Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 02:42 PM UTC

PDB ID	:	9M2W / pdb_00009m2w
EMDB ID	:	EMD-63592
Title	:	The cryo-EM structure of 26S proteasome-Midnolin complex in the MD state
Authors	:	Wang, H.Y.; Xu, W.Q.
Deposited on	:	2025-02-28
Resolution	:	3.31 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

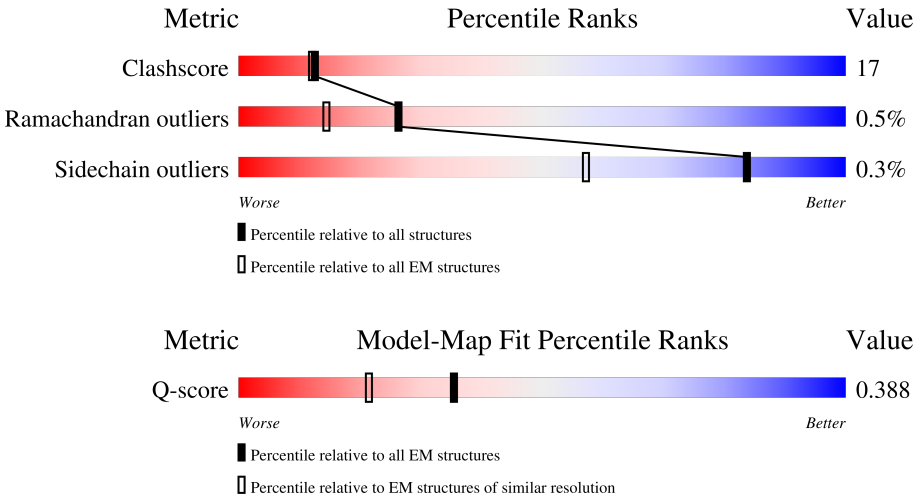
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.31 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14550 (2.81 - 3.81)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	63% 31% • •
2	B	440	60% 29% • 9%
3	C	406	65% 27% 8%
4	D	418	63% 27% 9%

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Mol	Chain	Length	Quality of chain
5	E	389	60% 20% 19%
6	F	439	53% 23% 24%
7	G	246	74% 23%
7	g	246	70% 26%
8	H	234	77% 21%
8	h	234	78% 19%
9	I	261	72% 23% 5%
9	i	261	75% 19% 6%
10	J	248	71% 24%
10	j	248	73% 20% 7%
11	K	241	74% 24%
11	k	241	75% 20% 6%
12	L	263	62% 29% 10%
12	l	263	70% 19% 10%
13	M	255	78% 16% 5%
13	m	255	72% 22% 6%
14	N	239	67% 16% 16%
14	n	239	72% 12% 16%
15	O	277	66% 14% 20%
15	o	277	68% 12% 21%
16	P	205	77% 23%
16	p	205	86% 13%
17	Q	201	79% 19%
17	q	201	86% 11%
18	R	263	63% 14% 24%

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Mol	Chain	Length	Quality of chain
18	r	263	63% 13% 24%
19	S	241	78% 11% 12%
19	s	241	76% 12% 12%
20	T	264	64% 17% 19%
20	t	264	66% 15% 19%
21	U	953	58% 26% 16%
22	V	534	55% 23% 21%
23	W	456	60% 39%
24	X	422	66% 23% 10%
25	Y	389	64% 33%
26	Z	324	62% 27% 11%
27	a	376	61% 38%
28	b	377	32% 18% 50%
29	c	310	67% 21% 12%
30	d	350	51% 15% 34%
31	e	70	34% 19% 46%
32	f	908	56% 40%
33	v	15	73% 27%
34	u	491	6% 92%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	ATP	A	501	-	-	X	-
35	ATP	C	501	-	-	X	-
35	ATP	F	501	-	-	X	-
36	ADP	D	501	-	-	X	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 98427 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	414	3062	1925	542	581	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	401	2901	1806	504	582	9	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	372	2723	1718	486	506	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	2777	1747	483	539	8	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	314	2324	1448	426	438	12	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	333	2421	1510	430	468	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	239	Total	C	N	O	S	0	0
			1798	1144	305	337	12		
7	g	235	Total	C	N	O	S	0	0
			1765	1124	297	332	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	230	Total	C	N	O	S	0	0
			1745	1117	294	329	5		
8	h	227	Total	C	N	O	S	0	0
			1679	1070	287	318	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	247	Total	C	N	O	S	0	0
			1900	1206	322	362	10		
9	i	246	Total	C	N	O	S	0	0
			1851	1165	319	359	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1839	1152	327	355	5		
10	j	231	Total	C	N	O	S	0	0
			1622	1014	293	310	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	237	Total	C	N	O	S	0	0
			1773	1114	295	354	10		
11	k	227	Total	C	N	O	S	0	0
			1677	1059	275	335	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1847	1157	332	347	11		
12	l	237	Total	C	N	O	S	0	0
			1831	1150	330	341	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	241	Total	C	N	O	S	0	0
			1843	1171	319	343	10		
13	m	240	Total	C	N	O	S	0	0
			1833	1164	311	348	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	200	Total	C	N	O	S	0	0
			1482	927	255	288	12		
14	n	201	Total	C	N	O	S	0	0
			1488	935	257	284	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	221	Total	C	N	O	S	0	0
			1637	1033	282	310	12		
15	o	220	Total	C	N	O	S	0	0
			1629	1027	278	312	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	204	Total	C	N	O	S	0	0
			1553	996	262	276	19		
16	p	204	Total	C	N	O	S	0	0
			1579	1006	264	290	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	197	Total	C	N	O	S	0	0
			1559	1002	267	281	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	197	Total	C	N	O	S	0	0
			1551	996	267	280	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	201	Total	C	N	O	S	0	0
			1536	970	271	286	9		
18	r	200	Total	C	N	O	S	0	0
			1540	973	273	285	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	213	Total	C	N	O	S	0	0
			1627	1032	284	301	10		
19	s	212	Total	C	N	O	S	0	0
			1620	1030	277	303	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	215	Total	C	N	O	S	0	0
			1674	1057	288	317	12		
20	t	215	Total	C	N	O	S	0	0
			1663	1052	289	310	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	803	Total	C	N	O	S	0	0
			5845	3671	1007	1130	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	420	Total	C	N	O	S	0	0
			3053	1923	532	593	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	456	Total	C	N	O	S	0	0
			3348	2085	584	663	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	381	Total	C	N	O	S	0	0
			2804	1765	480	550	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	379	Total	C	N	O	S	0	0
			2990	1901	512	564	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	287	Total	C	N	O	S	0	0
			2081	1318	361	399	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	373	Total	C	N	O	S	0	0
			2676	1691	456	518	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	189	Total	C	N	O	S	0	0
			1336	823	246	263	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	274	Total	C	N	O	S	0	0
			2008	1274	348	380	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	232	Total	C	N	O	S	0	0
			1772	1143	289	333	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
31	e	38	Total	C	N	O	0	0
			280	165	49	66		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	879	Total	C	N	O	S	0	0
			6339	3965	1079	1264	31		

- Molecule 33 is a protein called Substrate.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	v	15	Total	C	N	O	0	0
			75	45	15	15		

- Molecule 34 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	37	Total	C	N	O	S	0	0
			320	189	78	52	1		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	0	MET	-	initiating methionine	UNP Q504T8
u	469	GLY	-	expression tag	UNP Q504T8
u	470	SER	-	expression tag	UNP Q504T8
u	471	ASP	-	expression tag	UNP Q504T8
u	472	TYR	-	expression tag	UNP Q504T8
u	473	LYS	-	expression tag	UNP Q504T8
u	474	ASP	-	expression tag	UNP Q504T8
u	475	ASP	-	expression tag	UNP Q504T8
u	476	ASP	-	expression tag	UNP Q504T8
u	477	ASP	-	expression tag	UNP Q504T8
u	478	LYS	-	expression tag	UNP Q504T8
u	479	GLY	-	expression tag	UNP Q504T8

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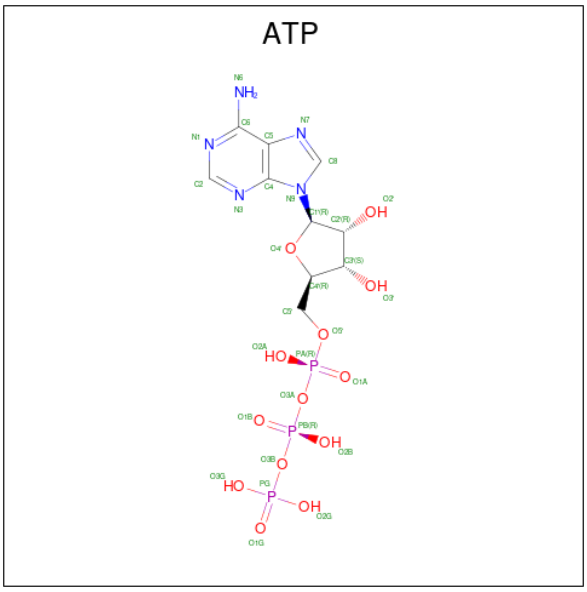
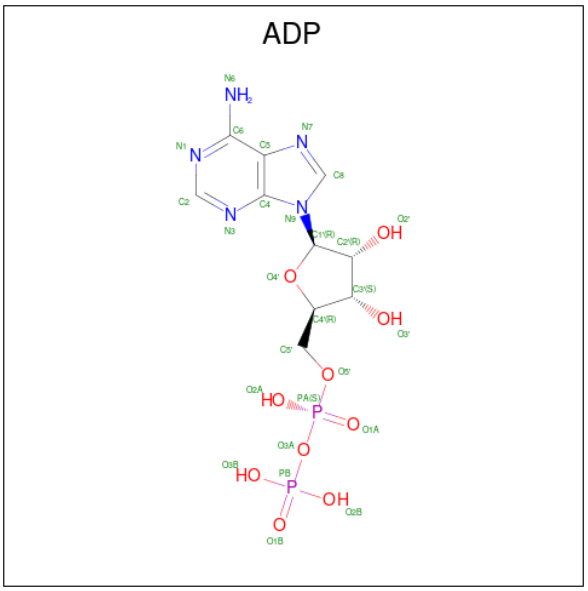
Chain	Residue	Modelled	Actual	Comment	Reference
u	480	SER	-	expression tag	UNP Q504T8
u	481	HIS	-	expression tag	UNP Q504T8
u	482	HIS	-	expression tag	UNP Q504T8
u	483	HIS	-	expression tag	UNP Q504T8
u	484	HIS	-	expression tag	UNP Q504T8
u	485	HIS	-	expression tag	UNP Q504T8
u	486	HIS	-	expression tag	UNP Q504T8
u	487	HIS	-	expression tag	UNP Q504T8
u	488	HIS	-	expression tag	UNP Q504T8
u	489	HIS	-	expression tag	UNP Q504T8
u	490	HIS	-	expression tag	UNP Q504T8

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



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

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



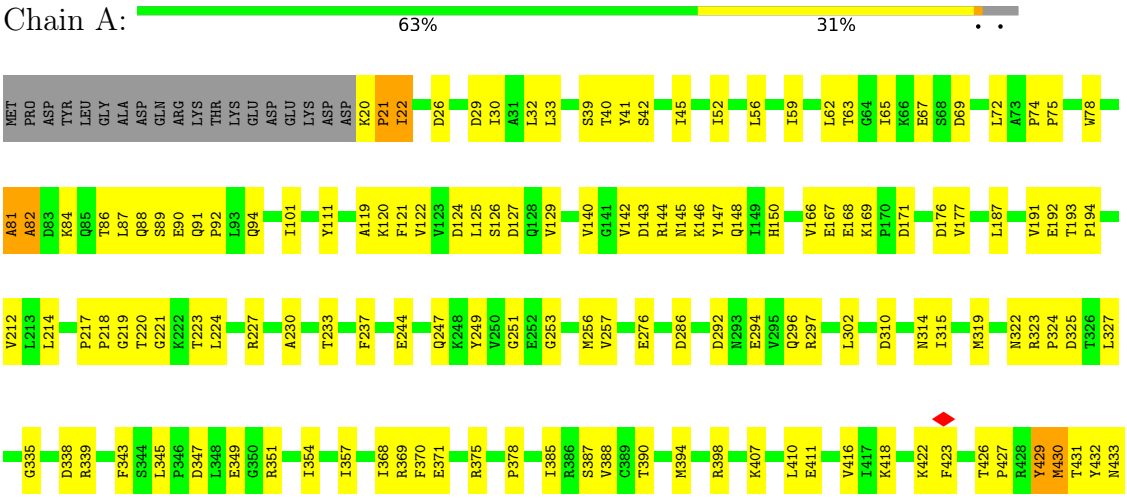
Mol	Chain	Residues	Atoms					AltConf
36	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

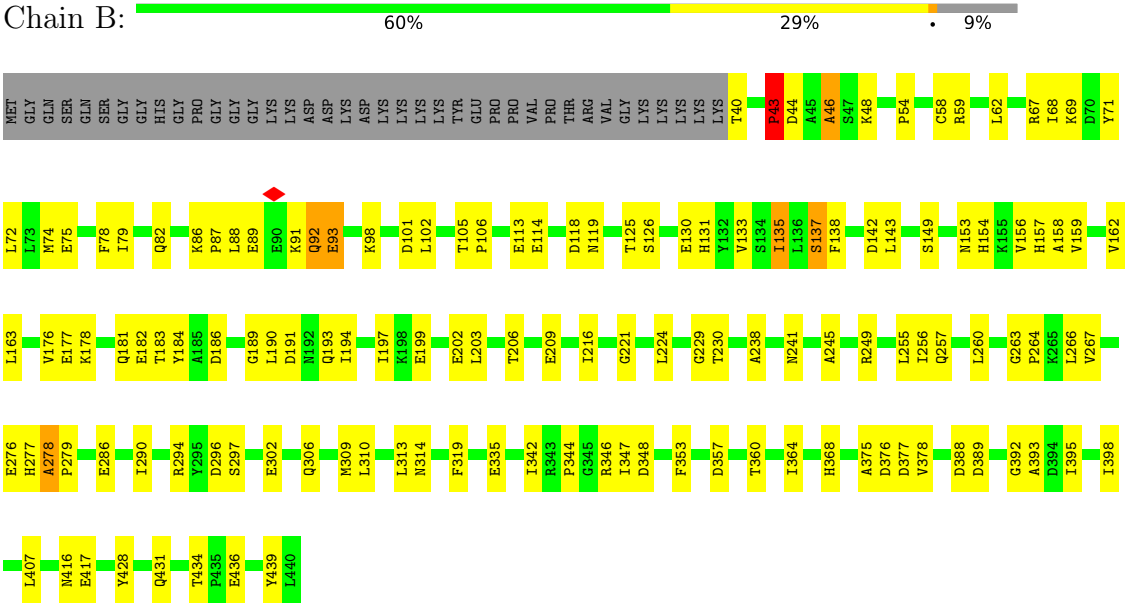
• Molecule 1: 26S proteasome regulatory subunit 7

Chain A:



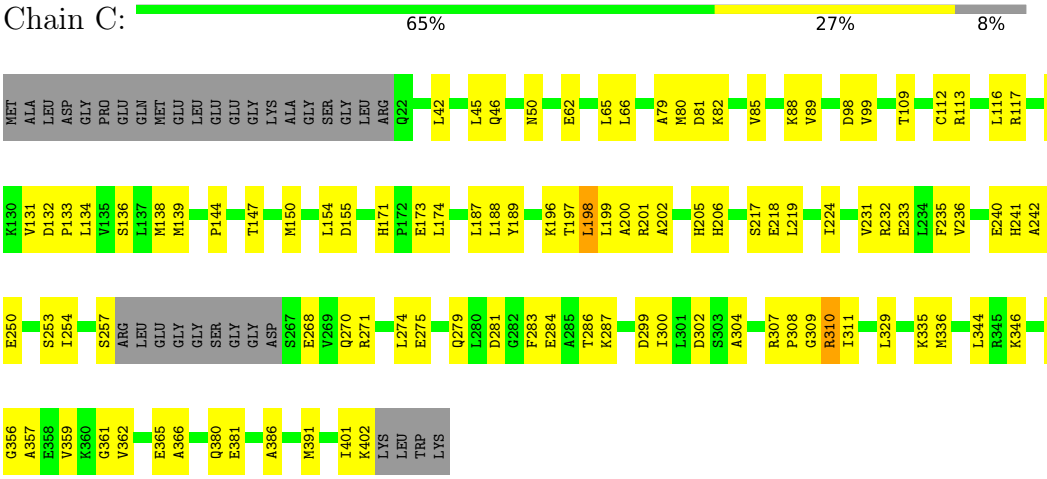
• Molecule 2: 26S proteasome regulatory subunit 4

Chain B:



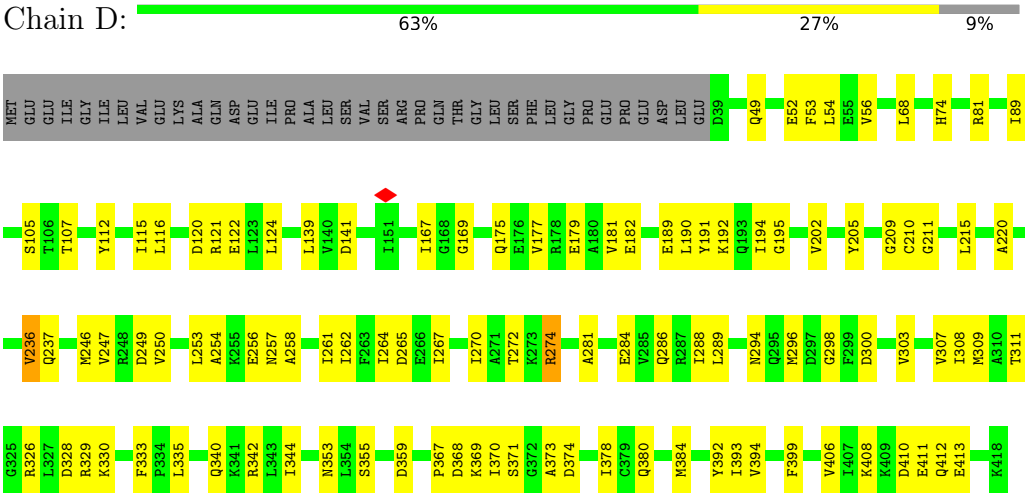
• Molecule 3: 26S proteasome regulatory subunit 8

Chain C:



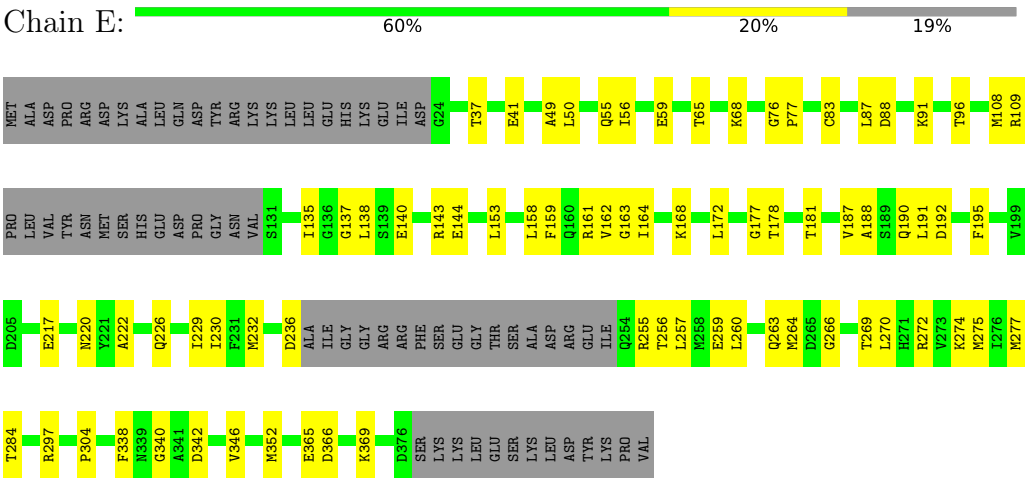
• Molecule 4: 26S proteasome regulatory subunit 6B

Chain D:



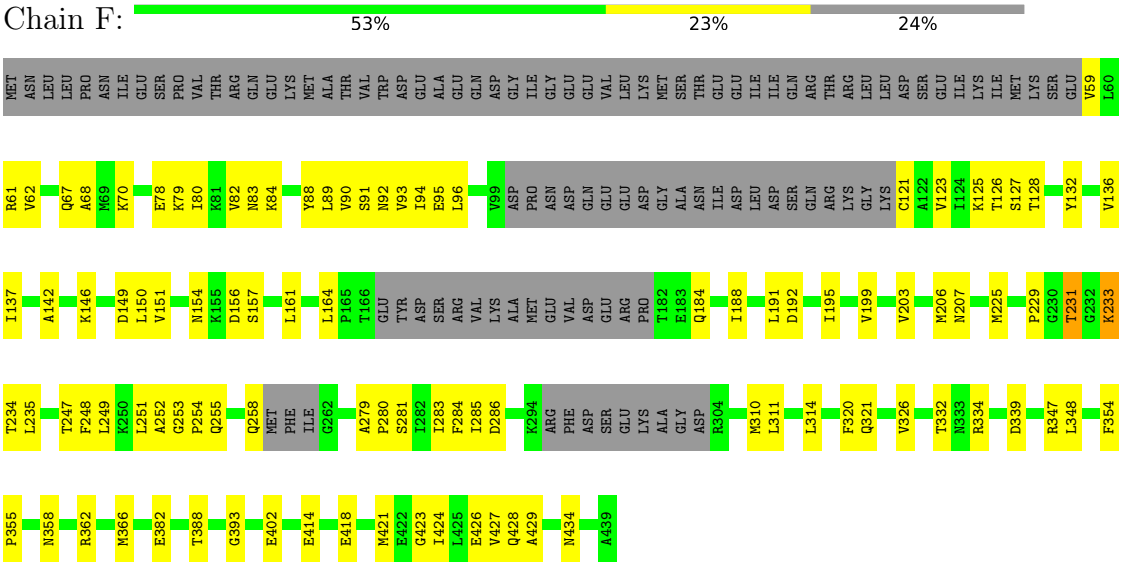
• Molecule 5: 26S proteasome regulatory subunit 10B

Chain E:



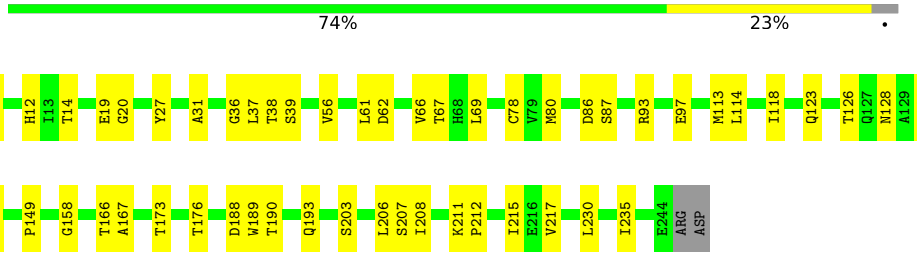
• Molecule 6: 26S proteasome regulatory subunit 6A

Chain F:



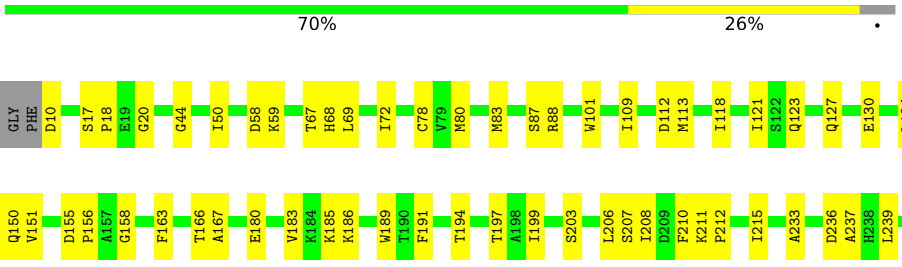
• Molecule 7: Proteasome subunit alpha type-6

Chain G:



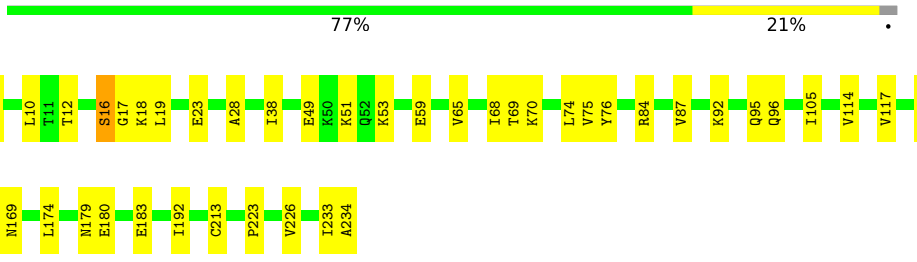
• Molecule 7: Proteasome subunit alpha type-6

Chain g:



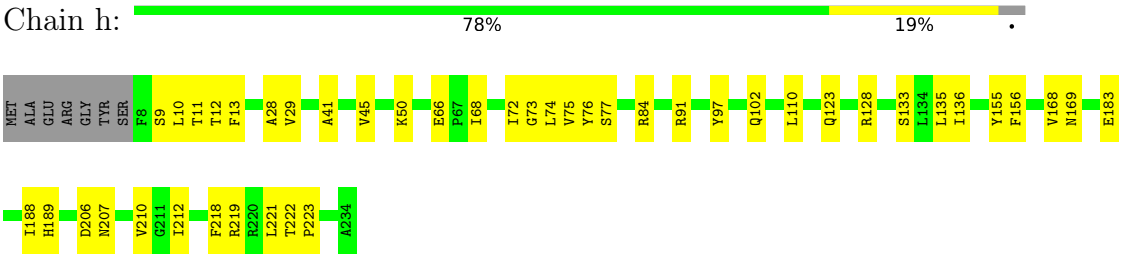
• Molecule 8: Proteasome subunit alpha type-2

Chain H:



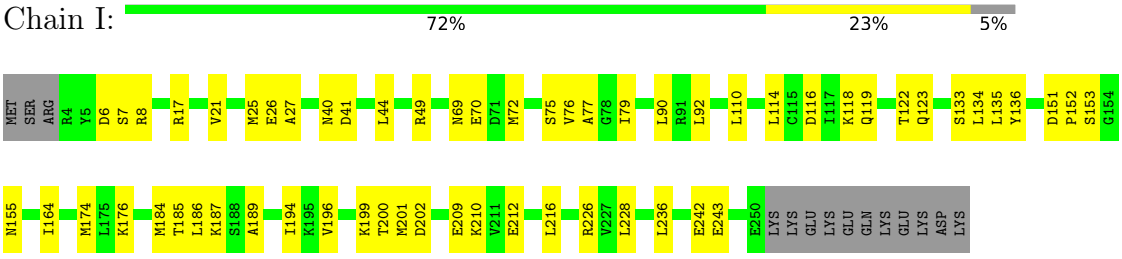
• Molecule 8: Proteasome subunit alpha type-2

Chain h:



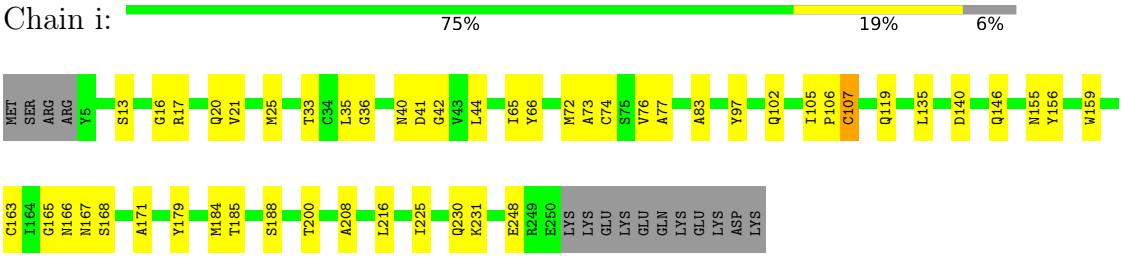
• Molecule 9: Proteasome subunit alpha type-4

Chain I:



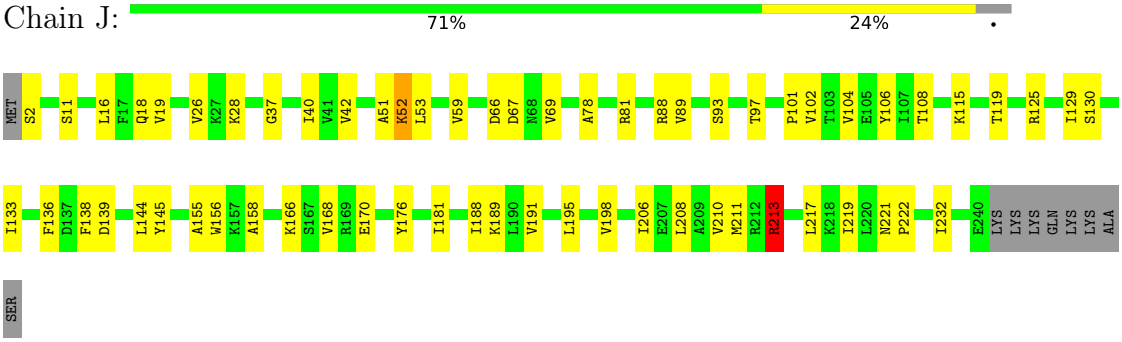
• Molecule 9: Proteasome subunit alpha type-4

Chain i:



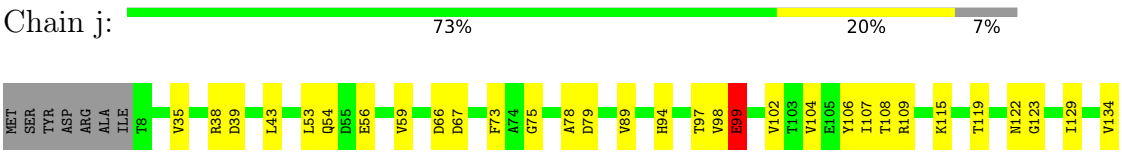
• Molecule 10: Proteasome subunit alpha type-7

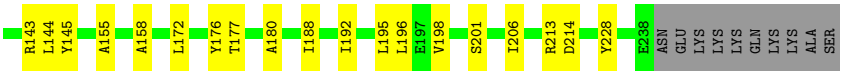
Chain J:



• Molecule 10: Proteasome subunit alpha type-7

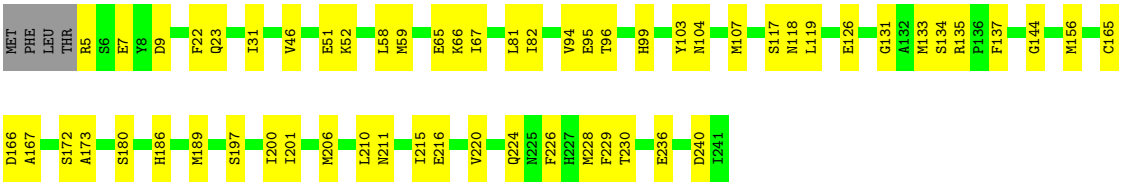
Chain j:





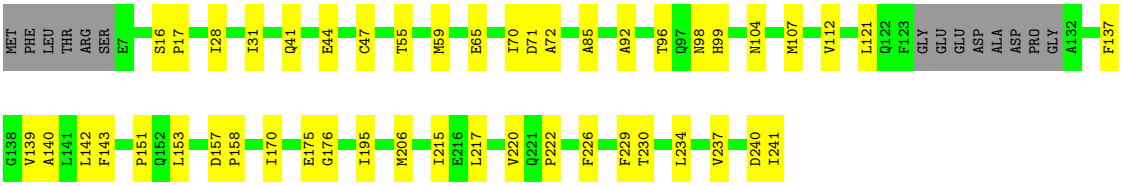
• Molecule 11: Proteasome subunit alpha type-5

Chain K:



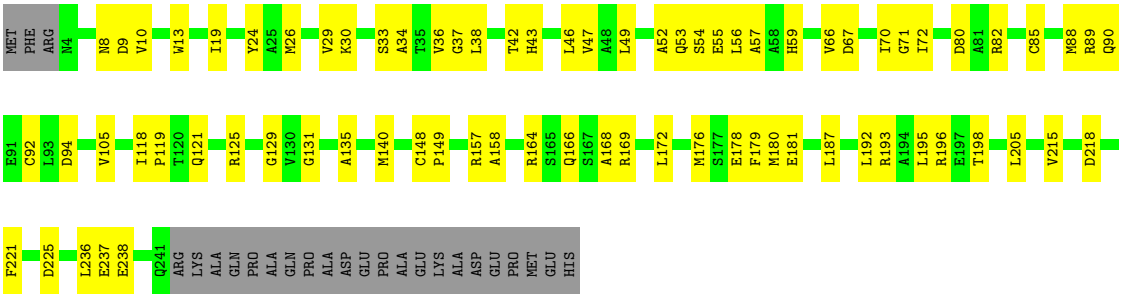
• Molecule 11: Proteasome subunit alpha type-5

Chain k:



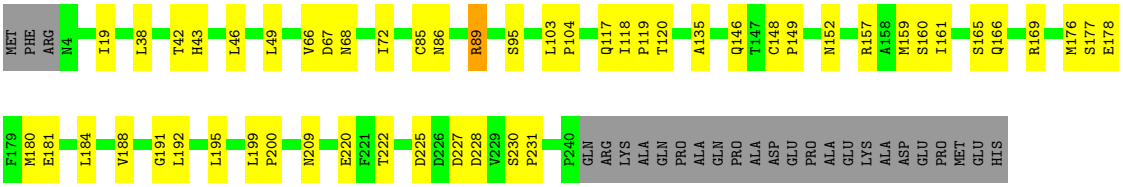
• Molecule 12: Proteasome subunit alpha type-1

Chain L:



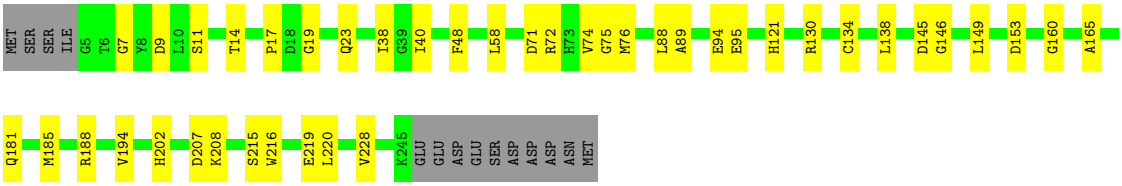
• Molecule 12: Proteasome subunit alpha type-1

Chain l:



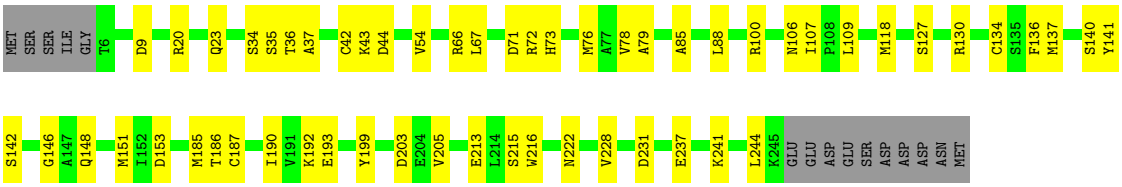
• Molecule 13: Proteasome subunit alpha type-3

Chain M:



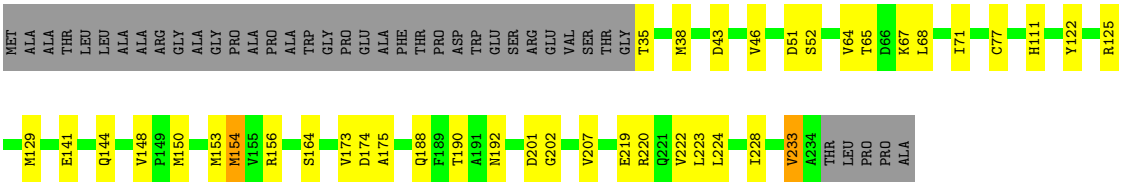
• Molecule 13: Proteasome subunit alpha type-3

Chain m:



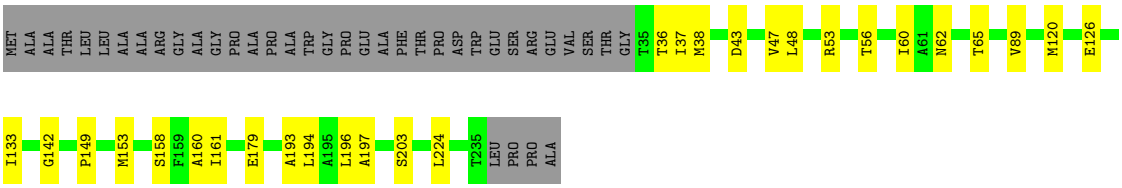
• Molecule 14: Proteasome subunit beta type-6

Chain N:



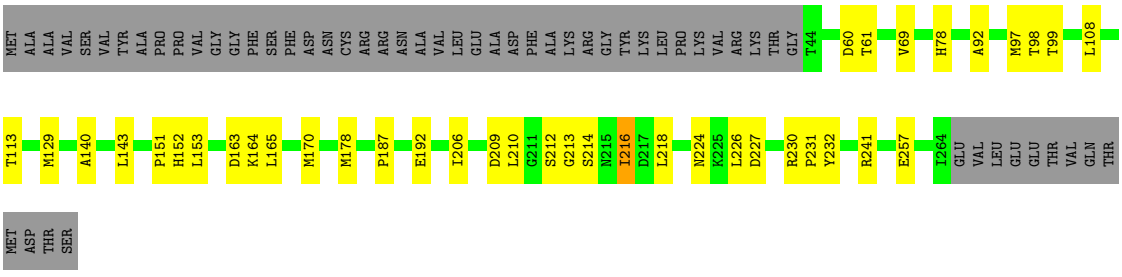
• Molecule 14: Proteasome subunit beta type-6

Chain n:



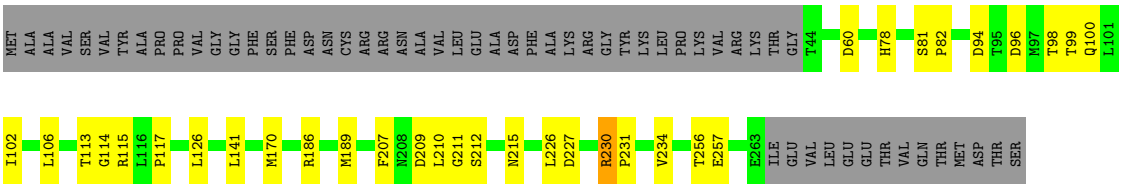
• Molecule 15: Proteasome subunit beta type-7

Chain O:



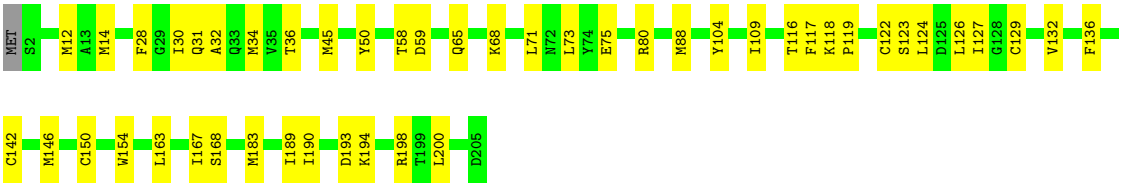
• Molecule 15: Proteasome subunit beta type-7

Chain o:



• Molecule 16: Proteasome subunit beta type-3

Chain P:



• Molecule 16: Proteasome subunit beta type-3

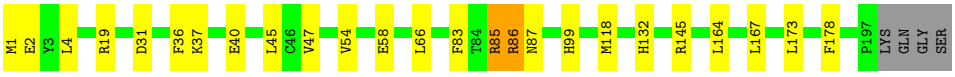
Chain p:

• Molecule 17: Proteasome subunit beta type-2

Chain Q:

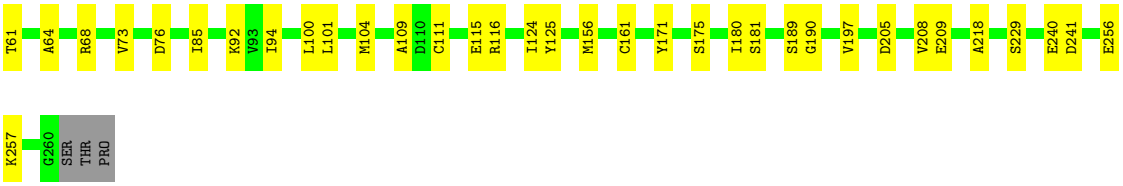
• Molecule 17: Proteasome subunit beta type-2

Chain q:



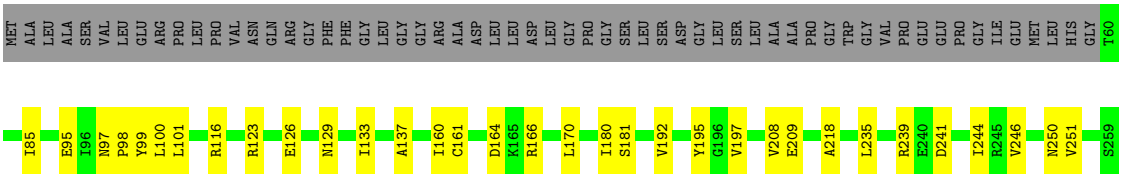
• Molecule 18: Proteasome subunit beta type-5

Chain R:



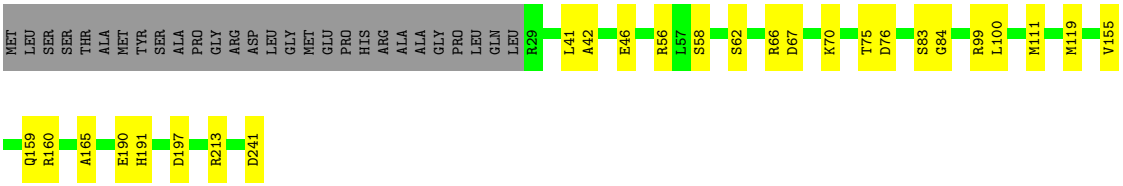
• Molecule 18: Proteasome subunit beta type-5

Chain r:



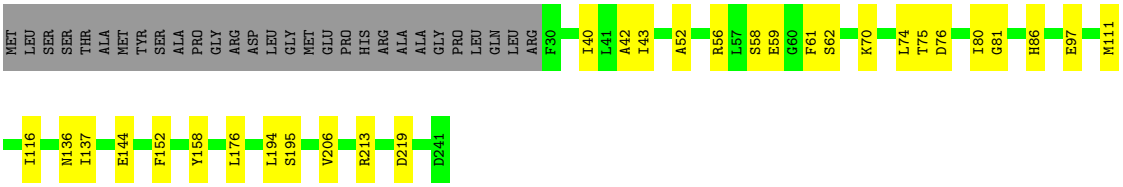
• Molecule 19: Proteasome subunit beta type-1

Chain S:



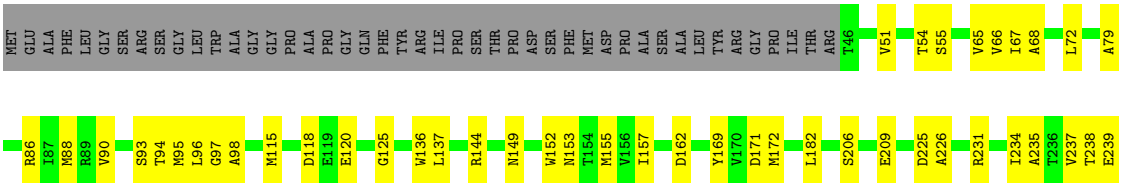
• Molecule 19: Proteasome subunit beta type-1

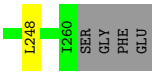
Chain s:



• Molecule 20: Proteasome subunit beta type-4

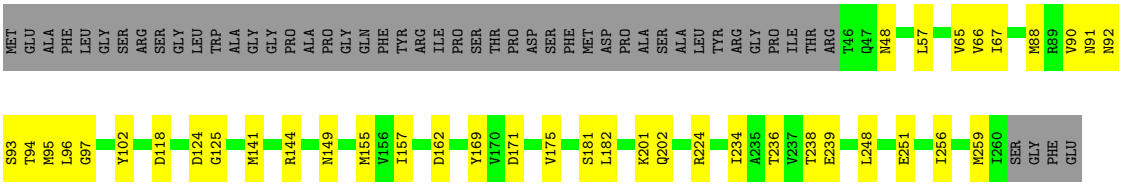
Chain T:





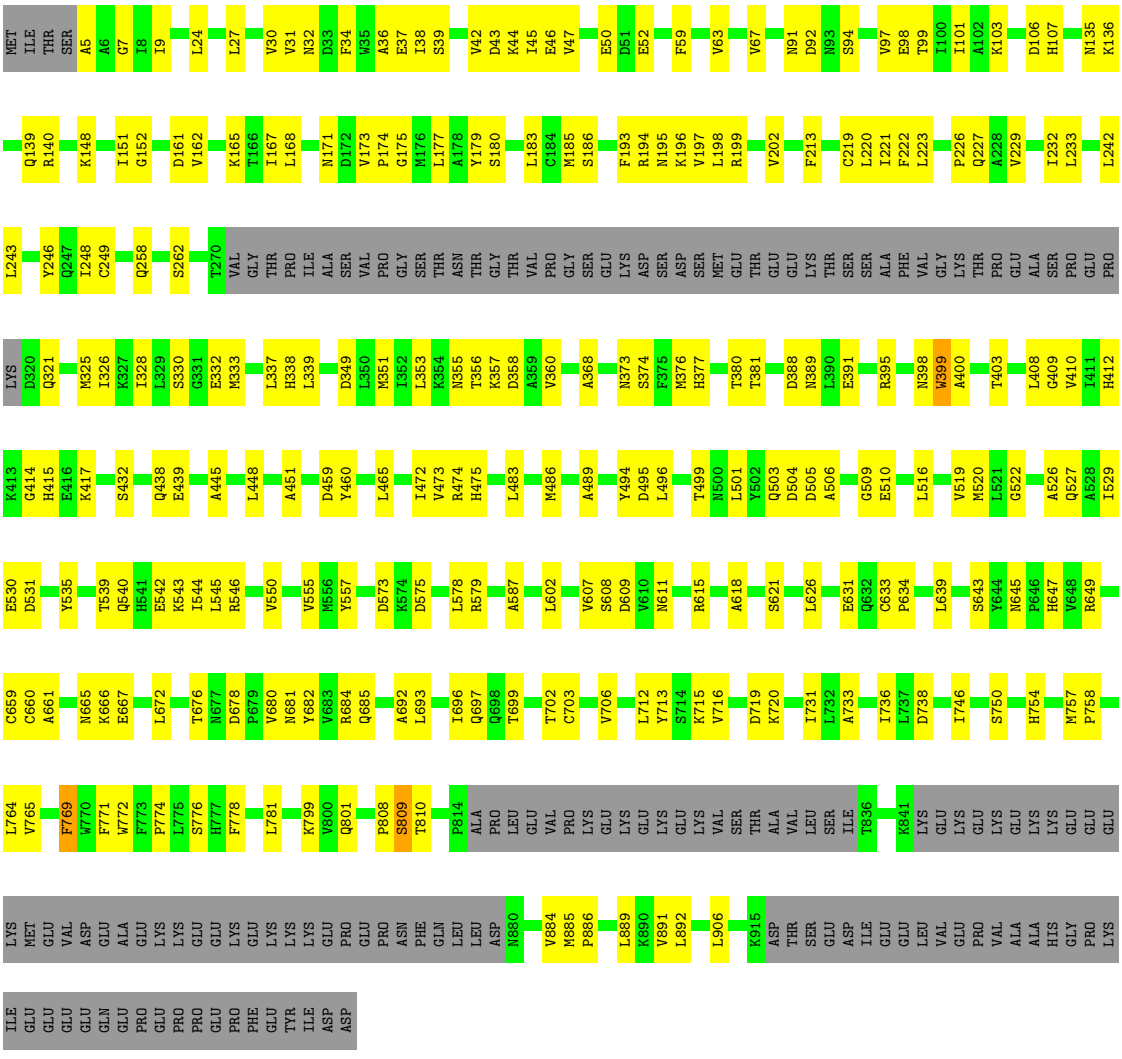
• Molecule 20: Proteasome subunit beta type-4

Chain t:



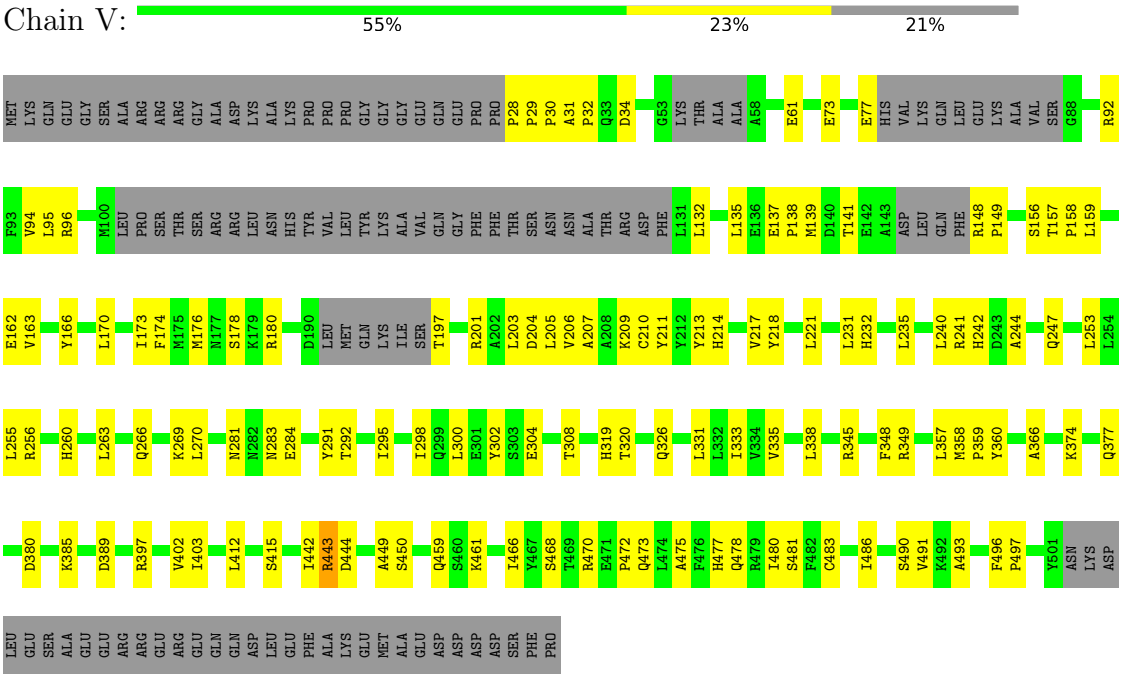
• Molecule 21: 26S proteasome non-ATPase regulatory subunit 1

