



Full wwPDB EM Validation Report ⓘ

Apr 5, 2026 – 10:31 PM UTC

PDB ID : 9MBQ / pdb_00009mbq
EMDB ID : EMD-63777
Title : Substrate-engaged human 26S proteasome bound to midnolin with RPT5 at top of spiral staircase
Authors : Zhu, C.; Qin, L.; Liang, L.
Deposited on : 2025-03-17
Resolution : 3.08 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:

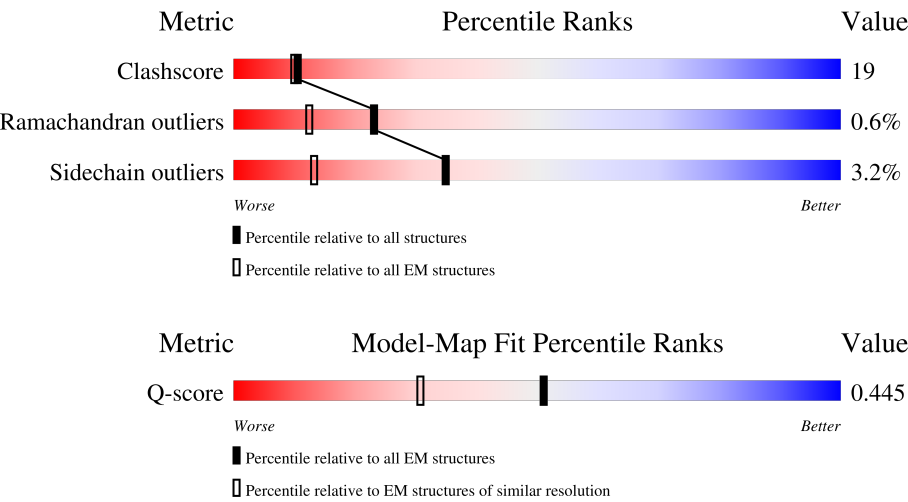
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 3.08 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.



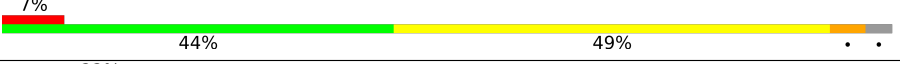



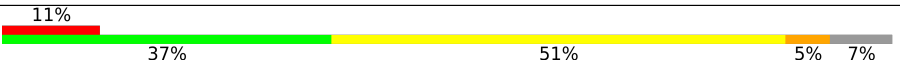
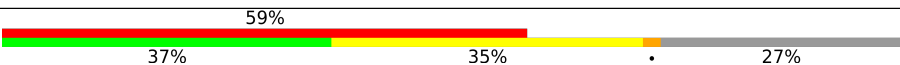
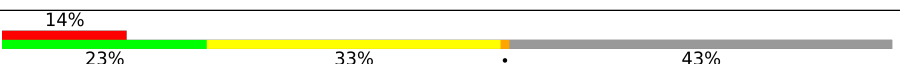
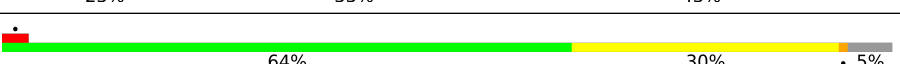
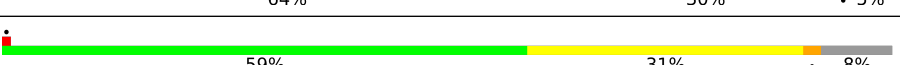
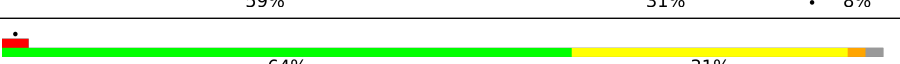
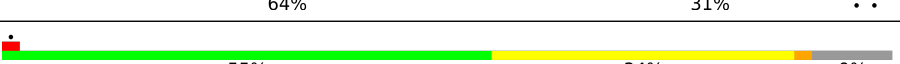
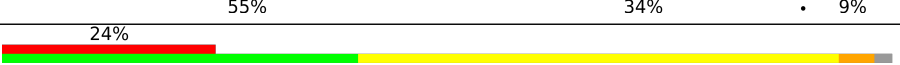

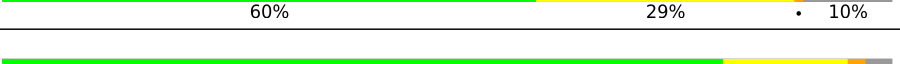



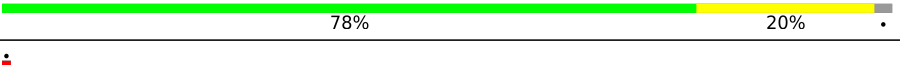


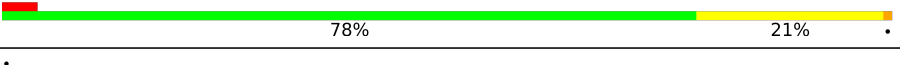


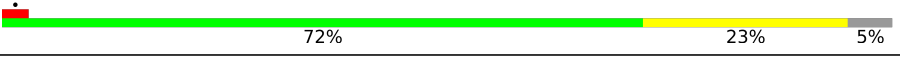

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14000 (2.58 - 3.58)

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

Mol	Chain	Length	Quality of chain
1	U	921	
2	V	480	
3	W	456	
4	X	422	














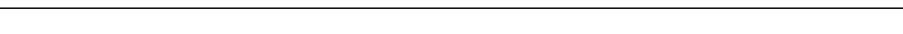





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Mol	Chain	Length	Quality of chain
5	Y	389	
6	Z	324	
7	a	376	
8	b	377	
9	c	310	
10	d	350	
11	e	70	
12	A	433	
13	B	440	
14	C	406	
15	D	418	
16	E	389	
17	F	439	
18	G	245	
18	g	245	
19	H	233	
19	h	233	
20	I	260	
20	i	260	
21	J	247	
21	j	247	
22	K	240	
22	k	240	
23	L	268	
23	l	268	

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Mol	Chain	Length	Quality of chain
24	M	254	
24	m	254	
25	N	238	
25	n	238	
26	O	276	
26	o	276	
27	P	204	
27	p	204	
28	Q	201	
28	q	201	
29	R	262	
29	r	262	
30	S	240	
30	s	240	
31	T	263	
31	t	263	
32	f	468	
33	x	908	
34	v	14	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 105726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	872	Total	C	N	O	S	0	0
			6828	4328	1157	1298	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	V	480	Total	C	N	O	S	0	0
			3852	2444	684	710	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	W	453	Total	C	N	O	S	0	0
			3679	2323	632	699	25		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Y	378	Total	C	N	O	S	0	0
			3109	1984	530	578	17		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 12 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	A	413	Total	C	N	O	S	0	0
			3229	2034	566	611	18		

- Molecule 13 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	B	405	Total	C	N	O	S	0	0
			3162	1994	538	615	15		

- Molecule 14 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	C	396	Total	C	N	O	S	0	0
			3107	1955	558	576	18		

- Molecule 15 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	D	380	Total	C	N	O	S	0	0
			3040	1923	524	580	13		

- Molecule 16 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	E	381	Total	C	N	O	S	0	0
			3031	1903	542	569	17		

- Molecule 17 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	395	Total	C	N	O	S	0	0
			3098	1951	533	596	18		

- Molecule 18 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	G	237	Total	C	N	O	S	0	0
			1809	1151	302	343	13		
18	g	240	Total	C	N	O	S	0	0
			1830	1163	306	348	13		

- Molecule 19 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	H	231	Total	C	N	O	S	0	0
			1714	1088	290	331	5		
19	h	229	Total	C	N	O	S	0	0
			1703	1083	286	329	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		

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

- Molecule 21 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	J	247	Total	C	N	O	S	0	0
			1844	1148	331	360	5		
21	j	239	Total	C	N	O	S	0	0
			1704	1056	308	335	5		

- Molecule 22 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	K	230	Total	C	N	O	S	0	0
			1746	1096	286	353	11		
22	k	228	Total	C	N	O	S	0	0
			1722	1080	284	348	10		

- Molecule 23 is a protein called Isoform Long of Proteasome subunit alpha type-1.

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

- Molecule 24 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		
24	m	240	Total	C	N	O	S	0	0
			1862	1181	317	353	11		

- Molecule 25 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	N	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		
25	n	197	Total	C	N	O	S	0	0
			1482	928	253	289	12		

- Molecule 26 is a protein called Proteasome subunit beta type-7.

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

- Molecule 27 is a protein called Proteasome subunit beta type-3.

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

- Molecule 28 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Q	199	Total	C	N	O	S	0	0
			1570	1006	265	290	9		
28	q	199	Total	C	N	O	S	0	0
			1574	1009	266	290	9		

- Molecule 29 is a protein called Proteasome subunit beta type-5.

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

- Molecule 30 is a protein called Proteasome subunit beta type-1.

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

- Molecule 31 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	T	215	Total	C	N	O	S	0	0
			1667	1052	285	318	12		
31	t	215	Total	C	N	O	S	0	0
			1673	1055	288	318	12		

- Molecule 32 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	42	Total	C	N	O	S	0	0
			367	222	86	58	1		

- Molecule 33 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	x	867	Total	C	N	O	S	0	0
			6723	4243	1141	1294	45		

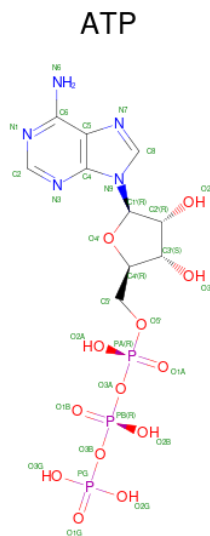
- Molecule 34 is a protein called substrate peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	v	14	Total	C	N	O	0	0
			70	42	14	14		

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃) (labeled as "Ligand of Interest" by depositor).

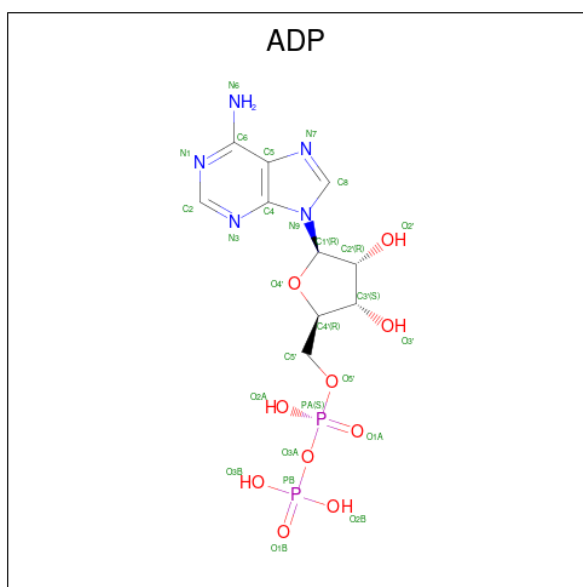


Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total 31	C 10	N 5	O 13	P 3	0
36	B	1	Total 31	C 10	N 5	O 13	P 3	0
36	C	1	Total 31	C 10	N 5	O 13	P 3	0
36	F	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
37	A	1	Total Mg 1 1	0
37	B	1	Total Mg 1 1	0
37	C	1	Total Mg 1 1	0
37	F	1	Total Mg 1 1	0

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



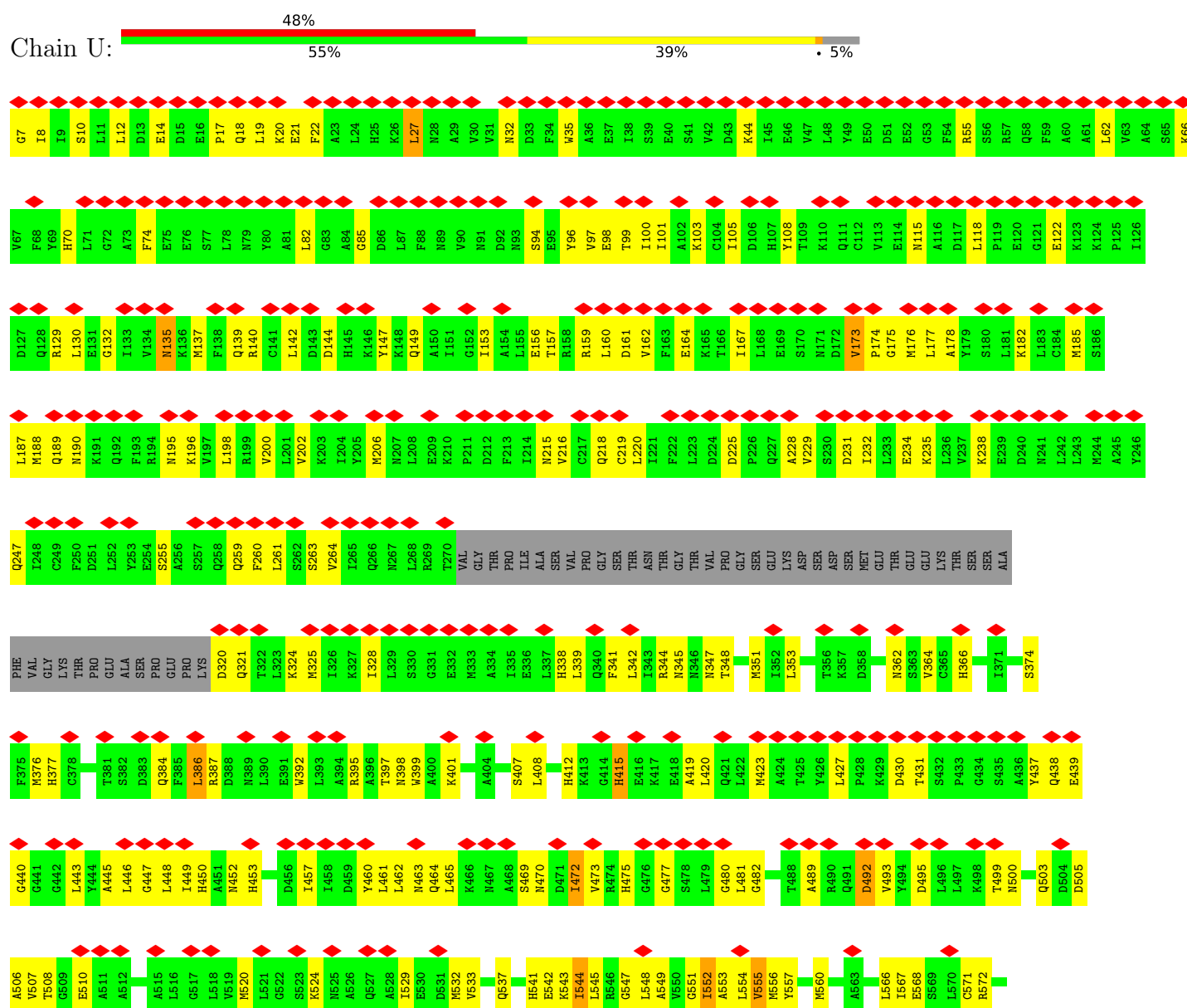
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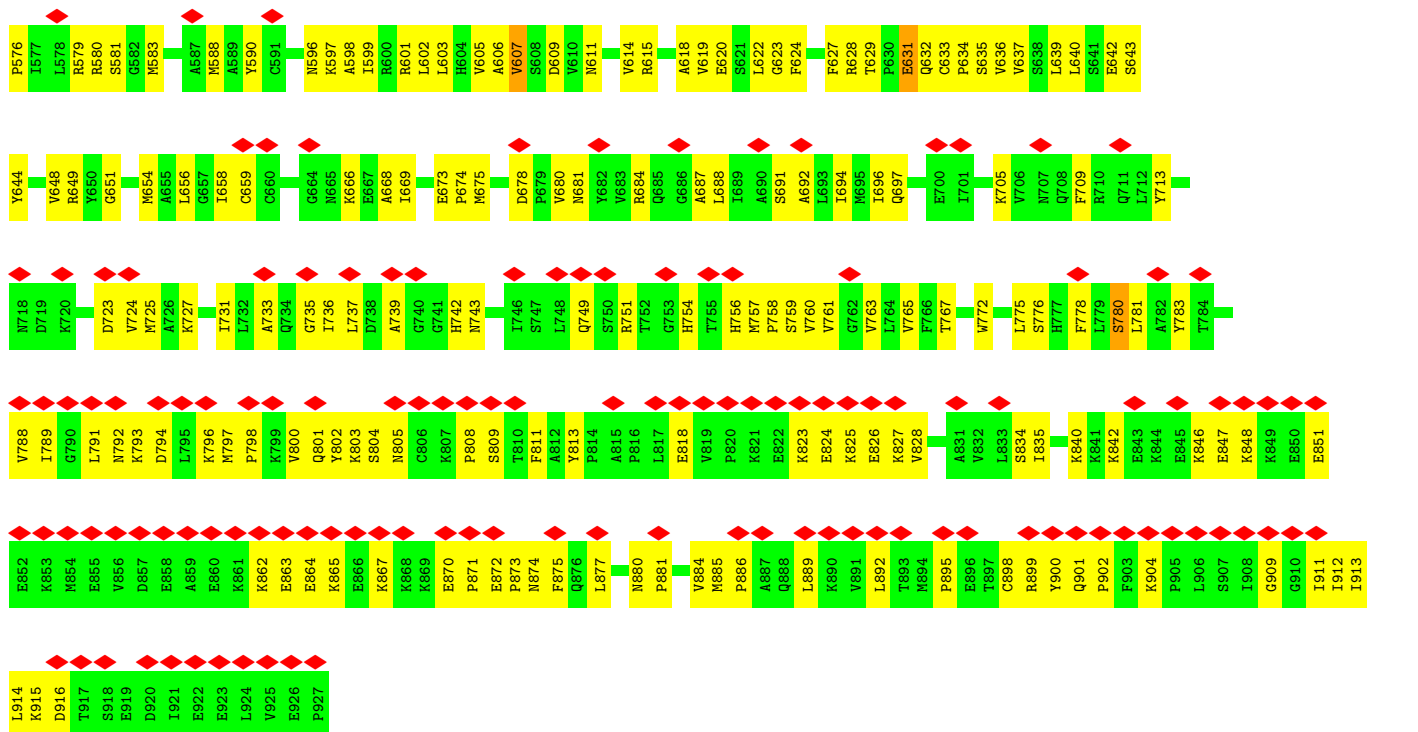
Mol	Chain	Residues	Atoms				AltConf
39	O	1	Total	C	N	O	0
			34	26	3	5	
39	R	1	Total	C	N	O	0
			34	26	3	5	
39	n	1	Total	C	N	O	0
			34	26	3	5	
39	o	1	Total	C	N	O	0
			34	26	3	5	
39	r	1	Total	C	N	O	0
			34	26	3	5	

3 Residue-property plots

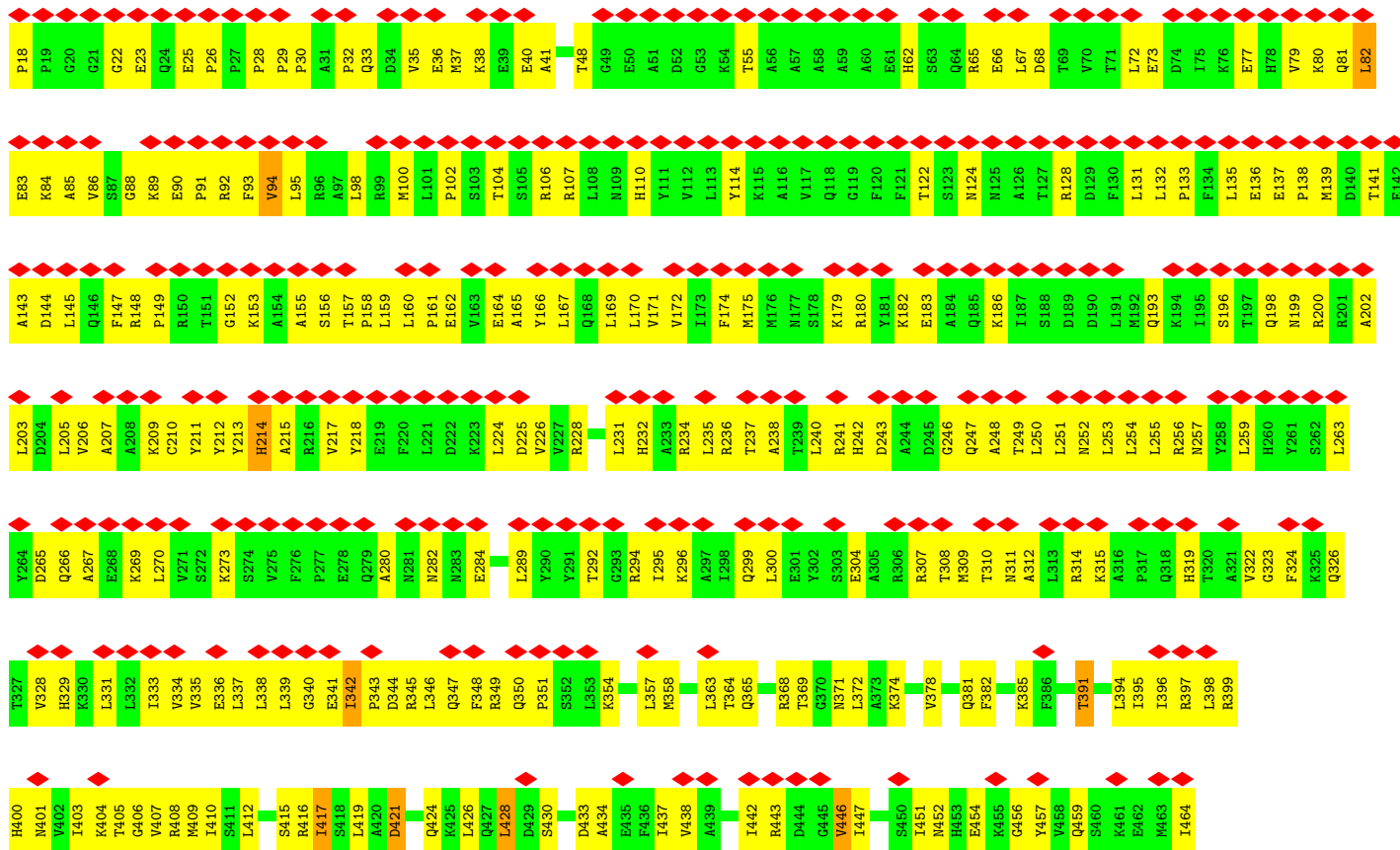
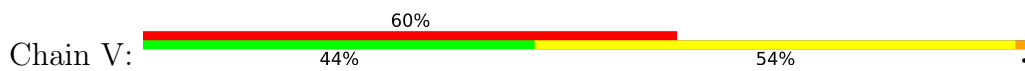
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

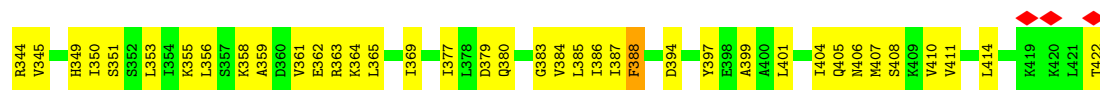
- Molecule 1: 26S proteasome non-ATPase regulatory subunit 1



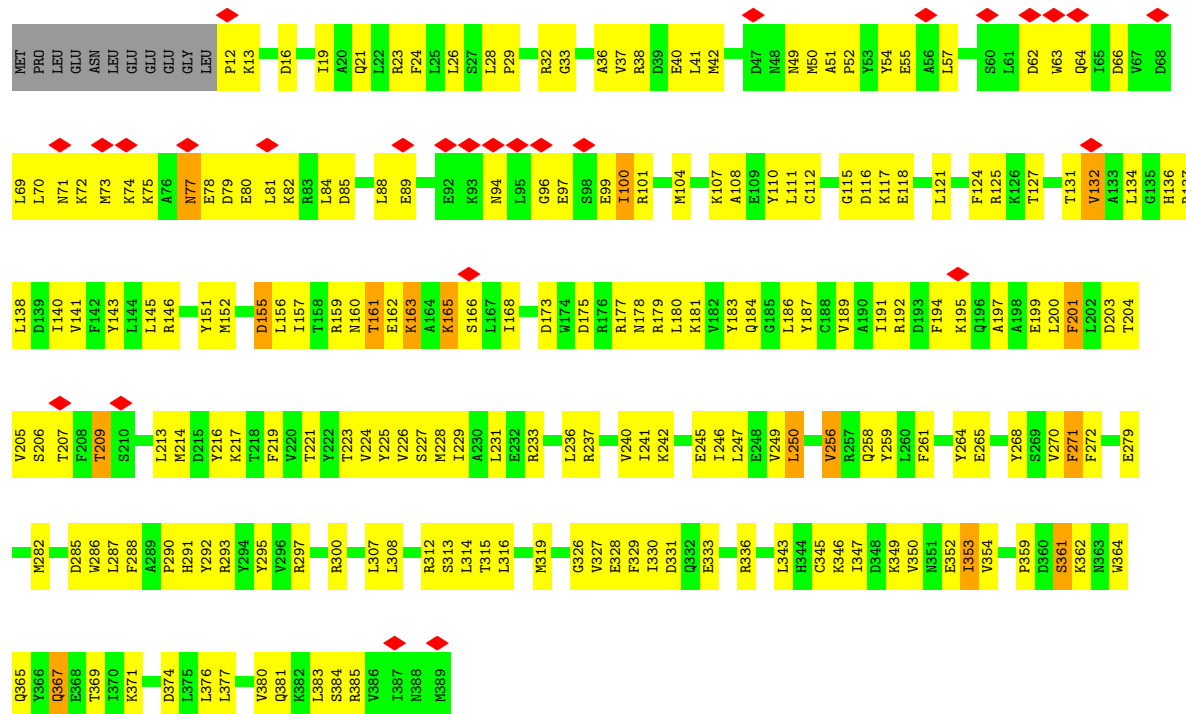
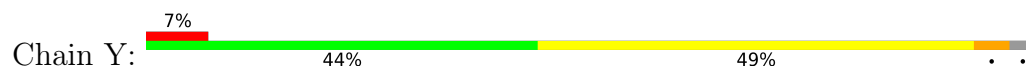


