	0.53
32:U:346:ASN:OD1	32:U:346:ASN:O	2.27	0.53
1:A:190:VAL:HG11	1:A:212:VAL:HG11	1.90	0.53
2:B:222:VAL:HG23	2:B:328:ILE:HG23	1.91	0.53
10:j:107:ILE:O	10:j:111:ILE:HG13	2.09	0.53
13:m:90:ILE:CD1	13:m:118:TYR:CE2	2.92	0.53
34:f:208:LEU:HD23	34:f:211:ILE:HD11	1.89	0.53
34:f:266:LEU:HD23	34:f:297:MET:CE	2.38	0.53
1:A:81:ALA:HB1	2:B:138:PHE:HD2	1.72	0.53
3:C:242:ALA:HB3	3:C:243:PRO:HD3	1.90	0.53
6:F:111:ILE:HG12	6:F:113:LEU:H	1.73	0.53
6:F:194:GLN:OE1	6:F:194:GLN:N	2.37	0.53
8:H:230:ALA:CB	23:X:87:ARG:CZ	2.84	0.53
10:J:59:VAL:HG12	10:J:59:VAL:O	2.08	0.53
16:P:33:MET:O	18:r:167:ARG:NH1	2.42	0.53
22:W:90:LEU:HA	22:W:93:ARG:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:138:VAL:O	22:W:138:VAL:HG12	2.08	0.53
22:W:198:ASP:C	22:W:198:ASP:OD1	2.51	0.53
22:W:314:LEU:HD22	22:W:381:LEU:HD11	1.89	0.53
22:W:373:ILE:HA	26:a:326:GLU:HB3	1.89	0.53
24:Y:125:ARG:NH1	24:Y:125:ARG:HB2	2.24	0.53
15:o:74:LEU:CD2	15:o:75:PRO:HD2	2.38	0.53
34:f:228:LYS:HD3	34:f:228:LYS:N	2.24	0.53
34:f:594:LEU:C	34:f:594:LEU:HD23	2.33	0.53
34:f:799:VAL:HG21	34:f:821:LEU:HG	1.91	0.53
1:A:111:TYR:CZ	1:A:125:LEU:HD21	2.44	0.53
10:J:5:ARG:O	10:J:123:GLY:N	2.42	0.53
11:K:29:GLU:OE1	11:K:29:GLU:HA	2.08	0.53
17:Q:11:ASP:O	17:Q:11:ASP:OD1	2.27	0.53
17:Q:13:VAL:HG11	17:Q:105:ALA:HB1	1.91	0.53
17:Q:184:ASP:CG	17:Q:189:HIS:HE2	2.16	0.53
22:W:425:LEU:CD2	25:Z:248:ALA:HB1	2.39	0.53
22:W:446:ILE:HD13	25:Z:211:TYR:HB3	1.90	0.53
24:Y:70:LEU:O	24:Y:74:LYS:HG3	2.08	0.53
26:a:43:ASP:C	26:a:43:ASP:OD1	2.50	0.53
13:m:108:LEU:HD13	13:m:139:SER:HB3	1.91	0.53
17:q:60:ILE:HD13	17:q:84:THR:OG1	2.07	0.53
20:t:91:TRP:HE3	20:t:92:LEU:HD12	1.72	0.53
2:B:314:ASN:C	2:B:314:ASN:OD1	2.52	0.53
8:H:74:VAL:HG22	8:H:75:TYR:H	1.72	0.53
20:T:63:LEU:HD13	20:T:110:MET:HE2	1.91	0.53
21:V:114:TYR:HA	21:V:135:LEU:HD13	1.89	0.53
21:V:243:ASP:OD1	21:V:243:ASP:C	2.51	0.53
21:V:255:LEU:HD21	21:V:271:VAL:CG1	2.39	0.53
22:W:436:MET:HE2	33:c:225:TRP:CZ3	2.44	0.53
16:p:70:LEU:CD1	16:p:81:ILE:HD13	2.38	0.53
34:f:89:MET:O	34:f:89:MET:HE3	2.09	0.53
2:B:388:ASP:OD2	2:B:423:LYS:NZ	2.39	0.53
4:D:96:VAL:HG13	4:D:96:VAL:O	2.08	0.53
7:G:86:ASP:HB3	7:G:134:LEU:HD22	1.89	0.53
12:L:36:VAL:HG12	12:L:37:GLY:N	2.23	0.53
16:P:150:GLU:OE2	19:S:185:ARG:NE	2.34	0.53
17:Q:35:MET:HE3	17:Q:45:LEU:CG	2.37	0.53
11:k:210:LEU:HD22	11:k:238:ILE:HD12	1.91	0.53
34:f:404:ASP:OD1	34:f:405:HIS:ND1	2.40	0.53
9:I:162:THR:OG1	9:I:163:CYS:N	2.40	0.53
22:W:47:LEU:CD1	22:W:70:VAL:HG22	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:365:ILE:HD11	26:a:312:MET:CE	2.38	0.53
22:W:453:HIS:C	22:W:456:GLN:HE21	2.16	0.53
7:g:86:ASP:OD1	13:m:120:HIS:NE2	2.42	0.53
7:g:155:ASP:OD1	7:g:159:TYR:O	2.27	0.53
32:U:748:LEU:HD12	32:U:760:VAL:HG22	1.91	0.53
33:c:229:LEU:HD22	33:c:305:ASP:OD1	2.09	0.53
2:B:288:ASP:OD1	2:B:289:ALA:N	2.42	0.53
4:D:120:ASP:OD1	33:c:282:ARG:NH2	2.42	0.53
20:T:59:ASP:HB3	20:T:106:LEU:HD22	1.90	0.53
22:W:115:ILE:HG12	22:W:120:ILE:HG21	1.90	0.53
22:W:129:ARG:HG3	22:W:129:ARG:NH1	2.23	0.53
22:W:453:HIS:CE1	25:Z:221:PRO:HG3	2.44	0.53
24:Y:383:LEU:HD23	24:Y:383:LEU:O	2.09	0.53
26:a:183:VAL:O	26:a:183:VAL:HG13	2.08	0.53
28:d:208:PHE:CE1	28:d:212:LEU:HD21	2.43	0.53
12:l:159:MET:HE2	13:m:58:TYR:HE1	1.73	0.53
18:r:6:ALA:HA	18:r:14:ILE:O	2.09	0.53
20:t:67:LEU:HD11	20:t:88:ILE:HD12	1.91	0.53
17:Q:170:ARG:NH2	18:r:141:ASP:OD1	2.38	0.52
22:W:202:THR:HA	22:W:205:ILE:CG2	2.34	0.52
25:Z:23:PHE:CD2	25:Z:126:VAL:HG21	2.45	0.52
7:g:155:ASP:OD1	7:g:155:ASP:N	2.41	0.52
34:f:226:TYR:HA	34:f:229:VAL:HG12	1.91	0.52
2:B:250:VAL:HG21	2:B:270:LEU:HD12	1.91	0.52
21:V:234:ARG:O	21:V:237:THR:HG22	2.10	0.52
22:W:103:LYS:HA	22:W:106:GLN:OE1	2.09	0.52
22:W:198:ASP:OD1	22:W:198:ASP:O	2.27	0.52
10:j:50:VAL:O	10:j:51:ALA:HB3	2.09	0.52
11:k:46:VAL:O	11:k:219:THR:HG23	2.08	0.52
14:n:166:GLU:OE2	20:t:37:ARG:NH1	2.38	0.52
15:o:79:THR:HG22	15:o:83:MET:HE3	1.91	0.52
32:U:185:MET:HE2	32:U:185:MET:CA	2.39	0.52
32:U:904:LYS:NZ	32:U:911:ILE:O	2.36	0.52
33:c:113:HIS:CE1	33:c:126:ASP:OD1	2.63	0.52
34:f:282:PHE:HA	34:f:294:MET:HE1	1.90	0.52
2:B:250:VAL:HG21	2:B:270:LEU:CD1	2.40	0.52
3:C:160:GLU:OE1	3:C:315:ILE:HD13	2.10	0.52
3:C:346:LYS:HD3	3:C:346:LYS:C	2.34	0.52
15:O:36:HIS:HB3	15:O:57:THR:HG21	1.91	0.52
21:V:292:THR:HA	21:V:295:ILE:HG22	1.92	0.52
22:W:55:ARG:HD3	22:W:96:GLN:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:213:PHE:CZ	22:W:219:THR:HG21	2.44	0.52
27:b:171:VAL:HG13	27:b:171:VAL:O	2.09	0.52
32:U:516:LEU:CB	32:U:532:MET:HE1	2.39	0.52
2:B:49:LEU:HD21	34:f:669:GLU:OE1	2.09	0.52
3:C:371:LEU:HD23	3:C:371:LEU:C	2.34	0.52
22:W:316:ARG:NE	22:W:383:ASP:OD2	2.43	0.52
22:W:432:LEU:O	22:W:436:MET:HG3	2.09	0.52
9:i:194:ILE:HD12	9:i:236:LEU:HB3	1.92	0.52
10:j:29:GLY:O	10:j:163:ARG:HG3	2.08	0.52
1:A:393:GLY:HA3	2:B:216:ILE:HD13	1.92	0.52
2:B:380:LEU:HA	2:B:383:LEU:HD12	1.91	0.52
5:E:115:VAL:O	5:E:115:VAL:HG23	2.09	0.52
22:W:60:MET:CA	22:W:97:LEU:HD12	2.38	0.52
28:d:341:GLU:HA	28:d:341:GLU:OE2	2.08	0.52
33:c:130:GLN:NE2	33:c:134:GLU:OE2	2.32	0.52
33:c:163:ILE:HG23	33:c:174:PRO:HB3	1.92	0.52
34:f:795:GLY:O	34:f:799:VAL:HG23	2.09	0.52
4:D:231:VAL:HG11	5:E:262:ASN:CG	2.34	0.52
10:J:9:VAL:HG22	11:K:23:GLN:OE1	2.10	0.52
21:V:254:LEU:HD23	21:V:270:LEU:HD21	1.91	0.52
22:W:33:LYS:HD3	22:W:36:LYS:HE2	1.91	0.52
22:W:60:MET:HE3	22:W:60:MET:H	1.74	0.52
22:W:199:TYR:HD2	22:W:233:LEU:CD1	2.22	0.52
22:W:431:LYS:HG3	25:Z:236:LEU:CD2	2.40	0.52
28:d:232:LEU:HD23	28:d:232:LEU:O	2.10	0.52
7:g:79:VAL:HG23	7:g:139:ILE:HB	1.92	0.52
10:j:33:VAL:CG1	10:j:191:VAL:HG13	2.38	0.52
17:q:3:TYR:N	17:q:18:ASP:OD2	2.42	0.52
32:U:573:ASP:OD1	32:U:574:LYS:N	2.42	0.52
32:U:678:ASP:OD1	32:U:679:PRO:HD2	2.10	0.52
34:f:78:LEU:HD23	34:f:78:LEU:C	2.35	0.52
2:B:118:ASP:O	2:B:119:ASN:OD1	2.28	0.52
3:C:66:LEU:HD22	4:D:138:ALA:HB1	1.91	0.52
6:F:275:ALA:HB1	6:F:281:SER:OG	2.09	0.52
7:G:7:ALA:N	7:G:10:ASP:OD1	2.42	0.52
10:J:121:SER:HB3	10:J:124:ARG:HD2	1.92	0.52
12:L:84:LEU:O	12:L:88:MET:HG3	2.09	0.52
15:O:2:THR:N	15:O:170:SER:OG	2.39	0.52
18:R:36:ILE:N	18:R:44:GLY:O	2.42	0.52
22:W:24:VAL:HG11	22:W:62:SER:HB3	1.92	0.52
22:W:67:LEU:HD12	22:W:90:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:276:LEU:CD2	22:W:353:ASP:HB3	2.40	0.52
26:a:130:VAL:HG22	26:a:134:THR:HG23	1.90	0.52
22:W:180:LYS:HE2	22:W:180:LYS:H	1.75	0.52
22:W:214:PHE:HB3	22:W:223:LYS:CG	2.35	0.52
22:W:326:MET:HE2	22:W:326:MET:CA	2.32	0.52
22:W:326:MET:HA	22:W:326:MET:CE	2.24	0.52
22:W:439:VAL:O	22:W:443:THR:HG23	2.08	0.52
23:X:267:VAL:HG11	23:X:291:ALA:CB	2.39	0.52
16:p:36:THR:O	16:p:36:THR:CG2	2.58	0.52
14:N:49:SER:HG	14:N:52:ASP:CG	2.17	0.52
27:b:15:TYR:CE2	27:b:116:PRO:HD3	2.45	0.52
7:g:138:MET:HE2	7:g:140:LEU:HD13	1.92	0.52
12:l:94:ASP:C	12:l:94:ASP:OD1	2.52	0.52
12:l:165:SER:OG	12:l:169:ARG:NH2	2.43	0.52
34:f:584:SER:O	34:f:588:ARG:N	2.34	0.52
5:E:385:ASP:OD1	5:E:386:TYR:N	2.44	0.52
8:H:230:ALA:O	8:H:231:ALA:O	2.27	0.52
16:P:179:VAL:HG13	16:P:179:VAL:O	2.09	0.52
17:Q:19:ARG:NH2	17:Q:177:THR:HG21	2.25	0.52
17:Q:108:ASP:OD1	17:Q:109:GLU:N	2.43	0.52
22:W:87:ILE:HG12	22:W:104:MET:HE2	1.91	0.52
28:d:143:LEU:O	28:d:147:ILE:HG12	2.10	0.52
8:h:67:ILE:HG21	8:h:109:LEU:HD21	1.91	0.52
34:f:257:ARG:NH1	34:f:280:ASP:OD2	2.43	0.52
2:B:348:ASP:N	2:B:348:ASP:OD1	2.43	0.51
11:K:18:GLU:OE1	11:K:18:GLU:N	2.43	0.51
16:P:58:ASP:OD2	16:P:102:TYR:HA	2.11	0.51
22:W:68:VAL:HA	22:W:71:VAL:HG12	1.90	0.51
28:d:154:TRP:CZ2	28:d:158:ARG:HG3	2.45	0.51
16:p:189:ILE:HG22	16:p:194:ILE:HD13	1.90	0.51
32:U:743:ASN:C	32:U:786:THR:HG22	2.35	0.51
34:f:251:CYS:O	34:f:255:VAL:HG13	2.09	0.51
3:C:154:LEU:HD12	3:C:154:LEU:N	2.25	0.51
10:J:207:GLU:O	10:J:208:LEU:HD22	2.10	0.51
22:W:163:ALA:CB	22:W:196:VAL:HG11	2.40	0.51
22:W:181:GLU:H	22:W:181:GLU:CD	2.17	0.51
22:W:408:ARG:HG2	22:W:408:ARG:NH1	2.24	0.51
28:d:226:ILE:O	28:d:226:ILE:HG22	2.10	0.51
13:m:176:ILE:O	13:m:179:LEU:HB2	2.11	0.51
15:o:184:LEU:HD13	15:o:184:LEU:C	2.35	0.51
4:D:96:VAL:O	4:D:100:THR:OG1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ARG:NH2	10:J:58:THR:HG22	2.26	0.51
19:S:13:LEU:HD13	19:S:145:LEU:HD13	1.92	0.51
21:V:72:LEU:HD22	21:V:147:PHE:CE2	2.45	0.51
22:W:112:VAL:HG21	22:W:128:LEU:HD12	1.91	0.51
23:X:332:GLU:OE2	23:X:368:MET:HE3	2.10	0.51
5:E:76:GLY:N	5:E:77:PRO:HD2	2.25	0.51
5:E:135:ILE:HD12	5:E:135:ILE:N	2.25	0.51
13:M:35:THR:HG21	13:M:200:VAL:HG21	1.92	0.51
20:T:51:LEU:HD21	20:T:110:MET:HE3	1.92	0.51
22:W:41:GLN:O	22:W:44:ILE:HG12	2.10	0.51
22:W:177:MET:HE2	22:W:181:GLU:HB2	1.92	0.51
22:W:178:GLU:HB3	22:W:181:GLU:OE1	2.09	0.51
23:X:160:MET:SD	23:X:162:ASP:OD2	2.68	0.51
24:Y:197:ALA:HB3	24:Y:226:VAL:HG21	1.92	0.51
27:b:57:ASP:O	27:b:58:CYS:SG	2.68	0.51
32:U:101:ILE:HG12	32:U:137:MET:HE3	1.92	0.51
32:U:573:ASP:OD1	32:U:575:ASP:N	2.40	0.51
5:E:76:GLY:N	5:E:77:PRO:CD	2.73	0.51
12:L:154:PHE:HB3	13:M:58:TYR:CE1	2.45	0.51
14:N:63:GLN:HE21	14:N:83:LEU:HD22	1.73	0.51
22:W:49:SER:O	22:W:53:GLN:HG3	2.11	0.51
22:W:146:THR:HG21	22:W:169:LEU:HD11	1.92	0.51
22:W:212:LYS:HD2	22:W:212:LYS:C	2.34	0.51
24:Y:352:GLU:O	24:Y:353:ILE:HD13	2.11	0.51
25:Z:69:PHE:CD2	27:b:96:ALA:HA	2.46	0.51
32:U:233:LEU:HD11	32:U:325:MET:CE	2.41	0.51
32:U:620:GLU:OE2	32:U:767:THR:HG21	2.11	0.51
32:U:899:ARG:NH2	32:U:900:TYR:OH	2.44	0.51
34:f:208:LEU:HD22	34:f:213:GLN:O	2.10	0.51
2:B:410:ARG:HH22	3:C:167:LEU:HD11	1.75	0.51
4:D:337:ASP:OD1	4:D:337:ASP:N	2.35	0.51
6:F:358:ASN:O	6:F:361:ALA:N	2.43	0.51
8:H:24:ALA:O	8:H:28:VAL:HG23	2.10	0.51
19:S:176:LYS:HE2	19:S:208:VAL:HG11	1.91	0.51
23:X:126:ARG:NH2	23:X:156:GLU:OE2	2.43	0.51
26:a:280:MET:HE1	26:a:296:ILE:CD1	2.32	0.51
28:d:282:ILE:O	28:d:283:LEU:HB2	2.10	0.51
9:i:201:MET:HG3	9:i:201:MET:O	2.11	0.51
11:k:121:LEU:HD23	11:k:123:PHE:HE2	1.76	0.51
15:o:188:ARG:HB3	15:o:189:PRO:HD3	1.92	0.51
24:Y:228:MET:HE1	24:Y:259:TYR:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:21:ASP:OD1	25:Z:21:ASP:C	2.53	0.51
28:d:98:LEU:HD21	28:d:115:GLU:HB3	1.93	0.51
14:n:93:GLU:HA	14:n:93:GLU:OE1	2.11	0.51
19:s:201:GLU:HA	19:s:201:GLU:OE2	2.10	0.51
34:f:433:LEU:HA	34:f:444:ALA:CB	2.41	0.51
4:D:194:ILE:HG13	4:D:196:ILE:HG22	1.92	0.51
16:P:188:ILE:HD13	16:P:197:ARG:NH1	2.26	0.51
22:W:317:TRP:CE2	22:W:355:LYS:HE3	2.45	0.51
22:W:395:ASN:OD1	22:W:399:ASN:ND2	2.44	0.51
25:Z:48:LEU:HD21	25:Z:92:VAL:HG11	1.93	0.51
26:a:68:GLU:HG3	26:a:71:VAL:HG23	1.92	0.51
27:b:147:GLU:O	27:b:148:VAL:HG12	2.11	0.51
18:r:41:TYR:HE2	18:r:105:TRP:O	1.93	0.51
32:U:142:LEU:O	32:U:142:LEU:HD23	2.09	0.51
34:f:373:ALA:HB2	34:f:760:PHE:CD1	2.45	0.51
2:B:65:LEU:HD23	2:B:68:ILE:HD11	1.91	0.51
4:D:213:THR:O	4:D:213:THR:HG22	2.10	0.51
22:W:83:LEU:HD11	22:W:87:ILE:HD11	1.93	0.51
25:Z:45:LYS:O	25:Z:46:LYS:HB2	2.11	0.51
26:a:130:VAL:O	26:a:134:THR:N	2.36	0.51
27:b:156:PHE:CZ	27:b:160:LEU:HD11	2.46	0.51
8:h:110:VAL:HG22	8:h:135:ILE:HD13	1.93	0.51
19:s:186:ASP:C	19:s:186:ASP:OD1	2.53	0.51
34:f:485:LEU:HD21	34:f:497:VAL:HG13	1.93	0.51
34:f:489:TYR:O	34:f:490:ALA:C	2.52	0.51
1:A:166:VAL:O	1:A:168:GLU:N	2.44	0.51
3:C:135:VAL:HA	3:C:138:MET:HE1	1.92	0.51
11:K:191:LEU:O	11:K:195:ILE:HG13	2.10	0.51
21:V:320:THR:O	21:V:321:ALA:HB3	2.11	0.51
22:W:60:MET:H	22:W:60:MET:CE	2.23	0.51
22:W:124:LEU:HD12	22:W:124:LEU:O	2.10	0.51
22:W:399:ASN:O	22:W:400:LYS:HB3	2.10	0.51
7:g:54:LYS:NZ	7:g:63:SER:O	2.42	0.51
32:U:188:MET:SD	32:U:188:MET:O	2.69	0.51
32:U:788:VAL:HB	32:U:884:VAL:HG21	1.93	0.51
3:C:287:LYS:NZ	3:C:288:ASN:OD1	2.44	0.50
8:H:62:HIS:CD2	8:H:219:ARG:CZ	2.94	0.50
11:K:46:VAL:HG12	11:K:220:VAL:HG13	1.93	0.50
19:S:91:MET:HE3	19:S:95:ILE:HD12	1.92	0.50
21:V:255:LEU:HD21	21:V:271:VAL:HG12	1.93	0.50
25:Z:34:ARG:HD3	25:Z:60:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:191:ILE:HG13	25:Z:192:THR:N	2.27	0.50
26:a:141:MET:CE	26:a:141:MET:H	2.23	0.50
26:a:360:VAL:HG22	33:c:308:VAL:HG13	1.92	0.50
28:d:339:VAL:HG21	33:c:303:MET:HE1	1.93	0.50
10:j:115:LYS:NZ	10:j:147:THR:OG1	2.43	0.50
11:k:51:GLU:HG3	11:k:206:MET:HE3	1.91	0.50
18:r:155:ASP:OD1	18:r:158:ARG:NH2	2.43	0.50
32:U:7:GLY:O	32:U:10:SER:N	2.44	0.50
32:U:550:VAL:HG21	32:U:768:GLN:CD	2.36	0.50
34:f:270:LEU:HD22	34:f:301:HIS:ND1	2.27	0.50
1:A:101:ILE:HG23	1:A:137:GLY:H	1.75	0.50
3:C:138:MET:SD	3:C:138:MET:N	2.85	0.50
3:C:338:LEU:HD13	3:C:342:ILE:HD13	1.92	0.50
9:I:48:GLU:OE2	9:I:50:ARG:NH1	2.44	0.50
26:a:279:GLU:OE2	26:a:279:GLU:HA	2.11	0.50
29:e:48:VAL:HG23	29:e:48:VAL:O	2.09	0.50
8:h:90:ARG:HB3	15:o:66:LEU:HD11	1.93	0.50
32:U:177:LEU:CD1	32:U:201:LEU:CD2	2.89	0.50
2:B:61:LYS:O	2:B:65:LEU:HD12	2.12	0.50
2:B:201:VAL:HG11	2:B:239:VAL:HG21	1.93	0.50
6:F:398:ALA:HB1	6:F:427:VAL:HG22	1.93	0.50
13:M:219:LEU:HD12	13:M:219:LEU:N	2.27	0.50
26:a:208:GLU:OE2	26:a:267:GLN:NE2	2.41	0.50
15:o:25:MET:HG2	19:s:188:TYR:CE2	2.47	0.50
32:U:420:LEU:HD21	32:U:457:ILE:CD1	2.41	0.50
34:f:130:ALA:HB3	34:f:139:CYS:SG	2.52	0.50
3:C:381:GLU:OE1	3:C:381:GLU:N	2.39	0.50
4:D:407:ILE:O	4:D:407:ILE:CG2	2.54	0.50
13:M:39:ILE:HG13	13:M:176:ILE:HD11	1.94	0.50
18:R:13:VAL:HG13	18:R:180:VAL:HB	1.92	0.50
21:V:121:PHE:CE2	21:V:167:LEU:HD12	2.47	0.50
22:W:188:GLU:OE1	22:W:191:ARG:NH2	2.44	0.50
22:W:226:TYR:CD1	22:W:226:TYR:C	2.87	0.50
22:W:278:PRO:HG3	22:W:357:ARG:NH2	2.23	0.50
23:X:394:ASP:OD1	23:X:394:ASP:N	2.42	0.50
15:o:214:THR:HG22	15:o:215:GLU:N	2.26	0.50
33:c:25:VAL:O	33:c:25:VAL:HG12	2.11	0.50
33:c:226:MET:O	33:c:230:THR:HG23	2.11	0.50
2:B:232:LYS:NZ	35:B:501:ATP:O2G	2.45	0.50
4:D:162:VAL:HG23	4:D:162:VAL:O	2.10	0.50
21:V:391:THR:O	21:V:392:TYR:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:214:PHE:HA	22:W:219:THR:OG1	2.12	0.50
22:W:320:LEU:HD12	22:W:324:TYR:CE1	2.45	0.50
26:a:68:GLU:OE2	26:a:70:ARG:N	2.32	0.50
10:j:121:SER:OG	10:j:122:ASN:N	2.45	0.50
17:q:160:LEU:O	17:q:164:LEU:HG	2.12	0.50
33:c:64:ASP:N	33:c:64:ASP:OD1	2.45	0.50
1:A:234:ASP:C	1:A:234:ASP:OD1	2.54	0.50
7:G:84:THR:CG2	13:M:156:VAL:HG23	2.41	0.50
21:V:409:MET:O	21:V:409:MET:HE3	2.11	0.50
22:W:43:VAL:HA	22:W:46:THR:CG2	2.42	0.50
22:W:199:TYR:O	22:W:202:THR:N	2.43	0.50
24:Y:279:GLU:OE1	24:Y:296:VAL:HG21	2.12	0.50
8:h:117:MET:O	8:h:121:THR:HG23	2.11	0.50
12:l:72:ILE:HG21	12:l:88:MET:CE	2.42	0.50
15:o:192:VAL:O	15:o:192:VAL:CG2	2.56	0.50
17:q:84:THR:HG22	17:q:118:MET:HE1	1.94	0.50
32:U:427:LEU:CD1	32:U:438:GLN:HG2	2.42	0.50
7:G:214:GLU:O	7:G:215:ILE:HG23	2.12	0.50
22:W:22:ALA:O	22:W:25:ASP:OD1	2.30	0.50
22:W:250:ILE:C	22:W:253:THR:HG23	2.36	0.50
22:W:403:PHE:C	22:W:403:PHE:CD1	2.88	0.50
22:W:448:LYS:O	22:W:452:ILE:HG22	2.11	0.50
23:X:338:VAL:CG2	23:X:353:LEU:HD13	2.42	0.50
19:s:37:THR:OG1	19:s:38:ARG:N	2.45	0.50
34:f:778:LEU:O	34:f:779:CYS:C	2.53	0.50
5:E:339:ASN:OD1	5:E:342:ASP:OD1	2.30	0.50
13:M:165:ILE:HG23	13:M:165:ILE:O	2.11	0.50
14:N:66:PHE:CZ	14:N:70:GLU:OE1	2.64	0.50
21:V:463:MET:SD	21:V:463:MET:C	2.95	0.50
22:W:102:ALA:O	22:W:106:GLN:HG2	2.12	0.50
22:W:233:LEU:O	22:W:233:LEU:HD12	2.11	0.50
22:W:299:ILE:HG22	22:W:302:TYR:CD1	2.46	0.50
27:b:150:THR:OG1	27:b:154:THR:HG22	2.11	0.50
28:d:219:ASP:OD1	28:d:220:ILE:N	2.44	0.50
28:d:346:LEU:HD23	28:d:346:LEU:O	2.12	0.50
18:r:21:ALA:CB	18:r:32:VAL:HG21	2.41	0.50
34:f:516:GLY:HA3	34:f:557:TRP:HB2	1.94	0.50
1:A:187:LEU:HD23	1:A:225:CYS:SG	2.51	0.50
2:B:322:ARG:HG3	2:B:325:VAL:HG22	1.94	0.50
5:E:242:ARG:NE	5:E:286:ASP:OD2	2.45	0.50
21:V:94:VAL:HG11	21:V:202:ALA:HB1	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:445:LEU:HD12	25:Z:229:GLN:OE1	2.11	0.50
26:a:140:GLU:OE1	26:a:140:GLU:N	2.44	0.50
27:b:154:THR:O	27:b:158:ASN:OD1	2.30	0.50
7:g:189:TRP:HZ3	7:g:197:THR:HG1	1.60	0.50
15:o:12:GLY:HA2	15:o:109:PRO:HB3	1.93	0.50
34:f:648:ALA:O	34:f:649:HIS:C	2.50	0.50
8:H:220:LEU:HG	8:H:224:GLU:OE2	2.12	0.49
13:M:39:ILE:HD12	13:M:193:VAL:HG22	1.93	0.49
22:W:146:THR:HG21	22:W:169:LEU:CD2	2.31	0.49
22:W:202:THR:O	22:W:205:ILE:HG22	2.12	0.49
22:W:263:TRP:CZ2	22:W:295:LYS:HE2	2.47	0.49
2:B:107:MET:HG2	2:B:160:ILE:HD11	1.94	0.49
3:C:186:VAL:HG12	3:C:187:LEU:N	2.26	0.49
15:O:71:THR:HG23	15:O:73:ARG:HH11	1.77	0.49
17:Q:35:MET:CE	17:Q:45:LEU:HD11	2.42	0.49
22:W:205:ILE:CD1	22:W:208:LYS:HD3	2.16	0.49
22:W:400:LYS:O	22:W:400:LYS:CG	2.58	0.49
24:Y:205:VAL:O	24:Y:216:TYR:OH	2.28	0.49
25:Z:49:ASP:C	25:Z:49:ASP:OD1	2.55	0.49
26:a:240:PHE:CZ	26:a:268:LEU:CD1	2.96	0.49
28:d:133:GLY:O	28:d:134:THR:C	2.55	0.49
8:h:173:LEU:O	8:h:177:TYR:N	2.44	0.49
34:f:596:ASP:OD2	34:f:608:LYS:NZ	2.41	0.49
2:B:364:ILE:HG22	2:B:395:ILE:HG21	1.94	0.49
14:N:136:ILE:HD12	14:N:160:ALA:HB1	1.93	0.49
20:T:136:SER:HB3	20:T:154:LEU:CD1	2.43	0.49
22:W:223:LYS:HG2	22:W:227:TYR:HE2	1.77	0.49
26:a:70:ARG:O	26:a:71:VAL:C	2.54	0.49
27:b:93:ALA:O	27:b:97:LEU:HG	2.13	0.49
12:l:72:ILE:HG22	12:l:134:ILE:HG13	1.93	0.49
18:r:3:THR:HG21	18:r:164:ALA:HB3	1.94	0.49
1:A:125:LEU:CD2	1:A:149:ILE:HD12	2.42	0.49
1:A:366:ARG:NE	1:A:366:ARG:HA	2.26	0.49
2:B:112:LEU:HD22	2:B:144:LEU:HD23	1.93	0.49
4:D:370:ILE:CD1	4:D:407:ILE:HD13	2.42	0.49
9:I:37:ILE:CD1	9:I:44:LEU:HD11	2.41	0.49
25:Z:187:LEU:HD13	26:a:374:ILE:HB	1.94	0.49
26:a:162:TYR:C	26:a:162:TYR:CD1	2.89	0.49
28:d:184:GLU:OE1	28:d:184:GLU:N	2.45	0.49
28:d:254:GLU:O	28:d:257:THR:OG1	2.26	0.49
32:U:339:LEU:HD11	32:U:343:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:446:LEU:HD22	32:U:461:LEU:HD11	1.95	0.49
33:c:207:TYR:O	33:c:209:LYS:NZ	2.43	0.49
33:c:244:VAL:HG11	33:c:291:LEU:HG	1.94	0.49
34:f:471:LEU:O	34:f:471:LEU:HD23	2.12	0.49
34:f:827:PRO:CB	34:f:829:MET:HE3	2.42	0.49
2:B:56:THR:O	2:B:57:GLN:C	2.55	0.49
11:K:235:GLU:HA	11:K:238:ILE:HG22	1.95	0.49
15:O:105:ASP:OD1	15:O:107:THR:OG1	2.27	0.49
21:V:497:PRO:O	21:V:498:PRO:C	2.54	0.49
22:W:267:LEU:O	22:W:270:VAL:HG12	2.11	0.49
24:Y:203:ASP:OD1	24:Y:203:ASP:C	2.56	0.49
24:Y:336:ARG:O	24:Y:339:ALA:HB3	2.12	0.49
26:a:80:ILE:HD13	26:a:100:THR:HG21	1.94	0.49
27:b:138:VAL:HG22	27:b:139:ASP:N	2.27	0.49
28:d:116:LEU:HD21	28:d:150:ILE:HD12	1.93	0.49
33:c:102:THR:O	33:c:102:THR:OG1	2.29	0.49
33:c:118:PHE:O	33:c:121:TRP:NE1	2.36	0.49
34:f:239:TYR:CE1	34:f:664:GLU:HG2	2.47	0.49
6:F:248:PHE:C	6:F:249:LEU:HD12	2.38	0.49
22:W:140:ILE:HB	22:W:141:GLU:OE1	2.13	0.49
25:Z:259:VAL:HG13	33:c:291:LEU:HD13	1.93	0.49
26:a:244:ASN:OD1	26:a:244:ASN:N	2.43	0.49
27:b:32:ALA:O	27:b:36:VAL:HG23	2.11	0.49
7:g:166:THR:OG1	7:g:167:ALA:N	2.45	0.49
8:h:202:MET:HE3	8:h:229:LEU:CD2	2.43	0.49
11:k:85:ALA:O	11:k:89:ILE:HG13	2.12	0.49
14:n:28:ALA:O	20:t:179:ARG:NH1	2.44	0.49
15:o:92:GLN:OE1	15:o:92:GLN:HA	2.12	0.49
32:U:236:LEU:CD1	32:U:248:ILE:HD12	2.42	0.49
5:E:190:GLN:HA	5:E:190:GLN:NE2	2.27	0.49
10:J:192:ILE:O	10:J:196:LEU:HD23	2.13	0.49
11:K:145:GLY:HA2	11:K:220:VAL:HG11	1.94	0.49
21:V:288:TYR:CD1	21:V:288:TYR:C	2.91	0.49
26:a:162:TYR:O	26:a:165:THR:OG1	2.27	0.49
27:b:61:LEU:O	27:b:62:THR:OG1	2.24	0.49
28:d:194:LEU:HD13	28:d:256:TYR:CD1	2.48	0.49
12:l:158:ALA:HB1	12:l:172:LEU:HD22	1.93	0.49
14:n:50:ALA:O	14:n:54:GLN:HG3	2.13	0.49
32:U:416:GLU:OE1	32:U:416:GLU:O	2.30	0.49
34:f:446:LEU:O	34:f:450:ILE:HG12	2.13	0.49
34:f:858:LYS:O	34:f:858:LYS:CD	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:40:VAL:HG13	7:G:202:LEU:HD13	1.94	0.49
24:Y:98:SER:O	24:Y:102:ASP:N	2.38	0.49
27:b:10:VAL:CG2	27:b:33:VAL:HG11	2.43	0.49
28:d:237:MET:HE2	28:d:237:MET:HA	1.94	0.49
7:g:22:LEU:HD12	8:h:78:MET:HE1	1.94	0.49
10:j:59:VAL:HG23	10:j:59:VAL:O	2.12	0.49
19:s:176:LYS:O	19:s:180:ILE:HG12	2.13	0.49
34:f:270:LEU:O	34:f:273:ASN:N	2.45	0.49
4:D:96:VAL:O	4:D:96:VAL:CG1	2.59	0.49
22:W:290:ILE:O	22:W:293:ASP:HB2	2.13	0.49
22:W:381:LEU:HD23	22:W:381:LEU:C	2.38	0.49
31:z:52:THR:O	31:z:55:GLY:N	2.46	0.49
32:U:695:MET:O	32:U:695:MET:CE	2.61	0.49
33:c:279:ASP:OD1	33:c:279:ASP:C	2.55	0.49
34:f:463:LEU:HD13	34:f:497:VAL:HG22	1.95	0.49
13:M:192:GLU:OE1	13:M:192:GLU:HA	2.13	0.49
17:Q:184:ASP:OD2	17:Q:189:HIS:NE2	2.39	0.49
22:W:362:ASN:O	22:W:366:MET:HG2	2.13	0.49
26:a:21:VAL:HG21	26:a:44:PHE:CD1	2.48	0.49
27:b:10:VAL:HG22	27:b:33:VAL:HG11	1.93	0.49
9:i:230:GLN:OE1	9:i:230:GLN:N	2.43	0.49
32:U:695:MET:CE	32:U:706:VAL:HG13	2.43	0.49
33:c:94:LYS:O	33:c:98:MET:HG2	2.13	0.49
2:B:260:LEU:HD23	2:B:260:LEU:C	2.38	0.48
3:C:252:ASP:OD1	3:C:253:SER:N	2.45	0.48
11:K:233:GLU:OE1	11:K:237:VAL:HG13	2.13	0.48
13:M:39:ILE:CG1	13:M:176:ILE:HD11	2.43	0.48
20:T:25:ASP:C	20:T:25:ASP:OD1	2.56	0.48
27:b:16:MET:HE2	27:b:16:MET:N	2.28	0.48
32:U:594:GLY:HA2	32:U:625:ILE:HG22	1.94	0.48
32:U:717:ILE:HD12	32:U:731:ILE:CG1	2.43	0.48
34:f:53:GLN:NE2	34:f:57:GLU:OE1	2.46	0.48
34:f:56:LEU:CD2	34:f:78:LEU:HD12	2.42	0.48
34:f:870:THR:O	34:f:872:VAL:HG12	2.12	0.48
1:A:380:SER:HB2	1:A:384:GLU:HG2	1.95	0.48
1:A:383:ALA:HB1	2:B:344:PRO:HB2	1.95	0.48
2:B:49:LEU:HD11	34:f:669:GLU:OE1	2.13	0.48
2:B:93:GLU:O	2:B:94:GLU:HB3	2.14	0.48
4:D:83:GLN:HG2	4:D:140:VAL:HG13	1.94	0.48
5:E:39:GLN:OE1	6:F:73:ILE:HD13	2.13	0.48
12:L:99:PHE:CD1	20:t:87:ALA:HB1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:226:TYR:HE1	22:W:230:MET:CE	2.25	0.48
24:Y:141:VAL:HG11	24:Y:164:ALA:HB2	1.94	0.48
25:Z:199:LYS:NZ	26:a:364:GLU:OE1	2.43	0.48
25:Z:217:THR:HG21	25:Z:219:LYS:HE3	1.94	0.48
18:r:68:GLU:HG3	18:r:74:ARG:HG3	1.94	0.48
32:U:185:MET:HE2	32:U:185:MET:HA	1.94	0.48
33:c:27:THR:HG23	33:c:176:GLN:O	2.14	0.48
22:W:38:GLY:O	22:W:39:ARG:NH1	2.45	0.48
22:W:40:LEU:HD22	22:W:41:GLN:OE1	2.14	0.48
22:W:108:CYS:HB3	22:W:128:LEU:HD11	1.95	0.48
22:W:314:LEU:HD13	26:a:309:LEU:HD23	1.95	0.48
7:g:61:LEU:HD23	7:g:62:ASP:N	2.27	0.48
33:c:88:ASP:OD1	33:c:88:ASP:C	2.57	0.48
1:A:199:GLU:HA	1:A:199:GLU:OE2	2.13	0.48
2:B:164:MET:HE2	2:B:164:MET:N	2.29	0.48
2:B:174:MET:HE3	2:B:248:LEU:HD13	1.96	0.48
5:E:126:ASP:C	5:E:126:ASP:OD1	2.56	0.48
8:H:147:GLN:OE1	8:H:157:TRP:NE1	2.43	0.48
18:R:139:VAL:HG23	17:q:141:SER:HB3	1.95	0.48
22:W:299:ILE:HG22	22:W:302:TYR:HB2	1.95	0.48
22:W:317:TRP:CZ3	22:W:358:VAL:HG11	2.48	0.48
32:U:703:CYS:HB2	32:U:706:VAL:HG23	1.95	0.48
34:f:339:ILE:O	34:f:339:ILE:HG13	2.13	0.48
4:D:326:ARG:O	4:D:327:LEU:C	2.57	0.48
4:D:352:MET:HE1	5:E:164:ILE:CG2	2.44	0.48
6:F:175:MET:SD	6:F:251:LEU:HD21	2.53	0.48
6:F:284:PHE:CZ	6:F:286:ASP:OD1	2.67	0.48
12:L:118:ILE:HD13	12:L:118:ILE:N	2.28	0.48
17:Q:101:ASN:C	17:Q:102:LEU:HD23	2.39	0.48