Chain U:



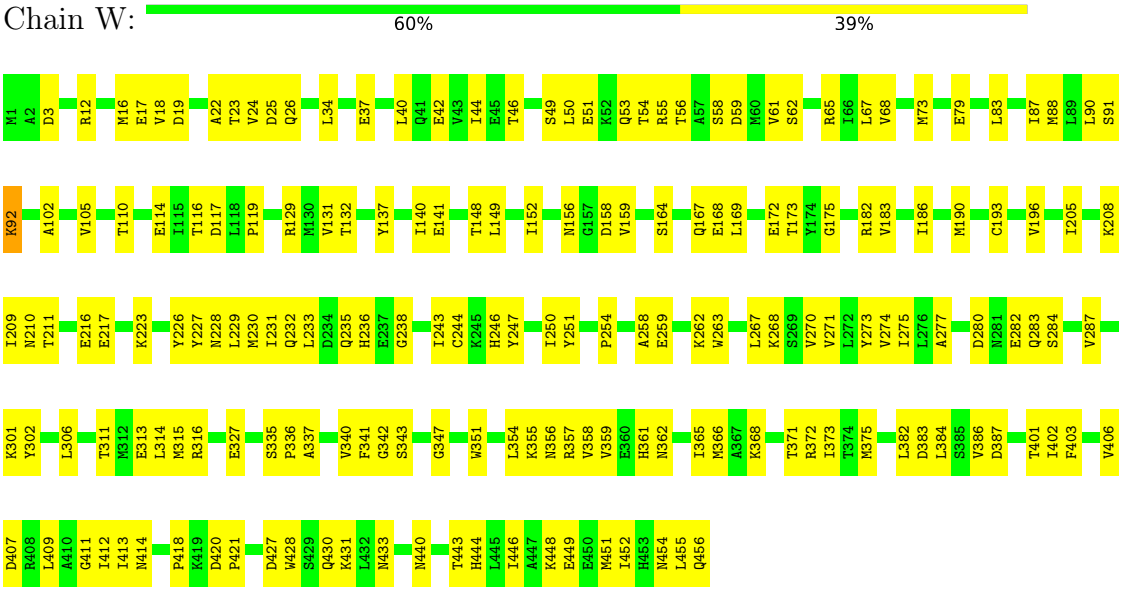
• Molecule 22: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



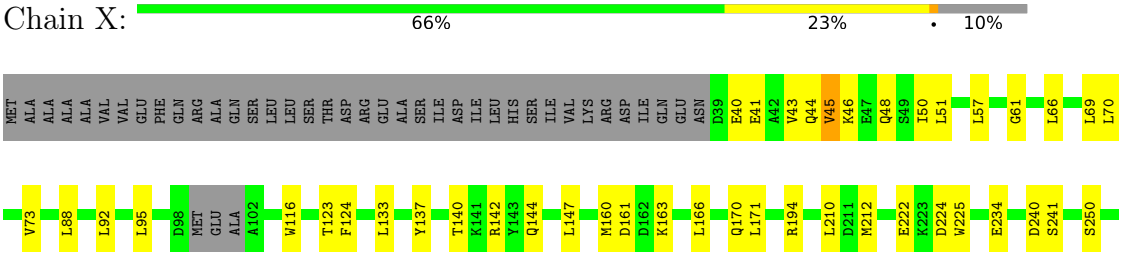
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 12

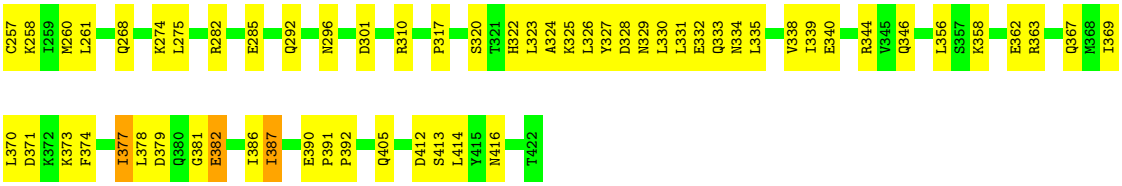
Chain W:



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

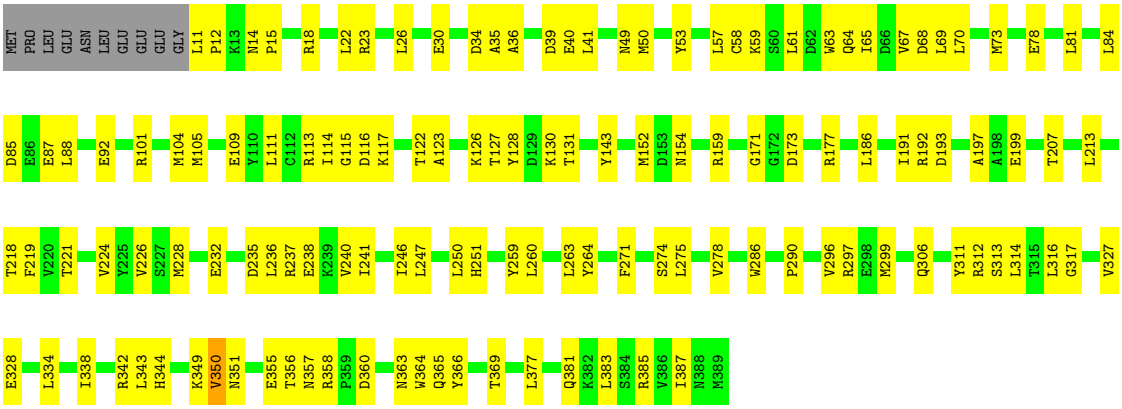
Chain X:





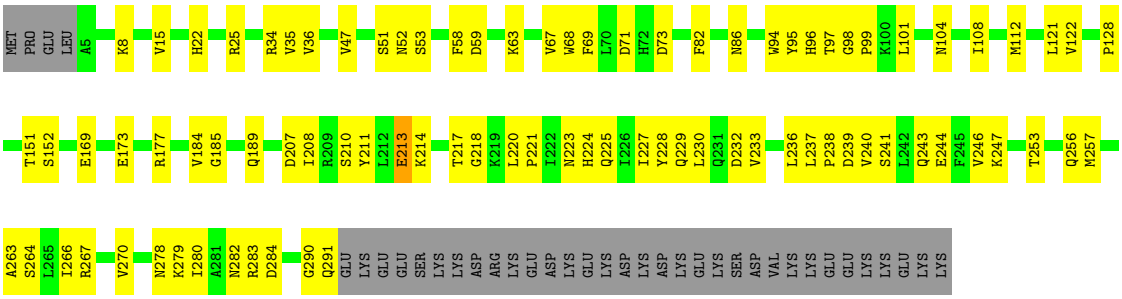
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 6

Chain Y:



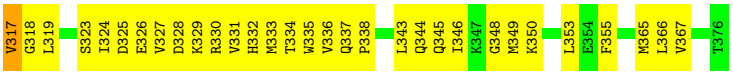
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:



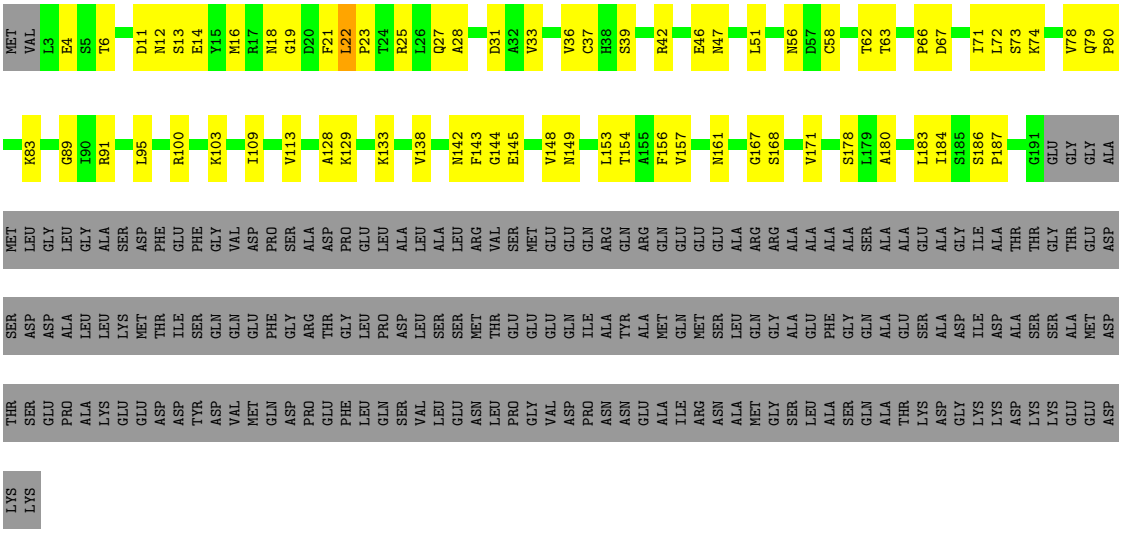
• Molecule 27: 26S proteasome non-ATPase regulatory subunit 13

Chain a:



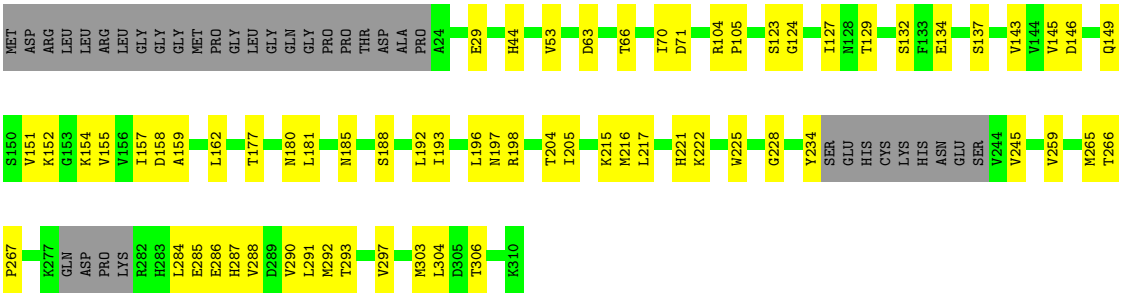
• Molecule 28: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



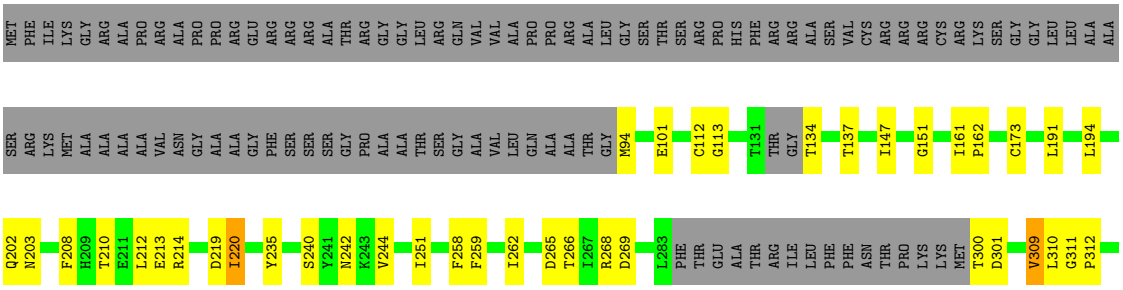
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 14

Chain c:



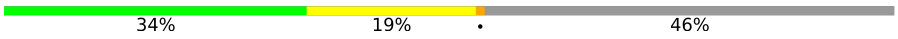
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 8

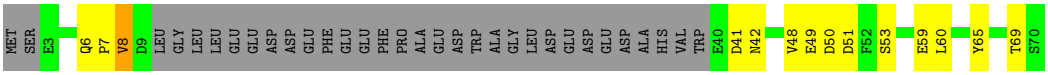
Chain d:



• Molecule 31: 26S proteasome complex subunit SEM1

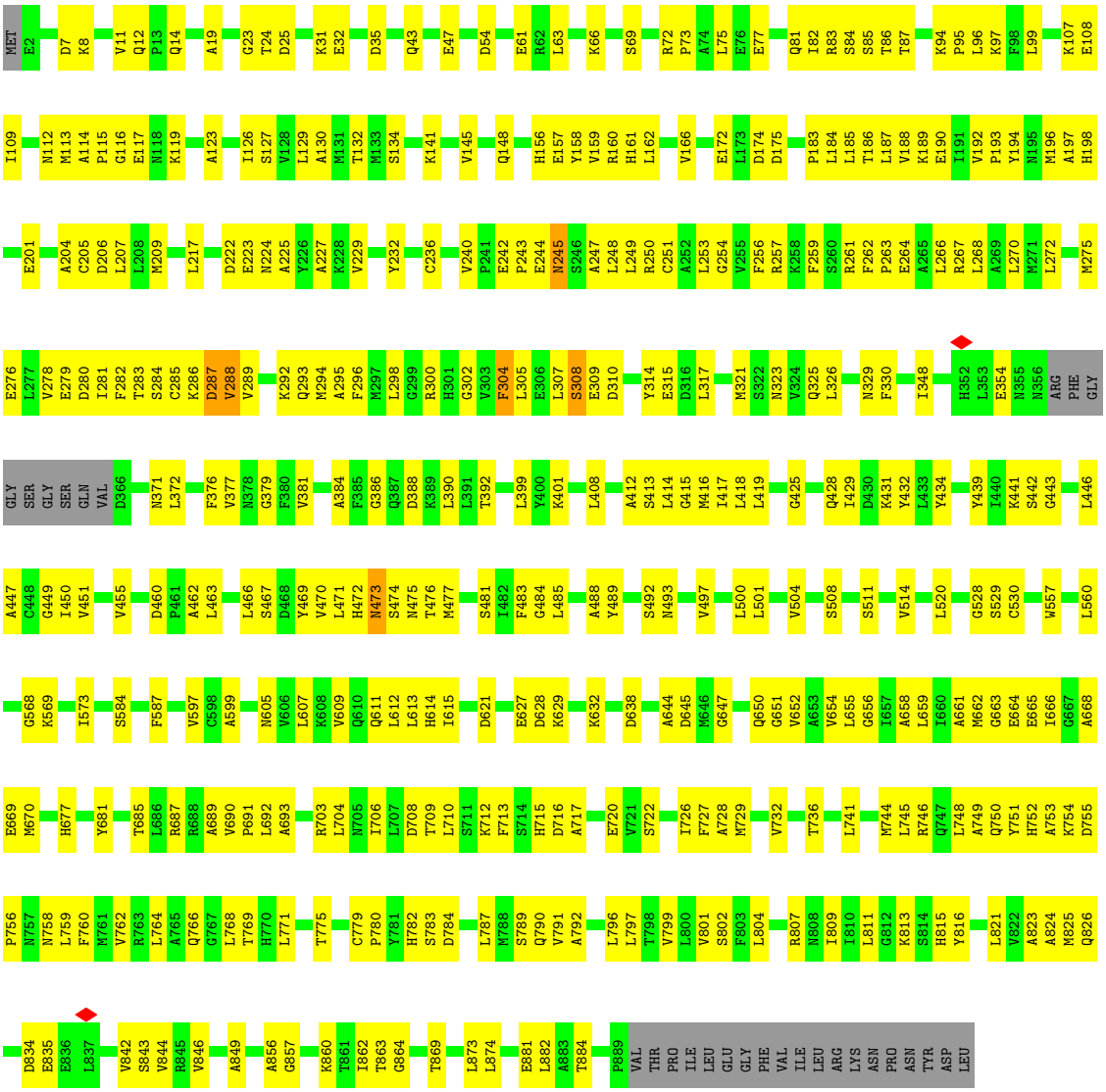
Chain e:





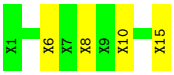
• Molecule 32: 26S proteasome non-ATPase regulatory subunit 2

Chain f:



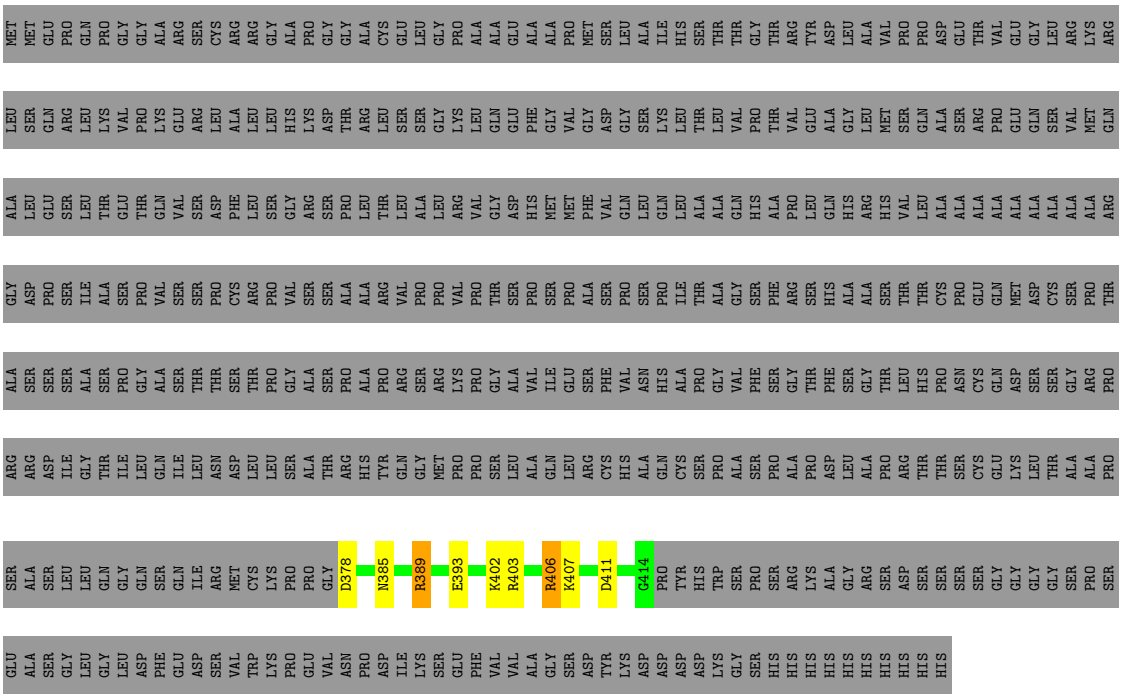
• Molecule 33: Substrate

Chain v:



• Molecule 34: Midnolin

Chain u: 6% 92%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	468422	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.551	Depositor
Minimum map value	-0.112	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	445.19998, 445.19998, 445.19998	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.39	0/3113	0.57	0/4227
2	B	0.38	0/2943	0.60	5/4005 (0.1%)
3	C	0.24	0/2759	0.45	1/3737 (0.0%)
4	D	0.19	0/2823	0.39	0/3838
5	E	0.13	0/2352	0.31	0/3179
6	F	0.23	0/2451	0.45	2/3322 (0.1%)
7	G	0.34	0/1830	0.42	0/2482
7	g	0.25	0/1797	0.33	0/2443
8	H	0.34	0/1784	0.41	0/2423
8	h	0.26	0/1715	0.36	0/2334
9	I	0.31	0/1930	0.39	0/2609
9	i	0.26	0/1879	0.39	0/2545
10	J	0.33	0/1865	0.43	0/2524
10	j	0.23	0/1645	0.32	0/2247
11	K	0.30	0/1800	0.37	0/2437
11	k	0.25	0/1702	0.34	0/2309
12	L	0.32	0/1882	0.43	0/2549
12	l	0.26	0/1866	0.35	0/2527
13	M	0.33	0/1878	0.43	0/2535
13	m	0.25	0/1868	0.30	0/2526
14	N	0.39	0/1507	0.44	0/2042
14	n	0.34	0/1514	0.42	2/2051 (0.1%)
15	O	0.31	0/1664	0.32	0/2257
15	o	0.31	0/1656	0.35	1/2246 (0.0%)
16	P	0.34	0/1581	0.37	0/2135
16	p	0.31	0/1608	0.38	0/2170
17	Q	0.34	0/1592	0.33	0/2156
17	q	0.32	0/1584	0.37	0/2148
18	R	0.32	0/1567	0.27	0/2118
18	r	0.32	0/1571	0.34	0/2123
19	S	0.33	0/1657	0.31	0/2233
19	s	0.36	0/1650	0.36	0/2227

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	T	0.34	0/1707	0.39	0/2312
20	t	0.34	0/1696	0.31	0/2297
21	U	0.16	0/5935	0.33	0/8069
22	V	0.18	0/3104	0.38	0/4225
23	W	0.17	0/3386	0.36	0/4596
24	X	0.25	0/2839	0.45	2/3851 (0.1%)
25	Y	0.20	0/3042	0.36	0/4110
26	Z	0.23	0/2118	0.42	1/2891 (0.0%)
27	a	0.20	0/2725	0.42	1/3722 (0.0%)
28	b	0.15	0/1353	0.36	0/1846
29	c	0.17	0/2043	0.36	0/2784
30	d	0.14	0/1803	0.33	0/2447
31	e	0.37	0/282	0.75	1/378 (0.3%)
32	f	0.51	1/6432 (0.0%)	0.89	8/8752 (0.1%)
34	u	0.84	0/319	1.44	0/419
All	All	0.30	1/99817 (0.0%)	0.45	24/135403 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	f	245	ASN	C-O	5.37	1.30	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	142	GLY	CA-C-N	7.91	127.52	119.92
14	n	142	GLY	C-N-CA	7.91	127.52	119.92
3	C	198	LEU	N-CA-C	-7.60	102.94	111.07
32	f	288	VAL	N-CA-C	6.83	116.96	110.74
32	f	287	ASP	N-CA-C	-6.58	104.11	111.28
32	f	247	ALA	CA-C-N	-6.44	112.25	122.17
32	f	247	ALA	C-N-CA	-6.44	112.25	122.17
32	f	247	ALA	CA-C-O	-6.41	115.25	121.02
2	B	43	PRO	CA-C-N	6.06	129.90	120.75
2	B	43	PRO	C-N-CA	6.06	129.90	120.75
24	X	116	TRP	O-C-N	5.81	128.05	122.07
2	B	92	GLN	CA-C-N	5.64	132.31	121.54
2	B	92	GLN	C-N-CA	5.64	132.31	121.54
2	B	43	PRO	N-CA-CB	-5.62	97.35	103.25
26	Z	213	GLU	N-CA-C	-5.56	105.37	111.82
32	f	587	PHE	CA-C-O	-5.56	113.13	119.41
15	o	231	PRO	CA-C-O	-5.44	113.84	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	f	310	ASP	N-CA-C	-5.38	105.53	111.71
31	e	6	GLN	CB-CA-C	5.34	117.28	110.98
6	F	233	LYS	CA-C-N	-5.25	113.25	120.28
6	F	233	LYS	C-N-CA	-5.25	113.25	120.28
32	f	584	SER	O-C-N	5.16	128.73	122.85
27	a	243	GLY	N-CA-C	-5.08	106.60	112.50
24	X	301	ASP	CB-CA-C	5.02	119.12	110.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3062	0	2938	181	0
2	B	2901	0	2696	157	0
3	C	2723	0	2645	149	0
4	D	2777	0	2566	103	0
5	E	2324	0	2231	61	0
6	F	2421	0	2294	92	0
7	G	1798	0	1776	52	0
7	g	1765	0	1729	61	0
8	H	1745	0	1692	37	0
8	h	1679	0	1596	36	0
9	I	1900	0	1880	60	0
9	i	1851	0	1777	52	0
10	J	1839	0	1805	62	0
10	j	1622	0	1464	42	0
11	K	1773	0	1728	59	0
11	k	1677	0	1611	36	0
12	L	1847	0	1811	75	0
12	l	1831	0	1800	40	0
13	M	1843	0	1800	38	0
13	m	1833	0	1773	49	0
14	N	1482	0	1442	35	0
14	n	1488	0	1457	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	O	1637	0	1642	45	0
15	o	1629	0	1623	31	0
16	P	1553	0	1574	40	0
16	p	1579	0	1590	29	0
17	Q	1559	0	1560	32	0
17	q	1551	0	1542	24	0
18	R	1536	0	1488	38	0
18	r	1540	0	1503	22	0
19	S	1627	0	1617	20	0
19	s	1620	0	1609	34	0
20	T	1674	0	1643	47	0
20	t	1663	0	1629	32	0
21	U	5845	0	5485	210	0
22	V	3053	0	2786	109	0
23	W	3348	0	3119	151	0
24	X	2804	0	2685	79	0
25	Y	2990	0	2888	111	0
26	Z	2081	0	1915	99	0
27	a	2676	0	2390	126	0
28	b	1336	0	1269	61	0
29	c	2008	0	1887	51	0
30	d	1772	0	1701	63	0
31	e	280	0	213	17	0
32	f	6339	0	5975	508	0
33	v	75	0	17	6	0
34	u	320	0	351	24	0
35	A	31	0	12	15	0
35	B	31	0	12	6	0
35	C	31	0	12	19	0
35	F	31	0	12	11	0
36	D	27	0	12	13	0
All	All	98427	0	94272	3233	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 17.