• Molecule 2: 26S proteasome non-ATPase regulatory subunit 3

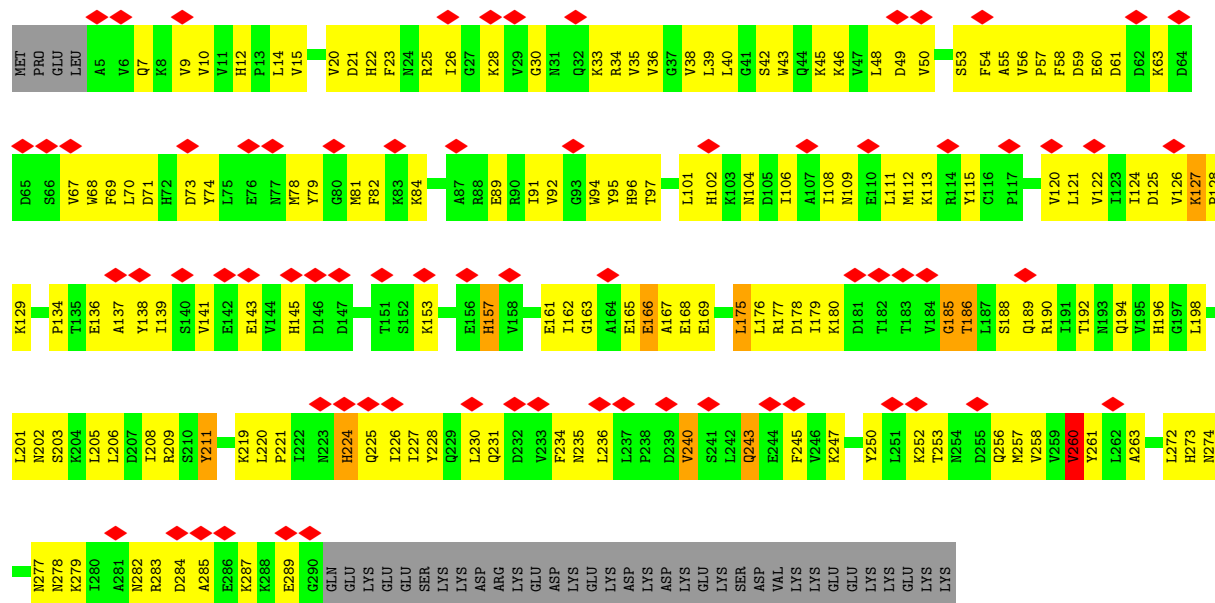




• Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

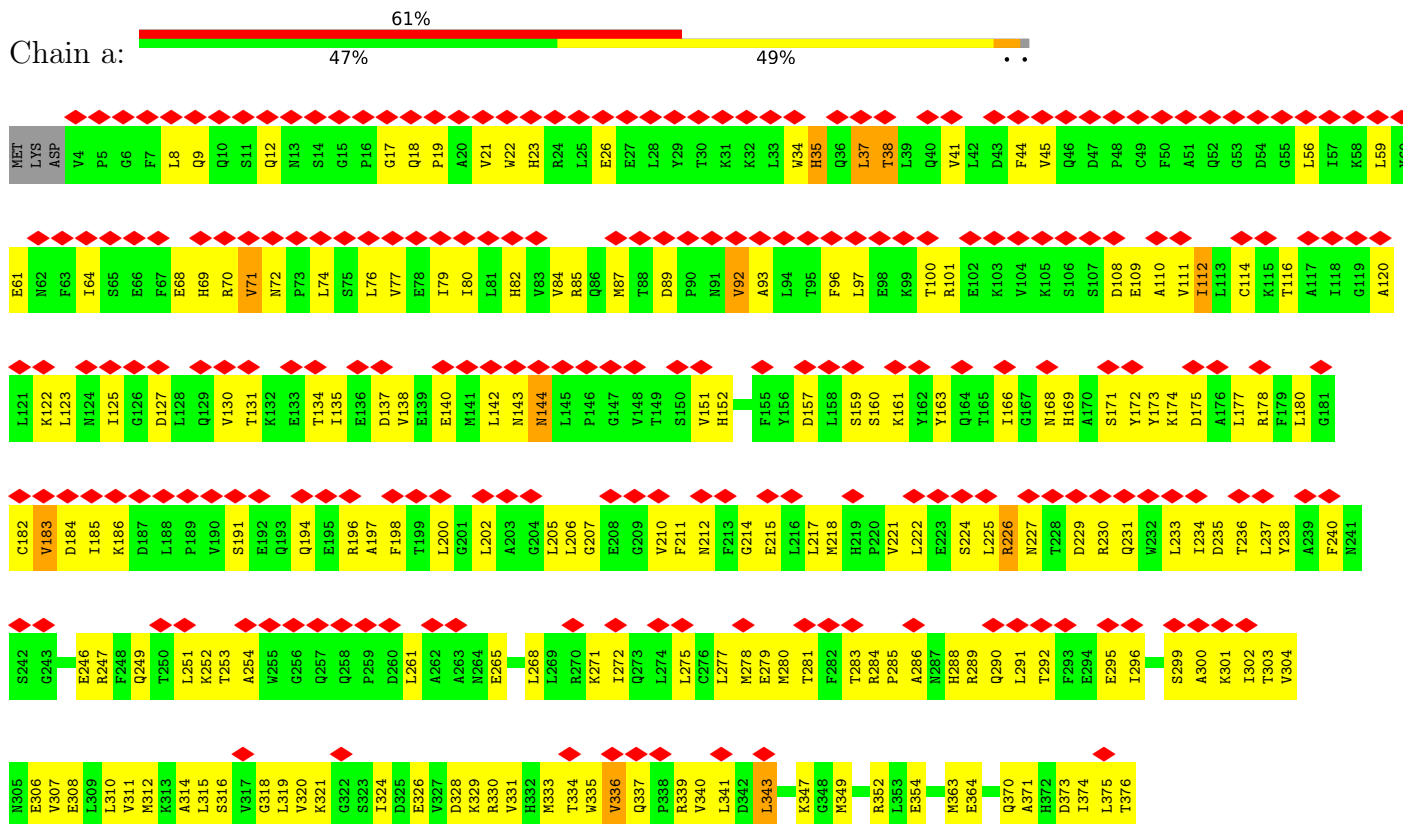


• Molecule 6: 26S proteasome non-ATPase regulatory subunit 7



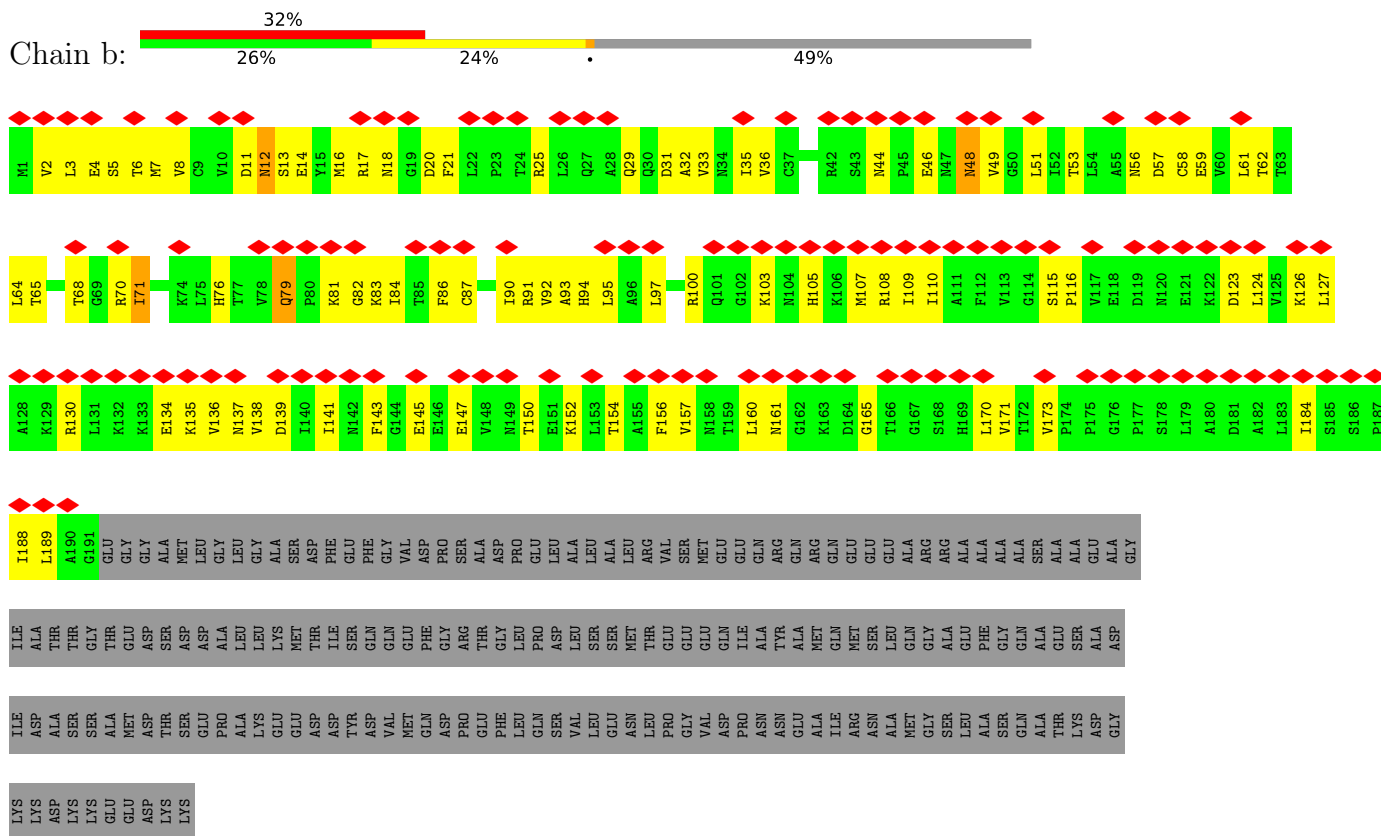
• Molecule 7: 26S proteasome non-ATPase regulatory subunit 13

Chain a:

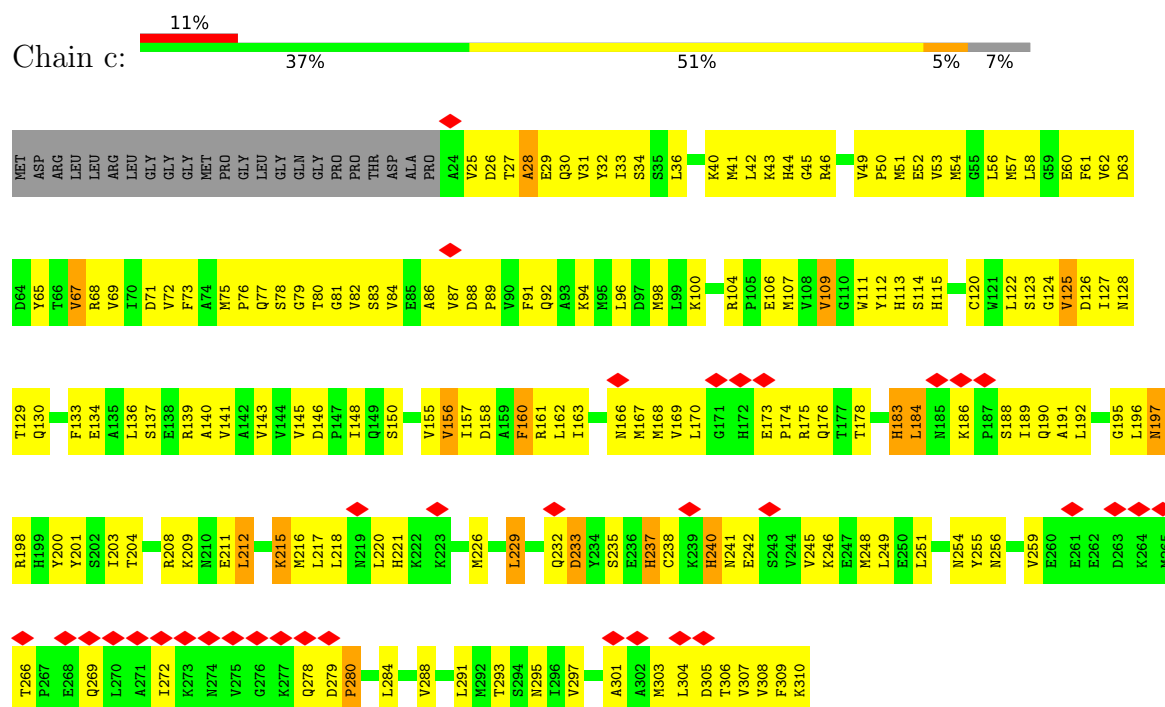


• Molecule 8: 26S proteasome non-ATPase regulatory subunit 4

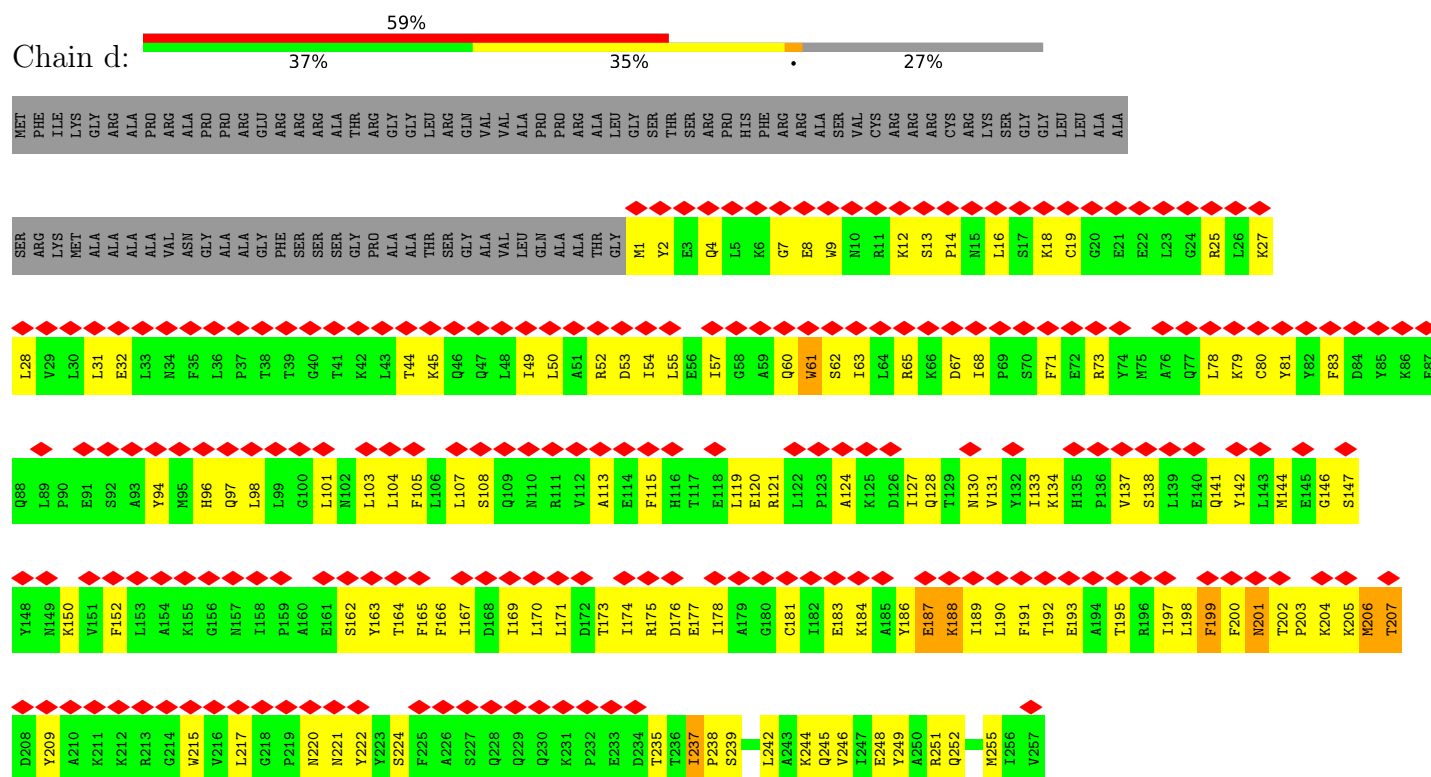
Chain b:



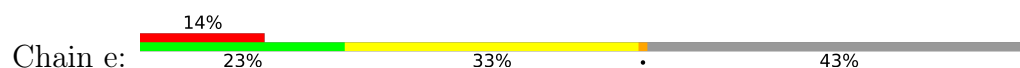
- Molecule 9: 26S proteasome non-ATPase regulatory subunit 14



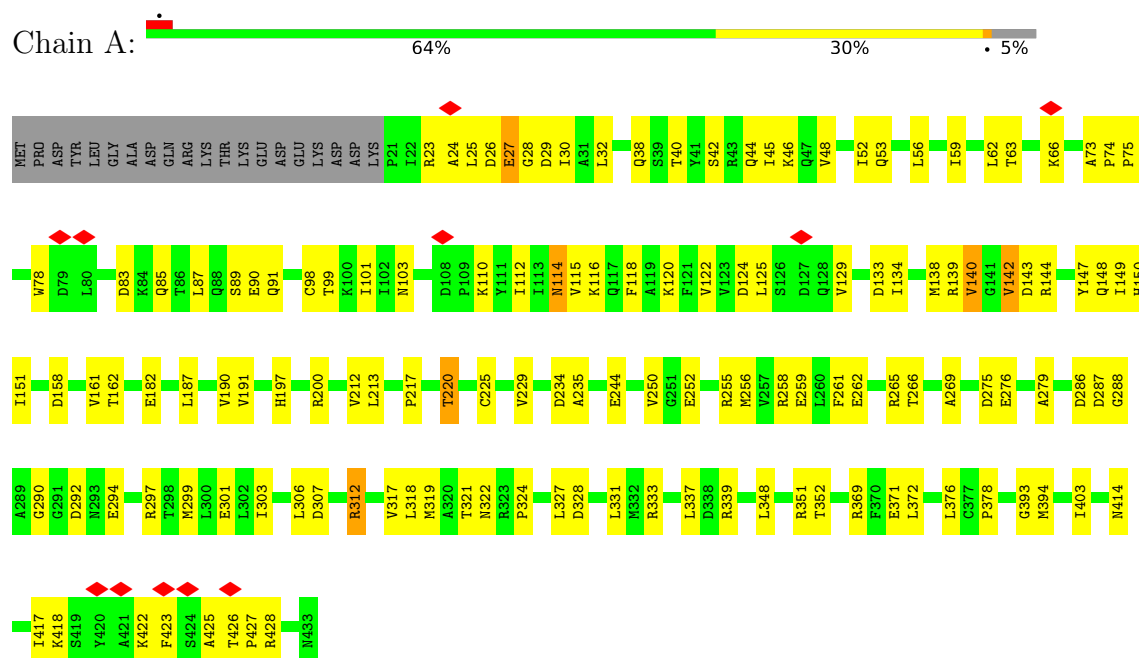
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8



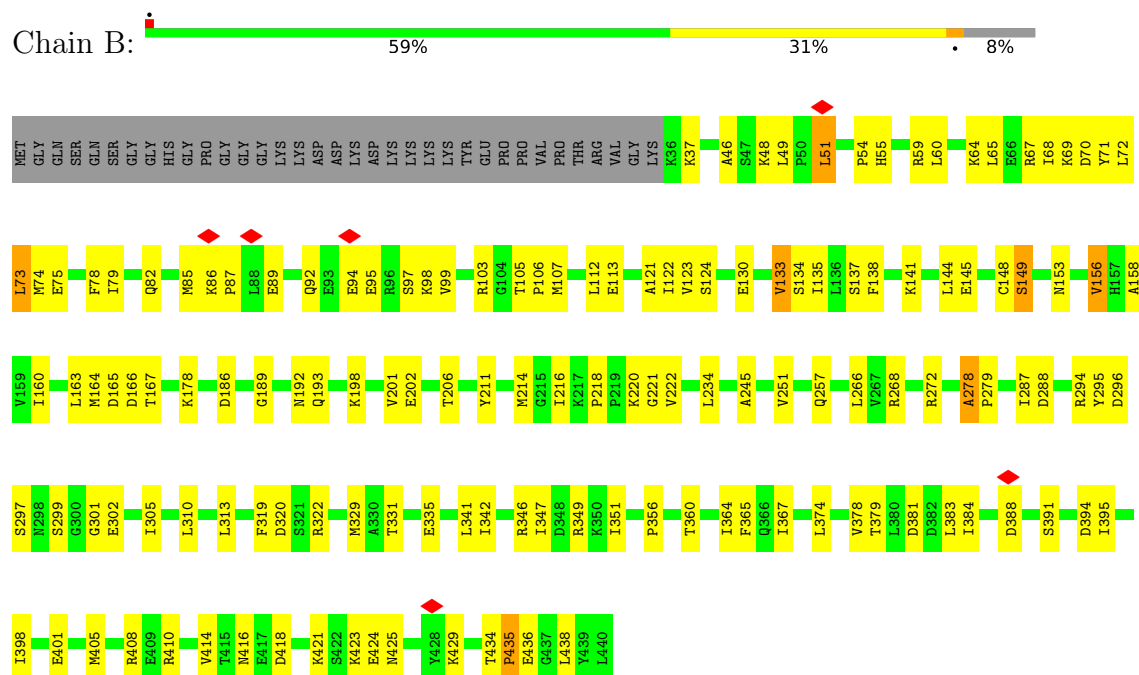
- Molecule 11: 26S proteasome complex subunit SEM1



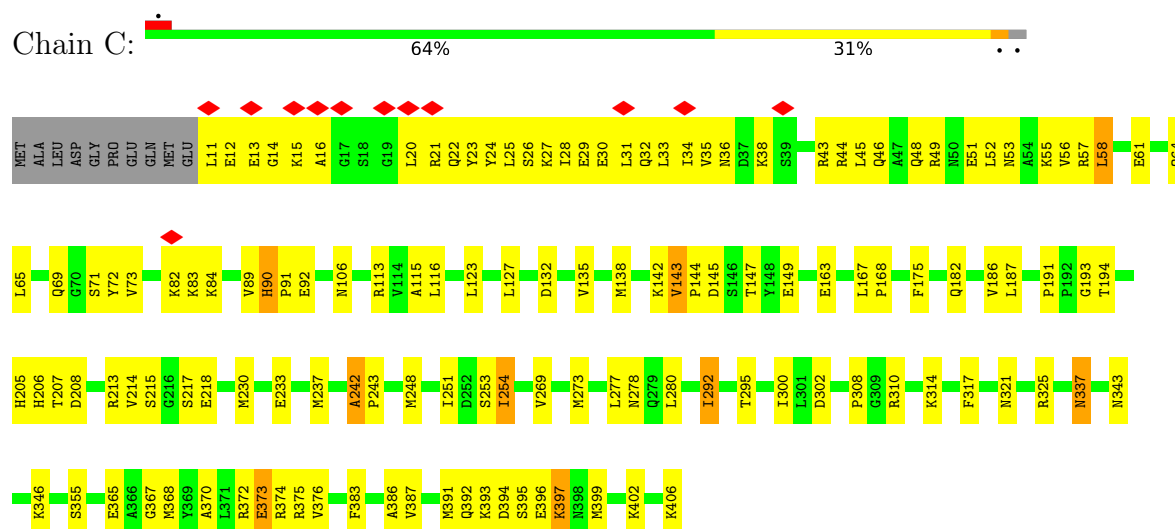
- Molecule 12: 26S proteasome regulatory subunit 7



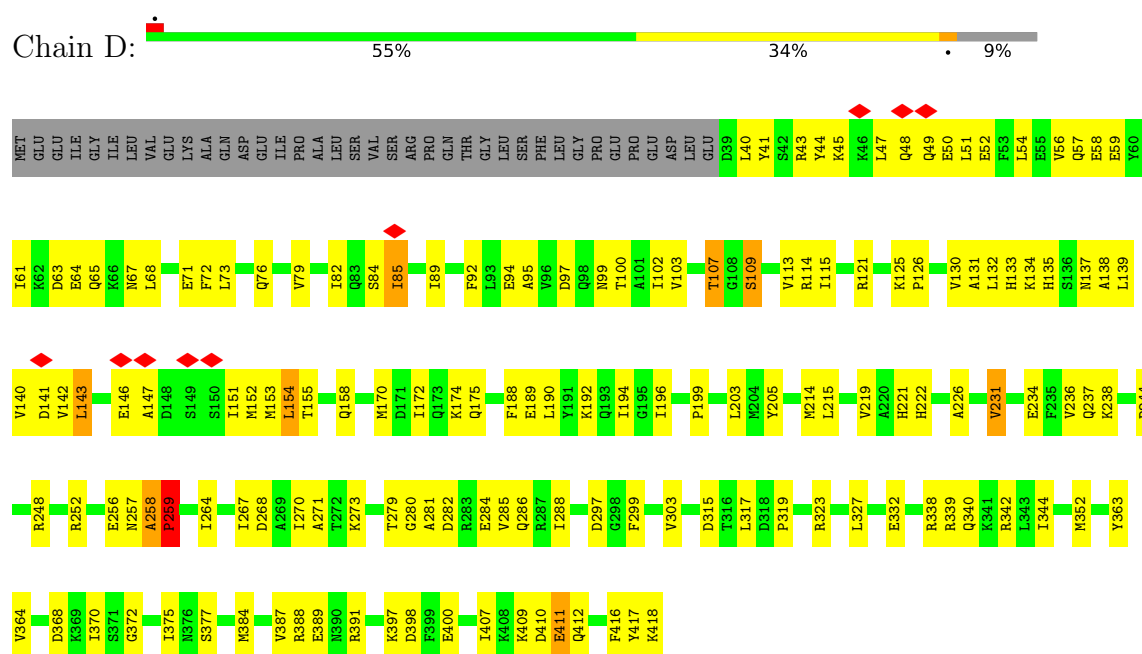
- Molecule 13: 26S proteasome regulatory subunit 4



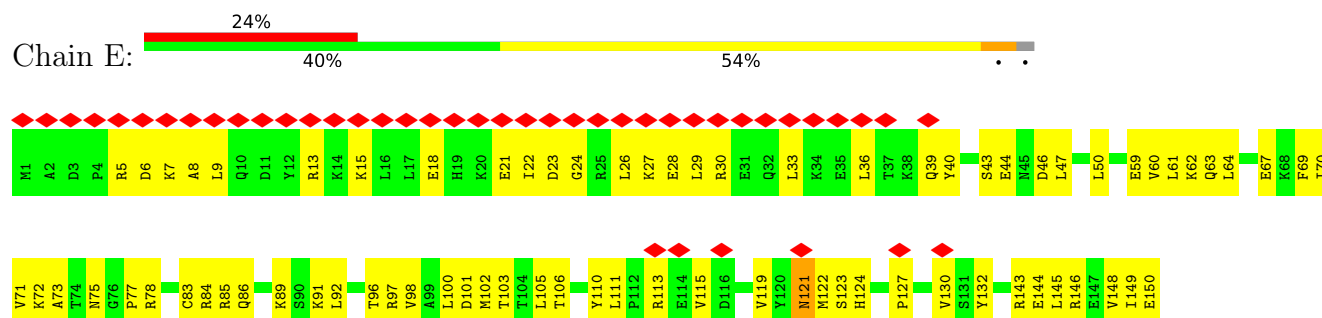
- Molecule 14: 26S proteasome regulatory subunit 8