20:T:199:ILE:HG22	20:T:199:ILE:O	2.13	0.48
3:C:346:LYS:HE2	3:C:346:LYS:HA	1.96	0.48
6:F:366:MET:HG2	6:F:396:CYS:HB2	1.94	0.48
8:H:123:SER:OG	8:H:124:GLY:N	2.47	0.48
21:V:290:TYR:CD1	21:V:290:TYR:C	2.92	0.48
22:W:194:LEU:CD1	22:W:229:LEU:HD12	2.44	0.48
23:X:125:LEU:HD23	23:X:129:LEU:HD13	1.96	0.48
28:d:297:LYS:C	28:d:297:LYS:HD3	2.39	0.48
17:q:4:LEU:HD22	17:q:45:LEU:HB3	1.96	0.48
32:U:738:ASP:OD1	32:U:738:ASP:N	2.43	0.48
2:B:70:ASP:O	2:B:74:MET:HG3	2.14	0.48
2:B:250:VAL:HG13	2:B:254:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:59:LEU:HD12	4:D:72:PHE:CE1	2.48	0.48
14:N:86:GLU:HA	14:N:86:GLU:OE2	2.14	0.48
22:W:287:VAL:HG23	22:W:306:LEU:CD1	2.38	0.48
23:X:327:TYR:C	23:X:327:TYR:CD1	2.92	0.48
24:Y:350:VAL:HG13	24:Y:351:ASN:OD1	2.13	0.48
27:b:125:VAL:HG13	27:b:159:THR:HG21	1.96	0.48
12:l:109:VAL:HA	12:l:112:ILE:HD12	1.95	0.48
34:f:703:ARG:HD2	34:f:706:ILE:HD12	1.95	0.48
8:H:122:GLN:NE2	9:I:121:TYR:HE2	2.12	0.48
12:L:220:GLU:O	12:L:222:THR:HG23	2.14	0.48
18:R:175:VAL:HG11	18:R:196:LEU:HD11	1.96	0.48
21:V:67:LEU:O	21:V:71:THR:HG23	2.14	0.48
22:W:132:THR:HG22	22:W:138:VAL:HG11	1.96	0.48
25:Z:148:GLY:O	25:Z:150:PRO:HD2	2.14	0.48
18:r:8:LYS:CG	18:r:13:VAL:HG12	2.44	0.48
32:U:139:GLN:NE2	32:U:143:ASP:OD2	2.47	0.48
32:U:198:LEU:HB3	32:U:223:LEU:HD21	1.96	0.48
2:B:53:THR:O	2:B:55:HIS:N	2.47	0.48
6:F:370:SER:O	6:F:370:SER:OG	2.24	0.48
9:I:8:ARG:HG2	9:I:11:ILE:HD13	1.95	0.48
9:I:109:GLN:NE2	9:I:109:GLN:CA	2.67	0.48
11:K:38:ILE:HG23	11:K:181:LEU:HD11	1.95	0.48
17:Q:38:MET:HE3	17:Q:44:LEU:HD22	1.95	0.48
21:V:309:MET:HE3	21:V:331:LEU:HD23	1.95	0.48
24:Y:314:LEU:HD21	24:Y:318:TYR:CD1	2.42	0.48
25:Z:44:GLN:O	25:Z:45:LYS:HG2	2.13	0.48
29:e:20:GLU:OE1	29:e:21:GLU:N	2.45	0.48
31:z:31:MET:HE1	31:z:91:GLY:HA2	1.96	0.48
32:U:339:LEU:CD1	32:U:343:ILE:HD11	2.44	0.48
6:F:83:ASN:O	6:F:83:ASN:ND2	2.47	0.48
12:L:13:TRP:HB2	13:M:22:GLN:OE1	2.13	0.48
20:T:27:LEU:HD13	20:T:27:LEU:C	2.39	0.48
21:V:497:PRO:O	21:V:499:LYS:N	2.46	0.48
22:W:115:ILE:HG12	22:W:120:ILE:HG22	1.96	0.48
22:W:219:THR:O	22:W:223:LYS:HB2	2.13	0.48
27:b:55:ALA:O	27:b:56:ASN:C	2.55	0.48
15:o:162:ALA:O	15:o:166:ASN:ND2	2.47	0.48
20:t:5:MET:HE1	20:t:30:TYR:CE1	2.49	0.48
33:c:75:MET:SD	33:c:92:GLN:NE2	2.87	0.48
5:E:161:ARG:HH21	22:W:136:ILE:HD11	1.78	0.47
6:F:141:ASP:N	6:F:141:ASP:OD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:17:SER:OG	7:G:18:PRO:HD2	2.13	0.47
22:W:129:ARG:NH1	22:W:149:LEU:HD23	2.27	0.47
22:W:183:VAL:HG12	22:W:187:LEU:HD13	1.96	0.47
22:W:363:ILE:HG12	22:W:378:MET:CE	2.44	0.47
24:Y:59:LYS:C	24:Y:59:LYS:HD3	2.39	0.47
11:k:195:ILE:CD1	11:k:217:LEU:HD11	2.44	0.47
12:l:172:LEU:HD23	12:l:179:PHE:CZ	2.49	0.47
32:U:142:LEU:HD23	32:U:142:LEU:C	2.39	0.47
32:U:557:TYR:CD1	32:U:557:TYR:C	2.91	0.47
34:f:239:TYR:CZ	34:f:664:GLU:HG2	2.49	0.47
34:f:686:LEU:O	34:f:690:VAL:HG23	2.14	0.47
5:E:109:ARG:NH2	6:F:114:ASP:O	2.47	0.47
5:E:264:MET:HE1	5:E:277:MET:HE3	1.96	0.47
9:I:37:ILE:HD11	9:I:193:ALA:HB2	1.96	0.47
10:J:152:THR:HG22	11:K:82:ILE:HB	1.96	0.47
11:K:50:VAL:HG22	11:K:51:GLU:N	2.29	0.47
22:W:108:CYS:CB	22:W:128:LEU:HD11	2.45	0.47
22:W:180:LYS:HE2	22:W:180:LYS:N	2.28	0.47
22:W:450:GLU:O	22:W:454:ASN:HB2	2.14	0.47
26:a:217:LEU:CD1	26:a:237:LEU:HB3	2.40	0.47
32:U:122:GLU:OE1	32:U:122:GLU:N	2.47	0.47
34:f:714:SER:OG	34:f:748:LEU:HD11	2.14	0.47
34:f:715:HIS:ND1	34:f:751:TYR:CD2	2.82	0.47
2:B:201:VAL:CG1	2:B:239:VAL:HG21	2.45	0.47
5:E:142:ILE:HD12	5:E:183:LEU:HD11	1.96	0.47
6:F:315:ASN:C	6:F:315:ASN:OD1	2.57	0.47
8:H:209:VAL:HG21	8:H:220:LEU:HD22	1.97	0.47
22:W:214:PHE:HD1	22:W:219:THR:CB	2.28	0.47
22:W:256:ILE:HD13	22:W:262:LYS:HD3	1.96	0.47
23:X:255:LEU:HD23	23:X:287:LEU:CB	2.44	0.47
24:Y:334:LEU:HB3	24:Y:347:ILE:HD11	1.96	0.47
25:Z:201:LEU:HD21	33:c:309:PHE:HE1	1.79	0.47
26:a:295:GLU:C	26:a:295:GLU:CD	2.82	0.47
9:i:53:HIS:ND1	9:i:54:LYS:N	2.62	0.47
17:q:177:THR:HG22	17:q:195:SER:OG	2.13	0.47
32:U:164:GLU:OE1	32:U:204:ILE:HD11	2.14	0.47
32:U:195:ASN:OD1	32:U:223:LEU:HD23	2.14	0.47
34:f:731:MET:O	34:f:733:GLY:N	2.47	0.47
13:M:139:SER:HA	13:M:216:VAL:HG11	1.94	0.47
15:O:164:ILE:HG23	15:O:171:GLY:HA2	1.96	0.47
18:R:180:VAL:HG22	18:R:185:TRP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:313:LEU:HB2	21:V:328:VAL:HG11	1.96	0.47
24:Y:315:THR:O	24:Y:318:TYR:N	2.46	0.47
25:Z:67:VAL:HG13	27:b:92:VAL:HG23	1.95	0.47
25:Z:213:GLU:O	25:Z:217:THR:HG22	2.14	0.47
26:a:17:GLY:C	26:a:19:PRO:HD2	2.39	0.47
28:d:167:TYR:O	28:d:170:GLN:OE1	2.33	0.47
32:U:405:THR:CG2	32:U:427:LEU:HD21	2.45	0.47
34:f:705:ASN:O	34:f:709:THR:HG22	2.14	0.47
2:B:202:GLU:O	2:B:206:THR:HG23	2.14	0.47
9:I:21:VAL:O	9:I:25:MET:HG3	2.13	0.47
12:L:171:TYR:CD1	12:L:194:ALA:HB2	2.49	0.47
22:W:39:ARG:CZ	22:W:39:ARG:HA	2.44	0.47
22:W:51:GLU:OE1	22:W:52:LYS:N	2.48	0.47
22:W:403:PHE:CE2	22:W:417:ARG:HD3	2.50	0.47
26:a:274:LEU:HD13	26:a:319:LEU:HD11	1.97	0.47
11:k:195:ILE:HD12	11:k:217:LEU:HD21	1.95	0.47
15:o:85:LYS:HE2	15:o:120:THR:HG23	1.97	0.47
19:s:145:LEU:HD23	19:s:178:VAL:HB	1.97	0.47
32:U:120:GLU:OE1	32:U:120:GLU:N	2.48	0.47
32:U:902:PRO:HB2	32:U:912:ILE:HD11	1.96	0.47
34:f:778:LEU:HD13	34:f:821:LEU:HD22	1.95	0.47
6:F:257:VAL:HG23	6:F:257:VAL:O	2.14	0.47
10:J:104:VAL:HG23	10:J:133:ILE:HG22	1.97	0.47
13:M:34:SER:OG	13:M:65:ARG:NH1	2.44	0.47
13:M:134:SER:OG	13:M:153:PRO:HD3	2.14	0.47
24:Y:88:LEU:O	24:Y:88:LEU:HD23	2.15	0.47
25:Z:173:GLU:HA	25:Z:173:GLU:OE1	2.13	0.47
26:a:72:ASN:O	26:a:75:SER:N	2.43	0.47
27:b:25:ARG:HH11	27:b:144:GLY:HA2	1.79	0.47
8:h:114:ALA:HB1	8:h:152:GLY:O	2.15	0.47
9:i:198:ASN:HB2	9:i:206:LEU:HD11	1.95	0.47
2:B:173:VAL:O	3:C:258:ARG:NH1	2.48	0.47
11:K:14:THR:HG23	11:K:22:PHE:HD2	1.80	0.47
11:K:31:ILE:HD11	11:K:158:PRO:CD	2.44	0.47
11:K:31:ILE:HG22	11:K:31:ILE:O	2.15	0.47
15:O:7:VAL:HG12	15:O:14:VAL:CG2	2.45	0.47
21:V:207:ALA:HA	21:V:210:CYS:SG	2.55	0.47
21:V:497:PRO:N	21:V:498:PRO:HD3	2.29	0.47
22:W:200:ILE:H	22:W:200:ILE:CD1	2.21	0.47
22:W:272:LEU:HD23	22:W:272:LEU:HA	1.72	0.47
22:W:346:GLU:HG3	22:W:350:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:50:ILE:HD12	23:X:69:LEU:HD21	1.97	0.47
23:X:243:ASP:OD1	23:X:243:ASP:N	2.47	0.47
26:a:140:GLU:O	26:a:143:ASN:ND2	2.47	0.47
26:a:142:LEU:HD22	26:a:152:HIS:NE2	2.30	0.47
27:b:4:GLU:OE1	27:b:108:ARG:NH1	2.40	0.47
32:U:408:LEU:HD23	32:U:426:TYR:CG	2.50	0.47
32:U:701:ILE:HD13	32:U:810:THR:HB	1.96	0.47
33:c:131:GLN:C	33:c:131:GLN:OE1	2.57	0.47
34:f:175:ASP:O	34:f:178:LYS:NZ	2.37	0.47
34:f:193:PRO:HA	34:f:196:MET:HG3	1.97	0.47
34:f:698:SER:OG	34:f:703:ARG:NE	2.47	0.47
34:f:850:VAL:HG22	34:f:863:THR:HG23	1.97	0.47
1:A:177:VAL:HG12	1:A:224:LEU:HD23	1.96	0.47
3:C:161:ILE:HG12	3:C:199:LEU:HD21	1.96	0.47
6:F:98:ASP:C	6:F:98:ASP:OD1	2.56	0.47
7:G:80:MET:HE2	7:G:138:MET:HA	1.96	0.47
24:Y:80:GLU:OE1	24:Y:83:ARG:NH1	2.48	0.47
26:a:141:MET:O	26:a:143:ASN:OD1	2.32	0.47
27:b:20:ASP:OD1	27:b:20:ASP:O	2.33	0.47
10:j:41:VAL:HG23	10:j:41:VAL:O	2.15	0.47
11:k:50:VAL:HG21	11:k:66:LYS:HB3	1.97	0.47
32:U:416:GLU:O	32:U:417:LYS:C	2.58	0.47
1:A:273:PHE:CZ	1:A:275:ASP:OD1	2.68	0.47
3:C:277:LEU:HD11	3:C:305:LEU:HD23	1.96	0.47
4:D:345:PHE:O	4:D:349:THR:HG23	2.14	0.47
22:W:315:MET:HE2	22:W:315:MET:HB3	1.78	0.47
23:X:365:LEU:HD22	23:X:385:LEU:HD11	1.96	0.47
24:Y:186:LEU:HD13	24:Y:214:MET:HE1	1.95	0.47
26:a:122:LYS:HE2	26:a:130:VAL:HG11	1.96	0.47
7:g:72:ILE:HD12	7:g:94:ALA:HB3	1.97	0.47
12:l:172:LEU:O	12:l:176:MET:HB2	2.15	0.47
14:n:21:THR:HG21	14:n:32:THR:HG21	1.95	0.47
18:r:158:ARG:HA	18:r:175:VAL:HG11	1.97	0.47
1:A:85:GLN:O	1:A:89:SER:N	2.46	0.47
1:A:262:GLU:O	1:A:266:THR:HG23	2.15	0.47
2:B:347:ILE:O	2:B:350:LYS:NZ	2.48	0.47
8:H:47:THR:CG2	8:H:74:VAL:HG21	2.45	0.47
9:I:37:ILE:CD1	9:I:193:ALA:HB2	2.45	0.47
10:J:42:VAL:CG1	10:J:191:VAL:HG21	2.43	0.47
15:O:39:SER:OG	15:O:42:ILE:N	2.48	0.47
16:P:187:HIS:CE1	16:P:196:THR:OG1	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:87:ILE:CA	22:W:104:MET:HE1	2.43	0.47
22:W:146:THR:HB	22:W:169:LEU:HD11	1.96	0.47
22:W:179:LYS:HD3	22:W:213:PHE:CD1	2.50	0.47
23:X:47:GLU:HA	23:X:50:ILE:HG22	1.96	0.47
24:Y:310:SER:O	24:Y:310:SER:OG	2.27	0.47
26:a:280:MET:SD	26:a:295:GLU:OE1	2.72	0.47
29:e:17:ASP:O	29:e:18:GLU:C	2.58	0.47
13:m:69:VAL:HG22	13:m:73:VAL:HG12	1.97	0.47
32:U:128:GLN:NE2	32:U:131:GLU:OE1	2.48	0.47
32:U:233:LEU:HD12	32:U:233:LEU:O	2.15	0.47
32:U:406:ALA:HA	32:U:445:ALA:HB2	1.96	0.47
34:f:278:VAL:HG12	34:f:305:LEU:HD12	1.96	0.47
2:B:53:THR:HB	2:B:54:PRO:HD2	1.97	0.46
5:E:240:GLY:O	5:E:241:ARG:C	2.58	0.46
9:I:92:LEU:CD2	16:P:72:LEU:HD21	2.45	0.46
22:W:64:SER:HB3	22:W:103:LYS:HD2	1.97	0.46
24:Y:285:ASP:O	24:Y:289:ALA:HB2	2.15	0.46
25:Z:38:VAL:HG21	25:Z:54:PHE:CZ	2.50	0.46
26:a:54:ASP:HB2	26:a:83:VAL:HG23	1.97	0.46
26:a:148:VAL:HG23	26:a:152:HIS:ND1	2.30	0.46
28:d:198:PHE:CE1	28:d:202:GLN:HG3	2.49	0.46
8:h:132:SER:OG	8:h:162:MET:HE1	2.15	0.46
13:m:182:LYS:O	13:m:182:LYS:HG2	2.15	0.46
18:r:43:LEU:HD12	18:r:43:LEU:O	2.15	0.46
34:f:307:LEU:HD12	34:f:311:VAL:HG11	1.97	0.46
1:A:364:VAL:HG22	1:A:365:GLU:N	2.31	0.46
2:B:55:HIS:O	2:B:61:LYS:NZ	2.46	0.46
2:B:125:THR:HG1	2:B:129:SER:HG	1.62	0.46
2:B:377:ASP:OD1	2:B:377:ASP:N	2.46	0.46
3:C:140:VAL:O	3:C:140:VAL:HG12	2.15	0.46
8:H:135:ILE:HD12	8:H:135:ILE:N	2.30	0.46
22:W:39:ARG:O	22:W:42:GLU:HG2	2.15	0.46
22:W:340:VAL:HG12	22:W:341:PHE:CE1	2.50	0.46
22:W:396:LEU:CD2	22:W:401:THR:HG21	2.45	0.46
23:X:259:ILE:HD11	23:X:291:ALA:HB2	1.97	0.46
24:Y:357:ASN:O	24:Y:358:ARG:C	2.58	0.46
26:a:232:TRP:HB2	26:a:254:ALA:HB1	1.95	0.46
9:i:25:MET:SD	9:i:152:PRO:HD2	2.55	0.46
34:f:564:LEU:HD11	34:f:794:ALA:HA	1.97	0.46
2:B:116:ILE:O	2:B:116:ILE:HG22	2.14	0.46
9:I:229:LYS:O	9:I:233:VAL:HG23	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:184:VAL:CG2	11:K:185:TYR:N	2.78	0.46
17:Q:27:GLN:O	17:q:170:ARG:NH1	2.48	0.46
17:Q:100:VAL:HB	17:Q:102:LEU:HD21	1.97	0.46
19:S:12:ILE:HD12	19:S:109:ILE:HD12	1.97	0.46
22:W:26:GLN:OE1	22:W:27:ARG:HD2	2.15	0.46
22:W:112:VAL:HG22	22:W:124:LEU:HD21	1.96	0.46
22:W:377:ARG:NH2	26:a:305:ASN:O	2.48	0.46
26:a:100:THR:O	26:a:104:VAL:HG22	2.16	0.46
28:d:189:HIS:HB3	28:d:223:ASN:OD1	2.15	0.46
9:i:139:TRP:CZ3	9:i:218:ARG:NH1	2.84	0.46
13:m:37:ILE:HD12	13:m:176:ILE:HD11	1.98	0.46
15:o:175:ASP:OD1	15:o:188:ARG:O	2.34	0.46
32:U:446:LEU:HD23	32:U:446:LEU:O	2.15	0.46
32:U:810:THR:HG1	32:U:811:PHE:HD1	1.59	0.46
34:f:869:THR:HG22	34:f:870:THR:N	2.30	0.46
2:B:118:ASP:OD1	2:B:118:ASP:N	2.48	0.46
3:C:218:GLU:O	3:C:221:GLN:HG2	2.15	0.46
4:D:415:GLU:CD	4:D:415:GLU:H	2.24	0.46
11:K:231:LYS:O	11:K:235:GLU:HG2	2.16	0.46
14:N:136:ILE:HG21	14:N:164:ALA:HB2	1.97	0.46
15:O:188:ARG:HB3	15:O:189:PRO:CD	2.46	0.46
22:W:377:ARG:CZ	26:a:308:GLU:OE1	2.63	0.46
24:Y:124:PHE:CB	24:Y:144:LEU:HD21	2.46	0.46
25:Z:182:THR:O	25:Z:183:THR:C	2.59	0.46
26:a:366:LEU:CD1	28:d:333:THR:HG23	2.46	0.46
27:b:58:CYS:SG	27:b:89:GLY:HA2	2.55	0.46
27:b:128:ALA:O	27:b:160:LEU:CD2	2.64	0.46
14:n:15:LEU:HD23	14:n:45:CYS:SG	2.55	0.46
20:t:156:LYS:HD2	20:t:156:LYS:C	2.40	0.46
32:U:695:MET:HE1	32:U:737:LEU:HD11	1.98	0.46
34:f:376:PHE:CE1	34:f:409:SER:HB3	2.51	0.46
4:D:293:LEU:CD1	4:D:320:ALA:HB1	2.46	0.46
4:D:407:ILE:O	4:D:408:LYS:C	2.57	0.46
6:F:70:LYS:HA	6:F:73:ILE:HG22	1.97	0.46
11:K:118:ASN:OD1	12:L:82:ARG:NH2	2.47	0.46
13:M:66:LEU:HD12	13:M:66:LEU:N	2.31	0.46
20:T:1:THR:N	20:T:105:PRO:O	2.45	0.46
22:W:61:VAL:HG13	22:W:62:SER:N	2.30	0.46
22:W:86:ASN:O	22:W:90:LEU:HG	2.16	0.46
22:W:199:TYR:HD2	22:W:233:LEU:HD13	1.81	0.46
23:X:170:GLN:OE1	23:X:192:SER:OG	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:339:ILE:O	23:X:339:ILE:HG22	2.16	0.46
27:b:24:THR:O	27:b:25:ARG:C	2.58	0.46
18:r:15:VAL:CG2	18:r:178:TYR:HB2	2.45	0.46
32:U:346:ASN:OD1	32:U:348:THR:HG23	2.14	0.46
34:f:220:ASP:OD1	34:f:220:ASP:N	2.49	0.46
1:A:76:ALA:O	1:A:79:ASP:OD2	2.33	0.46
5:E:171:LEU:HD12	5:E:277:MET:HB2	1.97	0.46
8:H:192:LEU:O	8:H:195:LYS:N	2.48	0.46
9:I:80:THR:O	9:I:83:ALA:HB3	2.16	0.46
21:V:222:ASP:OD1	21:V:222:ASP:N	2.49	0.46
22:W:61:VAL:O	22:W:65:ARG:HG2	2.16	0.46
24:Y:202:LEU:HD11	24:Y:227:SER:OG	2.15	0.46
28:d:180:GLU:N	28:d:180:GLU:OE1	2.49	0.46
9:i:92:LEU:HD13	9:i:96:ARG:NH2	2.29	0.46
11:k:24:VAL:O	11:k:28:ILE:HG12	2.15	0.46
14:n:161:LEU:O	14:n:165:MET:HG2	2.15	0.46
18:r:35:VAL:HG11	18:r:43:LEU:HD13	1.93	0.46
34:f:558:LEU:HB2	34:f:559:PRO:HD3	1.97	0.46
1:A:59:ILE:CD1	2:B:79:ILE:HD13	2.46	0.46
5:E:372:ARG:HG2	5:E:372:ARG:HH11	1.81	0.46
7:G:160:TYR:CD2	7:G:160:TYR:O	2.69	0.46
12:L:196:ARG:HB2	12:L:205:LEU:HD11	1.98	0.46
20:T:14:VAL:CG1	20:T:150:LEU:HD22	2.45	0.46
22:W:103:LYS:HA	22:W:106:GLN:CG	2.45	0.46
22:W:172:GLU:H	22:W:172:GLU:HG2	1.58	0.46
24:Y:279:GLU:OE2	29:e:52:PHE:HB3	2.16	0.46
26:a:240:PHE:CZ	26:a:268:LEU:HD12	2.51	0.46
27:b:124:LEU:HD23	27:b:152:LYS:O	2.15	0.46
10:j:51:ALA:C	10:j:53:LEU:H	2.23	0.46
34:f:394:ASP:CG	34:f:397:LYS:HZ3	2.24	0.46
34:f:826:GLN:OE1	34:f:826:GLN:HA	2.16	0.46
34:f:850:VAL:CG2	34:f:863:THR:HG23	2.45	0.46
7:G:67:THR:OG1	7:G:68:HIS:N	2.46	0.46
8:H:47:THR:HG21	8:H:74:VAL:HG21	1.98	0.46
8:H:134:LEU:CD1	8:H:162:MET:HE2	2.45	0.46
10:J:156:TRP:HA	11:K:59:MET:HA	1.97	0.46
11:K:225:ASN:OD1	11:K:225:ASN:N	2.48	0.46
13:M:52:LEU:HD13	13:M:206:ASP:OD2	2.15	0.46
17:Q:143:LEU:O	17:Q:147:TYR:HB3	2.16	0.46
22:W:186:ILE:HD12	22:W:209:ILE:HG12	1.98	0.46
22:W:235:GLN:HG3	22:W:243:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:449:GLU:OE2	25:Z:223:ASN:ND2	2.48	0.46
27:b:24:THR:O	27:b:27:GLN:N	2.31	0.46
28:d:116:LEU:HD21	28:d:150:ILE:HD11	1.97	0.46
10:j:127:PHE:O	10:j:149:PRO:HB3	2.16	0.46
32:U:668:ALA:HB1	32:U:694:ILE:HD13	1.98	0.46
33:c:299:CYS:O	33:c:303:MET:SD	2.74	0.46
34:f:87:THR:O	34:f:90:THR:OG1	2.32	0.46
34:f:253:LEU:HD23	34:f:253:LEU:O	2.15	0.46
34:f:519:ALA:HB3	34:f:557:TRP:O	2.15	0.46
1:A:103:ASN:OD1	1:A:104:ALA:N	2.49	0.46
1:A:401:ARG:NH2	1:A:408:ASP:OD1	2.49	0.46
2:B:342:ILE:HD12	2:B:342:ILE:O	2.15	0.46
4:D:185:LEU:HD12	4:D:185:LEU:N	2.31	0.46
14:N:136:ILE:O	14:N:140:VAL:HG22	2.16	0.46
21:V:451:ILE:HB	28:d:279:TYR:HA	1.98	0.46
22:W:139:GLU:CD	22:W:174:TYR:HD1	2.24	0.46
22:W:365:ILE:HD11	26:a:312:MET:HE1	1.98	0.46
22:W:394:SER:O	22:W:398:VAL:HG23	2.16	0.46
28:d:339:VAL:HG13	33:c:296:ILE:HG23	1.97	0.46
8:h:166:TYR:O	8:h:170:LYS:HG3	2.16	0.46
20:t:43:MET:HG2	20:t:44:ARG:N	2.30	0.46
32:U:889:LEU:HD11	32:U:909:GLY:HA2	1.98	0.46
34:f:270:LEU:O	34:f:271:MET:C	2.59	0.46
1:A:379:ASN:N	1:A:379:ASN:OD1	2.48	0.46
11:K:50:VAL:CG1	11:K:216:GLU:HG3	2.46	0.46
14:N:15:LEU:CD1	14:N:180:ILE:HD12	2.46	0.46
19:S:73:LYS:HE2	12:l:93:LEU:HD21	1.98	0.46
21:V:301:GLU:O	21:V:302:TYR:C	2.59	0.46
22:W:178:GLU:HB3	22:W:181:GLU:CD	2.41	0.46
24:Y:247:LEU:O	24:Y:251:HIS:ND1	2.49	0.46
26:a:18:GLN:N	26:a:19:PRO:HD2	2.30	0.46
26:a:186:LYS:O	26:a:187:ASP:C	2.59	0.46
17:q:59:TYR:HE2	17:q:87:ASN:HD22	1.63	0.46
33:c:130:GLN:HG3	33:c:162:LEU:HD11	1.97	0.46
1:A:59:ILE:HD13	2:B:79:ILE:HD13	1.98	0.45
1:A:168:GLU:HG3	1:A:168:GLU:O	2.16	0.45
2:B:88:LEU:HD22	34:f:681:TYR:CD1	2.50	0.45
2:B:184:TYR:HE2	2:B:194:ILE:HG23	1.81	0.45
2:B:254:GLU:O	2:B:254:GLU:HG2	2.15	0.45
3:C:140:VAL:O	3:C:140:VAL:CG1	2.63	0.45
5:E:384:LEU:HD23	5:E:384:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:329:ILE:HG22	6:F:330:ALA:N	2.31	0.45
8:H:122:GLN:NE2	9:I:121:TYR:CE2	2.84	0.45
9:I:44:LEU:C	9:I:44:LEU:HD12	2.41	0.45
15:O:3:THR:HG23	15:O:3:THR:O	2.16	0.45
17:Q:45:LEU:HD12	17:Q:45:LEU:N	2.31	0.45
19:S:26:ASP:C	19:S:26:ASP:OD1	2.59	0.45
21:V:302:TYR:CZ	21:V:338:LEU:HD13	2.51	0.45
21:V:341:GLU:O	21:V:342:ILE:HD13	2.17	0.45
21:V:435:GLU:OE1	28:d:279:TYR:CE2	2.68	0.45
22:W:369:TYR:CD2	26:a:312:MET:SD	3.09	0.45
23:X:123:THR:OG1	23:X:124:PHE:N	2.49	0.45
23:X:320:SER:HA	23:X:323:LEU:HD23	1.98	0.45
26:a:240:PHE:HZ	26:a:268:LEU:CD1	2.29	0.45
26:a:274:LEU:HD23	26:a:310:LEU:HD11	1.98	0.45
26:a:366:LEU:HD23	26:a:366:LEU:C	2.41	0.45
20:t:20:VAL:HG22	20:t:192:VAL:HG12	1.98	0.45
32:U:265:ILE:HD11	32:U:326:ILE:HD13	1.98	0.45
32:U:792:ASN:OD1	32:U:796:LYS:N	2.42	0.45
34:f:86:THR:OG1	34:f:87:THR:N	2.49	0.45
34:f:322:SER:OG	34:f:324:VAL:HB	2.16	0.45
34:f:372:LEU:O	34:f:375:SER:OG	2.29	0.45
34:f:603:SER:OG	34:f:604:GLY:N	2.49	0.45
6:F:134:LEU:HD23	6:F:160:ILE:HG23	1.98	0.45
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.98	0.45
15:O:16:GLY:HA2	15:O:175:ASP:O	2.16	0.45
22:W:250:ILE:HA	22:W:253:THR:HG23	1.97	0.45
22:W:371:THR:HG23	26:a:323:SER:CB	2.44	0.45
24:Y:18:ARG:O	24:Y:22:LEU:HG	2.16	0.45
24:Y:201:PHE:O	24:Y:205:VAL:HG23	2.16	0.45
26:a:368:GLU:OE1	26:a:369:HIS:N	2.49	0.45
27:b:15:TYR:C	27:b:16:MET:HE2	2.41	0.45
32:U:48:LEU:HD21	32:U:54:PHE:CD2	2.52	0.45
34:f:521:ALA:O	34:f:524:MET:HG2	2.16	0.45
3:C:155:ASP:O	3:C:159:LYS:HG3	2.16	0.45
3:C:376:VAL:O	3:C:376:VAL:CG1	2.64	0.45
8:H:34:SER:OG	8:H:47:THR:HG22	2.16	0.45
14:N:53:THR:HG22	14:N:99:ILE:HD11	1.99	0.45
15:O:49:THR:OG1	15:O:52:ASP:HB2	2.15	0.45
19:S:37:THR:OG1	19:S:38:ARG:N	2.50	0.45
22:W:34:LEU:HB2	22:W:43:VAL:HG13	1.97	0.45
22:W:72:LYS:CB	22:W:73:MET:HE2	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:76:GLU:HA	22:W:78:LYS:HZ1	1.81	0.45
22:W:80:TRP:NE1	22:W:120:ILE:HD11	2.30	0.45
22:W:160:LYS:HE2	22:W:160:LYS:HB2	1.71	0.45
22:W:235:GLN:OE1	22:W:350:ARG:NH2	2.49	0.45
22:W:256:ILE:O	22:W:262:LYS:HB2	2.16	0.45
22:W:314:LEU:HD22	22:W:381:LEU:HD21	1.98	0.45
22:W:396:LEU:HD22	22:W:401:THR:HG21	1.98	0.45
23:X:122:ARG:C	23:X:123:THR:HG1	2.21	0.45
24:Y:186:LEU:CD1	24:Y:214:MET:HE1	2.47	0.45
26:a:315:LEU:HD23	26:a:320:VAL:HG23	1.98	0.45
26:a:366:LEU:HD23	26:a:367:VAL:N	2.31	0.45
27:b:154:THR:HG23	27:b:155:ALA:N	2.32	0.45
32:U:628:ARG:NH1	32:U:749:GLN:OE1	2.49	0.45
34:f:485:LEU:C	34:f:485:LEU:CD2	2.89	0.45
34:f:502:LEU:N	34:f:503:PRO:HD2	2.31	0.45
34:f:747:GLN:O	34:f:750:GLN:HB2	2.16	0.45
34:f:846:VAL:HG21	34:f:872:VAL:HG21	1.98	0.45
1:A:303:ILE:HD11	1:A:331:LEU:HB2	1.98	0.45
4:D:162:VAL:O	4:D:162:VAL:CG2	2.63	0.45
4:D:230:VAL:HG12	4:D:231:VAL:N	2.31	0.45
5:E:338:PHE:CE2	5:E:374:VAL:HG23	2.51	0.45
8:H:74:VAL:HG22	8:H:75:TYR:N	2.31	0.45
9:I:105:ILE:HD13	9:I:110:LEU:HB2	1.97	0.45
14:N:49:SER:OG	14:N:52:ASP:CG	2.59	0.45
21:V:265:ASP:C	21:V:265:ASP:OD1	2.59	0.45
22:W:366:MET:SD	22:W:378:MET:HG3	2.56	0.45
24:Y:145:LEU:HG	24:Y:160:ASN:HB3	1.98	0.45
26:a:365:MET:HE2	26:a:365:MET:HA	1.97	0.45
11:k:185:TYR:CD1	11:k:185:TYR:C	2.94	0.45
11:k:210:LEU:C	11:k:210:LEU:HD23	2.41	0.45
13:m:39:ILE:HG21	13:m:193:VAL:CG2	2.47	0.45
32:U:660:CYS:O	32:U:694:ILE:HG12	2.17	0.45
34:f:170:TRP:CD1	34:f:170:TRP:C	2.94	0.45
34:f:715:HIS:ND1	34:f:751:TYR:HD2	2.14	0.45
4:D:155:THR:HA	4:D:159:LYS:HG3	1.99	0.45
9:I:43:VAL:CG2	9:I:145:PHE:HB3	2.47	0.45
10:J:206:ILE:HG22	10:J:207:GLU:N	2.32	0.45
14:N:38:ILE:HD13	14:N:61:THR:OG1	2.17	0.45
19:S:212:LYS:O	19:S:213:ASP:CB	2.64	0.45
22:W:40:LEU:O	22:W:43:VAL:HG23	2.16	0.45
22:W:299:ILE:CG2	22:W:302:TYR:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:324:TYR:O	22:W:328:LEU:HG	2.16	0.45
24:Y:351:ASN:OD1	24:Y:351:ASN:N	2.48	0.45
7:g:37:LEU:HD23	7:g:53:GLN:HB2	1.97	0.45
14:n:3:THR:HG22	14:n:161:LEU:HD23	1.98	0.45
17:q:103:LEU:HD23	17:q:116:TYR:O	2.16	0.45
32:U:48:LEU:C	32:U:48:LEU:HD23	2.41	0.45
34:f:731:MET:O	34:f:732:VAL:C	2.58	0.45
5:E:149:ILE:HD11	5:E:187:VAL:CG1	2.47	0.45
6:F:115:SER:OG	6:F:116:GLN:N	2.49	0.45
21:V:357:LEU:O	21:V:358:MET:C	2.60	0.45
22:W:73:MET:HE2	22:W:73:MET:H	1.81	0.45
22:W:298:GLU:O	22:W:300:PRO:HD3	2.17	0.45
22:W:432:LEU:HD22	33:c:309:PHE:HD2	1.80	0.45
24:Y:215:ASP:OD1	24:Y:215:ASP:C	2.59	0.45
25:Z:131:LEU:HD23	25:Z:196:HIS:ND1	2.31	0.45
25:Z:136:GLU:OE1	25:Z:136:GLU:N	2.50	0.45
28:d:104:ARG:NH1	28:d:106:SER:O	2.47	0.45
7:g:10:ASP:C	7:g:10:ASP:OD1	2.59	0.45
18:r:173:GLY:O	18:r:193:VAL:HG23	2.16	0.45
20:t:92:LEU:O	20:t:96:MET:HG2	2.16	0.45
33:c:304:LEU:O	33:c:308:VAL:HG23	2.16	0.45
34:f:201:GLU:C	34:f:201:GLU:CD	2.85	0.45
34:f:429:ILE:O	34:f:429:ILE:HG22	2.16	0.45
34:f:460:ASP:OD2	34:f:494:ARG:NH2	2.50	0.45
3:C:263:SER:OG	4:D:278:GLN:OE1	2.34	0.45
5:E:108:MET:HE2	6:F:111:ILE:HD13	1.98	0.45
5:E:349:GLU:OE2	6:F:350:ARG:NH1	2.49	0.45
6:F:279:ALA:HB1	6:F:280:PRO:CD	2.39	0.45
18:R:165:THR:HG23	18:R:172:GLY:HA2	1.98	0.45
22:W:234:ASP:HB2	22:W:243:ILE:HG12	1.99	0.45
10:j:43:LEU:HD21	10:j:72:ALA:CB	2.47	0.45
11:k:210:LEU:HD23	11:k:211:ASN:N	2.32	0.45
12:l:188:VAL:HG21	12:l:214:ILE:HD11	1.97	0.45
32:U:557:TYR:OH	32:U:757:MET:HB2	2.17	0.45
1:A:80:LEU:HD21	34:f:712:LYS:HA	1.99	0.45
3:C:153:GLY:C	3:C:154:LEU:HD12	2.42	0.45
4:D:370:ILE:HG12	4:D:374:ASP:HB2	1.99	0.45
6:F:321:GLN:HG3	6:F:321:GLN:O	2.16	0.45
21:V:243:ASP:O	21:V:247:GLN:NE2	2.43	0.45
22:W:68:VAL:O	22:W:71:VAL:HG12	2.16	0.45
22:W:256:ILE:HD13	22:W:262:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:326:MET:HE1	22:W:330:LYS:HG2	1.98	0.45
23:X:140:THR:O	23:X:141:LYS:C	2.60	0.45
23:X:256:LEU:HD22	23:X:319:ILE:HD12	1.97	0.45
24:Y:124:PHE:HB2	24:Y:144:LEU:HD21	1.98	0.45
25:Z:70:LEU:HD23	25:Z:70:LEU:C	2.41	0.45
7:g:72:ILE:HD11	7:g:78:CYS:SG	2.56	0.45
9:i:194:ILE:CD1	9:i:236:LEU:HB3	2.47	0.45
12:l:146:GLN:O	12:l:153:TYR:HA	2.16	0.45
17:q:35:MET:HE2	17:q:45:LEU:HD21	1.98	0.45
31:z:70:ARG:HD3	31:z:101:THR:OG1	2.17	0.45
32:U:410:VAL:HG23	32:U:448:LEU:HD13	1.99	0.45
34:f:192:VAL:O	34:f:196:MET:HG3	2.16	0.45
34:f:257:ARG:O	34:f:258:LYS:C	2.60	0.45
3:C:148:TYR:HB3	3:C:158:ILE:HD11	1.99	0.45
9:I:106:PRO:HG2	9:I:109:GLN:HB2	1.98	0.45
22:W:115:ILE:HG23	22:W:121:LYS:NZ	2.31	0.45
22:W:180:LYS:HD3	22:W:213:PHE:HZ	1.81	0.45
22:W:235:GLN:CD	22:W:350:ARG:HH21	2.25	0.45
22:W:401:THR:HG22	22:W:402:ILE:HG23	1.99	0.45
26:a:200:LEU:HD12	26:a:222:LEU:HD21	1.99	0.45
27:b:121:GLU:C	27:b:121:GLU:OE2	2.59	0.45
28:d:241:TYR:HA	28:d:244:VAL:HG12	1.99	0.45
28:d:266:THR:HA	28:d:269:ASP:OD2	2.15	0.45
10:j:134:VAL:HG12	10:j:144:LEU:HD13	1.99	0.45
14:n:39:HIS:CG	14:n:40:ASP:H	2.35	0.45
19:s:145:LEU:CD2	19:s:178:VAL:HB	2.47	0.45
8:H:64:VAL:HG12	8:H:74:VAL:HB	1.98	0.45
8:H:191:ILE:CD1	8:H:207:ILE:HD12	2.47	0.45
22:W:43:VAL:HA	22:W:46:THR:HG22	1.98	0.45
22:W:317:TRP:NE1	22:W:355:LYS:HE3	2.30	0.45
22:W:344:THR:HG21	22:W:346:GLU:HG2	1.97	0.45
24:Y:313:SER:OG	24:Y:314:LEU:N	2.50	0.45