All (3233) 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)
32:f:282:PHE:CE1	32:f:317:LEU:HD21	1.34	1.59
9:I:134:LEU:HD11	9:I:136:TYR:CZ	1.46	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:282:PHE:CZ	32:f:317:LEU:HD21	1.58	1.36
21:U:772:TRP:CD1	21:U:774:PRO:HD2	1.61	1.35
7:g:210:PHE:CE1	7:g:215:ILE:HD13	1.69	1.27
32:f:298:LEU:HD11	32:f:492:SER:O	1.32	1.24
32:f:282:PHE:CE1	32:f:317:LEU:CD2	2.20	1.22
32:f:282:PHE:CZ	32:f:317:LEU:CD2	2.23	1.22
32:f:416:MET:CE	32:f:801:VAL:HG23	1.69	1.21
32:f:245:ASN:HD22	32:f:256:PHE:CB	1.50	1.21
3:C:197:THR:HG23	3:C:200:ALA:CB	1.69	1.20
32:f:416:MET:HE1	32:f:801:VAL:HG23	1.19	1.17
20:T:95:MET:HE1	20:T:235:ALA:HB3	1.19	1.16
32:f:413:SER:O	32:f:417:ILE:HG12	1.41	1.16
32:f:560:LEU:HD22	32:f:782:HIS:CD2	1.81	1.16
27:a:38:THR:HG21	27:a:70:ARG:HG3	1.28	1.16
1:A:354:ILE:HD12	35:A:501:ATP:N6	1.58	1.15
15:o:60:ASP:OD2	15:o:212:SER:HB3	1.42	1.15
14:N:224:LEU:HD12	14:N:224:LEU:O	1.44	1.15
4:D:229:ARG:O	4:D:231:VAL:HG23	1.46	1.14
3:C:197:THR:CG2	3:C:200:ALA:HB3	1.77	1.13
34:u:402:LYS:HB3	34:u:406:ARG:NH2	1.62	1.13
32:f:245:ASN:ND2	32:f:256:PHE:HB2	1.63	1.13
8:h:222:THR:CG2	8:h:223:PRO:HD2	1.79	1.12
9:i:106:PRO:O	9:i:107:CYS:SG	2.07	1.12
3:C:281:ASP:CB	3:C:310:ARG:HH21	1.62	1.11
9:I:134:LEU:CD1	9:I:136:TYR:CZ	2.34	1.11
31:e:65:TYR:O	31:e:69:THR:HG23	1.49	1.11
32:f:379:GLY:HA2	32:f:417:ILE:HD13	1.16	1.10
3:C:197:THR:CG2	3:C:247:PHE:CE2	2.36	1.09
18:R:94:ILE:HD11	18:R:104:MET:HE1	1.24	1.08
32:f:300:ARG:CB	32:f:321:MET:CB	2.29	1.08
12:L:72:ILE:CD1	12:L:88:MET:HE1	1.82	1.08
12:L:72:ILE:HD11	12:L:88:MET:HE1	1.36	1.08
32:f:463:LEU:HB2	32:f:489:TYR:CE2	1.88	1.08
32:f:787:LEU:HD23	32:f:791:VAL:HG11	1.35	1.08
32:f:266:LEU:HB3	32:f:270:LEU:HD12	1.28	1.07
21:U:543:LYS:HE3	21:U:772:TRP:CZ3	1.88	1.07
8:h:222:THR:HG23	8:h:223:PRO:HD2	1.26	1.07
2:B:59:ARG:HE	32:f:188:VAL:HG12	0.92	1.07
32:f:787:LEU:HD23	32:f:791:VAL:CG1	1.84	1.07
32:f:266:LEU:CB	32:f:270:LEU:HD12	1.84	1.07
32:f:379:GLY:HA2	32:f:417:ILE:CD1	1.83	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:VAL:HG12	1:A:339:ARG:HB3	1.33	1.06
21:U:772:TRP:HE1	21:U:774:PRO:CG	1.68	1.06
32:f:245:ASN:HD22	32:f:256:PHE:HB2	0.93	1.06
32:f:463:LEU:HB2	32:f:489:TYR:CZ	1.90	1.06
1:A:69:ASP:HB2	3:C:82:LYS:CE	1.84	1.06
25:Y:224:VAL:CG2	25:Y:260:LEU:HD12	1.84	1.05
13:m:88:LEU:HD12	13:m:134:CYS:SG	1.97	1.05
32:f:325:GLN:HB2	32:f:329:ASN:ND2	1.72	1.05
2:B:59:ARG:NE	32:f:188:VAL:HG12	1.71	1.04
4:D:167:ILE:CB	36:D:501:ADP:HN61	1.71	1.04
15:O:210:LEU:HD23	19:s:61:PHE:CD1	1.93	1.04
1:A:33:LEU:HD22	3:C:174:LEU:HG	1.36	1.03
1:A:432:TYR:CE1	11:K:81:LEU:CD2	2.41	1.03
15:O:210:LEU:HD23	19:s:61:PHE:HD1	1.17	1.03
3:C:197:THR:HG21	3:C:247:PHE:CE2	1.93	1.03
32:f:463:LEU:HD13	32:f:497:VAL:HG22	1.38	1.03
15:O:210:LEU:CD2	19:s:61:PHE:HD1	1.71	1.02
26:Z:34:ARG:HA	26:Z:97:THR:OG1	1.59	1.02
21:U:772:TRP:CD1	21:U:774:PRO:CD	2.42	1.02
26:Z:237:LEU:HD13	26:Z:243:GLN:HE22	1.25	1.02
26:Z:237:LEU:HD11	26:Z:239:ASP:OD1	1.56	1.02
1:A:354:ILE:CD1	35:A:501:ATP:N6	2.21	1.02
1:A:41:TYR:OH	32:f:188:VAL:HG11	1.60	1.01
3:C:197:THR:HG21	3:C:247:PHE:HE2	1.25	1.01
16:P:12:MET:HE3	16:P:167:ILE:HG13	1.40	1.01
34:u:402:LYS:O	34:u:406:ARG:HG2	1.59	1.01
15:O:210:LEU:HG	19:s:61:PHE:CE1	1.95	1.01
21:U:543:LYS:NZ	21:U:772:TRP:CE3	2.28	1.01
13:M:48:PHE:HB2	13:M:215:SER:OG	1.58	1.01
16:P:12:MET:CE	16:P:167:ILE:HG13	1.91	1.01
32:f:245:ASN:ND2	32:f:256:PHE:CB	2.21	1.01
12:l:49:LEU:HD12	12:l:209:ASN:O	1.60	1.01
2:B:59:ARG:HE	32:f:188:VAL:CG1	1.72	1.00
32:f:416:MET:HE2	32:f:804:LEU:HG	1.41	1.00
23:W:440:ASN:O	23:W:443:THR:HG22	1.62	1.00
1:A:32:LEU:CD2	32:f:96:LEU:CB	2.41	0.99
32:f:282:PHE:HA	32:f:286:LYS:CB	1.91	0.99
13:M:216:TRP:CD1	13:M:228:VAL:HA	1.97	0.99
4:D:281:ALA:HB1	33:v:15:UNK:N	1.77	0.98
3:C:198:LEU:HD22	35:C:501:ATP:H2'	1.43	0.98
21:U:772:TRP:HE1	21:U:774:PRO:HG2	1.25	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:g:199:ILE:HG23	7:g:210:PHE:HZ	1.28	0.97
21:U:543:LYS:HE3	21:U:772:TRP:HZ3	1.28	0.97
32:f:282:PHE:CE1	32:f:317:LEU:HD11	1.99	0.96
1:A:33:LEU:HD11	2:B:407:LEU:HD11	1.46	0.96
20:T:95:MET:CE	20:T:235:ALA:HB3	1.96	0.96
32:f:283:THR:HA	32:f:816:TYR:CE1	2.01	0.96
9:i:73:ALA:HB2	9:i:225:ILE:CD1	1.96	0.96
18:R:94:ILE:HD11	18:R:104:MET:CE	1.96	0.95
1:A:354:ILE:HD12	35:A:501:ATP:HN61	1.23	0.95
3:C:197:THR:HG23	3:C:247:PHE:CE2	1.99	0.95
9:I:176:LYS:HA	10:J:53:LEU:HD11	1.47	0.95
32:f:348:ILE:HG23	32:f:754:LYS:HB2	1.49	0.95
7:G:217:VAL:CG1	7:G:230:LEU:HD12	1.95	0.95
21:U:772:TRP:NE1	21:U:774:PRO:HG2	1.81	0.95
21:U:772:TRP:NE1	21:U:774:PRO:CG	2.28	0.95
2:B:54:PRO:HA	32:f:835:GLU:HB2	1.48	0.95
21:U:772:TRP:NE1	21:U:774:PRO:HD2	1.81	0.95
3:C:197:THR:CG2	3:C:247:PHE:HE2	1.77	0.95
1:A:56:LEU:HD21	2:B:48:LYS:HE3	1.47	0.95
7:G:211:LYS:HG2	7:G:212:PRO:HD2	1.49	0.94
1:A:20:LYS:CB	1:A:21:PRO:HD3	1.97	0.94
1:A:56:LEU:HD11	2:B:48:LYS:HE3	1.46	0.94
2:B:58:CYS:SG	32:f:835:GLU:OE1	2.25	0.94
21:U:575:ASP:OD2	21:U:578:LEU:HD13	1.67	0.94
27:a:317:VAL:CG2	27:a:319:LEU:HD23	1.96	0.94
1:A:20:LYS:CB	1:A:21:PRO:CD	2.46	0.94
7:G:211:LYS:CG	7:G:212:PRO:HD2	1.97	0.94
1:A:20:LYS:HB2	1:A:21:PRO:CD	1.97	0.94
12:L:164:ARG:O	12:L:198:THR:HG23	1.68	0.94
4:D:167:ILE:CB	36:D:501:ADP:N6	2.30	0.93
21:U:543:LYS:CE	21:U:772:TRP:CE3	2.51	0.93
1:A:78:TRP:HA	1:A:81:ALA:HB3	1.50	0.93
2:B:125:THR:HG22	2:B:126:SER:H	1.29	0.93
6:F:235:LEU:HB2	35:F:501:ATP:H5'1	1.49	0.93
32:f:416:MET:HE2	32:f:804:LEU:CG	1.97	0.93
26:Z:214:LYS:CB	26:Z:221:PRO:CD	2.47	0.93
15:O:210:LEU:CD2	19:s:61:PHE:CD1	2.50	0.93
32:f:282:PHE:HE1	32:f:317:LEU:HD21	1.28	0.93
1:A:33:LEU:CD2	3:C:174:LEU:HG	1.98	0.92
12:L:125:ARG:HH11	12:L:125:ARG:HG2	1.33	0.92
25:Y:213:LEU:HD13	25:Y:219:PHE:HB2	1.49	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD11	2:B:48:LYS:CE	1.99	0.92
15:O:206:ILE:HG23	15:O:212:SER:O	1.68	0.92
32:f:283:THR:HA	32:f:816:TYR:CZ	2.04	0.92
3:C:198:LEU:HD12	3:C:201:ARG:HD2	1.51	0.91
3:C:357:ALA:N	35:C:501:ATP:H8	1.68	0.91
25:Y:224:VAL:HG23	25:Y:260:LEU:HD12	1.49	0.91
32:f:483:PHE:HZ	32:f:802:SER:OG	1.52	0.91
1:A:69:ASP:HB2	3:C:82:LYS:HE3	1.53	0.91
32:f:308:SER:O	32:f:309:GLU:HG2	1.69	0.91
32:f:462:ALA:CB	32:f:488:ALA:HB1	2.00	0.91
32:f:325:GLN:O	32:f:329:ASN:HB2	1.71	0.90
32:f:377:VAL:HG22	32:f:752:HIS:HD2	1.34	0.90
3:C:197:THR:O	3:C:200:ALA:HB3	1.69	0.90
32:f:282:PHE:HE1	32:f:317:LEU:HD11	1.32	0.90
21:U:575:ASP:OD2	21:U:578:LEU:CD1	2.20	0.90
32:f:462:ALA:CB	32:f:488:ALA:CB	2.50	0.90
14:n:38:MET:HG3	14:n:161:ILE:HG22	1.53	0.90
15:o:215:ASN:OD1	15:o:234:VAL:HG13	1.72	0.90
3:C:357:ALA:N	35:C:501:ATP:C8	2.39	0.90
1:A:30:ILE:HG21	3:C:171:HIS:CD2	2.06	0.89
2:B:59:ARG:HD2	32:f:188:VAL:HG13	1.51	0.89
1:A:32:LEU:HD23	32:f:96:LEU:CB	2.02	0.89
3:C:197:THR:HG23	3:C:200:ALA:HB3	1.37	0.89
3:C:198:LEU:HD12	3:C:201:ARG:CD	2.03	0.88
26:Z:237:LEU:HD11	26:Z:239:ASP:CG	1.98	0.88
32:f:462:ALA:HB1	32:f:488:ALA:CB	2.02	0.88
9:I:134:LEU:HD11	9:I:136:TYR:CE2	2.08	0.88
23:W:355:LYS:HE3	23:W:384:LEU:HD11	1.56	0.88
7:g:72:ILE:HG13	7:g:78:CYS:SG	2.13	0.88
21:U:543:LYS:CE	21:U:772:TRP:CZ3	2.55	0.88
10:j:102:VAL:HG11	10:j:107:ILE:HG13	1.54	0.88
21:U:772:TRP:NE1	21:U:774:PRO:CD	2.37	0.88
32:f:245:ASN:HD22	32:f:256:PHE:CA	1.85	0.88
32:f:530:CYS:SG	32:f:569:LYS:HG3	2.13	0.88
2:B:59:ARG:NE	32:f:188:VAL:CG1	2.31	0.88
7:g:199:ILE:HG23	7:g:210:PHE:CZ	2.08	0.87
9:i:97:TYR:CE1	9:i:105:ILE:HA	2.09	0.87
32:f:379:GLY:CA	32:f:417:ILE:HD13	2.04	0.87
32:f:434:TYR:CD1	34:u:385:ASN:ND2	2.43	0.87
1:A:20:LYS:HB3	1:A:21:PRO:HD3	1.55	0.87
9:I:134:LEU:CD1	9:I:136:TYR:CE1	2.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:34:ARG:HA	26:Z:97:THR:HG1	1.35	0.87
32:f:282:PHE:HE1	32:f:317:LEU:CD1	1.87	0.87
7:g:210:PHE:CE1	7:g:215:ILE:CD1	2.57	0.87
15:O:61:THR:OG1	15:O:214:SER:HB3	1.75	0.86
13:M:216:TRP:HD1	13:M:228:VAL:CA	1.87	0.86
32:f:463:LEU:CB	32:f:489:TYR:CZ	2.58	0.86
32:f:266:LEU:HB3	32:f:270:LEU:CD1	2.05	0.86
32:f:416:MET:CE	32:f:804:LEU:HG	2.04	0.86
15:o:60:ASP:OD2	15:o:212:SER:CB	2.23	0.86
19:s:144:GLU:N	19:s:144:GLU:OE1	2.09	0.86
1:A:432:TYR:CE1	11:K:81:LEU:HD21	2.10	0.86
1:A:322:ASN:OD1	1:A:323:ARG:HG2	1.75	0.86
32:f:245:ASN:ND2	32:f:256:PHE:N	2.22	0.86
32:f:377:VAL:HG22	32:f:752:HIS:CD2	2.11	0.86
32:f:386:GLY:HA2	32:f:418:LEU:HG	1.57	0.86
22:V:214:HIS:O	22:V:217:VAL:HG12	1.76	0.86
4:D:211:GLY:O	4:D:333:PHE:CD2	2.29	0.85
32:f:416:MET:CE	32:f:801:VAL:CG2	2.53	0.85
3:C:197:THR:CG2	3:C:247:PHE:CZ	2.58	0.85
27:a:38:THR:HG21	27:a:70:ARG:CG	2.05	0.85
32:f:217:LEU:CD2	32:f:244:GLU:OE1	2.24	0.85
32:f:434:TYR:HD1	34:u:385:ASN:HB3	1.41	0.85
3:C:197:THR:OG1	3:C:247:PHE:HZ	1.58	0.85
4:D:281:ALA:CB	33:v:15:UNK:N	2.38	0.85
1:A:354:ILE:CD1	35:A:501:ATP:HN62	1.87	0.85
3:C:197:THR:HG1	3:C:247:PHE:HZ	0.89	0.84
26:Z:214:LYS:CB	26:Z:221:PRO:N	2.41	0.84
32:f:287:ASP:OD2	32:f:816:TYR:CE1	2.29	0.84
32:f:412:ALA:HA	32:f:447:ALA:HB2	1.59	0.84
9:I:134:LEU:HD11	9:I:136:TYR:CE1	2.09	0.84
13:M:216:TRP:CD1	13:M:228:VAL:CA	2.59	0.84
32:f:467:SER:HA	32:f:500:LEU:HD21	1.58	0.84
8:H:183:GLU:OE1	8:H:183:GLU:N	2.09	0.84
1:A:432:TYR:HE1	11:K:81:LEU:HD21	1.43	0.84
13:m:78:VAL:HG11	13:m:85:ALA:HB2	1.59	0.84
32:f:282:PHE:HZ	32:f:317:LEU:CD2	1.90	0.84
2:B:335:GLU:OE1	2:B:335:GLU:N	2.11	0.84
13:m:42:CYS:SG	13:m:187:CYS:N	2.51	0.84
16:p:48:ARG:HG2	16:p:48:ARG:HH11	1.43	0.84
32:f:597:VAL:CB	32:f:638:ASP:OD2	2.26	0.83
32:f:326:LEU:O	32:f:330:PHE:CB	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:463:LEU:N	32:f:489:TYR:HE2	1.76	0.83
32:f:298:LEU:CD1	32:f:492:SER:O	2.23	0.83
13:M:216:TRP:CD1	13:M:228:VAL:CB	2.62	0.83
32:f:326:LEU:O	32:f:330:PHE:HB3	1.79	0.83
32:f:434:TYR:CD1	34:u:385:ASN:HB3	2.13	0.82
32:f:217:LEU:HD23	32:f:244:GLU:OE1	1.79	0.82
1:A:59:ILE:HD11	2:B:75:GLU:HG2	1.62	0.82
5:E:283:ASP:OD1	5:E:284:THR:HG23	1.79	0.82
32:f:276:GLU:OE1	32:f:276:GLU:N	2.12	0.82
7:g:78:CYS:SG	7:g:140:LEU:HD23	2.19	0.82
32:f:283:THR:HA	32:f:816:TYR:OH	1.79	0.82
25:Y:213:LEU:HD11	25:Y:219:PHE:HD1	1.45	0.82
26:Z:68:TRP:HB3	26:Z:104:ASN:HD21	1.45	0.82
32:f:811:LEU:HG	32:f:856:ALA:HB2	1.61	0.82
1:A:220:THR:O	35:A:501:ATP:H2	1.63	0.81
32:f:775:THR:O	32:f:775:THR:HG22	1.78	0.81
13:m:88:LEU:CD1	13:m:134:CYS:SG	2.68	0.81
1:A:56:LEU:HD11	2:B:48:LYS:NZ	1.96	0.81
26:Z:214:LYS:CB	26:Z:221:PRO:HD3	2.09	0.81
26:Z:104:ASN:ND2	26:Z:108:ILE:HD11	1.96	0.81
32:f:416:MET:HE1	32:f:801:VAL:CG2	2.08	0.81
4:D:231:VAL:O	4:D:231:VAL:HG12	1.79	0.81
11:K:224:GLN:N	11:K:224:GLN:OE1	2.14	0.81
10:j:102:VAL:HG11	10:j:107:ILE:CG1	2.10	0.80
32:f:463:LEU:N	32:f:489:TYR:CE2	2.48	0.80
1:A:33:LEU:HD22	3:C:174:LEU:CG	2.10	0.80
32:f:399:LEU:HD11	32:f:432:TYR:CE1	2.16	0.80
32:f:466:LEU:HD13	32:f:485:LEU:N	1.97	0.80
13:m:78:VAL:HG11	13:m:85:ALA:CB	2.12	0.80
9:I:69:ASN:OD1	9:I:70:GLU:N	2.15	0.80
32:f:309:GLU:HB2	32:f:314:TYR:CB	2.11	0.80
2:B:59:ARG:HD2	32:f:188:VAL:CG1	2.11	0.80
1:A:69:ASP:HB2	3:C:82:LYS:HE2	1.61	0.80
35:B:501:ATP:H5'2	3:C:307:ARG:NH1	1.95	0.80
32:f:224:ASN:OD1	32:f:225:ALA:N	2.14	0.79
9:I:134:LEU:HD11	9:I:136:TYR:OH	1.81	0.79
15:o:102:ILE:CD1	15:o:126:LEU:HG	2.11	0.79
32:f:466:LEU:HD13	32:f:484:GLY:C	2.07	0.79
8:h:222:THR:CG2	8:h:223:PRO:CD	2.61	0.79
32:f:245:ASN:ND2	32:f:256:PHE:CA	2.45	0.79
32:f:282:PHE:CZ	32:f:317:LEU:CG	2.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:209:GLY:O	4:D:371:SER:HB3	1.83	0.79
21:U:381:THR:HG21	21:U:415:HIS:NE2	1.98	0.79
25:Y:224:VAL:HG21	25:Y:260:LEU:HD12	1.61	0.79
26:Z:210:SER:HA	26:Z:213:GLU:CB	2.13	0.79
1:A:89:SER:HA	1:A:92:PRO:HG2	1.65	0.79
27:a:87:MET:HE1	27:a:94:LEU:HB3	1.65	0.79
27:a:317:VAL:HG13	27:a:318:GLY:H	1.45	0.79
7:g:210:PHE:HE1	7:g:215:ILE:HD13	1.41	0.79
2:B:125:THR:HG22	2:B:126:SER:N	1.98	0.78
32:f:463:LEU:CB	32:f:489:TYR:CE2	2.65	0.78
6:F:67:GLN:O	6:F:70:LYS:CB	2.31	0.78
19:s:74:LEU:O	19:s:75:THR:HG23	1.84	0.78
32:f:418:LEU:CD2	32:f:425:GLY:HA2	2.14	0.78
3:C:281:ASP:CB	3:C:310:ARG:NH2	2.43	0.78
28:b:25:ARG:HH22	28:b:145:GLU:N	1.82	0.78
1:A:56:LEU:CD1	2:B:48:LYS:HE3	2.13	0.78
24:X:358:LYS:O	24:X:362:GLU:HB2	1.83	0.78
20:t:66:VAL:HG22	20:t:236:THR:HG22	1.66	0.78
14:n:38:MET:CG	14:n:161:ILE:HG22	2.13	0.78
21:U:543:LYS:NZ	21:U:772:TRP:HE3	1.81	0.77
2:B:59:ARG:CD	32:f:188:VAL:HG13	2.14	0.77
3:C:197:THR:HG22	3:C:200:ALA:HB3	1.65	0.77
10:j:102:VAL:CG1	10:j:107:ILE:HG13	2.13	0.77
1:A:32:LEU:HD11	32:f:96:LEU:O	1.84	0.77
1:A:56:LEU:CD2	2:B:48:LYS:HE3	2.14	0.77
13:M:216:TRP:HD1	13:M:228:VAL:HA	1.37	0.77
20:t:238:THR:HG22	20:t:239:GLU:H	1.50	0.77
34:u:403:ARG:HA	34:u:406:ARG:HD2	1.65	0.77
23:W:409:LEU:CB	24:X:344:ARG:HB2	2.14	0.77
32:f:282:PHE:CE1	32:f:317:LEU:CD1	2.66	0.77
32:f:282:PHE:CE1	32:f:317:LEU:CG	2.66	0.77
24:X:369:ILE:HG22	24:X:370:LEU:HG	1.67	0.77
27:a:38:THR:CG2	27:a:70:ARG:HG3	2.11	0.77
7:g:210:PHE:CZ	7:g:215:ILE:HD13	2.19	0.77
17:Q:40:GLU:OE2	17:Q:40:GLU:N	2.15	0.77
9:i:159:TRP:CE2	10:j:54:GLN:OE1	2.38	0.77
2:B:393:ALA:HB2	35:B:501:ATP:H5'1	1.66	0.77
2:B:59:ARG:CD	32:f:188:VAL:CG1	2.63	0.76
26:Z:237:LEU:CD1	26:Z:239:ASP:CG	2.58	0.76
1:A:41:TYR:HE2	2:B:59:ARG:HB2	1.50	0.76
15:O:140:ALA:HB1	15:O:170:MET:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:151:PRO:O	15:O:152:HIS:ND1	2.16	0.76
23:W:401:THR:HG23	23:W:402:ILE:H	1.48	0.76
23:W:413:ILE:HD12	23:W:413:ILE:O	1.83	0.76
32:f:376:PHE:HE1	32:f:801:VAL:CG1	1.98	0.76
32:f:416:MET:CE	32:f:804:LEU:CD2	2.63	0.76
18:R:61:THR:HG23	18:R:229:SER:OG	1.86	0.76
20:T:153:ASN:HB3	20:T:155:MET:CE	2.14	0.76
32:f:720:GLU:OE2	32:f:753:ALA:HB1	1.84	0.76
20:t:238:THR:HG22	20:t:239:GLU:N	1.99	0.76
32:f:399:LEU:CD1	32:f:432:TYR:CE1	2.68	0.76
10:J:211:MET:HE1	10:J:217:LEU:CB	2.15	0.76
1:A:20:LYS:HB2	1:A:21:PRO:HD2	1.66	0.76
32:f:463:LEU:HB3	32:f:489:TYR:OH	1.86	0.76
32:f:483:PHE:HZ	32:f:802:SER:HG	0.77	0.76
9:I:226:ARG:HH12	9:I:228:LEU:CD2	1.99	0.76
21:U:772:TRP:HE1	21:U:774:PRO:CB	1.99	0.76
27:a:317:VAL:HG22	27:a:319:LEU:HD23	1.67	0.75
15:o:102:ILE:HG21	15:o:126:LEU:HD21	1.68	0.75
1:A:354:ILE:HD11	35:A:501:ATP:HN62	1.49	0.75
21:U:432:SER:HB3	21:U:438:GLN:OE1	1.87	0.75
7:g:123:GLN:HE22	7:g:127:GLN:HG2	1.50	0.75
7:G:217:VAL:HB	7:G:230:LEU:HD12	1.67	0.75
7:G:217:VAL:HG12	7:G:230:LEU:HD12	1.69	0.75
25:Y:213:LEU:HD11	25:Y:219:PHE:CD1	2.22	0.75
32:f:460:ASP:OD1	32:f:489:TYR:HE1	1.68	0.75
34:u:402:LYS:HB3	34:u:406:ARG:CZ	2.17	0.75
5:E:168:LYS:O	5:E:275:MET:N	2.20	0.75
27:a:325:ASP:N	27:a:330:ARG:O	2.20	0.75
32:f:466:LEU:CB	32:f:485:LEU:HG	2.17	0.75
13:m:9:ASP:O	13:m:23:GLN:NE2	2.20	0.75
17:Q:168:GLN:NE2	17:Q:175:LEU:O	2.20	0.75
32:f:713:PHE:CD1	32:f:753:ALA:HB2	2.21	0.75
32:f:708:ASP:OD1	32:f:709:THR:N	2.20	0.74
24:X:374:PHE:O	24:X:386:ILE:HG12	1.87	0.74
19:S:66:ARG:NH2	15:o:207:PHE:O	2.20	0.74
27:a:87:MET:SD	27:a:93:ALA:HB3	2.27	0.74
30:d:350:VAL:O	30:d:350:VAL:HG12	1.87	0.74
15:O:210:LEU:HG	19:s:61:PHE:HE1	1.52	0.74
32:f:384:ALA:HB2	32:f:419:LEU:O	1.87	0.74
26:Z:34:ARG:CA	26:Z:97:THR:OG1	2.36	0.74
32:f:560:LEU:HD13	32:f:782:HIS:NE2	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:791:VAL:O	32:f:797:LEU:HD21	1.87	0.74
20:T:238:THR:HG22	20:T:239:GLU:N	2.03	0.74
32:f:824:ALA:HB1	32:f:849:ALA:HB1	1.70	0.74
3:C:42:LEU:HD23	3:C:45:LEU:HD21	1.70	0.74
3:C:197:THR:HG23	3:C:247:PHE:CZ	2.21	0.74
29:c:266:THR:OG1	29:c:267:PRO:HD3	1.88	0.74
13:m:42:CYS:HB3	13:m:187:CYS:SG	2.27	0.74
14:N:68:LEU:HD11	14:N:220:ARG:NH2	2.02	0.74
1:A:212:VAL:HG12	1:A:339:ARG:CB	2.14	0.74
21:U:643:SER:O	21:U:649:ARG:NH1	2.21	0.74
22:V:473:GLN:NE2	30:d:333:THR:HG21	2.03	0.74
23:W:401:THR:HG23	23:W:402:ILE:N	2.02	0.74
9:I:6:ASP:O	9:I:7:SER:OG	2.02	0.74
25:Y:349:LYS:O	25:Y:351:ASN:N	2.20	0.74
9:i:159:TRP:CZ2	10:j:54:GLN:OE1	2.41	0.74
1:A:418:LYS:HA	1:A:422:LYS:HB2	1.68	0.73
26:Z:185:GLY:HA3	29:c:297:VAL:HG22	1.69	0.73
32:f:266:LEU:CB	32:f:270:LEU:CD1	2.63	0.73
32:f:415:GLY:O	32:f:451:VAL:HG22	1.86	0.73
3:C:198:LEU:CD1	3:C:201:ARG:HD2	2.18	0.73
7:G:217:VAL:CB	7:G:230:LEU:HD12	2.17	0.73
13:m:42:CYS:SG	13:m:185:MET:O	2.46	0.73
1:A:69:ASP:CB	3:C:82:LYS:HE2	2.18	0.73
14:N:219:GLU:OE1	14:N:219:GLU:N	2.20	0.73
16:P:126:LEU:HD12	16:P:127:ILE:HG23	1.69	0.73
32:f:463:LEU:CB	32:f:489:TYR:OH	2.35	0.73
24:X:166:LEU:O	24:X:170:GLN:HG3	1.89	0.73
32:f:560:LEU:HD22	32:f:782:HIS:HD2	1.47	0.73
32:f:766:GLN:HG3	32:f:768:LEU:HD12	1.69	0.73
32:f:463:LEU:CD1	32:f:497:VAL:HG22	2.16	0.73
17:Q:101:ASN:HB3	17:Q:132:HIS:CE1	2.24	0.73
31:e:65:TYR:O	31:e:69:THR:CG2	2.33	0.73
32:f:266:LEU:HB2	32:f:270:LEU:HD12	1.70	0.73
2:B:86:LYS:HA	32:f:621:ASP:O	1.89	0.73
4:D:211:GLY:O	4:D:333:PHE:HD2	1.70	0.73
27:a:147:GLY:O	27:a:149:THR:N	2.22	0.73
20:T:153:ASN:HB3	20:T:155:MET:HE3	1.69	0.72
32:f:281:ILE:O	32:f:281:ILE:HG22	1.89	0.72
12:l:165:SER:OG	12:l:169:ARG:NH2	2.22	0.72
1:A:41:TYR:OH	32:f:188:VAL:CG1	2.37	0.72
2:B:260:LEU:H	33:v:8:UNK:HA	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:37:CYS:SG	28:b:71:ILE:HG21	2.29	0.72
14:N:224:LEU:O	14:N:224:LEU:CD1	2.33	0.72
23:W:355:LYS:CE	23:W:384:LEU:HD11	2.19	0.72
32:f:787:LEU:HD23	32:f:791:VAL:HG12	1.72	0.72
18:R:94:ILE:CD1	18:R:104:MET:CE	2.66	0.72
32:f:413:SER:O	32:f:417:ILE:CG1	2.31	0.72
32:f:416:MET:CE	32:f:804:LEU:HD23	2.19	0.72
14:N:228:ILE:O	14:N:228:ILE:HG13	1.89	0.72
22:V:326:GLN:HE21	31:e:8:VAL:CB	2.03	0.72
13:m:42:CYS:SG	13:m:186:THR:C	2.72	0.72
29:c:193:ILE:O	29:c:197:ASN:N	2.22	0.72
9:I:134:LEU:HD12	9:I:136:TYR:CE1	2.25	0.72
9:i:73:ALA:CB	9:i:225:ILE:CD1	2.68	0.72
19:s:74:LEU:O	19:s:75:THR:CG2	2.38	0.72
22:V:214:HIS:O	22:V:217:VAL:CG1	2.37	0.72
21:U:573:ASP:CG	21:U:578:LEU:HD22	2.15	0.71
32:f:416:MET:SD	32:f:804:LEU:HG	2.30	0.71
32:f:597:VAL:CA	32:f:638:ASP:OD2	2.37	0.71
32:f:706:ILE:HD11	32:f:741:LEU:HG	1.72	0.71
34:u:403:ARG:O	34:u:406:ARG:HG3	1.90	0.71
4:D:210:CYS:SG	4:D:335:LEU:HD13	2.30	0.71
12:L:72:ILE:HD11	12:L:88:MET:CE	2.17	0.71
15:O:192:GLU:OE1	15:O:192:GLU:N	2.24	0.71
20:T:225:ASP:OD1	20:T:226:ALA:N	2.23	0.71
21:U:573:ASP:OD2	21:U:578:LEU:HD22	1.90	0.71
28:b:25:ARG:CZ	28:b:144:GLY:HA3	2.20	0.71
32:f:205:CYS:O	32:f:209:MET:N	2.23	0.71
32:f:470:VAL:CG1	32:f:501:LEU:HD23	2.20	0.71
9:i:73:ALA:HB2	9:i:225:ILE:HD13	1.70	0.71
13:m:67:LEU:HD13	13:m:215:SER:OG	1.90	0.71
23:W:375:MET:HE2	23:W:375:MET:HA	1.72	0.71
32:f:282:PHE:HE1	32:f:317:LEU:CD2	1.83	0.71
32:f:462:ALA:HB3	32:f:488:ALA:HB1	1.72	0.71
8:h:222:THR:HG22	8:h:223:PRO:HD2	1.71	0.71
20:T:238:THR:HG22	20:T:239:GLU:H	1.55	0.71
23:W:337:ALA:O	23:W:341:PHE:N	2.23	0.71
32:f:790:GLN:OE1	32:f:790:GLN:N	2.24	0.71
32:f:826:GLN:NE2	32:f:862:ILE:O	2.23	0.71
9:i:73:ALA:CB	9:i:225:ILE:HD11	2.20	0.71
9:i:216:LEU:HD12	9:i:225:ILE:HD12	1.72	0.71
16:p:65:GLN:NE2	17:q:86:ARG:HH11	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:s:56:ARG:O	19:s:70:LYS:NZ	2.23	0.71
1:A:33:LEU:CD1	2:B:407:LEU:HD11	2.21	0.71
8:H:10:LEU:HD12	8:H:19:LEU:HD13	1.72	0.71
18:R:64:ALA:HB2	18:R:73:VAL:HG23	1.72	0.71
22:V:385:LYS:O	22:V:389:ASP:N	2.21	0.71
4:D:167:ILE:CA	36:D:501:ADP:N6	2.54	0.71
32:f:245:ASN:HD21	32:f:256:PHE:H	1.36	0.71
7:g:158:GLY:O	8:h:84:ARG:NH2	2.23	0.71
32:f:267:ARG:NH1	32:f:296:PHE:O	2.22	0.71
8:H:51:LYS:HA	8:H:51:LYS:HE3	1.72	0.71
32:f:628:ASP:O	32:f:632:LYS:NZ	2.23	0.71
21:U:542:GLU:OE2	21:U:546:ARG:NE	2.24	0.70
21:U:543:LYS:CE	21:U:772:TRP:HE3	2.03	0.70
32:f:381:VAL:HG22	32:f:755:ASP:HB2	1.72	0.70
9:I:72:MET:HE2	9:I:110:LEU:HD23	1.73	0.70
18:R:94:ILE:CD1	18:R:104:MET:HE1	2.12	0.70
28:b:25:ARG:NH2	28:b:145:GLU:N	2.39	0.70
30:d:349:ILE:O	30:d:350:VAL:HG23	1.92	0.70
8:h:73:GLY:HA3	8:h:218:PHE:CE2	2.26	0.70
10:J:18:GLN:HA	10:J:18:GLN:NE2	2.06	0.70
25:Y:240:VAL:HG21	25:Y:260:LEU:HD11	1.72	0.70
4:D:250:VAL:O	4:D:254:ALA:N	2.24	0.70
13:m:192:LYS:NZ	13:m:193:GLU:OE2	2.18	0.70
1:A:286:ASP:OD1	1:A:296:GLN:NE2	2.24	0.70
3:C:197:THR:C	3:C:200:ALA:H	2.00	0.70
3:C:242:ALA:HB3	3:C:243:PRO:HD3	1.72	0.70
17:Q:60:ILE:HG21	17:Q:84:THR:HG22	1.74	0.70
18:R:76:ASP:OD1	18:R:92:LYS:NZ	2.24	0.70
30:d:240:SER:O	30:d:244:VAL:N	2.24	0.70
32:f:713:PHE:HD1	32:f:753:ALA:HB2	1.54	0.70
7:g:123:GLN:NE2	7:g:127:GLN:HG2	2.07	0.70
9:i:185:THR:O	9:i:188:SER:N	2.25	0.70
25:Y:207:THR:O	25:Y:207:THR:HG22	1.90	0.70
32:f:652:VAL:O	32:f:656:GLY:N	2.25	0.70
1:A:418:LYS:HD3	1:A:422:LYS:HG3	1.73	0.70
21:U:631:GLU:N	21:U:631:GLU:OE1	2.25	0.70
21:U:697:GLN:OE1	21:U:885:MET:HE1	1.91	0.70
3:C:197:THR:O	3:C:200:ALA:CB	2.38	0.70
32:f:569:LYS:O	32:f:599:ALA:HB1	1.90	0.70
35:C:501:ATP:O3G	35:C:501:ATP:H5'2	1.92	0.70
32:f:278:VAL:O	32:f:280:ASP:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:i:13:SER:OG	9:i:17:ARG:N	2.24	0.70
32:f:323:ASN:HB3	32:f:326:LEU:HD11	1.74	0.69
13:m:88:LEU:HD12	13:m:134:CYS:HG	1.57	0.69
1:A:432:TYR:HE1	11:K:81:LEU:CD2	1.96	0.69
3:C:197:THR:CG2	3:C:200:ALA:CB	2.44	0.69
9:I:226:ARG:NH1	9:I:228:LEU:CD2	2.56	0.69
32:f:281:ILE:HG23	32:f:284:SER:HB2	1.74	0.69
21:U:106:ASP:OD1	21:U:107:HIS:N	2.25	0.69
20:t:91:ASN:OD1	20:t:92:ASN:N	2.26	0.69
2:B:78:PHE:O	2:B:82:GLN:HB2	1.93	0.69
36:D:501:ADP:H8	36:D:501:ADP:H3'	1.57	0.69
12:L:66:VAL:HG21	12:L:72:ILE:HG13	1.73	0.69
32:f:416:MET:CE	32:f:804:LEU:CG	2.69	0.69
32:f:811:LEU:HG	32:f:856:ALA:CB	2.23	0.69
3:C:197:THR:O	3:C:200:ALA:N	2.25	0.69
32:f:728:ALA:HB1	32:f:751:TYR:CZ	2.27	0.69
1:A:20:LYS:HB2	1:A:21:PRO:HD3	1.68	0.69
1:A:30:ILE:HG21	3:C:171:HIS:NE2	2.08	0.69
25:Y:213:LEU:CD1	25:Y:219:PHE:HD1	2.06	0.69
7:g:72:ILE:CG1	7:g:78:CYS:SG	2.80	0.69
17:q:145:ARG:HD2	17:q:145:ARG:O	1.92	0.69
5:E:256:THR:O	5:E:260:LEU:N	2.26	0.69
6:F:231:THR:HG22	6:F:355:PRO:O	1.92	0.69
7:G:211:LYS:HG3	7:G:212:PRO:HD2	1.75	0.69
27:a:34:TRP:O	27:a:38:THR:HG23	1.92	0.69
8:h:102:GLN:NE2	15:o:100:GLN:OE1	2.26	0.69
1:A:176:ASP:O	1:A:357:ILE:HD13	1.93	0.69
26:Z:8:LYS:HB2	26:Z:47:VAL:HG23	1.72	0.69
32:f:148:GLN:N	32:f:148:GLN:OE1	2.25	0.69
32:f:172:GLU:OE1	32:f:172:GLU:N	2.25	0.69
32:f:475:ASN:OD1	32:f:514:VAL:HG21	1.93	0.69
6:F:234:THR:CG2	35:F:501:ATP:O1G	2.41	0.68
20:T:67:ILE:HB	20:T:95:MET:CE	2.22	0.68
32:f:245:ASN:ND2	32:f:256:PHE:H	1.89	0.68
32:f:614:HIS:O	32:f:629:LYS:NZ	2.26	0.68
21:U:227:GLN:OE1	21:U:227:GLN:N	2.26	0.68
32:f:560:LEU:CD2	32:f:782:HIS:CD2	2.68	0.68
22:V:204:ASP:O	22:V:207:ALA:HB3	1.93	0.68
12:l:157:ARG:NH1	12:l:176:MET:SD	2.66	0.68
1:A:45:ILE:HD11	2:B:62:LEU:HB2	1.75	0.68
2:B:143:LEU:O	2:B:163:LEU:HD13	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:86:ASP:OD2	7:G:132:ARG:NH2	2.27	0.68
12:L:66:VAL:HG21	12:L:72:ILE:CG1	2.24	0.68
25:Y:213:LEU:CD1	25:Y:219:PHE:CD1	2.77	0.68
27:a:87:MET:HE1	27:a:94:LEU:CA	2.24	0.68
32:f:119:LYS:O	32:f:123:ALA:N	2.27	0.68
3:C:45:LEU:HD12	3:C:46:GLN:N	2.08	0.68
12:L:192:LEU:HD13	12:L:236:LEU:HD22	1.75	0.68
32:f:416:MET:HE1	32:f:804:LEU:HD23	1.75	0.68
1:A:59:ILE:HD11	2:B:75:GLU:CG	2.24	0.68
6:F:234:THR:HG23	35:F:501:ATP:O1G	1.93	0.68
19:s:176:LEU:HD23	19:s:206:VAL:HG12	1.76	0.68
13:M:216:TRP:NE1	13:M:228:VAL:CB	2.57	0.68
21:U:573:ASP:OD2	21:U:578:LEU:CD2	2.42	0.68
32:f:466:LEU:HB2	32:f:485:LEU:CD2	2.24	0.68
32:f:475:ASN:ND2	32:f:511:SER:OG	2.27	0.68
6:F:188:ILE:CD1	6:F:195:ILE:HD11	2.24	0.68
21:U:808:PRO:O	21:U:810:THR:N	2.27	0.68
2:B:278:ALA:HB1	2:B:279:PRO:HD2	1.74	0.67
2:B:364:ILE:O	2:B:368:HIS:CD2	2.47	0.67
10:j:192:ILE:O	10:j:196:LEU:HG	1.92	0.67
32:f:379:GLY:CA	32:f:417:ILE:CD1	2.67	0.67
4:D:373:ALA:HA	36:D:501:ADP:O2'	1.94	0.67
7:G:86:ASP:OD1	13:M:121:HIS:HE1	1.76	0.67
2:B:58:CYS:SG	32:f:835:GLU:CD	2.77	0.67
4:D:384:MET:SD	5:E:164:ILE:HG21	2.34	0.67
36:D:501:ADP:H3'	36:D:501:ADP:C8	2.29	0.67
14:N:51:ASP:OD1	14:N:67:LYS:NZ	2.27	0.67
27:a:240:PHE:O	27:a:244:ASN:HA	1.93	0.67
34:u:403:ARG:HA	34:u:406:ARG:CG	2.23	0.67
34:u:403:ARG:HA	34:u:406:ARG:HG3	1.75	0.67
3:C:197:THR:HG23	3:C:200:ALA:HB1	1.71	0.67
6:F:231:THR:HG21	6:F:354:PHE:O	1.95	0.67
7:G:128:ASN:OD1	8:H:127:VAL:HG23	1.94	0.67
22:V:214:HIS:C	22:V:217:VAL:HG12	2.18	0.67
32:f:717:ALA:HB2	32:f:760:PHE:CE2	2.30	0.67
1:A:84:LYS:O	1:A:88:GLN:N	2.27	0.67
32:f:309:GLU:HA	32:f:314:TYR:CB	2.25	0.67
32:f:418:LEU:HD23	32:f:425:GLY:HA2	1.77	0.67
34:u:403:ARG:HA	34:u:406:ARG:CD	2.24	0.67
29:c:306:THR:OG1	30:d:334:GLU:CB	2.43	0.67
32:f:434:TYR:HD1	34:u:385:ASN:CB	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a:244:ASN:CB	27:a:276:CYS:HA	2.25	0.67
32:f:254:GLY:HA2	32:f:285:CYS:SG	2.35	0.67
12:L:181:GLU:N	12:L:181:GLU:OE2	2.27	0.67
20:T:171:ASP:OD1	20:T:172:MET:N	2.28	0.67
12:l:148:CYS:SG	12:l:152:ASN:O	2.50	0.67
26:Z:69:PHE:CE1	28:b:95:LEU:HD22	2.29	0.67
32:f:112:ASN:OD1	32:f:113:MET:N	2.28	0.67
32:f:117:GLU:OE1	32:f:117:GLU:N	2.26	0.67
32:f:787:LEU:CD2	32:f:791:VAL:HG11	2.17	0.67
2:B:59:ARG:H	32:f:184:LEU:HD22	1.61	0.66
1:A:32:LEU:HG	32:f:96:LEU:CB	2.26	0.66
3:C:268:GLU:OE2	3:C:271:ARG:NE	2.28	0.66
15:O:140:ALA:HB1	15:O:170:MET:HE3	1.75	0.66
23:W:356:ASN:OD1	23:W:357:ARG:N	2.29	0.66
32:f:470:VAL:HG13	32:f:501:LEU:HD23	1.76	0.66
16:p:65:GLN:NE2	17:q:86:ARG:NH1	2.42	0.66
16:p:193:ASP:OD1	16:p:194:LYS:N	2.28	0.66
1:A:176:ASP:OD1	1:A:177:VAL:N	2.29	0.66
24:X:325:LYS:O	24:X:329:ASN:N	2.26	0.66
32:f:611:GLN:O	32:f:615:ILE:N	2.28	0.66
10:J:26:VAL:HG11	10:J:130:SER:HB3	1.77	0.66
21:U:326:ILE:O	21:U:330:SER:CB	2.44	0.66
21:U:472:ILE:O	21:U:475:HIS:NE2	2.28	0.66
7:g:78:CYS:SG	7:g:138:MET:HE2	2.36	0.66
23:W:223:LYS:O	23:W:227:TYR:N	2.25	0.66
34:u:402:LYS:CB	34:u:406:ARG:NH2	2.51	0.66
14:N:207:VAL:HG13	14:N:223:LEU:O	1.95	0.66
27:a:87:MET:HE1	27:a:94:LEU:CB	2.25	0.66
18:r:161:CYS:HB3	18:r:170:LEU:HD13	1.76	0.66
3:C:356:GLY:C	35:C:501:ATP:C8	2.74	0.66
27:a:325:ASP:O	27:a:329:LYS:N	2.28	0.66
32:f:381:VAL:HA	32:f:755:ASP:OD2	1.96	0.66
7:g:203:SER:O	7:g:207:SER:N	2.27	0.66
2:B:183:THR:O	2:B:238:ALA:HB1	1.96	0.66
4:D:406:VAL:O	4:D:408:LYS:NZ	2.22	0.66
24:X:331:LEU:O	24:X:335:LEU:N	2.28	0.66
29:c:158:ASP:OD1	29:c:159:ALA:N	2.28	0.66
32:f:466:LEU:HB3	32:f:485:LEU:HG	1.77	0.66
11:k:41:GLN:NE2	11:k:151:PRO:O	2.28	0.66
2:B:125:THR:CG2	2:B:126:SER:H	2.07	0.66
7:G:203:SER:O	7:G:207:SER:N	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:49:GLU:OE2	8:H:51:LYS:N	2.29	0.66
32:f:710:LEU:HD23	32:f:784:ASP:OD1	1.96	0.66
1:A:82:ALA:HA	1:A:86:THR:HG21	1.77	0.66
21:U:769:PHE:CD2	21:U:776:SER:HB3	2.31	0.66
27:a:244:ASN:CB	27:a:276:CYS:CB	2.73	0.66
32:f:99:LEU:HD12	32:f:99:LEU:O	1.95	0.66
32:f:418:LEU:HD22	32:f:425:GLY:HA2	1.78	0.66
1:A:221:GLY:HA2	35:A:501:ATP:H5'1	1.77	0.65
12:L:125:ARG:HG2	12:L:125:ARG:NH1	2.07	0.65
23:W:407:ASP:O	23:W:412:ILE:N	2.28	0.65
24:X:323:LEU:HD11	24:X:327:TYR:CZ	2.30	0.65
27:a:129:GLN:O	27:a:132:LYS:N	2.28	0.65
13:m:35:SER:OG	13:m:66:ARG:NH1	2.29	0.65
1:A:69:ASP:CA	3:C:82:LYS:HE2	2.26	0.65
2:B:86:LYS:CB	32:f:621:ASP:O	2.45	0.65
21:U:626:LEU:O	21:U:633:CYS:SG	2.53	0.65
28:b:16:MET:HA	28:b:25:ARG:HD2	1.78	0.65
24:X:405:GLN:NE2	29:c:265:MET:SD	2.68	0.65
3:C:357:ALA:CA	35:C:501:ATP:H8	2.09	0.65
14:N:153:MET:HE1	20:T:51:VAL:HG11	1.78	0.65
3:C:197:THR:HA	3:C:200:ALA:HB2	1.79	0.65
23:W:316:ARG:NH1	23:W:383:ASP:OD1	2.29	0.65
26:Z:237:LEU:CD1	26:Z:239:ASP:OD1	2.38	0.65
12:l:227:ASP:OD1	12:l:228:ASP:N	2.29	0.65
12:L:72:ILE:CG1	12:L:88:MET:HE1	2.27	0.65
22:V:162:GLU:O	22:V:166:TYR:N	2.29	0.65
27:a:317:VAL:HG21	27:a:319:LEU:CD2	2.27	0.65
3:C:88:LYS:NZ	3:C:89:VAL:O	2.20	0.65
30:d:346:LEU:O	30:d:349:ILE:HG12	1.97	0.65
1:A:94:GLN:OE1	1:A:94:GLN:N	2.29	0.65
28:b:100:ARG:O	28:b:103:LYS:NZ	2.30	0.65
1:A:432:TYR:CE1	11:K:81:LEU:HD23	2.28	0.65
3:C:42:LEU:O	3:C:45:LEU:HG	1.97	0.65
13:M:11:SER:OG	13:M:14:THR:HG23	1.96	0.65
20:T:144:ARG:NH2	20:T:149:ASN:OD1	2.29	0.65
2:B:87:PRO:O	2:B:89:GLU:HG3	1.96	0.64
6:F:235:LEU:CB	35:F:501:ATP:H5'1	2.25	0.64
7:G:217:VAL:CG1	7:G:230:LEU:CD1	2.73	0.64
9:I:72:MET:CE	9:I:110:LEU:HD23	2.27	0.64
27:a:317:VAL:CG2	27:a:319:LEU:CD2	2.74	0.64
16:p:48:ARG:HG2	16:p:48:ARG:NH1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:309:GLU:CB	32:f:314:TYR:CB	2.76	0.64
12:l:43:HIS:CE1	12:l:184:LEU:HD11	2.31	0.64
1:A:368:ILE:HD11	1:A:370:PHE:CE1	2.32	0.64
11:K:95:GLU:OE1	11:K:107:MET:HE1	1.97	0.64
19:S:190:GLU:OE2	19:S:191:HIS:N	2.30	0.64
20:T:96:LEU:HD13	20:T:157:ILE:HD13	1.79	0.64
11:k:157:ASP:HB2	11:k:158:PRO:HD2	1.79	0.64
12:l:43:HIS:NE2	12:l:184:LEU:HD11	2.13	0.64
1:A:32:LEU:CG	32:f:96:LEU:CB	2.74	0.64
3:C:299:ASP:OD1	3:C:300:ILE:N	2.31	0.64
16:P:109:ILE:HB	16:P:122:CYS:SG	2.38	0.64
20:T:67:ILE:HD13	20:T:95:MET:SD	2.37	0.64
24:X:324:ALA:O	24:X:328:ASP:N	2.28	0.64
27:a:244:ASN:CB	27:a:276:CYS:CA	2.75	0.64
27:a:317:VAL:HG21	27:a:319:LEU:HD23	1.79	0.64
32:f:323:ASN:O	32:f:326:LEU:HG	1.98	0.64
32:f:416:MET:HE3	32:f:801:VAL:HG23	1.76	0.64
32:f:469:TYR:HB2	32:f:481:SER:CB	2.28	0.64
10:j:35:VAL:HG22	10:j:158:ALA:HB1	1.80	0.64
2:B:376:ASP:OD1	2:B:377:ASP:N	2.30	0.64
3:C:198:LEU:CD2	35:C:501:ATP:N3	2.60	0.64
28:b:186:SER:HB2	28:b:187:PRO:HD3	1.79	0.64
32:f:282:PHE:CZ	32:f:317:LEU:HG	2.31	0.64
7:g:210:PHE:HE1	7:g:215:ILE:CD1	2.05	0.64
8:h:222:THR:HG22	8:h:223:PRO:CD	2.27	0.64
9:i:72:MET:HE1	9:i:105:ILE:HG23	1.79	0.64
21:U:52:GLU:OE1	21:U:52:GLU:N	2.31	0.64
32:f:217:LEU:HD21	32:f:244:GLU:OE1	1.95	0.64
17:Q:146:TYR:HB2	17:Q:159:LEU:HD11	1.80	0.64
25:Y:224:VAL:HG23	25:Y:260:LEU:CD1	2.23	0.64
32:f:384:ALA:CB	32:f:419:LEU:O	2.45	0.64
26:Z:68:TRP:HB3	26:Z:104:ASN:ND2	2.13	0.64
31:e:50:ASP:OD1	31:e:51:ASP:N	2.31	0.64
9:i:35:LEU:CB	9:i:163:CYS:HB3	2.28	0.64
12:L:67:ASP:OD2	12:L:92:CYS:HB3	1.97	0.63
17:Q:154:GLU:OE1	17:Q:154:GLU:N	2.30	0.63
23:W:172:GLU:OE2	23:W:182:ARG:NH1	2.31	0.63
24:X:166:LEU:O	24:X:170:GLN:CG	2.46	0.63
32:f:325:GLN:CB	32:f:329:ASN:ND2	2.56	0.63
32:f:416:MET:HE3	32:f:801:VAL:CG2	2.28	0.63
9:I:226:ARG:NH1	9:I:228:LEU:HD23	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:325:GLN:HB2	32:f:329:ASN:CG	2.23	0.63
16:p:65:GLN:HE22	17:q:86:ARG:HH11	1.46	0.63
7:G:190:THR:OG1	7:G:193:GLN:HG2	1.98	0.63
23:W:235:GLN:O	23:W:238:GLY:N	2.30	0.63
32:f:416:MET:HE2	32:f:804:LEU:CD2	2.27	0.63
32:f:466:LEU:CD1	32:f:484:GLY:C	2.72	0.63
7:g:58:ASP:OD1	7:g:59:LYS:N	2.31	0.63
1:A:429:TYR:C	1:A:431:THR:H	2.06	0.63
6:F:90:VAL:HG21	6:F:150:LEU:HD21	1.79	0.63
30:d:349:ILE:O	30:d:350:VAL:CG2	2.46	0.63
32:f:415:GLY:O	32:f:451:VAL:CG2	2.47	0.63
11:k:47:CYS:SG	11:k:195:ILE:HG12	2.37	0.63
3:C:356:GLY:C	35:C:501:ATP:N7	2.56	0.63
20:T:237:VAL:O	20:T:238:THR:OG1	2.14	0.63
32:f:54:ASP:O	32:f:97:LYS:NZ	2.29	0.63
32:f:323:ASN:HB3	32:f:326:LEU:CD1	2.29	0.63
32:f:758:ASN:N	32:f:809:ILE:HG22	2.13	0.63
2:B:182:GLU:OE1	2:B:184:TYR:N	2.31	0.63
21:U:799:LYS:O	21:U:801:GLN:NE2	2.32	0.63
27:a:149:THR:O	27:a:153:SER:N	2.31	0.63
15:O:206:ILE:HD11	15:O:216:ILE:HG12	1.80	0.63
21:U:494:TYR:CE1	21:U:516:LEU:HD11	2.34	0.63
23:W:452:ILE:O	23:W:456:GLN:N	2.31	0.63
32:f:659:LEU:O	32:f:663:GLY:N	2.32	0.63
6:F:414:GLU:N	6:F:414:GLU:OE1	2.31	0.63
24:X:332:GLU:N	24:X:332:GLU:OE1	2.31	0.63
20:t:181:SER:O	20:t:182:LEU:HD12	1.98	0.63
17:Q:60:ILE:CG2	17:Q:84:THR:HG22	2.29	0.63
22:V:207:ALA:HB1	22:V:211:TYR:CZ	2.33	0.63
2:B:263:GLY:O	2:B:266:LEU:N	2.30	0.62
3:C:198:LEU:HD22	35:C:501:ATP:C2'	2.24	0.62
24:X:346:GLN:HG3	24:X:381:GLY:HA2	1.80	0.62
25:Y:186:LEU:HD21	25:Y:213:LEU:HD21	1.81	0.62
27:a:303:THR:O	27:a:307:VAL:N	2.28	0.62
32:f:77:GLU:OE2	32:f:83:ARG:N	2.32	0.62
32:f:292:LYS:O	32:f:294:MET:HE3	1.99	0.62
32:f:493:ASN:ND2	32:f:529:SER:HB2	2.15	0.62
32:f:557:TRP:HZ2	32:f:799:VAL:HG11	1.65	0.62
17:q:36:PHE:HE2	17:q:58:GLU:OE2	1.81	0.62
23:W:61:VAL:O	23:W:65:ARG:N	2.29	0.62
22:V:135:LEU:HD21	22:V:178:SER:OG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:330:ILE:N	30:d:331:PRO:HD2	2.14	0.62
32:f:281:ILE:HG22	32:f:285:CYS:H	1.63	0.62
32:f:326:LEU:O	32:f:330:PHE:N	2.31	0.62
10:J:42:VAL:HG21	10:J:188:ILE:CD1	2.28	0.62
32:f:493:ASN:ND2	32:f:529:SER:CB	2.62	0.62
11:K:228:MET:HA	11:K:228:MET:HE2	1.81	0.62
20:T:98:ALA:HB1	20:T:155:MET:HE1	1.82	0.62
34:u:389:ARG:NE	34:u:393:GLU:OE1	2.30	0.62
21:U:607:VAL:O	21:U:615:ARG:NH2	2.32	0.62
22:V:477:HIS:ND1	22:V:478:GLN:OE1	2.32	0.62
32:f:87:THR:HG21	32:f:113:MET:SD	2.40	0.62
6:F:255:GLN:O	6:F:258:GLN:NE2	2.33	0.62
17:Q:108:ASP:OD1	17:Q:109:GLU:N	2.33	0.62
18:R:256:GLU:OE1	18:R:257:LYS:N	2.32	0.62
20:T:96:LEU:HD12	20:T:97:GLY:N	2.13	0.62
27:a:112:ILE:HG22	27:a:151:VAL:HG21	1.81	0.62
12:l:49:LEU:HB2	12:l:195:LEU:HD21	1.80	0.62
10:J:211:MET:CE	10:J:217:LEU:CB	2.77	0.62
25:Y:68:ASP:OD1	25:Y:69:LEU:N	2.33	0.62
32:f:326:LEU:HD12	32:f:455:VAL:HG22	1.82	0.62
32:f:376:PHE:HE1	32:f:801:VAL:HG12	1.65	0.62
7:G:188:ASP:OD1	7:G:189:TRP:N	2.33	0.62
21:U:24:LEU:HD12	21:U:59:PHE:CG	2.35	0.62
23:W:401:THR:CG2	23:W:402:ILE:H	2.12	0.62
32:f:462:ALA:HB1	32:f:488:ALA:HB2	1.80	0.62
32:f:463:LEU:CA	32:f:489:TYR:CE2	2.83	0.62
11:k:220:VAL:HG22	11:k:226:PHE:HA	1.82	0.62
12:l:103:LEU:HD23	12:l:104:PRO:O	1.99	0.62
2:B:87:PRO:O	2:B:89:GLU:N	2.33	0.61
17:Q:60:ILE:HG21	17:Q:84:THR:CG2	2.30	0.61
21:U:415:HIS:O	21:U:417:LYS:N	2.32	0.61
30:d:340:ILE:HG23	30:d:344:ARG:CZ	2.30	0.61
1:A:32:LEU:HD21	32:f:96:LEU:CB	2.29	0.61
23:W:273:TYR:OH	23:W:287:VAL:HG12	1.99	0.61
7:g:50:ILE:HG13	7:g:141:ILE:HD13	1.81	0.61
1:A:387:SER:HB2	2:B:344:PRO:HB3	1.81	0.61
7:G:93:ARG:NH2	7:G:97:GLU:OE2	2.33	0.61
15:O:210:LEU:HG	19:s:61:PHE:CD1	2.35	0.61
21:U:678:ASP:OD1	21:U:680:VAL:N	2.32	0.61
21:U:772:TRP:HE1	21:U:774:PRO:HB2	1.65	0.61
28:b:72:LEU:HD12	28:b:73:SER:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:257:ARG:NH2	32:f:275:MET:HB2	2.16	0.61
17:q:164:LEU:HD22	17:q:178:PHE:CE2	2.36	0.61
22:V:281:ASN:OD1	22:V:284:GLU:N	2.31	0.61
32:f:434:TYR:CD1	34:u:385:ASN:CB	2.82	0.61
13:m:231:ASP:N	13:m:231:ASP:OD1	2.32	0.61
2:B:46:ALA:HB2	2:B:178:LYS:HA	1.82	0.61
7:g:123:GLN:NE2	7:g:127:GLN:CG	2.64	0.61
1:A:276:GLU:OE1	2:B:310:LEU:HB3	2.00	0.61
8:H:10:LEU:CD1	8:H:19:LEU:HD13	2.29	0.61
15:O:210:LEU:CG	19:s:61:PHE:CD1	2.84	0.61
23:W:228:ASN:O	23:W:232:GLN:N	2.24	0.61
32:f:287:ASP:OD2	32:f:816:TYR:CZ	2.53	0.61
32:f:446:LEU:HD11	32:f:483:PHE:CD2	2.35	0.61
32:f:729:MET:SD	32:f:729:MET:N	2.73	0.61
16:p:122:CYS:HG	16:p:131:MET:C	2.09	0.61
13:M:216:TRP:HE1	13:M:228:VAL:CB	2.14	0.61
29:c:180:ASN:OD1	29:c:181:LEU:N	2.34	0.61
9:i:163:CYS:SG	9:i:171:ALA:HB3	2.41	0.61
7:G:158:GLY:O	8:H:84:ARG:NH2	2.34	0.61
16:P:30:ILE:HG22	16:P:31:GLN:H	1.65	0.61
32:f:418:LEU:HD21	32:f:428:GLN:NE2	2.14	0.61
32:f:463:LEU:CA	32:f:489:TYR:HE2	2.14	0.61
32:f:466:LEU:HB2	32:f:485:LEU:HG	1.83	0.61
32:f:732:VAL:HG13	32:f:732:VAL:O	2.00	0.61
9:i:97:TYR:CZ	9:i:106:PRO:HD3	2.36	0.61
2:B:102:LEU:HD12	2:B:137:SER:HB2	1.83	0.61
3:C:217:SER:OG	3:C:218:GLU:N	2.28	0.61
10:J:176:TYR:CZ	10:J:181:ILE:HD11	2.36	0.61
16:P:50:TYR:CD2	16:P:190:ILE:HD11	2.35	0.61
21:U:333:MET:SD	21:U:333:MET:N	2.73	0.61
22:V:210:CYS:O	22:V:214:HIS:ND1	2.34	0.61
25:Y:275:LEU:HD23	31:e:60:LEU:HD21	1.83	0.61
27:a:291:LEU:HD12	27:a:295:GLU:OE1	2.01	0.61
30:d:235:TYR:O	30:d:240:SER:N	2.34	0.61
31:e:41:ASP:OD1	31:e:42:ASN:N	2.33	0.61
32:f:309:GLU:CA	32:f:314:TYR:CB	2.79	0.61
34:u:402:LYS:HB3	34:u:406:ARG:HH21	1.57	0.61
1:A:219:GLY:C	35:A:501:ATP:H5'2	2.26	0.61
4:D:190:LEU:HD23	4:D:190:LEU:H	1.65	0.61
4:D:211:GLY:O	4:D:333:PHE:CE2	2.53	0.61
14:N:68:LEU:O	14:N:68:LEU:HD12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:348:ILE:HG23	32:f:754:LYS:CB	2.28	0.61
32:f:460:ASP:OD1	32:f:489:TYR:CE1	2.52	0.61
23:W:373:ILE:CB	23:W:413:ILE:HD11	2.31	0.60
6:F:188:ILE:HD11	6:F:195:ILE:HD11	1.82	0.60
20:T:118:ASP:N	20:T:118:ASP:OD1	2.32	0.60
26:Z:51:SER:OG	26:Z:52:ASN:N	2.33	0.60
27:a:317:VAL:HG13	27:a:318:GLY:N	2.14	0.60
20:t:118:ASP:N	20:t:118:ASP:OD1	2.34	0.60
1:A:432:TYR:CD1	11:K:81:LEU:HD23	2.36	0.60
8:H:38:ILE:CD1	8:H:174:LEU:HD11	2.31	0.60
9:I:186:LEU:O	9:I:189:ALA:N	2.34	0.60
15:o:102:ILE:HD12	15:o:126:LEU:HG	1.83	0.60
20:t:238:THR:CG2	20:t:239:GLU:H	2.13	0.60
2:B:54:PRO:CA	32:f:835:GLU:HB2	2.28	0.60
2:B:58:CYS:HG	32:f:835:GLU:CD	2.09	0.60
21:U:221:ILE:HD12	21:U:222:PHE:CD1	2.37	0.60
22:V:61:GLU:OE1	22:V:61:GLU:N	2.31	0.60
10:J:189:LYS:HB3	10:J:232:ILE:HD11	1.82	0.60
13:M:94:GLU:OE1	13:M:95:GLU:N	2.34	0.60
23:W:402:ILE:HD12	23:W:403:PHE:H	1.67	0.60
32:f:325:GLN:O	32:f:329:ASN:CB	2.47	0.60
11:k:217:LEU:HD22	11:k:230:THR:HG21	1.82	0.60
2:B:153:ASN:OD1	2:B:154:HIS:N	2.35	0.60
6:F:80:ILE:HG22	6:F:80:ILE:O	2.02	0.60
21:U:609:ASP:O	21:U:615:ARG:NH1	2.34	0.60
32:f:282:PHE:HZ	32:f:317:LEU:HG	1.63	0.60
32:f:706:ILE:HD11	32:f:741:LEU:CG	2.31	0.60
10:j:109:ARG:NH2	18:r:129:ASN:OD1	2.35	0.60
20:t:93:SER:O	20:t:94:THR:OG1	2.19	0.60
3:C:250:GLU:OE1	3:C:250:GLU:N	2.33	0.60
18:R:60:THR:OG1	18:R:92:LYS:NZ	2.29	0.60
17:q:85:ARG:HH11	17:q:85:ARG:HG3	1.66	0.60
1:A:65:ILE:O	1:A:65:ILE:HG22	2.02	0.60
2:B:181:GLN:OE1	2:B:182:GLU:N	2.35	0.60
19:S:159:GLN:NE2	19:S:160:ARG:O	2.35	0.60
20:T:67:ILE:HB	20:T:95:MET:HE2	1.83	0.60
24:X:344:ARG:HA	24:X:382:GLU:HA	1.83	0.60
28:b:161:ASN:OD1	28:b:167:GLY:N	2.34	0.60
32:f:298:LEU:O	32:f:302:GLY:N	2.35	0.60
9:i:140:ASP:OD1	9:i:146:GLN:NE2	2.35	0.60
11:k:65:GLU:OE1	11:k:65:GLU:N	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HG	2:B:79:ILE:HG23	1.84	0.60
1:A:429:TYR:O	1:A:431:THR:N	2.27	0.60
3:C:187:LEU:HD13	3:C:188:LEU:N	2.17	0.60
23:W:337:ALA:O	23:W:342:GLY:N	2.35	0.60
32:f:441:LYS:CD	32:f:477:MET:HE1	2.32	0.60
32:f:729:MET:O	32:f:732:VAL:HG12	2.01	0.60
1:A:69:ASP:HA	3:C:82:LYS:HE2	1.84	0.60
12:L:49:LEU:HB2	12:L:195:LEU:HD21	1.84	0.60
14:N:188:GLN:NE2	14:N:192:ASN:OD1	2.35	0.60
15:O:61:THR:HG1	15:O:214:SER:HB3	1.64	0.60
22:V:444:ASP:OD1	22:V:444:ASP:N	2.35	0.60
22:V:470:ARG:HH21	30:d:329:THR:H	1.49	0.60
23:W:314:LEU:HD23	23:W:315:MET:N	2.17	0.60
25:Y:365:GLN:O	25:Y:369:THR:HG23	2.01	0.60
27:a:109:GLU:OE1	27:a:109:GLU:N	2.35	0.60
8:h:12:THR:CG2	9:i:20:GLN:OE1	2.50	0.60
17:q:37:LYS:NZ	17:q:40:GLU:OE1	2.34	0.60
4:D:371:SER:N	4:D:374:ASP:OD2	2.34	0.59
11:K:226:PHE:O	11:K:228:MET:N	2.34	0.59
14:N:38:MET:HE1	14:N:190:THR:HA	1.84	0.59
22:V:73:GLU:O	22:V:77:GLU:N	2.35	0.59
10:J:18:GLN:HA	10:J:18:GLN:HE21	1.66	0.59
23:W:440:ASN:O	23:W:443:THR:CG2	2.43	0.59
25:Y:171:GLY:O	25:Y:177:ARG:NH2	2.35	0.59
14:n:38:MET:HE1	14:n:193:ALA:HB3	1.83	0.59
3:C:155:ASP:OD1	3:C:155:ASP:N	2.35	0.59
11:K:94:VAL:HG22	18:R:124:ILE:HD11	1.85	0.59
14:N:52:SER:HB2	14:N:65:THR:H	1.66	0.59
23:W:34:LEU:O	23:W:44:ILE:HD11	2.02	0.59
23:W:343:SER:O	23:W:347:GLY:N	2.33	0.59
28:b:25:ARG:HH22	28:b:145:GLU:H	1.49	0.59
32:f:253:LEU:HD23	32:f:256:PHE:CG	2.38	0.59
32:f:282:PHE:HZ	32:f:317:LEU:CG	2.10	0.59
13:m:76:MET:HE3	13:m:78:VAL:CG2	2.32	0.59
21:U:489:ALA:HA	21:U:520:MET:HE1	1.83	0.59
21:U:765:VAL:HG11	21:U:778:PHE:CG	2.37	0.59
25:Y:296:VAL:CG2	31:e:60:LEU:HD22	2.32	0.59
32:f:483:PHE:HZ	32:f:802:SER:CB	2.15	0.59
11:K:95:GLU:CD	11:K:107:MET:HE1	2.27	0.59
21:U:495:ASP:OD1	21:U:496:LEU:N	2.35	0.59
21:U:681:ASN:HA	21:U:684:ARG:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:304:GLU:OE2	22:V:304:GLU:N	2.30	0.59
26:Z:214:LYS:CB	26:Z:221:PRO:CG	2.80	0.59
30:d:309:VAL:HG22	30:d:310:LEU:H	1.67	0.59
7:g:127:GLN:OE1	8:h:128:ARG:NH1	2.36	0.59
17:q:19:ARG:NH2	17:q:31:ASP:OD1	2.35	0.59
22:V:244:ALA:O	22:V:247:GLN:NE2	2.35	0.59
12:L:9:ASP:OD1	12:L:10:VAL:N	2.35	0.59
14:N:43:ASP:N	14:N:43:ASP:OD1	2.33	0.59
15:O:210:LEU:CG	19:s:61:PHE:CE1	2.80	0.59
25:Y:238:GLU:C	25:Y:238:GLU:OE1	2.45	0.59
27:a:324:ILE:HD12	27:a:331:VAL:HA	1.83	0.59
17:q:1:MET:HE3	17:q:1:MET:C	2.27	0.59
9:I:26:GLU:OE1	9:I:27:ALA:N	2.36	0.59
10:J:115:LYS:HZ1	10:J:129:ILE:HD12	1.68	0.59
24:X:322:HIS:O	24:X:326:LEU:N	2.32	0.59
25:Y:173:ASP:N	25:Y:173:ASP:OD1	2.34	0.59
25:Y:241:ILE:O	25:Y:247:LEU:HD11	2.02	0.59
29:c:265:MET:HA	29:c:265:MET:HE3	1.85	0.59
1:A:87:LEU:HA	1:A:90:GLU:HB2	1.83	0.59
25:Y:316:LEU:HD12	25:Y:317:GLY:N	2.17	0.59
26:Z:96:HIS:ND1	26:Z:97:THR:O	2.33	0.59
26:Z:257:MET:HA	26:Z:257:MET:HE2	1.83	0.59
10:j:177:THR:OG1	10:j:180:ALA:HB2	2.02	0.59
28:b:161:ASN:ND2	28:b:168:SER:OG	2.36	0.59
14:n:224:LEU:C	14:n:224:LEU:HD12	2.28	0.59
16:p:31:GLN:OE1	16:p:31:GLN:HA	2.01	0.59
1:A:430:MET:SD	11:K:59:MET:HE1	2.43	0.58
3:C:336:MET:HE2	3:C:336:MET:HA	1.85	0.58
8:H:69:THR:HG22	8:H:70:LYS:H	1.68	0.58
18:R:240:GLU:OE1	18:R:241:ASP:N	2.35	0.58
27:a:313:LYS:HA	27:a:316:SER:OG	2.03	0.58
18:R:61:THR:HG22	18:R:190:GLY:CA	2.33	0.58
21:U:135:ASN:O	21:U:139:GLN:NE2	2.36	0.58
32:f:605:ASN:OD1	32:f:609:VAL:N	2.31	0.58
7:g:149:PRO:O	7:g:150:GLN:NE2	2.36	0.58
7:g:210:PHE:CD1	7:g:215:ILE:CG2	2.86	0.58
15:o:102:ILE:HD13	15:o:126:LEU:HG	1.86	0.58
31:e:49:GLU:O	31:e:53:SER:N	2.36	0.58
32:f:287:ASP:OD2	32:f:816:TYR:CD1	2.57	0.58
32:f:446:LEU:CD1	32:f:483:PHE:CD2	2.87	0.58
4:D:167:ILE:HA	36:D:501:ADP:N6	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:153:ASP:OD1	13:M:153:ASP:N	2.36	0.58
27:a:175:ASP:OD1	27:a:176:ALA:N	2.37	0.58
32:f:293:GLN:OE1	32:f:295:ALA:N	2.35	0.58
32:f:560:LEU:HD22	32:f:782:HIS:NE2	2.14	0.58
1:A:394:MET:HE2	1:A:394:MET:HA	1.85	0.58
2:B:313:LEU:HD21	2:B:346:ARG:CZ	2.34	0.58
5:E:140:GLU:N	5:E:140:GLU:OE1	2.36	0.58
18:R:60:THR:O	18:R:189:SER:N	2.36	0.58
20:T:238:THR:CG2	20:T:239:GLU:H	2.17	0.58
23:W:229:LEU:O	23:W:233:LEU:N	2.36	0.58
32:f:283:THR:CA	32:f:816:TYR:CE1	2.82	0.58
17:q:1:MET:HE3	17:q:2:GLU:N	2.18	0.58
11:K:5:ARG:NH2	11:K:7:GLU:OE1	2.37	0.58
1:A:369:ARG:NH1	11:K:206:MET:O	2.36	0.58
35:B:501:ATP:O2G	3:C:310:ARG:NH2	2.36	0.58
14:N:68:LEU:HD12	14:N:68:LEU:C	2.29	0.58
21:U:765:VAL:HG11	21:U:778:PHE:CD1	2.39	0.58
26:Z:67:VAL:HG11	28:b:95:LEU:HD13	1.86	0.58
28:b:66:PRO:O	28:b:67:ASP:OD1	2.22	0.58
32:f:762:VAL:O	32:f:771:LEU:N	2.33	0.58
11:k:104:ASN:OD1	18:r:116:ARG:NH2	2.36	0.58
9:I:44:LEU:HD21	9:I:189:ALA:HB1	1.85	0.58
20:T:95:MET:CE	20:T:235:ALA:CB	2.76	0.58
21:U:373:ASN:OD1	21:U:374:SER:N	2.37	0.58
21:U:645:ASN:OD1	21:U:647:HIS:N	2.36	0.58
30:d:300:THR:OG1	30:d:301:ASP:N	2.37	0.58
7:g:112:ASP:OD1	7:g:113:MET:N	2.37	0.58
20:t:238:THR:CG2	20:t:239:GLU:N	2.66	0.58
1:A:322:ASN:OD1	1:A:323:ARG:N	2.37	0.58
4:D:309:MET:HA	4:D:309:MET:HE3	1.86	0.58
7:G:12:HIS:NE2	13:M:7:GLY:O	2.37	0.58
11:K:210:LEU:HD13	11:K:211:ASN:N	2.19	0.58
22:V:470:ARG:O	22:V:473:GLN:N	2.33	0.58
32:f:251:CYS:O	32:f:253:LEU:HD12	2.03	0.58
32:f:399:LEU:HD12	32:f:432:TYR:CE1	2.38	0.58
32:f:869:THR:HG22	32:f:882:LEU:HB3	1.86	0.58
3:C:131:VAL:HG23	3:C:134:LEU:HD13	1.86	0.57
3:C:197:THR:HA	3:C:200:ALA:CB	2.34	0.57
6:F:235:LEU:HD22	35:F:501:ATP:H2'	1.85	0.57
2:B:193:GLN:OE1	2:B:193:GLN:N	2.36	0.57
13:M:71:ASP:OD1	13:M:72:ARG:N	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:58:THR:HG23	16:P:59:ASP:N	2.18	0.57
21:U:167:ILE:HD12	21:U:168:LEU:HD13	1.86	0.57
24:X:160:MET:HA	24:X:160:MET:HE3	1.86	0.57
25:Y:14:ASN:CB	25:Y:15:PRO:HD3	2.34	0.57
27:a:228:THR:O	27:a:230:ARG:NH2	2.37	0.57
29:c:124:GLY:O	29:c:127:ILE:HG22	2.04	0.57
13:m:71:ASP:OD1	13:m:72:ARG:N	2.34	0.57
1:A:40:THR:OG1	32:f:132:THR:CB	2.53	0.57
2:B:276:GLU:OE1	2:B:277:HIS:ND1	2.37	0.57
5:E:178:THR:OG1	5:E:340:GLY:N	2.31	0.57
16:P:65:GLN:OE1	17:Q:86:ARG:NH2	2.36	0.57
21:U:7:GLY:N	30:d:173:CYS:SG	2.77	0.57
21:U:696:ILE:HD13	21:U:736:ILE:O	2.04	0.57
24:X:45:VAL:O	24:X:45:VAL:HG23	2.05	0.57
32:f:745:LEU:O	32:f:749:ALA:N	2.35	0.57
20:t:67:ILE:HD13	20:t:95:MET:SD	2.44	0.57
36:D:501:ADP:C8	36:D:501:ADP:C3'	2.86	0.57
6:F:418:GLU:OE1	6:F:418:GLU:N	2.31	0.57
18:R:61:THR:HG22	18:R:190:GLY:H	1.69	0.57
20:T:120:GLU:C	20:T:120:GLU:OE1	2.47	0.57
26:Z:246:VAL:HG23	26:Z:247:LYS:HD2	1.87	0.57
27:a:365:MET:SD	27:a:366:LEU:N	2.77	0.57
32:f:415:GLY:HA2	32:f:429:ILE:HD11	1.86	0.57
13:m:54:VAL:HG13	13:m:54:VAL:O	2.04	0.57
17:q:4:LEU:HD11	17:q:47:VAL:HG13	1.86	0.57
19:s:74:LEU:C	19:s:75:THR:HG23	2.28	0.57
6:F:154:ASN:OD1	6:F:156:ASP:N	2.36	0.57
15:O:206:ILE:CD1	15:O:216:ILE:HG12	2.33	0.57
19:S:58:SER:OG	19:S:62:SER:O	2.20	0.57
20:T:152:TRP:CD2	20:T:172:MET:HE1	2.40	0.57
25:Y:152:MET:O	25:Y:152:MET:HE3	2.04	0.57
3:C:197:THR:O	3:C:200:ALA:CA	2.52	0.57
3:C:329:LEU:HD22	3:C:344:LEU:HD22	1.85	0.57
5:E:188:ALA:O	5:E:192:ASP:N	2.37	0.57
6:F:146:LYS:N	6:F:146:LYS:HD3	2.20	0.57
6:F:252:ALA:N	6:F:255:GLN:OE1	2.37	0.57
8:H:127:VAL:O	8:H:127:VAL:HG13	2.03	0.57
9:I:209:GLU:OE1	9:I:209:GLU:N	2.37	0.57
26:Z:214:LYS:CB	26:Z:221:PRO:HG3	2.35	0.57
32:f:670:MET:HE1	32:f:704:LEU:HA	1.86	0.57
32:f:821:LEU:HD13	32:f:882:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:ASP:OD1	3:C:99:VAL:N	2.37	0.57
3:C:356:GLY:HA3	35:C:501:ATP:N7	2.20	0.57
21:U:510:GLU:OE1	21:U:510:GLU:N	2.36	0.57
21:U:666:LYS:NZ	21:U:702:THR:O	2.30	0.57
30:d:259:PHE:O	30:d:262:ILE:HD12	2.03	0.57
32:f:294:MET:HE2	32:f:807:ARG:NH1	2.20	0.57
32:f:354:GLU:HG2	32:f:729:MET:HE2	1.87	0.57
32:f:809:ILE:HG23	32:f:809:ILE:O	2.05	0.57
10:J:26:VAL:HG11	10:J:130:SER:CB	2.34	0.57
25:Y:126:LYS:O	25:Y:126:LYS:NZ	2.34	0.57
29:c:29:GLU:O	29:c:204:THR:OG1	2.21	0.57
1:A:56:LEU:HD21	2:B:48:LYS:CE	2.27	0.57
5:E:37:THR:O	5:E:41:GLU:N	2.33	0.57
21:U:659:CYS:SG	21:U:660:CYS:N	2.78	0.57
32:f:446:LEU:CD1	32:f:483:PHE:HD2	2.17	0.57
2:B:86:LYS:CA	32:f:621:ASP:O	2.53	0.57
7:G:211:LYS:HG2	7:G:212:PRO:CD	2.31	0.57
20:T:72:LEU:HD11	20:T:79:ALA:HB1	1.85	0.57
23:W:22:ALA:O	23:W:26:GLN:NE2	2.38	0.57
23:W:251:TYR:C	23:W:254:PRO:HD2	2.29	0.57
23:W:273:TYR:O	23:W:277:ALA:N	2.37	0.57
25:Y:232:GLU:O	25:Y:236:LEU:N	2.35	0.57
32:f:19:ALA:O	32:f:23:GLY:N	2.38	0.57
7:g:78:CYS:SG	7:g:140:LEU:CD2	2.91	0.57
7:g:210:PHE:CE1	7:g:215:ILE:HG21	2.39	0.57
1:A:52:ILE:HD12	2:B:68:ILE:HG22	1.86	0.56
4:D:175:GLN:NE2	4:D:179:GLU:OE2	2.38	0.56
6:F:347:ARG:O	6:F:348:LEU:HD22	2.04	0.56
7:G:62:ASP:OD2	13:M:160:GLY:C	2.48	0.56
20:T:152:TRP:O	20:T:153:ASN:ND2	2.38	0.56
24:X:369:ILE:CG2	24:X:370:LEU:HG	2.35	0.56
30:d:349:ILE:C	30:d:350:VAL:HG23	2.30	0.56
17:q:85:ARG:HH11	17:q:85:ARG:CG	2.18	0.56
16:P:59:ASP:OD2	16:P:104:TYR:N	2.34	0.56
23:W:254:PRO:O	23:W:258:ALA:N	2.38	0.56
24:X:268:GLN:N	24:X:268:GLN:OE1	2.38	0.56
26:Z:59:ASP:CG	28:b:95:LEU:HD21	2.30	0.56
30:d:191:LEU:HA	30:d:194:LEU:HD12	1.86	0.56
12:l:148:CYS:HB2	12:l:149:PRO:HD2	1.87	0.56
1:A:32:LEU:CD1	32:f:96:LEU:O	2.54	0.56
1:A:62:LEU:HG	2:B:79:ILE:CG2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:HA	2:B:138:PHE:O	2.05	0.56
1:A:143:ASP:OD1	1:A:144:ARG:N	2.38	0.56
8:H:6:TYR:O	8:H:7:SER:OG	2.18	0.56
19:S:99:ARG:HE	19:S:119:MET:HE2	1.68	0.56
20:T:238:THR:CG2	20:T:239:GLU:N	2.69	0.56
21:U:195:ASN:OD1	21:U:196:LYS:N	2.38	0.56
21:U:575:ASP:OD2	21:U:578:LEU:HD12	2.01	0.56
23:W:280:ASP:C	23:W:280:ASP:OD1	2.47	0.56
23:W:313:GLU:C	23:W:365:ILE:HD12	2.29	0.56
24:X:224:ASP:OD1	24:X:225:TRP:N	2.39	0.56
24:X:258:LYS:HA	24:X:261:LEU:HD12	1.86	0.56
25:Y:240:VAL:CG2	25:Y:260:LEU:HD11	2.36	0.56
25:Y:312:ARG:NH1	25:Y:312:ARG:O	2.38	0.56
27:a:87:MET:HE1	27:a:94:LEU:HA	1.87	0.56
28:b:25:ARG:NH2	28:b:144:GLY:CA	2.68	0.56
32:f:376:PHE:HE1	32:f:801:VAL:HB	1.71	0.56
32:f:466:LEU:HB2	32:f:485:LEU:CG	2.35	0.56
7:G:56:VAL:HG23	7:G:61:LEU:HD22	1.87	0.56
10:J:166:LYS:O	10:J:166:LYS:NZ	2.38	0.56
21:U:330:SER:O	21:U:332:GLU:N	2.35	0.56
26:Z:238:PRO:CB	27:a:286:ALA:HB2	2.34	0.56
27:a:293:PHE:N	27:a:328:ASP:O	2.38	0.56
32:f:670:MET:HE1	32:f:704:LEU:N	2.21	0.56
3:C:173:GLU:OE1	3:C:173:GLU:N	2.35	0.56
3:C:198:LEU:HD23	35:C:501:ATP:C2	2.39	0.56
4:D:307:VAL:O	4:D:308:ILE:HD13	2.06	0.56
26:Z:104:ASN:HD22	26:Z:108:ILE:HD11	1.71	0.56
29:c:286:GLU:OE1	29:c:287:HIS:N	2.35	0.56
32:f:466:LEU:HB2	32:f:485:LEU:HD21	1.86	0.56
32:f:557:TRP:CZ2	32:f:799:VAL:HG11	2.40	0.56
9:i:163:CYS:SG	9:i:171:ALA:CB	2.93	0.56
2:B:130:GLU:O	2:B:131:HIS:ND1	2.39	0.56
4:D:261:ILE:O	4:D:262:ILE:HD13	2.05	0.56
5:E:83:CYS:SG	5:E:87:LEU:HB2	2.45	0.56
7:G:217:VAL:HG12	7:G:230:LEU:CD1	2.33	0.56
16:P:50:TYR:HD2	16:P:190:ILE:HD11	1.70	0.56
21:U:693:LEU:O	21:U:696:ILE:HG22	2.06	0.56
25:Y:199:GLU:C	25:Y:199:GLU:OE1	2.49	0.56
26:Z:253:THR:OG1	30:d:330:ILE:HD11	2.05	0.56
7:g:210:PHE:CD1	7:g:215:ILE:HG21	2.41	0.56
12:l:49:LEU:CD1	12:l:209:ASN:O	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:ALA:O	2:B:378:VAL:HG22	2.06	0.56
6:F:91:SER:O	6:F:151:VAL:N	2.36	0.56
21:U:769:PHE:CD1	21:U:769:PHE:C	2.84	0.56
26:Z:25:ARG:NH2	29:c:71:ASP:OD2	2.38	0.56
28:b:39:SER:OG	28:b:42:ARG:NH2	2.38	0.56
2:B:58:CYS:SG	32:f:835:GLU:OE2	2.61	0.56
3:C:198:LEU:HA	3:C:201:ARG:HG2	1.87	0.56
35:C:501:ATP:H2'	35:C:501:ATP:N3	2.20	0.56
4:D:384:MET:HA	4:D:384:MET:HE3	1.88	0.56
23:W:254:PRO:HB2	23:W:263:TRP:CB	2.35	0.56
27:a:302:ILE:HG21	27:a:310:LEU:HD12	1.88	0.56
12:l:166:GLN:OE1	12:l:169:ARG:NH1	2.38	0.56
34:u:402:LYS:O	34:u:406:ARG:CG	2.46	0.56
7:G:206:LEU:HB3	7:G:208:ILE:CD1	2.36	0.56
23:W:254:PRO:HB2	23:W:263:TRP:CD1	2.41	0.56
23:W:428:TRP:CH2	29:c:245:VAL:HG11	2.41	0.56
27:a:4:VAL:HB	27:a:5:PRO:HD3	1.88	0.56
32:f:244:GLU:HA	32:f:248:LEU:HD12	1.88	0.56
7:g:130:GLU:OE2	13:m:127:SER:OG	2.23	0.56
4:D:94:GLU:OE1	4:D:94:GLU:N	2.39	0.56
17:Q:39:SER:HB3	17:Q:40:GLU:OE2	2.06	0.56