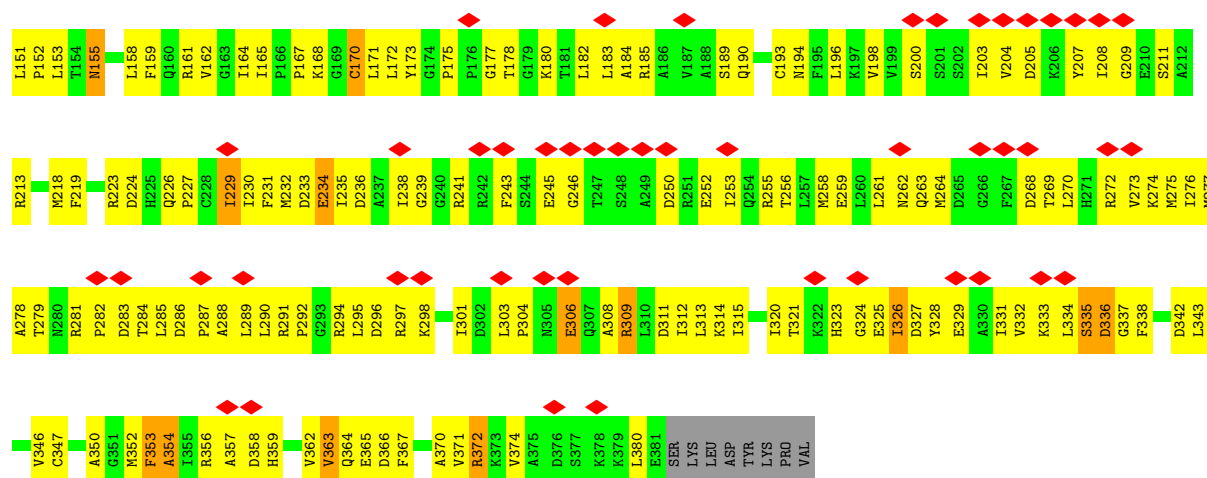


- Molecule 15: 26S proteasome regulatory subunit 6B

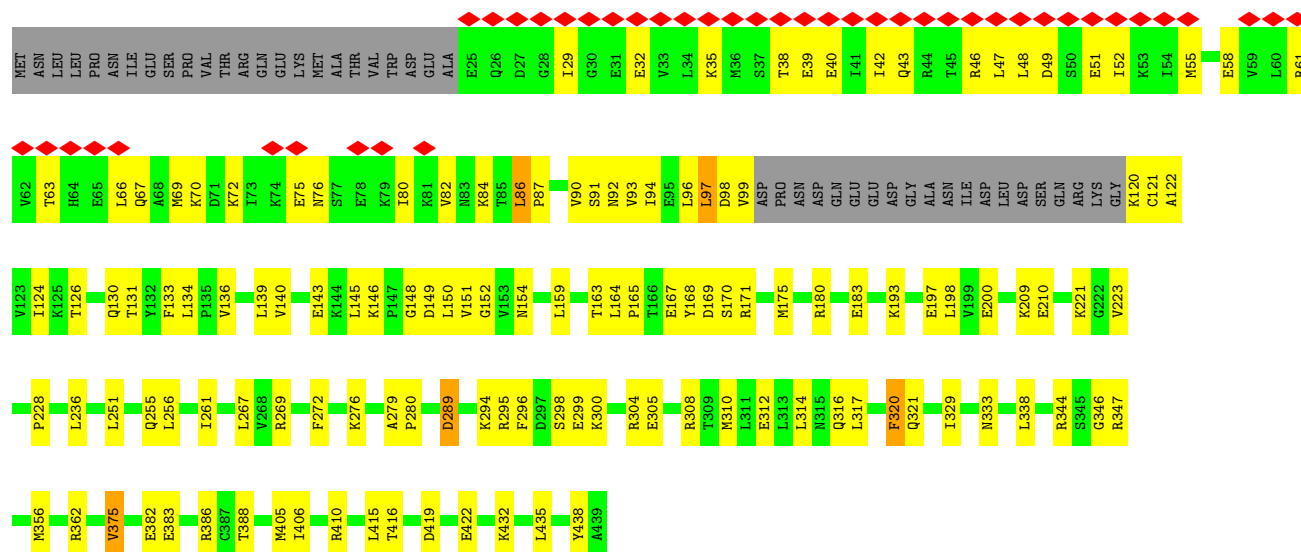


- Molecule 16: 26S proteasome regulatory subunit 10B

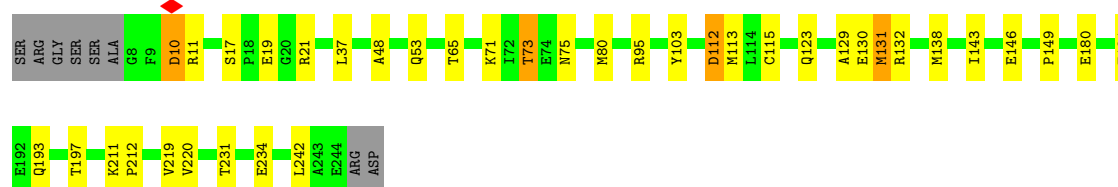
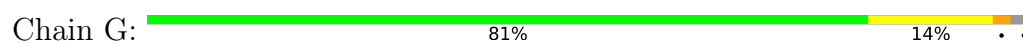




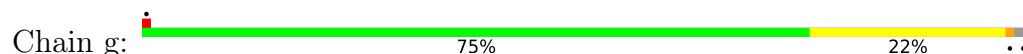
• Molecule 17: 26S proteasome regulatory subunit 6A

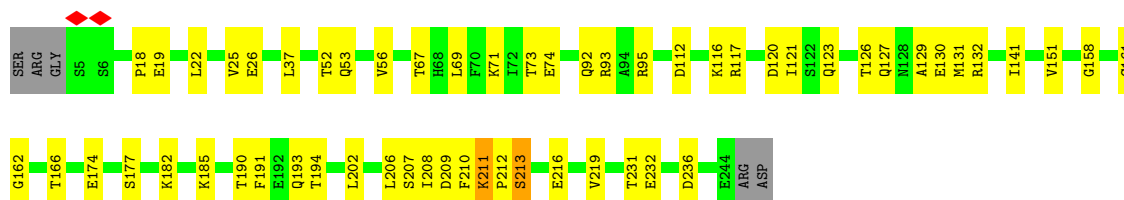


• Molecule 18: Proteasome subunit alpha type-6



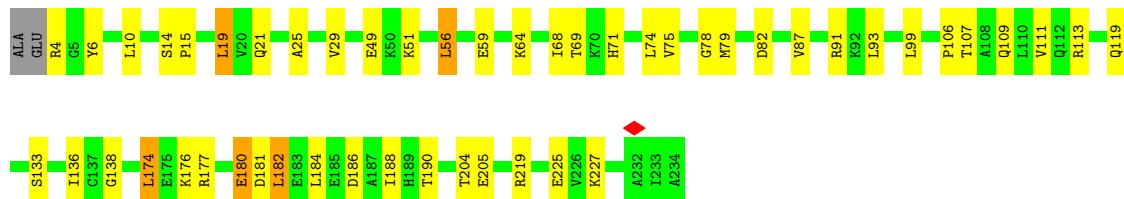
• Molecule 18: Proteasome subunit alpha type-6





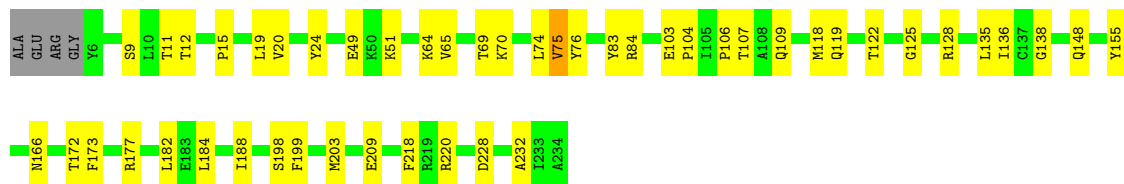
• Molecule 19: Proteasome subunit alpha type-2

Chain H: 78% 19% ..



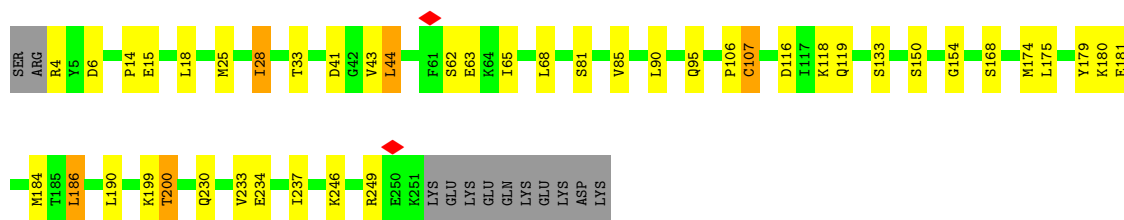
• Molecule 19: Proteasome subunit alpha type-2

Chain h: 78% 20% .



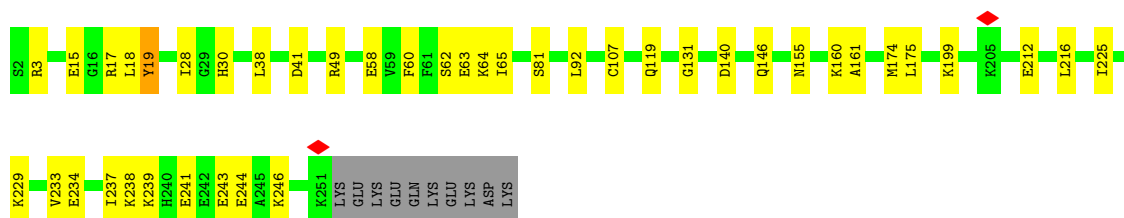
• Molecule 20: Proteasome subunit alpha type-4

Chain I: 78% 15% 5% .



• Molecule 20: Proteasome subunit alpha type-4

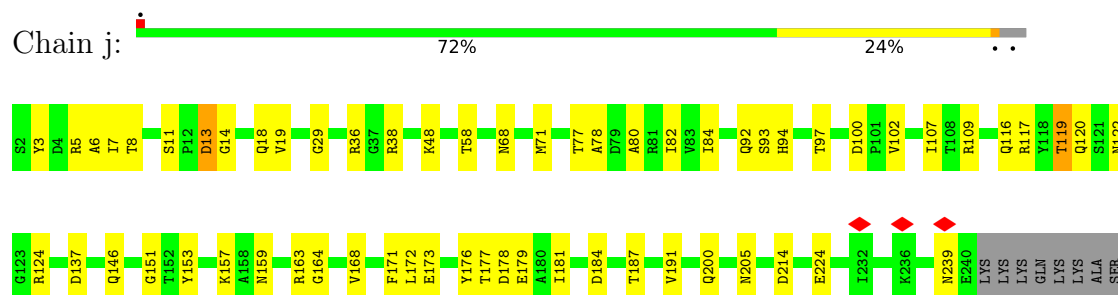
Chain i: 80% 16% .



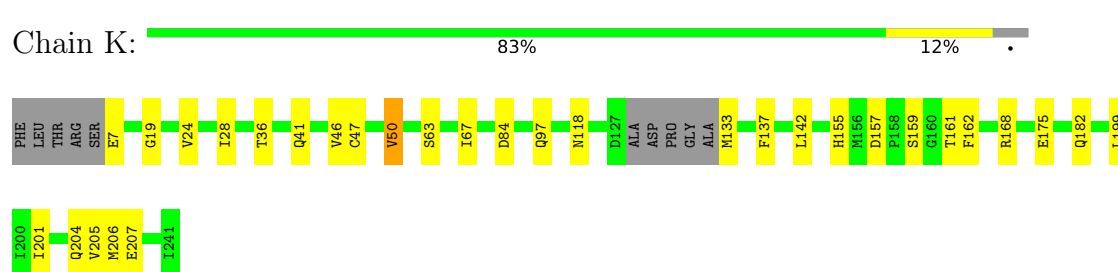
- Molecule 21: Proteasome subunit alpha type-7



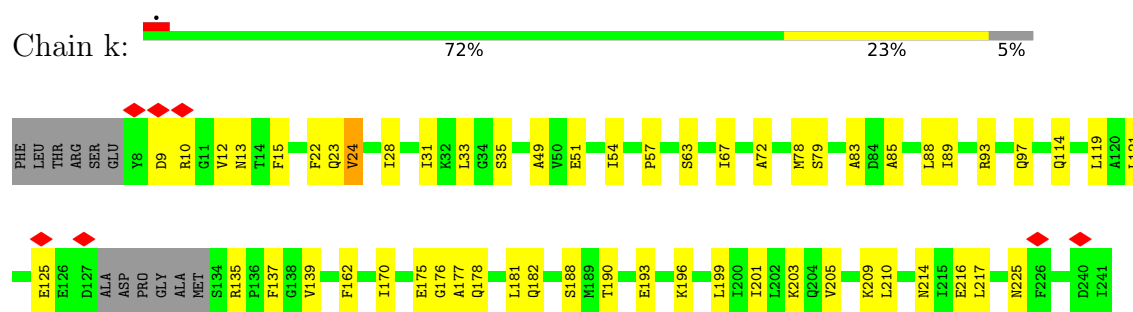
- Molecule 21: Proteasome subunit alpha type-7



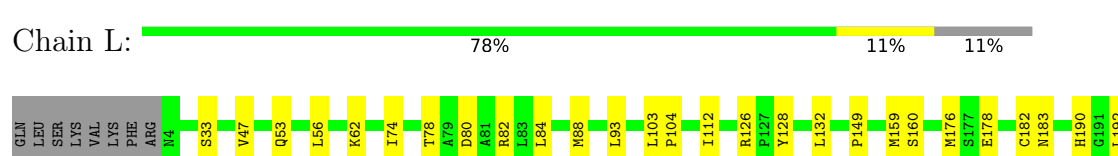
- Molecule 22: Proteasome subunit alpha type-5

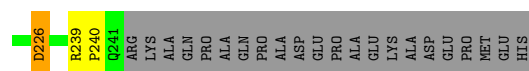


- Molecule 22: Proteasome subunit alpha type-5

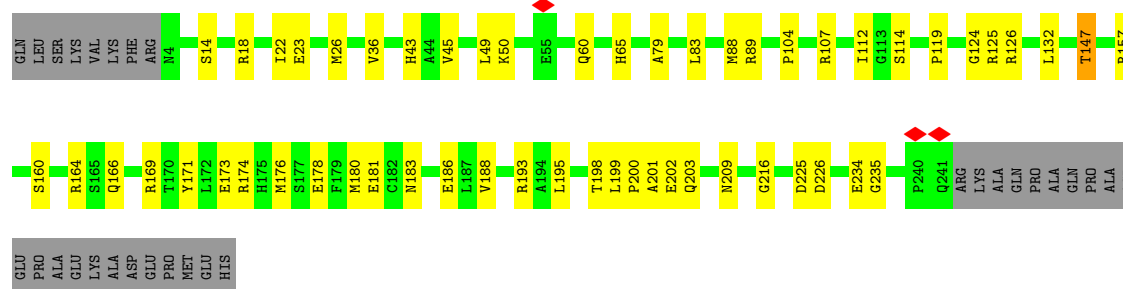


- Molecule 23: Isoform Long of Proteasome subunit alpha type-1

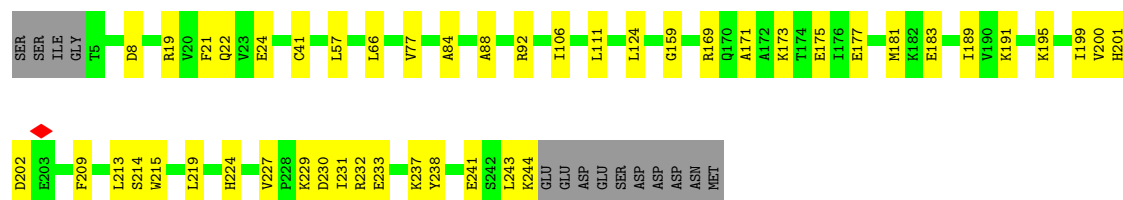
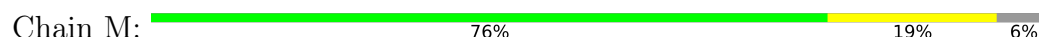




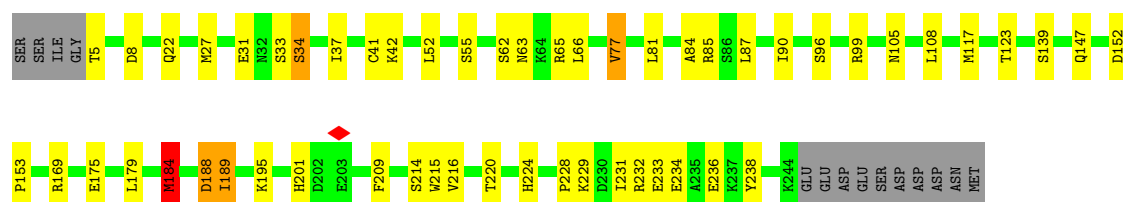
- Molecule 23: Isoform Long of Proteasome subunit alpha type-1



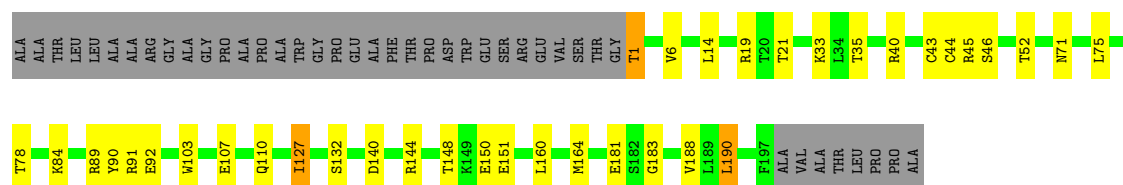
- Molecule 24: Proteasome subunit alpha type-3



- Molecule 24: Proteasome subunit alpha type-3

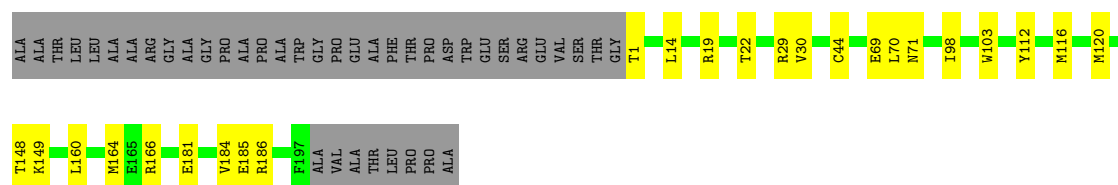


- Molecule 25: Proteasome subunit beta type-6



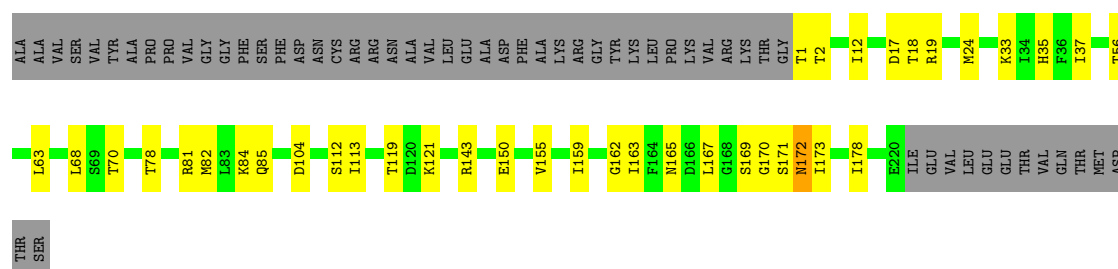
- Molecule 25: Proteasome subunit beta type-6

Chain n:  73% 10% 17%



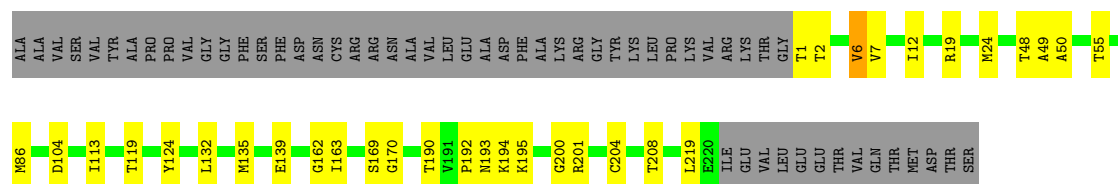
- Molecule 26: Proteasome subunit beta type-7

Chain O:  66% 13% 20%




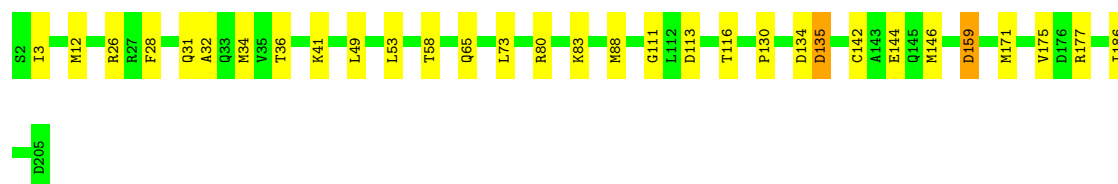
- Molecule 26: Proteasome subunit beta type-7

Chain o:  68% 12% 20%




- Molecule 27: Proteasome subunit beta type-3

Chain P:  85% 14% .




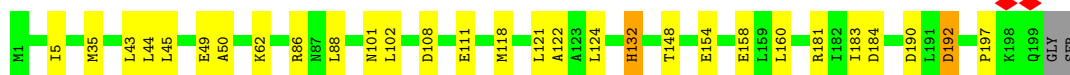
- Molecule 27: Proteasome subunit beta type-3

Chain p:  86% 13% .




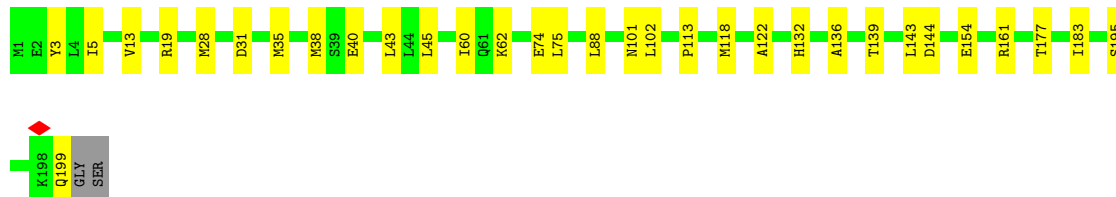
- Molecule 28: Proteasome subunit beta type-2

Chain Q:  85% 13% ..



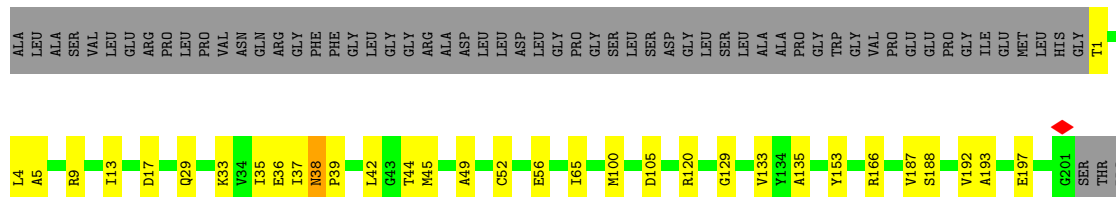
• Molecule 28: Proteasome subunit beta type-2

Chain q:  83% 16% .