25:Z:73:ASP:OD1	25:Z:73:ASP:C	2.60	0.45
28:d:188:MET:HE1	28:d:192:LEU:HG	1.99	0.45
7:g:60:LEU:HD13	13:m:162:GLY:O	2.17	0.45
10:j:35:VAL:HG21	10:j:187:THR:CG2	2.46	0.45
19:s:12:ILE:HD12	19:s:109:ILE:HG22	1.98	0.45
32:U:342:LEU:HD23	32:U:743:ASN:OD1	2.16	0.45
2:B:234:LEU:N	35:B:501:ATP:O1A	2.49	0.44
3:C:233:GLU:HA	3:C:236:VAL:HG22	1.99	0.44
4:D:316:THR:O	4:D:316:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:37:ILE:CD1	8:H:190:ALA:HB2	2.46	0.44
14:N:115:VAL:HA	14:N:120:MET:O	2.17	0.44
16:P:119:PHE:CD1	16:P:119:PHE:C	2.94	0.44
19:S:17:GLY:HA3	19:S:20:PHE:CE2	2.52	0.44
20:T:99:ARG:HG2	20:T:104:ASN:O	2.17	0.44
21:V:332:LEU:HA	21:V:335:VAL:HG12	1.99	0.44
22:W:226:TYR:CE1	22:W:230:MET:CG	3.00	0.44
22:W:314:LEU:CD2	22:W:381:LEU:HD11	2.47	0.44
22:W:393:LEU:HD23	22:W:413:ILE:HD13	1.99	0.44
24:Y:42:MET:HE3	24:Y:42:MET:HA	1.98	0.44
24:Y:201:PHE:HB3	24:Y:223:THR:CG2	2.46	0.44
24:Y:204:THR:O	24:Y:204:THR:CG2	2.63	0.44
26:a:4:VAL:N	26:a:5:PRO:HD2	2.32	0.44
28:d:88:LEU:HD11	28:d:139:GLN:HG3	1.99	0.44
8:h:138:TRP:CD1	8:h:138:TRP:C	2.95	0.44
8:h:191:ILE:HG22	8:h:195:LYS:HD2	1.99	0.44
16:p:12:ALA:HB3	16:p:136:VAL:CG2	2.48	0.44
19:s:199:THR:OG1	19:s:200:LYS:N	2.50	0.44
32:U:126:ILE:HD12	32:U:126:ILE:N	2.33	0.44
32:U:459:ASP:C	32:U:459:ASP:OD1	2.59	0.44
32:U:653:ALA:HB2	32:U:675:MET:HE1	1.99	0.44
34:f:387:GLN:OE1	34:f:387:GLN:N	2.49	0.44
34:f:704:LEU:H	34:f:704:LEU:HD12	1.82	0.44
2:B:410:ARG:HA	2:B:410:ARG:NE	2.32	0.44
3:C:182:GLN:HB2	3:C:285:ALA:HB1	1.98	0.44
9:I:90:LEU:HD11	9:I:114:LEU:HD22	1.98	0.44
9:I:174:MET:CE	9:I:195:LYS:HE2	2.46	0.44
13:M:216:VAL:HG13	13:M:216:VAL:O	2.16	0.44
13:M:219:LEU:N	13:M:219:LEU:CD1	2.81	0.44
18:R:67:TYR:CD1	18:R:67:TYR:C	2.95	0.44
21:V:404:LYS:HZ2	21:V:441:ALA:HB1	1.82	0.44
22:W:97:LEU:O	22:W:101:VAL:HG23	2.17	0.44
22:W:226:TYR:HE1	22:W:230:MET:SD	2.40	0.44
22:W:250:ILE:HA	22:W:253:THR:CG2	2.47	0.44
24:Y:24:PHE:O	24:Y:27:SER:HB3	2.17	0.44
27:b:143:PHE:CG	27:b:144:GLY:N	2.85	0.44
29:e:41:ASP:O	29:e:42:ASN:HB3	2.18	0.44
18:r:137:TYR:O	18:r:138:GLY:C	2.60	0.44
32:U:31:VAL:HG13	32:U:32:ASN:N	2.33	0.44
32:U:143:ASP:O	32:U:145:HIS:ND1	2.50	0.44
32:U:450:HIS:NE2	32:U:457:ILE:HG13	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:266:LEU:HD23	34:f:297:MET:HE2	1.99	0.44
1:A:105:ASP:OD1	1:A:105:ASP:O	2.35	0.44
2:B:133:VAL:HG11	2:B:157:HIS:HB2	2.00	0.44
2:B:431:GLN:O	2:B:432:GLU:HB2	2.17	0.44
3:C:151:ILE:O	3:C:151:ILE:CG2	2.61	0.44
3:C:328:ILE:HA	3:C:331:ILE:HG22	1.99	0.44
5:E:143:ARG:HG2	5:E:143:ARG:HH11	1.82	0.44
5:E:283:ASP:OD1	5:E:284:THR:N	2.50	0.44
8:H:227:ASP:CB	23:X:84:LYS:HE3	2.47	0.44
9:I:166:ASN:OD1	9:I:167:ASN:N	2.50	0.44
10:J:10:PHE:CE2	11:K:27:ALA:HA	2.52	0.44
13:M:53:VAL:HG22	13:M:208:ALA:O	2.18	0.44
14:N:31:VAL:HG21	20:T:212:ALA:HB2	1.99	0.44
14:N:40:ASP:C	14:N:41:ARG:HG2	2.43	0.44
15:O:25:MET:HE2	19:S:188:TYR:OH	2.17	0.44
17:Q:117:TYR:CE2	17:Q:132:HIS:CE1	3.05	0.44
23:X:97:LEU:HD23	23:X:132:ARG:CG	2.47	0.44
25:Z:45:LYS:O	25:Z:45:LYS:CG	2.65	0.44
13:m:220:THR:HG22	13:m:225:GLU:OE2	2.17	0.44
15:o:13:ILE:HG22	15:o:14:VAL:N	2.33	0.44
32:U:253:TYR:CE2	32:U:334:ALA:HB3	2.53	0.44
34:f:316:ASP:OD1	34:f:316:ASP:C	2.60	0.44
6:F:250:LYS:O	6:F:251:LEU:HG	2.18	0.44
7:G:42:VAL:CG2	7:G:198:ALA:HB2	2.48	0.44
10:J:10:PHE:CE1	10:J:16:LEU:HD11	2.52	0.44
11:K:66:LYS:O	11:K:66:LYS:HG2	2.16	0.44
22:W:67:LEU:HD13	22:W:90:LEU:HD22	1.98	0.44
23:X:384:VAL:HG12	23:X:385:LEU:N	2.32	0.44
24:Y:154:ASN:OD1	24:Y:154:ASN:C	2.60	0.44
24:Y:320:ALA:O	24:Y:324:GLY:N	2.51	0.44
26:a:179:PHE:O	26:a:183:VAL:HG12	2.16	0.44
27:b:90:ILE:HG23	27:b:131:LEU:HD11	1.99	0.44
14:n:107:GLN:OE1	14:n:107:GLN:N	2.50	0.44
17:q:85:ARG:HA	17:q:118:MET:HE1	2.00	0.44
34:f:349:TYR:CZ	34:f:763:ARG:CD	3.01	0.44
1:A:120:LYS:HD2	6:F:90:VAL:HG21	1.99	0.44
1:A:177:VAL:HG12	1:A:224:LEU:CD2	2.47	0.44
7:G:80:MET:CE	7:G:138:MET:HA	2.47	0.44
9:I:122:THR:O	9:I:122:THR:OG1	2.36	0.44
15:O:2:THR:N	15:O:130:SER:OG	2.50	0.44
15:O:188:ARG:HB3	15:O:189:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:122:THR:HG21	21:V:150:ARG:HB2	1.99	0.44
21:V:237:THR:CG2	21:V:238:ALA:N	2.80	0.44
22:W:81:ASP:O	22:W:85:GLU:HG2	2.17	0.44
22:W:180:LYS:HD3	22:W:213:PHE:CZ	2.53	0.44
22:W:354:LEU:O	22:W:358:VAL:HG12	2.18	0.44
23:X:100:GLU:OE1	23:X:100:GLU:N	2.51	0.44
24:Y:162:GLU:OE1	24:Y:162:GLU:O	2.35	0.44
25:Z:26:ILE:O	25:Z:29:VAL:HB	2.17	0.44
26:a:158:LEU:HD23	26:a:158:LEU:C	2.43	0.44
27:b:109:ILE:N	27:b:137:ASN:O	2.41	0.44
27:b:189:LEU:C	27:b:189:LEU:HD12	2.42	0.44
28:d:309:VAL:HG22	28:d:317:SER:H	1.83	0.44
10:j:136:PHE:CD1	10:j:136:PHE:N	2.86	0.44
32:U:676:THR:O	32:U:676:THR:HG22	2.17	0.44
33:c:41:MET:CE	33:c:57:MET:CE	2.95	0.44
33:c:134:GLU:OE1	33:c:162:LEU:HD12	2.18	0.44
34:f:141:LYS:C	34:f:141:LYS:HD3	2.43	0.44
34:f:249:LEU:HD22	34:f:272:LEU:HB2	1.99	0.44
2:B:163:LEU:C	2:B:164:MET:HE2	2.42	0.44
2:B:168:ASP:OD1	2:B:172:THR:OG1	2.35	0.44
3:C:186:VAL:HG11	3:C:315:ILE:HD11	1.99	0.44
4:D:60:TYR:OH	32:U:640:LEU:HD13	2.16	0.44
4:D:352:MET:HE2	4:D:379:CYS:SG	2.58	0.44
22:W:44:ILE:HG13	22:W:45:GLU:OE2	2.18	0.44
22:W:448:LYS:HB2	22:W:448:LYS:NZ	2.32	0.44
23:X:84:LYS:HE2	23:X:84:LYS:HA	2.00	0.44
24:Y:381:GLN:OE1	24:Y:381:GLN:HA	2.17	0.44
26:a:37:LEU:HD21	26:a:64:ILE:HD13	1.98	0.44
27:b:22:LEU:HB3	27:b:23:PRO:CD	2.47	0.44
28:d:221:GLN:OE1	28:d:221:GLN:N	2.44	0.44
7:g:174:GLU:OE1	7:g:174:GLU:N	2.43	0.44
19:s:75:TYR:CD2	19:s:83:MET:HE2	2.53	0.44
32:U:227:GLN:OE1	32:U:230:SER:OG	2.34	0.44
1:A:299:MET:CE	1:A:328:ASP:OD2	2.65	0.44
3:C:299:ASP:OD1	3:C:300:ILE:N	2.51	0.44
5:E:284:THR:O	5:E:284:THR:OG1	2.33	0.44
5:E:355:ILE:O	5:E:358:ASP:N	2.49	0.44
17:Q:11:ASP:OD1	17:Q:11:ASP:C	2.61	0.44
21:V:205:LEU:HD23	21:V:245:ASP:OD2	2.18	0.44
21:V:327:THR:O	21:V:330:LYS:HG2	2.17	0.44
22:W:33:LYS:N	22:W:36:LYS:HZ3	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:241:ILE:HD11	24:Y:261:PHE:CD2	2.53	0.44
25:Z:62:ASP:N	25:Z:62:ASP:OD1	2.47	0.44
26:a:70:ARG:HA	26:a:73:PRO:HG3	1.99	0.44
9:i:98:LEU:O	9:i:102:GLN:HA	2.18	0.44
9:i:198:ASN:CA	9:i:206:LEU:HD11	2.48	0.44
6:F:278:LYS:O	6:F:279:ALA:HB3	2.18	0.44
7:G:86:ASP:CB	7:G:134:LEU:HD22	2.47	0.44
13:M:52:LEU:HD22	13:M:206:ASP:OD2	2.17	0.44
21:V:496:PHE:C	21:V:498:PRO:CD	2.90	0.44
22:W:225:LYS:O	22:W:229:LEU:HD23	2.17	0.44
24:Y:45:VAL:O	24:Y:49:ASN:N	2.48	0.44
27:b:11:ASP:O	27:b:29:GLN:NE2	2.49	0.44
27:b:128:ALA:HA	27:b:160:LEU:HD21	2.00	0.44
27:b:154:THR:O	27:b:157:VAL:HG12	2.17	0.44
7:g:16:PHE:HE1	8:h:78:MET:HE3	1.83	0.44
14:n:175:ILE:HD11	14:n:195:ILE:HG23	1.98	0.44
20:t:45:VAL:HG13	20:t:67:LEU:HG	2.00	0.44
32:U:236:LEU:O	32:U:239:GLU:O	2.36	0.44
32:U:349:ASP:O	32:U:352:ILE:HG22	2.17	0.44
32:U:527:GLN:NE2	32:U:531:ASP:OD2	2.51	0.44
32:U:717:ILE:HD12	32:U:731:ILE:HG12	1.99	0.44
2:B:139:VAL:O	2:B:139:VAL:HG23	2.18	0.44
5:E:191:LEU:HD23	5:E:193:CYS:SG	2.57	0.44
6:F:253:GLY:HA3	6:F:290:ALA:HB3	1.99	0.44
7:G:191:PHE:CD1	7:G:193:GLN:HB2	2.53	0.44
21:V:392:TYR:O	21:V:396:ILE:HG12	2.17	0.44
22:W:205:ILE:C	22:W:208:LYS:HG3	2.43	0.44
22:W:226:TYR:O	22:W:230:MET:HG2	2.18	0.44
23:X:212:MET:HE2	23:X:212:MET:HA	2.00	0.44
26:a:45:VAL:HG12	26:a:82:HIS:ND1	2.33	0.44
28:d:88:LEU:HD11	28:d:139:GLN:CG	2.48	0.44
16:p:87:MET:HE1	16:p:131:VAL:HB	2.00	0.44
17:q:44:LEU:HD12	17:q:104:LEU:HD12	2.00	0.44
17:q:66:LEU:HD21	17:q:70:ARG:NH2	2.32	0.44
17:q:153:ARG:O	17:q:157:VAL:HG23	2.18	0.44
33:c:118:PHE:N	33:c:118:PHE:CD1	2.83	0.44
34:f:426:LEU:N	34:f:426:LEU:HD23	2.33	0.44
1:A:299:MET:SD	1:A:299:MET:C	3.00	0.43
2:B:230:THR:HG21	2:B:353:PHE:O	2.18	0.43
4:D:205:TYR:CZ	4:D:332:GLU:OE2	2.70	0.43
4:D:370:ILE:HG13	4:D:407:ILE:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:399:VAL:HG23	6:F:427:VAL:HG21	1.99	0.43
8:H:176:ARG:NH2	23:X:162:ASP:OD1	2.50	0.43
17:Q:121:LEU:O	17:Q:122:ALA:HB3	2.16	0.43
18:R:4:THR:OG1	18:R:129:VAL:O	2.35	0.43
21:V:409:MET:HE3	21:V:409:MET:CA	2.48	0.43
23:X:296:ASN:C	23:X:296:ASN:OD1	2.61	0.43
25:Z:259:VAL:CG1	33:c:291:LEU:HD13	2.48	0.43
15:o:114:ILE:N	15:o:114:ILE:HD12	2.32	0.43
18:r:14:ILE:CD1	18:r:153:ALA:HB1	2.48	0.43
34:f:208:LEU:CD1	34:f:217:LEU:HD12	2.48	0.43
34:f:783:SER:O	34:f:783:SER:OG	2.34	0.43
34:f:905:ASN:OD1	34:f:905:ASN:N	2.50	0.43
1:A:255:ARG:NH1	1:A:255:ARG:HG2	2.33	0.43
2:B:275:GLU:N	2:B:275:GLU:CD	2.75	0.43
2:B:313:LEU:HD23	2:B:313:LEU:C	2.43	0.43
5:E:193:CYS:SG	5:E:229:ILE:HD11	2.58	0.43
5:E:217:GLU:CD	5:E:217:GLU:C	2.87	0.43
5:E:270:LEU:HG	5:E:273:VAL:CG1	2.48	0.43
6:F:134:LEU:HG	6:F:159:LEU:HD23	2.00	0.43
9:I:90:LEU:CG	9:I:114:LEU:HD22	2.48	0.43
16:P:34:VAL:O	16:P:35:THR:HG23	2.17	0.43
16:P:167:SER:OG	16:P:199:LEU:HD13	2.17	0.43
20:T:27:LEU:HD13	20:T:28:GLY:N	2.33	0.43
21:V:65:ARG:HA	21:V:65:ARG:CZ	2.48	0.43
21:V:132:LEU:N	21:V:133:PRO:HD2	2.33	0.43
21:V:438:VAL:O	21:V:442:ILE:HG22	2.18	0.43
22:W:88:MET:HE1	22:W:92:LYS:NZ	2.33	0.43
22:W:322:GLU:OE1	22:W:322:GLU:HA	2.17	0.43
23:X:136:LEU:O	23:X:140:THR:HG23	2.18	0.43
26:a:211:PHE:N	26:a:211:PHE:CD1	2.86	0.43
26:a:217:LEU:HD11	26:a:237:LEU:CB	2.43	0.43
7:g:220:VAL:HG22	7:g:227:PHE:HA	1.99	0.43
19:s:34:SER:OG	19:s:35:ILE:N	2.51	0.43
32:U:481:LEU:HD23	32:U:481:LEU:C	2.42	0.43
34:f:865:PHE:C	34:f:865:PHE:CD1	2.96	0.43
1:A:238:ILE:HG13	1:A:270:CYS:SG	2.57	0.43
1:A:277:ILE:HG22	1:A:321:THR:CG2	2.48	0.43
2:B:164:MET:HE2	2:B:164:MET:HA	2.00	0.43
5:E:338:PHE:CZ	5:E:374:VAL:HG23	2.53	0.43
6:F:188:ILE:HG23	6:F:235:LEU:CD2	2.48	0.43
9:I:167:ASN:HB2	9:I:200:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:78:LYS:HA	22:W:78:LYS:HD3	1.81	0.43
22:W:128:LEU:O	22:W:132:THR:HG23	2.19	0.43
22:W:146:THR:CB	22:W:169:LEU:HD11	2.48	0.43
23:X:289:CYS:SG	23:X:305:ALA:HB2	2.58	0.43
25:Z:244:GLU:OE1	25:Z:244:GLU:N	2.47	0.43
26:a:218:MET:SD	26:a:218:MET:O	2.76	0.43
26:a:278:MET:HE2	26:a:319:LEU:HB3	2.00	0.43
15:o:188:ARG:HB3	15:o:189:PRO:CD	2.48	0.43
31:z:66:VAL:CG2	31:z:71:LEU:HD21	2.48	0.43
34:f:110:TYR:O	34:f:111:GLU:C	2.62	0.43
34:f:805:ASP:O	34:f:808:ASN:OD1	2.36	0.43
3:C:390:VAL:HA	3:C:393:LYS:HG2	2.00	0.43
7:G:163:PHE:CG	7:G:166:THR:OG1	2.71	0.43
8:H:35:VAL:HG12	8:H:36:GLY:N	2.34	0.43
22:W:31:CYS:HA	22:W:43:VAL:HG12	1.99	0.43
22:W:72:LYS:NZ	22:W:73:MET:HE1	2.33	0.43
22:W:365:ILE:HD11	26:a:312:MET:HE2	2.00	0.43
24:Y:178:ASN:O	24:Y:182:VAL:HG23	2.17	0.43
25:Z:67:VAL:HG11	27:b:91:ARG:HB3	2.00	0.43
29:e:59:GLU:C	29:e:59:GLU:CD	2.86	0.43
7:g:143:ILE:HG12	7:g:220:VAL:CG1	2.48	0.43
7:g:214:GLU:O	7:g:215:ILE:HG23	2.17	0.43
8:h:71:ILE:HG23	8:h:136:CYS:O	2.19	0.43
11:k:231:LYS:O	11:k:235:GLU:HG3	2.18	0.43
32:U:114:GLU:O	32:U:118:LEU:HD13	2.19	0.43
32:U:322:THR:O	32:U:326:ILE:HG13	2.18	0.43
32:U:356:THR:HG21	32:U:734:GLN:OE1	2.18	0.43
1:A:382:GLY:HA3	35:A:501:ATP:C8	2.54	0.43
2:B:193:GLN:HG3	2:B:351:ILE:CG2	2.48	0.43
2:B:270:LEU:HD23	2:B:270:LEU:C	2.44	0.43
2:B:379:THR:OG1	2:B:416:ASN:ND2	2.51	0.43
5:E:354:ALA:HB1	5:E:361:PHE:O	2.17	0.43
8:H:114:ALA:O	8:H:117:MET:N	2.50	0.43
14:N:148:MET:HE3	14:N:153:CYS:SG	2.58	0.43
22:W:149:LEU:HD12	22:W:149:LEU:O	2.18	0.43
22:W:453:HIS:CA	22:W:456:GLN:HE21	2.32	0.43
26:a:138:VAL:O	26:a:138:VAL:HG13	2.19	0.43
26:a:141:MET:O	26:a:143:ASN:N	2.51	0.43
28:d:126:LEU:H	28:d:126:LEU:HD12	1.83	0.43
8:h:43:VAL:HG21	8:h:136:CYS:CB	2.45	0.43
15:o:79:THR:O	15:o:83:MET:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:U:405:THR:HG21	32:U:427:LEU:HD21	2.01	0.43
34:f:150:GLU:OE2	34:f:151:LEU:N	2.51	0.43
34:f:659:LEU:HG	34:f:696:LEU:HD21	2.00	0.43
34:f:707:LEU:HD22	34:f:741:LEU:HD13	2.01	0.43
34:f:827:PRO:HB2	34:f:829:MET:HE3	2.00	0.43
1:A:225:CYS:O	1:A:229:VAL:HG23	2.19	0.43
4:D:318:ASP:OD1	4:D:320:ALA:CB	2.66	0.43
6:F:183:GLU:OE1	6:F:238:ARG:CZ	2.67	0.43
8:H:28:VAL:HG11	8:H:132:SER:OG	2.19	0.43
8:H:64:VAL:HG23	8:H:64:VAL:O	2.19	0.43
12:L:19:ILE:HD12	12:L:22:ILE:HD12	2.01	0.43
18:R:140:MET:O	18:R:144:TYR:N	2.50	0.43
18:R:183:ASP:OD1	18:R:183:ASP:O	2.36	0.43
22:W:98:LYS:NZ	22:W:137:TYR:HB3	2.33	0.43
22:W:346:GLU:HG3	22:W:350:ARG:HH12	1.84	0.43
22:W:430:GLN:HA	22:W:430:GLN:OE1	2.18	0.43
26:a:68:GLU:CG	26:a:71:VAL:HG23	2.47	0.43
26:a:295:GLU:C	26:a:295:GLU:OE2	2.62	0.43
28:d:236:LEU:HD23	28:d:237:MET:HE2	2.00	0.43
29:e:48:VAL:O	29:e:48:VAL:CG2	2.66	0.43
9:i:216:LEU:CD1	9:i:225:ILE:HG12	2.49	0.43
18:r:15:VAL:HG11	18:r:103:CYS:SG	2.58	0.43
32:U:151:ILE:CG2	32:U:152:GLY:N	2.81	0.43
32:U:233:LEU:HD23	32:U:268:LEU:HD11	2.01	0.43
2:B:164:MET:HE2	2:B:164:MET:CA	2.49	0.43
2:B:431:GLN:C	2:B:432:GLU:HG3	2.43	0.43
3:C:234:LEU:HD21	3:C:246:ILE:HG21	1.99	0.43
4:D:412:GLN:OE1	8:H:52:LYS:CB	2.66	0.43
6:F:137:ILE:O	6:F:160:ILE:HG12	2.19	0.43
8:H:161:ALA:O	8:H:166:TYR:HB2	2.18	0.43
9:I:44:LEU:HD22	9:I:190:LEU:HD22	2.01	0.43
10:J:35:VAL:HG22	10:J:42:VAL:CG1	2.48	0.43
10:J:104:VAL:HG11	10:J:143:ARG:CB	2.49	0.43
15:O:4:ILE:HD12	15:O:45:CYS:CB	2.45	0.43
15:O:203:TYR:OH	19:S:174:LEU:HD12	2.18	0.43
18:R:5:LEU:HD11	18:R:140:MET:HG3	1.99	0.43
21:V:443:ARG:HA	28:d:277:LYS:HD2	2.01	0.43
22:W:27:ARG:NE	22:W:30:GLU:OE1	2.50	0.43
22:W:152:ILE:HD13	22:W:152:ILE:N	2.32	0.43
22:W:194:LEU:HD12	22:W:229:LEU:CD1	2.46	0.43
22:W:348:GLU:OE1	22:W:348:GLU:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:446:ILE:HD13	25:Z:211:TYR:CB	2.49	0.43
26:a:18:GLN:N	26:a:19:PRO:CD	2.82	0.43
26:a:122:LYS:HE2	26:a:130:VAL:HG21	2.01	0.43
27:b:120:ASN:C	27:b:120:ASN:OD1	2.61	0.43
9:i:83:ALA:O	9:i:87:THR:HG23	2.19	0.43
10:j:44:GLY:CA	10:j:208:LEU:HD23	2.49	0.43
13:m:87:LEU:HD13	13:m:135:PHE:CE2	2.53	0.43
18:r:14:ILE:HD12	18:r:153:ALA:HB1	2.00	0.43
32:U:52:GLU:OE1	32:U:52:GLU:N	2.51	0.43
32:U:234:GLU:OE1	32:U:271:VAL:HG11	2.18	0.43
32:U:262:SER:HA	32:U:265:ILE:HG22	1.99	0.43
34:f:334:ALA:C	34:f:340:MET:SD	3.01	0.43
34:f:515:ALA:O	34:f:518:THR:OG1	2.33	0.43
1:A:303:ILE:HG22	1:A:336:ARG:HH21	1.84	0.43
1:A:303:ILE:HG22	1:A:336:ARG:NH2	2.34	0.43
2:B:371:ARG:C	2:B:372:MET:HG2	2.44	0.43
2:B:401:GLU:O	2:B:405:MET:HG2	2.19	0.43
3:C:160:GLU:CD	3:C:160:GLU:C	2.87	0.43
3:C:188:LEU:HD22	3:C:317:PHE:CZ	2.53	0.43
14:N:64:LEU:HD11	14:N:75:PRO:HB2	2.01	0.43
16:P:187:HIS:CE1	16:P:196:THR:HG1	2.36	0.43
21:V:453:HIS:HB3	28:d:283:LEU:HB3	2.00	0.43
24:Y:354:VAL:O	24:Y:355:GLU:C	2.61	0.43
26:a:129:GLN:CD	26:a:130:VAL:HG12	2.43	0.43
9:i:174:MET:HE1	9:i:199:LYS:HB2	2.00	0.43
17:q:13:VAL:HG11	17:q:105:ALA:CB	2.47	0.43
33:c:120:CYS:SG	33:c:156:VAL:HG12	2.59	0.43
2:B:220:LYS:HB2	2:B:348:ASP:OD1	2.19	0.43
4:D:98:GLN:O	4:D:99:ASN:HB2	2.18	0.43
5:E:300:HIS:CE1	5:E:302:ASP:OD1	2.72	0.43
19:S:114:ASP:N	19:S:114:ASP:OD1	2.49	0.43
21:V:275:VAL:O	21:V:275:VAL:HG13	2.19	0.43
22:W:44:ILE:HG13	22:W:45:GLU:N	2.34	0.43
22:W:50:LEU:O	22:W:54:THR:OG1	2.27	0.43
22:W:431:LYS:HG3	25:Z:236:LEU:HD22	2.00	0.43
22:W:436:MET:HE3	33:c:309:PHE:CZ	2.50	0.43
23:X:77:LEU:HD13	23:X:116:TRP:HE1	1.83	0.43
23:X:80:ILE:HG22	23:X:81:SER:N	2.33	0.43
26:a:116:THR:OG1	26:a:158:LEU:HD12	2.19	0.43
9:i:174:MET:HE1	9:i:199:LYS:CB	2.48	0.43
32:U:698:GLN:OE1	32:U:702:THR:HG21	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:367:ILE:HD13	2:B:367:ILE:HA	1.96	0.43
6:F:224:LEU:HB2	6:F:348:LEU:HD13	1.99	0.43
9:I:192:LEU:O	9:I:196:VAL:HG23	2.18	0.43
16:P:24:ASP:OD1	16:P:40:LYS:NZ	2.47	0.43
17:Q:18:ASP:C	17:Q:18:ASP:OD1	2.62	0.43
22:W:103:LYS:HA	22:W:106:GLN:HG2	2.01	0.43
22:W:204:ILE:HD13	22:W:204:ILE:N	2.33	0.43
22:W:422:ASN:OD1	33:c:234:TYR:HB3	2.19	0.43
22:W:431:LYS:HZ3	22:W:431:LYS:HB2	1.83	0.43
26:a:71:VAL:O	26:a:72:ASN:C	2.62	0.43
27:b:78:VAL:O	27:b:79:GLN:C	2.61	0.43
28:d:241:TYR:HE2	28:d:271:ILE:HG22	1.78	0.43
19:s:127:VAL:HG22	19:s:127:VAL:O	2.18	0.43
31:z:52:THR:HG23	31:z:55:GLY:H	1.83	0.43
32:U:793:LYS:NZ	32:U:914:LEU:O	2.44	0.43
32:U:891:VAL:O	32:U:891:VAL:HG12	2.19	0.43
34:f:124:ASP:OD2	34:f:147:SER:HB2	2.19	0.43
34:f:374:SER:HA	34:f:377:VAL:HG12	2.01	0.43
2:B:182:GLU:HB3	2:B:186:ASP:HB2	2.01	0.42
4:D:119:ILE:HD11	4:D:140:VAL:O	2.19	0.42
5:E:215:ILE:HD12	5:E:256:THR:HG23	2.01	0.42
5:E:270:LEU:HG	5:E:273:VAL:HG13	2.01	0.42
10:J:35:VAL:HG13	10:J:191:VAL:HG22	1.99	0.42
10:J:155:ALA:HB3	11:K:63:SER:CB	2.49	0.42
11:K:142:LEU:HD22	11:K:153:LEU:HD11	2.01	0.42
15:O:136:MET:HE3	20:T:179:ARG:CZ	2.49	0.42
21:V:495:ARG:O	21:V:497:PRO:HD3	2.19	0.42
22:W:160:LYS:HD3	22:W:160:LYS:H	1.84	0.42
22:W:177:MET:HE2	22:W:181:GLU:HB3	2.00	0.42
22:W:275:ILE:HG23	22:W:309:PHE:CE2	2.54	0.42
22:W:393:LEU:HD12	22:W:393:LEU:O	2.18	0.42
23:X:264:PRO:O	23:X:267:VAL:HG12	2.19	0.42
23:X:384:VAL:HG12	23:X:385:LEU:H	1.84	0.42
25:Z:149:THR:HG22	26:a:178:ARG:HA	1.99	0.42
26:a:81:LEU:HD13	26:a:117:ALA:HB2	2.01	0.42
14:n:91:TYR:O	14:n:95:LEU:HB2	2.18	0.42
16:p:34:VAL:HG12	16:p:35:THR:HG23	2.00	0.42
18:r:84:LEU:O	18:r:88:VAL:HG12	2.18	0.42
31:z:56:LEU:HD23	31:z:56:LEU:HA	1.89	0.42
1:A:284:ARG:NH1	1:A:296:GLN:HG2	2.35	0.42
2:B:119:ASN:OD1	2:B:119:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:LEU:HB2	2:B:346:ARG:HD2	2.00	0.42
3:C:192:PRO:CA	3:C:296:ASN:OD1	2.67	0.42
6:F:289:ASP:HA	6:F:338:LEU:HD21	2.01	0.42
9:I:105:ILE:HG23	9:I:105:ILE:O	2.18	0.42
10:J:103:THR:HG23	10:J:106:TYR:H	1.84	0.42
12:L:49:LEU:HD11	12:L:199:LEU:CD2	2.49	0.42
13:M:39:ILE:HD13	13:M:179:LEU:CD2	2.49	0.42
17:Q:4:LEU:HD22	17:Q:45:LEU:HD23	2.01	0.42
18:R:38:ILE:HD13	18:R:60:LEU:HD23	2.00	0.42
21:V:264:TYR:CD2	21:V:298:ILE:HG21	2.54	0.42
22:W:362:ASN:HA	22:W:365:ILE:CG2	2.49	0.42
23:X:297:ARG:O	23:X:337:ARG:NH1	2.52	0.42
25:Z:64:ASP:OD1	25:Z:64:ASP:C	2.61	0.42
25:Z:101:LEU:CD1	25:Z:105:ASP:OD2	2.67	0.42
26:a:188:LEU:HB2	26:a:189:PRO:HD2	2.01	0.42
10:j:43:LEU:HD21	10:j:72:ALA:HB2	2.00	0.42
11:k:33:LEU:O	11:k:53:ARG:NH2	2.46	0.42
18:r:71:ASN:OD1	18:r:71:ASN:N	2.51	0.42
32:U:471:ASP:CG	32:U:507:VAL:HG12	2.44	0.42
32:U:560:MET:O	32:U:590:TYR:CZ	2.72	0.42
34:f:450:ILE:HD13	34:f:450:ILE:N	2.34	0.42
1:A:177:VAL:O	1:A:177:VAL:HG23	2.19	0.42
1:A:369:ARG:O	1:A:372:LEU:N	2.53	0.42
2:B:51:LEU:H	2:B:51:LEU:HD22	1.84	0.42
2:B:234:LEU:HD12	2:B:234:LEU:C	2.43	0.42
3:C:187:LEU:CD1	3:C:306:LEU:HD21	2.48	0.42
4:D:45:LYS:C	32:U:187:LEU:HD11	2.43	0.42
9:I:116:ASP:OD1	10:J:82:ILE:HD11	2.19	0.42
10:J:141:THR:CB	10:J:143:ARG:HH12	2.32	0.42
10:J:158:ALA:HB1	10:J:172:LEU:HD13	2.01	0.42
13:M:70:ASP:OD1	13:M:71:ARG:N	2.44	0.42
20:T:79:ASP:OD1	20:T:79:ASP:N	2.51	0.42
22:W:223:LYS:HG2	22:W:227:TYR:CE2	2.54	0.42
22:W:396:LEU:HD22	22:W:401:THR:CG2	2.50	0.42
24:Y:112:CYS:SG	24:Y:113:ARG:N	2.93	0.42
25:Z:149:THR:HB	25:Z:150:PRO:HD3	2.00	0.42
25:Z:215:VAL:HG13	25:Z:222:ILE:CD1	2.48	0.42
26:a:72:ASN:C	26:a:74:LEU:N	2.75	0.42
26:a:89:ASP:HB2	26:a:92:VAL:HG12	2.00	0.42
26:a:123:LEU:HD12	26:a:131:THR:HG22	2.00	0.42
7:g:87:SER:O	7:g:91:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:195:VAL:HG21	7:g:238:HIS:NE2	2.34	0.42
19:s:14:ALA:HA	19:s:22:ILE:O	2.19	0.42
19:s:75:TYR:CG	19:s:83:MET:HE2	2.53	0.42
32:U:233:LEU:HD21	32:U:268:LEU:HD21	2.01	0.42
32:U:360:VAL:HG23	32:U:365:CYS:HB3	2.01	0.42
32:U:672:LEU:HD21	32:U:690:ALA:HB3	2.00	0.42
32:U:720:LYS:HD3	32:U:720:LYS:C	2.44	0.42
34:f:413:SER:N	34:f:819:TYR:OH	2.52	0.42
2:B:380:LEU:HG	2:B:381:ASP:OD1	2.20	0.42
4:D:395:LEU:HD22	4:D:395:LEU:N	2.34	0.42
8:H:67:ILE:HD11	8:H:73:LEU:CD2	2.46	0.42
11:K:50:VAL:HG22	11:K:51:GLU:H	1.84	0.42
12:L:70:ILE:HD13	12:L:108:LEU:HD23	2.01	0.42
13:M:83:ASP:N	13:M:83:ASP:OD1	2.52	0.42
17:Q:5:ILE:HG21	17:Q:160:LEU:CD1	2.49	0.42
20:T:10:SER:HB3	20:T:139:THR:O	2.20	0.42
20:T:67:LEU:HA	20:T:70:MET:HG2	2.01	0.42
21:V:300:LEU:O	21:V:301:GLU:OE2	2.37	0.42
22:W:396:LEU:HD22	22:W:401:THR:HB	2.01	0.42
23:X:218:HIS:O	23:X:218:HIS:CG	2.72	0.42
24:Y:48:ASN:HB3	24:Y:50:MET:SD	2.59	0.42
28:d:197:LEU:HD21	28:d:260:ILE:HD13	2.01	0.42
28:d:282:ILE:CG2	28:d:283:LEU:N	2.80	0.42
9:i:11:ILE:HG22	10:j:7:ILE:CG2	2.49	0.42
15:o:123:LEU:HD22	15:o:124:PRO:HD2	2.00	0.42
33:c:25:VAL:HG11	33:c:201:TYR:OH	2.19	0.42
34:f:422:VAL:HG21	34:f:457:ASN:OD1	2.18	0.42
34:f:571:GLU:N	34:f:600:TYR:OH	2.52	0.42
34:f:608:LYS:HA	34:f:608:LYS:HE3	1.99	0.42
34:f:866:GLN:OE1	34:f:866:GLN:N	2.52	0.42
34:f:870:THR:O	34:f:872:VAL:N	2.49	0.42
1:A:364:VAL:HG22	1:A:368:ILE:HD11	2.01	0.42
9:I:107:CYS:O	9:I:110:LEU:N	2.52	0.42
12:L:116:THR:O	12:L:116:THR:HG22	2.19	0.42
14:N:67:HIS:O	14:N:71:LEU:HD23	2.19	0.42
17:Q:101:ASN:HB3	17:Q:132:HIS:CE1	2.54	0.42
18:R:181:ARG:NH2	18:R:186:ILE:HG21	2.34	0.42
22:W:30:GLU:OE2	22:W:34:LEU:HD11	2.18	0.42
22:W:65:ARG:HA	22:W:68:VAL:CG1	2.49	0.42
22:W:339:ASP:OD1	22:W:339:ASP:N	2.51	0.42
22:W:355:LYS:O	22:W:358:VAL:CG1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:370:ILE:HD13	24:Y:370:ILE:HA	1.96	0.42
25:Z:149:THR:CB	25:Z:150:PRO:CD	2.97	0.42
26:a:76:LEU:O	26:a:79:ILE:HG12	2.20	0.42
28:d:128:PHE:CG	28:d:129:LEU:HD12	2.55	0.42
7:g:41:ALA:HB2	7:g:50:ILE:HG22	2.01	0.42
7:g:50:ILE:HG23	7:g:141:ILE:HG21	2.01	0.42
8:h:104:ILE:HG23	8:h:104:ILE:O	2.19	0.42
12:l:22:ILE:O	12:l:26:MET:HG2	2.19	0.42
13:m:115:VAL:O	13:m:119:VAL:HG23	2.20	0.42
18:r:78:ALA:HB2	18:r:113:TYR:OH	2.19	0.42
32:U:746:ILE:HD11	32:U:779:LEU:HD21	2.02	0.42
33:c:266:THR:HG23	33:c:267:PRO:HD2	2.02	0.42
34:f:102:HIS:O	34:f:102:HIS:CG	2.73	0.42
34:f:659:LEU:HD21	34:f:797:LEU:HD21	2.01	0.42
34:f:805:ASP:O	34:f:806:VAL:C	2.62	0.42
2:B:203:LEU:N	2:B:204:PRO:HD2	2.34	0.42
2:B:278:ALA:CB	2:B:279:PRO:CD	2.93	0.42
4:D:384:MET:CE	5:E:167:PRO:CD	2.97	0.42
6:F:341:ALA:O	6:F:347:ARG:HD2	2.19	0.42
6:F:415:LEU:HD22	6:F:415:LEU:N	2.34	0.42
8:H:47:THR:HG21	8:H:74:VAL:CG2	2.49	0.42
12:L:49:LEU:HD23	12:L:49:LEU:C	2.44	0.42
17:Q:105:ALA:HA	17:Q:114:ALA:O	2.19	0.42
22:W:340:VAL:HG12	22:W:341:PHE:CD1	2.55	0.42
26:a:44:PHE:O	26:a:45:VAL:C	2.62	0.42
27:b:8:VAL:HB	27:b:50:GLY:O	2.20	0.42
27:b:121:GLU:O	27:b:125:VAL:HG23	2.20	0.42
27:b:178:SER:O	27:b:179:LEU:C	2.61	0.42
28:d:261:ASP:O	28:d:265:ASP:OD2	2.38	0.42
9:i:72:MET:HE2	9:i:72:MET:HB3	1.98	0.42
11:k:167:ALA:HB3	12:l:56:LEU:HD13	2.01	0.42
12:l:43:HIS:CD2	12:l:184:LEU:HD13	2.55	0.42
13:m:39:ILE:HD11	13:m:181:MET:CB	2.49	0.42
18:r:15:VAL:O	18:r:15:VAL:HG23	2.20	0.42
19:s:186:ASP:OD1	19:s:188:TYR:N	2.52	0.42
32:U:139:GLN:CD	32:U:143:ASP:OD2	2.63	0.42
32:U:188:MET:SD	32:U:188:MET:C	3.02	0.42
32:U:536:ALA:CB	32:U:578:LEU:HD21	2.50	0.42