21:U:587:ALA:HB2	21:U:621:SER:CB	2.36	0.56
26:Z:189:GLN:N	26:Z:189:GLN:OE1	2.38	0.56
32:f:272:LEU:HA	32:f:275:MET:HE3	1.88	0.56
32:f:471:LEU:CD2	32:f:504:VAL:HG22	2.35	0.56
32:f:766:GLN:CG	32:f:768:LEU:HD12	2.36	0.56
18:r:239:ARG:HH21	18:r:244:ILE:HD13	1.69	0.56
18:R:115:GLU:OE1	18:R:115:GLU:N	2.39	0.55
21:U:59:PHE:O	21:U:63:VAL:HG23	2.06	0.55
27:a:68:GLU:O	27:a:69:HIS:ND1	2.39	0.55
29:c:104:ARG:NE	29:c:105:PRO:O	2.37	0.55
32:f:706:ILE:HD11	32:f:741:LEU:CD2	2.35	0.55
3:C:335:LYS:NZ	4:D:194:ILE:O	2.29	0.55
10:J:52:LYS:HG3	10:J:53:LEU:HG	1.87	0.55
13:M:38:ILE:HG22	13:M:165:ALA:CB	2.37	0.55
22:V:205:LEU:HD22	22:V:205:LEU:H	1.69	0.55
26:Z:67:VAL:CG1	28:b:95:LEU:HD13	2.36	0.55
32:f:414:LEU:HD21	32:f:428:GLN:O	2.05	0.55
12:l:46:LEU:H	12:l:46:LEU:HD23	1.71	0.55
13:m:100:ARG:NH1	13:m:106:ASN:OD1	2.39	0.55
1:A:325:ASP:OD1	1:A:325:ASP:N	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:THR:HG23	2:B:184:TYR:N	2.21	0.55
3:C:197:THR:O	3:C:201:ARG:N	2.39	0.55
7:G:56:VAL:HG13	7:G:56:VAL:O	2.06	0.55
21:U:579:ARG:NH2	21:U:611:ASN:OD1	2.39	0.55
24:X:140:THR:OG1	24:X:142:ARG:NH1	2.39	0.55
26:Z:68:TRP:CB	26:Z:104:ASN:HD21	2.15	0.55
13:m:109:LEU:HD22	13:m:140:SER:HB3	1.86	0.55
16:p:149:MET:HA	16:p:149:MET:HE3	1.88	0.55
21:U:183:LEU:O	21:U:186:SER:OG	2.21	0.55
23:W:55:ARG:NH2	23:W:58:SER:OG	2.40	0.55
28:b:4:GLU:OE1	28:b:6:THR:OG1	2.23	0.55
32:f:650:GLN:O	32:f:654:VAL:N	2.32	0.55
9:i:35:LEU:HD12	9:i:35:LEU:C	2.32	0.55
1:A:351:ARG:NH1	1:A:378:PRO:O	2.39	0.55
2:B:229:GLY:HA3	3:C:307:ARG:HD2	1.89	0.55
3:C:356:GLY:CA	35:C:501:ATP:N7	2.70	0.55
20:T:95:MET:HE1	20:T:235:ALA:CB	2.13	0.55
23:W:73:MET:N	23:W:73:MET:SD	2.80	0.55
27:a:246:GLU:O	27:a:249:GLN:N	2.40	0.55
32:f:783:SER:HG	32:f:790:GLN:HE21	1.55	0.55
13:m:216:TRP:CD1	13:m:228:VAL:HG12	2.41	0.55
21:U:30:VAL:O	21:U:30:VAL:HG23	2.05	0.55
28:b:178:SER:OG	28:b:183:LEU:HD21	2.06	0.55
2:B:241:ASN:O	2:B:241:ASN:ND2	2.40	0.55
10:J:42:VAL:HG22	10:J:210:VAL:HG12	1.87	0.55
24:X:390:GLU:N	24:X:391:PRO:CD	2.70	0.55
1:A:33:LEU:HD11	2:B:407:LEU:CD1	2.29	0.55
17:Q:94:SER:OG	17:Q:95:ARG:N	2.40	0.55
32:f:414:LEU:HD22	32:f:432:TYR:HE2	1.71	0.55
32:f:726:ILE:HD11	32:f:727:PHE:CZ	2.41	0.55
9:i:35:LEU:HB2	9:i:163:CYS:HB3	1.88	0.55
12:l:181:GLU:OE1	12:l:181:GLU:N	2.33	0.55
18:r:235:LEU:HD23	18:r:246:VAL:HG11	1.89	0.55
10:J:18:GLN:HE21	10:J:18:GLN:CA	2.18	0.55
10:J:108:THR:HG21	10:J:145:TYR:HB2	1.89	0.55
27:a:107:SER:OG	27:a:109:GLU:OE1	2.25	0.55
27:a:219:HIS:CE1	27:a:221:VAL:HG22	2.41	0.55
29:c:123:SER:OG	29:c:124:GLY:N	2.38	0.55
32:f:692:LEU:HD22	32:f:712:LYS:HZ2	1.72	0.55
1:A:33:LEU:HD22	3:C:174:LEU:CD1	2.37	0.55
3:C:275:GLU:C	3:C:275:GLU:OE1	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:242:GLU:OE1	9:I:243:GLU:N	2.40	0.55
21:U:5:ALA:HB2	21:U:34:PHE:CG	2.42	0.55
21:U:573:ASP:CG	21:U:578:LEU:CD2	2.80	0.55
32:f:388:ASP:OD1	32:f:392:THR:HG23	2.07	0.55
10:j:102:VAL:HG13	10:j:106:TYR:HD2	1.72	0.55
10:j:122:ASN:OD1	10:j:123:GLY:N	2.39	0.55
9:I:212:GLU:OE1	9:I:212:GLU:N	2.40	0.54
16:P:45:MET:HA	16:P:45:MET:HE3	1.87	0.54
23:W:53:GLN:O	23:W:56:THR:OG1	2.22	0.54
23:W:87:ILE:O	23:W:90:LEU:N	2.40	0.54
32:f:66:LYS:O	32:f:69:SER:OG	2.26	0.54
32:f:597:VAL:C	32:f:638:ASP:OD2	2.50	0.54
13:m:140:SER:OG	13:m:141:TYR:N	2.40	0.54
2:B:186:ASP:OD1	2:B:186:ASP:N	2.41	0.54
3:C:131:VAL:HG13	3:C:131:VAL:O	2.06	0.54
10:J:108:THR:HG21	10:J:145:TYR:CB	2.37	0.54
11:K:210:LEU:HD21	11:K:215:ILE:HG21	1.89	0.54
21:U:43:ASP:OD1	21:U:43:ASP:N	2.40	0.54
22:V:201:ARG:O	22:V:205:LEU:HD23	2.07	0.54
26:Z:263:ALA:O	26:Z:266:ILE:HG13	2.07	0.54
32:f:87:THR:OG1	32:f:109:ILE:O	2.21	0.54
32:f:261:ARG:CZ	32:f:295:ALA:HB2	2.36	0.54
32:f:376:PHE:CE1	32:f:801:VAL:HB	2.42	0.54
32:f:716:ASP:OD1	32:f:716:ASP:O	2.26	0.54
19:s:56:ARG:NH2	19:s:219:ASP:OD1	2.38	0.54
4:D:367:PRO:C	4:D:368:ASP:OD1	2.51	0.54
21:U:50:GLU:OE1	21:U:50:GLU:N	2.33	0.54
22:V:170:LEU:O	22:V:173:ILE:N	2.40	0.54
26:Z:34:ARG:CA	26:Z:97:THR:HG1	2.16	0.54
26:Z:63:LYS:O	28:b:91:ARG:NH2	2.40	0.54
32:f:186:THR:HG23	32:f:197:ALA:HB3	1.90	0.54
13:m:42:CYS:SG	13:m:187:CYS:CA	2.95	0.54
1:A:69:ASP:CB	3:C:82:LYS:CE	2.69	0.54
2:B:229:GLY:CA	3:C:307:ARG:HD2	2.36	0.54
3:C:357:ALA:CA	35:C:501:ATP:C8	2.88	0.54
4:D:167:ILE:CA	36:D:501:ADP:HN62	2.20	0.54
13:M:48:PHE:HB2	13:M:215:SER:HG	1.67	0.54
27:a:261:LEU:O	27:a:265:GLU:N	2.40	0.54
32:f:376:PHE:CE1	32:f:801:VAL:HG12	2.42	0.54
32:f:441:LYS:HD3	32:f:477:MET:CE	2.38	0.54
9:i:74:CYS:SG	9:i:135:LEU:O	2.57	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:176:LYS:CA	10:J:53:LEU:HD11	2.29	0.54
18:R:104:MET:HB2	18:R:111:CYS:HB3	1.89	0.54
22:V:483:CYS:O	22:V:486:ILE:HG22	2.07	0.54
24:X:386:ILE:C	24:X:387:ILE:HD12	2.32	0.54
32:f:376:PHE:HE1	32:f:801:VAL:CB	2.20	0.54
32:f:469:TYR:HB2	32:f:481:SER:HB3	1.90	0.54
32:f:755:ASP:OD1	32:f:756:PRO:HD2	2.07	0.54
32:f:809:ILE:HD11	32:f:857:GLY:HA2	1.90	0.54
11:k:28:ILE:O	11:k:31:ILE:HG22	2.07	0.54
1:A:347:ASP:OD1	1:A:349:GLU:N	2.40	0.54
32:f:257:ARG:CZ	32:f:275:MET:HB2	2.37	0.54
32:f:664:GLU:OE2	32:f:668:ALA:N	2.40	0.54
32:f:790:GLN:HG2	32:f:791:VAL:HG23	1.90	0.54
13:m:42:CYS:SG	13:m:43:LYS:N	2.80	0.54
20:t:201:LYS:HG2	20:t:202:GLN:N	2.22	0.54
12:L:8:ASN:C	12:L:8:ASN:OD1	2.51	0.54
21:U:213:PHE:HB3	21:U:248:ILE:HD12	1.90	0.54
23:W:371:THR:H	27:a:326:GLU:HG2	1.73	0.54
32:f:372:LEU:HD21	32:f:797:LEU:HD13	1.89	0.54
1:A:145:ASN:N	1:A:145:ASN:OD1	2.40	0.54
3:C:144:PRO:O	3:C:205:HIS:ND1	2.36	0.54
22:V:481:SER:HB2	30:d:344:ARG:HH21	1.72	0.54
10:J:16:LEU:O	10:J:19:VAL:HG22	2.08	0.54
10:J:181:ILE:O	10:J:181:ILE:HG22	2.08	0.54
19:S:56:ARG:O	19:S:70:LYS:NZ	2.38	0.54
21:U:357:LYS:O	21:U:360:VAL:HG23	2.07	0.54
23:W:216:GLU:OE1	23:W:216:GLU:N	2.34	0.54
25:Y:299:MET:HA	25:Y:299:MET:HE3	1.88	0.54
26:Z:267:ARG:HA	26:Z:267:ARG:NE	2.23	0.54
30:d:350:VAL:O	30:d:350:VAL:CG1	2.55	0.54
32:f:61:GLU:O	32:f:66:LYS:NZ	2.40	0.54
32:f:77:GLU:O	32:f:83:ARG:NE	2.40	0.54
32:f:416:MET:HE1	32:f:804:LEU:CD2	2.37	0.54
9:i:248:GLU:N	9:i:248:GLU:OE1	2.38	0.54
15:o:81:SER:HB2	15:o:82:PRO:CD	2.38	0.54
1:A:220:THR:O	35:A:501:ATP:C2	2.54	0.54
2:B:176:VAL:HG21	2:B:249:ARG:NH1	2.22	0.54
4:D:122:GLU:OE2	4:D:122:GLU:N	2.33	0.54
4:D:296:MET:HE1	4:D:326:ARG:HA	1.89	0.54
8:H:38:ILE:HD11	8:H:174:LEU:HD11	1.91	0.54
9:I:216:LEU:C	9:I:216:LEU:HD23	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:213:ARG:NE	16:p:151:GLU:OE2	2.31	0.54
25:Y:88:LEU:O	25:Y:92:GLU:N	2.35	0.54
27:a:72:ASN:ND2	27:a:104:VAL:O	2.40	0.54
10:J:66:ASP:OD1	10:J:67:ASP:N	2.36	0.53
12:L:80:ASP:OD2	12:L:129:GLY:N	2.41	0.53
21:U:587:ALA:HB2	21:U:621:SER:HB3	1.89	0.53
22:V:207:ALA:HA	22:V:210:CYS:SG	2.48	0.53
26:Z:69:PHE:CD1	28:b:95:LEU:HD22	2.43	0.53
30:d:345:GLN:OE1	30:d:349:ILE:HD11	2.08	0.53
32:f:471:LEU:HD23	32:f:504:VAL:HG22	1.90	0.53
1:A:368:ILE:HD11	1:A:370:PHE:CZ	2.43	0.53
2:B:44:ASP:HA	2:B:177:GLU:CB	2.37	0.53
10:J:26:VAL:CG1	10:J:130:SER:HB3	2.37	0.53
12:L:37:GLY:C	12:L:38:LEU:HD12	2.34	0.53
18:R:104:MET:HB2	18:R:111:CYS:SG	2.49	0.53
20:T:96:LEU:HD13	20:T:157:ILE:CD1	2.37	0.53
21:U:376:MET:HE1	21:U:738:ASP:O	2.08	0.53
22:V:304:GLU:O	22:V:308:THR:HG22	2.09	0.53
28:b:142:ASN:N	28:b:171:VAL:O	2.39	0.53
1:A:56:LEU:CD2	2:B:48:LYS:HG3	2.38	0.53
1:A:432:TYR:CD1	11:K:81:LEU:CD2	2.88	0.53
2:B:296:ASP:OD1	2:B:297:SER:N	2.36	0.53
3:C:199:LEU:O	3:C:199:LEU:HD13	2.09	0.53
22:V:326:GLN:NE2	31:e:8:VAL:CB	2.70	0.53
9:i:35:LEU:HD12	9:i:36:GLY:N	2.24	0.53
6:F:68:ALA:O	6:F:70:LYS:N	2.40	0.53
9:I:44:LEU:HD12	9:I:44:LEU:O	2.08	0.53
10:J:51:ALA:O	10:J:53:LEU:N	2.41	0.53
22:V:203:LEU:HA	22:V:206:VAL:HG12	1.89	0.53
28:b:18:ASN:O	28:b:25:ARG:HG2	2.07	0.53
32:f:198:HIS:ND1	32:f:201:GLU:OE2	2.37	0.53
32:f:223:GLU:O	32:f:227:ALA:N	2.41	0.53
32:f:441:LYS:HD3	32:f:477:MET:HE1	1.89	0.53
14:n:53:ARG:HE	14:n:60:ILE:HD11	1.73	0.53
19:s:194:LEU:HD12	19:s:195:SER:H	1.73	0.53
1:A:251:GLY:N	1:A:294:GLU:OE2	2.41	0.53
4:D:68:LEU:O	4:D:68:LEU:HD13	2.07	0.53
4:D:231:VAL:O	5:E:255:ARG:NH2	2.41	0.53
24:X:50:ILE:HG23	24:X:69:LEU:HD21	1.89	0.53
3:C:147:THR:HG23	3:C:202:ALA:HB2	1.90	0.53
3:C:391:MET:N	3:C:391:MET:SD	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:314:LEU:O	6:F:347:ARG:NH2	2.41	0.53
10:J:210:VAL:HG23	10:J:210:VAL:O	2.08	0.53
20:T:206:SER:N	20:T:209:GLU:OE1	2.36	0.53
21:U:353:LEU:O	21:U:356:THR:OG1	2.24	0.53
21:U:388:ASP:OD1	21:U:389:ASN:N	2.41	0.53
26:Z:184:VAL:HG12	29:c:297:VAL:HG21	1.90	0.53
28:b:25:ARG:NH2	28:b:145:GLU:H	2.04	0.53
29:c:159:ALA:N	29:c:205:ILE:HD11	2.24	0.53
32:f:254:GLY:CA	32:f:285:CYS:SG	2.97	0.53
32:f:790:GLN:O	32:f:797:LEU:HD23	2.09	0.53
11:k:71:ASP:OD1	11:k:72:ALA:N	2.36	0.53
16:p:180:VAL:O	16:p:180:VAL:HG12	2.08	0.53
1:A:176:ASP:OD1	1:A:177:VAL:HG23	2.09	0.53
3:C:307:ARG:NH1	3:C:309:GLY:HA3	2.23	0.53
6:F:156:ASP:OD1	6:F:157:SER:N	2.42	0.53
6:F:393:GLY:HA3	35:F:501:ATP:C8	2.44	0.53
8:H:59:GLU:OE1	8:H:59:GLU:N	2.39	0.53
22:V:260:HIS:O	22:V:263:LEU:HD21	2.09	0.53
32:f:245:ASN:ND2	32:f:253:LEU:HA	2.24	0.53
32:f:530:CYS:HG	32:f:569:LYS:HG3	1.70	0.53
32:f:784:ASP:O	32:f:787:LEU:HD11	2.09	0.53
7:g:194:THR:O	7:g:197:THR:OG1	2.24	0.53
18:r:239:ARG:NH2	18:r:244:ILE:HD13	2.23	0.53
1:A:90:GLU:OE2	2:B:156:VAL:HG11	2.08	0.53
4:D:353:ASN:ND2	5:E:161:ARG:O	2.37	0.53
14:N:129:MET:HG3	14:N:150:MET:HE1	1.90	0.53
23:W:443:THR:HG23	23:W:444:HIS:N	2.23	0.53
7:g:123:GLN:HE22	7:g:127:GLN:CG	2.17	0.53
12:l:86:ASN:C	12:l:86:ASN:OD1	2.51	0.53
12:l:177:SER:OG	12:l:178:GLU:OE2	2.25	0.53
1:A:191:VAL:HG23	1:A:192:GLU:N	2.24	0.53
1:A:371:GLU:OE1	1:A:371:GLU:N	2.35	0.53
6:F:225:MET:HE3	6:F:233:LYS:CB	2.39	0.53
17:Q:84:THR:OG1	17:Q:118:MET:HE1	2.09	0.53
27:a:38:THR:HG21	27:a:70:ARG:CD	2.39	0.53
32:f:72:ARG:NH1	32:f:86:THR:OG1	2.36	0.53
3:C:299:ASP:OD1	3:C:300:ILE:HG23	2.09	0.53
5:E:59:GLU:OE2	5:E:96:THR:N	2.42	0.53
5:E:236:ASP:O	5:E:281:ARG:NH2	2.42	0.53
12:L:8:ASN:OD1	12:L:9:ASP:N	2.42	0.53
15:O:69:VAL:O	19:s:213:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:448:LEU:HD23	21:U:483:LEU:HD23	1.91	0.53
30:d:258:PHE:CE1	30:d:262:ILE:HD11	2.43	0.53
32:f:192:VAL:HB	32:f:193:PRO:HD3	1.90	0.53
32:f:386:GLY:HA2	32:f:418:LEU:CG	2.36	0.53
11:k:31:ILE:HD11	11:k:140:ALA:N	2.23	0.53
4:D:257:ASN:OD1	4:D:258:ALA:N	2.42	0.52
9:I:118:LYS:O	9:I:122:THR:HG23	2.09	0.52
12:L:47:VAL:HG12	12:L:195:LEU:HD22	1.91	0.52
21:U:173:VAL:HG22	21:U:177:LEU:HD22	1.90	0.52
21:U:633:CYS:SG	21:U:659:CYS:HB2	2.49	0.52
23:W:402:ILE:HD11	23:W:418:PRO:HG3	1.90	0.52
25:Y:207:THR:O	25:Y:207:THR:CG2	2.56	0.52
32:f:408:LEU:HG	32:f:443:GLY:N	2.24	0.52
32:f:469:TYR:CB	32:f:481:SER:HB3	2.39	0.52
7:g:191:PHE:O	7:g:194:THR:OG1	2.21	0.52
4:D:177:VAL:O	4:D:181:VAL:HG12	2.09	0.52
11:K:65:GLU:OE1	11:K:66:LYS:N	2.42	0.52
15:O:218:LEU:HD12	15:O:232:TYR:CD2	2.45	0.52
16:P:30:ILE:O	16:P:31:GLN:C	2.51	0.52
24:X:391:PRO:HG2	24:X:392:PRO:HD3	1.91	0.52
27:a:276:CYS:SG	27:a:277:LEU:N	2.82	0.52
15:o:102:ILE:CD1	15:o:126:LEU:CG	2.86	0.52
1:A:126:SER:O	1:A:129:VAL:HG22	2.10	0.52
12:L:52:ALA:HB2	12:L:59:HIS:CE1	2.44	0.52
21:U:91:ASN:HB3	21:U:97:VAL:HG21	1.90	0.52
24:X:334:ASN:O	24:X:338:VAL:HG22	2.10	0.52
26:Z:214:LYS:CB	26:Z:220:LEU:C	2.82	0.52
29:c:145:VAL:HG22	29:c:146:ASP:H	1.75	0.52
7:g:83:MET:HE2	7:g:135:GLY:HA3	1.90	0.52
1:A:41:TYR:CE2	2:B:59:ARG:HB2	2.37	0.52
1:A:218:PRO:HA	35:A:501:ATP:O1G	2.10	0.52
2:B:74:MET:HE2	32:f:613:LEU:HD13	1.90	0.52
2:B:135:ILE:CB	2:B:159:VAL:HB	2.40	0.52
6:F:90:VAL:CG2	6:F:150:LEU:HD21	2.38	0.52
12:L:49:LEU:HD23	12:L:49:LEU:C	2.34	0.52
12:L:192:LEU:CD1	12:L:236:LEU:HD22	2.37	0.52
21:U:505:ASP:OD1	21:U:506:ALA:N	2.42	0.52
25:Y:104:MET:HG3	25:Y:127:THR:HG22	1.90	0.52
30:d:340:ILE:O	30:d:344:ARG:HD2	2.10	0.52
4:D:342:ARG:NH2	24:X:234:GLU:OE2	2.41	0.52
7:G:78:CYS:SG	7:G:138:MET:HG3	2.49	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:90:ASP:OD1	17:Q:91:CYS:N	2.43	0.52
19:S:197:ASP:N	19:S:197:ASP:OD1	2.40	0.52
21:U:501:LEU:HD21	21:U:535:TYR:CG	2.45	0.52
32:f:32:GLU:HA	32:f:82:ILE:HD11	1.90	0.52
14:n:38:MET:SD	14:n:161:ILE:HG22	2.49	0.52
23:W:420:ASP:C	23:W:420:ASP:OD1	2.53	0.52
27:a:68:GLU:O	27:a:70:ARG:NH2	2.41	0.52
28:b:46:GLU:OE1	28:b:46:GLU:N	2.37	0.52
29:c:129:THR:O	29:c:132:SER:OG	2.26	0.52
29:c:216:MET:SD	29:c:216:MET:C	2.93	0.52
32:f:326:LEU:HD12	32:f:455:VAL:CG2	2.40	0.52
32:f:862:ILE:HG22	32:f:863:THR:H	1.75	0.52
7:g:166:THR:OG1	7:g:167:ALA:N	2.41	0.52
8:h:135:LEU:C	8:h:136:ILE:HD12	2.35	0.52
11:k:142:LEU:HD22	11:k:153:LEU:HD11	1.90	0.52
3:C:302:ASP:OD1	3:C:304:ALA:N	2.39	0.52
7:G:86:ASP:OD1	13:M:121:HIS:CE1	2.62	0.52
12:L:54:SER:OG	12:L:55:GLU:N	2.42	0.52
25:Y:358:ARG:NH1	25:Y:358:ARG:O	2.43	0.52
27:a:7:PHE:O	27:a:11:SER:HB3	2.09	0.52
27:a:346:ILE:HA	27:a:349:MET:HE3	1.91	0.52
30:d:328:THR:C	30:d:329:THR:HG23	2.34	0.52
2:B:78:PHE:CE1	2:B:82:GLN:OE1	2.63	0.52
3:C:198:LEU:O	3:C:201:ARG:HG2	2.09	0.52
4:D:231:VAL:O	4:D:231:VAL:CG1	2.52	0.52
5:E:222:ALA:CB	5:E:230:ILE:HD11	2.40	0.52
18:R:61:THR:HG22	18:R:190:GLY:N	2.25	0.52
25:Y:101:ARG:NE	25:Y:130:LYS:O	2.43	0.52
32:f:775:THR:O	32:f:775:THR:CG2	2.50	0.52
17:q:83:PHE:CZ	17:q:87:ASN:ND2	2.78	0.52
35:B:501:ATP:O1A	35:B:501:ATP:O3'	2.25	0.52
4:D:181:VAL:HG13	4:D:182:GLU:N	2.25	0.52
5:E:264:MET:HA	5:E:269:THR:HG21	1.91	0.52
6:F:94:ILE:N	6:F:123:VAL:O	2.42	0.52
6:F:150:LEU:HD22	6:F:164:LEU:CB	2.40	0.52
10:J:69:VAL:HG22	10:J:104:VAL:HG12	1.92	0.52
16:P:123:SER:OG	16:P:124:LEU:N	2.43	0.52
21:U:27:LEU:HD11	21:U:63:VAL:HG22	1.90	0.52
22:V:333:ILE:O	22:V:360:TYR:OH	2.28	0.52
23:W:454:ASN:ND2	26:Z:101:LEU:O	2.39	0.52
32:f:664:GLU:OE1	32:f:665:GLU:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:220:VAL:CG2	11:k:226:PHE:HD1	2.23	0.52
15:o:94:ASP:O	15:o:98:THR:HG22	2.10	0.52
1:A:230:ALA:O	1:A:233:THR:HG22	2.09	0.52
6:F:231:THR:HB	6:F:354:PHE:CB	2.41	0.52
7:G:14:THR:HG21	7:G:126:THR:O	2.11	0.52
9:I:202:ASP:C	9:I:202:ASP:OD1	2.53	0.52
11:K:65:GLU:OE1	11:K:67:ILE:N	2.43	0.52
16:P:193:ASP:OD1	16:P:194:LYS:N	2.42	0.52
21:U:5:ALA:HB2	21:U:34:PHE:CD1	2.45	0.52
25:Y:271:PHE:O	25:Y:274:SER:OG	2.22	0.52
30:d:309:VAL:HG22	30:d:310:LEU:N	2.25	0.52
32:f:706:ILE:HG21	32:f:787:LEU:HD13	1.92	0.52
5:E:236:ASP:OD1	5:E:281:ARG:NH2	2.41	0.51
6:F:195:ILE:O	6:F:199:VAL:HG23	2.10	0.51
6:F:203:VAL:O	6:F:207:ASN:N	2.36	0.51
24:X:327:TYR:O	24:X:331:LEU:N	2.42	0.51
27:a:94:LEU:HD23	27:a:94:LEU:H	1.75	0.51
32:f:157:GLU:OE1	32:f:157:GLU:N	2.37	0.51
9:i:76:VAL:HG21	9:i:83:ALA:CB	2.41	0.51
15:o:106:LEU:HD22	15:o:117:PRO:HB3	1.92	0.51
16:p:193:ASP:OD1	16:p:193:ASP:C	2.52	0.51
2:B:183:THR:N	2:B:241:ASN:OD1	2.43	0.51
6:F:191:LEU:N	6:F:191:LEU:HD23	2.25	0.51
21:U:98:GLU:OE1	21:U:98:GLU:N	2.44	0.51
28:b:128:ALA:HB3	28:b:156:PHE:CE1	2.45	0.51
32:f:81:GLN:O	32:f:85:SER:HB2	2.10	0.51
32:f:308:SER:C	32:f:309:GLU:HG2	2.35	0.51
32:f:703:ARG:NH2	32:f:787:LEU:O	2.42	0.51
11:k:16:SER:HB2	11:k:17:PRO:HD2	1.92	0.51
15:o:113:THR:OG1	15:o:114:GLY:N	2.43	0.51
3:C:361:GLY:HA3	4:D:324:PRO:HB3	1.92	0.51
35:C:501:ATP:N3	35:C:501:ATP:C2'	2.72	0.51
4:D:394:VAL:HG12	4:D:399:PHE:CE2	2.45	0.51
5:E:153:LEU:O	5:E:226:GLN:NE2	2.44	0.51
7:G:123:GLN:O	7:G:126:THR:HG22	2.10	0.51
12:L:38:LEU:HD21	12:L:179:PHE:CZ	2.44	0.51
12:L:225:ASP:OD1	12:L:225:ASP:N	2.43	0.51
17:Q:38:MET:HE1	17:Q:61:GLN:HA	1.92	0.51
27:a:52:GLN:O	27:a:56:LEU:HG	2.10	0.51
29:c:185:ASN:O	29:c:188:SER:N	2.43	0.51
32:f:294:MET:SD	32:f:807:ARG:NH2	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:309:GLU:OE1	32:f:315:GLU:HG2	2.09	0.51
32:f:472:HIS:CE1	32:f:474:SER:HB3	2.45	0.51
32:f:670:MET:HE1	32:f:704:LEU:CA	2.40	0.51
32:f:736:THR:O	32:f:746:ARG:NH2	2.41	0.51
32:f:834:ASP:OD1	32:f:834:ASP:N	2.42	0.51
11:k:44:GLU:O	11:k:222:PRO:HD3	2.10	0.51
11:k:175:GLU:OE1	11:k:176:GLY:N	2.44	0.51
16:p:45:MET:HE1	16:p:68:LYS:HA	1.93	0.51
6:F:283:ILE:HG22	6:F:285:ILE:HD11	1.93	0.51
12:L:125:ARG:NH1	12:L:125:ARG:CG	2.73	0.51
18:R:94:ILE:HG12	18:R:104:MET:HE2	1.91	0.51
23:W:230:MET:SD	23:W:231:ILE:N	2.84	0.51
25:Y:11:LEU:CB	25:Y:12:PRO:HD3	2.40	0.51
32:f:35:ASP:HB2	32:f:82:ILE:CD1	2.40	0.51
9:i:119:GLN:HG3	10:j:78:ALA:HB1	1.93	0.51
1:A:219:GLY:HA2	35:A:501:ATP:H5'2	1.92	0.51
2:B:58:CYS:SG	32:f:184:LEU:HD21	2.50	0.51
3:C:198:LEU:CD2	35:C:501:ATP:C2	2.93	0.51
4:D:355:SER:OG	4:D:394:VAL:O	2.20	0.51
6:F:382:GLU:OE1	6:F:382:GLU:N	2.38	0.51
7:G:20:GLY:HA3	8:H:28:ALA:HB2	1.92	0.51
14:N:201:ASP:OD1	14:N:202:GLY:N	2.43	0.51
19:S:100:LEU:HD13	19:S:111:MET:HE3	1.91	0.51
23:W:314:LEU:HD23	23:W:315:MET:C	2.36	0.51
25:Y:192:ARG:NH2	25:Y:290:PRO:O	2.43	0.51
25:Y:328:GLU:OE1	25:Y:328:GLU:N	2.37	0.51
27:a:50:PHE:O	27:a:52:GLN:N	2.43	0.51
32:f:282:PHE:HE1	32:f:317:LEU:CG	2.12	0.51
32:f:759:LEU:HD22	32:f:809:ILE:HD12	1.90	0.51
19:s:97:GLU:OE1	19:s:97:GLU:HA	2.10	0.51
9:I:44:LEU:HD12	9:I:44:LEU:C	2.36	0.51
13:M:219:GLU:OE1	13:M:220:LEU:N	2.44	0.51
15:O:98:THR:HG23	15:O:129:MET:HE1	1.92	0.51
14:n:224:LEU:HD12	14:n:224:LEU:O	2.11	0.51
1:A:314:ASN:C	1:A:315:ILE:HD13	2.35	0.51
1:A:335:GLY:N	1:A:338:ASP:OD1	2.40	0.51
14:N:71:ILE:HD11	14:N:77:CYS:HB3	1.92	0.51
21:U:575:ASP:CG	21:U:578:LEU:HD13	2.35	0.51
21:U:672:LEU:O	21:U:676:THR:N	2.44	0.51
22:V:138:PRO:O	22:V:141:THR:OG1	2.22	0.51
23:W:254:PRO:HB2	23:W:263:TRP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:40:GLU:OE1	24:X:41:GLU:HG2	2.11	0.51
24:X:44:GLN:O	24:X:46:LYS:N	2.44	0.51
25:Y:105:MET:HA	25:Y:127:THR:HG21	1.91	0.51
25:Y:237:ARG:NE	25:Y:264:TYR:OH	2.36	0.51
28:b:113:VAL:HG13	28:b:142:ASN:CG	2.35	0.51
32:f:294:MET:HE2	32:f:807:ARG:CZ	2.40	0.51
5:E:135:ILE:HB	5:E:138:LEU:HD21	1.93	0.51
15:O:140:ALA:HB1	15:O:170:MET:HE1	1.90	0.51
21:U:680:VAL:O	21:U:684:ARG:HG3	2.11	0.51
25:Y:81:LEU:HD21	25:Y:111:LEU:HD21	1.92	0.51
32:f:296:PHE:HE1	32:f:298:LEU:HD12	1.74	0.51
32:f:862:ILE:HG22	32:f:863:THR:N	2.25	0.51
34:u:403:ARG:C	34:u:406:ARG:HG3	2.35	0.51
1:A:67:GLU:H	3:C:81:ASP:CB	2.24	0.51
2:B:357:ASP:OD1	2:B:357:ASP:N	2.43	0.51
21:U:175:GLY:O	21:U:179:TYR:N	2.44	0.51
26:Z:244:GLU:OE1	26:Z:244:GLU:N	2.43	0.51
32:f:198:HIS:CD2	32:f:240:VAL:HG13	2.46	0.51
13:m:78:VAL:HG11	13:m:85:ALA:HB1	1.91	0.51
1:A:171:ASP:OD1	1:A:171:ASP:O	2.29	0.51
1:A:217:PRO:O	1:A:220:THR:HG23	2.11	0.51
1:A:310:ASP:C	1:A:310:ASP:OD1	2.53	0.51
2:B:202:GLU:O	2:B:206:THR:HG23	2.10	0.51
3:C:362:VAL:HG23	3:C:386:ALA:HB1	1.93	0.51
4:D:189:GLU:OE1	4:D:189:GLU:N	2.36	0.51
6:F:362:ARG:NE	6:F:388:THR:O	2.44	0.51
9:I:151:ASP:OD1	9:I:153:SER:N	2.44	0.51
15:O:97:MET:C	15:O:97:MET:SD	2.94	0.51
24:X:378:LEU:O	25:Y:313:SER:HB3	2.11	0.51
25:Y:224:VAL:CG2	25:Y:260:LEU:CD1	2.74	0.51
28:b:14:GLU:OE1	28:b:14:GLU:N	2.42	0.51
32:f:416:MET:HB2	32:f:450:ILE:HG21	1.91	0.51
32:f:434:TYR:CD1	34:u:385:ASN:CG	2.89	0.51
32:f:873:LEU:C	32:f:874:LEU:HD12	2.36	0.51
10:j:145:TYR:CE1	10:j:155:ALA:HB2	2.45	0.51
5:E:365:GLU:OE2	5:E:365:GLU:N	2.29	0.50
6:F:234:THR:HG21	35:F:501:ATP:O1G	2.11	0.50
9:I:184:MET:HE2	9:I:184:MET:HA	1.93	0.50
23:W:302:TYR:CZ	23:W:306:LEU:HD21	2.45	0.50
23:W:407:ASP:N	23:W:412:ILE:O	2.44	0.50
32:f:376:PHE:CE1	32:f:801:VAL:CG1	2.88	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:h:68:ILE:HD11	8:h:74:LEU:HD13	1.93	0.50
9:i:208:ALA:CB	9:i:230:GLN:HE22	2.23	0.50
12:l:66:VAL:HG23	12:l:72:ILE:HG22	1.92	0.50
6:F:231:THR:CG2	6:F:355:PRO:O	2.59	0.50
12:L:180:MET:HA	12:L:180:MET:HE3	1.93	0.50
17:Q:181:ARG:NH1	17:Q:190:ASP:OD1	2.43	0.50
21:U:885:MET:O	21:U:889:LEU:N	2.37	0.50
22:V:473:GLN:HE22	30:d:333:THR:HG21	1.75	0.50
25:Y:355:GLU:OE1	25:Y:355:GLU:N	2.44	0.50
11:k:85:ALA:HB2	11:k:139:VAL:HG21	1.92	0.50
16:p:65:GLN:HE21	17:q:86:ARG:NH1	2.10	0.50
19:s:40:ILE:HD12	19:s:52:ALA:O	2.11	0.50
2:B:428:TYR:O	2:B:431:GLN:NE2	2.44	0.50
5:E:232:MET:SD	5:E:232:MET:N	2.74	0.50
22:V:470:ARG:HA	26:Z:257:MET:HG3	1.92	0.50
24:X:194:ARG:HG2	24:X:210:LEU:HD21	1.93	0.50
32:f:467:SER:CA	32:f:500:LEU:HD21	2.36	0.50
32:f:779:CYS:SG	32:f:780:PRO:HD3	2.51	0.50
7:g:211:LYS:HB2	7:g:212:PRO:HD2	1.93	0.50
11:k:240:ASP:OD1	11:k:241:ILE:N	2.44	0.50
15:o:102:ILE:HD13	15:o:126:LEU:CG	2.41	0.50
1:A:82:ALA:HB2	2:B:137:SER:O	2.11	0.50
2:B:224:LEU:N	2:B:224:LEU:HD12	2.26	0.50
2:B:224:LEU:HD23	2:B:353:PHE:CZ	2.47	0.50
3:C:79:ALA:CB	3:C:85:VAL:HG12	2.41	0.50
6:F:251:LEU:N	6:F:284:PHE:O	2.38	0.50
6:F:286:ASP:C	6:F:286:ASP:OD1	2.53	0.50
6:F:421:MET:HE3	12:L:30:LYS:HZ1	1.77	0.50
12:L:72:ILE:HG13	12:L:88:MET:HE1	1.94	0.50
23:W:336:PRO:O	23:W:340:VAL:HG22	2.12	0.50
27:a:41:VAL:O	27:a:45:VAL:HG23	2.12	0.50
29:c:303:MET:SD	29:c:304:LEU:N	2.85	0.50
9:i:44:LEU:C	9:i:44:LEU:HD12	2.37	0.50
12:l:67:ASP:OD1	12:l:68:ASN:N	2.35	0.50
1:A:187:LEU:O	1:A:191:VAL:HG22	2.11	0.50
2:B:142:ASP:OD1	2:B:142:ASP:N	2.39	0.50
3:C:335:LYS:NZ	3:C:335:LYS:O	2.39	0.50
12:L:37:GLY:O	12:L:38:LEU:HD12	2.10	0.50
16:P:116:THR:HG22	16:P:117:PHE:N	2.25	0.50
21:U:173:VAL:HA	21:U:177:LEU:HB3	1.92	0.50
21:U:398:ASN:O	21:U:399:TRP:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:466:ILE:O	22:V:466:ILE:HG23	2.12	0.50
23:W:335:SER:N	23:W:336:PRO:HD2	2.26	0.50
23:W:362:ASN:O	23:W:366:MET:HG2	2.12	0.50
26:Z:220:LEU:HB3	26:Z:223:ASN:CB	2.42	0.50
27:a:112:ILE:HG22	27:a:151:VAL:CG2	2.41	0.50
28:b:25:ARG:CZ	28:b:144:GLY:CA	2.89	0.50
30:d:161:ILE:HD12	30:d:162:PRO:N	2.26	0.50
7:g:189:TRP:HB3	7:g:194:THR:HG23	1.93	0.50
10:j:104:VAL:O	10:j:108:THR:HG23	2.10	0.50
12:l:85:CYS:SG	12:l:89:ARG:NH1	2.84	0.50
1:A:119:ALA:HB1	6:F:127:SER:OG	2.11	0.50
3:C:116:LEU:HD11	3:C:121:TYR:HA	1.93	0.50
3:C:224:ILE:CB	33:v:10:UNK:HA	2.41	0.50
4:D:412:GLN:O	8:H:53:LYS:NZ	2.44	0.50
5:E:257:LEU:HD23	5:E:257:LEU:H	1.76	0.50
19:S:75:THR:OG1	19:S:76:ASP:N	2.44	0.50
23:W:148:THR:O	23:W:152:ILE:HG23	2.11	0.50
9:i:33:THR:OG1	9:i:166:ASN:OD1	2.29	0.50
13:m:42:CYS:SG	13:m:187:CYS:HA	2.51	0.50
3:C:197:THR:CA	3:C:200:ALA:CB	2.90	0.50
32:f:126:ILE:HG23	32:f:127:SER:N	2.27	0.50
32:f:470:VAL:HG11	32:f:501:LEU:HD23	1.91	0.50
8:h:11:THR:O	8:h:11:THR:HG22	2.11	0.50
34:u:403:ARG:CA	34:u:406:ARG:HG3	2.41	0.50
2:B:40:THR:N	2:B:276:GLU:OE2	2.45	0.50
3:C:359:VAL:O	3:C:362:VAL:HG12	2.12	0.50
4:D:205:TYR:HA	4:D:312:ASN:CG	2.36	0.50
6:F:421:MET:CE	12:L:30:LYS:NZ	2.74	0.50
21:U:602:LEU:HD23	21:U:602:LEU:C	2.37	0.50
26:Z:185:GLY:O	26:Z:189:GLN:NE2	2.44	0.50
29:c:265:MET:SD	29:c:265:MET:N	2.84	0.50
30:d:112:CYS:SG	30:d:113:GLY:N	2.85	0.50
7:g:210:PHE:CD1	7:g:215:ILE:HG23	2.46	0.50
1:A:433:ASN:HB2	11:K:82:ILE:HD11	1.93	0.50
12:L:42:THR:HG1	12:L:43:HIS:CE1	2.29	0.50
21:U:376:MET:HB3	21:U:377:HIS:CE1	2.47	0.50
23:W:137:TYR:HB2	23:W:140:ILE:HD13	1.93	0.50
23:W:193:CYS:HA	23:W:196:VAL:HG23	1.93	0.50
28:b:113:VAL:HG13	28:b:142:ASN:OD1	2.12	0.50
11:k:55:THR:HG22	11:k:59:MET:CE	2.41	0.50
11:k:98:ASN:OD1	11:k:99:HIS:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:88:MET:HE2	20:t:90:VAL:HG22	1.93	0.50
5:E:159:PHE:O	5:E:163:GLY:N	2.45	0.49
7:G:114:LEU:HD23	7:G:114:LEU:C	2.36	0.49
10:J:88:ARG:NH1	17:Q:69:MET:O	2.45	0.49
15:O:69:VAL:HG22	19:s:213:ARG:O	2.12	0.49
22:V:478:GLN:HA	22:V:481:SER:OG	2.12	0.49
27:a:80:ILE:HA	27:a:83:VAL:HG22	1.93	0.49
27:a:163:TYR:O	27:a:166:ILE:O	2.30	0.49
27:a:313:LYS:O	27:a:316:SER:HB2	2.11	0.49
32:f:371:ASN:ND2	32:f:401:LYS:O	2.45	0.49
32:f:647:GLY:O	32:f:651:GLY:N	2.39	0.49
15:o:81:SER:HB2	15:o:82:PRO:HD2	1.94	0.49
6:F:92:ASN:C	6:F:92:ASN:OD1	2.55	0.49
12:L:70:ILE:HD11	12:L:105:VAL:HG22	1.94	0.49
18:R:68:ARG:NH2	18:R:205:ASP:OD1	2.44	0.49
18:R:101:LEU:HB2	18:R:161:CYS:SG	2.52	0.49
20:T:153:ASN:CB	20:T:155:MET:HE3	2.37	0.49
30:d:202:GLN:C	30:d:203:ASN:OD1	2.55	0.49
32:f:11:VAL:HG23	32:f:12:GLN:N	2.27	0.49
32:f:597:VAL:O	32:f:638:ASP:OD2	2.29	0.49
32:f:615:ILE:HA	32:f:629:LYS:HZ1	1.78	0.49
32:f:655:LEU:O	32:f:658:ALA:HB3	2.13	0.49
20:t:234:ILE:HD12	20:t:248:LEU:HD12	1.94	0.49
1:A:39:SER:HB2	1:A:42:SER:HB2	1.93	0.49
9:I:116:ASP:OD1	10:J:81:ARG:NH1	2.42	0.49
15:O:187:PRO:HB3	20:t:259:MET:HE1	1.94	0.49
29:c:143:VAL:CG1	29:c:157:ILE:HD11	2.43	0.49
32:f:644:ALA:O	32:f:645:ASP:OD1	2.29	0.49
32:f:665:GLU:CD	32:f:665:GLU:H	2.20	0.49
9:i:165:GLY:N	9:i:168:SER:OG	2.45	0.49
11:k:107:MET:HE2	11:k:112:VAL:HG22	1.93	0.49
11:k:206:MET:HE3	11:k:215:ILE:HG22	1.93	0.49
12:l:120:THR:O	12:l:120:THR:OG1	2.30	0.49
2:B:314:ASN:OD1	2:B:314:ASN:C	2.56	0.49
4:D:321:LEU:HD23	4:D:321:LEU:O	2.12	0.49
6:F:229:PRO:O	35:F:501:ATP:O1B	2.31	0.49
8:H:137:CYS:SG	8:H:138:GLY:N	2.85	0.49
10:J:115:LYS:NZ	10:J:129:ILE:HD12	2.28	0.49
11:K:133:MET:SD	11:K:135:ARG:NH1	2.86	0.49
12:L:46:LEU:HD23	12:L:46:LEU:H	1.77	0.49
17:Q:109:GLU:H	17:Q:109:GLU:CD	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:764:LEU:HD13	32:f:769:THR:HG22	1.95	0.49
8:h:29:VAL:HG13	8:h:77:SER:O	2.11	0.49
1:A:124:ASP:OD1	1:A:125:LEU:N	2.44	0.49
5:E:283:ASP:OD1	5:E:284:THR:N	2.45	0.49
10:J:115:LYS:HD2	10:J:129:ILE:HD11	1.94	0.49
21:U:439:GLU:HG3	21:U:473:VAL:HG21	1.93	0.49
22:V:358:MET:N	22:V:359:PRO:CD	2.75	0.49
24:X:416:ASN:ND2	26:Z:284:ASP:OD2	2.45	0.49
26:Z:96:HIS:HD2	26:Z:121:LEU:HD11	1.77	0.49
30:d:258:PHE:CD1	30:d:258:PHE:C	2.89	0.49
32:f:31:LYS:HE3	32:f:82:ILE:HG13	1.93	0.49
32:f:325:GLN:O	32:f:329:ASN:N	2.42	0.49
32:f:434:TYR:HD1	34:u:385:ASN:CG	2.20	0.49
32:f:463:LEU:HA	32:f:485:LEU:CD2	2.42	0.49
9:i:73:ALA:HB2	9:i:225:ILE:HD11	1.77	0.49
13:m:203:ASP:O	13:m:205:VAL:N	2.46	0.49
16:p:48:ARG:NH1	16:p:48:ARG:CG	2.72	0.49
17:q:85:ARG:CG	17:q:85:ARG:NH1	2.73	0.49
10:J:158:ALA:O	11:K:58:LEU:HD13	2.12	0.49
15:O:210:LEU:HD22	15:O:210:LEU:N	2.28	0.49
23:W:301:LYS:NZ	23:W:327:GLU:OE1	2.38	0.49
24:X:133:LEU:HD11	24:X:137:TYR:CZ	2.47	0.49
26:Z:230:LEU:HA	26:Z:233:VAL:HG22	1.93	0.49
28:b:51:LEU:C	28:b:51:LEU:HD12	2.36	0.49
32:f:463:LEU:N	32:f:489:TYR:OH	2.42	0.49
8:h:219:ARG:HH11	8:h:219:ARG:HG3	1.77	0.49
10:j:66:ASP:OD1	10:j:67:ASP:N	2.39	0.49
12:l:43:HIS:CD2	12:l:184:LEU:HD11	2.47	0.49
2:B:118:ASP:O	2:B:119:ASN:HB2	2.13	0.49
3:C:147:THR:CG2	3:C:202:ALA:HB2	2.42	0.49
3:C:197:THR:C	3:C:200:ALA:HB3	2.37	0.49
19:S:67:ASP:OD1	19:S:67:ASP:C	2.56	0.49
20:T:67:ILE:HB	20:T:95:MET:HE1	1.94	0.49
23:W:67:LEU:HD23	23:W:68:VAL:N	2.28	0.49
23:W:275:ILE:CG2	23:W:354:LEU:HD13	2.43	0.49
25:Y:57:LEU:HD23	25:Y:58:CYS:N	2.28	0.49
30:d:134:THR:O	30:d:137:THR:OG1	2.28	0.49
32:f:470:VAL:HG12	32:f:504:VAL:CG2	2.42	0.49
7:g:244:GLU:OE1	7:g:244:GLU:N	2.38	0.49
8:h:188:ILE:HD11	8:h:210:VAL:HG11	1.94	0.49
2:B:230:THR:HG21	2:B:353:PHE:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:THR:CA	3:C:200:ALA:HB3	2.42	0.49
8:H:68:ILE:HD11	8:H:87:VAL:HG23	1.94	0.49
8:H:192:ILE:HD11	8:H:234:ALA:HB1	1.95	0.49
11:K:22:PHE:O	11:K:23:GLN:HB2	2.12	0.49
18:R:240:GLU:OE1	18:R:240:GLU:N	2.46	0.49
22:V:207:ALA:HB1	22:V:211:TYR:OH	2.12	0.49
23:W:216:GLU:O	23:W:217:GLU:HG3	2.13	0.49
29:c:162:LEU:C	29:c:162:LEU:HD12	2.37	0.49
32:f:262:PHE:O	32:f:264:GLU:N	2.46	0.49
15:o:209:ASP:OD1	15:o:211:GLY:N	2.36	0.49
15:o:226:LEU:HD23	15:o:227:ASP:N	2.26	0.49
15:o:230:ARG:HH11	15:o:230:ARG:HG3	1.76	0.49
2:B:102:LEU:CD1	2:B:137:SER:HB2	2.42	0.49
2:B:434:THR:O	2:B:436:GLU:N	2.37	0.49
3:C:257:SER:O	3:C:257:SER:OG	2.16	0.49
4:D:236:VAL:HG12	4:D:237:GLN:N	2.28	0.49
9:I:186:LEU:O	9:I:189:ALA:HB3	2.13	0.49
11:K:46:VAL:HG11	11:K:144:GLY:HA3	1.94	0.49
22:V:292:THR:O	22:V:295:ILE:HG12	2.12	0.49
23:W:149:LEU:O	23:W:152:ILE:HG13	2.12	0.49
23:W:244:CYS:HB2	23:W:273:TYR:CB	2.41	0.49
23:W:274:VAL:HG23	23:W:275:ILE:N	2.28	0.49
23:W:372:ARG:CB	27:a:327:VAL:HG23	2.43	0.49
24:X:144:GLN:O	24:X:147:LEU:N	2.46	0.49
24:X:161:ASP:C	24:X:161:ASP:OD1	2.55	0.49
27:a:104:VAL:O	27:a:104:VAL:HG12	2.13	0.49
32:f:439:TYR:CD1	32:f:476:THR:HG21	2.48	0.49
32:f:658:ALA:O	32:f:661:ALA:N	2.45	0.49
32:f:664:GLU:OE2	32:f:669:GLU:N	2.33	0.49
7:g:87:SER:N	7:g:136:CYS:SG	2.86	0.49
10:j:59:VAL:O	10:j:59:VAL:HG13	2.13	0.49
10:j:144:LEU:HD23	10:j:144:LEU:O	2.13	0.49
4:D:359:ASP:OD2	24:X:274:LYS:NZ	2.40	0.49
4:D:380:GLN:OE1	5:E:164:ILE:HG23	2.13	0.49
9:I:122:THR:O	10:J:125:ARG:NH1	2.46	0.49
15:O:241:ARG:NH2	16:P:154:TRP:O	2.46	0.49
20:T:169:TYR:HB2	20:T:182:LEU:HD13	1.95	0.49
21:U:376:MET:HA	21:U:376:MET:HE3	1.95	0.49
21:U:573:ASP:OD1	21:U:575:ASP:N	2.45	0.49
25:Y:26:LEU:HD21	25:Y:36:ALA:HB3	1.95	0.49
25:Y:213:LEU:HD13	25:Y:219:PHE:CB	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Z:225:GLN:OE1	26:Z:229:GLN:CB	2.61	0.49
27:a:79:ILE:O	27:a:83:VAL:HG13	2.13	0.49
28:b:180:ALA:O	28:b:184:ILE:HG12	2.13	0.49
32:f:43:GLN:O	32:f:47:GLU:N	2.27	0.49
32:f:266:LEU:HD13	32:f:270:LEU:HG	1.95	0.49
32:f:863:THR:OG1	32:f:864:GLY:N	2.46	0.49
2:B:183:THR:HG23	2:B:184:TYR:H	1.78	0.48
3:C:62:GLU:O	3:C:65:LEU:HD23	2.13	0.48
4:D:202:VAL:HG13	4:D:308:ILE:HD12	1.95	0.48
12:L:42:THR:OG1	12:L:43:HIS:ND1	2.42	0.48
14:N:64:VAL:HG21	20:t:256:ILE:HG13	1.95	0.48
21:U:219:CYS:SG	21:U:220:LEU:N	2.86	0.48
22:V:496:PHE:N	22:V:497:PRO:CD	2.76	0.48
26:Z:22:HIS:ND1	26:Z:35:VAL:HG13	2.28	0.48
27:a:245:VAL:HG13	27:a:246:GLU:N	2.28	0.48
27:a:278:MET:C	27:a:278:MET:SD	2.95	0.48
31:e:49:GLU:OE2	31:e:53:SER:OG	2.23	0.48
32:f:198:HIS:CG	32:f:240:VAL:HG13	2.47	0.48
1:A:322:ASN:OD1	1:A:323:ARG:CG	2.56	0.48
4:D:74:HIS:NE2	26:Z:177:ARG:O	2.46	0.48
8:H:84:ARG:O	8:H:87:VAL:HG12	2.13	0.48
12:L:29:VAL:HG22	12:L:131:GLY:N	2.28	0.48
17:Q:85:ARG:HB2	17:Q:118:MET:HE2	1.95	0.48
21:U:892:LEU:HD11	21:U:906:LEU:HB3	1.93	0.48
23:W:148:THR:OG1	23:W:168:GLU:OE1	2.22	0.48
23:W:449:GLU:O	23:W:452:ILE:HG12	2.13	0.48
24:X:330:LEU:HD12	24:X:333:GLN:OE1	2.13	0.48
25:Y:263:LEU:HD21	25:Y:306:GLN:OE1	2.13	0.48
27:a:226:ARG:O	27:a:229:ASP:N	2.46	0.48
12:l:188:VAL:O	12:l:192:LEU:HG	2.13	0.48
17:q:167:LEU:HD23	17:q:167:LEU:C	2.37	0.48
3:C:307:ARG:HH21	3:C:310:ARG:NE	2.10	0.48
6:F:94:ILE:HD11	6:F:125:LYS:HB2	1.95	0.48
13:M:9:ASP:O	13:M:23:GLN:NE2	2.39	0.48
14:N:141:GLU:CD	14:N:141:GLU:C	2.82	0.48
18:R:109:ALA:HB2	19:S:155:VAL:HG23	1.94	0.48
22:V:281:ASN:OD1	22:V:283:ASN:N	2.46	0.48
23:W:347:GLY:O	23:W:351:TRP:N	2.44	0.48
28:b:28:ALA:O	28:b:31:ASP:OD1	2.30	0.48
8:h:206:ASP:OD1	8:h:207:ASN:N	2.45	0.48
10:j:172:LEU:O	10:j:176:TYR:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:n:43:ASP:C	14:n:43:ASP:OD1	2.56	0.48
16:p:149:MET:HE3	16:p:149:MET:CA	2.43	0.48
19:s:76:ASP:O	19:s:76:ASP:OD1	2.31	0.48
1:A:56:LEU:HD13	2:B:72:LEU:HD21	1.94	0.48
6:F:402:GLU:OE1	6:F:423:GLY:O	2.31	0.48
35:F:501:ATP:C2'	35:F:501:ATP:N3	2.76	0.48
9:I:92:LEU:HD12	16:P:73:LEU:HD11	1.94	0.48
12:L:166:GLN:OE1	12:L:169:ARG:NH1	2.46	0.48
12:L:178:GLU:OE1	12:L:178:GLU:N	2.42	0.48
13:M:138:LEU:O	13:M:149:LEU:HD12	2.14	0.48
21:U:325:MET:SD	21:U:328:ILE:HD11	2.53	0.48
21:U:349:ASP:OD1	21:U:351:MET:N	2.44	0.48
22:V:31:ALA:HB3	22:V:32:PRO:HD3	1.94	0.48
23:W:40:LEU:O	23:W:42:GLU:N	2.46	0.48
24:X:377:ILE:HG21	25:Y:311:TYR:CE1	2.48	0.48
25:Y:84:LEU:O	25:Y:87:GLU:HG2	2.13	0.48
26:Z:169:GLU:O	26:Z:173:GLU:N	2.46	0.48
26:Z:267:ARG:HH21	26:Z:270:VAL:HG11	1.78	0.48
27:a:244:ASN:CB	27:a:276:CYS:HB3	2.43	0.48
32:f:470:VAL:HG12	32:f:504:VAL:HG21	1.96	0.48
32:f:560:LEU:CD1	32:f:782:HIS:NE2	2.74	0.48
32:f:615:ILE:O	32:f:615:ILE:HG22	2.13	0.48
14:n:149:PRO:HD2	14:n:153:MET:HG3	1.96	0.48
1:A:244:GLU:O	1:A:247:GLN:NE2	2.47	0.48
2:B:105:THR:OG1	2:B:106:PRO:HD3	2.13	0.48
2:B:388:ASP:O	2:B:389:ASP:OD1	2.31	0.48
2:B:392:GLY:HA3	35:B:501:ATP:N7	2.29	0.48
4:D:296:MET:HE1	4:D:326:ARG:C	2.39	0.48
12:L:140:MET:HE1	20:T:125:GLY:HA3	1.95	0.48
23:W:210:ASN:OD1	23:W:211:THR:N	2.46	0.48
23:W:283:GLN:O	23:W:287:VAL:HG13	2.13	0.48
30:d:219:ASP:O	30:d:220:ILE:C	2.55	0.48
32:f:787:LEU:O	32:f:792:ALA:HB3	2.13	0.48
17:q:85:ARG:HA	17:q:118:MET:CE	2.44	0.48
4:D:120:ASP:OD1	4:D:122:GLU:OE2	2.31	0.48
4:D:281:ALA:HB2	33:v:15:UNK:N	2.25	0.48
6:F:310:MET:SD	6:F:311:LEU:N	2.87	0.48
21:U:258:GLN:OE1	21:U:262:SER:HB2	2.14	0.48
23:W:110:THR:O	23:W:114:GLU:CB	2.61	0.48
26:Z:71:ASP:C	26:Z:71:ASP:OD1	2.56	0.48
32:f:108:GLU:O	32:f:112:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:283:THR:O	32:f:816:TYR:CE1	2.66	0.48
32:f:416:MET:HE2	32:f:804:LEU:HD23	1.92	0.48
14:n:126:GLU:O	14:n:126:GLU:HG2	2.14	0.48
4:D:169:GLY:O	4:D:340:GLN:NE2	2.47	0.48
4:D:284:GLU:O	4:D:288:ILE:HG12	2.14	0.48
6:F:203:VAL:O	6:F:206:MET:N	2.46	0.48
13:M:202:HIS:NE2	13:M:207:ASP:OD2	2.46	0.48
21:U:633:CYS:HB2	21:U:634:PRO:HD3	1.96	0.48
22:V:92:ARG:HA	22:V:95:LEU:HD13	1.95	0.48
22:V:205:LEU:HD22	22:V:205:LEU:N	2.29	0.48
22:V:442:ILE:O	22:V:443:ARG:C	2.56	0.48
27:a:194:GLN:HA	27:a:225:LEU:HB3	1.95	0.48
28:b:79:GLN:CD	28:b:79:GLN:N	2.69	0.48
30:d:316:TYR:HA	30:d:319:ALA:HB2	1.96	0.48
32:f:8:LYS:O	32:f:12:GLN:N	2.40	0.48
7:g:78:CYS:SG	7:g:138:MET:CE	3.00	0.48
4:D:374:ASP:O	4:D:378:ILE:HG13	2.14	0.48
9:I:75:SER:O	9:I:134:LEU:HB2	2.14	0.48
11:K:165:CYS:SG	12:L:57:ALA:HB2	2.54	0.48
13:M:145:ASP:OD1	13:M:146:GLY:N	2.47	0.48
18:R:209:GLU:HA	18:R:209:GLU:OE2	2.13	0.48
21:U:167:ILE:HB	21:U:177:LEU:HD21	1.96	0.48
30:d:309:VAL:HG11	30:d:316:TYR:HE1	1.79	0.48
18:r:164:ASP:OD1	18:r:166:ARG:N	2.47	0.48
1:A:368:ILE:HD11	1:A:370:PHE:CD1	2.49	0.48
1:A:407:LYS:O	1:A:410:LEU:HD12	2.14	0.48
4:D:141:ASP:C	4:D:141:ASP:OD1	2.56	0.48
5:E:352:MET:HE2	5:E:352:MET:HA	1.94	0.48
9:I:174:MET:HE1	9:I:199:LYS:HB2	1.96	0.48
9:I:174:MET:SD	9:I:196:VAL:HG22	2.54	0.48
14:N:175:ALA:HB2	14:n:196:LEU:HD11	1.96	0.48
21:U:94:SER:OG	21:U:97:VAL:HG12	2.14	0.48
21:U:633:CYS:CB	21:U:659:CYS:SG	3.02	0.48
21:U:891:VAL:O	21:U:891:VAL:HG12	2.13	0.48
22:V:291:TYR:O	22:V:295:ILE:HG23	2.14	0.48
24:X:292:GLN:O	24:X:296:ASN:OD1	2.31	0.48
25:Y:311:TYR:CD2	25:Y:314:LEU:HD21	2.49	0.48
26:Z:267:ARG:CZ	29:c:292:MET:HA	2.43	0.48
28:b:58:CYS:SG	28:b:89:GLY:N	2.87	0.48
29:c:70:ILE:HG23	29:c:71:ASP:OD1	2.14	0.48
9:i:97:TYR:CE1	9:i:105:ILE:CA	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:121:LEU:HD23	11:k:121:LEU:H	1.79	0.48
11:k:206:MET:CE	11:k:215:ILE:HG22	2.44	0.48
12:l:220:GLU:O	12:l:222:THR:HG23	2.14	0.48
13:m:142:SER:O	13:m:146:GLY:N	2.40	0.48
15:o:209:ASP:OD1	15:o:210:LEU:N	2.47	0.48
16:p:34:MET:SD	16:p:34:MET:C	2.97	0.48
18:r:97:ASN:O	18:r:99:TYR:N	2.47	0.48
8:H:95:GLN:HG3	15:O:108:LEU:HD13	1.96	0.48
12:L:158:ALA:O	13:M:58:LEU:HD22	2.14	0.48
21:U:400:ALA:O	21:U:403:THR:OG1	2.28	0.48
23:W:91:SER:OG	23:W:92:LYS:N	2.47	0.48
24:X:240:ASP:O	24:X:241:SER:OG	2.27	0.48
24:X:310:ARG:NH1	24:X:310:ARG:O	2.47	0.48
24:X:346:GLN:CG	24:X:381:GLY:HA2	2.44	0.48
25:Y:263:LEU:HD23	25:Y:263:LEU:C	2.38	0.48
25:Y:275:LEU:HD23	31:e:60:LEU:CD2	2.44	0.48
32:f:222:ASP:C	32:f:222:ASP:OD1	2.56	0.48
2:B:264:PRO:HA	2:B:267:VAL:HG22	1.96	0.47
3:C:283:PHE:O	3:C:284:GLU:HG2	2.14	0.47
4:D:105:SER:HG	4:D:107:THR:HG1	1.62	0.47
18:R:100:LEU:HD23	18:R:161:CYS:O	2.14	0.47
20:T:88:MET:HE3	20:T:90:VAL:HB	1.96	0.47
21:U:459:ASP:OD1	21:U:460:TYR:N	2.47	0.47
26:Z:213:GLU:O	26:Z:218:GLY:N	2.47	0.47
32:f:14:GLN:OE1	32:f:63:LEU:HD11	2.14	0.47
32:f:287:ASP:HB2	32:f:816:TYR:CE1	2.49	0.47
7:g:67:THR:HG22	7:g:68:HIS:N	2.29	0.47
10:j:195:LEU:HD12	10:j:206:ILE:CG2	2.44	0.47
15:o:186:ARG:HG2	15:o:189:MET:HE3	1.95	0.47
2:B:202:GLU:OE1	2:B:203:LEU:N	2.47	0.47
6:F:332:THR:OG1	6:F:334:ARG:O	2.32	0.47
7:G:114:LEU:HD22	7:G:140:LEU:HD21	1.96	0.47
21:U:148:LYS:NZ	21:U:180:SER:OG	2.42	0.47
32:f:114:ALA:O	32:f:116:GLY:N	2.47	0.47
32:f:434:TYR:CG	32:f:434:TYR:O	2.67	0.47
14:n:179:GLU:HA	14:n:179:GLU:OE2	2.13	0.47
3:C:154:LEU:N	3:C:154:LEU:HD23	2.29	0.47
6:F:61:ARG:N	6:F:61:ARG:HD2	2.29	0.47
6:F:434:ASN:N	6:F:434:ASN:OD1	2.47	0.47
12:L:121:GLN:OE1	13:M:130:ARG:NH1	2.48	0.47
16:P:58:THR:CG2	16:P:59:ASP:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:167:ILE:O	21:U:177:LEU:HD11	2.13	0.47
22:V:30:PRO:O	22:V:34:ASP:N	2.37	0.47
22:V:493:ALA:O	22:V:497:PRO:HD3	2.14	0.47
25:Y:356:THR:O	25:Y:357:ASN:ND2	2.47	0.47
32:f:266:LEU:HB2	32:f:270:LEU:CD1	2.37	0.47
32:f:326:LEU:O	32:f:330:PHE:HB2	2.12	0.47
1:A:56:LEU:CG	2:B:48:LYS:HE3	2.44	0.47
1:A:219:GLY:O	35:A:501:ATP:H5'2	2.14	0.47
4:D:215:LEU:C	4:D:215:LEU:HD13	2.40	0.47
4:D:264:ILE:HD12	4:D:265:ASP:H	1.79	0.47
9:I:7:SER:OG	9:I:8:ARG:N	2.48	0.47
9:I:135:LEU:HD21	9:I:164:ILE:CG2	2.43	0.47
11:K:133:MET:O	11:K:135:ARG:N	2.45	0.47
21:U:136:LYS:O	21:U:140:ARG:HG2	2.14	0.47
21:U:682:TYR:HA	21:U:685:GLN:OE1	2.14	0.47
22:V:156:SER:O	22:V:209:LYS:NZ	2.34	0.47
22:V:263:LEU:HG	30:d:210:THR:HG23	1.97	0.47
25:Y:109:GLU:OE2	25:Y:113:ARG:NH1	2.47	0.47
9:i:159:TRP:CD2	10:j:54:GLN:HB3	2.49	0.47
5:E:338:PHE:O	5:E:338:PHE:CD1	2.67	0.47
6:F:82:VAL:CB	6:F:161:LEU:HD22	2.45	0.47
6:F:191:LEU:HD23	6:F:191:LEU:H	1.78	0.47
12:L:66:VAL:CG2	12:L:72:ILE:HG12	2.43	0.47
15:O:92:ALA:HB1	16:P:129:CYS:SG	2.54	0.47
20:T:65:VAL:HG12	20:T:66:VAL:N	2.30	0.47
21:U:575:ASP:HB3	21:U:578:LEU:HD13	1.96	0.47
23:W:268:LYS:HA	23:W:271:VAL:HG12	1.96	0.47
23:W:451:MET:SD	23:W:451:MET:C	2.98	0.47
25:Y:360:ASP:HA	25:Y:364:TRP:CB	2.44	0.47
32:f:287:ASP:O	32:f:881:GLU:OE2	2.32	0.47
1:A:221:GLY:CA	35:A:501:ATP:H5'1	2.45	0.47
14:N:35:THR:OG1	14:N:67:LYS:NZ	2.42	0.47
21:U:373:ASN:OD1	21:U:373:ASN:C	2.58	0.47
21:U:602:LEU:HD21	21:U:618:ALA:O	2.15	0.47
26:Z:290:GLY:C	26:Z:291:GLN:HG3	2.39	0.47
28:b:27:GLN:O	28:b:31:ASP:OD1	2.33	0.47
28:b:56:ASN:N	28:b:83:LYS:O	2.42	0.47
32:f:416:MET:SD	32:f:801:VAL:HG23	2.54	0.47
13:m:137:MET:HG2	13:m:151:MET:HG3	1.96	0.47
13:m:153:ASP:OD1	13:m:153:ASP:N	2.42	0.47
14:n:47:VAL:C	14:n:48:LEU:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:GLU:OE1	3:C:386:ALA:CB	2.63	0.47
7:G:61:LEU:HD21	7:G:66:VAL:CG2	2.44	0.47
8:H:138:GLY:N	8:H:213:CYS:SG	2.88	0.47
10:J:145:TYR:CE1	10:J:155:ALA:HB2	2.50	0.47
11:K:172:SER:O	11:K:173:ALA:HB3	2.14	0.47
12:L:13:TRP:CD2	12:L:19:ILE:HD11	2.50	0.47
12:L:66:VAL:CG2	12:L:72:ILE:CG1	2.93	0.47
15:O:224:ASN:N	15:O:224:ASN:OD1	2.47	0.47
16:P:34:MET:SD	16:P:183:MET:HE1	2.54	0.47
21:U:376:MET:HE3	21:U:376:MET:CA	2.44	0.47
21:U:543:LYS:HZ3	21:U:772:TRP:HE3	1.59	0.47
21:U:697:GLN:OE1	21:U:697:GLN:HA	2.15	0.47
22:V:214:HIS:CA	22:V:217:VAL:HG12	2.44	0.47
22:V:214:HIS:HA	22:V:217:VAL:CG1	2.44	0.47
22:V:247:GLN:OE1	22:V:247:GLN:N	2.35	0.47
22:V:366:ALA:HB2	22:V:374:LYS:HZ2	1.80	0.47
22:V:472:PRO:HA	22:V:475:ALA:HB3	1.96	0.47
24:X:296:ASN:OD1	24:X:296:ASN:N	2.44	0.47
24:X:317:PRO:O	24:X:320:SER:N	2.48	0.47
27:a:53:GLY:O	27:a:57:ILE:HD12	2.14	0.47
27:a:345:GLN:O	27:a:348:GLY:N	2.47	0.47
29:c:159:ALA:CB	29:c:205:ILE:HD11	2.44	0.47
30:d:328:THR:O	30:d:329:THR:CG2	2.63	0.47
13:m:213:GLU:OE1	13:m:213:GLU:N	2.47	0.47
16:p:122:CYS:SG	16:p:123:SER:N	2.88	0.47
2:B:190:LEU:N	2:B:190:LEU:HD23	2.30	0.47
3:C:197:THR:HG21	3:C:247:PHE:CZ	2.32	0.47
12:L:66:VAL:HG21	12:L:72:ILE:HG12	1.95	0.47
12:L:192:LEU:HD12	12:L:193:ARG:N	2.30	0.47
21:U:602:LEU:HD11	21:U:621:SER:HB2	1.96	0.47
23:W:383:ASP:O	23:W:384:LEU:HG	2.15	0.47
28:b:31:ASP:OD1	28:b:31:ASP:N	2.43	0.47
28:b:153:LEU:O	28:b:157:VAL:N	2.44	0.47
31:e:41:ASP:O	31:e:42:ASN:ND2	2.44	0.47
32:f:159:VAL:HG13	32:f:160:ARG:NH1	2.30	0.47
32:f:715:HIS:O	32:f:716:ASP:CG	2.58	0.47
9:i:119:GLN:NE2	10:j:79:ASP:OD1	2.47	0.47
10:j:198:VAL:O	10:j:201:SER:OG	2.32	0.47
16:p:12:MET:HE3	16:p:146:MET:HE2	1.96	0.47
1:A:120:LYS:O	6:F:90:VAL:HG12	2.15	0.47
4:D:270:ILE:O	4:D:270:ILE:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:134:LEU:HD12	9:I:134:LEU:C	2.40	0.47
21:U:692:ALA:HB2	21:U:733:ALA:HB1	1.97	0.47
21:U:892:LEU:HD11	21:U:906:LEU:CB	2.44	0.47
22:V:94:VAL:O	22:V:94:VAL:HG22	2.15	0.47
22:V:412:LEU:C	22:V:412:LEU:HD13	2.40	0.47
23:W:152:ILE:O	23:W:156:ASN:N	2.48	0.47
24:X:386:ILE:O	24:X:387:ILE:HB	2.15	0.47
26:Z:246:VAL:HG21	30:d:331:PRO:HG3	1.97	0.47
26:Z:270:VAL:HG23	29:c:288:VAL:HG12	1.96	0.47
30:d:328:THR:O	30:d:329:THR:HG23	2.15	0.47
20:t:157:ILE:N	20:t:157:ILE:HD12	2.30	0.47
4:D:264:ILE:HG13	4:D:265:ASP:O	2.15	0.47
9:I:119:GLN:HG3	10:J:78:ALA:HB1	1.96	0.47
13:M:88:LEU:HD12	13:M:134:CYS:SG	2.55	0.47
15:O:164:LYS:O	15:O:165:LEU:HD23	2.15	0.47
25:Y:101:ARG:HA	25:Y:104:MET:HE2	1.97	0.47
27:a:122:LYS:CB	27:a:131:THR:HG22	2.45	0.47
32:f:35:ASP:CB	32:f:82:ILE:CD1	2.93	0.47
32:f:469:TYR:CB	32:f:481:SER:CB	2.90	0.47
32:f:717:ALA:HB2	32:f:760:PHE:CD2	2.49	0.47
7:g:80:MET:HA	7:g:80:MET:HE3	1.97	0.47
7:g:143:ILE:HD13	7:g:149:PRO:HA	1.97	0.47
14:n:36:THR:HG21	14:n:197:ALA:HB3	1.96	0.47
1:A:142:VAL:HG13	1:A:147:TYR:C	2.40	0.46
2:B:91:LYS:C	2:B:93:GLU:H	2.23	0.46
2:B:286:GLU:HA	2:B:286:GLU:OE1	2.14	0.46
7:G:86:ASP:CG	7:G:134:LEU:HD12	2.39	0.46
9:I:40:ASN:O	9:I:41:ASP:HB2	2.15	0.46
10:J:166:LYS:NZ	10:J:170:GLU:HB2	2.30	0.46
10:J:189:LYS:CB	10:J:232:ILE:HD11	2.46	0.46
11:K:133:MET:O	11:K:134:SER:HB2	2.15	0.46
11:K:197:SER:O	11:K:200:ILE:HG22	2.15	0.46
21:U:368:ALA:HB1	21:U:731:ILE:HG23	1.97	0.46
21:U:410:VAL:CG2	21:U:448:LEU:HD13	2.45	0.46
25:Y:218:THR:O	25:Y:221:THR:OG1	2.29	0.46
25:Y:228:MET:HE1	25:Y:259:TYR:CE2	2.50	0.46
26:Z:151:THR:O	26:Z:152:SER:C	2.58	0.46
31:e:59:GLU:O	31:e:60:LEU:HB3	2.14	0.46
32:f:158:TYR:HA	32:f:161:HIS:CD2	2.49	0.46
32:f:302:GLY:O	32:f:307:LEU:HD22	2.15	0.46
32:f:348:ILE:CG2	32:f:754:LYS:HB2	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:664:GLU:OE1	32:f:666:ILE:N	2.48	0.46
17:q:4:LEU:HD13	17:q:45:LEU:HB3	1.97	0.46
17:q:167:LEU:HD23	17:q:167:LEU:O	2.15	0.46
19:s:80:ILE:HD12	19:s:81:GLY:H	1.79	0.46
1:A:292:ASP:OD2	1:A:296:GLN:NE2	2.46	0.46
3:C:116:LEU:HD13	3:C:117:ARG:O	2.16	0.46
6:F:362:ARG:O	6:F:366:MET:HG3	2.15	0.46
12:L:26:MET:HE1	12:L:149:PRO:HD2	1.96	0.46
13:M:219:GLU:OE1	13:M:219:GLU:N	2.48	0.46
16:P:45:MET:HE1	16:P:68:LYS:CD	2.46	0.46
16:P:75:GLU:OE1	16:P:80:ARG:N	2.48	0.46
21:U:243:LEU:HD12	21:U:246:TYR:OH	2.15	0.46
28:b:25:ARG:NH2	28:b:144:GLY:C	2.73	0.46
30:d:161:ILE:HG13	30:d:162:PRO:HD3	1.97	0.46
32:f:764:LEU:N	32:f:769:THR:O	2.41	0.46
18:r:180:ILE:HG22	18:r:181:SER:N	2.31	0.46
2:B:306:GLN:OE1	2:B:306:GLN:N	2.41	0.46
4:D:220:ALA:HB2	4:D:227:PHE:CD2	2.50	0.46
8:H:179:ASN:OD1	8:H:180:GLU:N	2.47	0.46
10:J:93:SER:O	10:J:97:THR:HG23	2.15	0.46
22:V:490:SER:OG	22:V:491:VAL:N	2.47	0.46
24:X:57:LEU:O	24:X:61:GLY:N	2.48	0.46
7:g:185:LYS:O	7:g:186:LYS:C	2.58	0.46
12:l:46:LEU:HD22	12:l:135:ALA:CB	2.45	0.46
16:p:149:MET:HA	16:p:149:MET:CE	2.44	0.46
3:C:231:VAL:O	3:C:233:GLU:N	2.48	0.46
21:U:719:ASP:OD1	21:U:720:LYS:N	2.48	0.46
22:V:157:THR:N	22:V:158:PRO:CD	2.78	0.46
23:W:280:ASP:OD1	23:W:282:GLU:N	2.49	0.46
23:W:386:VAL:HG23	23:W:387:ASP:N	2.30	0.46
24:X:275:LEU:HD12	24:X:275:LEU:H	1.79	0.46
24:X:373:LYS:O	24:X:374:PHE:HB2	2.15	0.46
27:a:245:VAL:O	27:a:246:GLU:C	2.58	0.46
27:a:317:VAL:CG1	27:a:318:GLY:H	2.24	0.46
32:f:244:GLU:HG2	32:f:248:LEU:HD12	1.97	0.46
8:h:12:THR:HG23	9:i:20:GLN:OE1	2.16	0.46
4:D:328:ASP:O	4:D:330:LYS:NZ	2.44	0.46
5:E:222:ALA:HB2	5:E:230:ILE:HD11	1.95	0.46
6:F:184:GLN:CD	6:F:184:GLN:N	2.74	0.46
7:G:67:THR:HG22	7:G:69:LEU:H	1.79	0.46
7:G:78:CYS:SG	7:G:138:MET:SD	3.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:119:LEU:HD11	11:K:131:GLY:HA3	1.97	0.46
22:V:135:LEU:HD22	22:V:174:PHE:CE1	2.51	0.46
22:V:302:TYR:CZ	22:V:338:LEU:HD22	2.51	0.46
25:Y:23:ARG:NH2	25:Y:40:GLU:OE2	2.48	0.46
27:a:281:THR:HG23	27:a:282:PHE:N	2.30	0.46
27:a:366:LEU:HD23	27:a:367:VAL:N	2.30	0.46
32:f:206:ASP:OD1	32:f:207:LEU:N	2.48	0.46
9:i:106:PRO:C	9:i:107:CYS:SG	2.93	0.46
9:i:231:LYS:C	9:i:231:LYS:HD3	2.41	0.46
3:C:253:SER:O	3:C:254:ILE:C	2.59	0.46
6:F:93:VAL:HG13	6:F:93:VAL:O	2.16	0.46
6:F:253:GLY:N	6:F:254:PRO:HD2	2.30	0.46
6:F:426:GLU:O	6:F:429:ALA:N	2.44	0.46
8:H:92:LYS:HE2	8:H:96:GLN:NE2	2.31	0.46
9:I:134:LEU:CD1	9:I:136:TYR:CE2	2.84	0.46
11:K:167:ALA:HB3	12:L:56:LEU:HD13	1.96	0.46
12:L:90:GLN:NE2	12:L:94:ASP:OD2	2.48	0.46
15:O:209:ASP:CB	15:O:210:LEU:HD22	2.46	0.46
15:O:209:ASP:HB3	15:O:210:LEU:HD22	1.98	0.46
23:W:440:ASN:C	23:W:443:THR:HG22	2.35	0.46
26:Z:36:VAL:HB	26:Z:58:PHE:CG	2.51	0.46
32:f:31:LYS:HD2	32:f:82:ILE:HG21	1.98	0.46
32:f:677:HIS:ND1	32:f:677:HIS:O	2.49	0.46
32:f:681:TYR:OH	32:f:687:ARG:NH1	2.44	0.46
9:i:21:VAL:O	9:i:25:MET:HG2	2.16	0.46
2:B:439:TYR:CD1	2:B:439:TYR:C	2.93	0.46
6:F:358:ASN:O	6:F:362:ARG:N	2.42	0.46
7:G:206:LEU:HB3	7:G:208:ILE:HD12	1.97	0.46
13:M:38:ILE:HG22	13:M:165:ALA:HB2	1.97	0.46
21:U:757:MET:N	21:U:758:PRO:CD	2.79	0.46
25:Y:78:GLU:HA	25:Y:81:LEU:HD12	1.96	0.46
25:Y:296:VAL:HG21	31:e:60:LEU:HD22	1.96	0.46
26:Z:35:VAL:O	26:Z:96:HIS:HA	2.16	0.46
27:a:145:LEU:N	27:a:146:PRO:HD3	2.31	0.46
31:e:60:LEU:HG	31:e:60:LEU:O	2.13	0.46
32:f:629:LYS:HA	32:f:632:LYS:HG2	1.98	0.46
9:i:166:ASN:OD1	9:i:167:ASN:N	2.48	0.46
10:j:99:GLU:HA	10:j:99:GLU:OE2	2.15	0.46
11:k:41:GLN:OE1	11:k:153:LEU:N	2.48	0.46
1:A:276:GLU:OE1	2:B:310:LEU:CB	2.63	0.46
7:G:113:MET:HE3	15:O:113:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:16:SER:OG	8:H:17:GLY:N	2.49	0.46
14:N:219:GLU:N	14:N:219:GLU:CD	2.73	0.46
18:R:60:THR:C	18:R:61:THR:HG23	2.40	0.46
21:U:249:CYS:HB2	21:U:328:ILE:HD12	1.98	0.46
21:U:545:LEU:HD21	21:U:578:LEU:HD12	1.98	0.46
23:W:446:ILE:HA	23:W:449:GLU:HG2	1.97	0.46
27:a:18:GLN:O	27:a:21:VAL:HG12	2.15	0.46
30:d:214:ARG:HD2	30:d:214:ARG:O	2.16	0.46
30:d:251:ILE:HG23	30:d:251:ILE:O	2.16	0.46
1:A:30:ILE:CG2	3:C:171:HIS:CD2	2.92	0.46
9:I:123:GLN:NE2	10:J:125:ARG:O	2.49	0.46
15:O:97:MET:HE3	15:O:98:THR:N	2.31	0.46
17:Q:56:PHE:CZ	17:Q:88:LEU:HD13	2.50	0.46
22:V:213:TYR:O	22:V:217:VAL:HG12	2.15	0.46
22:V:255:LEU:HD11	22:V:266:GLN:CD	2.41	0.46
23:W:183:VAL:HA	23:W:186:ILE:HG22	1.98	0.46
32:f:706:ILE:HD11	32:f:741:LEU:HD21	1.98	0.46
9:i:225:ILE:HG23	9:i:225:ILE:O	2.16	0.46
18:r:85:ILE:O	18:r:85:ILE:HG22	2.15	0.46
1:A:45:ILE:HD11	2:B:62:LEU:CA	2.46	0.46
1:A:433:ASN:C	11:K:66:LYS:HZ3	2.23	0.46
8:H:105:ILE:HG23	8:H:105:ILE:O	2.16	0.46
21:U:185:MET:HE1	21:U:194:ARG:HD3	1.98	0.46
21:U:486:MET:C	21:U:486:MET:SD	2.99	0.46
22:V:159:LEU:O	22:V:163:VAL:HG23	2.15	0.46
26:Z:82:PHE:O	26:Z:86:ASN:N	2.47	0.46
28:b:18:ASN:OD1	28:b:19:GLY:N	2.49	0.46
32:f:442:SER:OG	32:f:476:THR:O	2.30	0.46
7:g:88:ARG:HB3	13:m:118:MET:HE1	1.98	0.46
9:i:97:TYR:OH	9:i:106:PRO:HD3	2.16	0.46
10:j:102:VAL:HG11	10:j:107:ILE:CD1	2.46	0.46
13:m:78:VAL:HG12	13:m:79:ALA:N	2.30	0.46
3:C:240:GLU:OE1	3:C:241:HIS:ND1	2.49	0.45
11:K:103:TYR:CE1	19:S:119:MET:HE3	2.51	0.45
13:M:76:MET:HE1	13:M:89:ALA:HA	1.97	0.45
16:P:12:MET:SD	16:P:150:CYS:SG	3.14	0.45
21:U:339:LEU:HD21	21:U:415:HIS:HD2	1.81	0.45
23:W:50:LEU:O	23:W:54:THR:HG23	2.15	0.45
25:Y:236:LEU:O	25:Y:240:VAL:HG12	2.15	0.45
26:Z:128:PRO:O	29:c:215:LYS:NZ	2.38	0.45
27:a:303:THR:OG1	27:a:306:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:309:VAL:HG22	30:d:310:LEU:HG	1.97	0.45
32:f:728:ALA:HB2	32:f:750:GLN:CD	2.40	0.45
12:l:227:ASP:OD1	12:l:227:ASP:C	2.59	0.45
15:o:102:ILE:CD1	15:o:126:LEU:CD2	2.93	0.45
1:A:388:VAL:HB	1:A:416:VAL:HG21	1.98	0.45
3:C:50:ASN:OD1	21:U:639:LEU:HD11	2.16	0.45
7:G:6:SER:OG	7:G:7:ALA:N	2.49	0.45
9:I:134:LEU:HD11	9:I:136:TYR:HH	1.81	0.45
10:J:166:LYS:HZ1	10:J:170:GLU:HB2	1.80	0.45
21:U:409:GLY:HA3	21:U:445:ALA:HB1	1.98	0.45
21:U:509:GLY:HA3	21:U:544:ILE:CD1	2.46	0.45
24:X:48:GLN:OE1	24:X:48:GLN:N	2.47	0.45
27:a:167:GLY:O	27:a:168:ASN:C	2.60	0.45
27:a:323:SER:OG	27:a:332:HIS:O	2.33	0.45
30:d:94:MET:HA	30:d:94:MET:HE3	1.98	0.45
32:f:418:LEU:HD23	32:f:425:GLY:CA	2.46	0.45
32:f:470:VAL:CG2	32:f:485:LEU:CD1	2.95	0.45
32:f:475:ASN:HD21	32:f:511:SER:CB	2.28	0.45
7:g:10:ASP:OD2	7:g:17:SER:HB2	2.14	0.45
8:h:222:THR:HG22	8:h:223:PRO:N	2.32	0.45
4:D:191:TYR:O	4:D:195:GLY:N	2.46	0.45
5:E:263:GLN:OE1	5:E:263:GLN:N	2.40	0.45
5:E:366:ASP:OD1	5:E:369:LYS:NZ	2.48	0.45
8:H:23:GLU:OE1	8:H:23:GLU:HA	2.17	0.45
10:J:139:ASP:C	10:J:139:ASP:OD1	2.58	0.45
21:U:771:PHE:HA	29:c:177:THR:HG23	1.98	0.45
22:V:139:MET:SD	22:V:139:MET:N	2.90	0.45
22:V:333:ILE:HD11	22:V:357:LEU:HD11	1.97	0.45
23:W:335:SER:N	23:W:336:PRO:CD	2.80	0.45
23:W:455:LEU:C	23:W:455:LEU:HD12	2.42	0.45
27:a:71:VAL:HG23	27:a:71:VAL:O	2.16	0.45
27:a:218:MET:SD	27:a:218:MET:C	2.99	0.45
27:a:293:PHE:HB3	27:a:329:LYS:HD3	1.99	0.45
32:f:728:ALA:HB2	32:f:750:GLN:HG2	1.98	0.45
9:i:208:ALA:HB1	9:i:230:GLN:HE22	1.82	0.45
10:j:56:GLU:O	10:j:59:VAL:HG12	2.16	0.45
10:j:73:PHE:HD2	10:j:129:ILE:HD11	1.81	0.45
17:q:54:VAL:O	17:q:58:GLU:HG2	2.16	0.45
18:r:100:LEU:HD22	18:r:160:ILE:HD11	1.98	0.45
19:s:219:ASP:OD1	19:s:219:ASP:N	2.49	0.45
4:D:369:LYS:HD3	4:D:369:LYS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:99:HIS:HB3	11:K:107:MET:HE2	1.99	0.45
15:O:78:HIS:HB3	15:O:99:THR:HG21	1.98	0.45
16:P:14:MET:HE1	16:P:167:ILE:HA	1.97	0.45
16:P:28:PHE:HD2	16:P:36:THR:HG22	1.82	0.45
19:S:41:LEU:HD22	19:S:42:ALA:N	2.32	0.45
23:W:16:MET:HE3	23:W:23:THR:OG1	2.16	0.45
23:W:275:ILE:HG23	23:W:354:LEU:HD13	1.98	0.45
23:W:401:THR:CG2	23:W:402:ILE:N	2.68	0.45
24:X:344:ARG:N	24:X:382:GLU:O	2.49	0.45
26:Z:225:GLN:HA	26:Z:228:TYR:CZ	2.51	0.45
26:Z:237:LEU:HD12	26:Z:237:LEU:O	2.15	0.45
29:c:290:VAL:HG13	29:c:291:LEU:N	2.31	0.45