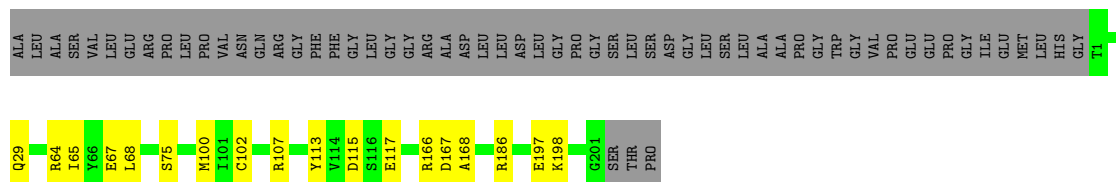
• Molecule 29: Proteasome subunit beta type-5

Chain R:  64% 12% 23%




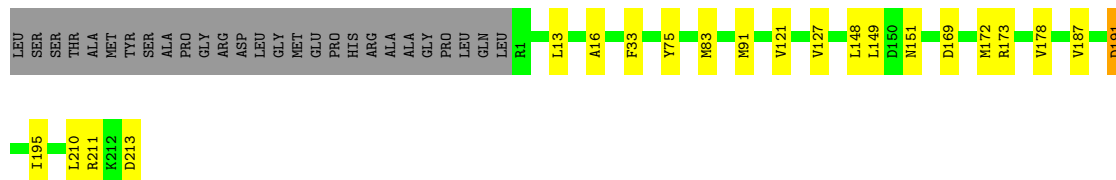
• Molecule 29: Proteasome subunit beta type-5

Chain r:  70% 7% 23%



• Molecule 30: Proteasome subunit beta type-1

Chain S:  80% 8% 11%



• Molecule 30: Proteasome subunit beta type-1

F124	D125	G128	S129	Y130	Q131	M144	L145	L148	L149	D150	E162	D169	R173	K176	D177	V178	E184	R185	Y188	T189	G190	D191	T199	K200	V208	R211	K212	D213																	
LEU	SER	THR	ALA	NET	TYR	SER	ALA	GLY	ARG	ASP	LEU	GLY	MET	GLU	PRO	HIS	ARG	ALA	ALA	GLY	PRO	LEU	GLN	LEU	R1	F2	S3	P4	A16	G17	E18	T27	R28	F33	D39	F57	D60	T65	E69	M83	A87	K118	V121	Y122	I123

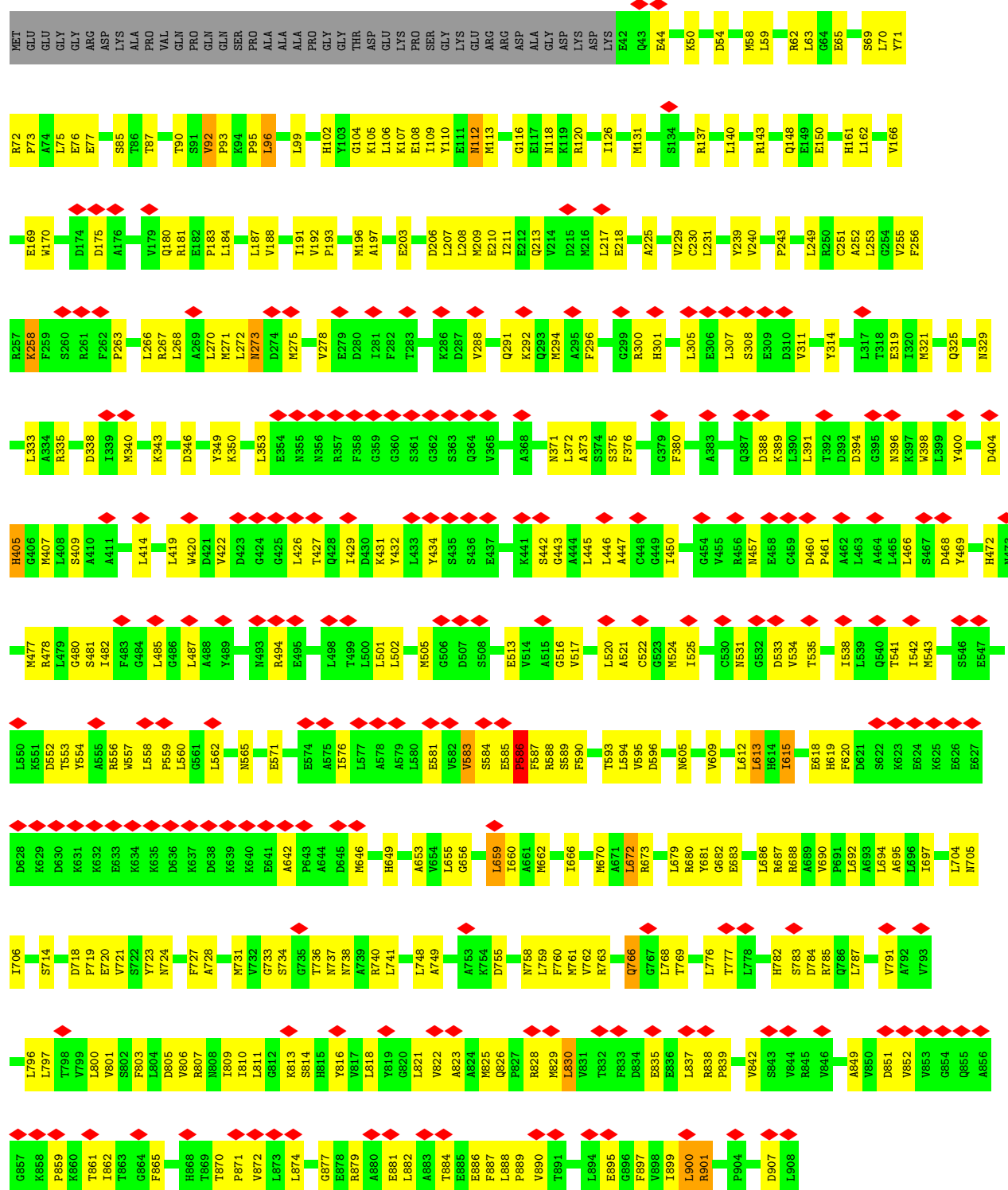
L92	M96	R100	S101	M108	T109	M110	V111	T112	D117	Y124	L137	Y144	L150	V153	T163	L168	R179	F187	T191	V192	V197	E206	J215	SER	GLY	PHE	GLU

R41	R45	T49	D59	L63	Q69	P85	R86	L92	R100	L106	W107	N108	T109	M110	L122	G123	Y124	A131	P135	S136	L137	R151	E155	F156	Q157	P158	V159	Y177	F187	T207	M208	W209	L215	SER	GLY	PHE	GLU									
ALA	LEU	GLY	SER	ARG	GLY	LEU	TRP	ALA	GLY	GLY	PRO	ALA	PRO	GLY	GLN	PHE	TYR	ARG	TLE	PRO	SER	PHE	MET	ASP	PRO	ALA	SER	ALA	LEU	TYR	ARG	GLY	PRO	TLE	THR	ARG	T1	T9	S10	K15	V20	V21	D25	M26	L27	A34

[illegible]

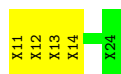
SER	ARG	LYS	ALA	GLY	GLY	ARG	SER	ASP	ASP	LYS	ALA	SER	SER	SER	SER	PRO	VAL	GLN	PRO	GLY	GLY	LEU	GLY	LEU	ASP	PHE	GLU	ASP	LYS	SER	VAL	TRP	ARG	LYS	PRO	GLU	GLY	VAL	ASN	PRO	ASP	ASP	LYS	LYS	LYS	SER	GLU	PHE	VAL	VAL	ALA
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• Molecule 33: 26S proteasome non-ATPase regulatory subunit 2



- Molecule 34: substrate peptide

Chain v:  71% 29%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23186	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.757	Depositor
Minimum map value	-1.033	Depositor
Average map value	0.022	Depositor
Map value standard deviation	0.105	Depositor
Recommended contour level	0.42	Depositor
Map size (Å)	510.0, 510.0, 510.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.21	0/6945	0.47	0/9382
2	V	0.21	0/3929	0.53	0/5309
3	W	0.25	0/3726	0.63	1/5006 (0.0%)
4	X	0.22	0/3053	0.54	2/4115 (0.0%)
5	Y	0.29	0/3167	0.66	0/4266
6	Z	0.28	0/2324	0.64	1/3150 (0.0%)
7	a	0.26	1/3053 (0.0%)	0.57	0/4133
8	b	0.19	0/1478	0.48	1/2001 (0.0%)
9	c	0.28	0/2302	0.68	1/3110 (0.0%)
10	d	0.30	0/2162	0.62	2/2919 (0.1%)
11	e	0.32	0/338	0.65	0/450
12	A	0.22	0/3283	0.53	2/4433 (0.0%)
13	B	0.22	0/3208	0.55	1/4327 (0.0%)
14	C	0.21	0/3148	0.50	0/4228
15	D	0.27	0/3090	0.56	0/4168
16	E	0.28	0/3077	0.70	3/4141 (0.1%)
17	F	0.20	0/3137	0.49	0/4223
18	G	0.28	0/1842	0.51	0/2500
18	g	0.15	0/1863	0.38	0/2527
19	H	0.23	0/1750	0.47	0/2379
19	h	0.25	0/1740	0.44	1/2368 (0.0%)
20	I	0.31	0/1925	0.51	0/2606
20	i	0.19	0/1942	0.46	0/2628
21	J	0.18	0/1869	0.43	0/2531
21	j	0.24	0/1728	0.54	0/2358
22	K	0.16	0/1772	0.37	0/2397
22	k	0.16	0/1747	0.38	0/2364
23	L	0.16	0/1885	0.39	1/2552 (0.0%)
23	l	0.17	0/1885	0.41	0/2552
24	M	0.23	0/1891	0.48	0/2552
24	m	0.23	0/1897	0.49	0/2559
25	N	0.19	0/1508	0.41	0/2040

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
25	n	0.19	0/1508	0.39	0/2040
26	O	0.17	0/1670	0.39	0/2265
26	o	0.18	0/1670	0.44	0/2265
27	P	0.16	0/1620	0.38	0/2184
27	p	0.17	0/1620	0.39	0/2184
28	Q	0.16	0/1603	0.39	0/2174
28	q	0.16	0/1607	0.37	0/2178
29	R	0.34	0/1579	0.54	0/2134
29	r	0.17	0/1579	0.36	0/2134
30	S	0.16	0/1671	0.36	0/2253
30	s	0.16	0/1671	0.36	0/2253
31	T	0.19	0/1700	0.41	0/2305
31	t	0.16	0/1706	0.36	0/2312
32	f	0.17	0/371	0.33	0/492
33	x	0.21	0/6836	0.45	0/9244
All	All	0.22	1/107075 (0.0%)	0.50	16/144691 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	G	0	1
33	x	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	a	226	ARG	CG-CD	-5.09	1.37	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	c	169	VAL	N-CA-C	-7.68	106.00	113.53
10	d	204	LYS	N-CA-C	-7.63	103.22	112.54
16	E	353	PHE	N-CA-C	-7.19	104.64	113.19
10	d	16	LEU	N-CA-C	-6.55	105.92	114.04
16	E	354	ALA	N-CA-C	-6.17	104.46	111.07
3	W	256	ILE	N-CA-C	-6.17	107.48	113.53
8	b	79	GLN	CA-CB-CG	5.80	125.70	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Z	260	VAL	N-CA-C	5.59	115.72	110.30
12	A	114	ASN	CA-C-N	-5.47	116.50	121.65
12	A	114	ASN	C-N-CA	-5.47	116.50	121.65
19	h	15	PRO	CA-N-CD	-5.42	104.41	112.00
23	L	226	ASP	CB-CA-C	-5.19	110.17	117.23
16	E	363	VAL	N-CA-C	5.18	115.11	107.75
4	X	317	PRO	CA-C-N	5.07	131.10	121.97
4	X	317	PRO	C-N-CA	5.07	131.10	121.97
13	B	435	PRO	CA-N-CD	-5.03	104.97	112.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	G	132	ARG	Sidechain
33	x	901	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6828	0	6886	330	0
2	V	3852	0	3893	302	0
3	W	3679	0	3795	334	0
4	X	3009	0	3113	156	0
5	Y	3109	0	3109	227	0
6	Z	2281	0	2312	207	0
7	a	2995	0	3012	204	0
8	b	1458	0	1505	89	0
9	c	2260	0	2276	197	0
10	d	2116	0	2146	145	0
11	e	334	0	294	30	0
12	A	3229	0	3262	119	0
13	B	3162	0	3224	155	0
14	C	3107	0	3224	121	0
15	D	3040	0	3076	166	0
16	E	3031	0	3103	273	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	F	3098	0	3187	126	0
18	G	1809	0	1781	24	0
18	g	1830	0	1807	42	0
19	H	1714	0	1617	42	0
19	h	1703	0	1597	41	0
20	I	1895	0	1833	29	0
20	i	1912	0	1851	26	0
21	J	1844	0	1747	31	0
21	j	1704	0	1517	47	0
22	K	1746	0	1695	18	0
22	k	1722	0	1673	40	0
23	L	1850	0	1822	20	0
23	l	1850	0	1822	48	0
24	M	1856	0	1816	28	0
24	m	1862	0	1827	35	0
25	N	1482	0	1450	20	0
25	n	1482	0	1450	18	0
26	O	1643	0	1644	30	0
26	o	1643	0	1644	29	0
27	P	1591	0	1609	22	0
27	p	1591	0	1609	19	0
28	Q	1570	0	1547	17	0
28	q	1574	0	1558	23	0
29	R	1548	0	1499	25	0
29	r	1548	0	1499	15	0
30	S	1641	0	1618	14	0
30	s	1641	0	1618	29	0
31	T	1667	0	1628	21	0
31	t	1673	0	1639	25	0
32	f	367	0	387	15	0
33	x	6723	0	6741	390	0
34	v	70	0	23	5	0
35	c	1	0	0	0	0
36	A	31	0	12	1	0
36	B	31	0	12	1	0
36	C	31	0	12	0	0
36	F	31	0	12	0	0
37	A	1	0	0	0	0
37	B	1	0	0	0	0
37	C	1	0	0	0	0
37	F	1	0	0	0	0
38	D	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	E	27	0	12	3	0
39	N	34	0	41	3	0
39	O	34	0	41	4	0
39	R	34	0	41	3	0
39	n	34	0	41	3	0
39	o	34	0	41	7	0
39	r	34	0	41	0	0
All	All	105726	0	105303	3975	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 19.