34:f:685:THR:HG23	34:f:686:LEU:N	2.35	0.42
34:f:731:MET:HE1	34:f:796:LEU:CD2	2.50	0.42
1:A:406:GLU:O	1:A:410:LEU:HD22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:115:ILE:HD11	2:B:144:LEU:HB3	2.01	0.42
4:D:293:LEU:HD13	4:D:320:ALA:HB1	2.02	0.42
4:D:374:ASP:O	4:D:377:SER:N	2.51	0.42
5:E:313:LEU:HD11	5:E:331:ILE:CG2	2.50	0.42
6:F:265:ALA:HB1	6:F:312:GLU:HG3	2.01	0.42
12:L:229:VAL:HG12	12:L:233:LEU:HD12	2.02	0.42
13:M:110:HIS:NE2	14:N:70:GLU:OE2	2.52	0.42
22:W:54:THR:HG22	22:W:59:ASP:CB	2.41	0.42
22:W:112:VAL:HG11	22:W:125:ILE:CG1	2.48	0.42
25:Z:149:THR:CB	25:Z:150:PRO:HD3	2.49	0.42
26:a:205:LEU:C	26:a:206:LEU:HD22	2.44	0.42
26:a:217:LEU:HD21	26:a:237:LEU:HD22	2.02	0.42
29:e:51:ASP:O	29:e:52:PHE:C	2.61	0.42
7:g:29:PHE:CZ	7:g:155:ASP:HB2	2.55	0.42
19:s:212:LYS:HD3	19:s:212:LYS:N	2.34	0.42
32:U:229:VAL:HG21	32:U:252:LEU:HD11	2.02	0.42
34:f:94:LYS:N	34:f:95:PRO:HD2	2.35	0.42
1:A:365:GLU:OE1	1:A:405:THR:HB	2.19	0.42
2:B:260:LEU:HD23	2:B:261:GLY:N	2.34	0.42
4:D:393:ILE:HG22	4:D:394:VAL:N	2.34	0.42
5:E:197:LYS:HG3	6:F:320:PHE:CD2	2.54	0.42
6:F:430:LYS:NZ	11:K:18:GLU:HA	2.35	0.42
9:I:121:TYR:HE2	9:I:128:ARG:O	2.03	0.42
9:I:215:THR:HG23	9:I:228:LEU:HD11	2.02	0.42
15:O:175:ASP:OD1	15:O:188:ARG:HA	2.19	0.42
21:V:206:VAL:O	21:V:210:CYS:SG	2.75	0.42
21:V:258:TYR:CE2	21:V:266:GLN:HB3	2.55	0.42
21:V:496:PHE:C	21:V:498:PRO:HD2	2.45	0.42
22:W:178:GLU:HB3	22:W:181:GLU:OE2	2.20	0.42
22:W:210:ASN:OD1	22:W:212:LYS:HB3	2.19	0.42
22:W:304:ASP:HB3	22:W:324:TYR:OH	2.20	0.42
24:Y:144:LEU:HB3	24:Y:160:ASN:OD1	2.20	0.42
26:a:8:LEU:HD21	26:a:60:TYR:HE2	1.83	0.42
26:a:97:LEU:HD12	26:a:121:LEU:CD1	2.49	0.42
26:a:218:MET:O	26:a:219:HIS:C	2.63	0.42
28:d:332:SER:OG	33:c:307:VAL:HG21	2.20	0.42
29:e:42:ASN:HD21	29:e:44:ASP:HB2	1.83	0.42
8:h:106:THR:O	8:h:110:VAL:HG23	2.20	0.42
11:k:77:ALA:HB3	11:k:142:LEU:HB2	2.01	0.42
20:t:12:LEU:C	20:t:12:LEU:HD12	2.45	0.42
32:U:374:SER:HB2	32:U:407:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:c:73:PHE:CD1	33:c:73:PHE:O	2.72	0.42
34:f:772:GLY:CA	34:f:776:LEU:HD12	2.50	0.42
6:F:198:LEU:HD23	6:F:198:LEU:C	2.45	0.42
6:F:431:LYS:NZ	6:F:432:LYS:O	2.52	0.42
7:G:33:ASN:N	7:G:33:ASN:OD1	2.51	0.42
10:J:55:ASP:C	10:J:55:ASP:OD1	2.63	0.42
11:K:164:GLN:CD	11:K:164:GLN:C	2.88	0.42
11:K:202:LEU:O	11:K:206:MET:HG3	2.20	0.42
14:N:23:THR:O	14:N:23:THR:OG1	2.31	0.42
17:Q:9:GLY:HA3	17:Q:12:TYR:CZ	2.55	0.42
21:V:409:MET:HE3	21:V:409:MET:C	2.45	0.42
22:W:297:GLU:C	22:W:297:GLU:CD	2.88	0.42
23:X:141:LYS:HD2	23:X:143:TYR:CZ	2.55	0.42
25:Z:10:VAL:O	25:Z:10:VAL:HG23	2.19	0.42
26:a:148:VAL:HG23	26:a:148:VAL:O	2.19	0.42
26:a:179:PHE:HA	26:a:182:CYS:SG	2.60	0.42
28:d:248:LYS:HD2	28:d:248:LYS:O	2.20	0.42
11:k:121:LEU:HD12	12:l:79:ALA:CB	2.49	0.42
15:o:178:VAL:O	15:o:178:VAL:HG23	2.20	0.42
32:U:889:LEU:HD11	32:U:909:GLY:CA	2.49	0.42
1:A:366:ARG:NE	1:A:366:ARG:CA	2.83	0.42
2:B:53:THR:O	2:B:54:PRO:C	2.62	0.42
4:D:58:GLU:O	4:D:62:LYS:HG3	2.20	0.42
4:D:353:ASN:O	4:D:354:LEU:C	2.62	0.42
7:G:123:GLN:HA	7:G:126:THR:HG22	2.01	0.42
13:M:211:LEU:HD23	13:M:213:LEU:HD11	2.01	0.42
17:Q:172:ILE:HG12	17:q:173:LEU:HD12	2.01	0.42
21:V:259:LEU:O	21:V:260:HIS:C	2.63	0.42
21:V:391:THR:O	21:V:394:LEU:N	2.50	0.42
22:W:59:ASP:O	22:W:63:THR:OG1	2.25	0.42
22:W:299:ILE:H	22:W:299:ILE:HD12	1.85	0.42
24:Y:246:ILE:O	24:Y:250:LEU:HD12	2.20	0.42
26:a:31:LYS:HG3	26:a:33:LEU:HD21	2.01	0.42
26:a:288:HIS:O	26:a:289:ARG:C	2.63	0.42
28:d:147:ILE:O	28:d:150:ILE:HG13	2.20	0.42
14:n:53:THR:HG22	14:n:97:ALA:HB1	2.02	0.42
32:U:9:ILE:HD13	32:U:27:LEU:HD21	2.02	0.42
32:U:332:GLU:C	32:U:332:GLU:CD	2.88	0.42
2:B:53:THR:C	2:B:55:HIS:N	2.78	0.41
3:C:237:MET:HE3	3:C:237:MET:HB3	1.93	0.41
9:I:28:ILE:C	9:I:30:HIS:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:51:ASN:HB3	9:I:56:LEU:HD13	2.02	0.41
9:I:192:LEU:HD12	9:I:196:VAL:HG23	2.02	0.41
10:J:40:ILE:CD1	10:J:210:VAL:HG13	2.40	0.41
13:M:229:LYS:HD2	13:M:229:LYS:O	2.19	0.41
16:P:26:ARG:HB2	16:P:181:GLY:O	2.20	0.41
21:V:336:GLU:O	21:V:339:LEU:N	2.45	0.41
22:W:297:GLU:C	22:W:297:GLU:OE2	2.63	0.41
22:W:424:LEU:HD12	22:W:424:LEU:HA	1.82	0.41
25:Z:131:LEU:HG	25:Z:196:HIS:ND1	2.35	0.41
27:b:25:ARG:O	27:b:28:ALA:N	2.53	0.41
19:s:15:ILE:HG22	19:s:135:PHE:HB2	2.02	0.41
9:I:217:THR:OG1	9:I:224:VAL:HG12	2.20	0.41
15:O:25:MET:HE3	19:S:187:VAL:CG2	2.44	0.41
15:O:31:ASN:OD1	15:O:188:ARG:NH1	2.50	0.41
15:O:31:ASN:O	15:O:31:ASN:CG	2.63	0.41
15:O:152:ALA:O	15:O:156:VAL:HG23	2.20	0.41
16:P:116:PHE:N	16:P:116:PHE:CD1	2.88	0.41
21:V:108:LEU:HD22	21:V:113:LEU:HD11	2.02	0.41
22:W:41:GLN:HA	22:W:44:ILE:HG12	2.02	0.41
22:W:231:ILE:HD13	22:W:247:TYR:CD2	2.54	0.41
22:W:321:VAL:O	22:W:325:GLY:HA3	2.20	0.41
23:X:122:ARG:O	23:X:124:PHE:N	2.52	0.41
23:X:264:PRO:HB2	23:X:295:LYS:HB2	2.01	0.41
24:Y:201:PHE:CB	24:Y:223:THR:HG23	2.49	0.41
24:Y:315:THR:HG22	24:Y:317:GLY:H	1.85	0.41
25:Z:189:GLN:O	25:Z:193:ASN:ND2	2.52	0.41
26:a:18:GLN:O	26:a:21:VAL:HG22	2.19	0.41
26:a:136:GLU:HG3	26:a:137:ASP:N	2.35	0.41
27:b:97:LEU:HD12	27:b:98:LYS:N	2.35	0.41
8:h:73:LEU:HD11	8:h:135:ILE:HG12	2.01	0.41
12:l:172:LEU:HD23	12:l:179:PHE:CE2	2.56	0.41
16:p:70:LEU:HD12	16:p:81:ILE:HD13	2.01	0.41
32:U:34:PHE:CD1	32:U:34:PHE:N	2.89	0.41
32:U:86:ASP:O	32:U:88:PHE:N	2.52	0.41
32:U:220:LEU:O	32:U:224:ASP:N	2.53	0.41
32:U:676:THR:O	32:U:676:THR:CG2	2.68	0.41
34:f:131:MET:SD	34:f:161:HIS:CG	3.13	0.41
34:f:213:GLN:OE1	34:f:213:GLN:HA	2.19	0.41
34:f:527:VAL:O	34:f:529:SER:N	2.53	0.41
34:f:781:TYR:CZ	34:f:788:MET:HG2	2.55	0.41
1:A:161:VAL:O	1:A:161:VAL:CG1	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:PRO:O	1:A:379:ASN:C	2.63	0.41
2:B:390:LEU:HD21	2:B:398:ILE:HD12	2.02	0.41
5:E:50:LEU:HD23	5:E:50:LEU:HA	1.96	0.41
5:E:373:LYS:O	5:E:376:ASP:N	2.53	0.41
6:F:362:ARG:NH1	6:F:389:ASP:HA	2.35	0.41
7:G:180:GLU:HA	8:H:55:LEU:HD21	2.03	0.41
8:H:37:ILE:HG22	8:H:38:LYS:N	2.35	0.41
8:H:94:GLN:HG3	15:O:66:LEU:HD13	2.02	0.41
11:K:167:ALA:HB3	12:L:56:LEU:HD13	2.01	0.41
13:M:19:ARG:NE	13:M:24:GLU:OE2	2.54	0.41
16:P:58:ASP:OD2	16:P:102:TYR:CA	2.68	0.41
21:V:437:ILE:HD12	28:d:239:GLY:HA3	2.02	0.41
22:W:21:SER:O	22:W:24:VAL:HG22	2.21	0.41
22:W:68:VAL:HG23	22:W:107:GLN:HG3	2.02	0.41
22:W:146:THR:HB	22:W:169:LEU:CD1	2.50	0.41
22:W:196:VAL:O	22:W:197:LYS:HB2	2.21	0.41
26:a:80:ILE:O	26:a:83:VAL:HG12	2.20	0.41
26:a:245:VAL:HG22	26:a:272:ILE:HG23	2.01	0.41
27:b:108:ARG:NH2	27:b:139:ASP:OD2	2.53	0.41
18:r:41:TYR:CE2	18:r:105:TRP:O	2.73	0.41
19:s:124:PHE:CD2	19:s:130:TYR:HB3	2.55	0.41
31:z:100:PRO:HG3	33:c:136:LEU:HD12	2.01	0.41
32:U:35:TRP:CD1	32:U:35:TRP:C	2.99	0.41
32:U:788:VAL:CG2	32:U:884:VAL:HG21	2.51	0.41
34:f:861:THR:O	34:f:862:ILE:HG23	2.19	0.41
1:A:234:ASP:OD1	1:A:234:ASP:O	2.38	0.41
1:A:295:VAL:HA	1:A:298:THR:HG22	2.03	0.41
2:B:53:THR:CB	2:B:54:PRO:HD2	2.50	0.41
2:B:109:VAL:O	2:B:109:VAL:HG12	2.20	0.41
10:J:71:MET:HE3	10:J:131:ALA:HB2	2.02	0.41
14:N:31:VAL:O	14:N:31:VAL:HG13	2.19	0.41
14:N:84:PHE:CE2	14:N:101:ILE:HD11	2.54	0.41
22:W:317:TRP:CE2	22:W:355:LYS:CE	3.03	0.41
22:W:451:MET:O	22:W:455:LEU:HD13	2.20	0.41
26:a:44:PHE:O	26:a:47:ASP:N	2.49	0.41
26:a:83:VAL:CG1	26:a:84:VAL:N	2.82	0.41
28:d:232:LEU:HD23	28:d:232:LEU:C	2.45	0.41
7:g:171:LYS:HG2	7:g:205:VAL:HB	2.02	0.41
9:i:224:VAL:O	9:i:224:VAL:HG23	2.20	0.41
11:k:52:LYS:HE3	11:k:216:GLU:HG2	2.01	0.41
11:k:226:PHE:CD1	11:k:226:PHE:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:50:LYS:HE3	12:l:211:SER:HB2	2.02	0.41
16:p:137:VAL:HG22	16:p:146:TYR:CZ	2.55	0.41
32:U:21:GLU:N	32:U:21:GLU:CD	2.78	0.41
32:U:98:GLU:O	32:U:101:ILE:HG22	2.21	0.41
33:c:131:GLN:C	33:c:131:GLN:CD	2.89	0.41
34:f:418:LEU:O	34:f:419:LEU:C	2.63	0.41
34:f:707:LEU:CD2	34:f:741:LEU:HD13	2.50	0.41
6:F:113:LEU:HD13	6:F:135:PRO:HG3	2.03	0.41
17:Q:119:ASP:OD1	17:Q:121:LEU:N	2.40	0.41
21:V:169:LEU:O	21:V:173:ILE:HG13	2.20	0.41
21:V:240:LEU:HD11	32:U:69:TYR:OH	2.20	0.41
21:V:451:ILE:O	28:d:280:GLU:N	2.53	0.41
23:X:138:PHE:C	23:X:138:PHE:CD1	2.98	0.41
24:Y:201:PHE:HE2	24:Y:222:TYR:HB3	1.85	0.41
25:Z:22:HIS:CE1	25:Z:35:VAL:CG1	3.03	0.41
26:a:9:GLN:OE1	26:a:9:GLN:HA	2.21	0.41
26:a:240:PHE:CZ	26:a:268:LEU:HD13	2.56	0.41
27:b:115:SER:O	27:b:151:GLU:OE1	2.37	0.41
28:d:236:LEU:HD23	28:d:236:LEU:C	2.46	0.41
9:i:216:LEU:HD12	9:i:225:ILE:HG13	2.03	0.41
13:m:17:ASP:OD1	13:m:17:ASP:N	2.44	0.41
14:n:27:ILE:HD12	20:t:178:TYR:O	2.20	0.41
16:p:57:THR:HG23	16:p:58:ASP:N	2.35	0.41
19:s:189:THR:OG1	19:s:190:GLY:N	2.53	0.41
31:z:31:MET:HE1	31:z:90:VAL:O	2.20	0.41
34:f:48:GLU:O	34:f:52:LEU:HD23	2.21	0.41
34:f:115:PRO:HA	34:f:119:LYS:HB2	2.02	0.41
2:B:234:LEU:HD22	35:B:501:ATP:H2'	2.03	0.41
3:C:273:MET:HE1	3:C:302:ASP:CB	2.51	0.41
6:F:257:VAL:O	6:F:257:VAL:CG2	2.68	0.41
8:H:71:ILE:HD13	8:H:109:LEU:HD23	2.01	0.41
9:I:170:ALA:HB3	9:I:199:LYS:HZ1	1.85	0.41
11:K:76:CYS:HA	11:K:142:LEU:O	2.21	0.41
11:K:197:SER:O	11:K:200:ILE:HG22	2.20	0.41
12:L:157:ARG:HG2	13:M:57:LEU:O	2.20	0.41
18:R:3:THR:HG22	18:R:18:ASP:OD2	2.20	0.41
21:V:382:PHE:CD1	21:V:382:PHE:N	2.88	0.41
22:W:283:GLN:CD	22:W:283:GLN:C	2.88	0.41
22:W:305:LEU:HD12	22:W:305:LEU:HA	1.83	0.41
23:X:267:VAL:HG11	23:X:291:ALA:HB3	2.02	0.41
25:Z:6:VAL:O	25:Z:6:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:77:VAL:HG11	26:a:113:LEU:HB3	2.02	0.41
14:n:2:THR:N	14:n:170:SER:O	2.53	0.41
14:n:13:VAL:HG21	14:n:102:ALA:HB1	2.02	0.41
19:s:51:VAL:HG23	19:s:198:VAL:HG21	2.02	0.41
32:U:2:ILE:HG22	32:U:3:THR:HG23	2.02	0.41
32:U:35:TRP:HA	32:U:38:ILE:CG2	2.50	0.41
32:U:164:GLU:CD	32:U:204:ILE:HD11	2.46	0.41
32:U:678:ASP:OD1	32:U:679:PRO:CD	2.68	0.41
34:f:616:CYS:HA	34:f:650:GLN:HE21	1.86	0.41
1:A:81:ALA:HB2	2:B:137:SER:C	2.46	0.41
2:B:49:LEU:HD11	34:f:669:GLU:CD	2.46	0.41
2:B:70:ASP:OD1	2:B:70:ASP:C	2.63	0.41
3:C:27:LYS:HD3	4:D:44:TYR:CE1	2.56	0.41
3:C:196:LYS:NZ	3:C:295:THR:O	2.53	0.41
3:C:241:HIS:CD2	3:C:241:HIS:N	2.89	0.41
6:F:358:ASN:O	6:F:359:GLU:C	2.64	0.41
17:Q:6:GLY:HA3	17:Q:115:LEU:HD21	2.02	0.41
18:R:175:VAL:O	18:R:175:VAL:HG13	2.21	0.41
22:W:51:GLU:OE1	22:W:93:ARG:NH1	2.54	0.41
22:W:393:LEU:O	22:W:397:VAL:HG23	2.21	0.41
24:Y:198:ALA:HA	24:Y:226:VAL:HG13	2.03	0.41
25:Z:183:THR:O	25:Z:184:VAL:C	2.63	0.41
28:d:156:ILE:HG23	28:d:157:LEU:N	2.36	0.41
8:h:49:LYS:O	8:h:49:LYS:CG	2.68	0.41
11:k:214:ASN:OD1	11:k:215:ILE:HG23	2.21	0.41
13:m:34:SER:OG	13:m:35:THR:N	2.54	0.41
17:q:67:TYR:CD1	17:q:67:TYR:C	2.99	0.41
32:U:399:TRP:CZ2	32:U:507:VAL:HG21	2.56	0.41
32:U:701:ILE:HD13	32:U:810:THR:CB	2.50	0.41
34:f:257:ARG:CZ	34:f:280:ASP:OD2	2.68	0.41
34:f:540:GLN:O	34:f:543:MET:SD	2.79	0.41
34:f:834:ASP:OD1	34:f:834:ASP:N	2.41	0.41
1:A:113:ILE:CD1	1:A:123:VAL:HG21	2.51	0.41
2:B:240:ALA:HB2	2:B:247:PHE:CD2	2.55	0.41
2:B:269:GLU:OE1	2:B:269:GLU:HA	2.21	0.41
4:D:103:VAL:O	4:D:103:VAL:HG23	2.20	0.41
4:D:257:ASN:N	4:D:257:ASN:OD1	2.53	0.41
4:D:322:LEU:HD22	4:D:330:LYS:HE3	2.02	0.41
6:F:45:THR:HG23	6:F:46:ARG:N	2.34	0.41
6:F:369:HIS:HB2	6:F:396:CYS:SG	2.60	0.41
8:H:38:LYS:HA	8:H:43:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:81:SER:HB2	18:R:121:ARG:HE	1.84	0.41
21:V:491:VAL:CG1	28:d:350:VAL:HG13	2.49	0.41
22:W:355:LYS:O	22:W:358:VAL:HG13	2.21	0.41
23:X:316:ASP:OD1	23:X:316:ASP:C	2.62	0.41
26:a:27:GLU:O	26:a:30:THR:OG1	2.25	0.41
26:a:132:LYS:O	26:a:136:GLU:HG2	2.21	0.41
27:b:11:ASP:OD1	27:b:11:ASP:C	2.63	0.41
27:b:15:TYR:CD2	27:b:116:PRO:HD3	2.55	0.41
27:b:116:PRO:HD3	27:b:146:GLU:HG3	2.02	0.41
7:g:38:THR:HG23	7:g:202:LEU:HD11	2.03	0.41
7:g:80:MET:CB	7:g:87:SER:OG	2.69	0.41
11:k:110:GLU:O	11:k:113:THR:HG22	2.21	0.41
12:l:134:ILE:HB	12:l:145:PHE:HB2	2.02	0.41
13:m:150:MET:O	13:m:157:SER:HA	2.20	0.41
17:q:42:ILE:HG22	17:q:43:LEU:N	2.36	0.41
32:U:757:MET:SD	32:U:757:MET:C	3.04	0.41
34:f:228:LYS:HD3	34:f:228:LYS:H	1.86	0.41
34:f:842:VAL:N	34:f:870:THR:OG1	2.37	0.41
34:f:858:LYS:O	34:f:858:LYS:CG	2.68	0.41
1:A:86:THR:HG22	2:B:136:LEU:HB3	2.03	0.41
1:A:164:MET:HE2	1:A:164:MET:HB3	1.97	0.41
2:B:112:LEU:HB2	2:B:150:VAL:HG11	2.02	0.41
2:B:380:LEU:HD23	2:B:380:LEU:N	2.36	0.41
2:B:381:ASP:OD1	2:B:381:ASP:N	2.53	0.41
2:B:436:GLU:OE1	2:B:436:GLU:CA	2.69	0.41
3:C:73:VAL:HG21	4:D:102:ILE:HG23	2.03	0.41
3:C:298:ILE:HG23	3:C:299:ASP:N	2.36	0.41
3:C:325:ARG:O	3:C:328:ILE:HG22	2.21	0.41
3:C:370:ALA:HB2	3:C:382:ASP:OD2	2.21	0.41
5:E:81:VAL:HB	5:E:105:LEU:O	2.21	0.41
5:E:109:ARG:NH2	6:F:113:LEU:O	2.38	0.41
5:E:135:ILE:HD12	5:E:135:ILE:H	1.86	0.41
6:F:206:MET:HE2	6:F:327:LYS:HG3	2.03	0.41
7:G:155:ASP:OD1	7:G:159:TYR:N	2.48	0.41
9:I:53:HIS:ND1	9:I:54:LYS:N	2.69	0.41
10:J:73:PHE:HA	10:J:130:SER:O	2.21	0.41
11:K:88:LEU:HD22	11:K:116:VAL:HG13	2.02	0.41
12:L:36:VAL:CG1	12:L:37:GLY:N	2.82	0.41
13:M:87:LEU:HD13	13:M:135:PHE:CE1	2.56	0.41
14:N:165:MET:HG2	14:N:172:GLY:HA2	2.02	0.41
15:O:160:ILE:CG2	15:O:174:ILE:HG12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:43:LEU:HD21	17:Q:181:ARG:HD2	2.01	0.41
18:R:94:MET:HE3	18:R:94:MET:HB2	1.95	0.41
21:V:71:THR:HG21	21:V:107:ARG:CD	2.51	0.41
21:V:125:ASN:O	21:V:128:ARG:N	2.51	0.41
21:V:176:MET:SD	21:V:217:VAL:HG23	2.61	0.41
21:V:357:LEU:C	21:V:359:PRO:HD2	2.45	0.41
22:W:75:TYR:C	22:W:77:ALA:H	2.29	0.41
22:W:205:ILE:CA	22:W:208:LYS:HD2	2.18	0.41
22:W:218:ASN:O	22:W:220:GLU:N	2.53	0.41
22:W:267:LEU:HD23	22:W:267:LEU:HA	1.81	0.41
23:X:267:VAL:HG11	23:X:291:ALA:HB1	2.02	0.41
24:Y:83:ARG:HD2	24:Y:87:GLU:HG2	2.03	0.41
24:Y:387:ILE:HD12	24:Y:388:ASN:N	2.36	0.41
26:a:139:GLU:N	26:a:141:MET:SD	2.94	0.41
26:a:265:GLU:OE2	26:a:265:GLU:HA	2.21	0.41
29:e:21:GLU:CD	29:e:21:GLU:C	2.89	0.41
29:e:51:ASP:O	29:e:53:SER:N	2.54	0.41
29:e:52:PHE:HA	29:e:55:GLN:HG3	2.02	0.41
9:i:11:ILE:HG22	10:j:7:ILE:HG23	2.03	0.41
15:o:213:LEU:HD21	16:p:200:LYS:HB3	2.02	0.41
18:r:161:ILE:HG21	18:r:175:VAL:HG13	2.03	0.41
32:U:412:HIS:N	32:U:412:HIS:CD2	2.89	0.41
32:U:486:MET:HE1	32:U:781:LEU:HD11	2.02	0.41
32:U:545:LEU:HD23	32:U:545:LEU:HA	1.97	0.41
34:f:186:THR:O	34:f:190:GLU:HG2	2.21	0.41
34:f:221:ILE:O	34:f:222:ASP:HB3	2.21	0.41
34:f:282:PHE:HA	34:f:294:MET:CE	2.51	0.41
34:f:347:ASP:N	34:f:347:ASP:OD1	2.53	0.41
34:f:377:VAL:HG23	34:f:767:GLY:CA	2.50	0.41
1:A:187:LEU:CD2	1:A:225:CYS:SG	3.09	0.41
2:B:93:GLU:C	2:B:95:GLU:H	2.28	0.41
2:B:133:VAL:HG11	2:B:157:HIS:O	2.21	0.41
15:O:14:VAL:CG2	15:O:156:VAL:HG21	2.48	0.41
25:Z:183:THR:O	25:Z:185:GLY:N	2.54	0.41
26:a:133:GLU:O	26:a:137:ASP:OD2	2.39	0.41
26:a:201:GLY:O	26:a:205:LEU:HD13	2.21	0.41
20:t:166:ARG:NE	20:t:189:ILE:HD11	2.35	0.41
32:U:229:VAL:HA	32:U:232:ILE:HG22	2.03	0.41
32:U:423:MET:HE2	32:U:427:LEU:HD23	2.03	0.41
32:U:627:PHE:CD1	32:U:627:PHE:C	2.99	0.41
34:f:324:VAL:HG13	34:f:325:GLN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:f:345:PRO:CD	34:f:390:LEU:HD11	2.51	0.41
1:A:81:ALA:CB	2:B:138:PHE:HB3	2.48	0.40
1:A:241:ILE:HG13	2:B:314:ASN:HD21	1.83	0.40
2:B:437:GLY:HA2	10:J:76:LEU:HD23	2.03	0.40
6:F:178:ASP:C	6:F:178:ASP:OD1	2.63	0.40
6:F:194:GLN:HG3	6:F:352:ILE:CG2	2.51	0.40
19:S:74:MET:HG3	12:l:93:LEU:HD11	2.02	0.40
21:V:293:GLY:C	21:V:309:MET:HE2	2.46	0.40
21:V:368:ARG:HH11	21:V:368:ARG:HG3	1.86	0.40
22:W:86:ASN:OD1	22:W:90:LEU:CD1	2.69	0.40
22:W:177:MET:HG2	22:W:182:ARG:HG2	2.03	0.40
22:W:223:LYS:CE	22:W:253:THR:HG22	2.50	0.40
22:W:368:LYS:HZ3	22:W:368:LYS:HB2	1.87	0.40
25:Z:167:ALA:O	33:c:42:LEU:HD23	2.20	0.40
26:a:153:SER:O	26:a:157:ASP:OD2	2.39	0.40
28:d:196:LEU:HD22	28:d:212:LEU:CD1	2.51	0.40
9:i:224:VAL:O	9:i:224:VAL:CG2	2.69	0.40
14:n:39:HIS:CE1	14:n:75:PRO:HD3	2.56	0.40
17:q:11:ASP:OD1	17:q:11:ASP:N	2.52	0.40
20:t:59:ASP:HB3	20:t:106:LEU:HD22	2.03	0.40
31:z:35:ILE:O	31:z:35:ILE:HG22	2.21	0.40
32:U:138:PHE:CZ	32:U:162:VAL:HG11	2.56	0.40
32:U:633:CYS:O	32:U:637:VAL:HG22	2.21	0.40
34:f:183:PRO:HA	34:f:186:THR:OG1	2.21	0.40
1:A:301:GLU:HA	1:A:301:GLU:OE2	2.22	0.40
6:F:79:LYS:HA	6:F:82:VAL:HG12	2.03	0.40
6:F:124:ILE:HD12	6:F:153:VAL:HG11	2.03	0.40
6:F:253:GLY:N	6:F:254:PRO:HD2	2.36	0.40
10:J:33:VAL:HG12	10:J:34:GLY:N	2.35	0.40
11:K:149:LYS:HB2	11:K:149:LYS:HE2	1.93	0.40
12:L:74:ILE:HD13	12:L:81:ALA:CB	2.51	0.40
17:Q:115:LEU:HD12	17:Q:116:TYR:N	2.36	0.40
17:Q:124:LEU:HD23	17:Q:124:LEU:C	2.46	0.40
21:V:392:TYR:CE1	21:V:396:ILE:HG13	2.55	0.40
22:W:115:ILE:CD1	22:W:116:THR:H	2.31	0.40
22:W:188:GLU:OE2	22:W:191:ARG:CZ	2.68	0.40
24:Y:148:GLY:HA2	24:Y:156:LEU:HD23	2.04	0.40
26:a:113:LEU:HA	26:a:116:THR:HG22	2.03	0.40
26:a:245:VAL:HG22	26:a:272:ILE:CG2	2.51	0.40
27:b:180:ALA:O	27:b:183:LEU:HB2	2.21	0.40
28:d:334:GLU:OE1	28:d:334:GLU:N	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:l:9:ASP:HB2	12:l:12:VAL:HG23	2.03	0.40
12:l:40:SER:HB3	12:l:187:LEU:HD22	2.03	0.40
19:s:100:ARG:HD3	19:s:100:ARG:O	2.22	0.40
32:U:357:LYS:HE2	32:U:389:ASN:CG	2.46	0.40
32:U:377:HIS:ND1	32:U:382:SER:OG	2.55	0.40
32:U:757:MET:SD	32:U:758:PRO:N	2.94	0.40
2:B:166:ASP:OD1	2:B:167:THR:N	2.54	0.40
2:B:417:GLU:HA	2:B:420:LYS:HG2	2.03	0.40
3:C:136:SER:C	3:C:139:MET:HE1	2.46	0.40
4:D:83:GLN:HG2	4:D:140:VAL:CG1	2.51	0.40
9:I:28:ILE:HD13	9:I:28:ILE:N	2.36	0.40
10:J:91:CYS:SG	10:J:107:ILE:HD13	2.62	0.40
22:W:314:LEU:HD11	26:a:312:MET:CG	2.52	0.40
26:a:80:ILE:HD13	26:a:100:THR:CG2	2.51	0.40
15:o:91:TYR:CB	15:o:95:ILE:HD12	2.51	0.40
32:U:164:GLU:OE2	32:U:204:ILE:HD11	2.21	0.40
32:U:462:LEU:HD23	32:U:462:LEU:C	2.47	0.40
34:f:300:ARG:CZ	34:f:826:GLN:HG3	2.51	0.40
34:f:343:LYS:HB2	34:f:381:VAL:HG11	2.04	0.40
1:A:97:ARG:HD2	1:A:115:VAL:HG11	2.03	0.40
2:B:105:THR:OG1	2:B:106:PRO:HD3	2.21	0.40
2:B:431:GLN:O	2:B:432:GLU:CB	2.69	0.40
6:F:136:VAL:O	6:F:136:VAL:HG23	2.21	0.40
6:F:175:MET:SD	6:F:251:LEU:CD2	3.10	0.40
6:F:188:ILE:HG23	6:F:235:LEU:HD21	2.02	0.40
16:P:111:LEU:HD12	16:P:189:ILE:HG22	2.03	0.40
21:V:223:LYS:O	21:V:226:VAL:HG22	2.21	0.40
21:V:374:LYS:O	21:V:378:VAL:HG13	2.22	0.40
22:W:412:ILE:HD13	26:a:327:VAL:HG21	2.03	0.40
23:X:333:GLN:HA	23:X:336:ILE:HG22	2.02	0.40
26:a:255:TRP:CD1	26:a:255:TRP:C	3.00	0.40
27:b:3:LEU:HB3	27:b:105:HIS:CD2	2.56	0.40
27:b:20:ASP:OD1	27:b:20:ASP:C	2.65	0.40
28:d:137:THR:HG1	28:d:140:GLN:HB2	1.87	0.40
10:j:125:ARG:NH1	10:j:126:PRO:O	2.55	0.40
11:k:28:ILE:CD1	11:k:158:PRO:HD2	2.52	0.40
13:m:24:GLU:O	13:m:28:LYS:HG2	2.22	0.40
13:m:238:TYR:CD1	13:m:238:TYR:C	2.99	0.40
19:s:46:LEU:CD1	19:s:52:ILE:HG22	2.50	0.40
34:f:234:THR:O	34:f:237:VAL:HG12	2.22	0.40
34:f:826:GLN:HB3	34:f:827:PRO:CD	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:LEU:O	3:C:52:LEU:HD23	2.22	0.40
3:C:214:VAL:HG12	3:C:215:SER:N	2.36	0.40
4:D:119:ILE:HD11	4:D:140:VAL:C	2.47	0.40
5:E:169:GLY:HA2	5:E:275:MET:O	2.21	0.40
5:E:178:THR:OG1	5:E:301:ILE:HG22	2.21	0.40
5:E:346:VAL:CG2	5:E:374:VAL:HG21	2.51	0.40
11:K:74:ILE:HD13	11:K:109:VAL:HG22	2.04	0.40
12:L:7:ASP:OD1	12:L:7:ASP:N	2.54	0.40
12:L:171:TYR:O	12:L:174:ARG:HB2	2.21	0.40
15:O:85:LYS:NZ	15:O:120:THR:HG22	2.36	0.40
21:V:160:LEU:O	21:V:163:VAL:HG12	2.22	0.40
22:W:55:ARG:HH22	22:W:93:ARG:NH2	2.18	0.40
22:W:213:PHE:CZ	22:W:219:THR:CG2	3.04	0.40
22:W:250:ILE:CA	22:W:253:THR:HG23	2.52	0.40
22:W:265:GLN:HE21	22:W:336:PRO:HG2	1.82	0.40
22:W:293:ASP:O	22:W:296:LEU:HB3	2.22	0.40
22:W:438:LEU:HB3	25:Z:233:VAL:CG2	2.51	0.40
25:Z:246:VAL:HG22	28:d:330:ILE:HG13	2.04	0.40
26:a:366:LEU:HD11	28:d:333:THR:HG23	2.03	0.40
12:l:150:SER:O	12:l:151:ALA:HB3	2.22	0.40
14:n:99:ILE:HG22	14:n:100:ILE:N	2.37	0.40
16:p:26:ARG:HG3	16:p:182:MET:HG3	2.02	0.40
17:q:158:GLU:CD	17:q:158:GLU:C	2.90	0.40
19:s:190:GLY:O	19:s:211:ARG:O	2.39	0.40
32:U:551:GLY:O	32:U:555:VAL:HG23	2.21	0.40
32:U:567:ILE:CD1	32:U:585:THR:HB	2.50	0.40
33:c:127:ILE:HG23	33:c:162:LEU:HD22	2.02	0.40
34:f:487:LEU:HD22	34:f:822:VAL:HG12	2.03	0.40
34:f:574:GLU:CD	34:f:575:ALA:N	2.79	0.40
34:f:840:LEU:HD21	34:f:887:PHE:CZ	2.57	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	388/433 (90%)	354 (91%)	34 (9%)	0	100	100
2	B	391/440 (89%)	341 (87%)	48 (12%)	2 (0%)	25	50
3	C	387/406 (95%)	349 (90%)	38 (10%)	0	100	100
4	D	378/418 (90%)	352 (93%)	25 (7%)	1 (0%)	37	60
5	E	387/403 (96%)	362 (94%)	25 (6%)	0	100	100
6	F	413/439 (94%)	382 (92%)	30 (7%)	1 (0%)	44	66
7	G	238/246 (97%)	222 (93%)	15 (6%)	1 (0%)	30	55
7	g	238/246 (97%)	233 (98%)	5 (2%)	0	100	100
8	H	227/234 (97%)	217 (96%)	10 (4%)	0	100	100
8	h	227/234 (97%)	218 (96%)	9 (4%)	0	100	100
9	I	245/261 (94%)	228 (93%)	17 (7%)	0	100	100
9	i	245/261 (94%)	237 (97%)	8 (3%)	0	100	100
10	J	230/248 (93%)	216 (94%)	14 (6%)	0	100	100
10	j	230/248 (93%)	222 (96%)	7 (3%)	1 (0%)	30	55
11	K	231/241 (96%)	217 (94%)	14 (6%)	0	100	100
11	k	231/241 (96%)	223 (96%)	8 (4%)	0	100	100
12	L	231/263 (88%)	222 (96%)	9 (4%)	0	100	100
12	l	231/263 (88%)	221 (96%)	10 (4%)	0	100	100
13	M	237/255 (93%)	230 (97%)	7 (3%)	0	100	100
13	m	237/255 (93%)	234 (99%)	3 (1%)	0	100	100
14	N	200/239 (84%)	196 (98%)	4 (2%)	0	100	100
14	n	200/239 (84%)	195 (98%)	5 (2%)	0	100	100
15	O	218/277 (79%)	209 (96%)	9 (4%)	0	100	100
15	o	218/277 (79%)	210 (96%)	7 (3%)	1 (0%)	25	50
16	P	202/205 (98%)	190 (94%)	12 (6%)	0	100	100
16	p	202/205 (98%)	192 (95%)	10 (5%)	0	100	100
17	Q	194/201 (96%)	185 (95%)	8 (4%)	1 (0%)	25	50
17	q	194/201 (96%)	184 (95%)	10 (5%)	0	100	100
18	R	198/263 (75%)	191 (96%)	7 (4%)	0	100	100
18	r	198/263 (75%)	186 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	210/241 (87%)	202 (96%)	8 (4%)	0	100	100
19	s	210/241 (87%)	203 (97%)	7 (3%)	0	100	100
20	T	210/264 (80%)	199 (95%)	10 (5%)	1 (0%)	25	50
20	t	210/264 (80%)	195 (93%)	15 (7%)	0	100	100
21	V	440/534 (82%)	413 (94%)	25 (6%)	2 (0%)	25	50
22	W	438/456 (96%)	411 (94%)	27 (6%)	0	100	100
23	X	382/422 (90%)	364 (95%)	18 (5%)	0	100	100
24	Y	378/389 (97%)	356 (94%)	21 (6%)	1 (0%)	37	60
25	Z	284/324 (88%)	258 (91%)	23 (8%)	3 (1%)	12	30
26	a	371/376 (99%)	325 (88%)	44 (12%)	2 (0%)	25	50
27	b	189/377 (50%)	151 (80%)	37 (20%)	1 (0%)	25	50
28	d	268/350 (77%)	246 (92%)	20 (8%)	2 (1%)	19	41
29	e	46/70 (66%)	37 (80%)	8 (17%)	1 (2%)	5	16
31	z	79/468 (17%)	78 (99%)	1 (1%)	0	100	100
32	U	812/953 (85%)	762 (94%)	49 (6%)	1 (0%)	48	72
33	c	279/310 (90%)	257 (92%)	21 (8%)	1 (0%)	30	55
34	f	832/908 (92%)	779 (94%)	53 (6%)	0	100	100
All	All	13284/15352 (86%)	12454 (94%)	807 (6%)	23 (0%)	45	66