32:f:462:ALA:CB	32:f:488:ALA:HB2	2.40	0.45
32:f:670:MET:HE1	32:f:703:ARG:C	2.41	0.45
9:i:102:GLN:NE2	16:p:65:GLN:OE1	2.50	0.45
1:A:59:ILE:CD1	2:B:75:GLU:HB3	2.46	0.45
5:E:144:GLU:OE1	5:E:297:ARG:NH1	2.50	0.45
11:K:5:ARG:HG3	11:K:9:ASP:OD2	2.17	0.45
12:L:53:GLN:OE1	12:L:54:SER:N	2.49	0.45
12:L:218:ASP:OD1	12:L:218:ASP:C	2.59	0.45
15:O:212:SER:OG	15:O:213:GLY:N	2.49	0.45
21:U:522:GLY:N	21:U:555:VAL:O	2.48	0.45
21:U:526:ALA:O	21:U:530:GLU:HG3	2.17	0.45
25:Y:152:MET:HE1	25:Y:154:ASN:HB3	1.99	0.45
27:a:87:MET:HE3	27:a:90:PRO:HA	1.98	0.45
27:a:218:MET:O	27:a:219:HIS:C	2.60	0.45
32:f:304:PHE:CB	32:f:314:TYR:CB	2.94	0.45
32:f:325:GLN:CD	32:f:329:ASN:HD22	2.23	0.45
32:f:449:GLY:HA3	32:f:484:GLY:HA2	1.98	0.45
32:f:470:VAL:CG2	32:f:485:LEU:HD12	2.46	0.45
32:f:611:GLN:NE2	32:f:612:LEU:HD23	2.32	0.45
9:i:179:TYR:HD2	10:j:53:LEU:HD11	1.81	0.45
3:C:147:THR:HA	3:C:150:MET:HE3	1.98	0.45
5:E:158:LEU:O	5:E:162:VAL:HG23	2.17	0.45
5:E:277:MET:SD	5:E:277:MET:N	2.80	0.45
7:G:190:THR:O	7:G:193:GLN:HB2	2.16	0.45
9:I:6:ASP:O	9:I:7:SER:CB	2.64	0.45
12:L:46:LEU:HD22	12:L:135:ALA:CB	2.46	0.45
14:N:207:VAL:CG1	14:N:222:VAL:HG13	2.46	0.45
15:O:60:ASP:HB2	15:O:212:SER:HB3	1.98	0.45
21:U:543:LYS:HE2	21:U:772:TRP:CE3	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:267:LEU:HA	23:W:270:VAL:HG22	1.97	0.45
27:a:210:VAL:HG22	27:a:211:PHE:H	1.82	0.45
28:b:11:ASP:OD1	28:b:12:ASN:N	2.49	0.45
32:f:748:LEU:O	32:f:748:LEU:HD22	2.16	0.45
7:g:123:GLN:CD	7:g:123:GLN:C	2.85	0.45
8:h:12:THR:HG22	8:h:13:PHE:N	2.31	0.45
9:i:35:LEU:HB3	9:i:163:CYS:HB3	1.99	0.45
20:t:162:ASP:O	20:t:162:ASP:OD1	2.35	0.45
4:D:274:ARG:N	4:D:286:GLN:OE1	2.45	0.45
6:F:89:LEU:HD21	6:F:128:THR:CG2	2.47	0.45
7:G:118:ILE:HG21	7:G:138:MET:CE	2.47	0.45
9:I:194:ILE:CD1	9:I:236:LEU:HD12	2.46	0.45
11:K:96:THR:HA	11:K:107:MET:CE	2.46	0.45
24:X:346:GLN:CD	24:X:381:GLY:HA2	2.42	0.45
25:Y:349:LYS:O	25:Y:350:VAL:HG12	2.16	0.45
26:Z:243:GLN:H	27:a:286:ALA:HB1	1.82	0.45
32:f:72:ARG:HB3	32:f:73:PRO:HD3	1.98	0.45
32:f:789:SER:O	32:f:796:LEU:N	2.50	0.45
12:l:225:ASP:OD1	12:l:225:ASP:N	2.49	0.45
13:m:20:ARG:HH11	13:m:20:ARG:HG3	1.82	0.45
20:t:169:TYR:HB2	20:t:182:LEU:HD21	1.99	0.45
14:N:111:HIS:NE2	14:N:154:MET:HE1	2.32	0.45
21:U:391:GLU:HB3	21:U:395:ARG:HE	1.81	0.45
21:U:703:CYS:SG	21:U:706:VAL:HG13	2.57	0.45
21:U:808:PRO:O	21:U:809:SER:C	2.60	0.45
24:X:363:ARG:O	24:X:367:GLN:HB2	2.17	0.45
26:Z:52:ASN:OD1	26:Z:53:SER:N	2.50	0.45
26:Z:71:ASP:OD1	26:Z:73:ASP:N	2.49	0.45
32:f:224:ASN:OD1	32:f:224:ASN:C	2.57	0.45
32:f:245:ASN:HD21	32:f:253:LEU:HA	1.82	0.45
7:g:17:SER:HB2	7:g:18:PRO:HD2	1.99	0.45
8:h:50:LYS:N	8:h:207:ASN:O	2.50	0.45
16:p:116:THR:OG1	16:p:117:PHE:N	2.50	0.45
5:E:56:ILE:HD13	5:E:56:ILE:N	2.32	0.45
6:F:96:LEU:HG	6:F:137:ILE:HD11	1.99	0.45
7:G:143:ILE:HD13	7:G:149:PRO:HA	1.98	0.45
14:N:233:VAL:HG23	14:n:158:SER:OG	2.16	0.45
16:P:88:MET:HE1	16:P:132:VAL:HG22	1.98	0.45
18:R:256:GLU:C	18:R:256:GLU:CD	2.85	0.45
21:U:168:LEU:HD12	21:U:171:ASN:HD21	1.82	0.45
21:U:633:CYS:HB3	21:U:659:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:750:SER:OG	21:U:754:HIS:N	2.49	0.45
22:V:132:LEU:O	22:V:135:LEU:N	2.50	0.45
22:V:300:LEU:HD12	22:V:300:LEU:N	2.32	0.45
23:W:359:VAL:HG13	23:W:382:LEU:HD21	1.99	0.45
27:a:212:ASN:HB3	27:a:215:GLU:HB3	1.98	0.45
32:f:791:VAL:O	32:f:797:LEU:CD2	2.63	0.45
16:p:189:ILE:HG22	16:p:196:THR:HB	1.99	0.45
1:A:256:MET:HE2	1:A:256:MET:HA	1.99	0.45
3:C:80:MET:N	3:C:80:MET:SD	2.89	0.45
3:C:133:PRO:HD2	3:C:134:LEU:HD12	1.99	0.45
5:E:172:LEU:C	5:E:172:LEU:HD12	2.42	0.45
10:J:115:LYS:NZ	10:J:129:ILE:CD1	2.80	0.45
11:K:52:LYS:NZ	11:K:216:GLU:OE1	2.38	0.45
18:R:125:TYR:CD1	18:R:125:TYR:C	2.95	0.45
21:U:713:TYR:O	21:U:716:VAL:HG12	2.17	0.45
21:U:772:TRP:NE1	21:U:774:PRO:CB	2.75	0.45
23:W:173:THR:O	23:W:175:GLY:N	2.49	0.45
23:W:205:ILE:O	23:W:209:ILE:HG12	2.17	0.45
23:W:452:ILE:O	23:W:455:LEU:HG	2.16	0.45
25:Y:152:MET:HE3	25:Y:152:MET:C	2.42	0.45
25:Y:296:VAL:HG23	31:e:60:LEU:HD22	1.98	0.45
30:d:258:PHE:CD1	30:d:262:ILE:HD11	2.51	0.45
30:d:311:GLY:N	30:d:312:PRO:HD2	2.32	0.45
32:f:201:GLU:HA	32:f:204:ALA:HB3	1.98	0.45
32:f:229:VAL:HG21	32:f:607:LEU:HD23	1.99	0.45
32:f:689:ALA:O	32:f:693:ALA:HB3	2.16	0.45
32:f:857:GLY:O	32:f:860:LYS:HG2	2.16	0.45
11:k:237:VAL:HA	11:k:240:ASP:OD2	2.17	0.45
20:t:162:ASP:OD1	20:t:162:ASP:C	2.60	0.45
1:A:26:ASP:H	1:A:29:ASP:HB2	1.81	0.44
1:A:45:ILE:HD11	2:B:62:LEU:CB	2.44	0.44
1:A:52:ILE:HD11	2:B:69:LYS:N	2.32	0.44
2:B:264:PRO:O	2:B:267:VAL:HG22	2.17	0.44
3:C:329:LEU:CD2	3:C:344:LEU:HD22	2.47	0.44
4:D:115:ILE:HG22	4:D:139:LEU:HB3	1.98	0.44
35:F:501:ATP:H2'	35:F:501:ATP:N3	2.32	0.44
11:K:99:HIS:CB	11:K:107:MET:HE2	2.47	0.44
13:M:74:VAL:HG12	13:M:75:GLY:N	2.32	0.44
14:N:71:ILE:HD11	14:N:77:CYS:CB	2.47	0.44
18:R:208:VAL:HG23	18:R:209:GLU:N	2.32	0.44
22:V:206:VAL:O	22:V:209:LYS:HG3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:158:ASP:OD1	23:W:159:VAL:N	2.48	0.44
25:Y:122:THR:O	25:Y:123:ALA:C	2.60	0.44
25:Y:383:LEU:O	25:Y:387:ILE:HG22	2.17	0.44
26:Z:237:LEU:HD12	26:Z:237:LEU:C	2.41	0.44
20:t:57:LEU:N	20:t:57:LEU:HD12	2.32	0.44
20:t:65:VAL:HG12	20:t:66:VAL:N	2.32	0.44
3:C:201:ARG:NH1	4:D:300:ASP:OD1	2.50	0.44
3:C:401:ILE:O	3:C:402:LYS:CB	2.65	0.44
4:D:370:ILE:HG23	4:D:374:ASP:HB2	1.99	0.44
7:G:27:TYR:CE2	13:M:17:PRO:HA	2.52	0.44
9:I:200:THR:HG23	9:I:201:MET:N	2.33	0.44
22:V:255:LEU:HD12	22:V:269:LYS:HE2	1.99	0.44
22:V:333:ILE:HD12	22:V:360:TYR:CD2	2.52	0.44
23:W:3:ASP:C	23:W:3:ASP:OD1	2.60	0.44
23:W:25:ASP:N	23:W:25:ASP:OD1	2.48	0.44
23:W:259:GLU:HG2	23:W:262:LYS:HB3	1.98	0.44
28:b:4:GLU:CD	28:b:6:THR:HG1	2.24	0.44
32:f:528:GLY:O	32:f:569:LYS:HE2	2.18	0.44
8:h:45:VAL:HG22	8:h:212:ILE:HG22	1.99	0.44
10:j:104:VAL:HG11	10:j:143:ARG:HB2	1.98	0.44
2:B:86:LYS:CB	32:f:621:ASP:CB	2.95	0.44
3:C:134:LEU:HD12	3:C:134:LEU:H	1.81	0.44
3:C:254:ILE:O	3:C:254:ILE:HD12	2.17	0.44
4:D:102:ILE:HD13	4:D:112:TYR:HA	1.99	0.44
4:D:121:ARG:O	4:D:124:LEU:N	2.50	0.44
9:I:76:VAL:HG22	9:I:77:ALA:N	2.31	0.44
16:P:30:ILE:O	16:P:32:ALA:N	2.51	0.44
17:Q:4:LEU:HD11	17:Q:47:VAL:HG13	1.97	0.44
19:S:241:ASP:OD1	19:S:241:ASP:N	2.50	0.44
21:U:242:LEU:HD21	21:U:321:GLN:HG2	1.99	0.44
21:U:575:ASP:CB	21:U:578:LEU:HD13	2.48	0.44
21:U:769:PHE:O	21:U:769:PHE:CG	2.69	0.44
23:W:140:ILE:HG22	23:W:141:GLU:N	2.33	0.44
26:Z:8:LYS:CB	26:Z:47:VAL:HG23	2.43	0.44
29:c:217:LEU:O	29:c:221:HIS:CE1	2.70	0.44
32:f:441:LYS:CG	32:f:477:MET:HE1	2.47	0.44
32:f:815:HIS:CE1	32:f:821:LEU:HD23	2.53	0.44
11:k:137:PHE:O	11:k:158:PRO:HB3	2.18	0.44
12:l:38:LEU:HD11	12:l:191:GLY:CA	2.47	0.44
12:l:118:ILE:HG22	12:l:119:PRO:HD3	1.98	0.44
20:t:251:GLU:OE1	20:t:251:GLU:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG12	1:A:237:PHE:O	2.17	0.44
1:A:168:GLU:OE1	1:A:169:LYS:N	2.51	0.44
2:B:133:VAL:HG11	2:B:157:HIS:O	2.18	0.44
4:D:53:PHE:O	4:D:56:VAL:HG12	2.18	0.44
4:D:249:ASP:O	4:D:253:LEU:N	2.35	0.44
5:E:153:LEU:CD2	5:E:191:LEU:HD11	2.47	0.44
7:G:80:MET:HB3	7:G:87:SER:HB2	1.98	0.44
17:Q:95:ARG:HG3	17:Q:96:THR:HG23	2.00	0.44
21:U:229:VAL:HA	21:U:232:ILE:HG22	1.99	0.44
23:W:131:VAL:CG2	23:W:140:ILE:HG23	2.47	0.44
25:Y:84:LEU:O	25:Y:85:ASP:C	2.60	0.44
26:Z:256:GLN:OE1	30:d:330:ILE:HG21	2.18	0.44
32:f:129:LEU:HD23	32:f:130:ALA:HB2	2.00	0.44
7:g:67:THR:HG22	7:g:69:LEU:H	1.83	0.44
8:h:123:GLN:NE2	8:h:123:GLN:O	2.50	0.44
20:t:48:ASN:N	20:t:48:ASN:OD1	2.50	0.44
1:A:146:LYS:O	1:A:148:GLN:N	2.51	0.44
2:B:59:ARG:NE	32:f:188:VAL:HG13	2.19	0.44
2:B:101:ASP:OD1	2:B:102:LEU:N	2.50	0.44
3:C:308:PRO:HA	3:C:311:ILE:O	2.18	0.44
4:D:102:ILE:HD11	4:D:112:TYR:HD1	1.83	0.44
5:E:172:LEU:HD23	5:E:278:ALA:HB1	1.98	0.44
10:J:59:VAL:HG13	10:J:59:VAL:O	2.17	0.44
12:L:85:CYS:SG	12:L:89:ARG:NE	2.90	0.44
14:N:173:VAL:HG23	14:N:174:ASP:N	2.32	0.44
15:O:163:ASP:C	15:O:163:ASP:OD1	2.61	0.44
18:R:156:MET:O	18:R:175:SER:N	2.51	0.44
19:S:46:GLU:CD	19:S:46:GLU:C	2.85	0.44
21:U:173:VAL:N	21:U:174:PRO:HD3	2.32	0.44
21:U:499:THR:O	21:U:503:GLN:NE2	2.51	0.44
26:Z:282:ASN:O	26:Z:284:ASP:N	2.50	0.44
27:a:38:THR:HG21	27:a:70:ARG:HD2	1.97	0.44
29:c:134:GLU:O	29:c:137:SER:O	2.35	0.44
32:f:156:HIS:O	32:f:159:VAL:HG12	2.17	0.44
32:f:287:ASP:OD1	32:f:881:GLU:OE1	2.35	0.44
32:f:627:GLU:O	32:f:627:GLU:CD	2.60	0.44
32:f:650:GLN:O	32:f:654:VAL:HG23	2.17	0.44
8:h:155:TYR:CG	8:h:155:TYR:O	2.70	0.44
10:j:94:HIS:O	10:j:97:THR:O	2.35	0.44
10:j:108:THR:HG21	10:j:145:TYR:CD2	2.53	0.44
10:j:188:ILE:O	10:j:192:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:r:123:ARG:NH1	18:r:126:GLU:OE1	2.50	0.44
1:A:426:THR:HB	1:A:427:PRO:HD3	1.98	0.44
4:D:254:ALA:HA	4:D:258:ALA:O	2.17	0.44
5:E:65:THR:N	5:E:68:LYS:O	2.45	0.44
12:L:215:VAL:HG13	12:L:215:VAL:O	2.17	0.44
14:N:35:THR:OG1	14:N:51:ASP:OD1	2.33	0.44
22:V:197:THR:HG1	22:V:242:HIS:CE1	2.32	0.44
22:V:255:LEU:HD23	22:V:255:LEU:C	2.43	0.44
23:W:117:ASP:OD1	23:W:117:ASP:N	2.50	0.44
23:W:129:ARG:HA	23:W:132:THR:HG23	2.00	0.44
23:W:168:GLU:HG2	23:W:169:LEU:N	2.32	0.44
24:X:282:ARG:HA	24:X:285:GLU:OE1	2.18	0.44
25:Y:39:ASP:OD1	25:Y:40:GLU:N	2.50	0.44
27:a:32:LYS:C	27:a:33:LEU:HD22	2.43	0.44
27:a:67:PHE:O	27:a:69:HIS:NE2	2.50	0.44
30:d:309:VAL:HG13	30:d:310:LEU:N	2.31	0.44
7:g:210:PHE:O	7:g:239:LEU:HD21	2.18	0.44
13:m:241:LYS:HA	13:m:244:LEU:HD12	1.99	0.44
1:A:62:LEU:O	2:B:79:ILE:HD13	2.17	0.44
1:A:101:ILE:HD11	1:A:140:VAL:HG11	2.00	0.44
1:A:219:GLY:CA	35:A:501:ATP:H5'2	2.48	0.44
3:C:81:ASP:O	3:C:82:LYS:HG2	2.18	0.44
8:H:18:LYS:CE	9:I:79:ILE:HD12	2.47	0.44
16:P:126:LEU:HD12	16:P:126:LEU:C	2.42	0.44
17:Q:20:VAL:O	17:Q:20:VAL:HG13	2.18	0.44
20:T:54:THR:OG1	20:T:55:SER:N	2.43	0.44
20:T:93:SER:O	20:T:94:THR:OG1	2.28	0.44
20:T:162:ASP:C	20:T:162:ASP:OD1	2.59	0.44
23:W:227:TYR:O	23:W:230:MET:HG3	2.18	0.44
26:Z:98:GLY:O	26:Z:99:PRO:C	2.60	0.44
27:a:157:ASP:O	27:a:160:SER:OG	2.27	0.44
32:f:257:ARG:HD2	32:f:289:VAL:HG22	1.99	0.44
7:g:20:GLY:HA3	8:h:28:ALA:HB2	2.00	0.44
1:A:45:ILE:CD1	2:B:62:LEU:HA	2.48	0.44
1:A:385:ILE:O	1:A:388:VAL:HG12	2.18	0.44
2:B:113:GLU:O	2:B:114:GLU:C	2.61	0.44
5:E:135:ILE:HG22	5:E:135:ILE:O	2.17	0.44
19:S:76:ASP:N	19:S:76:ASP:OD1	2.49	0.44
20:T:231:ARG:HA	20:T:248:LEU:O	2.17	0.44
21:U:757:MET:SD	21:U:758:PRO:N	2.91	0.44
22:V:338:LEU:O	22:V:338:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:37:GLU:O	23:W:44:ILE:HD13	2.17	0.44
23:W:259:GLU:O	23:W:263:TRP:HB3	2.17	0.44
23:W:433:ASN:OD1	23:W:433:ASN:C	2.61	0.44
24:X:66:LEU:O	24:X:70:LEU:HD23	2.17	0.44
27:a:18:GLN:N	27:a:19:PRO:CD	2.81	0.44
27:a:269:LEU:O	27:a:272:ILE:HG13	2.18	0.44
32:f:262:PHE:HB2	32:f:263:PRO:HD3	2.00	0.44
32:f:399:LEU:HD12	32:f:432:TYR:HE1	1.81	0.44
1:A:294:GLU:O	1:A:297:ARG:HG2	2.17	0.44
4:D:392:TYR:CD1	4:D:392:TYR:C	2.96	0.44
5:E:153:LEU:O	5:E:272:ARG:NH1	2.51	0.44
5:E:187:VAL:HG12	5:E:195:PHE:HE2	1.82	0.44
7:G:130:GLU:HA	7:G:130:GLU:OE2	2.18	0.44
10:J:101:PRO:HG3	10:J:138:PHE:CE1	2.53	0.44
10:J:221:ASN:OD1	10:J:222:PRO:N	2.51	0.44
11:K:236:GLU:O	11:K:240:ASP:OD2	2.36	0.44
15:O:257:GLU:OE2	16:P:198:ARG:NE	2.51	0.44
21:U:712:LEU:HA	21:U:715:LYS:HG2	2.00	0.44
22:V:197:THR:OG1	22:V:242:HIS:NE2	2.40	0.44
25:Y:14:ASN:CB	25:Y:143:TYR:CZ	3.01	0.44
25:Y:122:THR:O	25:Y:126:LYS:N	2.40	0.44
26:Z:253:THR:O	26:Z:257:MET:HG2	2.18	0.44
27:a:343:LEU:CG	27:a:344:GLN:H	2.30	0.44
32:f:415:GLY:CA	32:f:451:VAL:HG23	2.48	0.44
32:f:446:LEU:HD13	32:f:483:PHE:CD2	2.53	0.44
32:f:469:TYR:HB2	32:f:481:SER:HB2	1.99	0.44
32:f:779:CYS:N	32:f:780:PRO:HD2	2.32	0.44
8:h:75:VAL:HG22	8:h:76:TYR:N	2.32	0.44
13:m:44:ASP:OD1	13:m:44:ASP:N	2.48	0.44
15:o:78:HIS:CB	15:o:99:THR:HG21	2.48	0.44
20:t:144:ARG:HD2	20:t:149:ASN:O	2.18	0.44
2:B:183:THR:O	2:B:238:ALA:CB	2.66	0.43
3:C:357:ALA:HA	35:C:501:ATP:C8	2.53	0.43
6:F:154:ASN:OD1	6:F:157:SER:N	2.47	0.43
7:G:173:THR:O	7:G:176:THR:HG22	2.18	0.43
24:X:371:ASP:C	24:X:371:ASP:OD1	2.59	0.43
25:Y:338:ILE:HG13	25:Y:343:LEU:HD23	1.99	0.43
27:a:51:ALA:O	27:a:85:ARG:NE	2.50	0.43
27:a:305:ASN:O	27:a:309:LEU:HG	2.18	0.43
29:c:44:HIS:NE2	29:c:53:VAL:HG21	2.33	0.43
30:d:330:ILE:N	30:d:331:PRO:CD	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:185:LEU:O	32:f:189:LYS:HB3	2.18	0.43
32:f:193:PRO:O	32:f:196:MET:HG2	2.18	0.43
32:f:295:ALA:O	32:f:296:PHE:C	2.61	0.43
32:f:560:LEU:CD2	32:f:782:HIS:NE2	2.79	0.43
7:g:208:ILE:HD11	7:g:210:PHE:HB3	1.99	0.43
11:k:229:PHE:N	11:k:229:PHE:CD1	2.86	0.43
14:n:38:MET:HG3	14:n:160:ALA:O	2.18	0.43
14:n:62:ASN:ND2	14:n:65:THR:OG1	2.51	0.43
1:A:390:THR:HA	2:B:216:ILE:HD12	1.99	0.43
2:B:416:ASN:OD1	2:B:417:GLU:N	2.50	0.43
8:H:168:VAL:HG13	8:H:169:ASN:N	2.34	0.43
10:J:119:THR:O	10:J:119:THR:HG22	2.18	0.43
10:J:208:LEU:O	10:J:219:ILE:HD12	2.18	0.43
16:P:12:MET:HE3	16:P:167:ILE:CG1	2.29	0.43
16:P:88:MET:HE1	16:P:132:VAL:CG2	2.48	0.43
20:T:68:ALA:HB2	20:T:234:ILE:HD13	1.99	0.43
21:U:527:GLN:O	21:U:530:GLU:HG3	2.18	0.43
23:W:18:VAL:HG23	23:W:19:ASP:N	2.33	0.43
23:W:51:GLU:O	23:W:54:THR:OG1	2.33	0.43
23:W:311:THR:O	23:W:313:GLU:N	2.50	0.43
23:W:411:GLY:O	23:W:412:ILE:HG23	2.17	0.43
25:Y:30:GLU:OE1	25:Y:30:GLU:N	2.42	0.43
25:Y:128:TYR:O	25:Y:131:THR:HG23	2.19	0.43
26:Z:36:VAL:HA	26:Z:95:TYR:O	2.18	0.43
27:a:87:MET:SD	27:a:94:LEU:N	2.91	0.43
30:d:309:VAL:HG11	30:d:316:TYR:CE1	2.53	0.43
9:i:41:ASP:OD1	9:i:42:GLY:N	2.51	0.43
11:k:143:PHE:O	11:k:153:LEU:HD12	2.18	0.43
15:o:226:LEU:HD23	15:o:226:LEU:C	2.43	0.43
2:B:245:ALA:HB1	2:B:279:PRO:O	2.18	0.43
5:E:229:ILE:HG23	5:E:274:LYS:O	2.18	0.43
6:F:402:GLU:OE2	6:F:426:GLU:OE1	2.35	0.43
6:F:421:MET:CE	12:L:30:LYS:HZ2	2.31	0.43
8:H:38:ILE:HD12	8:H:174:LEU:HD11	1.98	0.43
10:J:136:PHE:CD1	10:J:213:ARG:O	2.71	0.43
11:K:229:PHE:O	11:K:230:THR:OG1	2.32	0.43
15:O:178:MET:HE3	20:t:224:ARG:HE	1.83	0.43
23:W:355:LYS:O	23:W:358:VAL:HG22	2.19	0.43
26:Z:278:ASN:OD1	26:Z:279:LYS:N	2.51	0.43
27:a:336:VAL:HG22	27:a:337:GLN:N	2.33	0.43
30:d:101:GLU:N	30:d:101:GLU:OE1	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:113:MET:SD	32:f:113:MET:C	3.02	0.43
32:f:283:THR:HA	32:f:816:TYR:HE1	1.70	0.43
32:f:690:VAL:CG2	32:f:691:PRO:HD3	2.48	0.43
12:l:95:SER:HB2	12:l:103:LEU:HD12	2.00	0.43
13:m:222:ASN:OD1	13:m:222:ASN:O	2.36	0.43
3:C:79:ALA:HB1	3:C:85:VAL:HG12	2.01	0.43
6:F:247:THR:HG23	6:F:247:THR:O	2.17	0.43
11:K:65:GLU:OE1	11:K:65:GLU:C	2.61	0.43
11:K:166:ASP:OD1	11:K:166:ASP:N	2.47	0.43
13:M:181:GLN:O	13:M:185:MET:HG3	2.18	0.43
16:P:168:SER:HB2	16:P:200:LEU:HD13	2.01	0.43
17:Q:104:LEU:HD13	17:Q:104:LEU:C	2.42	0.43
21:U:30:VAL:O	21:U:30:VAL:CG2	2.65	0.43
21:U:451:ALA:HB1	21:U:781:LEU:HD22	2.00	0.43
23:W:102:ALA:O	23:W:105:VAL:HG22	2.19	0.43
23:W:251:TYR:O	23:W:254:PRO:HD2	2.17	0.43
25:Y:41:LEU:C	25:Y:41:LEU:HD13	2.43	0.43
25:Y:50:MET:HA	25:Y:53:TYR:CE2	2.54	0.43
27:a:350:LYS:HA	27:a:353:LEU:O	2.19	0.43
28:b:78:VAL:N	28:b:79:GLN:OE1	2.52	0.43
28:b:148:VAL:HG13	28:b:148:VAL:O	2.18	0.43
30:d:309:VAL:HG13	30:d:310:LEU:H	1.83	0.43
32:f:174:ASP:OD1	32:f:175:ASP:N	2.51	0.43
32:f:244:GLU:HA	32:f:248:LEU:HB2	2.00	0.43
32:f:266:LEU:O	32:f:268:LEU:HD23	2.17	0.43
32:f:466:LEU:HD22	32:f:481:SER:HA	1.99	0.43
32:f:611:GLN:O	32:f:615:ILE:HG13	2.18	0.43
10:j:134:VAL:HG22	10:j:144:LEU:HD12	1.99	0.43
18:r:208:VAL:HG23	18:r:209:GLU:N	2.32	0.43
19:s:59:GLU:C	19:s:59:GLU:CD	2.86	0.43
1:A:398:ARG:NH1	2:B:199:GLU:OE2	2.51	0.43
2:B:342:ILE:HA	2:B:347:ILE:HD13	2.00	0.43
3:C:198:LEU:O	3:C:201:ARG:CG	2.65	0.43
6:F:79:LYS:O	6:F:161:LEU:HD23	2.18	0.43
8:H:136:ILE:HG22	8:H:137:CYS:O	2.18	0.43
11:K:220:VAL:HG13	11:K:220:VAL:O	2.18	0.43
26:Z:68:TRP:CG	26:Z:104:ASN:HD21	2.36	0.43
27:a:198:PHE:CE1	27:a:202:LEU:HD11	2.53	0.43
29:c:198:ARG:CZ	29:c:198:ARG:HA	2.49	0.43
30:d:330:ILE:H	30:d:330:ILE:HD12	1.83	0.43
32:f:99:LEU:HD12	32:f:99:LEU:C	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:473:ASN:OD1	32:f:473:ASN:N	2.41	0.43
32:f:611:GLN:HE21	32:f:615:ILE:HD12	1.83	0.43
7:g:155:ASP:HB3	7:g:156:PRO:HD2	2.01	0.43
7:g:206:LEU:O	7:g:207:SER:OG	2.30	0.43
10:j:89:VAL:HG22	17:q:66:LEU:HD21	2.00	0.43
16:p:88:MET:CE	16:p:130:PRO:HB2	2.48	0.43
4:D:410:ASP:O	4:D:411:GLU:HB3	2.18	0.43
9:I:90:LEU:HD21	9:I:114:LEU:HD22	2.01	0.43
9:I:176:LYS:HA	10:J:53:LEU:CD1	2.34	0.43
12:L:24:TYR:N	12:L:24:TYR:CD1	2.87	0.43
12:L:47:VAL:CG1	12:L:195:LEU:HD22	2.48	0.43
12:L:71:GLY:HA3	12:L:221:PHE:CZ	2.53	0.43
22:V:298:ILE:HG23	30:d:213:GLU:CD	2.44	0.43
22:V:300:LEU:HD11	22:V:397:ARG:CZ	2.48	0.43
23:W:254:PRO:HB2	23:W:263:TRP:CG	2.54	0.43
32:f:573:ILE:HG21	32:f:599:ALA:HB2	2.00	0.43
13:m:237:GLU:OE1	13:m:237:GLU:N	2.49	0.43
14:n:36:THR:HG22	14:n:194:LEU:HD22	2.01	0.43
19:s:42:ALA:O	19:s:43:ILE:HD12	2.18	0.43
19:s:86:HIS:HB3	20:t:175:VAL:HG13	2.01	0.43
19:s:194:LEU:HD12	19:s:195:SER:N	2.33	0.43
4:D:192:LYS:O	4:D:192:LYS:HD3	2.19	0.43
6:F:83:ASN:HA	6:F:88:TYR:CD1	2.54	0.43
6:F:233:LYS:N	35:F:501:ATP:O2B	2.51	0.43
7:G:36:GLY:C	7:G:37:LEU:HD22	2.44	0.43
7:G:166:THR:HG22	7:G:167:ALA:N	2.33	0.43
22:V:266:GLN:O	22:V:270:LEU:HG	2.19	0.43
23:W:443:THR:CG2	23:W:444:HIS:N	2.82	0.43
24:X:171:LEU:HD21	24:X:210:LEU:HA	2.01	0.43
26:Z:15:VAL:HG22	26:Z:51:SER:O	2.19	0.43
26:Z:208:ILE:HA	26:Z:211:TYR:CE2	2.54	0.43
32:f:266:LEU:HD23	32:f:268:LEU:HD23	2.00	0.43
7:g:44:GLY:HA3	7:g:194:THR:HG21	2.01	0.43
14:n:53:ARG:HE	14:n:60:ILE:CD1	2.31	0.43
19:s:137:ILE:HG23	19:s:137:ILE:O	2.19	0.43
1:A:74:PRO:HA	1:A:75:PRO:HD3	1.90	0.43
1:A:224:LEU:HD22	35:A:501:ATP:H2'	2.00	0.43
1:A:257:VAL:HG11	1:A:302:LEU:HA	2.00	0.43
4:D:229:ARG:O	4:D:230:VAL:C	2.61	0.43
5:E:50:LEU:HD21	6:F:78:GLU:HG2	2.00	0.43
5:E:88:ASP:HB3	5:E:91:LYS:HG2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:75:VAL:HG22	8:H:76:TYR:H	1.84	0.43
10:J:37:GLY:N	10:J:40:ILE:O	2.47	0.43
10:J:108:THR:HG22	10:J:133:ILE:HD13	2.01	0.43
11:K:104:ASN:OD1	18:R:116:ARG:NH2	2.47	0.43
11:K:118:ASN:OD1	12:L:82:ARG:NH2	2.49	0.43
21:U:339:LEU:HD22	21:U:414:GLY:HA3	2.01	0.43
22:V:331:LEU:O	22:V:335:VAL:HG23	2.19	0.43
23:W:356:ASN:OD1	23:W:356:ASN:C	2.62	0.43
25:Y:316:LEU:HD13	25:Y:327:VAL:HG11	2.01	0.43
25:Y:363:ASN:O	25:Y:366:TYR:N	2.49	0.43
27:a:35:HIS:CG	27:a:36:GLN:N	2.87	0.43
32:f:325:GLN:CD	32:f:329:ASN:ND2	2.77	0.43
32:f:441:LYS:HG2	32:f:477:MET:HE1	2.00	0.43
32:f:609:VAL:O	32:f:613:LEU:N	2.33	0.43
14:n:53:ARG:NH1	14:n:203:SER:O	2.52	0.43
16:p:122:CYS:SG	16:p:131:MET:O	2.60	0.43
19:s:152:PHE:CE2	19:s:158:TYR:HB3	2.54	0.43
20:t:96:LEU:HD12	20:t:97:GLY:H	1.84	0.43
1:A:324:PRO:HA	1:A:327:LEU:HD23	2.01	0.43
4:D:192:LYS:O	4:D:195:GLY:N	2.52	0.43
5:E:108:MET:O	5:E:109:ARG:C	2.61	0.43
6:F:80:ILE:O	6:F:84:LYS:HG2	2.18	0.43
6:F:96:LEU:CG	6:F:137:ILE:HD11	2.48	0.43
8:H:114:VAL:HA	8:H:117:VAL:HG12	2.01	0.43
10:J:191:VAL:HG11	10:J:208:LEU:HD21	2.01	0.43
21:U:408:LEU:C	21:U:408:LEU:HD13	2.44	0.43
21:U:886:PRO:HA	21:U:889:LEU:HD12	2.01	0.43
22:V:29:PRO:N	22:V:30:PRO:CD	2.82	0.43
22:V:231:LEU:O	22:V:235:LEU:HG	2.19	0.43
23:W:148:THR:HB	23:W:168:GLU:OE2	2.18	0.43
26:Z:207:ASP:HA	26:Z:210:SER:HB2	2.01	0.43
32:f:815:HIS:NE2	32:f:821:LEU:HD23	2.33	0.43
8:h:9:SER:C	8:h:10:LEU:HD22	2.43	0.43
9:i:184:MET:O	9:i:185:THR:C	2.62	0.43
17:q:99:HIS:ND1	17:q:99:HIS:O	2.50	0.43
18:r:166:ARG:HH11	18:r:166:ARG:HG3	1.83	0.43
1:A:45:ILE:CD1	2:B:62:LEU:CA	2.97	0.43
2:B:135:ILE:CB	2:B:159:VAL:CG2	2.97	0.43
4:D:246:MET:SD	4:D:247:VAL:N	2.92	0.43
6:F:89:LEU:HD23	6:F:126:THR:HB	2.00	0.43
10:J:89:VAL:HG22	17:Q:66:LEU:HD21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:195:LEU:HD13	10:J:206:ILE:HD12	2.00	0.43
13:M:11:SER:OG	13:M:14:THR:CG2	2.66	0.43
21:U:337:LEU:HD12	21:U:338:HIS:N	2.34	0.43
21:U:519:VAL:C	21:U:520:MET:HE2	2.44	0.43
21:U:539:THR:OG1	21:U:540:GLN:N	2.51	0.43
22:V:468:SER:O	22:V:468:SER:OG	2.35	0.43
23:W:131:VAL:HG21	23:W:140:ILE:HG23	2.00	0.43
23:W:371:THR:O	23:W:414:ASN:HA	2.19	0.43
26:Z:112:MET:HA	26:Z:112:MET:HE3	2.01	0.43
26:Z:121:LEU:HD12	26:Z:122:VAL:N	2.34	0.43
26:Z:232:ASP:HB3	27:a:338:PRO:HG3	2.01	0.43
27:a:35:HIS:O	27:a:38:THR:OG1	2.23	0.43
29:c:154:LYS:O	29:c:155:VAL:C	2.62	0.43
30:d:208:PHE:HE1	30:d:212:LEU:HD11	1.84	0.43
12:l:19:ILE:CD1	13:m:130:ARG:CZ	2.97	0.43
1:A:33:LEU:CD1	3:C:174:LEU:HG	2.49	0.42
1:A:146:LYS:O	1:A:147:TYR:CD2	2.72	0.42
1:A:223:THR:HG22	1:A:227:ARG:HH21	1.83	0.42
1:A:253:GLY:O	1:A:257:VAL:HG23	2.19	0.42
1:A:292:ASP:HB3	2:B:302:GLU:HG2	2.01	0.42
1:A:375:ARG:CD	11:K:173:ALA:HB2	2.49	0.42
3:C:206:HIS:ND1	3:C:206:HIS:N	2.66	0.42
4:D:267:ILE:H	4:D:311:THR:CB	2.32	0.42
4:D:344:ILE:HG12	36:D:501:ADP:C2	2.54	0.42
5:E:177:GLY:O	5:E:181:THR:N	2.52	0.42
6:F:59:VAL:O	6:F:62:VAL:HG12	2.18	0.42
10:J:104:VAL:O	10:J:108:THR:HG23	2.19	0.42
12:L:46:LEU:HD22	12:L:135:ALA:HB3	2.00	0.42
17:Q:43:LEU:HD12	17:Q:183:ILE:HD11	2.00	0.42
21:U:380:THR:O	21:U:381:THR:OG1	2.34	0.42
22:V:240:LEU:O	22:V:241:ARG:C	2.63	0.42
22:V:481:SER:HB2	30:d:344:ARG:NH2	2.33	0.42
23:W:23:THR:HG23	23:W:24:VAL:N	2.34	0.42
23:W:247:TYR:HA	23:W:250:ILE:HG12	2.00	0.42
25:Y:49:ASN:HA	25:Y:114:ILE:HA	2.01	0.42
10:j:97:THR:O	10:j:98:VAL:C	2.61	0.42
15:o:102:ILE:HD13	15:o:126:LEU:CD2	2.49	0.42
16:p:12:MET:HE2	16:p:146:MET:HB3	2.01	0.42
34:u:406:ARG:HG2	34:u:406:ARG:H	1.42	0.42
1:A:65:ILE:HD12	32:f:662:MET:HG2	2.01	0.42
2:B:137:SER:OG	2:B:138:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:156:VAL:HG13	2:B:158:ALA:H	1.84	0.42
3:C:133:PRO:O	3:C:136:SER:OG	2.35	0.42
9:I:49:ARG:N	9:I:210:LYS:O	2.41	0.42
10:J:213:ARG:HD2	10:J:213:ARG:C	2.44	0.42
16:P:45:MET:HE3	16:P:71:LEU:HD23	2.01	0.42
23:W:59:ASP:O	23:W:62:SER:OG	2.27	0.42
23:W:196:VAL:O	23:W:196:VAL:HG12	2.19	0.42
25:Y:197:ALA:HB3	25:Y:226:VAL:HG21	2.00	0.42
27:a:32:LYS:O	27:a:33:LEU:HD22	2.18	0.42
27:a:129:GLN:C	27:a:131:THR:N	2.76	0.42
32:f:304:PHE:CB	32:f:314:TYR:HA	2.49	0.42
32:f:713:PHE:HB3	32:f:749:ALA:HB1	2.00	0.42
8:h:66:GLU:OE2	8:h:91:ARG:NE	2.49	0.42
10:j:43:LEU:N	10:j:43:LEU:HD23	2.34	0.42
10:j:115:LYS:O	10:j:119:THR:HG23	2.19	0.42
12:l:46:LEU:HD23	12:l:46:LEU:N	2.33	0.42
13:m:107:ILE:O	13:m:107:ILE:HG23	2.19	0.42
4:D:296:MET:HE1	4:D:326:ARG:CA	2.49	0.42
4:D:370:ILE:CG2	4:D:374:ASP:HB2	2.50	0.42
6:F:93:VAL:HG12	6:F:149:ASP:OD1	2.20	0.42
10:J:156:TRP:CZ2	11:K:59:MET:HE3	2.54	0.42
12:L:33:SER:OG	12:L:34:ALA:N	2.51	0.42
12:L:66:VAL:HG11	12:L:88:MET:HE2	2.01	0.42
21:U:24:LEU:HD12	21:U:59:PHE:CD1	2.54	0.42
21:U:161:ASP:OD1	21:U:161:ASP:N	2.47	0.42
21:U:465:LEU:HD21	21:U:474:ARG:HD2	2.01	0.42
21:U:526:ALA:O	21:U:529:ILE:HG12	2.19	0.42
21:U:544:ILE:CG2	21:U:545:LEU:N	2.81	0.42
22:V:135:LEU:HD22	22:V:174:PHE:CZ	2.54	0.42
22:V:214:HIS:HA	22:V:217:VAL:HG12	2.01	0.42
23:W:284:SER:O	23:W:287:VAL:HG22	2.19	0.42
27:a:345:GLN:O	27:a:349:MET:HE3	2.19	0.42
28:b:21:PHE:HB2	28:b:25:ARG:HA	2.01	0.42
32:f:35:ASP:CG	32:f:82:ILE:HD12	2.44	0.42
32:f:141:LYS:O	32:f:145:VAL:HG12	2.19	0.42
32:f:520:LEU:HD13	32:f:560:LEU:HD23	2.01	0.42
10:j:94:HIS:ND1	10:j:102:VAL:HG22	2.34	0.42
18:r:197:VAL:HG11	18:r:218:ALA:HA	2.01	0.42
1:A:56:LEU:HD22	2:B:48:LYS:HG3	2.01	0.42
3:C:66:LEU:HD13	4:D:116:LEU:HD22	2.00	0.42
3:C:198:LEU:HD12	3:C:201:ARG:NE	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:137:ILE:HD13	6:F:142:ALA:CB	2.50	0.42
13:M:40:ILE:HD11	13:M:194:VAL:CG2	2.50	0.42
16:P:126:LEU:CD1	16:P:127:ILE:HG23	2.45	0.42
23:W:16:MET:HE1	23:W:26:GLN:HB2	2.01	0.42
23:W:46:THR:O	23:W:49:SER:OG	2.29	0.42
24:X:326:LEU:O	24:X:330:LEU:N	2.32	0.42
26:Z:51:SER:O	26:Z:52:ASN:C	2.62	0.42
26:Z:224:HIS:O	26:Z:227:ILE:N	2.47	0.42
13:m:199:TYR:HB3	13:m:244:LEU:HD11	2.00	0.42
15:o:96:ASP:O	15:o:100:GLN:HG3	2.19	0.42
18:r:97:ASN:OD1	18:r:98:PRO:HD2	2.20	0.42
34:u:403:ARG:CA	34:u:406:ARG:CG	2.94	0.42
1:A:63:THR:HA	2:B:79:ILE:HD13	2.02	0.42
1:A:193:THR:N	1:A:194:PRO:HD2	2.33	0.42
2:B:221:GLY:O	2:B:348:ASP:N	2.52	0.42
3:C:270:GLN:O	3:C:274:LEU:HD23	2.19	0.42
5:E:113:ARG:NH2	6:F:95:GLU:OE1	2.52	0.42
8:H:74:LEU:HD12	8:H:135:LEU:O	2.19	0.42
10:J:52:LYS:C	10:J:52:LYS:HD3	2.44	0.42
18:R:104:MET:HB2	18:R:111:CYS:CB	2.49	0.42
21:U:661:ALA:C	21:U:746:ILE:HD11	2.45	0.42
23:W:210:ASN:OD1	23:W:210:ASN:C	2.62	0.42
24:X:358:LYS:O	24:X:362:GLU:CB	2.62	0.42
25:Y:358:ARG:NH2	25:Y:360:ASP:OD1	2.53	0.42
27:a:78:GLU:O	27:a:82:HIS:ND1	2.49	0.42
30:d:202:GLN:O	30:d:203:ASN:OD1	2.37	0.42
32:f:232:TYR:O	32:f:236:CYS:SG	2.77	0.42
32:f:463:LEU:HD22	32:f:497:VAL:CG2	2.49	0.42
32:f:825:MET:O	32:f:849:ALA:HA	2.19	0.42
7:g:112:ASP:OD2	15:o:115:ARG:NH2	2.52	0.42
10:j:192:ILE:HD13	10:j:228:TYR:HB3	2.02	0.42
15:o:256:THR:HG22	15:o:257:GLU:N	2.35	0.42
2:B:189:GLY:HA3	2:B:360:THR:HG22	2.02	0.42
3:C:198:LEU:HD22	35:C:501:ATP:N3	2.33	0.42
11:K:133:MET:HE1	11:K:137:PHE:CE2	2.55	0.42
12:L:26:MET:N	12:L:26:MET:HE2	2.34	0.42
12:L:38:LEU:HB3	12:L:187:LEU:HD11	2.00	0.42
14:N:35:THR:O	14:N:164:SER:N	2.52	0.42
18:R:171:TYR:CE2	18:R:181:SER:HB3	2.54	0.42
20:T:237:VAL:HG22	20:T:238:THR:N	2.35	0.42
22:V:231:LEU:HD11	22:V:247:GLN:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:480:ILE:HG21	26:Z:264:SER:HB3	2.01	0.42
24:X:51:LEU:HD11	24:X:88:LEU:HD13	2.02	0.42
25:Y:49:ASN:O	25:Y:53:TYR:CD2	2.73	0.42
25:Y:159:ARG:NE	25:Y:159:ARG:HA	2.34	0.42
25:Y:343:LEU:O	25:Y:344:HIS:C	2.62	0.42
32:f:308:SER:O	32:f:309:GLU:CG	2.53	0.42
32:f:379:GLY:HA2	32:f:417:ILE:HD11	1.89	0.42
32:f:568:GLY:C	32:f:599:ALA:O	2.62	0.42
8:h:219:ARG:NH1	8:h:221:LEU:HD23	2.34	0.42
18:r:97:ASN:OD1	18:r:98:PRO:N	2.52	0.42
2:B:74:MET:O	2:B:78:PHE:N	2.53	0.42
2:B:149:SER:O	2:B:163:LEU:HG	2.19	0.42
2:B:194:ILE:HA	2:B:197:ILE:HG22	2.01	0.42
3:C:235:PHE:CD2	3:C:279:GLN:HG3	2.55	0.42
5:E:137:GLY:C	5:E:138:LEU:HD22	2.45	0.42
10:J:42:VAL:HG21	10:J:188:ILE:HD13	2.02	0.42
10:J:102:VAL:HG23	10:J:106:TYR:HD2	1.85	0.42
11:K:7:GLU:OE1	11:K:7:GLU:HA	2.19	0.42
13:M:94:GLU:OE1	13:M:94:GLU:C	2.63	0.42
16:P:163:LEU:HD23	16:P:189:ILE:HD13	2.02	0.42
21:U:98:GLU:HA	21:U:101:ILE:HG12	2.02	0.42
21:U:527:GLN:NE2	21:U:531:ASP:OD2	2.53	0.42
22:V:263:LEU:HA	22:V:266:GLN:CD	2.45	0.42
25:Y:65:ILE:C	25:Y:67:VAL:H	2.28	0.42
26:Z:95:TYR:CB	26:Z:122:VAL:HG23	2.49	0.42
32:f:283:THR:O	32:f:816:TYR:HE1	2.03	0.42
32:f:813:LYS:NZ	32:f:823:ALA:O	2.51	0.42
10:j:213:ARG:O	10:j:214:ASP:OD1	2.37	0.42
14:n:56:THR:O	14:n:56:THR:HG22	2.20	0.42
3:C:109:THR:O	3:C:112:CYS:SG	2.71	0.42
4:D:89:ILE:HG22	4:D:90:GLY:N	2.35	0.42
5:E:56:ILE:HD12	6:F:132:TYR:CE1	2.54	0.42
11:K:118:ASN:OD1	12:L:82:ARG:NH1	2.52	0.42
18:R:61:THR:CG2	18:R:190:GLY:HA3	2.49	0.42
21:U:162:VAL:HA	21:U:165:LYS:HG2	2.01	0.42
21:U:503:GLN:O	21:U:504:ASP:OD1	2.37	0.42
21:U:884:VAL:HG13	21:U:889:LEU:HD21	2.02	0.42
22:V:253:LEU:O	22:V:256:ARG:HG2	2.20	0.42
23:W:12:ARG:O	23:W:16:MET:HG2	2.20	0.42
23:W:193:CYS:O	23:W:196:VAL:HB	2.19	0.42
29:c:155:VAL:O	29:c:155:VAL:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:d:311:GLY:N	30:d:312:PRO:CD	2.81	0.42
32:f:842:VAL:O	32:f:843:SER:HB3	2.20	0.42
8:h:188:ILE:HG23	8:h:189:HIS:N	2.35	0.42
9:i:65:ILE:HG22	9:i:66:TYR:N	2.35	0.42
10:j:75:GLY:HA3	10:j:129:ILE:HD12	2.02	0.42
13:m:42:CYS:HB2	13:m:190:ILE:HG13	2.01	0.42
1:A:249:TYR:HA	33:v:6:UNK:HA	2.02	0.42
3:C:189:TYR:O	3:C:189:TYR:CG	2.72	0.42
4:D:81:ARG:HD3	29:c:151:VAL:HG12	2.00	0.42
4:D:211:GLY:HA2	36:D:501:ADP:H5'2	2.02	0.42
5:E:257:LEU:H	5:E:257:LEU:CD2	2.32	0.42
6:F:192:ASP:HA	6:F:195:ILE:HD12	2.01	0.42
6:F:281:SER:OG	6:F:326:VAL:HG13	2.20	0.42
7:G:114:LEU:HD23	7:G:114:LEU:O	2.18	0.42
9:I:136:TYR:CD1	9:I:136:TYR:N	2.87	0.42
10:J:28:LYS:O	10:J:28:LYS:CG	2.68	0.42
18:R:180:ILE:HG22	18:R:181:SER:N	2.35	0.42
21:U:44:LYS:O	21:U:47:VAL:HG22	2.20	0.42
21:U:91:ASN:CB	21:U:97:VAL:HG21	2.49	0.42
21:U:198:LEU:HD22	21:U:223:LEU:HB2	2.02	0.42
22:V:28:PRO:N	22:V:29:PRO:CD	2.83	0.42
23:W:226:TYR:CD1	23:W:226:TYR:C	2.97	0.42
24:X:356:LEU:O	24:X:358:LYS:N	2.53	0.42
25:Y:57:LEU:O	25:Y:61:LEU:O	2.38	0.42
26:Z:267:ARG:O	26:Z:270:VAL:HG12	2.20	0.42
27:a:218:MET:SD	27:a:218:MET:O	2.77	0.42
27:a:323:SER:H	27:a:333:MET:HA	1.85	0.42
29:c:284:LEU:HD23	29:c:284:LEU:C	2.45	0.42
30:d:268:ARG:O	30:d:269:ASP:OD1	2.37	0.42
32:f:94:LYS:N	32:f:95:PRO:CD	2.83	0.42
32:f:184:LEU:O	32:f:188:VAL:HG22	2.19	0.42
32:f:268:LEU:HD23	32:f:268:LEU:H	1.85	0.42
32:f:446:LEU:HD13	32:f:483:PHE:HD2	1.83	0.42
9:i:76:VAL:HG22	9:i:77:ALA:N	2.35	0.42
10:j:75:GLY:CA	10:j:129:ILE:HD12	2.50	0.42
11:k:234:LEU:HA	11:k:237:VAL:HG22	2.02	0.42
12:l:117:GLN:O	12:l:120:THR:HG22	2.20	0.42
20:t:141:MET:HE3	20:t:171:ASP:O	2.20	0.42
1:A:410:LEU:HD12	1:A:411:GLU:N	2.35	0.42
2:B:98:LYS:O	2:B:102:LEU:HG	2.20	0.42
2:B:256:ILE:O	2:B:257:GLN:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ILE:O	2:B:256:ILE:HG22	2.20	0.42
3:C:253:SER:C	3:C:254:ILE:HG13	2.44	0.42
5:E:190:GLN:N	5:E:190:GLN:OE1	2.52	0.42
6:F:83:ASN:OD1	6:F:84:LYS:N	2.53	0.42
8:H:223:PRO:HA	8:H:226:VAL:HG12	2.02	0.42
21:U:550:VAL:HG13	21:U:764:LEU:HD21	2.02	0.42
24:X:391:PRO:CG	24:X:392:PRO:HD3	2.50	0.42
27:a:334:THR:OG1	27:a:335:TRP:N	2.53	0.42
30:d:161:ILE:N	30:d:162:PRO:CD	2.83	0.42
30:d:242:ASN:OD1	30:d:242:ASN:C	2.63	0.42
32:f:75:LEU:HD12	32:f:77:GLU:HG2	2.01	0.42
32:f:84:SER:OG	32:f:115:PRO:HB3	2.20	0.42
32:f:242:GLU:HB2	32:f:243:PRO:HD3	2.02	0.42
32:f:261:ARG:NH2	32:f:295:ALA:HB2	2.35	0.42
32:f:826:GLN:OE1	32:f:826:GLN:N	2.53	0.42
8:h:218:PHE:CD1	8:h:218:PHE:C	2.97	0.42
11:k:55:THR:HG22	11:k:59:MET:HE2	2.02	0.42
1:A:91:GLN:N	1:A:92:PRO:HD2	2.34	0.41
1:A:119:ALA:HB3	1:A:121:PHE:HE1	1.85	0.41
2:B:91:LYS:O	2:B:93:GLU:N	2.53	0.41
3:C:117:ARG:HB3	3:C:122:THR:H	1.84	0.41
4:D:294:ASN:O	4:D:298:GLY:CA	2.68	0.41
4:D:294:ASN:O	4:D:298:GLY:N	2.53	0.41
4:D:371:SER:HB2	4:D:374:ASP:OD2	2.20	0.41
6:F:248:PHE:C	6:F:249:LEU:HD22	2.45	0.41
6:F:427:VAL:HG13	6:F:428:GLN:N	2.35	0.41
17:Q:43:LEU:O	17:Q:104:LEU:HD22	2.20	0.41
20:T:98:ALA:CB	20:T:155:MET:HE1	2.50	0.41
20:T:136:TRP:CE3	20:T:137:LEU:HD22	2.55	0.41
22:V:402:VAL:HG13	22:V:403:ILE:HD12	2.02	0.41
22:V:473:GLN:CD	26:Z:257:MET:SD	3.03	0.41
23:W:420:ASP:OD1	23:W:421:PRO:O	2.38	0.41
24:X:212:MET:HE1	24:X:250:SER:HA	2.02	0.41
24:X:222:GLU:O	24:X:222:GLU:CD	2.63	0.41
25:Y:70:LEU:HD22	25:Y:73:MET:HE2	2.02	0.41
28:b:143:PHE:CE1	28:b:183:LEU:HD22	2.55	0.41
7:g:180:GLU:HA	7:g:183:VAL:HG12	2.01	0.41
8:h:41:ALA:HB3	8:h:183:GLU:HA	2.02	0.41
9:i:155:ASN:OD1	9:i:156:TYR:N	2.53	0.41
11:k:217:LEU:CD2	11:k:230:THR:HG21	2.50	0.41
12:l:146:GLN:OE1	12:l:159:MET:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:CD1	2:B:48:LYS:CE	2.81	0.41
35:B:501:ATP:O3'	35:B:501:ATP:PA	2.78	0.41
3:C:113:ARG:NH2	3:C:129:ASN:O	2.53	0.41
3:C:138:MET:O	3:C:139:MET:C	2.63	0.41
4:D:167:ILE:C	36:D:501:ADP:HN62	2.28	0.41
6:F:150:LEU:HD23	6:F:150:LEU:C	2.45	0.41
11:K:165:CYS:SG	12:L:57:ALA:CB	3.08	0.41
21:U:381:THR:HG22	21:U:412:HIS:CG	2.54	0.41
23:W:16:MET:HE1	23:W:26:GLN:OE1	2.20	0.41
23:W:406:VAL:HA	23:W:413:ILE:HA	2.02	0.41
25:Y:59:LYS:HZ2	25:Y:59:LYS:C	2.28	0.41
25:Y:334:LEU:HD23	25:Y:343:LEU:HD21	2.03	0.41
25:Y:350:VAL:HG13	25:Y:351:ASN:N	2.35	0.41
28:b:62:THR:HG22	28:b:74:LYS:CD	2.50	0.41
32:f:846:VAL:O	32:f:846:VAL:CG1	2.67	0.41
15:o:102:ILE:HD13	15:o:126:LEU:HD21	2.01	0.41
19:s:80:ILE:HD11	19:s:136:ASN:HB3	2.01	0.41
34:u:407:LYS:HE2	34:u:411:ASP:OD2	2.20	0.41
1:A:127:ASP:OD1	1:A:127:ASP:N	2.53	0.41
2:B:67:ARG:NH2	2:B:71:TYR:OH	2.51	0.41
2:B:294:ARG:O	2:B:294:ARG:HG3	2.20	0.41
5:E:55:GLN:C	5:E:56:ILE:HD13	2.45	0.41
6:F:424:ILE:O	6:F:427:VAL:HG12	2.19	0.41
7:G:31:ALA:HA	13:M:19:GLY:O	2.21	0.41
9:I:21:VAL:O	9:I:25:MET:HG3	2.19	0.41
11:K:117:SER:OG	11:K:156:MET:HE3	2.19	0.41
12:L:158:ALA:HB1	12:L:172:LEU:HD13	2.03	0.41
15:O:230:ARG:CB	15:O:231:PRO:HD3	2.51	0.41
21:U:42:VAL:HA	21:U:45:ILE:HG22	2.01	0.41
21:U:355:ASN:O	21:U:358:ASP:OD1	2.38	0.41
22:V:218:TYR:O	22:V:221:LEU:N	2.53	0.41
22:V:415:SER:O	22:V:459:GLN:O	2.38	0.41
25:Y:297:ARG:NH1	31:e:48:VAL:O	2.53	0.41
27:a:113:LEU:HA	27:a:151:VAL:HG23	2.01	0.41
27:a:234:ILE:HA	27:a:237:LEU:HD12	2.01	0.41
27:a:290:GLN:O	27:a:290:GLN:CG	2.68	0.41
32:f:162:LEU:O	32:f:166:VAL:HG22	2.19	0.41
32:f:372:LEU:CD2	32:f:797:LEU:HD13	2.50	0.41
32:f:692:LEU:HD22	32:f:712:LYS:NZ	2.35	0.41
32:f:869:THR:HG23	32:f:884:THR:HA	2.02	0.41
9:i:13:SER:HG	9:i:16:GLY:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:k:44:GLU:O	11:k:222:PRO:CD	2.68	0.41
11:k:140:ALA:O	11:k:170:ILE:HD12	2.20	0.41
12:l:180:MET:HA	12:l:180:MET:HE3	2.02	0.41
13:m:34:SER:OG	13:m:35:SER:N	2.53	0.41
16:p:30:ILE:HD12	16:p:35:VAL:HG21	2.02	0.41
18:r:250:ASN:OD1	18:r:251:VAL:N	2.53	0.41
3:C:132:ASP:CB	3:C:133:PRO:HD3	2.50	0.41
9:I:44:LEU:CD2	9:I:189:ALA:HB1	2.50	0.41
11:K:31:ILE:C	11:K:31:ILE:HD12	2.45	0.41
17:Q:172:ILE:HG22	17:q:173:LEU:HG	2.01	0.41
21:U:31:VAL:HG13	21:U:32:ASN:N	2.35	0.41
21:U:92:ASP:OD1	21:U:92:ASP:N	2.52	0.41
22:V:148:ARG:HB3	22:V:149:PRO:HD3	2.03	0.41
23:W:448:LYS:O	23:W:452:ILE:HG23	2.21	0.41
24:X:194:ARG:CG	24:X:210:LEU:HD21	2.50	0.41
27:a:148:VAL:HG13	27:a:149:THR:N	2.35	0.41
28:b:12:ASN:HA	28:b:80:PRO:HB3	2.03	0.41
29:c:192:LEU:O	29:c:196:LEU:HD12	2.19	0.41
7:g:236:ASP:OD1	7:g:237:ALA:N	2.54	0.41
8:h:29:VAL:HG11	8:h:133:SER:CB	2.51	0.41
8:h:168:VAL:HG13	8:h:169:ASN:N	2.35	0.41
9:i:171:ALA:HB2	9:i:200:THR:HG21	2.03	0.41
13:m:76:MET:HE3	13:m:78:VAL:HG22	2.00	0.41
2:B:209:GLU:N	32:f:722:SER:OG	2.52	0.41
3:C:197:THR:CB	3:C:247:PHE:HZ	2.32	0.41
3:C:198:LEU:HD23	35:C:501:ATP:N3	2.33	0.41
4:D:122:GLU:H	4:D:122:GLU:CD	2.25	0.41
8:H:141:GLU:O	8:H:141:GLU:CD	2.63	0.41
12:L:237:GLU:OE1	12:L:238:GLU:N	2.54	0.41
16:P:45:MET:HE1	16:P:68:LYS:HD2	2.02	0.41
17:Q:38:MET:HE2	17:Q:64:VAL:HG21	2.01	0.41
18:R:197:VAL:HG11	18:R:218:ALA:HA	2.02	0.41
20:T:136:TRP:HE3	20:T:137:LEU:HD22	1.85	0.41
21:U:199:ARG:HA	21:U:202:VAL:HG22	2.03	0.41
22:V:232:HIS:HA	22:V:235:LEU:HG	2.03	0.41
22:V:486:ILE:HG21	25:Y:377:LEU:HD21	2.01	0.41
23:W:227:TYR:O	23:W:228:ASN:C	2.63	0.41
24:X:378:LEU:O	24:X:379:ASP:HB3	2.21	0.41
25:Y:41:LEU:HD13	25:Y:41:LEU:O	2.19	0.41
28:b:18:ASN:O	28:b:25:ARG:CG	2.68	0.41
28:b:22:LEU:CB	28:b:23:PRO:CD	2.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:b:113:VAL:O	28:b:142:ASN:HA	2.21	0.41
29:c:222:LYS:O	29:c:228:GLY:HA3	2.21	0.41
30:d:147:ILE:O	30:d:151:GLY:N	2.54	0.41
32:f:185:LEU:O	32:f:189:LYS:N	2.42	0.41
32:f:706:ILE:CG2	32:f:787:LEU:HD22	2.50	0.41
10:j:38:ARG:O	10:j:39:ASP:OD1	2.38	0.41
13:m:109:LEU:HD23	13:m:148:GLN:HB2	2.01	0.41
15:o:141:LEU:N	15:o:170:MET:HE1	2.35	0.41
16:p:58:THR:HG23	16:p:59:ASP:N	2.33	0.41
19:s:76:ASP:OD1	19:s:76:ASP:C	2.64	0.41
2:B:143:LEU:O	2:B:163:LEU:CD1	2.66	0.41
2:B:156:VAL:O	2:B:156:VAL:HG22	2.21	0.41
3:C:346:LYS:O	3:C:350:LEU:HG	2.19	0.41
3:C:380:GLN:HG2	3:C:381:GLU:N	2.35	0.41
5:E:270:LEU:HD22	5:E:270:LEU:N	2.35	0.41
7:G:19:GLU:O	7:G:20:GLY:C	2.64	0.41
14:N:111:HIS:CD2	14:N:154:MET:HE1	2.55	0.41
14:N:141:GLU:OE2	14:N:156:ARG:NH2	2.54	0.41
19:S:41:LEU:HD23	19:S:165:ALA:HB2	2.02	0.41
21:U:98:GLU:CD	21:U:99:THR:HG23	2.46	0.41
21:U:608:SER:O	21:U:609:ASP:C	2.64	0.41
21:U:772:TRP:CE2	21:U:774:PRO:HG2	2.52	0.41
22:V:176:MET:O	22:V:180:ARG:HG2	2.20	0.41
22:V:231:LEU:HD21	22:V:247:GLN:O	2.21	0.41
22:V:345:ARG:HD3	22:V:349:ARG:H	1.84	0.41
23:W:243:ILE:HA	23:W:246:HIS:CD2	2.56	0.41
24:X:412:ASP:OD1	24:X:412:ASP:C	2.64	0.41
24:X:414:LEU:HD22	25:Y:383:LEU:HD11	2.02	0.41
25:Y:63:TRP:O	25:Y:64:GLN:C	2.62	0.41
27:a:187:ASP:OD1	27:a:187:ASP:N	2.53	0.41
29:c:221:HIS:HA	29:c:225:TRP:HB2	2.01	0.41
32:f:24:THR:HG23	32:f:25:ASP:N	2.35	0.41
32:f:379:GLY:CA	32:f:417:ILE:HD11	2.49	0.41
6:F:249:LEU:HB2	6:F:283:ILE:HA	2.03	0.41
10:J:144:LEU:CD2	10:J:156:TRP:HB2	2.51	0.41
11:K:126:GLU:O	11:K:126:GLU:HG2	2.19	0.41
15:O:143:LEU:O	15:O:153:LEU:HD12	2.21	0.41
20:T:88:MET:HE2	20:T:88:MET:HB3	2.01	0.41
22:V:348:PHE:O	22:V:349:ARG:C	2.64	0.41
23:W:190:MET:HA	23:W:205:ILE:HD13	2.02	0.41
23:W:205:ILE:O	23:W:208:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:X:92:LEU:HA	24:X:95:LEU:HD12	2.03	0.41
24:X:257:CYS:HA	24:X:260:MET:HG2	2.02	0.41
25:Y:34:ASP:OD1	25:Y:35:ALA:N	2.53	0.41
27:a:106:SER:O	27:a:107:SER:C	2.63	0.41
27:a:217:LEU:O	27:a:222:LEU:HD11	2.20	0.41
27:a:266:ALA:O	27:a:269:LEU:HG	2.21	0.41
28:b:129:LYS:O	28:b:133:LYS:HG2	2.21	0.41
32:f:205:CYS:O	32:f:209:MET:O	2.39	0.41
32:f:560:LEU:CD2	32:f:782:HIS:HD2	2.23	0.41
7:g:233:ALA:HA	7:g:236:ASP:OD2	2.20	0.41
8:h:72:ILE:HG21	8:h:110:LEU:HD23	2.02	0.41
14:n:89:VAL:HG13	14:n:120:MET:CE	2.50	0.41
15:o:98:THR:HG23	15:o:99:THR:N	2.35	0.41
16:p:51:ILE:O	16:p:51:ILE:HG13	2.19	0.41
19:s:111:MET:HE3	19:s:116:ILE:HG13	2.02	0.41
1:A:345:LEU:H	1:A:345:LEU:HD12	1.84	0.41
5:E:217:GLU:O	5:E:220:ASN:OD1	2.39	0.41
11:K:119:LEU:O	11:K:119:LEU:HD12	2.21	0.41
12:L:26:MET:SD	12:L:148:CYS:SG	3.18	0.41
12:L:36:VAL:HG12	12:L:37:GLY:N	2.35	0.41
21:U:103:LYS:HA	21:U:106:ASP:OD2	2.21	0.41
21:U:193:PHE:O	21:U:197:VAL:HG22	2.21	0.41
21:U:645:ASN:OD1	21:U:645:ASN:C	2.63	0.41
21:U:757:MET:HG3	21:U:758:PRO:HD3	2.02	0.41
21:U:809:SER:OG	21:U:810:THR:N	2.53	0.41
23:W:243:ILE:HG13	23:W:244:CYS:N	2.35	0.41
23:W:373:ILE:O	23:W:413:ILE:HG13	2.21	0.41
25:Y:116:ASP:OD1	25:Y:117:LYS:N	2.50	0.41
25:Y:235:ASP:N	25:Y:235:ASP:OD1	2.53	0.41
26:Z:283:ARG:O	26:Z:284:ASP:C	2.62	0.41
29:c:151:VAL:HG13	29:c:152:LYS:N	2.36	0.41
32:f:645:ASP:OD1	32:f:645:ASP:C	2.64	0.41
7:g:141:ILE:HG22	7:g:151:VAL:HG22	2.02	0.41
12:l:230:SER:N	12:l:231:PRO:HD2	2.36	0.41
13:m:78:VAL:HG22	13:m:136:PHE:HB3	2.03	0.41
18:r:133:ILE:HD11	18:r:137:ALA:CB	2.51	0.41
1:A:21:PRO:HB2	1:A:22:ILE:H	1.66	0.41
1:A:56:LEU:HD21	2:B:48:LYS:HG3	2.02	0.41
1:A:220:THR:HG21	1:A:343:PHE:O	2.21	0.41
2:B:74:MET:CE	32:f:613:LEU:HD13	2.50	0.41
2:B:395:ILE:HA	2:B:398:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:233:GLU:O	3:C:236:VAL:HG12	2.21	0.41
5:E:49:ALA:HB1	6:F:136:VAL:HG11	2.03	0.41
5:E:259:GLU:O	5:E:263:GLN:OE1	2.38	0.41
7:G:93:ARG:O	7:G:97:GLU:HG2	2.20	0.41
9:I:151:ASP:OD2	9:I:155:ASN:O	2.39	0.41
13:M:188:ARG:HA	13:M:216:TRP:HH2	1.86	0.41
14:N:148:VAL:O	14:N:148:VAL:HG12	2.21	0.41
17:Q:137:PHE:HB3	18:r:192:VAL:HG21	2.03	0.41
18:R:73:VAL:O	18:R:73:VAL:HG13	2.20	0.41
18:R:85:ILE:O	18:R:85:ILE:HG22	2.21	0.41
19:S:41:LEU:HD22	19:S:42:ALA:H	1.85	0.41
20:T:54:THR:O	20:T:86:ARG:NH2	2.54	0.41
21:U:9:ILE:HG22	21:U:37:GLU:OE2	2.21	0.41
21:U:43:ASP:O	21:U:46:GLU:HG3	2.21	0.41
21:U:106:ASP:OD1	21:U:106:ASP:C	2.63	0.41
21:U:699:THR:OG1	21:U:702:THR:HG23	2.20	0.41
22:V:95:LEU:O	22:V:96:ARG:C	2.64	0.41
22:V:157:THR:N	22:V:158:PRO:HD3	2.36	0.41
22:V:319:HIS:O	22:V:320:THR:C	2.63	0.41
23:W:79:GLU:O	23:W:83:LEU:HD23	2.21	0.41
23:W:116:THR:HG23	23:W:119:PRO:CD	2.51	0.41
23:W:427:ASP:OD1	23:W:430:GLN:NE2	2.54	0.41
23:W:430:GLN:HG2	23:W:431:LYS:N	2.35	0.41
25:Y:18:ARG:O	25:Y:22:LEU:HD23	2.21	0.41
25:Y:246:ILE:HG22	25:Y:250:LEU:HD23	2.03	0.41
26:Z:213:GLU:O	26:Z:217:THR:N	2.54	0.41
27:a:291:LEU:O	27:a:330:ARG:HA	2.20	0.41
28:b:33:VAL:HA	28:b:36:VAL:HG12	2.02	0.41
29:c:149:GLN:HA	29:c:154:LYS:HG2	2.03	0.41
32:f:183:PRO:O	32:f:187:LEU:HD23	2.21	0.41
32:f:205:CYS:SG	32:f:206:ASP:N	2.94	0.41
32:f:288:VAL:HG22	32:f:881:GLU:HB2	2.03	0.41
32:f:434:TYR:O	32:f:434:TYR:CD2	2.74	0.41
32:f:470:VAL:CG1	32:f:504:VAL:HG21	2.50	0.41
32:f:732:VAL:O	32:f:732:VAL:CG1	2.68	0.41
12:l:160:SER:O	12:l:161:ILE:HD13	2.20	0.41
13:m:67:LEU:HD13	13:m:215:SER:HG	1.83	0.41
20:t:96:LEU:HD11	20:t:155:MET:HG3	2.02	0.41
1:A:143:ASP:O	1:A:147:TYR:N	2.50	0.41
1:A:148:GLN:O	1:A:150:HIS:ND1	2.54	0.41
1:A:166:VAL:HG13	1:A:167:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ILE:HD13	1:A:315:ILE:N	2.36	0.41
2:B:191:ASP:O	2:B:194:ILE:HG13	2.20	0.41
2:B:294:ARG:NE	2:B:294:ARG:HA	2.36	0.41
2:B:306:GLN:O	2:B:310:LEU:HG	2.20	0.41
4:D:202:VAL:HG23	4:D:329:ARG:O	2.21	0.41
4:D:264:ILE:CD1	5:E:255:ARG:NH2	2.84	0.41
4:D:392:TYR:CD1	4:D:393:ILE:N	2.88	0.41
5:E:153:LEU:HD22	5:E:191:LEU:HD11	2.03	0.41
6:F:320:PHE:CG	6:F:321:GLN:N	2.89	0.41
8:H:65:VAL:O	8:H:65:VAL:HG23	2.21	0.41
9:I:133:SER:HB3	9:I:152:PRO:HD3	2.02	0.41
12:L:196:ARG:HB2	12:L:205:LEU:HD12	2.03	0.41
15:O:226:LEU:HD12	15:O:227:ASP:N	2.35	0.41
19:S:83:SER:OG	19:S:84:GLY:N	2.54	0.41
21:U:50:GLU:HG2	21:U:50:GLU:O	2.19	0.41
21:U:151:ILE:HG13	21:U:152:GLY:N	2.36	0.41
21:U:226:PRO:HA	21:U:229:VAL:HG12	2.03	0.41
22:V:137:GLU:N	22:V:138:PRO:CD	2.84	0.41
24:X:405:GLN:NE2	29:c:265:MET:HE1	2.36	0.41
24:X:413:SER:CB	26:Z:280:ILE:HD11	2.51	0.41
25:Y:116:ASP:OD1	25:Y:116:ASP:N	2.53	0.41
25:Y:191:ILE:HG22	25:Y:193:ASP:H	1.86	0.41
27:a:300:ALA:O	27:a:302:ILE:HG23	2.20	0.41
27:a:343:LEU:HG	27:a:344:GLN:H	1.86	0.41
29:c:63:ASP:O	29:c:66:THR:O	2.39	0.41
32:f:130:ALA:O	32:f:134:SER:HB2	2.21	0.41
32:f:249:LEU:HD12	32:f:250:ARG:N	2.35	0.41
9:i:40:ASN:H	9:i:184:MET:CB	2.34	0.41
12:l:199:LEU:HB2	12:l:200:PRO:HD2	2.02	0.41
18:r:241:ASP:OD1	18:r:241:ASP:C	2.64	0.41
19:s:58:SER:HB2	19:s:62:SER:O	2.20	0.41
3:C:42:LEU:CD2	3:C:45:LEU:HD21	2.44	0.40
4:D:344:ILE:CD1	36:D:501:ADP:H2	2.35	0.40
5:E:76:GLY:N	5:E:77:PRO:CD	2.83	0.40
6:F:121:CYS:N	6:F:137:ILE:HD12	2.36	0.40
7:G:38:THR:HG22	7:G:39:SER:N	2.37	0.40
14:N:71:ILE:O	14:N:71:ILE:HG22	2.20	0.40
14:N:122:TYR:O	14:N:125:ARG:HG3	2.21	0.40
16:P:117:PHE:CD2	16:P:119:PRO:HD3	2.56	0.40
17:Q:118:MET:O	17:Q:132:HIS:HE1	2.03	0.40
20:T:238:THR:HG22	20:T:239:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:17:GLU:OE2	23:W:18:VAL:HG13	2.22	0.40
23:W:87:ILE:O	23:W:88:MET:C	2.64	0.40
23:W:131:VAL:O	23:W:131:VAL:HG13	2.21	0.40
24:X:339:ILE:HG23	24:X:340:GLU:N	2.36	0.40
25:Y:191:ILE:N	25:Y:191:ILE:HD12	2.36	0.40
28:b:109:ILE:HB	28:b:138:VAL:HG22	2.02	0.40
30:d:265:ASP:OD1	30:d:266:THR:HG23	2.21	0.40
32:f:259:PHE:N	32:f:259:PHE:CD1	2.89	0.40
32:f:431:LYS:HE3	32:f:432:TYR:CZ	2.57	0.40
32:f:745:LEU:N	32:f:745:LEU:HD22	2.36	0.40
11:k:229:PHE:O	11:k:230:THR:C	2.64	0.40
13:m:36:THR:OG1	13:m:37:ALA:N	2.53	0.40
14:n:153:MET:HE3	20:t:102:TYR:HD2	1.85	0.40
1:A:63:THR:HA	2:B:79:ILE:CD1	2.51	0.40
1:A:214:LEU:N	1:A:319:MET:O	2.42	0.40
2:B:255:LEU:HD22	2:B:255:LEU:N	2.37	0.40
2:B:290:ILE:HD12	2:B:309:MET:HG3	2.04	0.40
2:B:364:ILE:O	2:B:368:HIS:HD2	2.01	0.40
4:D:49:GLN:O	4:D:52:GLU:HG3	2.22	0.40
4:D:253:LEU:HA	4:D:256:GLU:HB3	2.03	0.40
5:E:304:PRO:HG2	5:E:338:PHE:O	2.21	0.40
6:F:90:VAL:CG2	6:F:150:LEU:CD2	2.99	0.40
6:F:279:ALA:HB3	6:F:280:PRO:HD3	2.03	0.40
11:K:186:HIS:O	11:K:189:MET:HG3	2.20	0.40
12:L:157:ARG:CZ	12:L:176:MET:HE2	2.51	0.40
16:P:117:PHE:O	16:P:118:LYS:C	2.63	0.40
16:P:142:CYS:O	16:P:146:MET:HE2	2.21	0.40
21:U:665:ASN:C	21:U:667:GLU:H	2.29	0.40
21:U:892:LEU:C	21:U:892:LEU:HD12	2.47	0.40
22:V:449:ALA:C	22:V:450:SER:HG	2.25	0.40
22:V:459:GLN:HB3	22:V:461:LYS:HD3	2.03	0.40
23:W:443:THR:O	23:W:446:ILE:HG12	2.22	0.40
24:X:413:SER:HB2	26:Z:280:ILE:HD11	2.02	0.40
26:Z:238:PRO:CG	27:a:286:ALA:HB2	2.51	0.40
26:Z:240:VAL:HG12	26:Z:241:SER:N	2.37	0.40
7:g:101:TRP:CD1	7:g:101:TRP:C	3.00	0.40
7:g:109:ILE:O	7:g:109:ILE:HG23	2.21	0.40
7:g:118:ILE:HA	7:g:121:ILE:HG12	2.03	0.40
7:g:163:PHE:HD2	7:g:166:THR:HG21	1.86	0.40
8:h:97:TYR:CD1	8:h:97:TYR:C	2.99	0.40
14:n:37:ILE:HG13	14:n:133:ILE:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:t:124:ASP:OD1	20:t:125:GLY:N	2.54	0.40
2:B:434:THR:HG21	9:I:17:ARG:HH21	1.86	0.40
3:C:286:THR:OG1	3:C:287:LYS:N	2.52	0.40
3:C:351:MET:N	3:C:352:PRO:HD3	2.36	0.40
7:G:215:ILE:HD11	7:G:235:ILE:HD11	2.03	0.40
9:I:79:ILE:N	9:I:79:ILE:HD13	2.36	0.40
10:J:168:VAL:HG23	10:J:198:VAL:HG21	2.04	0.40
13:M:207:ASP:O	13:M:208:LYS:HB2	2.21	0.40
21:U:36:ALA:HA	21:U:39:SER:HB3	2.04	0.40
25:Y:53:TYR:O	25:Y:63:TRP:CH2	2.74	0.40
25:Y:111:LEU:O	25:Y:115:GLY:N	2.44	0.40
27:a:18:GLN:N	27:a:19:PRO:HD2	2.37	0.40
27:a:245:VAL:CG1	27:a:246:GLU:N	2.85	0.40
28:b:13:SER:O	28:b:16:MET:N	2.54	0.40
28:b:62:THR:OG1	28:b:63:THR:N	2.53	0.40
28:b:148:VAL:O	28:b:149:ASN:C	2.63	0.40
28:b:154:THR:O	28:b:157:VAL:HB	2.21	0.40
32:f:94:LYS:N	32:f:95:PRO:HD2	2.35	0.40
12:l:46:LEU:HD22	12:l:135:ALA:HB3	2.02	0.40
14:n:48:LEU:HD12	14:n:48:LEU:N	2.36	0.40
14:n:153:MET:HE3	20:t:102:TYR:CD2	2.57	0.40
18:r:95:GLU:OE1	18:r:101:LEU:HD21	2.20	0.40
1:A:111:TYR:O	1:A:122:VAL:HA	2.21	0.40
3:C:116:LEU:HD13	3:C:116:LEU:C	2.47	0.40
4:D:54:LEU:C	4:D:54:LEU:HD13	2.46	0.40
5:E:342:ASP:O	5:E:346:VAL:HG23	2.21	0.40
8:H:12:THR:O	8:H:19:LEU:CD2	2.69	0.40
11:K:180:SER:HB3	11:K:201:ILE:HD12	2.02	0.40
14:N:46:VAL:HG11	14:N:144:GLN:O	2.22	0.40
16:P:14:MET:HG3	16:P:136:PHE:HB3	2.02	0.40
17:Q:13:VAL:HG23	17:Q:183:ILE:HB	2.03	0.40
20:T:115:MET:HE1	20:T:136:TRP:CZ2	2.57	0.40
21:U:24:LEU:HD12	21:U:59:PHE:CD2	2.56	0.40
21:U:233:LEU:HD11	21:U:249:CYS:SG	2.61	0.40
24:X:161:ASP:O	24:X:163:LYS:N	2.54	0.40
27:a:112:ILE:CG2	27:a:151:VAL:HG21	2.49	0.40
28:b:4:GLU:N	28:b:47:ASN:OD1	2.46	0.40
29:c:259:VAL:HG11	29:c:287:HIS:HE1	1.87	0.40
29:c:293:THR:O	29:c:297:VAL:HG23	2.21	0.40
29:c:306:THR:HB	30:d:331:PRO:HA	2.04	0.40
32:f:7:ASP:O	32:f:11:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:685:THR:HA	32:f:689:ALA:HB3	2.02	0.40
13:m:73:HIS:ND1	13:m:73:HIS:O	2.55	0.40
3:C:365:GLU:OE1	3:C:366:ALA:N	2.54	0.40
4:D:270:ILE:O	4:D:289:LEU:HD12	2.21	0.40
5:E:266:GLY:O	5:E:269:THR:HG23	2.22	0.40
6:F:339:ASP:N	6:F:339:ASP:OD1	2.53	0.40
9:I:185:THR:O	9:I:187:LYS:N	2.55	0.40
10:J:2:SER:CB	10:J:11:SER:HA	2.52	0.40
11:K:51:GLU:HB2	11:K:206:MET:HE3	2.03	0.40
12:L:118:ILE:HB	12:L:119:PRO:HD3	2.04	0.40
12:L:168:ALA:HB2	12:L:198:THR:OG1	2.22	0.40
15:O:230:ARG:HB2	15:O:231:PRO:HD3	2.03	0.40
21:U:38:ILE:CD1	21:U:67:VAL:HG22	2.52	0.40
22:V:377:GLN:O	22:V:380:ASP:OD1	2.39	0.40
23:W:164:SER:O	23:W:167:GLN:HG2	2.22	0.40
23:W:361:HIS:O	23:W:365:ILE:HG12	2.21	0.40
24:X:69:LEU:O	24:X:73:VAL:HG22	2.21	0.40
24:X:123:THR:HG23	24:X:124:PHE:N	2.36	0.40
24:X:391:PRO:N	24:X:392:PRO:CD	2.85	0.40
25:Y:275:LEU:HA	25:Y:278:VAL:HG12	2.04	0.40
25:Y:342:ARG:O	25:Y:343:LEU:HB3	2.21	0.40
25:Y:381:GLN:O	25:Y:385:ARG:HG2	2.21	0.40
26:Z:36:VAL:HG13	26:Z:94:TRP:HE3	1.86	0.40
26:Z:189:GLN:N	29:c:234:TYR:OH	2.55	0.40
26:Z:233:VAL:O	26:Z:236:LEU:HD23	2.22	0.40
27:a:87:MET:SD	27:a:93:ALA:C	3.05	0.40
27:a:353:LEU:O	27:a:355:PHE:N	2.50	0.40
32:f:190:GLU:O	32:f:194:TYR:HA	2.21	0.40
32:f:744:MET:O	32:f:748:LEU:HB3	2.22	0.40
11:k:70:ILE:HD12	11:k:92:ALA:HB3	2.03	0.40
11:k:96:THR:HG22	11:k:112:VAL:HG22	2.03	0.40
12:l:42:THR:HG1	12:l:43:HIS:CE1	2.25	0.40
12:l:118:ILE:N	12:l:119:PRO:CD	2.85	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	412/433 (95%)	361 (88%)	45 (11%)	6 (2%)	8 33
2	B	399/440 (91%)	339 (85%)	50 (12%)	10 (2%)	4 24
3	C	368/406 (91%)	311 (84%)	54 (15%)	3 (1%)	16 45
4	D	378/418 (90%)	313 (83%)	60 (16%)	5 (1%)	9 35
5	E	306/389 (79%)	274 (90%)	31 (10%)	1 (0%)	36 66
6	F	323/439 (74%)	296 (92%)	26 (8%)	1 (0%)	36 66
7	G	237/246 (96%)	219 (92%)	18 (8%)	0	100 100
7	g	233/246 (95%)	222 (95%)	10 (4%)	1 (0%)	30 60
8	H	228/234 (97%)	205 (90%)	21 (9%)	2 (1%)	14 43
8	h	225/234 (96%)	212 (94%)	13 (6%)	0	100 100
9	I	245/261 (94%)	227 (93%)	18 (7%)	0	100 100
9	i	244/261 (94%)	222 (91%)	21 (9%)	1 (0%)	30 60
10	J	237/248 (96%)	216 (91%)	19 (8%)	2 (1%)	16 45
10	j	229/248 (92%)	214 (93%)	14 (6%)	1 (0%)	30 60
11	K	235/241 (98%)	217 (92%)	18 (8%)	0	100 100
11	k	223/241 (92%)	212 (95%)	11 (5%)	0	100 100
12	L	236/263 (90%)	223 (94%)	13 (6%)	0	100 100
12	l	235/263 (89%)	226 (96%)	9 (4%)	0	100 100
13	M	239/255 (94%)	225 (94%)	14 (6%)	0	100 100
13	m	238/255 (93%)	219 (92%)	19 (8%)	0	100 100
14	N	198/239 (83%)	181 (91%)	16 (8%)	1 (0%)	24 56
14	n	199/239 (83%)	182 (92%)	17 (8%)	0	100 100
15	O	219/277 (79%)	201 (92%)	17 (8%)	1 (0%)	24 56
15	o	218/277 (79%)	207 (95%)	11 (5%)	0	100 100
16	P	202/205 (98%)	186 (92%)	16 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	p	202/205 (98%)	188 (93%)	14 (7%)	0	100	100
17	Q	195/201 (97%)	182 (93%)	13 (7%)	0	100	100
17	q	195/201 (97%)	185 (95%)	10 (5%)	0	100	100
18	R	199/263 (76%)	190 (96%)	9 (4%)	0	100	100
18	r	198/263 (75%)	187 (94%)	11 (6%)	0	100	100
19	S	211/241 (88%)	202 (96%)	9 (4%)	0	100	100
19	s	210/241 (87%)	199 (95%)	11 (5%)	0	100	100
20	T	213/264 (81%)	200 (94%)	13 (6%)	0	100	100
20	t	213/264 (81%)	199 (93%)	14 (7%)	0	100	100
21	U	795/953 (83%)	725 (91%)	68 (9%)	2 (0%)	36	66
22	V	408/534 (76%)	351 (86%)	56 (14%)	1 (0%)	43	72
23	W	454/456 (100%)	401 (88%)	51 (11%)	2 (0%)	30	60
24	X	377/422 (89%)	344 (91%)	29 (8%)	4 (1%)	11	40
25	Y	377/389 (97%)	329 (87%)	47 (12%)	1 (0%)	36	66
26	Z	285/324 (88%)	236 (83%)	49 (17%)	0	100	100
27	a	371/376 (99%)	308 (83%)	59 (16%)	4 (1%)	11	40
28	b	187/377 (50%)	163 (87%)	23 (12%)	1 (0%)	24	56
29	c	268/310 (86%)	238 (89%)	30 (11%)	0	100	100
30	d	224/350 (64%)	197 (88%)	25 (11%)	2 (1%)	14	43
31	e	34/70 (49%)	25 (74%)	7 (21%)	2 (6%)	1	9
32	f	875/908 (96%)	746 (85%)	122 (14%)	7 (1%)	16	45
34	u	35/491 (7%)	35 (100%)	0	0	100	100
All	All	13032/15361 (85%)	11740 (90%)	1231 (9%)	61 (0%)	26	56