All (3975) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:482:ILE:CD1	33:x:517:VAL:HG12	1.58	1.34
13:B:85:MET:HE1	33:x:618:GLU:C	1.57	1.28
13:B:85:MET:HE3	33:x:619:HIS:CB	1.67	1.24
6:Z:257:MET:O	6:Z:257:MET:SD	1.96	1.23
3:W:363:ILE:HD12	3:W:392:PHE:CE1	1.73	1.23
33:x:482:ILE:HD11	33:x:517:VAL:CG1	1.69	1.22
5:Y:314:LEU:HD12	5:Y:319:MET:SD	1.82	1.20
7:a:363:MET:CE	9:c:304:LEU:HD22	1.72	1.20
33:x:252:ALA:C	33:x:256:PHE:CE1	2.22	1.18
2:V:494:MET:HE2	14:C:44:ARG:HG2	1.27	1.17
17:F:96:LEU:HD21	17:F:145:LEU:HD11	1.24	1.17
7:a:194:GLN:HB2	7:a:226:ARG:HD3	1.28	1.15
15:D:258:ALA:HB1	15:D:259:PRO:HD2	1.25	1.14
19:h:74:LEU:CD1	19:h:136:ILE:CD1	2.25	1.14
2:V:289:LEU:HD22	2:V:312:ALA:HB2	1.29	1.14
1:U:344:ARG:HD2	1:U:344:ARG:O	1.46	1.13
9:c:51:MET:HA	9:c:51:MET:HE3	1.23	1.12
33:x:252:ALA:HB1	33:x:256:PHE:CZ	1.83	1.12
19:h:74:LEU:HD12	19:h:136:ILE:CD1	1.77	1.11
5:Y:88:LEU:HD21	5:Y:99:GLU:CG	1.79	1.11
5:Y:314:LEU:CD1	5:Y:319:MET:SD	2.39	1.11
33:x:890:VAL:HG23	33:x:900:LEU:HA	1.19	1.10
13:B:67:ARG:NH1	33:x:239:TYR:HD1	1.49	1.09
6:Z:257:MET:HA	6:Z:257:MET:HE2	1.31	1.08
6:Z:120:VAL:HG22	6:Z:139:ILE:HD13	1.36	1.07
15:D:115:ILE:HD12	15:D:115:ILE:O	1.54	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:96:LEU:HD11	17:F:145:LEU:HD13	1.28	1.06
5:Y:97:GLU:OE2	5:Y:132:VAL:HB	1.53	1.06
19:h:74:LEU:HD12	19:h:136:ILE:HD13	1.10	1.05
7:a:373:ASP:CB	10:d:255:MET:HE1	1.87	1.05
19:h:74:LEU:CD1	19:h:136:ILE:HD13	1.86	1.04
16:E:231:PHE:HB3	16:E:276:ILE:HD13	1.37	1.03
2:V:476:PHE:CE2	6:Z:257:MET:HE3	1.92	1.03
5:Y:88:LEU:HD21	5:Y:99:GLU:HG3	1.30	1.03
5:Y:181:LYS:NZ	5:Y:219:PHE:CG	2.26	1.02
3:W:359:VAL:O	3:W:363:ILE:HG13	1.56	1.02
4:X:377:ILE:HB	4:X:388:PHE:HE1	1.21	1.02
7:a:231:GLN:HA	7:a:234:ILE:HG13	1.41	1.02
7:a:363:MET:HE1	9:c:304:LEU:HD22	1.42	1.01
10:d:205:LYS:HB3	10:d:209:TYR:CE2	1.94	1.01
2:V:476:PHE:CE2	6:Z:257:MET:CE	2.43	1.01
5:Y:88:LEU:CD2	5:Y:99:GLU:HG3	1.88	1.01
6:Z:120:VAL:CG2	6:Z:139:ILE:HD13	1.90	1.01
4:X:283:GLN:OE1	4:X:312:GLU:HG2	1.60	1.01
27:P:88:MET:HE3	27:P:130:PRO:CB	1.91	1.01
7:a:311:VAL:O	7:a:315:LEU:HD13	1.61	1.01
16:E:290:LEU:HD23	16:E:295:LEU:HD12	1.43	1.01
13:B:85:MET:CE	33:x:619:HIS:HB2	1.91	1.00
31:T:108:ASN:HB3	31:T:110:MET:HE2	1.42	1.00
33:x:482:ILE:HD12	33:x:517:VAL:HG12	1.40	1.00
3:W:142:ARG:HG2	3:W:146:THR:HG23	1.41	0.99
27:P:88:MET:HE3	27:P:130:PRO:HB3	1.38	0.99
10:d:190:LEU:CD1	10:d:192:THR:HG22	1.92	0.99
33:x:482:ILE:HD11	33:x:517:VAL:HG12	1.23	0.99
7:a:373:ASP:HB3	10:d:255:MET:HE1	0.99	0.98
7:a:373:ASP:HB3	10:d:255:MET:CE	1.93	0.98
6:Z:57:PRO:HD3	6:Z:74:TYR:CE1	1.97	0.98
13:B:85:MET:HE3	33:x:619:HIS:HB2	1.00	0.98
10:d:190:LEU:HD11	10:d:192:THR:HG22	1.47	0.97
9:c:246:LYS:HA	9:c:249:LEU:HD21	1.47	0.97
4:X:377:ILE:HB	4:X:388:PHE:CE1	1.99	0.96
9:c:168:MET:H	9:c:168:MET:HE3	1.30	0.96
7:a:215:GLU:HA	7:a:218:MET:SD	2.06	0.96
9:c:246:LYS:HA	9:c:249:LEU:CD2	1.95	0.96
33:x:659:LEU:HD22	33:x:662:MET:HE1	1.44	0.96
13:B:67:ARG:NH1	33:x:239:TYR:CD1	2.34	0.96
2:V:309:MET:O	2:V:309:MET:HE3	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:373:GLU:OE1	14:C:373:GLU:N	1.99	0.95
7:a:281:THR:OG1	7:a:333:MET:HE3	1.67	0.95
7:a:363:MET:SD	9:c:307:VAL:HG11	2.06	0.95
33:x:256:PHE:CE1	33:x:268:LEU:CD1	2.49	0.94
33:x:889:PRO:HA	33:x:900:LEU:HD23	1.47	0.94
15:D:115:ILE:HG22	15:D:139:LEU:HD23	1.48	0.94
2:V:62:HIS:HA	2:V:65:ARG:HD3	1.49	0.94
3:W:86:ASN:ND2	3:W:92:LYS:HE2	1.82	0.94
13:B:313:LEU:HD23	13:B:341:LEU:CD1	1.98	0.94
5:Y:291:HIS:O	5:Y:295:TYR:HB2	1.68	0.93
16:E:124:HIS:HE1	17:F:344:ARG:NH1	1.65	0.93
1:U:757:MET:SD	1:U:758:PRO:HD3	2.09	0.93
16:E:124:HIS:HE1	17:F:344:ARG:HH12	1.04	0.93
15:D:115:ILE:CG2	15:D:139:LEU:HD23	1.98	0.93
33:x:559:PRO:HG3	33:x:587:PHE:CZ	2.04	0.93
33:x:252:ALA:HB1	33:x:256:PHE:CE1	2.03	0.93
23:L:88:MET:HE3	23:L:112:ILE:HG13	1.50	0.93
13:B:85:MET:HE1	33:x:618:GLU:O	1.67	0.92
5:Y:181:LYS:NZ	5:Y:219:PHE:CD2	2.37	0.92
3:W:363:ILE:HD12	3:W:392:PHE:HE1	1.35	0.92
5:Y:194:PHE:CD1	5:Y:195:LYS:N	2.37	0.91
33:x:542:ILE:HD12	33:x:543:MET:HE2	1.50	0.91
13:B:71:TYR:HA	13:B:74:MET:CE	1.99	0.91
1:U:376:MET:SD	1:U:735:GLY:HA2	2.11	0.91
19:h:74:LEU:HD11	19:h:136:ILE:HD11	1.50	0.91
4:X:385:LEU:HD23	4:X:386:ILE:N	1.86	0.91
4:X:355:LYS:O	4:X:356:LEU:HD23	1.71	0.91
33:x:521:ALA:HA	33:x:524:MET:HE3	1.53	0.90
10:d:12:LYS:HZ1	10:d:14:PRO:HB3	1.37	0.90
10:d:12:LYS:NZ	10:d:14:PRO:HB3	1.87	0.90
33:x:442:SER:O	33:x:446:LEU:HD22	1.72	0.90
16:E:198:VAL:HB	16:E:235:ILE:HG13	1.53	0.90
2:V:186:LYS:HD2	2:V:203:LEU:HB3	1.54	0.90
3:W:436:MET:HG3	9:c:226:MET:HE3	1.54	0.89
17:F:209:LYS:HG2	17:F:210:GLU:OE2	1.72	0.89
1:U:803:LYS:HG2	1:U:875:PHE:HB3	1.54	0.89
1:U:503:GLN:NE2	1:U:508:THR:HG21	1.88	0.89
3:W:89:LEU:HD23	16:E:306:GLU:HG2	1.54	0.89
33:x:252:ALA:HB1	33:x:256:PHE:HZ	1.33	0.89
4:X:385:LEU:HD21	4:X:387:ILE:HD13	1.52	0.89
7:a:363:MET:CE	9:c:304:LEU:CD2	2.50	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:257:MET:SD	6:Z:257:MET:C	2.45	0.88
23:l:157:ARG:CD	23:l:176:MET:HE3	2.03	0.88
3:W:392:PHE:CE1	3:W:396:LEU:HD11	2.08	0.88
4:X:407:MET:HA	4:X:407:MET:HE3	1.56	0.88
5:Y:69:LEU:O	5:Y:73:MET:HE2	1.74	0.88
6:Z:257:MET:HA	6:Z:257:MET:CE	2.01	0.88
17:F:96:LEU:HD21	17:F:145:LEU:CD1	2.04	0.88
1:U:247:GLN:NE2	1:U:912:ILE:HA	1.89	0.87
24:M:41:CYS:SG	24:M:189:ILE:HG13	2.14	0.87
25:n:185:GLU:N	25:n:185:GLU:OE2	2.06	0.87
3:W:363:ILE:CD1	3:W:392:PHE:CE1	2.57	0.87
17:F:228:PRO:HB2	17:F:356:MET:HE2	1.55	0.87
13:B:85:MET:CE	33:x:618:GLU:C	2.46	0.87
33:x:291:GLN:HA	33:x:294:MET:SD	2.15	0.87
1:U:554:LEU:HA	1:U:588:MET:HE1	1.56	0.87
32:f:395:LEU:HD23	33:x:426:LEU:HD21	1.57	0.87
16:E:231:PHE:HB3	16:E:276:ILE:CD1	2.04	0.87
5:Y:88:LEU:HD21	5:Y:99:GLU:CD	1.99	0.86
3:W:95:SER:H	3:W:98:LYS:HB2	1.39	0.86
21:j:177:THR:HG23	21:j:179:GLU:HG2	1.55	0.86
1:U:619:VAL:O	1:U:622:LEU:HD13	1.76	0.86
13:B:85:MET:HE3	33:x:619:HIS:CA	2.05	0.86
23:l:157:ARG:HD2	23:l:176:MET:HE3	1.54	0.86
33:x:272:LEU:O	33:x:273:ASN:ND2	2.08	0.86
16:E:270:LEU:HB3	16:E:273:VAL:HB	1.58	0.86
33:x:822:VAL:HA	33:x:825:MET:SD	2.16	0.86
12:A:235:ALA:HB1	12:A:269:ALA:O	1.76	0.86
7:a:363:MET:HE3	9:c:304:LEU:HD22	1.58	0.85
12:A:182:GLU:OE2	12:A:182:GLU:N	2.09	0.85
16:E:124:HIS:CE1	17:F:344:ARG:HH12	1.92	0.85
13:B:313:LEU:CD2	13:B:341:LEU:HD13	2.04	0.85
33:x:335:ARG:HB2	33:x:340:MET:HE2	1.59	0.85
1:U:803:LYS:CG	1:U:875:PHE:HB3	2.05	0.85
16:E:353:PHE:HA	16:E:356:ARG:HB2	1.57	0.85
31:T:96:MET:HE1	31:T:110:MET:HE1	1.58	0.85
33:x:585:GLU:HA	33:x:588:ARG:HB3	1.57	0.85
6:Z:102:HIS:HD2	6:Z:104:ASN:HB3	1.40	0.85
3:W:141:GLU:OE1	3:W:142:ARG:N	2.09	0.85
6:Z:190:ARG:HD3	9:c:297:VAL:HG11	1.58	0.85
3:W:365:ILE:HD12	3:W:366:MET:N	1.91	0.85
10:d:195:THR:HG21	10:d:201:ASN:HB3	1.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:295:ARG:HH22	17:F:298:SER:HB2	1.41	0.85
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.58	0.85
1:U:532:MET:HG3	1:U:548:LEU:HD12	1.59	0.84
7:a:18:GLN:HG3	7:a:19:PRO:HD3	1.59	0.84
2:V:438:VAL:O	2:V:442:ILE:HD12	1.78	0.84
9:c:54:MET:HE2	9:c:86:ALA:HB3	1.58	0.84
10:d:205:LYS:HB3	10:d:209:TYR:HE2	1.43	0.84
16:E:353:PHE:HA	16:E:356:ARG:CB	2.07	0.84
33:x:890:VAL:HG23	33:x:900:LEU:CA	2.06	0.84
33:x:256:PHE:CE1	33:x:268:LEU:HD11	2.11	0.84
3:W:436:MET:HB3	9:c:226:MET:HG2	1.58	0.84
15:D:264:ILE:HG22	15:D:267:ILE:CG2	2.08	0.84
33:x:731:MET:N	33:x:731:MET:SD	2.51	0.84
7:a:197:ALA:HB1	7:a:222:LEU:HD12	1.57	0.84
13:B:71:TYR:HA	13:B:74:MET:HE1	1.59	0.84
2:V:100:MET:HG2	2:V:102:PRO:HD2	1.60	0.83
33:x:256:PHE:CZ	33:x:268:LEU:HD11	2.13	0.83
3:W:230:MET:SD	3:W:246:HIS:HB2	2.18	0.83
10:d:205:LYS:HB3	10:d:209:TYR:CD2	2.11	0.83
33:x:740:ARG:H	33:x:740:ARG:HE	1.25	0.83
33:x:252:ALA:C	33:x:256:PHE:HE1	1.82	0.83
15:D:384:MET:HE1	16:E:167:PRO:HG3	1.61	0.83
2:V:476:PHE:HE2	6:Z:257:MET:HE3	1.39	0.83
13:B:67:ARG:HH11	33:x:239:TYR:HD1	1.24	0.83
13:B:313:LEU:CD2	13:B:341:LEU:CD1	2.57	0.83
7:a:234:ILE:HD12	7:a:235:ASP:N	1.94	0.83
9:c:51:MET:HA	9:c:51:MET:CE	2.08	0.83
8:b:79:GLN:OE1	8:b:81:LYS:HB2	1.79	0.83
9:c:124:GLY:HA2	9:c:127:ILE:HD12	1.59	0.83
15:D:388:ARG:HH22	16:E:297:ARG:HG2	1.40	0.83
1:U:188:MET:SD	1:U:189:GLN:N	2.52	0.82
5:Y:197:ALA:O	5:Y:201:PHE:HB2	1.77	0.82
1:U:481:LEU:HD12	1:U:482:GLY:N	1.94	0.82
3:W:366:MET:HG3	3:W:378:MET:CE	2.10	0.82
7:a:373:ASP:O	10:d:255:MET:HE3	1.78	0.82
4:X:350:ILE:HD11	4:X:361:VAL:HG11	1.60	0.82
7:a:363:MET:HE3	9:c:304:LEU:CD2	2.10	0.82
16:E:371:VAL:HG23	16:E:372:ARG:N	1.94	0.82
33:x:727:PHE:O	33:x:731:MET:HE2	1.78	0.82
3:W:183:VAL:O	3:W:187:LEU:HD12	1.80	0.82
15:D:258:ALA:HB1	15:D:259:PRO:CD	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:h:74:LEU:HD11	19:h:136:ILE:CD1	2.05	0.82
1:U:173:VAL:HG12	1:U:175:GLY:H	1.44	0.81
33:x:110:TYR:HA	33:x:113:MET:HE1	1.61	0.81
1:U:532:MET:HG3	1:U:548:LEU:CD1	2.11	0.81
21:J:233:GLU:HA	21:J:236:LYS:HD3	1.62	0.81
9:c:61:PHE:CZ	9:c:139:ARG:HG3	2.14	0.81
15:D:264:ILE:HG22	15:D:267:ILE:HG22	1.63	0.81
23:L:88:MET:HE3	23:L:112:ILE:CG1	2.10	0.81
33:x:335:ARG:C	33:x:335:ARG:HE	1.89	0.81
3:W:343:SER:HB2	3:W:347:GLY:H	1.45	0.81
6:Z:79:TYR:CZ	6:Z:91:ILE:HG13	2.16	0.81
33:x:682:GLY:CA	33:x:686:LEU:HD11	2.11	0.81
16:E:329:GLU:HG3	16:E:333:LYS:NZ	1.96	0.80
1:U:386:LEU:C	1:U:387:ARG:HE	1.88	0.80
13:B:374:LEU:HD23	13:B:378:VAL:CG1	2.11	0.80
33:x:443:GLY:HA2	33:x:446:LEU:HD23	1.62	0.80
5:Y:80:GLU:O	5:Y:84:LEU:HD23	1.80	0.80
3:W:359:VAL:HG12	3:W:363:ILE:HD11	1.62	0.80
9:c:26:ASP:H	9:c:174:PRO:HD2	1.45	0.80
3:W:98:LYS:HE2	3:W:135:LYS:HA	1.64	0.80
5:Y:314:LEU:HD11	5:Y:319:MET:SD	2.21	0.80
2:V:289:LEU:HD22	2:V:312:ALA:CB	2.09	0.80
1:U:532:MET:HE1	1:U:551:GLY:C	2.06	0.80
5:Y:160:ASN:HA	5:Y:163:LYS:HB3	1.63	0.80
7:a:374:ILE:CD1	10:d:255:MET:HG3	2.12	0.80
16:E:36:LEU:HD21	17:F:70:LYS:HG3	1.64	0.79
21:j:8:THR:HB	22:k:135:ARG:HB3	1.63	0.79
15:D:99:ASN:HA	15:D:115:ILE:CD1	2.12	0.79
33:x:335:ARG:NE	33:x:335:ARG:O	2.14	0.79
2:V:289:LEU:CD2	2:V:312:ALA:HB2	2.12	0.79
6:Z:257:MET:HE2	6:Z:257:MET:CA	2.07	0.79
9:c:191:ALA:CB	9:c:196:LEU:HB2	2.11	0.79
16:E:275:MET:SD	16:E:277:MET:HB3	2.22	0.79
31:T:108:ASN:HB3	31:T:110:MET:CE	2.11	0.79
23:l:225:ASP:OD1	23:l:226:ASP:HB2	1.83	0.79
1:U:796:LYS:C	1:U:797:MET:HE3	2.08	0.79
2:V:324:PHE:HB2	11:e:5:LYS:HB2	1.64	0.79
1:U:220:LEU:HD11	1:U:229:VAL:HB	1.64	0.79
5:Y:297:ARG:HH11	11:e:52:PHE:HD1	1.29	0.79
3:W:104:MET:HG2	3:W:123:ARG:NH1	1.98	0.79
3:W:142:ARG:NH1	3:W:146:THR:HG21	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:184:LEU:HD22	9:c:204:THR:HA	1.65	0.79
29:R:45:MET:HG2	29:R:52:CYS:HB3	1.65	0.79
2:V:90:GLU:O	2:V:94:VAL:HB	1.81	0.79
16:E:239:GLY:HA2	16:E:253:ILE:HG22	1.64	0.79
1:U:17:PRO:HA	1:U:20:LYS:HG2	1.64	0.78
2:V:65:ARG:HH21	2:V:153:LYS:HE3	1.47	0.78
3:W:366:MET:HG3	3:W:378:MET:HE3	1.65	0.78
4:X:407:MET:HE1	9:c:255:TYR:CE2	2.18	0.78
5:Y:319:MET:HB2	5:Y:330:ILE:HD12	1.65	0.78
22:k:203:LYS:HB2	22:k:210:LEU:HD22	1.65	0.78
2:V:324:PHE:O	2:V:328:VAL:HG23	1.83	0.78
4:X:385:LEU:HD21	4:X:387:ILE:CD1	2.13	0.78
10:d:198:LEU:O	10:d:199:PHE:HB2	1.80	0.78
16:E:36:LEU:HD21	17:F:70:LYS:HD2	1.63	0.78
9:c:61:PHE:CE1	9:c:139:ARG:HG3	2.18	0.78
5:Y:24:PHE:CD2	5:Y:28:LEU:HD23	2.19	0.78
5:Y:97:GLU:HA	5:Y:101:ARG:HH21	1.48	0.78
16:E:124:HIS:CE1	17:F:344:ARG:NH1	2.51	0.78
33:x:252:ALA:O	33:x:256:PHE:CD1	2.37	0.78
33:x:589:SER:O	33:x:593:THR:HG23	1.84	0.78
6:Z:134:PRO:HG3	9:c:220:LEU:HD12	1.65	0.78
16:E:36:LEU:HD21	17:F:70:LYS:CG	2.14	0.78
26:O:2:THR:HG21	26:O:162:GLY:HA3	1.66	0.78
33:x:252:ALA:CB	33:x:256:PHE:CE1	2.67	0.78
1:U:886:PRO:O	1:U:889:LEU:HD22	1.84	0.78
5:Y:42:MET:SD	5:Y:42:MET:N	2.56	0.78
13:B:313:LEU:HD21	13:B:341:LEU:HD13	1.65	0.78
5:Y:97:GLU:CD	5:Y:132:VAL:HB	2.08	0.77
9:c:245:VAL:O	9:c:249:LEU:HD23	1.85	0.77
33:x:659:LEU:HD22	33:x:659:LEU:O	1.83	0.77
1:U:321:GLN:O	1:U:325:MET:HE3	1.85	0.77
9:c:163:ILE:HG21	9:c:198:ARG:O	1.85	0.77
16:E:371:VAL:HG23	16:E:372:ARG:H	1.50	0.77
28:Q:192:ASP:OD1	28:Q:192:ASP:N	2.16	0.77
3:W:436:MET:HG3	9:c:226:MET:CE	2.13	0.77
33:x:889:PRO:CA	33:x:900:LEU:HD23	2.14	0.77
16:E:371:VAL:CG2	16:E:372:ARG:H	1.97	0.77
9:c:60:GLU:HA	9:c:107:MET:HE3	1.65	0.77
23:L:84:LEU:O	23:L:88:MET:HG3	1.84	0.77
33:x:93:PRO:HB2	33:x:96:LEU:HB2	1.66	0.77
15:D:252:ARG:O	15:D:256:GLU:HG2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:329:GLU:HG3	16:E:333:LYS:HZ3	1.49	0.77
4:X:385:LEU:HD23	4:X:385:LEU:C	2.10	0.77
13:B:67:ARG:HG2	33:x:666:ILE:HG21	1.66	0.77
15:D:115:ILE:HG22	15:D:139:LEU:CD2	2.14	0.77
3:W:35:ALA:HA	3:W:48:LEU:HD13	1.66	0.77
33:x:559:PRO:HB2	33:x:594:LEU:HD11	1.66	0.77
1:U:553:ALA:O	1:U:588:MET:HE2	1.84	0.76
10:d:188:LYS:HB3	10:d:221:ASN:OD1	1.84	0.76
15:D:264:ILE:CG2	15:D:267:ILE:HG22	2.15	0.76
6:Z:79:TYR:CE1	6:Z:91:ILE:HG13	2.19	0.76
12:A:103:ASN:HD22	17:F:167:GLU:HG3	1.49	0.76
33:x:890:VAL:CG2	33:x:900:LEU:HA	2.11	0.76
3:W:124:LEU:O	3:W:128:LEU:HD23	1.85	0.76
2:V:225:ASP:HA	2:V:228:ARG:HG3	1.68	0.76
3:W:95:SER:HA	3:W:99:GLN:H	1.49	0.76
13:B:278:ALA:HB1	13:B:279:PRO:HD2	1.67	0.76
4:X:407:MET:HE1	9:c:255:TYR:HE2	1.49	0.76
33:x:270:LEU:HD12	33:x:787:LEU:HD12	1.67	0.76
3:W:231:ILE:HD11	3:W:246:HIS:HB3	1.65	0.76
15:D:99:ASN:HA	15:D:115:ILE:HD11	1.66	0.76
16:E:172:LEU:HG	16:E:276:ILE:HG23	1.66	0.76
33:x:887:PHE:CE2	33:x:900:LEU:HD13	2.20	0.76
34:v:13:UNK:O	34:v:14:UNK:C	2.32	0.76
5:Y:26:LEU:HD12	5:Y:36:ALA:HB3	1.66	0.76
16:E:236:ASP:HA	16:E:279:THR:OG1	1.86	0.76
1:U:344:ARG:HD2	1:U:344:ARG:C	2.11	0.76
13:B:85:MET:HE1	33:x:619:HIS:N	1.99	0.76
2:V:476:PHE:HB3	6:Z:260:VAL:HG21	1.68	0.75
4:X:266:ASP:HB3	4:X:270:LEU:HD13	1.66	0.75
23:l:88:MET:HE3	23:l:112:ILE:HD11	1.66	0.75
10:d:203:PRO:HG2	10:d:206:MET:H	1.51	0.75
33:x:482:ILE:CD1	33:x:517:VAL:CG1	2.38	0.75
7:a:373:ASP:C	10:d:255:MET:HE3	2.12	0.75
9:c:89:PRO:HA	9:c:92:GLN:HB2	1.68	0.75
15:D:92:PHE:HA	15:D:103:VAL:HG12	1.69	0.75
16:E:235:ILE:HB	16:E:277:MET:SD	2.27	0.75
1:U:554:LEU:HA	1:U:588:MET:CE	2.16	0.75
15:D:384:MET:CE	16:E:167:PRO:HG3	2.17	0.75
16:E:245:GLU:HG3	16:E:246:GLY:H	1.50	0.75
19:H:180:GLU:H	19:H:180:GLU:CD	1.93	0.75
33:x:446:LEU:HD11	33:x:480:GLY:HA2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:97:GLU:CD	5:Y:97:GLU:H	1.93	0.75
16:E:173:TYR:HE1	16:E:298:LYS:HB3	1.51	0.75
17:F:269:ARG:HG2	17:F:316:GLN:HE21	1.51	0.75
3:W:340:VAL:HG22	3:W:350:ARG:CZ	2.17	0.75
4:X:110:CYS:O	4:X:114:ILE:HG13	1.86	0.75
6:Z:28:LYS:H	9:c:104:ARG:HH22	1.35	0.75
16:E:193:CYS:SG	16:E:194:ASN:N	2.59	0.75
1:U:376:MET:HA	1:U:739:ALA:HA	1.67	0.74
1:U:553:ALA:C	1:U:588:MET:HE2	2.12	0.74
7:a:246:GLU:HA	7:a:246:GLU:OE2	1.85	0.74
17:F:406:ILE:HD13	17:F:422:GLU:HG2	1.69	0.74
2:V:159:LEU:HG	2:V:162:GLU:OE1	1.88	0.74
5:Y:163:LYS:O	5:Y:168:ILE:HG12	1.87	0.74
21:j:122:ASN:ND2	22:k:9:ASP:OD2	2.20	0.74
9:c:26:ASP:HB2	9:c:173:GLU:HA	1.69	0.74
33:x:482:ILE:HD11	33:x:517:VAL:CB	2.16	0.74
3:W:213:PHE:HB2	3:W:223:LYS:HE3	1.69	0.74
13:B:59:ARG:NH1	33:x:209:MET:SD	2.59	0.74
15:D:342:ARG:HG2	15:D:364:VAL:HG11	1.68	0.74
9:c:91:PHE:HA	9:c:94:LYS:HE2	1.68	0.74
15:D:99:ASN:H	15:D:115:ILE:HD11	1.52	0.74
1:U:232:ILE:HA	1:U:235:LYS:HD2	1.67	0.74
9:c:58:LEU:HG	9:c:106:GLU:HG3	1.69	0.74
1:U:803:LYS:HG2	1:U:875:PHE:O	1.88	0.74
10:d:19:CYS:SG	10:d:65:ARG:NH2	2.61	0.74
13:B:71:TYR:HA	13:B:74:MET:HE2	1.68	0.74
31:T:92:LEU:HD12	31:T:112:ILE:HD11	1.68	0.74
16:E:289:LEU:HD12	16:E:295:LEU:HD11	1.69	0.74
3:W:142:ARG:CG	3:W:146:THR:HG23	2.18	0.74
12:A:114:ASN:HB3	12:A:120:LYS:HZ3	1.53	0.74
1:U:206:MET:HE2	1:U:206:MET:HA	1.69	0.74
1:U:344:ARG:NH2	1:U:345:ASN:HB2	2.03	0.74
7:a:275:LEU:HD23	7:a:278:MET:HE3	1.68	0.74
13:B:85:MET:CE	33:x:619:HIS:N	2.51	0.74
14:C:242:ALA:HB1	14:C:243:PRO:HD2	1.67	0.74
33:x:683:GLU:O	33:x:686:LEU:HD12	1.88	0.74
8:b:87:CYS:SG	8:b:91:ARG:NH2	2.61	0.73
6:Z:256:GLN:NE2	6:Z:257:MET:HA	2.02	0.73
20:i:18:LEU:O	20:i:19:TYR:HB2	1.86	0.73
7:a:163:TYR:HB2	7:a:172:TYR:HB2	1.70	0.73
9:c:58:LEU:HD22	9:c:71:ASP:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:71:VAL:HG11	16:E:100:LEU:HD21	1.70	0.73
1:U:607:VAL:HG23	15:D:67:ASN:HD21	1.52	0.73
2:V:347:GLN:HG2	2:V:348:PHE:HD1	1.53	0.73
13:B:313:LEU:HD23	13:B:341:LEU:HD12	1.70	0.73
19:h:51:LYS:HE2	19:h:199:PHE:CZ	2.23	0.73
33:x:888:LEU:O	33:x:900:LEU:HB3	1.88	0.73
7:a:211:PHE:O	7:a:212:ASN:ND2	2.22	0.73
13:B:85:MET:CE	33:x:619:HIS:CA	2.66	0.73