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	65	LEU
25	Z	149	THR
2	B	278	ALA
24	Y	98	SER
25	Z	194	GLN
28	d	283	LEU
10	j	52	LYS
32	U	4	SER
28	d	282	ILE
29	e	41	ASP
4	D	327	LEU
21	V	469	THR
6	F	279	ALA
7	G	189	TRP

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Mol	Chain	Res	Type
25	Z	183	THR
26	a	70	ARG
15	o	172	SER
21	V	368	ARG
33	c	25	VAL
17	Q	25	ILE
26	a	71	VAL
27	b	22	LEU
20	T	31	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	333/372 (90%)	329 (99%)	4 (1%)	67	81
2	B	344/385 (89%)	332 (96%)	12 (4%)	31	55
3	C	340/352 (97%)	337 (99%)	3 (1%)	75	85
4	D	333/366 (91%)	330 (99%)	3 (1%)	75	85
5	E	341/353 (97%)	336 (98%)	5 (2%)	60	78
6	F	357/379 (94%)	351 (98%)	6 (2%)	56	76
7	G	164/210 (78%)	157 (96%)	7 (4%)	25	49
7	g	168/210 (80%)	166 (99%)	2 (1%)	67	81
8	H	150/191 (78%)	146 (97%)	4 (3%)	40	64
8	h	150/191 (78%)	146 (97%)	4 (3%)	40	64
9	I	166/221 (75%)	158 (95%)	8 (5%)	21	44
9	i	160/221 (72%)	159 (99%)	1 (1%)	84	90
10	J	136/211 (64%)	133 (98%)	3 (2%)	47	70
10	j	136/211 (64%)	135 (99%)	1 (1%)	81	89
11	K	159/203 (78%)	158 (99%)	1 (1%)	84	90
11	k	158/203 (78%)	156 (99%)	2 (1%)	65	80
12	L	161/224 (72%)	161 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	l	161/224 (72%)	159 (99%)	2 (1%)	67	81
13	M	162/212 (76%)	159 (98%)	3 (2%)	52	73
13	m	163/212 (77%)	161 (99%)	2 (1%)	67	81
14	N	141/181 (78%)	139 (99%)	2 (1%)	62	79
14	n	140/181 (77%)	138 (99%)	2 (1%)	62	79
15	O	158/228 (69%)	156 (99%)	2 (1%)	65	80
15	o	157/228 (69%)	157 (100%)	0	100	100
16	P	159/174 (91%)	157 (99%)	2 (1%)	65	80
16	p	156/174 (90%)	153 (98%)	3 (2%)	52	73
17	Q	149/171 (87%)	147 (99%)	2 (1%)	65	80
17	q	148/171 (86%)	146 (99%)	2 (1%)	62	79
18	R	139/202 (69%)	136 (98%)	3 (2%)	47	70
18	r	138/202 (68%)	136 (99%)	2 (1%)	62	79
19	S	158/199 (79%)	154 (98%)	4 (2%)	42	66
19	s	159/199 (80%)	155 (98%)	4 (2%)	42	66
20	T	151/215 (70%)	150 (99%)	1 (1%)	81	89
20	t	149/215 (69%)	147 (99%)	2 (1%)	65	80
21	V	389/460 (85%)	379 (97%)	10 (3%)	41	65
22	W	405/416 (97%)	393 (97%)	12 (3%)	36	60
23	X	330/362 (91%)	326 (99%)	4 (1%)	67	81
24	Y	335/344 (97%)	327 (98%)	8 (2%)	44	68
25	Z	257/295 (87%)	250 (97%)	7 (3%)	40	64
26	a	333/336 (99%)	324 (97%)	9 (3%)	40	64
27	b	167/312 (54%)	161 (96%)	6 (4%)	30	54
28	d	237/294 (81%)	233 (98%)	4 (2%)	56	76
29	e	43/63 (68%)	42 (98%)	1 (2%)	45	69
31	z	68/377 (18%)	67 (98%)	1 (2%)	60	78
32	U	695/816 (85%)	680 (98%)	15 (2%)	47	70
33	c	249/268 (93%)	242 (97%)	7 (3%)	38	63
34	f	704/763 (92%)	690 (98%)	14 (2%)	50	72
All	All	10556/12997 (81%)	10354 (98%)	202 (2%)	52	73