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	43	PRO
2	B	88	LEU
2	B	92	GLN
2	B	162	VAL
3	C	219	LEU
4	D	236	VAL
5	E	143	ARG

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Mol	Chain	Res	Type
8	H	16	SER
8	H	233	ILE
10	J	52	LYS
21	U	399	TRP
21	U	809	SER
22	V	443	ARG
23	W	368	LYS
24	X	45	VAL
24	X	377	ILE
27	a	317	VAL
30	d	220	ILE
31	e	8	VAL
32	f	279	GLU
9	i	107	CYS
1	A	22	ILE
1	A	82	ALA
1	A	430	MET
2	B	135	ILE
3	C	196	LYS
4	D	272	THR
4	D	413	GLU
6	F	231	THR
24	X	382	GLU
27	a	242	SER
28	b	22	LEU
31	e	7	PRO
32	f	107	LYS
32	f	305	LEU
32	f	508	SER
10	j	99	GLU
1	A	21	PRO
1	A	423	PHE
2	B	93	GLU
32	f	308	SER
32	f	844	VAL
1	A	81	ALA
4	D	274	ARG
10	J	213	ARG
23	W	92	LYS
27	a	244	ASN
30	d	309	VAL
2	B	46	ALA

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Mol	Chain	Res	Type
2	B	137	SER
2	B	278	ALA
2	B	319	PHE
27	a	148	VAL
3	C	232	ARG
24	X	387	ILE
32	f	304	PHE
7	g	134	LEU
14	N	233	VAL
25	Y	350	VAL
4	D	303	VAL
15	O	216	ILE