33:x:659:LEU:CD2	33:x:662:MET:HE1	2.16	0.73
3:W:392:PHE:HE1	3:W:396:LEU:HD11	1.54	0.73
1:U:225:ASP:OD2	1:U:228:ALA:HB2	1.89	0.73
15:D:115:ILE:HG22	15:D:139:LEU:CB	2.19	0.73
6:Z:226:ILE:HG23	6:Z:230:LEU:HD13	1.70	0.72
15:D:368:ASP:O	15:D:370:ILE:HD13	1.90	0.72
2:V:464:ILE:HG22	2:V:466:ILE:H	1.53	0.72
3:W:151:THR:HG23	3:W:152:ILE:HD12	1.71	0.72
16:E:97:ARG:HG2	16:E:111:LEU:HB2	1.72	0.72
20:I:28:ILE:HD13	20:I:133:SER:HB2	1.70	0.72
26:o:163:ILE:HG12	26:o:169:SER:HB3	1.70	0.72
2:V:81:GLN:HB2	2:V:85:ALA:HB3	1.72	0.72
2:V:84:LYS:HG3	2:V:88:GLY:HA2	1.70	0.72
4:X:345:VAL:HG12	4:X:385:LEU:HB3	1.72	0.72
16:E:36:LEU:HD21	17:F:70:LYS:CD	2.20	0.72
1:U:607:VAL:HG21	15:D:63:ASP:HB3	1.70	0.72
11:e:45:ASP:O	11:e:47:ASN:N	2.23	0.72
1:U:19:LEU:HD23	10:d:27:LYS:HZ1	1.55	0.72
3:W:98:LYS:HA	3:W:135:LYS:HE3	1.71	0.72
3:W:251:TYR:OH	3:W:267:LEU:HD23	1.89	0.72
7:a:84:VAL:HA	7:a:87:MET:HG3	1.72	0.72
15:D:153:MET:CE	15:D:226:ALA:HB1	2.20	0.72
12:A:287:ASP:HB2	16:E:207:TYR:HB2	1.70	0.72
2:V:494:MET:HE2	14:C:44:ARG:CG	2.16	0.71
13:B:374:LEU:HB3	13:B:378:VAL:HG11	1.71	0.71
16:E:204:VAL:HG12	16:E:253:ILE:HD12	1.72	0.71
21:J:64:ALA:O	21:J:88:ARG:NH1	2.23	0.71
1:U:247:GLN:HE22	1:U:912:ILE:HA	1.55	0.71
7:a:227:ASN:O	7:a:231:GLN:NE2	2.23	0.71
14:C:113:ARG:HB3	14:C:127:LEU:HB2	1.71	0.71
1:U:611:ASN:HB3	1:U:614:VAL:HG12	1.72	0.71
1:U:633:CYS:HB2	1:U:659:CYS:SG	2.31	0.71
16:E:350:ALA:HA	16:E:353:PHE:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:615:ILE:HD11	33:x:649:HIS:HD2	1.54	0.71
2:V:309:MET:HG2	2:V:331:LEU:HD11	1.71	0.71
16:E:198:VAL:HG12	16:E:200:SER:H	1.55	0.71
2:V:406:GLY:O	2:V:410:ILE:HD12	1.91	0.71
3:W:12:ARG:HB2	3:W:27:ARG:HH22	1.55	0.71
3:W:86:ASN:HD22	3:W:92:LYS:HE2	1.54	0.71
5:Y:201:PHE:HB3	5:Y:223:THR:HG22	1.73	0.71
30:s:18:GLU:OE1	30:s:118:LYS:NZ	2.23	0.71
33:x:253:LEU:HA	33:x:256:PHE:HD1	1.56	0.71
6:Z:165:GLU:CD	6:Z:166:GLU:HG2	2.15	0.71
15:D:99:ASN:CA	15:D:115:ILE:HD11	2.20	0.71
31:T:9:THR:O	31:T:41:ARG:NH2	2.24	0.71
33:x:252:ALA:C	33:x:256:PHE:CD1	2.68	0.71
33:x:791:VAL:HG12	33:x:823:ALA:HB1	1.72	0.71
1:U:873:PRO:C	1:U:875:PHE:H	1.98	0.71
4:X:328:ASP:OD1	4:X:364:LYS:NZ	2.23	0.71
16:E:371:VAL:CG2	16:E:372:ARG:N	2.54	0.71
32:f:386:ARG:HH22	32:f:389:ARG:HD3	1.56	0.71
5:Y:50:MET:HB2	5:Y:70:LEU:HB3	1.71	0.71
6:Z:256:GLN:HE21	6:Z:257:MET:HA	1.55	0.71
7:a:278:MET:HA	7:a:281:THR:HG22	1.72	0.71
7:a:363:MET:HE1	9:c:304:LEU:CD2	2.16	0.71
14:C:56:VAL:HG12	15:D:72:PHE:HD1	1.54	0.71
16:E:230:ILE:HB	16:E:273:VAL:HG13	1.73	0.71
5:Y:101:ARG:HH12	5:Y:136:HIS:HB3	1.55	0.70
7:a:231:GLN:HA	7:a:234:ILE:CG1	2.20	0.70
18:g:56:VAL:HG23	18:g:56:VAL:O	1.88	0.70
23:l:157:ARG:HD2	23:l:176:MET:CE	2.21	0.70
2:V:309:MET:HE2	2:V:328:VAL:CG1	2.21	0.70
7:a:131:THR:HA	7:a:134:THR:HG22	1.73	0.70
12:A:307:ASP:OD2	12:A:333:ARG:NH2	2.23	0.70
12:A:425:ALA:HB1	12:A:428:ARG:HB2	1.73	0.70
27:p:138:VAL:HB	27:p:146:MET:HE3	1.71	0.70
2:V:492:LYS:O	14:C:44:ARG:NH1	2.24	0.70
3:W:102:ALA:O	3:W:106:GLN:NE2	2.24	0.70
5:Y:118:GLU:OE1	5:Y:118:GLU:N	2.22	0.70
33:x:560:LEU:HD21	33:x:801:VAL:CB	2.20	0.70
7:a:278:MET:HB3	7:a:319:LEU:HD12	1.73	0.70
34:v:12:UNK:O	34:v:13:UNK:C	2.39	0.70
1:U:10:SER:HB2	10:d:73:ARG:HG3	1.72	0.70
3:W:340:VAL:HG12	3:W:341:PHE:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:190:LEU:HD13	10:d:192:THR:HG22	1.72	0.70
1:U:225:ASP:C	1:U:225:ASP:OD1	2.35	0.70
3:W:141:GLU:OE2	3:W:172:GLU:HA	1.92	0.70
5:Y:316:LEU:HD23	5:Y:319:MET:HG3	1.74	0.70
9:c:75:MET:CE	9:c:88:ASP:H	2.04	0.70
1:U:188:MET:SD	1:U:190:ASN:N	2.64	0.70
1:U:524:LYS:HG3	1:U:556:MET:HE1	1.72	0.70
3:W:104:MET:HA	3:W:107:GLN:HG2	1.74	0.70
14:C:374:ARG:HA	14:C:374:ARG:HH11	1.56	0.70
18:g:120:ASP:OD1	19:h:84:ARG:NH1	2.25	0.70
19:h:74:LEU:CD1	19:h:136:ILE:HD11	2.09	0.70
1:U:247:GLN:OE1	1:U:247:GLN:HA	1.91	0.70
33:x:521:ALA:CA	33:x:524:MET:HE3	2.21	0.70
1:U:140:ARG:NH1	14:C:15:LYS:HB2	2.07	0.70
5:Y:187:TYR:HE2	5:Y:200:LEU:HD22	1.57	0.70
8:b:16:MET:SD	8:b:16:MET:N	2.62	0.70
7:a:307:VAL:HA	7:a:310:LEU:HG	1.74	0.69
26:O:19:ARG:NH2	30:s:213:ASP:OD2	2.25	0.69
21:j:122:ASN:ND2	22:k:125:GLU:OE2	2.24	0.69
30:s:169:ASP:O	30:s:173:ARG:HG3	1.91	0.69
6:Z:67:VAL:HG22	8:b:92:VAL:HG23	1.72	0.69
6:Z:189:GLN:OE1	6:Z:189:GLN:N	2.22	0.69
12:A:114:ASN:HB3	12:A:120:LYS:HG2	1.74	0.69
33:x:620:PHE:HE2	33:x:649:HIS:HE2	1.39	0.69
3:W:1:MET:HE1	3:W:34:LEU:HG	1.74	0.69
7:a:328:ASP:OD2	7:a:330:ARG:HG2	1.92	0.69
16:E:281:ARG:HE	16:E:284:THR:HG22	1.57	0.69
17:F:91:SER:HB2	17:F:126:THR:HA	1.74	0.69
33:x:450:ILE:HD12	33:x:822:VAL:HG21	1.75	0.69
1:U:656:LEU:HD11	1:U:668:ALA:HB1	1.75	0.69
32:f:395:LEU:HD21	33:x:461:PRO:HA	1.72	0.69
1:U:344:ARG:C	1:U:344:ARG:CD	2.65	0.69
17:F:96:LEU:CD1	17:F:145:LEU:HD13	2.16	0.69
33:x:889:PRO:HA	33:x:900:LEU:HB3	1.75	0.69
1:U:796:LYS:O	1:U:797:MET:HE3	1.91	0.69
3:W:432:LEU:HB3	3:W:436:MET:HE1	1.73	0.69
7:a:324:ILE:HG23	7:a:331:VAL:HG12	1.73	0.69
10:d:205:LYS:O	10:d:209:TYR:N	2.22	0.69
13:B:434:THR:HB	13:B:435:PRO:HD3	1.74	0.69
21:j:146:GLN:OE1	21:j:159:ASN:ND2	2.25	0.69
3:W:375:MET:H	3:W:375:MET:HE3	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:432:LEU:C	3:W:436:MET:SD	2.75	0.69
8:b:3:LEU:HD23	8:b:44:ASN:HD21	1.56	0.69
13:B:78:PHE:HB2	33:x:613:LEU:HD11	1.73	0.69
16:E:33:LEU:HD23	16:E:36:LEU:HD23	1.73	0.69
16:E:198:VAL:HG22	16:E:218:MET:CE	2.22	0.69
33:x:686:LEU:HD12	33:x:687:ARG:N	2.07	0.69
1:U:140:ARG:NH2	14:C:12:GLU:O	2.26	0.69
2:V:94:VAL:HG22	2:V:137:GLU:HB3	1.72	0.69
8:b:97:LEU:HB3	8:b:107:MET:SD	2.33	0.69
13:B:54:PRO:HG3	13:B:60:LEU:HD23	1.75	0.69
16:E:223:ARG:NH2	16:E:269:THR:O	2.26	0.69
9:c:52:GLU:HB3	9:c:82:VAL:HG22	1.75	0.69
12:A:38:GLN:OE1	12:A:40:THR:N	2.25	0.69
16:E:289:LEU:O	16:E:295:LEU:HG	1.92	0.69
19:H:184:LEU:O	19:H:188:ILE:HG13	1.92	0.69
33:x:162:LEU:HD12	33:x:191:ILE:HD11	1.75	0.69
1:U:649:ARG:HB3	1:U:675:MET:HE1	1.73	0.69
7:a:254:ALA:HA	7:a:261:LEU:HD12	1.75	0.69
8:b:84:ILE:HD12	8:b:115:SER:HB2	1.75	0.69
9:c:161:ARG:HD3	9:c:201:TYR:HE1	1.58	0.69
10:d:183:GLU:OE2	10:d:215:TRP:NE1	2.26	0.69
13:B:329:MET:HE3	13:B:347:ILE:HG21	1.75	0.69
2:V:408:ARG:HD3	2:V:446:VAL:HG13	1.75	0.68
5:Y:250:LEU:HD11	5:Y:256:VAL:HB	1.75	0.68
17:F:39:GLU:HA	17:F:43:GLN:HG3	1.74	0.68
3:W:36:LYS:HG2	3:W:85:GLU:HG2	1.76	0.68
17:F:296:PHE:CE1	17:F:310:MET:HE2	2.28	0.68
13:B:124:SER:HA	13:B:130:GLU:HA	1.76	0.68
18:G:130:GLU:O	18:G:131:MET:HB3	1.93	0.68
18:g:236:ASP:C	18:g:236:ASP:OD1	2.37	0.68
2:V:307:ARG:NH1	2:V:308:THR:OG1	2.25	0.68
4:X:410:VAL:O	4:X:414:LEU:HD23	1.94	0.68
7:a:215:GLU:O	7:a:218:MET:SD	2.52	0.68
13:B:107:MET:HG2	13:B:160:ILE:HD11	1.74	0.68
15:D:384:MET:O	15:D:388:ARG:HG2	1.93	0.68
16:E:258:MET:HA	16:E:258:MET:HE2	1.74	0.68
4:X:268:GLN:HB3	4:X:288:LYS:HD2	1.75	0.68
12:A:393:GLY:HA3	13:B:216:ILE:HD13	1.74	0.68
14:C:368:MET:HE1	15:D:199:PRO:HD3	1.74	0.68
16:E:264:MET:HE3	16:E:270:LEU:HD12	1.73	0.68
17:F:51:GLU:HG3	17:F:55:MET:HG3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:69:MET:SD	17:F:69:MET:C	2.77	0.68
23:l:125:ARG:NH1	23:l:126:ARG:O	2.25	0.68
1:U:633:CYS:O	1:U:636:VAL:HG12	1.93	0.68
3:W:87:ILE:HG22	3:W:88:MET:H	1.57	0.68
4:X:408:SER:HA	4:X:411:VAL:HG12	1.74	0.68
9:c:196:LEU:O	9:c:197:ASN:C	2.37	0.68
12:A:418:LYS:HD3	12:A:422:LYS:HG3	1.76	0.68
29:R:166:ARG:NH1	28:q:144:ASP:OD2	2.26	0.68
6:Z:225:GLN:HG3	6:Z:226:ILE:HG12	1.75	0.68
8:b:100:ARG:HE	8:b:103:LYS:HA	1.59	0.68
8:b:100:ARG:NH1	8:b:105:HIS:O	2.26	0.68
12:A:244:GLU:OE1	13:B:268:ARG:NH2	2.26	0.68
16:E:168:LYS:HD2	16:E:264:MET:HE1	1.76	0.68
16:E:264:MET:HG3	16:E:270:LEU:HD11	1.76	0.68
5:Y:214:MET:N	5:Y:214:MET:SD	2.67	0.68
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.75	0.68
36:A:501:ATP:O1G	13:B:346:ARG:NH2	2.27	0.68
29:R:4:LEU:HD11	29:R:135:ALA:HB1	1.75	0.68
21:j:7:ILE:HD13	21:j:18:GLN:HB3	1.75	0.68
4:X:43:VAL:HB	4:X:76:PHE:HE1	1.59	0.68
5:Y:82:LYS:HE2	5:Y:107:LYS:HE2	1.76	0.68
18:g:132:ARG:NH1	24:m:123:THR:O	2.26	0.68
5:Y:69:LEU:C	5:Y:73:MET:HE2	2.19	0.67
5:Y:156:LEU:HA	5:Y:159:ARG:HB3	1.74	0.67
18:G:191:PHE:HE1	18:G:219:VAL:HG21	1.59	0.67
19:H:4:ARG:NH1	19:H:14:SER:OG	2.27	0.67
33:x:585:GLU:N	33:x:586:PRO:HD2	2.09	0.67
16:E:289:LEU:HD13	16:E:295:LEU:HD21	1.75	0.67
18:g:92:GLN:NE2	25:n:69:GLU:OE1	2.27	0.67
18:g:158:GLY:O	19:h:84:ARG:NH2	2.28	0.67
6:Z:9:VAL:HG12	6:Z:48:LEU:HB3	1.76	0.67
6:Z:209:ARG:HH12	7:a:354:GLU:HA	1.58	0.67
33:x:162:LEU:HD11	33:x:187:LEU:HD22	1.77	0.67
1:U:338:HIS:O	1:U:342:LEU:HG	1.93	0.67
10:d:200:PHE:HB3	10:d:203:PRO:HB3	1.76	0.67
28:Q:181:ARG:NH1	28:Q:190:ASP:OD1	2.28	0.67
22:k:12:VAL:HB	22:k:23:GLN:HG2	1.76	0.67
23:l:166:GLN:OE1	23:l:169:ARG:NH1	2.28	0.67
33:x:350:LYS:HB3	33:x:353:LEU:HD13	1.75	0.67
8:b:57:ASP:OD1	8:b:58:CYS:N	2.27	0.67
9:c:84:VAL:HG22	9:c:129:THR:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:560:LEU:HD21	33:x:801:VAL:HG21	1.76	0.67
1:U:552:ILE:HD11	1:U:566:LEU:HD11	1.75	0.67
1:U:803:LYS:HG2	1:U:875:PHE:CB	2.24	0.67
16:E:232:MET:HB3	16:E:235:ILE:HD11	1.77	0.67
33:x:849:ALA:HB2	33:x:879:ARG:HB2	1.77	0.67
1:U:19:LEU:HD23	10:d:27:LYS:NZ	2.09	0.67
1:U:321:GLN:C	1:U:325:MET:HE3	2.20	0.67
3:W:63:THR:HG22	3:W:67:LEU:HB2	1.77	0.67
3:W:115:ILE:HG21	3:W:120:ILE:HG23	1.76	0.67
16:E:309:ARG:H	16:E:312:ILE:HB	1.58	0.67
20:I:116:ASP:OD1	21:J:81:ARG:NH1	2.27	0.67
30:s:144:MET:HE1	30:s:185:ARG:HB2	1.75	0.67
1:U:599:ILE:HG13	15:D:56:VAL:HG11	1.77	0.67
15:D:99:ASN:N	15:D:115:ILE:HD11	2.10	0.67
16:E:352:MET:O	16:E:356:ARG:HG2	1.94	0.67
1:U:678:ASP:O	1:U:684:ARG:NH1	2.23	0.67
3:W:39:ARG:HG2	3:W:42:GLU:HB3	1.76	0.67
5:Y:192:ARG:HD3	5:Y:194:PHE:HB3	1.77	0.67
33:x:253:LEU:HA	33:x:256:PHE:CD1	2.30	0.67
33:x:560:LEU:HD21	33:x:801:VAL:HB	1.76	0.67
33:x:682:GLY:HA3	33:x:686:LEU:HD11	1.76	0.67
13:B:48:LYS:O	13:B:49:LEU:HD23	1.95	0.67
14:C:406:LYS:NZ	20:I:63:GLU:O	2.27	0.67
16:E:198:VAL:HG22	16:E:218:MET:HE1	1.76	0.67
25:N:71:ASN:O	25:N:71:ASN:ND2	2.27	0.67
6:Z:231:GLN:HA	6:Z:234:PHE:HB2	1.77	0.66
8:b:123:ASP:HA	8:b:126:LYS:HD3	1.77	0.66
13:B:329:MET:CE	13:B:347:ILE:HG21	2.25	0.66
15:D:153:MET:HE1	15:D:226:ALA:HB1	1.78	0.66
17:F:72:LYS:O	17:F:75:GLU:HG3	1.95	0.66
17:F:209:LYS:CG	17:F:210:GLU:OE2	2.43	0.66
33:x:560:LEU:HD21	33:x:801:VAL:CG2	2.25	0.66
1:U:219:CYS:SG	1:U:220:LEU:N	2.67	0.66
3:W:148:THR:O	3:W:152:ILE:HD13	1.95	0.66
7:a:8:LEU:HD11	7:a:26:GLU:HB3	1.76	0.66
7:a:319:LEU:H	7:a:319:LEU:HD23	1.60	0.66
9:c:246:LYS:CA	9:c:249:LEU:CD2	2.73	0.66
15:D:368:ASP:HB2	15:D:370:ILE:HD11	1.77	0.66
16:E:219:PHE:HZ	16:E:270:LEU:HD21	1.60	0.66
29:R:17:ASP:C	29:R:17:ASP:OD2	2.36	0.66
3:W:183:VAL:HB	3:W:209:ILE:HD11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:798:PRO:O	1:U:880:ASN:ND2	2.23	0.66
1:U:884:VAL:HG21	1:U:892:LEU:HD11	1.77	0.66
5:Y:134:LEU:O	5:Y:138:LEU:HD23	1.94	0.66
7:a:210:VAL:HG22	7:a:212:ASN:H	1.59	0.66
1:U:19:LEU:HD12	1:U:20:LYS:HD2	1.77	0.66
3:W:428:TRP:CZ2	9:c:309:PHE:HZ	2.13	0.66
4:X:266:ASP:HB3	4:X:270:LEU:CD1	2.24	0.66
5:Y:50:MET:HE3	5:Y:51:ALA:HB2	1.78	0.66
17:F:58:GLU:HG2	17:F:61:ARG:HD2	1.75	0.66
21:J:99:GLU:OE1	29:R:120:ARG:NH2	2.28	0.66
2:V:480:ILE:HG21	6:Z:260:VAL:HA	1.78	0.66
6:Z:120:VAL:HG23	6:Z:139:ILE:HD13	1.77	0.66
7:a:374:ILE:HD11	10:d:255:MET:HG3	1.77	0.66
16:E:261:LEU:HD12	16:E:264:MET:CB	2.26	0.66
25:N:91:ARG:HG3	25:N:92:GLU:HG2	1.77	0.66
29:r:113:TYR:CZ	29:r:115:ASP:OD2	2.49	0.66
2:V:89:LYS:HA	2:V:92:ARG:HB2	1.77	0.66
3:W:142:ARG:H	3:W:142:ARG:HD2	1.60	0.66
4:X:103:THR:HG23	4:X:106:GLU:HB2	1.77	0.66
9:c:191:ALA:HB3	9:c:196:LEU:HB2	1.76	0.66
14:C:337:ASN:OD1	14:C:337:ASN:N	2.28	0.66
15:D:258:ALA:CB	15:D:259:PRO:HD2	2.15	0.66
2:V:475:ALA:O	2:V:479:ARG:NH2	2.28	0.66
7:a:180:LEU:HD22	7:a:221:VAL:HG21	1.77	0.66
15:D:244:PRO:HD3	15:D:288:ILE:HG12	1.77	0.66
24:m:41:CYS:HB3	24:m:189:ILE:HD12	1.78	0.66
2:V:171:VAL:HA	2:V:174:PHE:CD2	2.31	0.66
22:k:78:MET:HE3	22:k:85:ALA:HB3	1.77	0.66
1:U:792:ASN:HD21	1:U:796:LYS:HE2	1.61	0.66
16:E:312:ILE:HA	16:E:315:ILE:HB	1.78	0.66
21:j:38:ARG:HE	21:j:38:ARG:H	1.44	0.66
2:V:329:HIS:O	2:V:333:ILE:HG13	1.96	0.65
3:W:340:VAL:HG22	3:W:350:ARG:NH1	2.12	0.65
5:Y:79:ASP:HA	5:Y:82:LYS:HB2	1.78	0.65
5:Y:285:ASP:OD1	5:Y:291:HIS:ND1	2.26	0.65
6:Z:192:THR:HA	7:a:375:LEU:HD21	1.76	0.65
7:a:279:GLU:OE1	7:a:339:ARG:NH2	2.29	0.65
12:A:62:LEU:HD23	13:B:79:ILE:HD13	1.77	0.65
1:U:825:LYS:HD2	1:U:827:LYS:H	1.61	0.65
3:W:82:LEU:HD13	3:W:86:ASN:OD1	1.95	0.65
3:W:104:MET:CG	3:W:123:ARG:NH1	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:43:TRP:HE1	6:Z:92:VAL:HG21	1.60	0.65
13:B:48:LYS:C	13:B:49:LEU:HD23	2.21	0.65
16:E:173:TYR:HB2	16:E:282:PRO:HB3	1.78	0.65
33:x:253:LEU:N	33:x:256:PHE:CE1	2.65	0.65
2:V:416:ARG:NH1	2:V:416:ARG:O	2.30	0.65
9:c:134:GLU:HB3	9:c:162:LEU:HD13	1.78	0.65
14:C:55:LYS:HG2	15:D:72:PHE:CE1	2.31	0.65
17:F:298:SER:HB3	17:F:300:LYS:HE3	1.78	0.65
24:m:188:ASP:N	24:m:188:ASP:OD1	2.27	0.65
33:x:253:LEU:N	33:x:256:PHE:HE1	1.94	0.65
3:W:79:GLU:HB2	3:W:130:MET:HE1	1.77	0.65
27:P:12:MET:HE3	27:P:171:MET:HG2	1.78	0.65
6:Z:235:ASN:HD21	7:a:352:ARG:HE	1.44	0.65
9:c:197:ASN:HD22	9:c:198:ARG:HD2	1.61	0.65
14:C:30:GLU:O	14:C:34:ILE:HG12	1.97	0.65
2:V:200:ARG:HH11	2:V:243:ASP:HA	1.62	0.65
11:e:42:ASN:O	11:e:42:ASN:ND2	2.25	0.65
16:E:60:VAL:HG13	16:E:98:VAL:HG21	1.78	0.65
7:a:194:GLN:HB2	7:a:226:ARG:CD	2.18	0.65
12:A:324:PRO:HA	12:A:327:LEU:HD23	1.79	0.65
16:E:219:PHE:CZ	16:E:270:LEU:HD21	2.32	0.65
17:F:48:LEU:O	17:F:52:ILE:N	2.29	0.65
2:V:170:LEU:HG	2:V:174:PHE:CZ	2.31	0.65
2:V:289:LEU:HA	2:V:292:THR:HG22	1.78	0.65
15:D:417:TYR:HA	19:H:79:MET:HA	1.77	0.65
17:F:299:GLU:OE1	17:F:304:ARG:NH2	2.29	0.65
28:Q:44:LEU:HD11	28:Q:102:LEU:HD13	1.79	0.65
22:k:24:VAL:O	22:k:28:ILE:HG12	1.95	0.65
33:x:900:LEU:HD12	33:x:900:LEU:N	2.12	0.65
1:U:32:ASN:O	1:U:35:TRP:NE1	2.29	0.65
7:a:272:ILE:HA	7:a:275:LEU:HD12	1.78	0.65
8:b:161:ASN:HB2	8:b:165:GLY:HA3	1.78	0.65
19:h:65:VAL:O	19:h:220:ARG:NH1	2.30	0.65
14:C:52:LEU:O	14:C:56:VAL:HG22	1.97	0.64
15:D:152:MET:SD	15:D:152:MET:N	2.61	0.64
15:D:258:ALA:O	15:D:259:PRO:C	2.40	0.64
20:I:119:GLN:HG3	21:J:78:ALA:HB1	1.80	0.64
18:g:37:LEU:HD22	18:g:53:GLN:HG3	1.78	0.64
33:x:887:PHE:HE2	33:x:900:LEU:HD13	1.62	0.64
3:W:103:LYS:O	3:W:107:GLN:NE2	2.26	0.64
5:Y:228:MET:HE1	5:Y:259:TYR:CZ	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:7:MET:HE2	8:b:97:LEU:HG	1.79	0.64
13:B:46:ALA:HB2	13:B:178:LYS:HA	1.78	0.64
25:N:150:GLU:N	25:N:150:GLU:OE2	2.29	0.64
27:P:177:ARG:NH2	30:s:150:ASP:OD2	2.27	0.64
33:x:443:GLY:HA2	33:x:446:LEU:CD2	2.27	0.64
2:V:249:THR:O	2:V:253:LEU:HD12	1.96	0.64
3:W:95:SER:N	3:W:98:LYS:HB2	2.11	0.64
7:a:77:VAL:HG21	7:a:110:ALA:HB1	1.78	0.64
9:c:62:VAL:HG22	9:c:63:ASP:H	1.63	0.64
10:d:52:ARG:C	10:d:52:ARG:HD3	2.21	0.64
5:Y:261:PHE:O	5:Y:265:GLU:HB2	1.98	0.64
1:U:709:PHE:CE1	1:U:713:TYR:CE1	2.86	0.64
3:W:141:GLU:OE1	3:W:142:ARG:CA	2.45	0.64
5:Y:51:ALA:HB1	5:Y:116:ASP:OD2	1.98	0.64
12:A:143:ASP:HB3	12:A:148:GLN:H	1.63	0.64
30:S:187:VAL:HG21	26:o:24:MET:SD	2.36	0.64
2:V:91:PRO:HG3	2:V:124:ASN:HB2	1.78	0.64
6:Z:178:ASP:HB2	6:Z:179:ILE:HD12	1.79	0.64
18:G:71:LYS:O	18:G:95:ARG:NH1	2.30	0.64
26:o:19:ARG:HB2	26:o:170:GLY:H	1.61	0.64
33:x:889:PRO:HA	33:x:900:LEU:CD2	2.24	0.64
1:U:386:LEU:HB3	1:U:387:ARG:NH2	2.13	0.64
2:V:400:HIS:NE2	10:d:141:GLN:OE1	2.30	0.64
4:X:137:TYR:HE2	4:X:145:GLU:HB2	1.63	0.64
6:Z:102:HIS:CD2	6:Z:104:ASN:HB3	2.30	0.64
12:A:158:ASP:O	12:A:162:THR:HG23	1.98	0.64
1:U:532:MET:HE1	1:U:552:ILE:N	2.11	0.64
12:A:56:LEU:HD22	13:B:48:LYS:NZ	2.13	0.64
22:k:78:MET:CE	22:k:85:ALA:HB3	2.27	0.64
33:x:755:ASP:OD1	33:x:758:ASN:ND2	2.30	0.64
33:x:888:LEU:HD23	33:x:901:ARG:O	1.98	0.64
5:Y:156:LEU:HD23	5:Y:159:ARG:HB3	1.78	0.64
5:Y:184:GLN:HB2	5:Y:201:PHE:HE2	1.62	0.64
6:Z:33:LYS:HD2	6:Z:34:ARG:HG2	1.80	0.64
6:Z:252:LYS:NZ	9:c:303:MET:HE2	2.13	0.64
7:a:292:THR:HG23	7:a:295:GLU:H	1.61	0.64
16:E:320:ILE:HG22	16:E:321:THR:H	1.63	0.64
27:P:144:GLU:HB3	30:s:144:MET:HG2	1.80	0.64
21:j:38:ARG:H	21:j:38:ARG:NE	1.96	0.64
33:x:256:PHE:CE1	33:x:268:LEU:HD12	2.32	0.64
3:W:142:ARG:O	3:W:145:LEU:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:101:ARG:HD3	7:a:114:CYS:HB3	1.79	0.63
7:a:292:THR:HA	7:a:330:ARG:HD2	1.78	0.63
12:A:322:ASN:HD22	13:B:294:ARG:HH22	1.46	0.63
12:A:369:ARG:NH1	22:K:206:MET:O	2.27	0.63