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	VAL
1	A	203	ASN
1	A	361	SER
1	A	406	GLU
2	B	94	GLU
2	B	130	GLU
2	B	151	LEU
2	B	207	HIS
2	B	290	ILE
2	B	346	ARG
2	B	351	ILE
2	B	357	ASP
2	B	366	GLN
2	B	372	MET
2	B	405	MET
2	B	411	ARG
3	C	165	ILE
3	C	250	GLU
3	C	379	THR
4	D	60	TYR
4	D	159	LYS
4	D	181	VAL
5	E	104	THR
5	E	108	MET
5	E	190	GLN
5	E	230	ILE
5	E	363	VAL
6	F	111	ILE
6	F	160	ILE
6	F	188	ILE
6	F	248	PHE
6	F	261	ILE
6	F	425	LEU
7	G	19	GLU
7	G	30	LYS
7	G	33	ASN
7	G	52	THR
7	G	115	CYS
7	G	219	VAL
7	G	230	LEU
8	H	15	SER
8	H	71	ILE

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Mol	Chain	Res	Type
8	H	121	THR
8	H	133	LEU
9	I	61	PHE
9	I	69	ASN
9	I	72	MET
9	I	92	LEU
9	I	100	GLN
9	I	147	LEU
9	I	187	LYS
9	I	201	MET
10	J	23	GLN
10	J	188	ILE
10	J	228	TYR
11	K	164	GLN
13	M	68	ASN
13	M	123	THR
13	M	185	THR
14	N	105	ASP
14	N	197	LYS
15	O	71	THR
15	O	218	THR
16	P	121	CYS
16	P	203	MET
17	Q	141	SER
17	Q	188	ILE
18	R	46	MET
18	R	83	LEU
18	R	100	THR
19	S	6	VAL
19	S	47	THR
19	S	50	THR
19	S	114	ASP
20	T	26	MET
21	V	100	MET
21	V	217	VAL
21	V	220	PHE
21	V	269	LYS
21	V	273	LYS
21	V	298	ILE
21	V	300	LEU
21	V	308	THR
21	V	320	THR