5.3.2 Protein sidechains (i)

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	302/372 (81%)	301 (100%)	1 (0%)	86	85
2	B	284/385 (74%)	283 (100%)	1 (0%)	84	83
3	C	268/352 (76%)	267 (100%)	1 (0%)	84	83
4	D	263/366 (72%)	263 (100%)	0	100	100
5	E	228/341 (67%)	228 (100%)	0	100	100
6	F	233/379 (62%)	233 (100%)	0	100	100
7	G	187/210 (89%)	187 (100%)	0	100	100
7	g	183/210 (87%)	183 (100%)	0	100	100
8	H	175/191 (92%)	174 (99%)	1 (1%)	78	80
8	h	162/191 (85%)	161 (99%)	1 (1%)	78	80
9	I	195/221 (88%)	195 (100%)	0	100	100
9	i	183/221 (83%)	183 (100%)	0	100	100
10	J	189/211 (90%)	188 (100%)	1 (0%)	81	82
10	j	143/211 (68%)	142 (99%)	1 (1%)	76	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	188/203 (93%)	188 (100%)	0	100	100
11	k	174/203 (86%)	174 (100%)	0	100	100
12	L	197/224 (88%)	197 (100%)	0	100	100
12	l	194/224 (87%)	193 (100%)	1 (0%)	81	82
13	M	186/212 (88%)	186 (100%)	0	100	100
13	m	186/212 (88%)	186 (100%)	0	100	100
14	N	151/181 (83%)	150 (99%)	1 (1%)	76	79
14	n	151/181 (83%)	151 (100%)	0	100	100
15	O	174/228 (76%)	174 (100%)	0	100	100
15	o	173/228 (76%)	172 (99%)	1 (1%)	78	80
16	P	163/174 (94%)	163 (100%)	0	100	100
16	p	170/174 (98%)	169 (99%)	1 (1%)	78	80
17	Q	163/171 (95%)	162 (99%)	1 (1%)	78	80
17	q	161/171 (94%)	158 (98%)	3 (2%)	50	68
18	R	150/202 (74%)	150 (100%)	0	100	100
18	r	152/202 (75%)	151 (99%)	1 (1%)	76	79
19	S	170/199 (85%)	170 (100%)	0	100	100
19	s	171/199 (86%)	171 (100%)	0	100	100
20	T	176/215 (82%)	176 (100%)	0	100	100
20	t	172/215 (80%)	172 (100%)	0	100	100
21	U	575/816 (70%)	573 (100%)	2 (0%)	86	85
22	V	283/460 (62%)	283 (100%)	0	100	100
23	W	326/416 (78%)	325 (100%)	1 (0%)	86	85
24	X	272/362 (75%)	271 (100%)	1 (0%)	84	83
25	Y	302/344 (88%)	300 (99%)	2 (1%)	76	79
26	Z	203/295 (69%)	203 (100%)	0	100	100
27	a	250/336 (74%)	250 (100%)	0	100	100
28	b	136/312 (44%)	136 (100%)	0	100	100
29	c	198/268 (74%)	197 (100%)	1 (0%)	81	82
30	d	177/294 (60%)	177 (100%)	0	100	100
31	e	26/63 (41%)	26 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	f	629/763 (82%)	627 (100%)	2 (0%)	86 85
34	u	33/398 (8%)	30 (91%)	3 (9%)	9 32
All	All	9827/13006 (76%)	9799 (100%)	28 (0%)	84 85

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	429	TYR
2	B	43	PRO
3	C	310	ARG
8	H	128	ARG
10	J	213	ARG
14	N	154	MET
17	Q	132	HIS
21	U	557	TYR
21	U	769	PHE
23	W	236	HIS
24	X	43	VAL
25	Y	251	HIS
25	Y	286	TRP
29	c	285	GLU
32	f	390	LEU
32	f	473	ASN
8	h	156	PHE
10	j	99	GLU
12	l	89	ARG
15	o	230	ARG
16	p	48	ARG
17	q	85	ARG
17	q	86	ARG
17	q	132	HIS
18	r	195	TYR
34	u	378	ASP
34	u	389	ARG
34	u	406	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	82	GLN

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Mol	Chain	Res	Type
2	B	120	HIS
2	B	368	HIS
3	C	332	HIS
4	D	221	HIS
4	D	340	GLN
6	F	184	GLN
6	F	258	GLN
6	F	358	ASN
8	H	102	GLN
8	H	166	ASN
9	I	102	GLN
10	J	18	GLN
12	L	59	HIS
12	L	146	GLN
13	M	121	HIS
15	O	78	HIS
17	Q	101	ASN
17	Q	132	HIS
19	S	64	HIS
19	S	180	GLN
21	U	346	ASN
22	V	282	ASN
22	V	326	GLN
25	Y	31	HIS
26	Z	24	ASN
26	Z	102	HIS
26	Z	104	ASN
26	Z	243	GLN
27	a	169	HIS
29	c	287	HIS
32	f	43	GLN
32	f	53	GLN
32	f	245	ASN
32	f	329	ASN
32	f	475	ASN
32	f	493	ASN
32	f	531	ASN
32	f	614	HIS
32	f	752	HIS
32	f	868	HIS
7	g	68	HIS
9	i	102	GLN

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Mol	Chain	Res	Type
9	i	109	GLN
9	i	230	GLN
10	j	15	HIS
13	m	102	ASN
13	m	121	HIS
14	n	62	ASN
16	p	65	GLN
17	q	27	GLN
17	q	174	ASN
17	q	189	HIS
20	t	126	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
35	ATP	A	501	-	32,33,33	0.51	0	48,52,52	0.67	0
35	ATP	C	501	-	32,33,33	0.52	0	48,52,52	0.55	0
35	ATP	B	501	-	32,33,33	0.54	0	48,52,52	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	ATP	F	501	-	32,33,33	0.50	0	48,52,52	0.60	0
36	ADP	D	501	-	28,29,29	0.46	0	43,45,45	0.52	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	ATP	A	501	-	-	7/22/38/38	0/3/3/3
35	ATP	C	501	-	-	10/22/38/38	0/3/3/3
35	ATP	B	501	-	-	8/22/38/38	0/3/3/3
35	ATP	F	501	-	-	11/22/38/38	0/3/3/3
36	ADP	D	501	-	-	9/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	A	501	ATP	PB-O3A-PA-O5'
35	A	501	ATP	O4'-C1'-N9-C8
35	B	501	ATP	C5'-O5'-PA-O1A
35	B	501	ATP	C5'-O5'-PA-O2A
35	B	501	ATP	C5'-O5'-PA-O3A
35	C	501	ATP	C5'-O5'-PA-O2A
35	C	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C5'-O5'-PA-O1A
35	F	501	ATP	C5'-O5'-PA-O2A
35	F	501	ATP	C5'-O5'-PA-O3A
35	F	501	ATP	C4'-C5'-O5'-PA
36	D	501	ADP	PA-O3A-PB-O3B
36	D	501	ADP	C5'-O5'-PA-O1A
36	D	501	ADP	C4'-C5'-O5'-PA
35	B	501	ATP	O4'-C4'-C5'-O5'
35	B	501	ATP	C3'-C4'-C5'-O5'
35	F	501	ATP	C3'-C4'-C5'-O5'
35	F	501	ATP	O4'-C4'-C5'-O5'
36	D	501	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
35	A	501	ATP	O4'-C1'-N9-C4
36	D	501	ADP	C3'-C4'-C5'-O5'
35	B	501	ATP	C4'-C5'-O5'-PA
35	C	501	ATP	C2'-C1'-N9-C8
35	C	501	ATP	C2'-C1'-N9-C4
35	F	501	ATP	PG-O3B-PB-O3A
35	C	501	ATP	PG-O3B-PB-O3A
36	D	501	ADP	C2'-C1'-N9-C8
35	A	501	ATP	PG-O3B-PB-O2B
35	A	501	ATP	PA-O3A-PB-O2B
35	C	501	ATP	PA-O3A-PB-O1B
35	C	501	ATP	C5'-O5'-PA-O1A
35	F	501	ATP	C2'-C1'-N9-C8
35	F	501	ATP	C2'-C1'-N9-C4
35	A	501	ATP	PA-O3A-PB-O1B
35	B	501	ATP	PB-O3A-PA-O1A
35	C	501	ATP	O4'-C4'-C5'-O5'
36	D	501	ADP	C2'-C1'-N9-C4
35	A	501	ATP	PG-O3B-PB-O1B
35	B	501	ATP	PB-O3A-PA-O2A
35	C	501	ATP	PA-O3A-PB-O2B
36	D	501	ADP	O4'-C1'-N9-C8
36	D	501	ADP	PA-O3A-PB-O1B
35	C	501	ATP	PG-O3B-PB-O1B
35	F	501	ATP	PG-O3B-PB-O1B
35	F	501	ATP	PB-O3A-PA-O1A

There are no ring outliers.