2:V:84:LYS:HE3	2:V:122:THR:HA	1.79	0.63
5:Y:88:LEU:CD2	5:Y:99:GLU:OE2	2.46	0.63
6:Z:33:LYS:O	6:Z:34:ARG:NE	2.30	0.63
6:Z:94:TRP:HB3	6:Z:112:MET:HE1	1.80	0.63
7:a:231:GLN:CA	7:a:234:ILE:HG13	2.25	0.63
7:a:370:GLN:O	10:d:251:ARG:NH1	2.31	0.63
16:E:229:ILE:HA	16:E:272:ARG:O	1.98	0.63
21:J:229:VAL:O	21:J:233:GLU:HG2	1.97	0.63
3:W:142:ARG:HG2	3:W:146:THR:CG2	2.23	0.63
4:X:410:VAL:HG12	4:X:414:LEU:HD21	1.81	0.63
5:Y:89:GLU:HB2	5:Y:100:ILE:HD13	1.80	0.63
6:Z:253:THR:O	6:Z:256:GLN:HG3	1.98	0.63
17:F:76:ASN:O	17:F:80:ILE:HG12	1.98	0.63
27:P:113:ASP:HB3	27:P:116:THR:O	1.98	0.63
33:x:720:GLU:O	33:x:724:ASN:ND2	2.29	0.63
9:c:139:ARG:HA	9:c:161:ARG:HH22	1.64	0.63
16:E:331:ILE:O	16:E:334:LEU:HD12	1.97	0.63
1:U:803:LYS:CD	1:U:875:PHE:HB3	2.28	0.63
4:X:137:TYR:HB3	4:X:146:ALA:HB2	1.79	0.63
9:c:266:THR:HB	9:c:269:GLN:HB2	1.80	0.63
3:W:296:LEU:H	3:W:296:LEU:HD12	1.63	0.63
29:R:1:THR:O	29:R:129:GLY:HA3	1.99	0.63
19:h:199:PHE:CD1	19:h:203:MET:HG2	2.33	0.63
33:x:211:ILE:HD12	33:x:213:GLN:H	1.64	0.63
3:W:186:ILE:O	3:W:189:GLN:HG2	1.99	0.63
3:W:432:LEU:O	3:W:436:MET:SD	2.57	0.63
7:a:284:ARG:HD2	7:a:288:HIS:HB3	1.81	0.63
8:b:32:ALA:O	8:b:35:ILE:HD12	1.98	0.63
10:d:195:THR:CG2	10:d:201:ASN:HB3	2.28	0.63
21:J:171:PHE:O	21:J:175:ASN:HB2	1.99	0.63
23:L:80:ASP:OD1	23:L:126:ARG:NH2	2.31	0.63
33:x:375:SER:HB3	33:x:398:TRP:HZ2	1.63	0.63
1:U:344:ARG:O	1:U:344:ARG:CD	2.34	0.63
1:U:503:GLN:HE21	1:U:508:THR:HG21	1.64	0.63
1:U:631:GLU:CD	1:U:631:GLU:H	2.06	0.63
2:V:29:PRO:HA	2:V:32:PRO:HG2	1.81	0.63
9:c:306:THR:HA	9:c:309:PHE:CZ	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:147:THR:HA	14:C:206:HIS:HE1	1.64	0.63
22:k:13:ASN:HB3	23:l:126:ARG:HB3	1.80	0.63
33:x:584:SER:HB2	33:x:586:PRO:HD2	1.79	0.63
13:B:112:LEU:HA	13:B:123:VAL:HG12	1.81	0.63
17:F:122:ALA:HB3	17:F:134:LEU:HD11	1.81	0.63
23:l:181:GLU:N	23:l:181:GLU:OE1	2.32	0.63
5:Y:152:MET:CG	5:Y:152:MET:O	2.47	0.62
16:E:261:LEU:HD12	16:E:264:MET:HB2	1.79	0.62
31:t:49:THR:HG22	31:t:85:PRO:HG3	1.80	0.62
2:V:77:GLU:HB2	2:V:86:VAL:HG21	1.81	0.62
4:X:310:ARG:HG2	4:X:314:ARG:HH21	1.64	0.62
5:Y:245:GLU:O	5:Y:249:VAL:HG22	2.00	0.62
10:d:78:LEU:HD13	10:d:98:LEU:HD11	1.79	0.62
1:U:803:LYS:HD3	1:U:875:PHE:HB3	1.81	0.62
3:W:12:ARG:HH21	3:W:54:THR:HB	1.63	0.62
4:X:397:TYR:HE2	5:Y:362:LYS:HD2	1.64	0.62
7:a:127:ASP:HB2	7:a:131:THR:HG21	1.79	0.62
15:D:114:ARG:NH1	15:D:114:ARG:HB3	2.15	0.62
22:k:209:LYS:O	22:k:214:ASN:ND2	2.31	0.62
2:V:33:GLN:NE2	2:V:83:GLU:O	2.32	0.62
4:X:94:ASP:O	4:X:98:ASP:HB2	1.99	0.62
13:B:99:VAL:O	13:B:103:ARG:HG2	2.00	0.62
8:b:4:GLU:C	8:b:4:GLU:OE2	2.41	0.62
16:E:72:LYS:NZ	16:E:73:ALA:O	2.26	0.62
16:E:289:LEU:CD1	16:E:295:LEU:HD11	2.28	0.62
24:M:214:SER:OG	24:M:224:HIS:NE2	2.29	0.62
9:c:309:PHE:O	9:c:309:PHE:HD2	1.83	0.62
10:d:181:CYS:O	10:d:186:TYR:HE2	1.82	0.62
14:C:365:GLU:HB3	14:C:386:ALA:HB1	1.82	0.62
16:E:159:PHE:HE2	16:E:167:PRO:HD3	1.64	0.62
16:E:353:PHE:HA	16:E:356:ARG:CG	2.29	0.62
16:E:353:PHE:CD1	16:E:356:ARG:HB2	2.34	0.62
33:x:252:ALA:CA	33:x:256:PHE:CE1	2.82	0.62
1:U:178:ALA:O	1:U:182:LYS:HG2	1.99	0.62
7:a:312:MET:HA	7:a:312:MET:HE3	1.82	0.62
33:x:466:LEU:HG	33:x:485:LEU:HG	1.81	0.62
33:x:822:VAL:HG22	33:x:825:MET:HE1	1.81	0.62
1:U:140:ARG:HH11	14:C:15:LYS:HB2	1.65	0.62
1:U:397:THR:O	9:c:176:GLN:NE2	2.32	0.62
4:X:401:LEU:O	4:X:405:GLN:HG2	2.00	0.62
5:Y:282:MET:HE2	5:Y:288:PHE:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:174:LYS:O	7:a:178:ARG:NH1	2.33	0.62
16:E:15:LYS:HG3	17:F:47:LEU:HD12	1.82	0.62
19:H:204:THR:HG22	19:H:205:GLU:H	1.64	0.62
29:R:49:ALA:HA	39:R:301:LDZ:H22	1.81	0.62
33:x:556:ARG:HA	33:x:587:PHE:CZ	2.35	0.62
33:x:887:PHE:CE2	33:x:900:LEU:HD22	2.35	0.62
1:U:675:MET:HG3	1:U:687:ALA:HB2	1.82	0.62
3:W:251:TYR:HD1	3:W:266:ALA:HB3	1.63	0.62
3:W:408:ARG:HG3	4:X:344:ARG:NH1	2.15	0.62
5:Y:73:MET:N	5:Y:73:MET:SD	2.73	0.62
5:Y:365:GLN:O	5:Y:369:THR:HG23	1.99	0.62
7:a:34:TRP:HE1	7:a:68:GLU:HA	1.64	0.62
7:a:302:ILE:HG12	7:a:306:GLU:OE2	2.00	0.62
9:c:75:MET:HE3	9:c:87:VAL:HG13	1.82	0.62
9:c:143:VAL:HG12	9:c:145:VAL:HG13	1.82	0.62
9:c:191:ALA:HB1	9:c:196:LEU:HB2	1.81	0.62
12:A:110:LYS:O	12:A:110:LYS:HD3	1.99	0.62
2:V:346:LEU:HB3	2:V:349:ARG:HE	1.65	0.62
6:Z:236:LEU:HD21	7:a:335:TRP:HB3	1.82	0.62
7:a:45:VAL:HG21	7:a:79:ILE:HG13	1.81	0.62
13:B:295:TYR:HE1	13:B:297:SER:HB2	1.64	0.62
16:E:151:LEU:HB3	16:E:158:LEU:HD12	1.81	0.62
19:h:64:LYS:HD2	19:h:76:TYR:HE1	1.63	0.62
23:l:225:ASP:OD1	23:l:226:ASP:N	2.33	0.62
33:x:300:ARG:NH2	33:x:897:PHE:O	2.32	0.62
33:x:686:LEU:HD12	33:x:687:ARG:H	1.65	0.62
2:V:322:VAL:O	11:e:6:GLN:HB3	2.00	0.61
5:Y:50:MET:CE	5:Y:51:ALA:HB2	2.30	0.61
5:Y:300:ARG:NH1	11:e:59:GLU:OE2	2.32	0.61
13:B:401:GLU:OE2	13:B:425:ASN:ND2	2.33	0.61
17:F:308:ARG:O	17:F:312:GLU:HG2	2.00	0.61
2:V:476:PHE:CD2	6:Z:257:MET:CE	2.83	0.61
3:W:445:LEU:HD11	6:Z:227:ILE:HA	1.82	0.61
6:Z:120:VAL:CG2	6:Z:139:ILE:CD1	2.74	0.61
13:B:251:VAL:HG13	14:C:278:ASN:HD22	1.65	0.61
33:x:740:ARG:HD2	33:x:741:LEU:H	1.65	0.61
1:U:606:ALA:O	1:U:615:ARG:NE	2.30	0.61
2:V:349:ARG:HB2	2:V:354:LYS:HD3	1.82	0.61
3:W:216:GLU:HG2	3:W:220:GLU:OE1	2.00	0.61
23:L:239:ARG:HD2	23:L:240:PRO:HD2	1.81	0.61
19:h:173:PHE:HE1	19:h:177:ARG:HH21	1.46	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:l:157:ARG:NE	23:l:176:MET:HE3	2.14	0.61
33:x:95:PRO:O	33:x:99:LEU:HD12	2.00	0.61
33:x:252:ALA:O	33:x:256:PHE:CE1	2.47	0.61
33:x:275:MET:HE2	33:x:275:MET:HA	1.81	0.61
3:W:95:SER:HA	3:W:99:GLN:N	2.15	0.61
4:X:365:LEU:O	4:X:369:ILE:HG12	1.99	0.61
14:C:367:GLY:HA3	15:D:196:ILE:HG21	1.81	0.61
16:E:198:VAL:HG22	16:E:218:MET:SD	2.41	0.61
33:x:542:ILE:CD1	33:x:543:MET:HE2	2.29	0.61
1:U:834:SER:OG	1:U:835:ILE:N	2.34	0.61
4:X:125:LEU:O	4:X:129:LEU:HG	2.00	0.61
9:c:145:VAL:HG12	9:c:157:ILE:HG23	1.82	0.61
30:S:148:LEU:HD23	30:S:178:VAL:HG12	1.82	0.61
1:U:503:GLN:OE1	1:U:505:ASP:HB2	1.99	0.61
8:b:109:ILE:HB	8:b:138:VAL:HG22	1.80	0.61
16:E:5:ARG:HB2	16:E:8:ALA:HB3	1.82	0.61
21:J:246:LYS:C	33:x:907:ASP:HB3	2.25	0.61
2:V:228:ARG:HD2	2:V:257:ASN:HD22	1.64	0.61
3:W:317:TRP:HD1	3:W:320:LEU:HD21	1.64	0.61
6:Z:10:VAL:HG23	6:Z:161:GLU:HG3	1.82	0.61
7:a:373:ASP:O	10:d:255:MET:CE	2.48	0.61
9:c:57:MET:HE3	9:c:143:VAL:HG21	1.83	0.61
14:C:145:ASP:OD2	14:C:145:ASP:N	2.31	0.61
16:E:275:MET:C	16:E:276:ILE:HD12	2.26	0.61
28:Q:154:GLU:O	28:Q:158:GLU:HG2	2.01	0.61
25:n:103:TRP:CZ2	25:n:181:GLU:HG3	2.36	0.61
3:W:1:MET:CE	3:W:34:LEU:HG	2.29	0.61
3:W:369:TYR:CD2	7:a:312:MET:HE1	2.36	0.61
7:a:363:MET:SD	9:c:307:VAL:CG1	2.87	0.61
31:T:100:ARG:NH1	31:T:101:SER:OG	2.33	0.61
19:h:119:GLN:HG3	20:i:81:SER:HB2	1.83	0.61
23:l:169:ARG:O	23:l:173:GLU:HG3	2.01	0.61
27:p:49:LEU:HD21	27:p:87:LEU:HD22	1.81	0.61
3:W:64:SER:HA	3:W:111:TYR:OH	2.00	0.61
4:X:317:PRO:HG2	4:X:319:ILE:HG12	1.81	0.61
4:X:406:ASN:O	4:X:410:VAL:HG23	2.01	0.61
16:E:170:CYS:HB2	16:E:298:LYS:HD2	1.83	0.61
18:g:112:ASP:OD1	18:g:112:ASP:N	2.33	0.61
32:f:395:LEU:HD21	33:x:461:PRO:CA	2.30	0.61
2:V:32:PRO:HB2	2:V:85:ALA:HB1	1.82	0.60
3:W:1:MET:HB3	3:W:43:VAL:HB	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:101:VAL:HG21	3:W:135:LYS:HD3	1.83	0.60
9:c:246:LYS:CA	9:c:249:LEU:HD21	2.26	0.60
13:B:167:THR:HG22	13:B:272:ARG:HH22	1.66	0.60
16:E:171:LEU:HB2	16:E:277:MET:O	2.01	0.60
16:E:353:PHE:CG	16:E:356:ARG:HB2	2.36	0.60
21:J:239:ASN:HA	21:J:243:LYS:HB3	1.83	0.60
33:x:373:ALA:HB2	33:x:760:PHE:HD1	1.64	0.60
3:W:326:MET:HE2	3:W:331:GLY:HA3	1.83	0.60
4:X:71:LYS:HA	4:X:74:ARG:HD3	1.83	0.60
4:X:251:LEU:O	4:X:255:LEU:HD12	2.01	0.60
5:Y:184:GLN:HB2	5:Y:201:PHE:CE2	2.37	0.60
5:Y:209:THR:HA	5:Y:213:LEU:HD12	1.82	0.60
8:b:25:ARG:HH12	8:b:145:GLU:HG3	1.66	0.60
9:c:46:ARG:O	9:c:46:ARG:HG3	2.01	0.60
12:A:112:ILE:HG12	12:A:122:VAL:HG22	1.83	0.60
12:A:116:LYS:HA	12:A:116:LYS:HE3	1.83	0.60
14:C:374:ARG:HA	14:C:374:ARG:NH1	2.16	0.60
29:R:45:MET:HE3	39:R:301:LDZ:H20	1.81	0.60
1:U:176:MET:N	1:U:176:MET:SD	2.73	0.60
4:X:422:THR:OXT	6:Z:283:ARG:NH2	2.33	0.60
5:Y:237:ARG:O	5:Y:242:LYS:HG2	2.01	0.60
10:d:171:LEU:O	10:d:175:ARG:HG2	2.01	0.60
13:B:60:LEU:O	13:B:64:LYS:HG3	2.01	0.60
33:x:106:LEU:HB3	33:x:126:ILE:HD11	1.83	0.60
33:x:587:PHE:HE1	33:x:590:PHE:HD1	1.48	0.60
1:U:765:VAL:HG11	1:U:778:PHE:HD1	1.66	0.60
15:D:417:TYR:HB3	19:H:79:MET:HG2	1.83	0.60
16:E:119:VAL:HA	16:E:123:SER:HB3	1.82	0.60
16:E:332:VAL:HA	16:E:335:SER:HB3	1.84	0.60
26:O:12:ILE:HD11	26:O:178:ILE:HD12	1.84	0.60
21:j:13:ASP:OD1	21:j:13:ASP:N	2.32	0.60
24:m:236:GLU:OE1	24:m:236:GLU:N	2.21	0.60
33:x:181:ARG:HH22	33:x:213:GLN:HE22	1.49	0.60
1:U:633:CYS:HB3	1:U:634:PRO:HD3	1.82	0.60
3:W:220:GLU:CG	3:W:221:LYS:H	2.14	0.60
3:W:228:ASN:O	3:W:232:GLN:NE2	2.35	0.60
3:W:340:VAL:HG12	3:W:341:PHE:CD2	2.36	0.60
17:F:228:PRO:HB2	17:F:356:MET:CE	2.30	0.60
33:x:346:ASP:HA	33:x:349:TYR:HB2	1.83	0.60
33:x:686:LEU:O	33:x:690:VAL:HG23	2.01	0.60
5:Y:383:LEU:HD22	6:Z:272:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:86:PHE:C	8:b:86:PHE:HD2	2.08	0.60
10:d:200:PHE:O	10:d:203:PRO:HB3	2.02	0.60
12:A:74:PRO:O	12:A:78:TRP:HD1	1.85	0.60
14:C:392:GLN:NE2	14:C:393:LYS:O	2.31	0.60
16:E:46:ASP:OD1	17:F:139:LEU:HD22	2.02	0.60
16:E:171:LEU:HA	16:E:276:ILE:O	2.01	0.60
16:E:211:SER:HB2	16:E:256:THR:HG21	1.82	0.60
18:g:56:VAL:O	18:g:56:VAL:CG2	2.49	0.60
23:l:178:GLU:HG2	23:l:178:GLU:O	2.01	0.60
33:x:683:GLU:N	33:x:686:LEU:HD11	2.17	0.60
3:W:267:LEU:HD11	3:W:296:LEU:HA	1.83	0.60
12:A:85:GLN:OE1	12:A:89:SER:OG	2.20	0.60
14:C:24:TYR:O	14:C:28:ILE:HG23	2.02	0.60
20:I:180:LYS:HE2	20:I:184:MET:HA	1.82	0.60
1:U:17:PRO:HB2	1:U:55:ARG:HH12	1.67	0.60
2:V:253:LEU:HB3	2:V:256:ARG:NH2	2.17	0.60
17:F:66:LEU:O	17:F:66:LEU:HD23	2.01	0.60
24:m:233:GLU:HA	24:m:236:GLU:OE1	2.02	0.60
2:V:231:LEU:HD11	2:V:250:LEU:HB3	1.84	0.60
2:V:476:PHE:CE2	6:Z:257:MET:HE1	2.34	0.60
2:V:494:MET:SD	14:C:44:ARG:HD2	2.42	0.60
5:Y:101:ARG:HA	5:Y:104:MET:HG2	1.83	0.60
5:Y:160:ASN:CA	5:Y:163:LYS:HB3	2.32	0.60
6:Z:256:GLN:HE22	6:Z:260:VAL:CG2	2.14	0.60
7:a:168:ASN:OD1	7:a:171:SER:OG	2.20	0.60
7:a:289:ARG:HD2	7:a:333:MET:SD	2.42	0.60
16:E:170:CYS:SG	16:E:171:LEU:N	2.74	0.60
16:E:353:PHE:HA	16:E:356:ARG:HG2	1.83	0.60
31:T:150:LEU:HD23	31:T:168:LEU:HD23	1.84	0.60
21:j:7:ILE:HG23	21:j:8:THR:HG23	1.84	0.60
24:m:179:LEU:HD22	24:m:184:MET:SD	2.42	0.60
1:U:623:GLY:HA3	1:U:658:ILE:HG13	1.84	0.60
2:V:65:ARG:NH2	2:V:205:LEU:HD21	2.17	0.60
3:W:194:LEU:HG	3:W:229:LEU:HD11	1.83	0.60
4:X:92:LEU:HD23	4:X:95:LEU:HD12	1.84	0.60
4:X:237:GLU:OE1	15:D:338:ARG:NH1	2.35	0.60
7:a:373:ASP:C	10:d:255:MET:CE	2.75	0.60
10:d:101:LEU:HD22	10:d:166:PHE:HE2	1.67	0.60
12:A:299:MET:HE1	12:A:328:ASP:CB	2.32	0.60
14:C:253:SER:O	14:C:254:ILE:HB	2.01	0.60
16:E:335:SER:O	16:E:337:GLY:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:252:ALA:CB	33:x:256:PHE:HE1	2.14	0.60
3:W:70:VAL:O	3:W:74:CYS:HB2	2.02	0.59
4:X:137:TYR:CE2	4:X:145:GLU:HB2	2.37	0.59
16:E:18:GLU:HA	16:E:21:GLU:HB3	1.84	0.59
20:I:33:THR:HG21	20:I:200:THR:HG21	1.84	0.59
22:K:182:GLN:HA	23:L:56:LEU:HD11	1.82	0.59
33:x:656:GLY:O	33:x:660:ILE:HG12	2.02	0.59
1:U:408:LEU:O	1:U:412:HIS:ND1	2.26	0.59
4:X:91:SER:O	4:X:95:LEU:HG	2.02	0.59
16:E:5:ARG:HH11	16:E:9:LEU:HB2	1.67	0.59
17:F:49:ASP:HA	17:F:52:ILE:HG12	1.83	0.59
31:t:157:GLN:HG3	31:t:157:GLN:O	2.02	0.59
33:x:442:SER:C	33:x:446:LEU:HD22	2.26	0.59
2:V:299:GLN:OE1	2:V:299:GLN:N	2.35	0.59
2:V:433:ASP:O	2:V:437:ILE:HG12	2.02	0.59
3:W:190:MET:HE3	3:W:206:SER:OG	2.01	0.59
9:c:49:VAL:HG23	9:c:50:PRO:HD3	1.85	0.59
16:E:325:GLU:HG2	16:E:326:ILE:N	2.18	0.59
33:x:887:PHE:CZ	33:x:900:LEU:HD13	2.36	0.59
1:U:571:CYS:HB3	1:U:572:ARG:NH2	2.17	0.59
2:V:28:PRO:O	2:V:32:PRO:HD2	2.02	0.59
4:X:410:VAL:HG12	4:X:414:LEU:CD2	2.32	0.59
7:a:306:GLU:OE1	7:a:310:LEU:HD23	2.02	0.59
12:A:252:GLU:O	12:A:256:MET:HG3	2.01	0.59
3:W:355:LYS:O	3:W:359:VAL:HG23	2.03	0.59
3:W:393:LEU:HA	3:W:396:LEU:HD12	1.84	0.59
5:Y:37:VAL:HB	5:Y:41:LEU:HG	1.84	0.59
5:Y:227:SER:O	5:Y:231:LEU:HB2	2.02	0.59
14:C:175:PHE:HD2	14:C:182:GLN:HG2	1.68	0.59
15:D:237:GLN:HA	16:E:213:ARG:HH21	1.68	0.59
16:E:198:VAL:HG12	16:E:200:SER:N	2.16	0.59
3:W:317:TRP:HB2	3:W:358:VAL:HG11	1.84	0.59
4:X:69:LEU:O	4:X:73:VAL:HG23	2.03	0.59
5:Y:189:VAL:HG23	5:Y:287:LEU:HD22	1.85	0.59
13:B:153:ASN:HD21	13:B:156:VAL:HG23	1.66	0.59
26:O:17:ASP:OD2	26:O:33:LYS:NZ	2.27	0.59
33:x:296:PHE:HZ	33:x:837:LEU:CD1	2.14	0.59
2:V:65:ARG:HH21	2:V:153:LYS:CE	2.16	0.59
3:W:186:ILE:O	3:W:190:MET:HG3	2.02	0.59
3:W:311:THR:HA	7:a:316:SER:HB3	1.85	0.59
3:W:317:TRP:CD1	3:W:320:LEU:HD11	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:112:ILE:HG13	7:a:138:VAL:HG13	1.85	0.59
8:b:13:SER:OG	8:b:16:MET:HE1	2.03	0.59
13:B:67:ARG:HG2	33:x:666:ILE:CG2	2.32	0.59
17:F:96:LEU:HD11	17:F:145:LEU:CD1	2.19	0.59
21:j:164:GLY:O	21:j:168:VAL:HG23	2.02	0.59
9:c:32:TYR:HB3	9:c:208:ARG:HB2	1.85	0.59
33:x:585:GLU:O	33:x:587:PHE:N	2.36	0.59
6:Z:179:ILE:HD13	9:c:218:LEU:CD1	2.33	0.59
9:c:168:MET:H	9:c:168:MET:CE	2.12	0.59
15:D:115:ILE:HG21	15:D:139:LEU:HD23	1.84	0.59
15:D:203:LEU:HB2	15:D:327:LEU:HD13	1.85	0.59
21:j:173:GLU:OE2	22:k:57:PRO:HD2	2.03	0.59
6:Z:81:MET:HA	6:Z:84:LYS:HG2	1.84	0.59
9:c:248:MET:HA	9:c:251:LEU:HB3	1.84	0.59
12:A:42:SER:O	12:A:46:LYS:HG3	2.03	0.59
17:F:32:GLU:HG2	17:F:39:GLU:HB3	1.84	0.59
33:x:469:TYR:CD2	33:x:477:MET:HE3	2.37	0.59
3:W:408:ARG:HG3	4:X:344:ARG:HH12	1.68	0.58
6:Z:257:MET:CE	6:Z:257:MET:CA	2.68	0.58
7:a:198:PHE:HB2	7:a:226:ARG:NH1	2.18	0.58
16:E:235:ILE:O	16:E:277:MET:HE1	2.03	0.58
33:x:380:PHE:HZ	33:x:821:LEU:HD12	1.68	0.58
2:V:98:LEU:HG	2:V:104:THR:HG22	1.85	0.58
2:V:495:ARG:HD3	2:V:497:PRO:HD2	1.85	0.58
3:W:36:LYS:HA	3:W:85:GLU:HA	1.85	0.58
3:W:45:GLU:HB2	3:W:92:LYS:HG2	1.85	0.58
6:Z:109:ASN:O	6:Z:113:LYS:HG2	2.03	0.58
7:a:247:ARG:HH12	7:a:251:LEU:HD13	1.69	0.58
12:A:143:ASP:OD1	12:A:144:ARG:N	2.35	0.58
13:B:65:LEU:O	13:B:68:ILE:HG22	2.03	0.58
13:B:234:LEU:HD22	36:B:501:ATP:H2'	1.84	0.58
31:T:96:MET:CE	31:T:110:MET:HE1	2.32	0.58
23:l:225:ASP:OD1	23:l:225:ASP:C	2.45	0.58
33:x:252:ALA:CB	33:x:256:PHE:CZ	2.74	0.58
2:V:159:LEU:HB2	2:V:209:LYS:HZ1	1.68	0.58
4:X:286:ALA:HA	4:X:309:TYR:HD2	1.68	0.58
6:Z:256:GLN:NE2	6:Z:257:MET:HE2	2.18	0.58
9:c:216:MET:O	9:c:220:LEU:HD23	2.03	0.58
16:E:89:LYS:HA	16:E:92:LEU:HG	1.85	0.58
1:U:532:MET:CG	1:U:548:LEU:HD12	2.32	0.58
3:W:251:TYR:HD1	3:W:266:ALA:CB	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:181:LYS:HG2	5:Y:213:LEU:HD22	1.85	0.58
19:H:91:ARG:HD3	26:O:68:LEU:HD23	1.85	0.58
22:k:97:GLN:HG3	29:r:65:ILE:HG12	1.85	0.58
33:x:206:ASP:O	33:x:210:GLU:HG2	2.03	0.58
2:V:180:ARG:NH1	2:V:183:GLU:OE1	2.35	0.58
3:W:141:GLU:OE1	3:W:141:GLU:C	2.46	0.58
5:Y:225:TYR:HB3	5:Y:295:TYR:OH	2.04	0.58
5:Y:336:ARG:HD2	11:e:52:PHE:HE2	1.67	0.58
6:Z:209:ARG:NH1	7:a:354:GLU:HA	2.18	0.58
8:b:130:ARG:NH1	8:b:134:GLU:OE2	2.36	0.58
13:B:374:LEU:HD23	13:B:378:VAL:HG12	1.84	0.58
15:D:418:LYS:HG2	19:H:78:GLY:O	2.04	0.58
16:E:320:ILE:HD11	16:E:347:CYS:SG	2.43	0.58
23:L:88:MET:CE	23:L:112:ILE:HG13	2.30	0.58
26:o:2:THR:HG21	26:o:162:GLY:HA3	1.84	0.58
33:x:225:ALA:O	33:x:229:VAL:HG23	2.03	0.58
1:U:220:LEU:CD1	1:U:229:VAL:HB	2.32	0.58
2:V:241:ARG:O	2:V:242:HIS:ND1	2.37	0.58
2:V:243:ASP:CG	2:V:247:GLN:H	2.10	0.58
6:Z:43:TRP:CZ2	6:Z:48:LEU:HD12	2.39	0.58
13:B:424:GLU:OE1	13:B:424:GLU:N	2.37	0.58
15:D:40:LEU:HA	15:D:43:ARG:HG3	1.85	0.58
19:H:10:LEU:HD13	19:H:21:GLN:HB2	1.84	0.58
3:W:47:LEU:HA	3:W:50:LEU:HD23	1.84	0.58
9:c:46:ARG:HA	9:c:49:VAL:HG13	1.86	0.58
13:B:103:ARG:HB2	13:B:160:ILE:HD12	1.84	0.58
16:E:205:ASP:HB2	16:E:209:GLY:H	1.67	0.58
16:E:320:ILE:HG21	16:E:362:VAL:CG1	2.34	0.58
20:i:238:LYS:HA	20:i:241:GLU:OE2	2.04	0.58
1:U:19:LEU:CD2	10:d:27:LYS:HZ1	2.16	0.58
2:V:94:VAL:HA	2:V:138:PRO:HD3	1.85	0.58
3:W:428:TRP:HZ2	9:c:309:PHE:HZ	1.52	0.58
4:X:385:LEU:CD2	4:X:387:ILE:HD13	2.30	0.58
5:Y:69:LEU:CA	5:Y:73:MET:HE2	2.34	0.58
8:b:86:PHE:C	8:b:86:PHE:CD2	2.82	0.58
12:A:255:ARG:O	12:A:259:GLU:HG2	2.04	0.58
16:E:155:ASN:HB2	16:E:158:LEU:HG	1.86	0.58
1:U:615:ARG:HD2	1:U:648:VAL:HG22	1.85	0.58
2:V:193:GLN:NE2	14:C:22:GLN:O	2.37	0.58
3:W:366:MET:HG3	3:W:378:MET:HE1	1.85	0.58
15:D:363:TYR:OH	15:D:400:GLU:OE1	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:q:38:MET:HE1	28:q:60:ILE:HG22	1.85	0.58