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Mol	Chain	Res	Type
21	V	338	LEU
22	W	54	THR
22	W	74	CYS
22	W	159	VAL
22	W	166	LEU
22	W	172	GLU
22	W	200	ILE
22	W	206	SER
22	W	271	VAL
22	W	274	VAL
22	W	299	ILE
22	W	385	SER
22	W	400	LYS
23	X	217	ILE
23	X	243	ASP
23	X	388	PHE
23	X	420	LYS
24	Y	26	LEU
24	Y	39	ASP
24	Y	117	LYS
24	Y	121	LEU
24	Y	143	TYR
24	Y	210	SER
24	Y	291	HIS
24	Y	357	ASN
25	Z	38	VAL
25	Z	116	CYS
25	Z	135	THR
25	Z	179	ILE
25	Z	190	ARG
25	Z	205	LEU
25	Z	214	LYS
26	a	21	VAL
26	a	83	VAL
26	a	89	ASP
26	a	105	LYS
26	a	127	ASP
26	a	229	ASP
26	a	336	VAL
26	a	358	THR
26	a	366	LEU
27	b	48	ASN

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Mol	Chain	Res	Type
27	b	51	LEU
27	b	90	ILE
27	b	100	ARG
27	b	161	ASN
27	b	189	LEU
28	d	94	MET
28	d	125	GLU
28	d	192	LEU
28	d	237	MET
29	e	20	GLU
7	g	51	VAL
7	g	175	SER
8	h	35	VAL
8	h	73	LEU
8	h	148	SER
8	h	212	CYS
9	i	75	SER
10	j	107	ILE
11	k	108	THR
11	k	206	MET
12	l	11	THR
12	l	88	MET
13	m	68	ASN
13	m	133	CYS
14	n	71	LEU
14	n	122	VAL
16	p	115	THR
16	p	125	LEU
16	p	189	ILE
17	q	41	LYS
17	q	148	THR
18	r	45	THR
18	r	74	ARG
19	s	35	ILE
19	s	37	THR
19	s	189	THR
19	s	199	THR
20	t	20	VAL
20	t	92	LEU
31	z	77	ASP
32	U	91	ASN
32	U	92	ASP

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Mol	Chain	Res	Type
32	U	105	ILE
32	U	109	THR
32	U	117	ASP
32	U	187	LEU
32	U	244	MET
32	U	325	MET
32	U	360	VAL
32	U	421	GLN
32	U	525	ASN
32	U	703	CYS
32	U	720	LYS
32	U	805	ASN
32	U	880	ASN
33	c	64	ASP
33	c	102	THR
33	c	109	VAL
33	c	141	VAL
33	c	205	ILE
33	c	265	MET
33	c	289	ASP
34	f	207	LEU
34	f	237	VAL
34	f	240	VAL
34	f	258	LYS
34	f	328	SER
34	f	388	ASP
34	f	465	LEU
34	f	517	VAL
34	f	681	TYR
34	f	712	LYS
34	f	731	MET
34	f	744	MET
34	f	813	LYS
34	f	842	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	84	GLN
2	B	314	ASN
2	B	366	GLN
3	C	205	HIS

*Continued on next page...*

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Mol	Chain	Res	Type
3	C	377	HIS
4	D	76	GLN
4	D	294	ASN
4	D	376	ASN
5	E	124	HIS
5	E	254	GLN
5	E	271	HIS
5	E	307	GLN
6	F	333	ASN
6	F	380	ASN
7	G	12	HIS
7	G	92	GLN
8	H	122	GLN
9	I	20	GLN
9	I	84	ASN
9	I	109	GLN
9	I	177	GLN
10	J	85	ASN
11	K	114	GLN
13	M	72	HIS
14	N	67	HIS
14	N	155	GLN
15	O	67	HIS
15	O	92	GLN
16	P	17	ASN
17	Q	8	GLN
17	Q	71	ASN
17	Q	82	ASN
17	Q	101	ASN
17	Q	132	HIS
17	Q	168	GLN
19	S	108	ASN
21	V	168	GLN
21	V	232	HIS
21	V	401	ASN
22	W	264	GLN
22	W	265	GLN
23	X	329	ASN
24	Y	280	GLN
24	Y	332	GLN
24	Y	357	ASN
25	Z	145	HIS

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Mol	Chain	Res	Type
25	Z	273	HIS
26	a	46	GLN
26	a	288	HIS
26	a	344	GLN
26	a	372	HIS
27	b	29	GLN
27	b	76	HIS
27	b	137	ASN
27	b	142	ASN
29	e	37	HIS
29	e	54	ASN
9	i	100	GLN
9	i	109	GLN
9	i	198	ASN
11	k	164	GLN
11	k	186	HIS
11	k	221	GLN
12	l	90	GLN
13	m	221	ASN
15	o	31	ASN
15	o	81	ASN
16	p	32	GLN
16	p	156	ASN
18	r	197	HIS
19	s	79	ASN
19	s	151	ASN
19	s	152	GLN
32	U	338	HIS
32	U	525	ASN
32	U	801	GLN
32	U	901	GLN
33	c	113	HIS
33	c	149	GLN
33	c	176	GLN
33	c	274	ASN
34	f	51	GLN
34	f	156	HIS
34	f	371	ASN
34	f	493	ASN
34	f	566	HIS
34	f	701	ASN
34	f	855	GLN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
37	ADP	E	401	-	24,29,29	0.87	0	29,45,45	1.17	1 (3%)
35	ATP	A	501	36	28,33,33	0.85	0	34,52,52	1.09	6 (17%)
35	ATP	F	501	36	28,33,33	1.20	2 (7%)	34,52,52	1.27	6 (17%)
35	ATP	B	501	36	28,33,33	0.85	1 (3%)	34,52,52	1.26	5 (14%)
35	ATP	D	502	36	28,33,33	0.84	0	34,52,52	1.17	4 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	ADP	E	401	-	-	4/12/32/32	0/3/3/3
35	ATP	A	501	36	-	3/18/38/38	0/3/3/3
35	ATP	F	501	36	-	4/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	B	501	36	-	3/18/38/38	0/3/3/3
35	ATP	D	502	36	-	3/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	F	501	ATP	PA-O3A	-3.70	1.55	1.59
35	F	501	ATP	PB-O3B	-3.38	1.55	1.59
35	B	501	ATP	PA-O3A	-2.24	1.57	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	501	ATP	C4'-O4'-C1'	-4.35	105.94	109.92
35	F	501	ATP	C4'-O4'-C1'	-4.27	106.01	109.92
37	E	401	ADP	N3-C2-N1	-4.05	123.18	128.67
35	D	502	ATP	C4'-O4'-C1'	-3.91	106.35	109.92
35	F	501	ATP	C5-C6-N6	2.41	123.98	120.31
35	B	501	ATP	O2'-C2'-C3'	-2.38	104.19	111.82
35	A	501	ATP	O3'-C3'-C2'	-2.38	104.19	111.82
35	F	501	ATP	O2'-C2'-C3'	-2.38	104.19	111.82
35	B	501	ATP	C5-C6-N6	2.33	123.86	120.31
35	B	501	ATP	O3'-C3'-C2'	-2.30	104.45	111.82
35	D	502	ATP	C5-C6-N6	2.27	123.77	120.31
35	A	501	ATP	C5-C6-N6	2.25	123.74	120.31
35	A	501	ATP	O2'-C2'-C3'	-2.19	104.78	111.82
35	A	501	ATP	C4'-O4'-C1'	-2.18	107.93	109.92
35	F	501	ATP	O3'-C3'-C2'	-2.18	104.84	111.82
35	B	501	ATP	O3'-C3'-C4'	-2.16	104.88	111.08
35	A	501	ATP	O4'-C1'-N9	-2.14	105.90	108.75
35	F	501	ATP	O3'-C3'-C4'	-2.06	105.16	111.08
35	D	502	ATP	O2'-C2'-C3'	-2.06	105.22	111.82
35	D	502	ATP	O3'-C3'-C2'	-2.02	105.33	111.82
35	F	501	ATP	O4'-C1'-N9	-2.01	106.08	108.75
35	A	501	ATP	O3'-C3'-C4'	-2.00	105.33	111.08

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	D	502	ATP	C5'-O5'-PA-O1A

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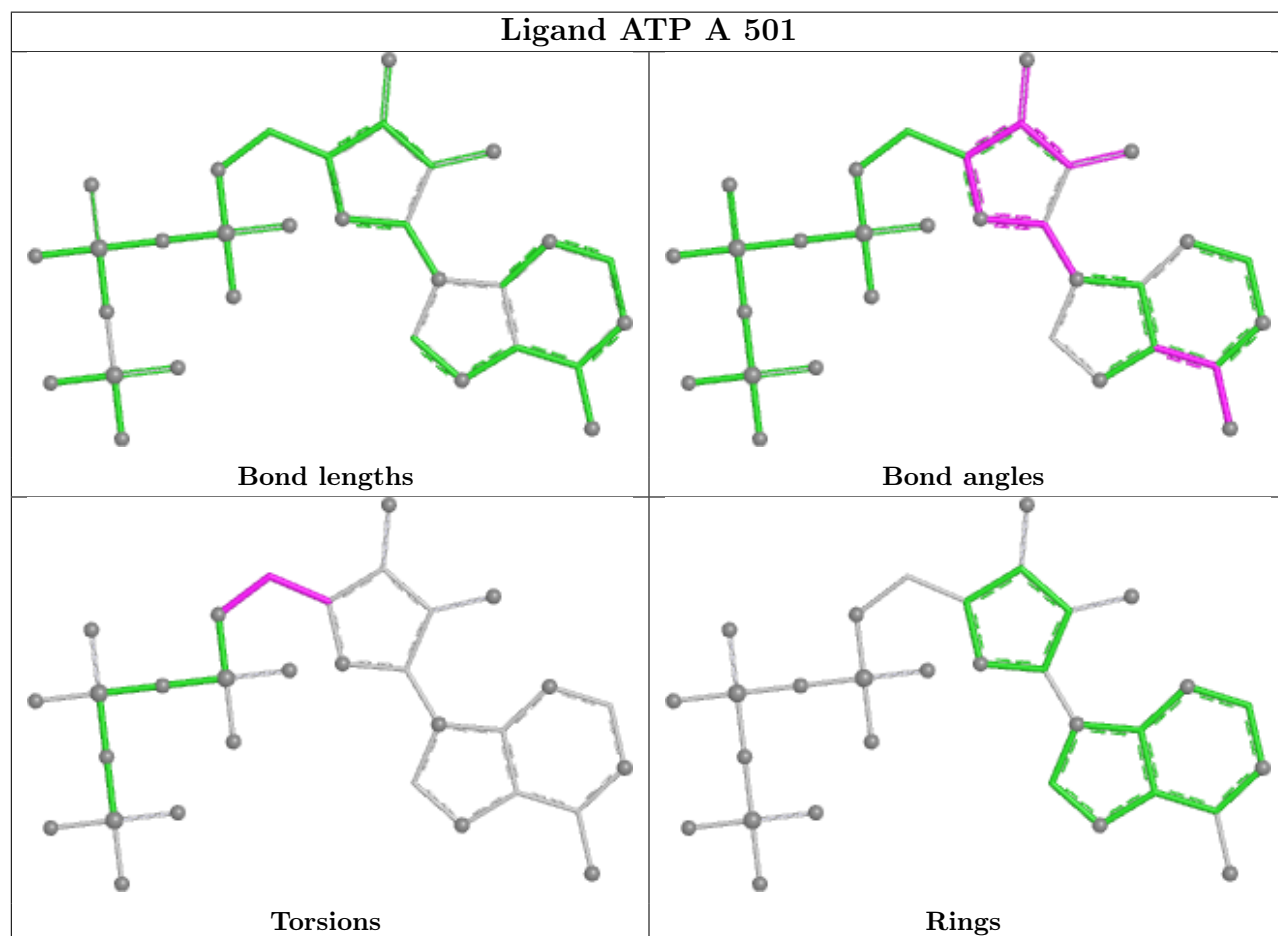
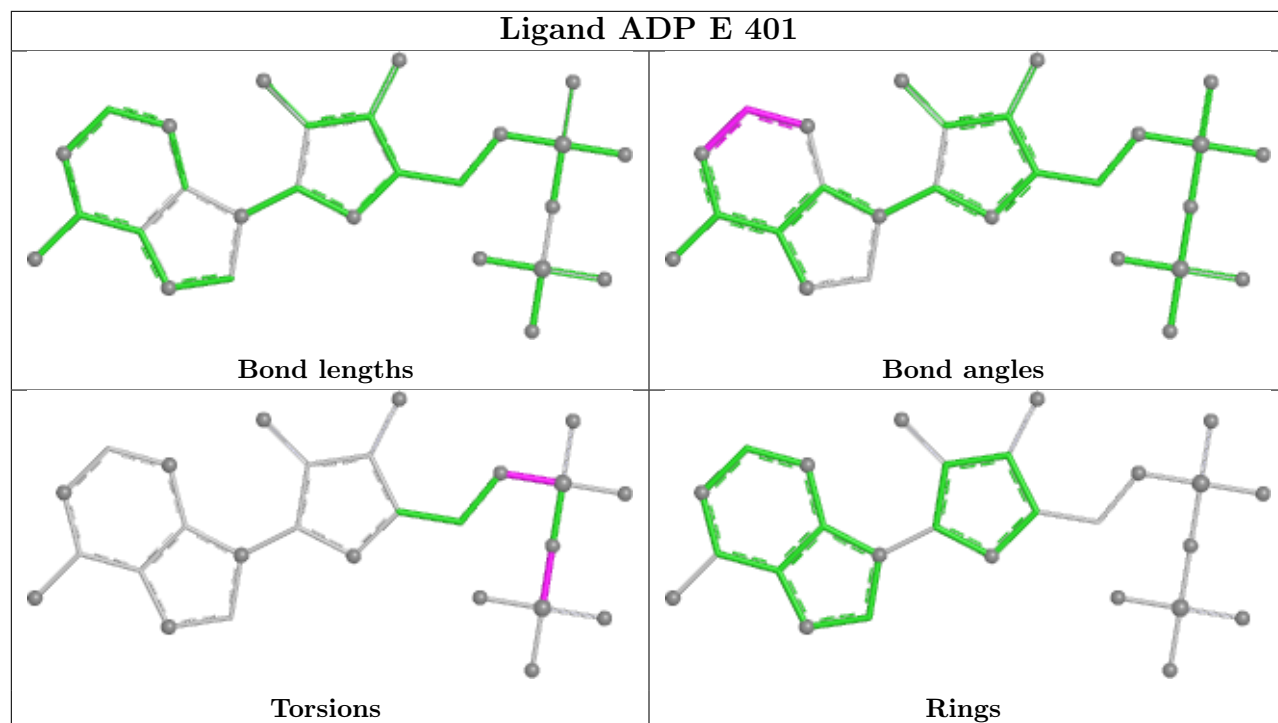
Mol	Chain	Res	Type	Atoms
35	D	502	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C5'-O5'-PA-O2A
35	F	501	ATP	C5'-O5'-PA-O3A
37	E	401	ADP	PA-O3A-PB-O2B
37	E	401	ADP	PA-O3A-PB-O3B
37	E	401	ADP	C5'-O5'-PA-O2A
37	E	401	ADP	C5'-O5'-PA-O3A
35	F	501	ATP	O4'-C4'-C5'-O5'
35	A	501	ATP	O4'-C4'-C5'-O5'
35	A	501	ATP	C3'-C4'-C5'-O5'
35	B	501	ATP	C3'-C4'-C5'-O5'
35	B	501	ATP	O4'-C4'-C5'-O5'
35	D	502	ATP	C3'-C4'-C5'-O5'
35	A	501	ATP	C4'-C5'-O5'-PA
35	B	501	ATP	C4'-C5'-O5'-PA
35	F	501	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

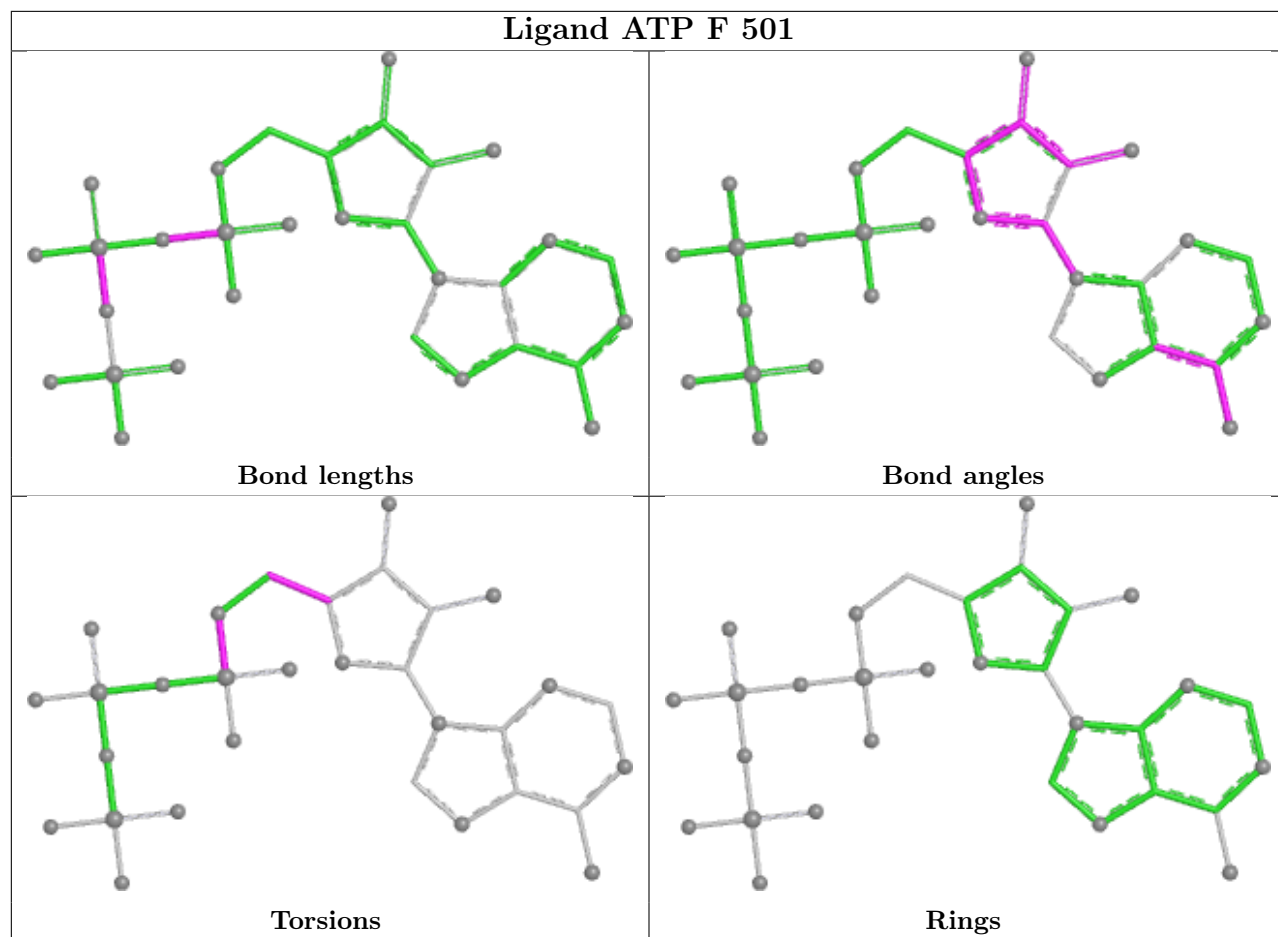
4 monomers are involved in 6 short contacts:

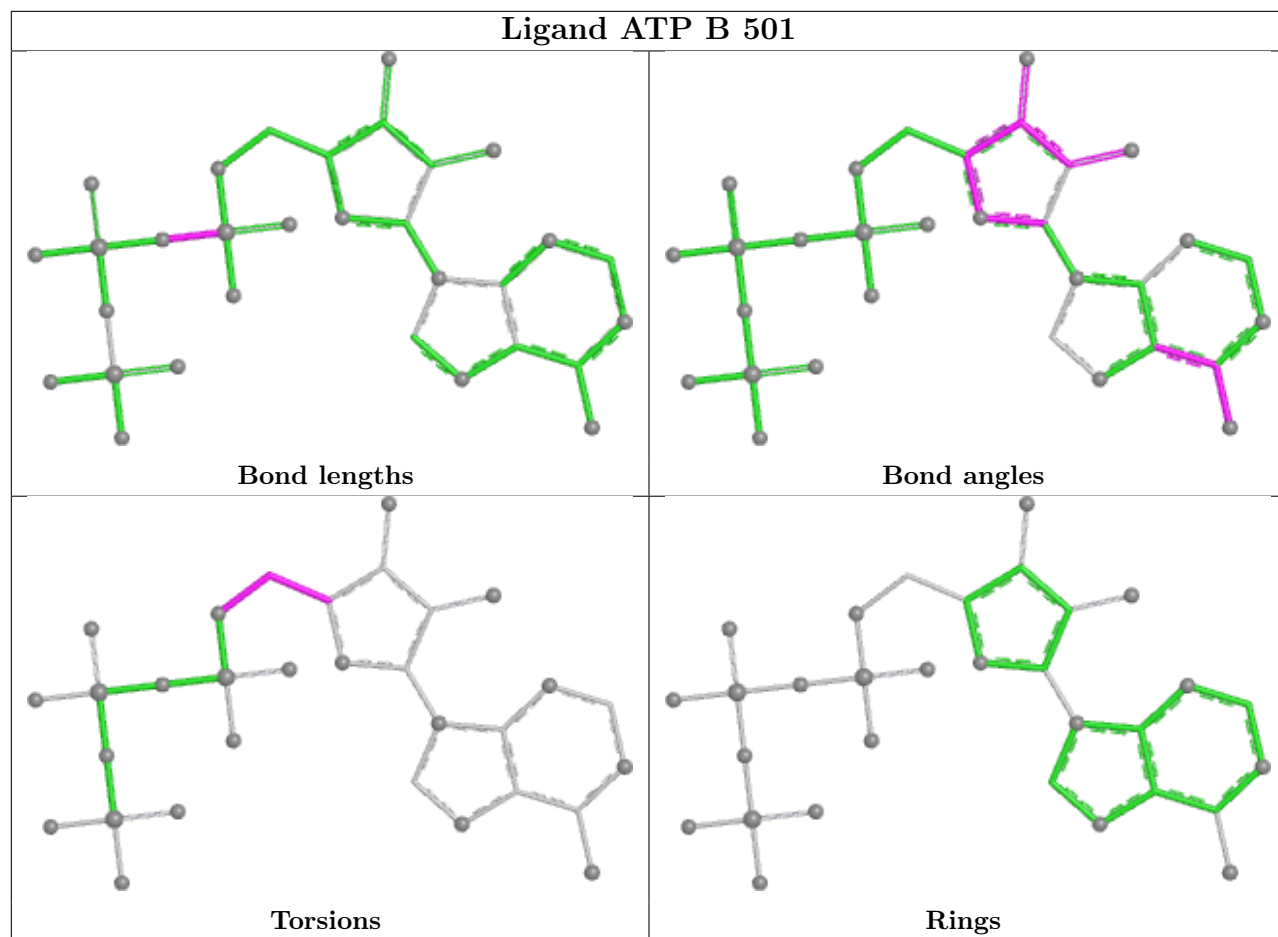
Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	E	401	ADP	1	0
35	A	501	ATP	1	0
35	F	501	ATP	1	0
35	B	501	ATP	3	0

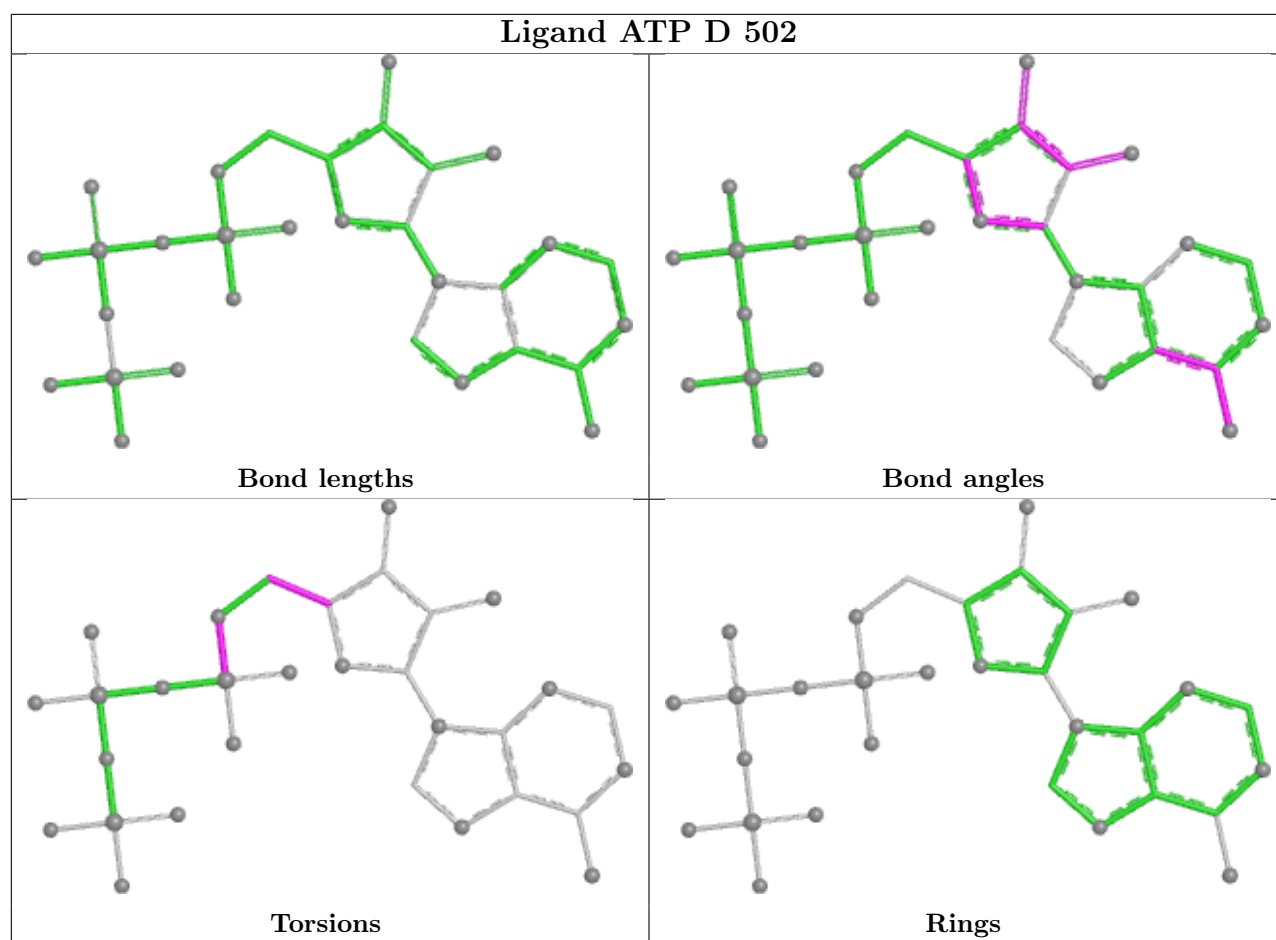
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



## Ligand ATP F 501







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

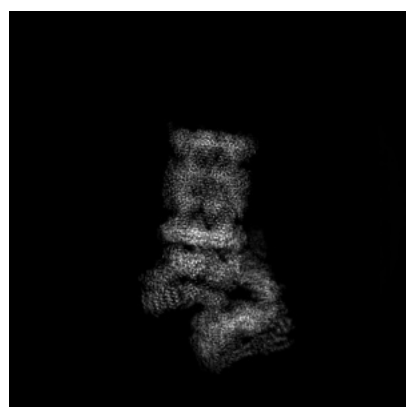
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-49509. These allow visual inspection of the internal detail of the map and identification of artifacts.