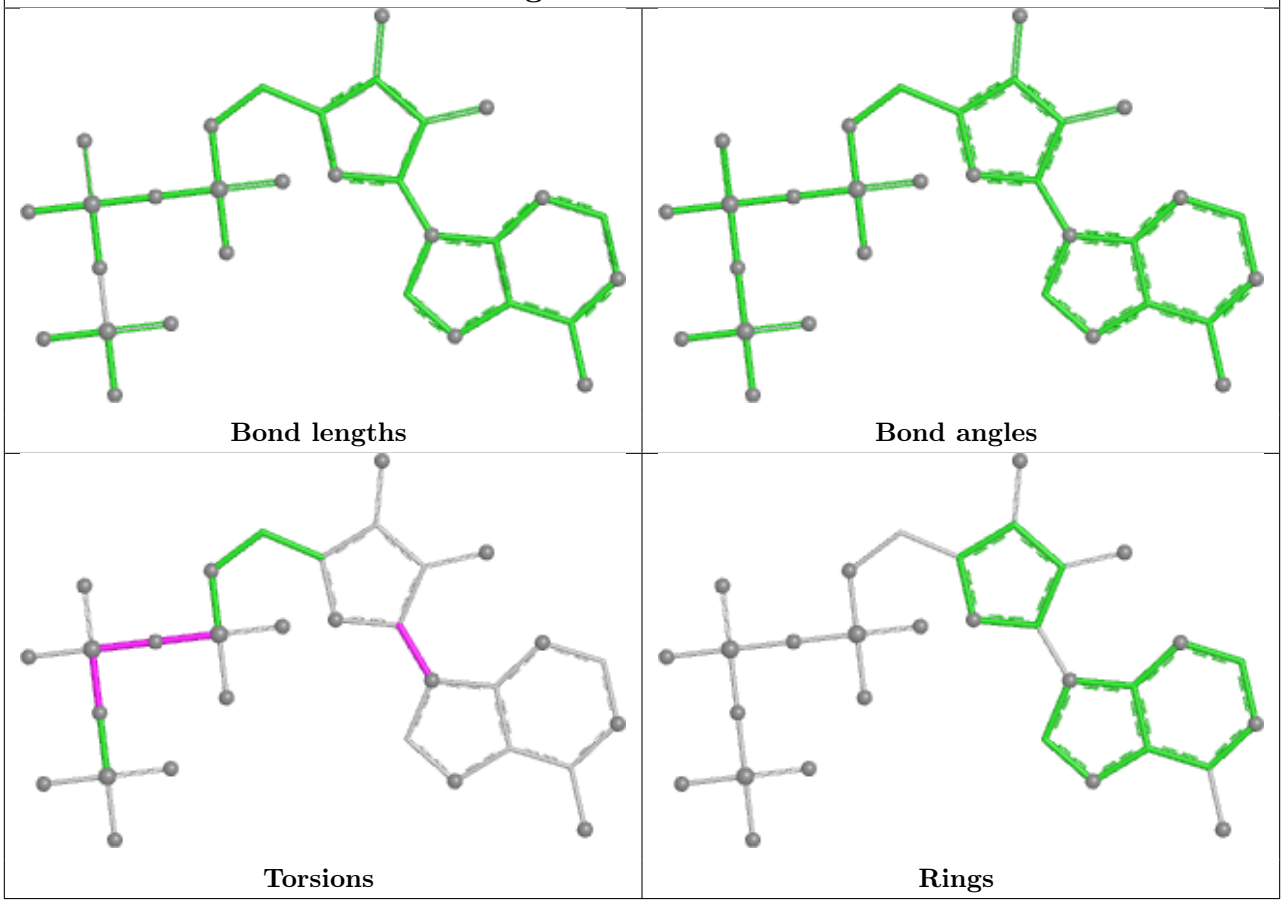
5 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	501	ATP	15	0
35	C	501	ATP	19	0
35	B	501	ATP	6	0
35	F	501	ATP	11	0
36	D	501	ADP	13	0

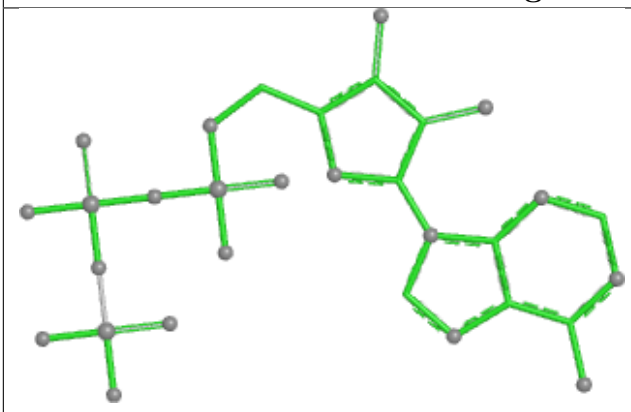
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

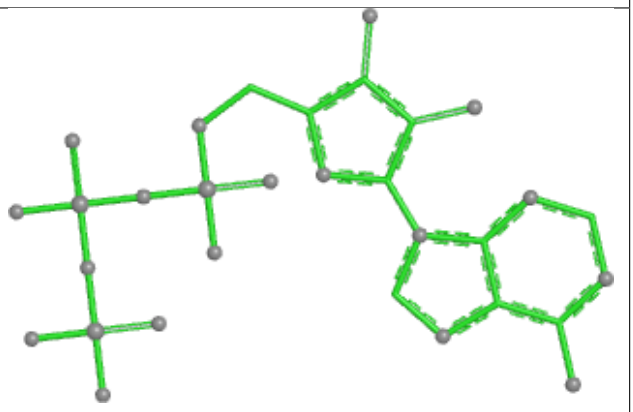
Ligand ATP A 501



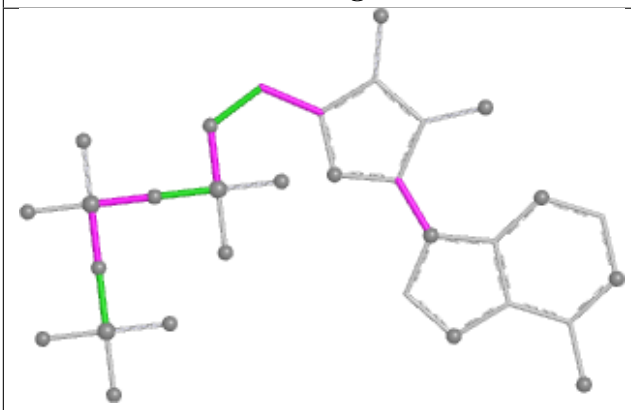
Ligand ATP C 501



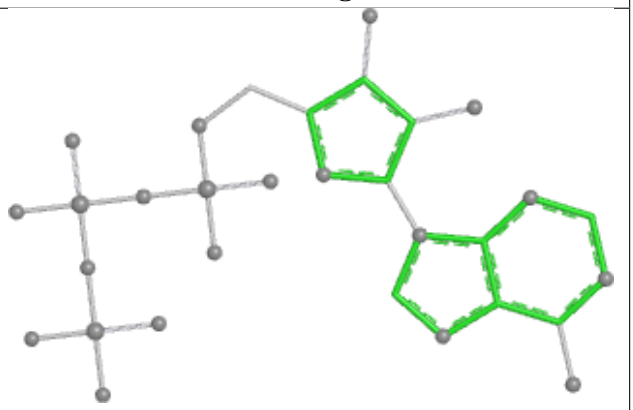
Bond lengths



Bond angles

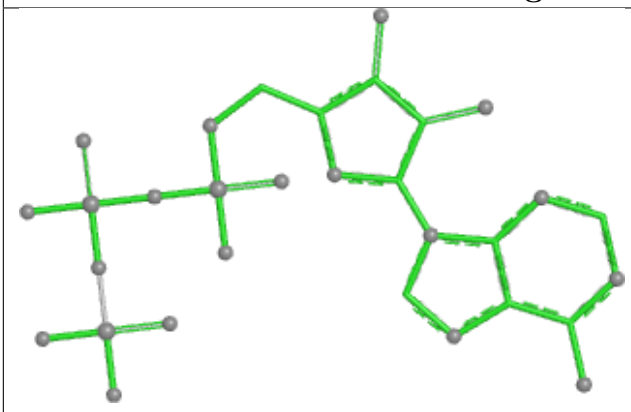


Torsions

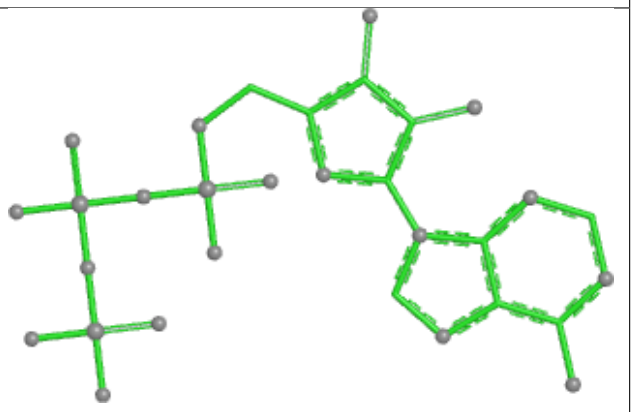


Rings

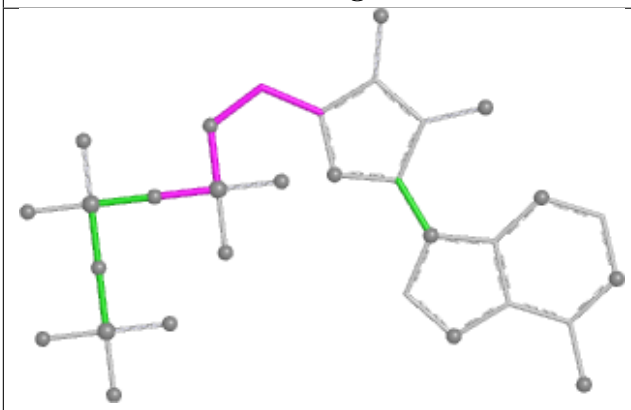
Ligand ATP B 501



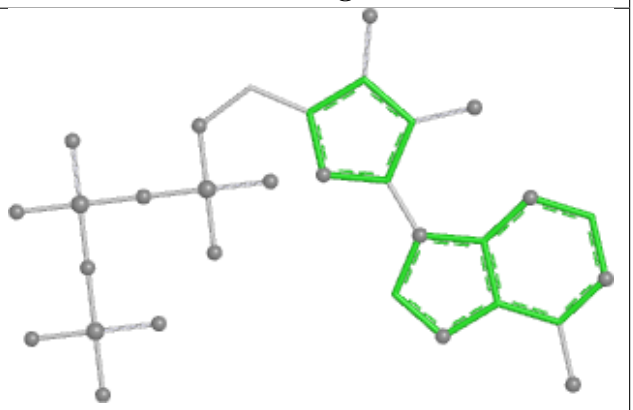
Bond lengths



Bond angles

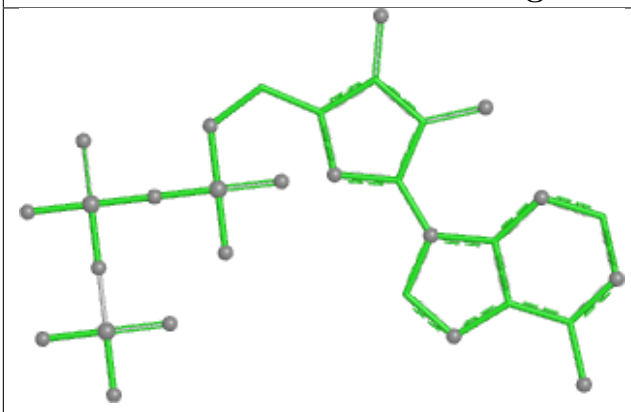


Torsions

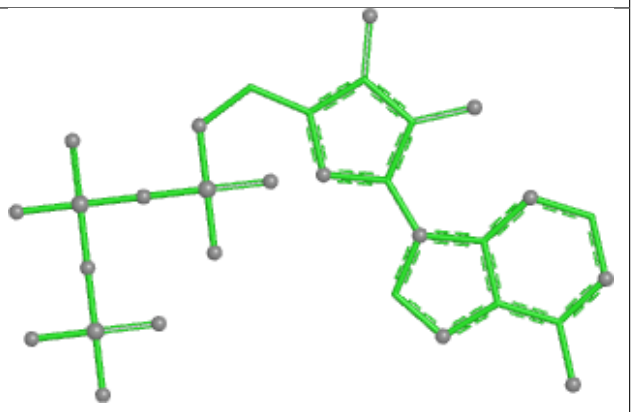


Rings

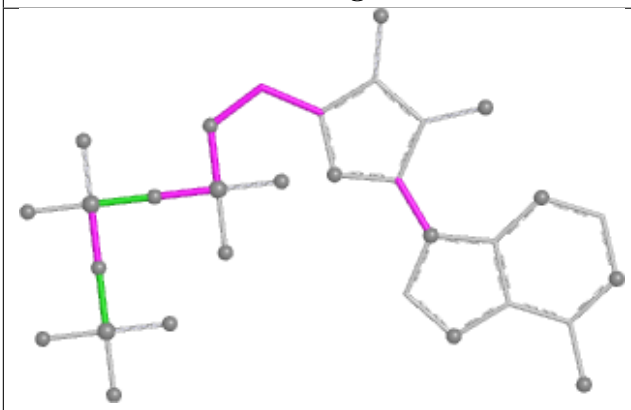
Ligand ATP F 501



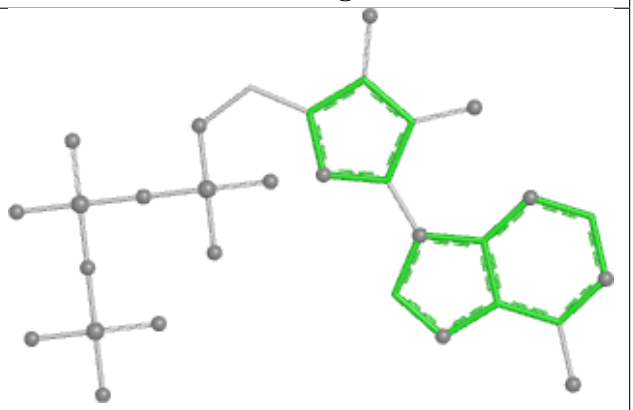
Bond lengths



Bond angles

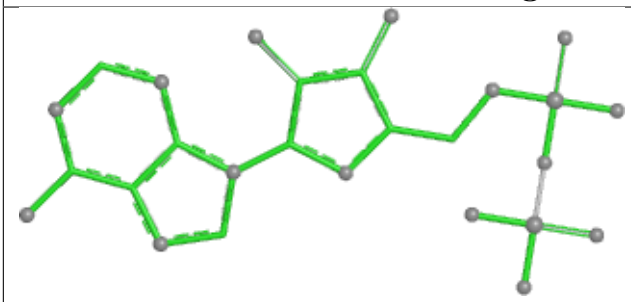


Torsions

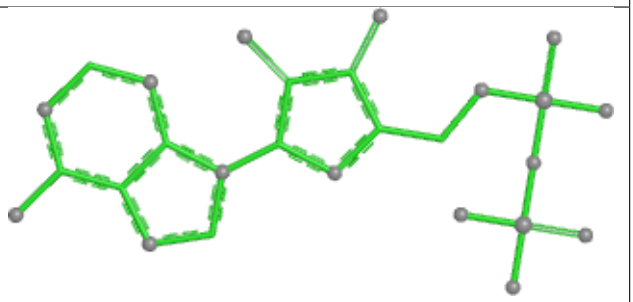


Rings

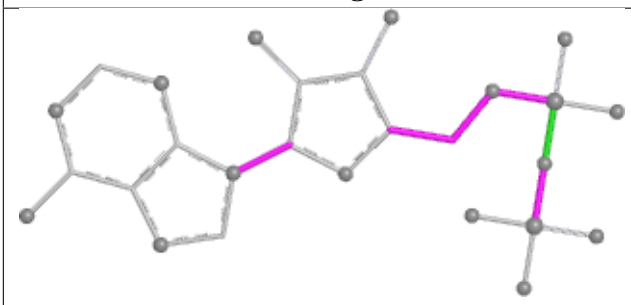
Ligand ADP D 501



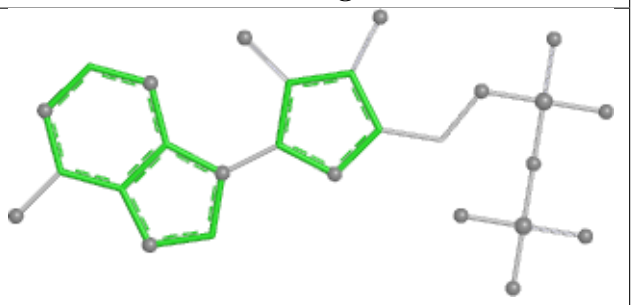
Bond lengths



Bond angles



Torsions



Rings

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.

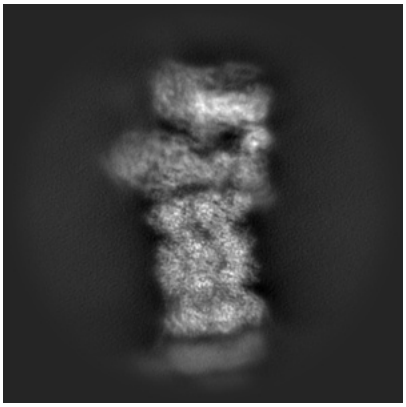
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-63592. These allow visual inspection of the internal detail of the map and identification of artifacts.

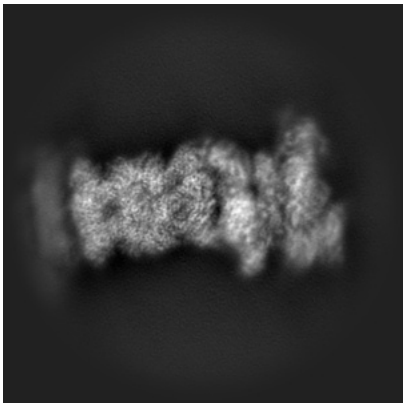
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

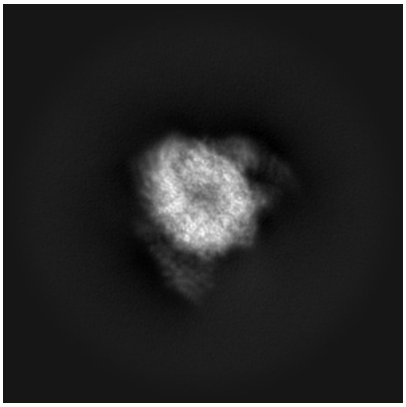
6.1.1 Primary map



X



Y

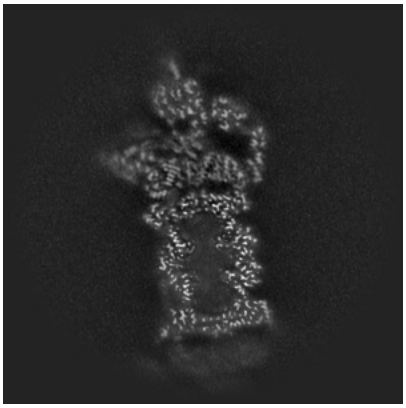


Z

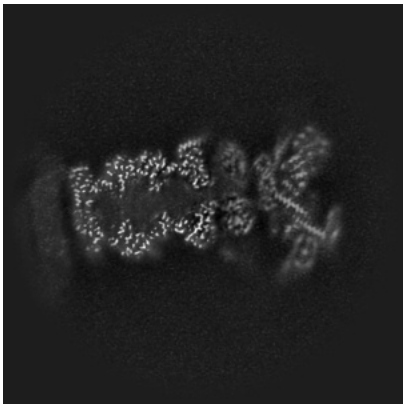
The images above show the map projected in three orthogonal directions.

6.2 Central slices

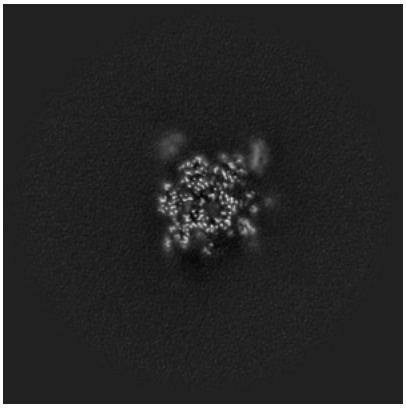
6.2.1 Primary map



X Index: 210



Y Index: 210

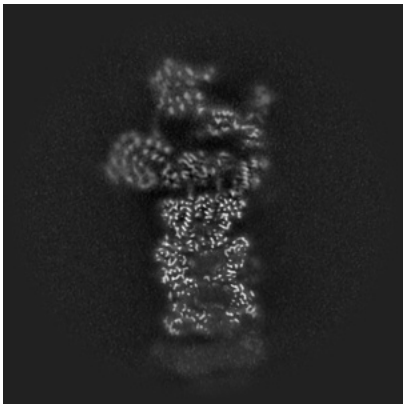


Z Index: 210

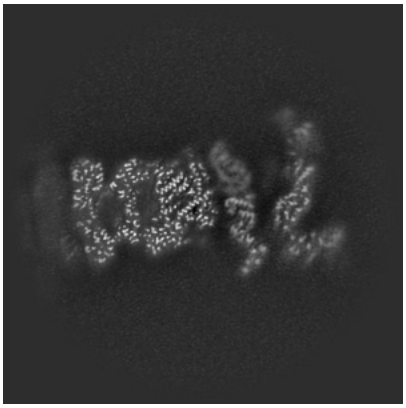
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

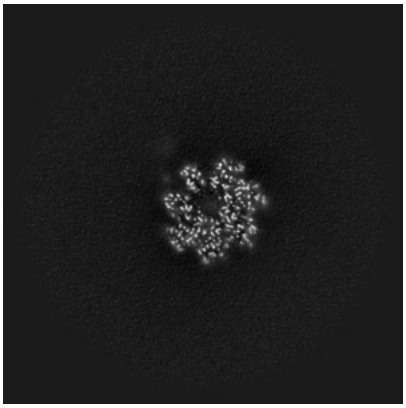
6.3.1 Primary map



X Index: 194



Y Index: 233

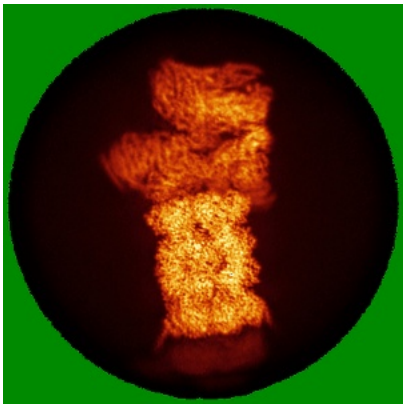


Z Index: 198

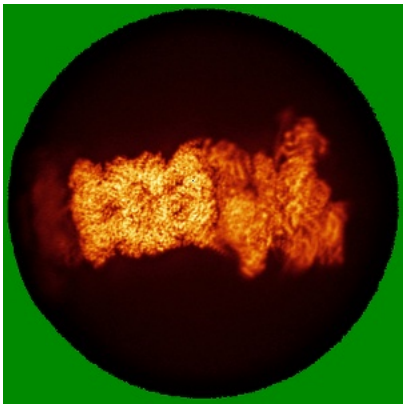
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

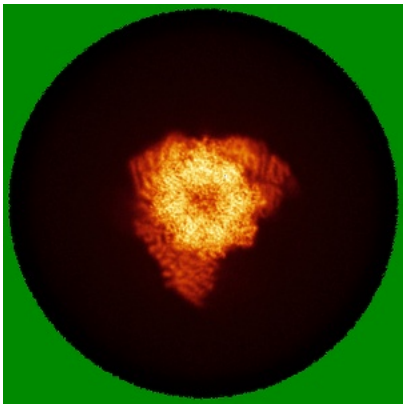
6.4.1 Primary map



X



Y

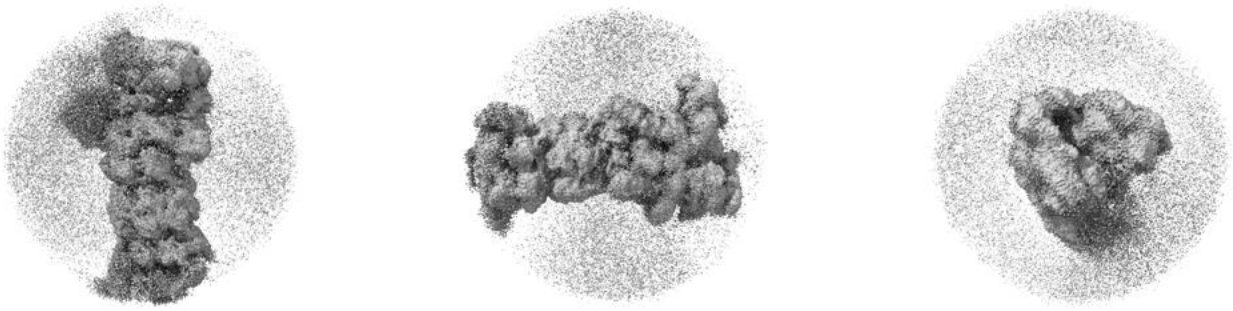


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

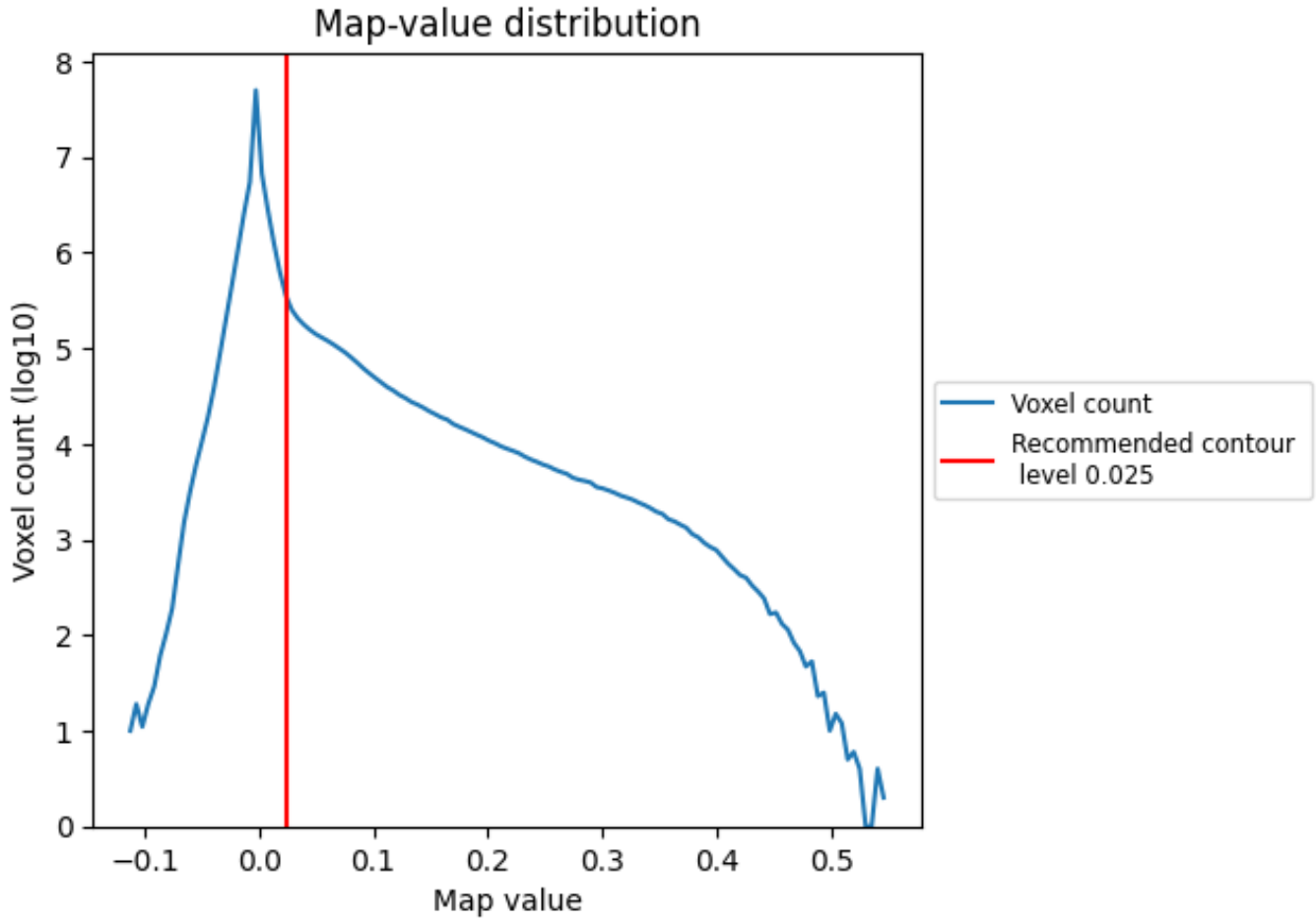
6.6 Mask visualisation (i)

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

7 Map analysis

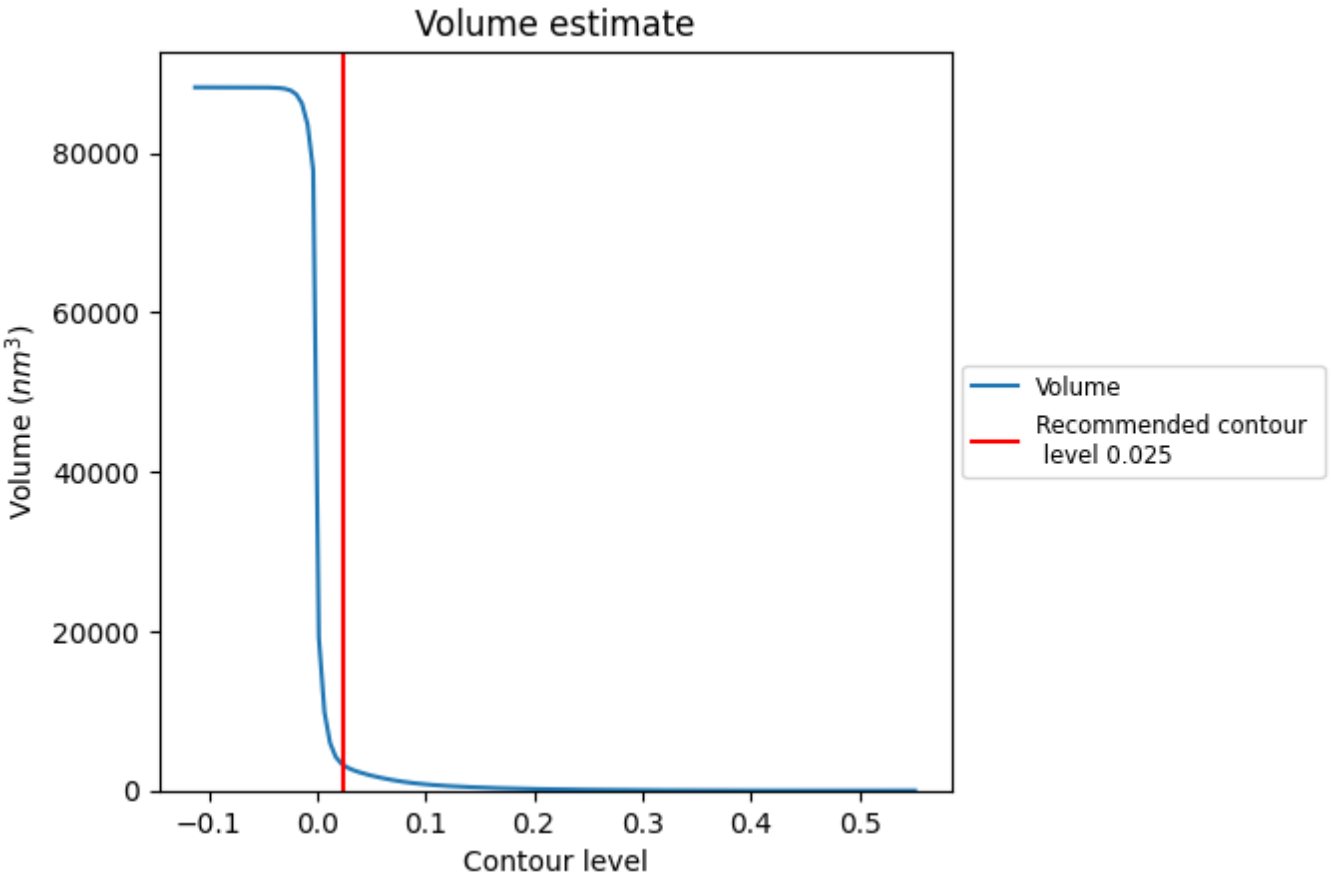
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

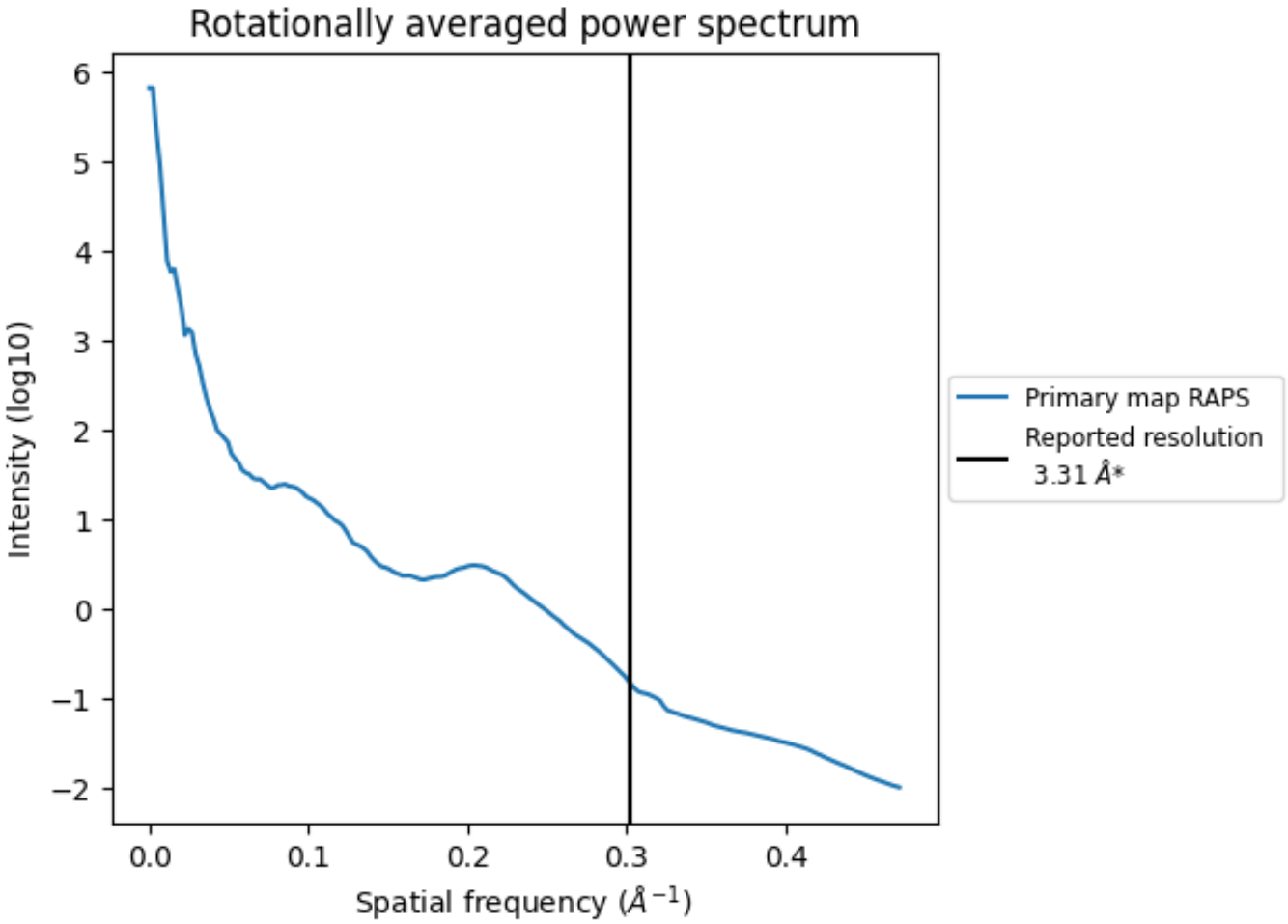
7.2 Volume estimate



The volume at the recommended contour level is 3154 nm^3; this corresponds to an approximate mass of 2849 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 (i)



*Reported resolution corresponds to spatial frequency of 0.302 Å^{-1}

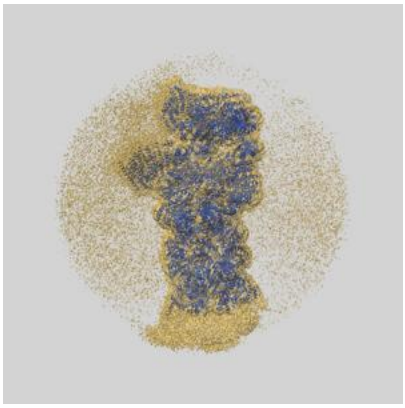
8 Fourier-Shell correlation

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

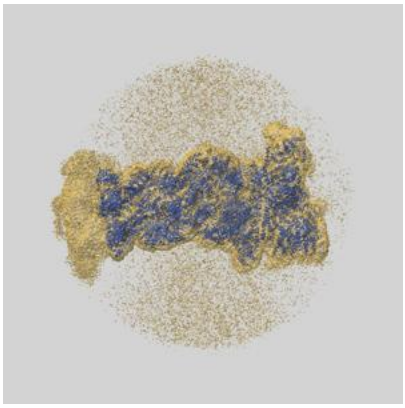
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-63592 and PDB model 9M2W. Per-residue inclusion information can be found in section 3 on page 13.

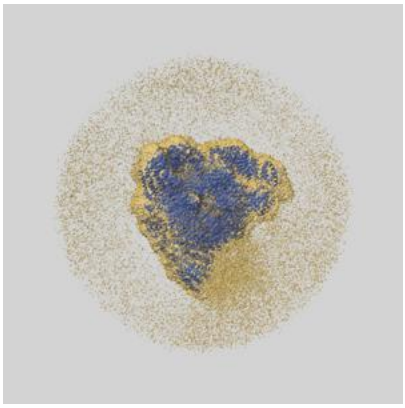
9.1 Map-model overlay



X



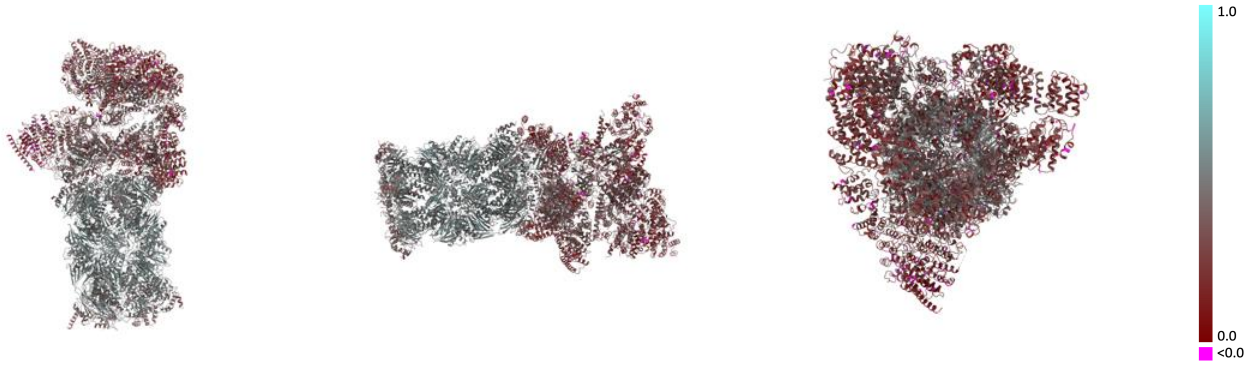
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.025 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.

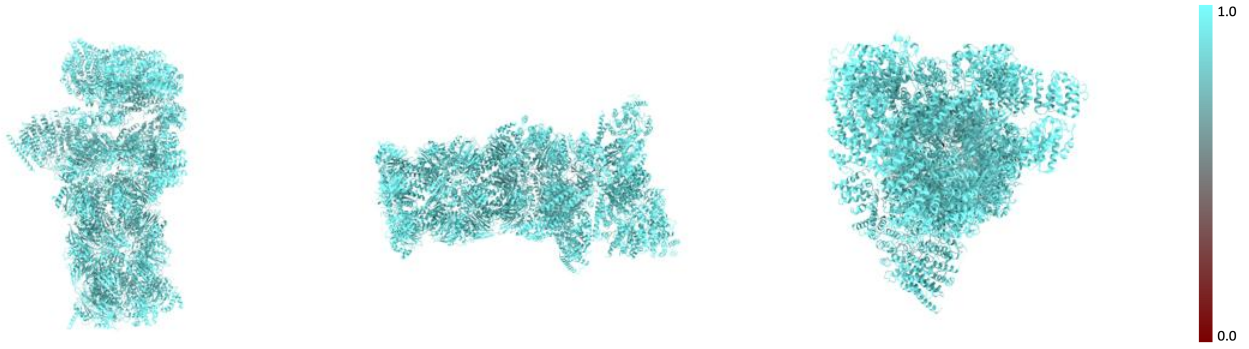
9.2 Q-score mapped to coordinate model



X Y Z

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

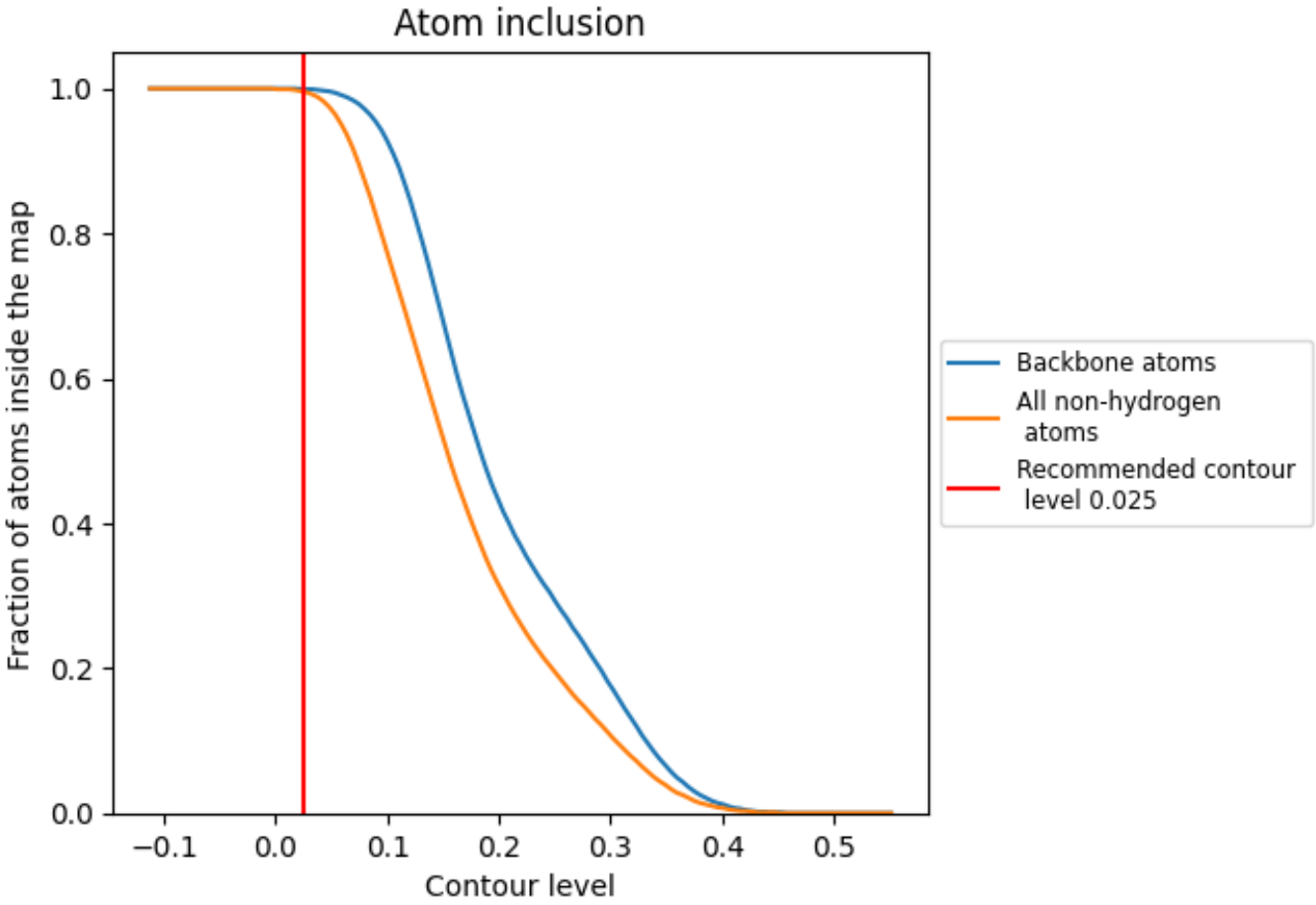
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.025).

9.4 Atom inclusion (i)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9960	0.3880
A	0.9830	0.3620
B	0.9790	0.3610
C	0.9910	0.3760
D	0.9850	0.3590
E	0.9980	0.2600
F	0.9950	0.3460
G	0.9980	0.4860
H	0.9900	0.4930
I	0.9950	0.4860
J	0.9970	0.4790
K	0.9960	0.4870
L	0.9980	0.4970
M	0.9950	0.4880
N	0.9990	0.5110
O	0.9990	0.5160
P	1.0000	0.5190
Q	0.9990	0.5210
R	0.9990	0.5230
S	0.9980	0.5170
T	0.9990	0.5130
U	0.9990	0.2940
V	0.9970	0.2690
W	0.9950	0.2530
X	0.9980	0.3150
Y	0.9970	0.3250
Z	0.9970	0.3030
a	0.9990	0.2410
b	0.9990	0.2280
c	0.9890	0.3120
d	0.9960	0.2420
e	0.9960	0.2740
f	0.9920	0.1960
g	0.9990	0.4570
h	0.9960	0.4660

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	1.0000	0.4440
j	0.9990	0.4450
k	1.0000	0.4600
l	0.9990	0.4730
m	0.9980	0.4680
n	0.9990	0.5090
o	1.0000	0.5140
p	1.0000	0.5050
q	1.0000	0.5120
r	1.0000	0.5180
s	0.9990	0.5200
t	0.9990	0.5150
u	0.9870	0.1290
v	1.0000	0.4210