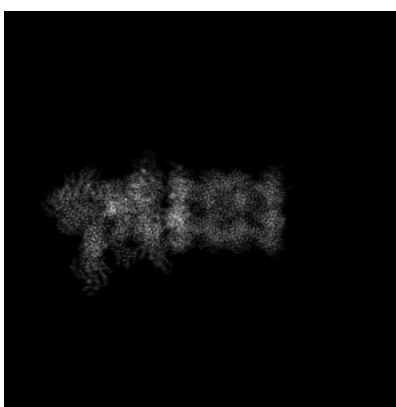
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

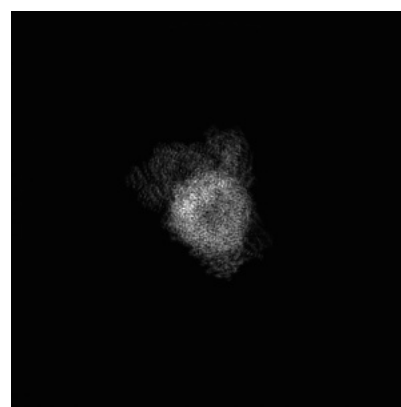
#### 6.1.1 Primary map



X



Y



Z

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

### 6.2 Central slices [i](#)

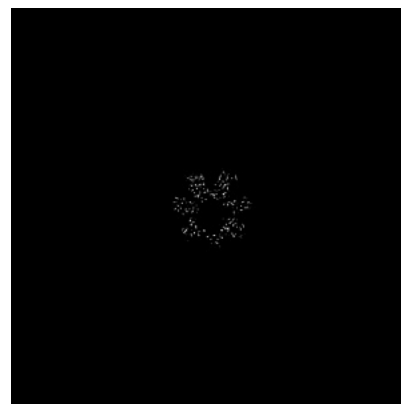
#### 6.2.1 Primary map



X Index: 301



Y Index: 301



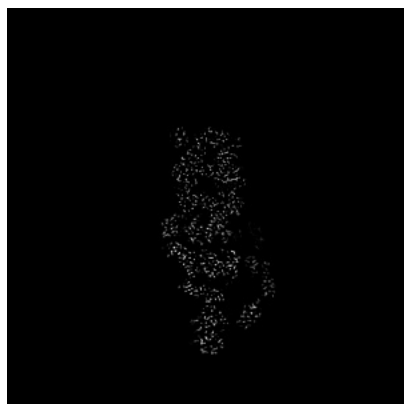
Z Index: 301



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: 273



Y Index: 319

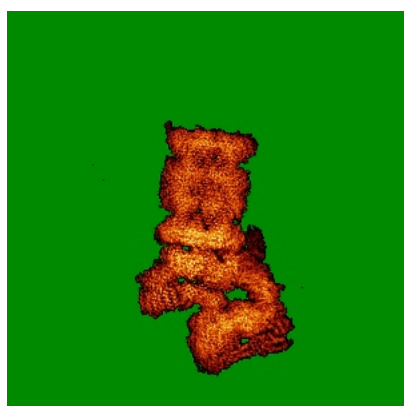


Z Index: 265

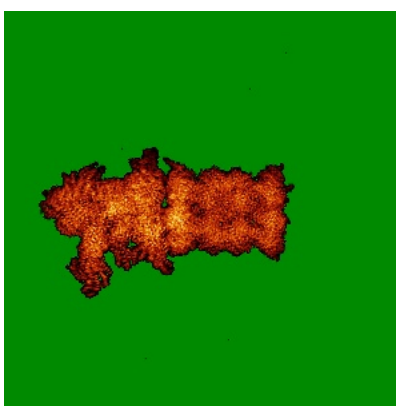
The images above show the largest variance slices of the map in three orthogonal directions.

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

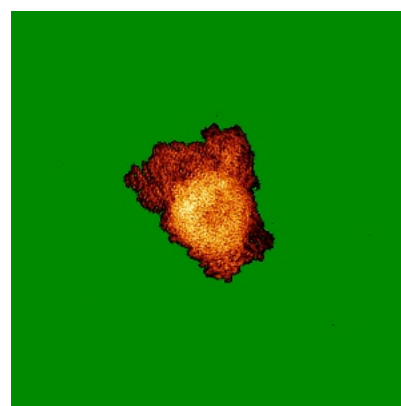
### 6.4.1 Primary map



X



Y

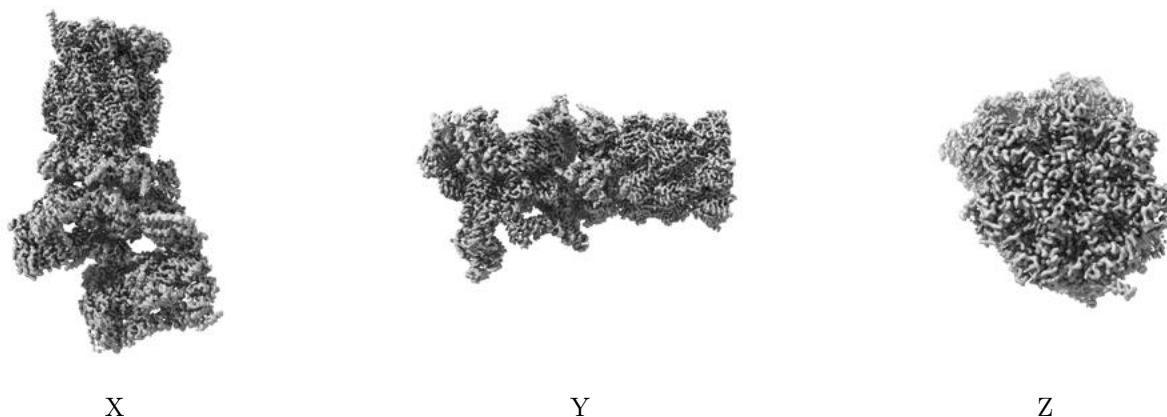


Z

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 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

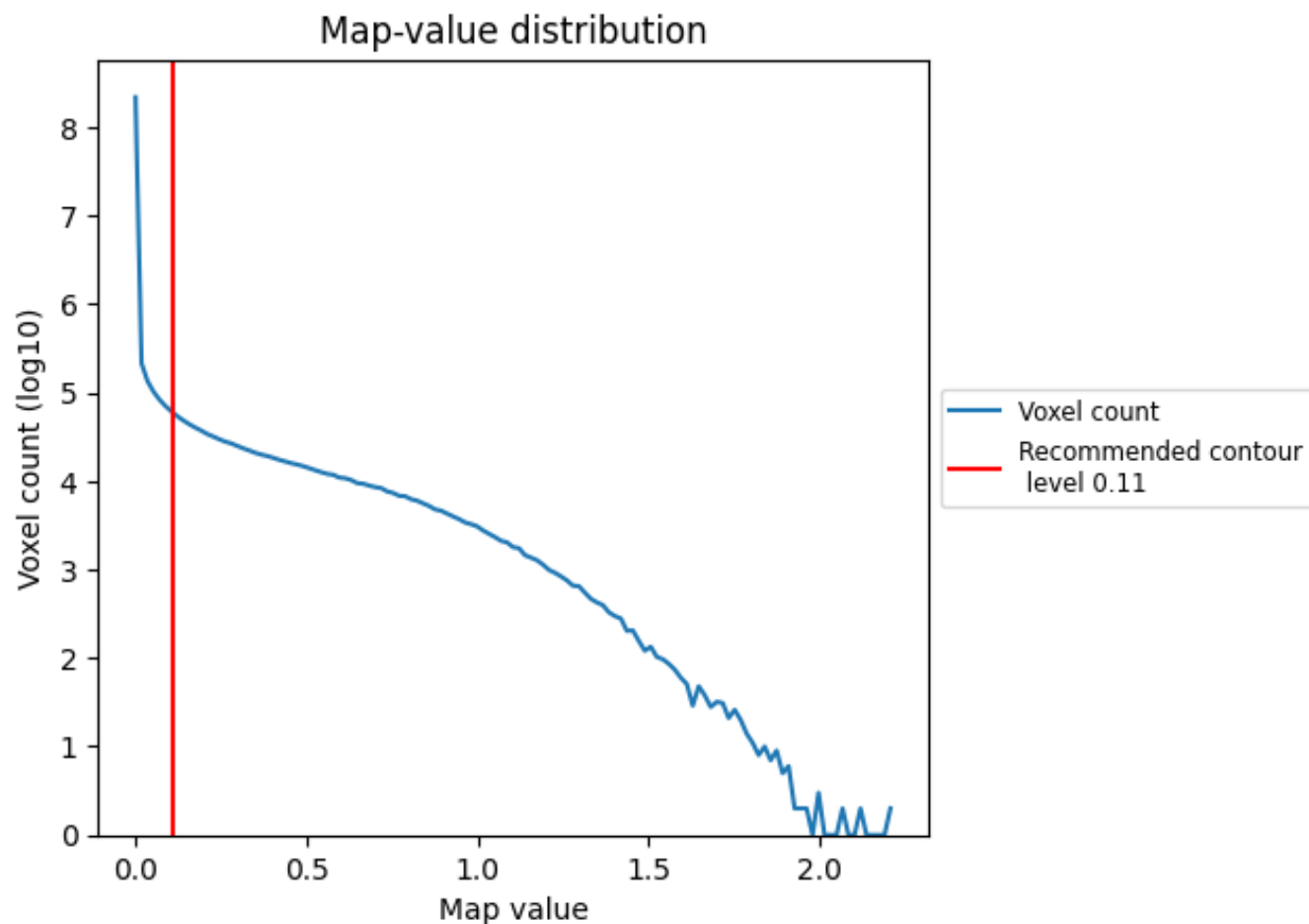
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

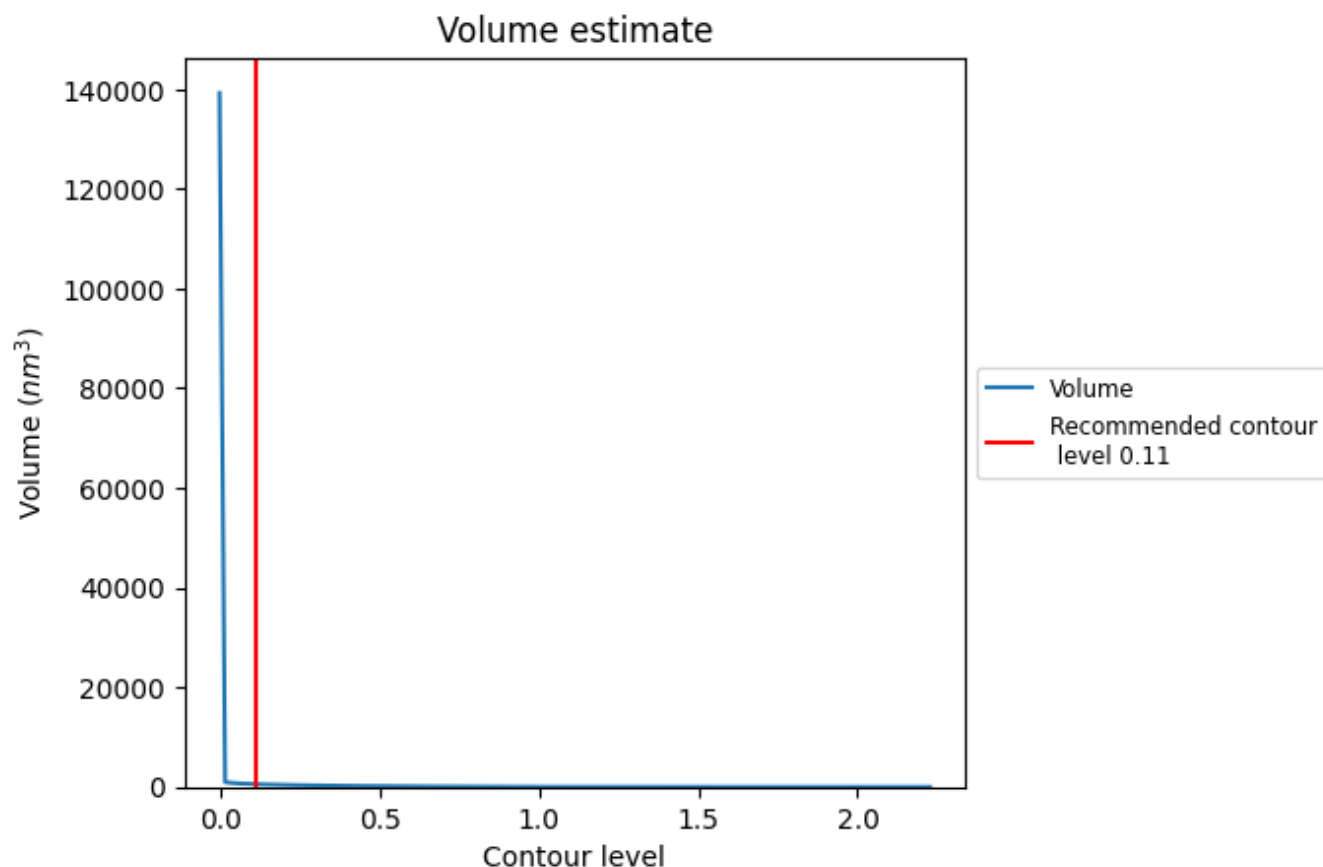
This section contains the results of statistical analysis of the map.

### 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.

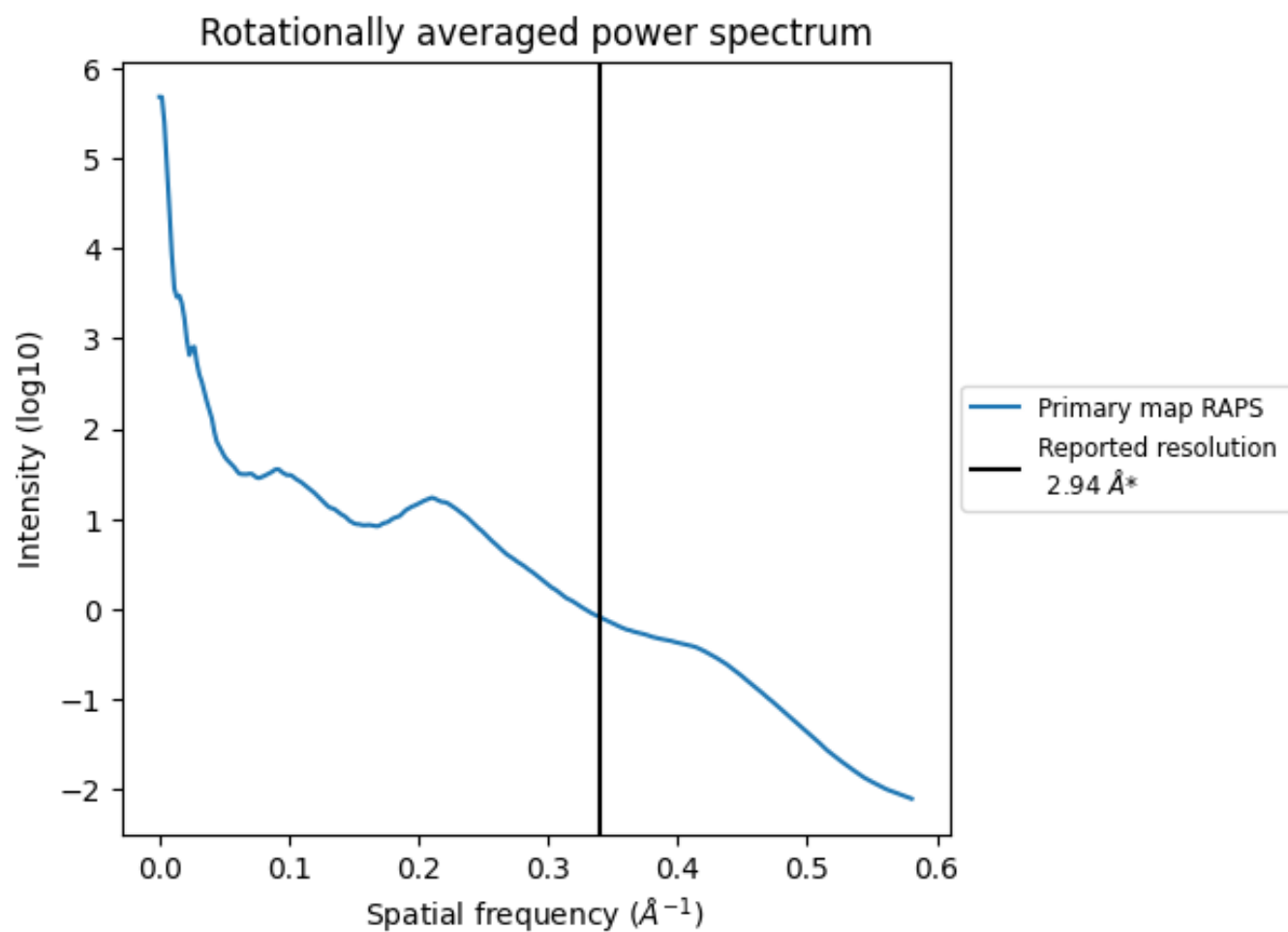
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 569  $\text{nm}^3$ ; this corresponds to an approximate mass of 514 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 0.340 Å<sup>-1</sup>

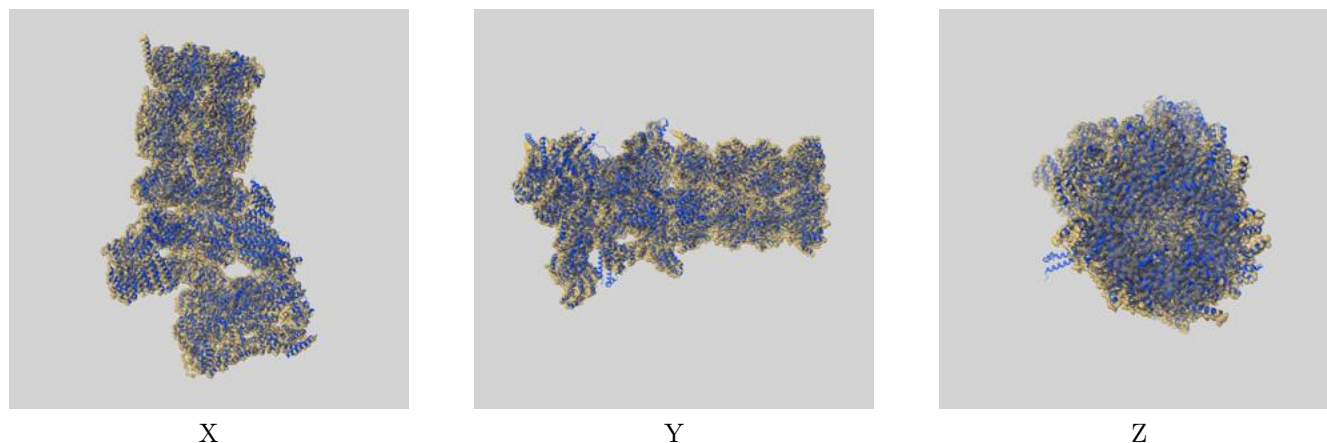
## 8 Fourier-Shell correlation ⓘ

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

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

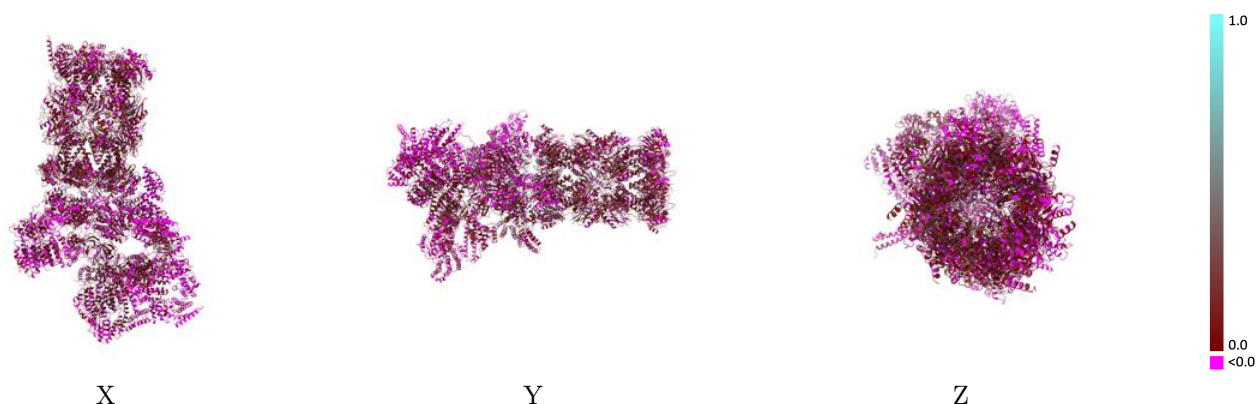
This section contains information regarding the fit between EMDB map EMD-49509 and PDB model 9NKI. Per-residue inclusion information can be found in section [3](#) on page [13](#).

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



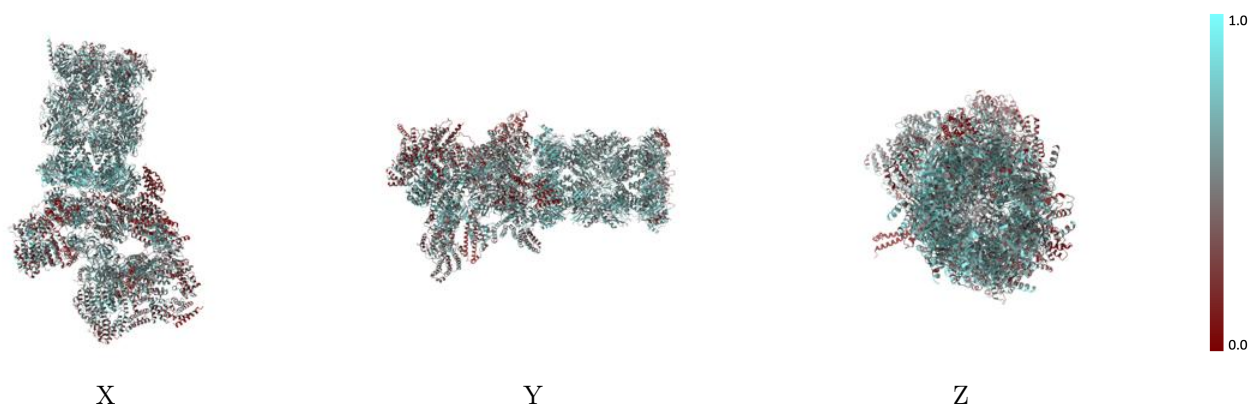
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

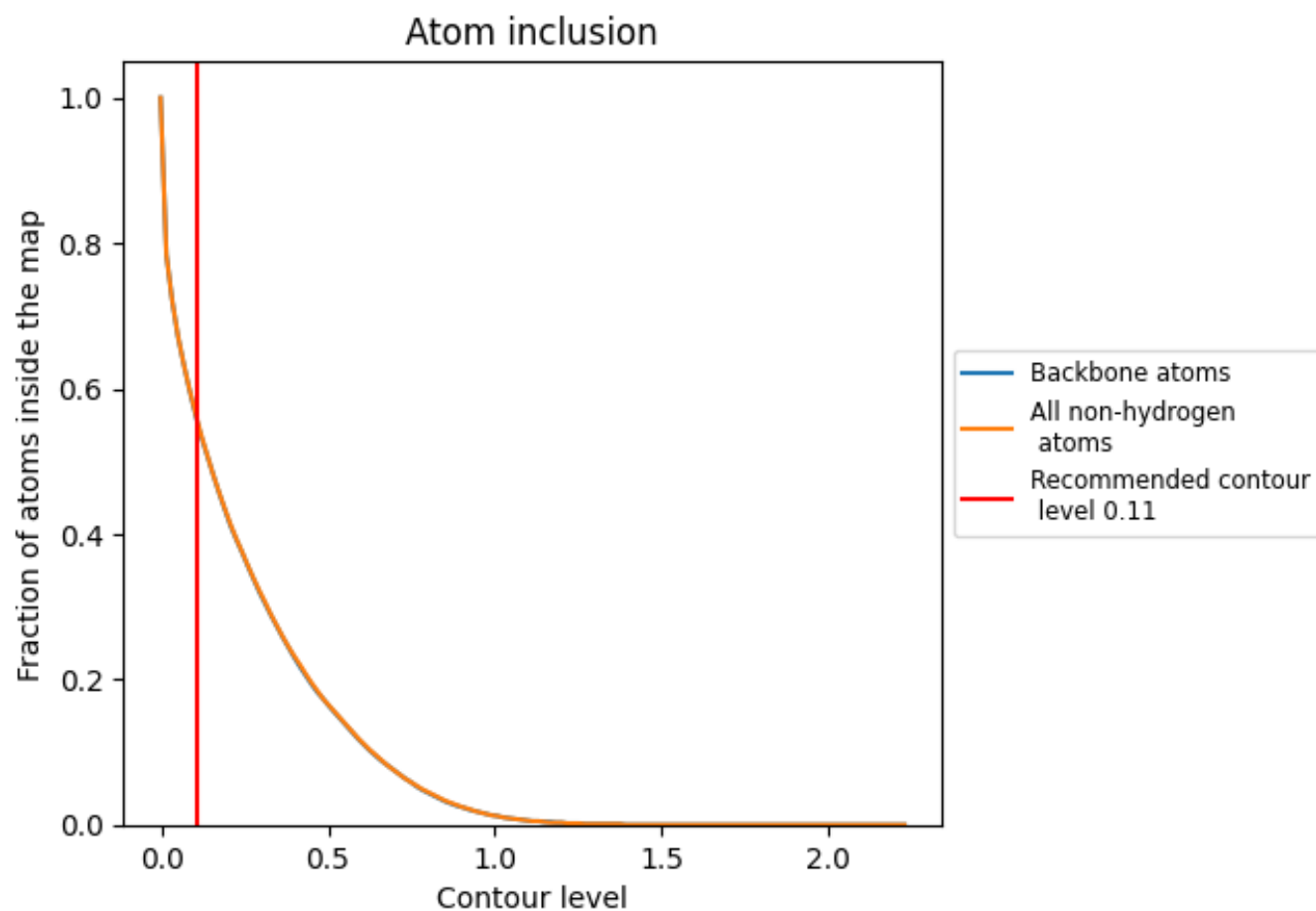
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.11).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 55% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5530	 0.1090
A	 0.5720	 0.1290
B	 0.5120	 0.0770
C	 0.4780	 0.0660
D	 0.5940	 0.1290
E	 0.5650	 0.1400
F	 0.5130	 0.1220
G	 0.7030	 0.1770
H	 0.7340	 0.1890
I	 0.6730	 0.1470
J	 0.6880	 0.1260
K	 0.6650	 0.1480
L	 0.7190	 0.1760
M	 0.6970	 0.1680
N	 0.6120	 0.1600
O	 0.6280	 0.1440
P	 0.5850	 0.1260
Q	 0.6000	 0.1180
R	 0.6000	 0.1110
S	 0.5920	 0.1620
T	 0.6210	 0.1430
U	 0.5350	 0.0880
V	 0.4600	 0.0390
W	 0.5510	 0.1450
X	 0.3610	 0.0240
Y	 0.5110	 0.0730
Z	 0.5910	 0.1270
a	 0.5020	 0.0680
b	 0.4300	 0.0320
c	 0.6090	 0.1450
d	 0.3720	 0.0070
e	 0.2950	 0.0400
f	 0.4580	 0.0460
g	 0.5780	 0.1480
h	 0.6190	 0.1490



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Chain	Atom inclusion	Q-score
i	 0.5650	 0.1080
j	 0.5520	 0.0850
k	 0.5120	 0.0800
l	 0.5760	 0.1200
m	 0.6010	 0.1490
n	 0.5970	 0.1310
o	 0.5960	 0.1520
p	 0.6030	 0.1280
q	 0.5900	 0.1070
r	 0.5880	 0.1280
s	 0.5970	 0.1390
t	 0.6210	 0.1730
v	 0.7000	 0.2410
z	 0.4910	 0.0950