1:U:235:LYS:HA	1:U:238:LYS:HD2	1.85	0.57
2:V:144:ASP:HB3	2:V:147:PHE:HB2	1.85	0.57
2:V:183:GLU:HA	2:V:186:LYS:HE2	1.86	0.57
2:V:396:ILE:HA	2:V:400:HIS:HE1	1.68	0.57
3:W:409:LEU:HD22	4:X:384:VAL:HG21	1.86	0.57
18:g:18:PRO:HB3	19:h:24:TYR:CZ	2.39	0.57
33:x:851:ASP:N	33:x:851:ASP:OD1	2.37	0.57
2:V:68:ASP:O	2:V:73:GLU:N	2.37	0.57
2:V:326:GLN:OE1	11:e:9:ASP:HB3	2.04	0.57
3:W:3:ASP:OD1	3:W:3:ASP:N	2.35	0.57
5:Y:88:LEU:CD2	5:Y:99:GLU:CG	2.61	0.57
6:Z:26:ILE:HG12	6:Z:35:VAL:HG11	1.85	0.57
6:Z:120:VAL:HA	6:Z:139:ILE:HD12	1.86	0.57
9:c:145:VAL:HG12	9:c:157:ILE:HD12	1.86	0.57
10:d:164:THR:HA	10:d:167:ILE:HG12	1.85	0.57
10:d:193:GLU:O	10:d:197:ILE:HG12	2.04	0.57
11:e:56:LEU:HD21	11:e:62:LYS:HG2	1.85	0.57
12:A:299:MET:HE1	12:A:328:ASP:HB2	1.85	0.57
13:B:78:PHE:C	13:B:78:PHE:CD2	2.80	0.57
15:D:297:ASP:OD2	15:D:323:ARG:NH2	2.37	0.57
17:F:32:GLU:HA	17:F:39:GLU:HG3	1.85	0.57
29:R:36:GLU:HA	29:R:42:LEU:HD23	1.86	0.57
33:x:734:SER:HB2	33:x:768:LEU:HD22	1.86	0.57
2:V:159:LEU:CB	2:V:209:LYS:HZ1	2.17	0.57
17:F:86:LEU:HB3	17:F:87:PRO:HD3	1.84	0.57
25:N:103:TRP:CH2	25:N:181:GLU:HG3	2.39	0.57
33:x:682:GLY:C	33:x:686:LEU:HD11	2.28	0.57
10:d:190:LEU:HD12	10:d:193:GLU:H	1.68	0.57
17:F:91:SER:OG	17:F:92:ASN:N	2.36	0.57
17:F:221:LYS:HD3	17:F:320:PHE:CZ	2.39	0.57
17:F:362:ARG:HE	17:F:388:THR:HG23	1.67	0.57
33:x:54:ASP:O	33:x:58:MET:HE3	2.05	0.57
1:U:548:LEU:O	1:U:552:ILE:HG22	2.04	0.57
1:U:904:LYS:HD3	1:U:912:ILE:HG23	1.86	0.57
7:a:320:VAL:HG21	7:a:333:MET:HB2	1.86	0.57
8:b:8:VAL:HA	8:b:110:ILE:HG13	1.87	0.57
8:b:36:VAL:HG21	8:b:110:ILE:HD13	1.87	0.57
13:B:49:LEU:HD12	13:B:51:LEU:HB2	1.85	0.57
16:E:325:GLU:HG2	16:E:327:ASP:H	1.70	0.57
17:F:272:PHE:O	17:F:276:LYS:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:187:LEU:HB3	3:W:226:TYR:HB3	1.86	0.57
6:Z:42:SER:OG	6:Z:43:TRP:N	2.38	0.57
7:a:35:HIS:CE1	8:b:17:ARG:HB2	2.40	0.57
12:A:426:THR:HB	12:A:427:PRO:HD3	1.85	0.57
15:D:153:MET:HE1	15:D:226:ALA:CB	2.35	0.57
1:U:603:LEU:O	1:U:607:VAL:HG12	2.05	0.57
2:V:175:MET:HE1	2:V:217:VAL:HG21	1.87	0.57
3:W:45:GLU:HG2	3:W:46:THR:H	1.69	0.57
6:Z:175:LEU:HD12	9:c:217:LEU:HD22	1.87	0.57
16:E:184:ALA:HB2	16:E:233:ASP:OD2	2.05	0.57
20:i:239:LYS:O	20:i:243:GLU:HG2	2.05	0.57
33:x:72:ARG:HE	33:x:75:LEU:HD12	1.70	0.57
2:V:289:LEU:HD23	2:V:289:LEU:C	2.30	0.57
3:W:202:THR:O	3:W:206:SER:OG	2.22	0.57
6:Z:39:LEU:HB2	6:Z:95:TYR:HD2	1.68	0.57
7:a:374:ILE:CG1	10:d:251:ARG:HA	2.34	0.57
15:D:409:LYS:C	15:D:411:GLU:OE1	2.48	0.57
16:E:232:MET:O	16:E:276:ILE:HB	2.05	0.57
29:R:9:ARG:HH11	29:R:9:ARG:HG3	1.70	0.57
19:h:69:THR:HG22	19:h:70:LYS:H	1.68	0.57
23:l:164:ARG:HG3	23:l:198:THR:HG23	1.87	0.57
24:m:31:GLU:OE2	24:m:169:ARG:NH2	2.34	0.57
25:n:160:LEU:O	25:n:164:MET:HG3	2.05	0.57
33:x:797:LEU:O	33:x:801:VAL:HG23	2.05	0.57
1:U:139:GLN:HA	1:U:142:LEU:HD12	1.86	0.57
2:V:231:LEU:O	2:V:235:LEU:HD13	2.05	0.57
3:W:363:ILE:CD1	3:W:392:PHE:CD1	2.87	0.57
4:X:192:SER:O	4:X:196:THR:HG22	2.04	0.57
4:X:239:TYR:CD1	4:X:243:ASP:HB3	2.39	0.57
8:b:48:ASN:OD1	8:b:48:ASN:N	2.37	0.57
13:B:113:GLU:HB3	13:B:122:ILE:HG23	1.86	0.57
18:G:193:GLN:O	18:G:197:THR:OG1	2.23	0.57
23:L:103:LEU:HD12	23:L:104:PRO:HD2	1.87	0.57
32:f:395:LEU:HD21	33:x:461:PRO:CB	2.34	0.57
33:x:266:LEU:HD22	33:x:294:MET:HB2	1.85	0.57
33:x:466:LEU:HD21	33:x:481:SER:HA	1.85	0.57
1:U:873:PRO:O	1:U:875:PHE:N	2.38	0.57
4:X:385:LEU:C	4:X:385:LEU:CD2	2.77	0.57
5:Y:246:ILE:O	5:Y:250:LEU:HB2	2.05	0.57
6:Z:258:VAL:HG12	9:c:291:LEU:HD13	1.87	0.57
10:d:206:MET:O	10:d:207:THR:C	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:142:VAL:HG13	12:A:147:TYR:HA	1.86	0.57
13:B:130:GLU:OE2	13:B:130:GLU:N	2.29	0.57
29:R:52:CYS:O	29:R:56:GLU:HG3	2.05	0.57
7:a:35:HIS:H	8:b:18:ASN:CG	2.13	0.56
7:a:134:THR:O	7:a:138:VAL:HG23	2.05	0.56
28:q:40:GLU:N	28:q:40:GLU:OE1	2.37	0.56
33:x:740:ARG:H	33:x:740:ARG:NE	2.00	0.56
1:U:198:LEU:HD13	1:U:219:CYS:HA	1.87	0.56
1:U:772:TRP:CD1	1:U:775:LEU:HG	2.40	0.56
2:V:139:MET:HA	2:V:143:ALA:HB2	1.86	0.56
2:V:251:LEU:O	2:V:255:LEU:HG	2.05	0.56
3:W:121:LYS:O	3:W:125:ILE:HG12	2.05	0.56
4:X:410:VAL:HG22	9:c:256:ASN:HD22	1.68	0.56
5:Y:291:HIS:CD2	5:Y:295:TYR:CD1	2.92	0.56
14:C:82:LYS:C	14:C:83:LYS:HD2	2.30	0.56
16:E:130:VAL:HG12	16:E:132:TYR:H	1.70	0.56
3:W:220:GLU:HG3	3:W:221:LYS:H	1.69	0.56
5:Y:77:ASN:HB2	5:Y:110:TYR:CZ	2.40	0.56
5:Y:197:ALA:O	5:Y:201:PHE:CB	2.51	0.56
7:a:284:ARG:HD3	7:a:285:PRO:HD2	1.85	0.56
13:B:301:GLY:O	13:B:305:ILE:HG12	2.05	0.56
14:C:251:ILE:HG22	14:C:295:THR:HB	1.86	0.56
16:E:334:LEU:HD13	16:E:371:VAL:HG12	1.87	0.56
18:G:180:GLU:HG2	19:H:56:LEU:HD21	1.87	0.56
19:H:182:LEU:HD22	19:H:186:ASP:OD2	2.05	0.56
25:N:45:ARG:HD2	25:N:52:THR:HB	1.88	0.56
2:V:250:LEU:HA	2:V:253:LEU:CD1	2.35	0.56
2:V:401:ASN:HD22	2:V:404:LYS:HB2	1.70	0.56
3:W:243:ILE:HG13	3:W:273:TYR:CE1	2.40	0.56
10:d:120:GLU:OE1	10:d:121:ARG:NH2	2.38	0.56
12:A:115:VAL:HG13	12:A:118:PHE:HB3	1.88	0.56
26:O:121:LYS:HZ2	31:t:215:ILE:HG21	1.70	0.56
18:g:185:LYS:O	18:g:185:LYS:HD3	2.06	0.56
28:q:5:ILE:HD11	28:q:143:LEU:HD11	1.87	0.56
33:x:469:TYR:HD2	33:x:477:MET:HE3	1.70	0.56
9:c:218:LEU:HA	9:c:221:HIS:CD2	2.40	0.56
9:c:240:HIS:C	9:c:240:HIS:ND1	2.63	0.56
13:B:295:TYR:CE1	13:B:297:SER:HB2	2.39	0.56
16:E:119:VAL:HG23	16:E:121:ASN:H	1.71	0.56
22:k:121:LEU:HD11	23:l:79:ALA:CB	2.36	0.56
33:x:72:ARG:NH2	33:x:118:ASN:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:559:PRO:HG3	33:x:587:PHE:HZ	1.63	0.56
33:x:587:PHE:CE1	33:x:590:PHE:HD1	2.24	0.56
1:U:802:TYR:HB3	1:U:895:PRO:HB3	1.88	0.56
6:Z:256:GLN:HE21	6:Z:257:MET:HE2	1.71	0.56
7:a:120:ALA:HA	7:a:123:LEU:HG	1.87	0.56
8:b:65:THR:HG21	8:b:70:ARG:HE	1.71	0.56
10:d:52:ARG:NH2	10:d:94:TYR:HB2	2.20	0.56
13:B:211:TYR:CE1	13:B:218:PRO:HB3	2.39	0.56
15:D:99:ASN:HB3	15:D:114:ARG:NH2	2.21	0.56
28:Q:49:GLU:HG3	28:Q:50:ALA:H	1.70	0.56
3:W:39:ARG:HG3	3:W:40:LEU:H	1.69	0.56
3:W:314:LEU:HD11	3:W:381:LEU:HD13	1.88	0.56
5:Y:297:ARG:HD3	11:e:52:PHE:CD1	2.41	0.56
7:a:343:LEU:O	7:a:347:LYS:HG2	2.06	0.56
9:c:81:GLY:HA2	9:c:86:ALA:HB2	1.87	0.56
9:c:125:VAL:HA	9:c:128:ASN:ND2	2.20	0.56
15:D:99:ASN:HA	15:D:115:ILE:HD12	1.86	0.56
27:p:12:MET:HE3	27:p:171:MET:HG2	1.87	0.56
33:x:502:LEU:HD11	33:x:533:ASP:OD2	2.05	0.56
2:V:228:ARG:HE	2:V:254:LEU:HD12	1.70	0.56
5:Y:141:VAL:O	5:Y:145:LEU:HD12	2.06	0.56
7:a:292:THR:O	7:a:296:ILE:HD12	2.06	0.56
9:c:245:VAL:HA	9:c:248:MET:HG3	1.88	0.56
10:d:200:PHE:CB	10:d:203:PRO:HB3	2.36	0.56
12:A:27:GLU:OE1	12:A:27:GLU:N	2.39	0.56
14:C:55:LYS:HA	14:C:58:LEU:HD23	1.87	0.56
15:D:40:LEU:C	15:D:40:LEU:HD12	2.31	0.56
16:E:234:GLU:H	16:E:278:ALA:H	1.54	0.56
19:H:49:GLU:HG3	19:H:51:LYS:HE2	1.88	0.56
18:g:67:THR:HG22	18:g:69:LEU:H	1.71	0.56
27:p:22:ILE:HG22	27:p:188:HIS:HB2	1.86	0.56
33:x:266:LEU:HD11	33:x:278:VAL:HG13	1.88	0.56
7:a:249:GLN:HA	7:a:252:LYS:HG2	1.88	0.56
12:A:103:ASN:ND2	17:F:167:GLU:HG3	2.20	0.56
12:A:150:HIS:C	12:A:151:ILE:HD12	2.31	0.56
13:B:141:LYS:HA	13:B:144:LEU:HD12	1.88	0.56
13:B:313:LEU:CD2	13:B:341:LEU:HD12	2.32	0.56
14:C:89:VAL:HG12	14:C:91:PRO:HD2	1.88	0.56
15:D:113:VAL:HG22	15:D:114:ARG:H	1.70	0.56
27:p:159:ASP:C	27:p:159:ASP:OD1	2.48	0.56
28:q:28:MET:HE1	29:r:113:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:300:LEU:HD13	10:d:113:ALA:HA	1.88	0.56
3:W:231:ILE:CD1	3:W:246:HIS:HB3	2.36	0.56
5:Y:282:MET:HE3	5:Y:292:TYR:HD1	1.71	0.56
7:a:112:ILE:HG21	7:a:151:VAL:HG23	1.87	0.56
8:b:56:ASN:HB3	8:b:83:LYS:H	1.71	0.56
17:F:69:MET:SD	17:F:70:LYS:N	2.79	0.56
24:M:219:LEU:HD23	24:M:219:LEU:H	1.70	0.56
31:t:9:THR:O	31:t:41:ARG:NH2	2.36	0.56
31:t:63:LEU:HD11	31:t:106:LEU:HD13	1.87	0.56
1:U:94:SER:HB3	1:U:97:VAL:HG12	1.87	0.55
1:U:161:ASP:OD1	1:U:162:VAL:N	2.39	0.55
3:W:127:THR:HG23	3:W:147:LYS:HE3	1.88	0.55
3:W:449:GLU:HA	3:W:452:ILE:HG12	1.88	0.55
4:X:51:LEU:HD23	4:X:88:LEU:HD13	1.88	0.55
9:c:45:GLY:O	9:c:49:VAL:HG13	2.06	0.55
10:d:52:ARG:HH22	10:d:94:TYR:HB2	1.72	0.55
13:B:70:ASP:O	13:B:74:MET:SD	2.64	0.55
24:m:117:MET:HE2	24:m:117:MET:HA	1.88	0.55
1:U:218:GLN:HA	1:U:754:HIS:NE2	2.21	0.55
3:W:183:VAL:O	3:W:187:LEU:CD1	2.51	0.55
3:W:395:ASN:OD1	3:W:396:LEU:N	2.39	0.55
6:Z:23:PHE:O	6:Z:26:ILE:HG13	2.07	0.55
6:Z:120:VAL:HG22	6:Z:139:ILE:CD1	2.24	0.55
7:a:169:HIS:NE2	7:a:207:GLY:HA2	2.20	0.55
16:E:353:PHE:CD2	16:E:357:ALA:HB3	2.41	0.55
17:F:175:MET:HE1	17:F:251:LEU:HD21	1.88	0.55
18:G:80:MET:SD	18:G:138:MET:HG3	2.46	0.55
30:S:172:MET:HE1	30:S:195:ILE:HG21	1.89	0.55
1:U:461:LEU:HD22	1:U:481:LEU:HB3	1.88	0.55
4:X:282:ARG:HA	4:X:285:GLU:HB2	1.89	0.55
6:Z:21:ASP:OD1	6:Z:22:HIS:N	2.39	0.55
6:Z:188:SER:O	6:Z:192:THR:HG23	2.06	0.55
6:Z:235:ASN:HD22	7:a:349:MET:HG2	1.72	0.55
12:A:262:GLU:O	12:A:266:THR:HG23	2.07	0.55
16:E:47:LEU:HD11	17:F:76:ASN:HD21	1.72	0.55
16:E:152:PRO:HG2	16:E:167:PRO:HD3	1.88	0.55
16:E:320:ILE:HG21	16:E:362:VAL:HG11	1.87	0.55
24:M:106:ILE:HD13	24:M:111:LEU:HB2	1.88	0.55
19:h:184:LEU:O	19:h:188:ILE:HG13	2.06	0.55
28:q:40:GLU:H	28:q:40:GLU:CD	2.13	0.55
2:V:446:VAL:HG12	2:V:447:ILE:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:317:TRP:CD1	3:W:320:LEU:HD21	2.41	0.55
3:W:443:THR:HG23	6:Z:208:ILE:HD11	1.86	0.55
9:c:269:GLN:HA	9:c:272:ILE:HG22	1.87	0.55
16:E:127:PRO:HG2	16:E:185:ARG:HD3	1.89	0.55
17:F:69:MET:HE1	17:F:70:LYS:HG3	1.89	0.55
20:I:181:GLU:OE2	20:I:181:GLU:C	2.49	0.55
24:M:213:LEU:HD12	24:M:232:ARG:HG3	1.87	0.55
27:P:49:LEU:HD12	27:P:111:GLY:HA3	1.87	0.55
27:P:135:ASP:OD1	27:P:135:ASP:N	2.40	0.55
18:g:190:THR:HG1	18:g:193:GLN:CD	2.13	0.55
21:j:7:ILE:HG21	21:j:119:THR:O	2.06	0.55
33:x:391:LEU:HG	33:x:398:TRP:HD1	1.72	0.55
33:x:513:GLU:OE2	33:x:816:TYR:OH	2.21	0.55
1:U:198:LEU:O	1:U:202:VAL:HG23	2.07	0.55
2:V:480:ILE:HG21	6:Z:260:VAL:HG22	1.89	0.55
3:W:241:LEU:O	3:W:245:LYS:HG2	2.06	0.55
3:W:363:ILE:HD12	3:W:392:PHE:CD1	2.34	0.55
7:a:172:TYR:HA	7:a:175:ASP:OD2	2.07	0.55
13:B:394:ASP:O	13:B:398:ILE:HG12	2.06	0.55
14:C:31:LEU:HB3	15:D:47:LEU:HB3	1.88	0.55
14:C:69:GLN:HE22	15:D:135:HIS:HB3	1.72	0.55
16:E:352:MET:C	16:E:354:ALA:N	2.65	0.55
17:F:296:PHE:CD1	17:F:310:MET:HE2	2.42	0.55
18:G:123:GLN:NE2	19:H:82:ASP:OD1	2.40	0.55
21:J:96:LEU:HD13	28:Q:62:LYS:HG3	1.88	0.55
28:Q:88:LEU:HB3	28:Q:122:ALA:HB2	1.87	0.55
19:h:65:VAL:HG23	19:h:209:GLU:HG2	1.88	0.55
2:V:79:VAL:HG22	2:V:80:LYS:H	1.71	0.55
3:W:231:ILE:HA	3:W:243:ILE:HG22	1.88	0.55
5:Y:319:MET:HB2	5:Y:330:ILE:CD1	2.35	0.55
12:A:26:ASP:O	12:A:29:ASP:N	2.34	0.55
33:x:140:LEU:HD22	33:x:166:VAL:HG12	1.89	0.55
1:U:398:ASN:H	1:U:401:LYS:HE2	1.72	0.55
2:V:48:THR:OG1	2:V:147:PHE:HZ	1.90	0.55
5:Y:194:PHE:HD1	5:Y:195:LYS:N	2.01	0.55
10:d:28:LEU:O	10:d:32:GLU:HG3	2.07	0.55
14:C:217:SER:O	15:D:248:ARG:NH2	2.40	0.55
14:C:280:LEU:HD23	14:C:310:ARG:HB3	1.88	0.55
18:G:112:ASP:OD2	18:G:112:ASP:N	2.35	0.55
21:J:105:GLU:OE2	21:J:109:ARG:NH2	2.28	0.55
1:U:74:PHE:CG	1:U:103:LYS:HE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:481:LEU:HD12	1:U:481:LEU:C	2.32	0.55
6:Z:28:LYS:N	9:c:104:ARG:HH22	2.05	0.55
9:c:57:MET:HE1	9:c:112:TYR:HB3	1.88	0.55
14:C:186:VAL:HG13	14:C:292:ILE:HG23	1.87	0.55
16:E:168:LYS:CD	16:E:264:MET:HE1	2.37	0.55
27:P:28:PHE:HB3	27:P:36:THR:HG22	1.89	0.55
19:h:11:THR:HG22	19:h:19:LEU:HD22	1.88	0.55
23:l:171:TYR:O	23:l:174:ARG:HG2	2.07	0.55
25:n:148:THR:HG22	25:n:149:LYS:H	1.72	0.55
33:x:520:LEU:O	33:x:524:MET:HE2	2.07	0.55
2:V:252:ASN:ND2	2:V:284:GLU:HG2	2.22	0.55
3:W:429:SER:HA	3:W:432:LEU:HD12	1.89	0.55
5:Y:361:SER:O	5:Y:364:TRP:N	2.37	0.55
9:c:75:MET:SD	9:c:76:PRO:HD2	2.47	0.55
13:B:92:GLN:CB	13:B:97:SER:H	2.20	0.55
13:B:374:LEU:HD23	13:B:378:VAL:HG11	1.85	0.55
16:E:275:MET:SD	16:E:275:MET:C	2.90	0.55
21:j:38:ARG:NH1	21:j:181:ILE:HA	2.21	0.55
5:Y:74:LYS:O	5:Y:78:GLU:HB2	2.07	0.55
5:Y:160:ASN:HA	5:Y:163:LYS:CB	2.37	0.55
6:Z:70:LEU:HD22	6:Z:71:ASP:H	1.72	0.55
6:Z:256:GLN:HE21	6:Z:257:MET:CA	2.19	0.55
10:d:190:LEU:HD11	10:d:192:THR:CG2	2.30	0.55
12:A:294:GLU:OE1	12:A:297:ARG:NH1	2.40	0.55
32:f:396:GLN:NE2	33:x:427:THR:OG1	2.39	0.55
1:U:791:LEU:HD22	1:U:797:MET:HE2	1.88	0.54
1:U:864:GLU:OE2	1:U:865:LYS:NZ	2.39	0.54
2:V:426:LEU:HB3	2:V:428:LEU:HD23	1.89	0.54
3:W:254:PRO:HD3	3:W:262:LYS:HZ3	1.72	0.54
3:W:352:LYS:O	3:W:356:ASN:ND2	2.39	0.54
6:Z:257:MET:HE1	6:Z:260:VAL:HG11	1.89	0.54
7:a:70:ARG:HH21	8:b:17:ARG:HG2	1.71	0.54
13:B:153:ASN:OD1	13:B:158:ALA:N	2.34	0.54
17:F:221:LYS:HD3	17:F:320:PHE:HZ	1.72	0.54
17:F:321:GLN:OE1	17:F:321:GLN:N	2.40	0.54
23:L:88:MET:HE3	23:L:112:ILE:CD1	2.37	0.54
30:s:148:LEU:HD23	30:s:178:VAL:HG12	1.89	0.54
33:x:852:VAL:HG13	33:x:859:PRO:HG3	1.89	0.54
4:X:66:LEU:O	4:X:70:LEU:HG	2.07	0.54
4:X:96:PHE:HD1	4:X:109:LEU:HD23	1.71	0.54
5:Y:161:THR:C	5:Y:165:LYS:HD3	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:55:ALA:O	6:Z:74:TYR:OH	2.24	0.54
6:Z:260:VAL:HG12	6:Z:261:TYR:N	2.21	0.54
8:b:51:LEU:H	8:b:62:THR:HG22	1.72	0.54
9:c:80:THR:O	9:c:83:SER:OG	2.21	0.54
10:d:45:LYS:O	10:d:49:ILE:HG13	2.07	0.54
22:K:118:ASN:OD1	23:L:82:ARG:NH2	2.40	0.54
20:i:119:GLN:HG3	21:j:78:ALA:HB1	1.89	0.54
26:o:49:ALA:HA	39:o:301:LDZ:H22	1.89	0.54
2:V:213:TYR:O	2:V:217:VAL:HG23	2.07	0.54
3:W:124:LEU:HB3	3:W:128:LEU:CD2	2.37	0.54
3:W:432:LEU:HD21	9:c:309:PHE:CE1	2.42	0.54
5:Y:136:HIS:O	5:Y:140:ILE:HG13	2.08	0.54
5:Y:279:GLU:O	5:Y:282:MET:HB3	2.08	0.54
7:a:131:THR:O	7:a:135:ILE:HD13	2.06	0.54
7:a:268:LEU:HA	7:a:271:LYS:HB2	1.89	0.54
10:d:104:LEU:HD22	10:d:163:TYR:HD2	1.72	0.54
14:C:23:TYR:O	14:C:27:LYS:HG2	2.07	0.54
27:P:65:GLN:OE1	28:Q:86:ARG:NH2	2.39	0.54
21:j:68:ASN:ND2	21:j:137:ASP:OD2	2.40	0.54
22:k:79:SER:HB2	22:k:170:ILE:HD12	1.89	0.54
33:x:278:VAL:HG12	33:x:305:LEU:HD11	1.89	0.54
33:x:419:LEU:HD11	33:x:822:VAL:HG13	1.88	0.54
33:x:522:CYS:O	33:x:525:ILE:HG22	2.06	0.54
5:Y:157:ILE:HA	5:Y:160:ASN:HD21	1.72	0.54
5:Y:224:VAL:HG21	5:Y:250:LEU:HD21	1.88	0.54
9:c:197:ASN:HD22	9:c:198:ARG:HH11	1.55	0.54
16:E:290:LEU:HD23	16:E:295:LEU:CD1	2.26	0.54
16:E:323:HIS:HB2	16:E:364:GLN:HE22	1.73	0.54
17:F:43:GLN:HG2	17:F:46:ARG:CZ	2.38	0.54
33:x:538:ILE:HD13	33:x:562:LEU:HB2	1.90	0.54
2:V:169:LEU:HD12	2:V:170:LEU:H	1.72	0.54
2:V:405:THR:HG22	2:V:409:MET:HE3	1.90	0.54
3:W:293:ASP:HB3	3:W:295:LYS:HE2	1.88	0.54
6:Z:252:LYS:HZ2	9:c:303:MET:CE	2.21	0.54
9:c:163:ILE:HD13	9:c:198:ARG:O	2.08	0.54
13:B:221:GLY:HA3	13:B:347:ILE:HA	1.89	0.54
16:E:101:ASP:HB3	16:E:106:THR:H	1.72	0.54
16:E:264:MET:HG2	16:E:270:LEU:HG	1.89	0.54
17:F:221:LYS:HD2	17:F:346:GLY:O	2.08	0.54
18:G:48:ALA:HB3	18:G:220:VAL:HG12	1.89	0.54
29:R:38:ASN:HD22	29:R:39:PRO:HD3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:h:51:LYS:HE2	19:h:199:PHE:CE2	2.42	0.54
1:U:532:MET:HE1	1:U:551:GLY:CA	2.38	0.54
2:V:29:PRO:HB2	2:V:33:GLN:NE2	2.23	0.54
3:W:127:THR:CG2	3:W:147:LYS:HE3	2.38	0.54
3:W:136:ILE:O	3:W:175:GLY:HA3	2.07	0.54
10:d:152:PHE:HE1	10:d:171:LEU:HD12	1.71	0.54
12:A:394:MET:HE2	13:B:216:ILE:HD11	1.89	0.54
14:C:73:VAL:HG23	14:C:127:LEU:HD12	1.90	0.54
16:E:338:PHE:CD2	16:E:343:LEU:HD21	2.43	0.54
17:F:438:TYR:OH	22:K:19:GLY:O	2.26	0.54
26:O:1:THR:N	39:O:301:LDZ:O33	2.34	0.54
30:S:33:PHE:CE1	26:o:24:MET:HE1	2.43	0.54
33:x:291:GLN:HA	33:x:294:MET:CE	2.36	0.54
33:x:482:ILE:HD11	33:x:517:VAL:HB	1.87	0.54
1:U:446:LEU:HD11	1:U:461:LEU:HD12	1.90	0.54
2:V:345:ARG:NH1	11:e:50:ASP:OD2	2.40	0.54
4:X:275:LEU:HD12	4:X:275:LEU:H	1.72	0.54
5:Y:327:VAL:O	5:Y:331:ASP:HB2	2.07	0.54
9:c:27:THR:O	9:c:29:GLU:N	2.41	0.54
10:d:131:VAL:HA	10:d:134:LYS:HB3	1.90	0.54
10:d:249:TYR:O	10:d:252:GLN:HG3	2.08	0.54
13:B:133:VAL:HG12	13:B:134:SER:H	1.72	0.54
26:o:48:THR:O	26:o:50:ALA:N	2.40	0.54
33:x:887:PHE:CZ	33:x:900:LEU:HB2	2.43	0.54
4:X:99:MET:SD	4:X:100:GLU:HG3	2.47	0.54
4:X:163:LYS:O	4:X:167:VAL:HG13	2.08	0.54
5:Y:228:MET:CE	5:Y:259:TYR:CZ	2.90	0.54
6:Z:165:GLU:O	6:Z:166:GLU:C	2.51	0.54
7:a:268:LEU:HD23	7:a:268:LEU:H	1.73	0.54
10:d:162:SER:OG	10:d:164:THR:OG1	2.23	0.54
16:E:203:ILE:HB	16:E:211:SER:HB3	1.90	0.54
16:E:281:ARG:CZ	16:E:283:ASP:HB3	2.38	0.54
30:s:4:PRO:O	31:t:100:ARG:NH1	2.40	0.54
33:x:319:GLU:OE2	33:x:325:GLN:NE2	2.39	0.54
33:x:376:PHE:HE1	33:x:818:LEU:HD21	1.73	0.54
1:U:801:GLN:HB3	1:U:877:LEU:HD22	1.88	0.54
2:V:65:ARG:NH2	2:V:153:LYS:HE3	2.22	0.54
2:V:484:LEU:O	2:V:488:ASN:ND2	2.41	0.54
3:W:307:LYS:O	3:W:313:GLU:HG3	2.08	0.54
6:Z:177:ARG:HA	6:Z:180:LYS:HD3	1.90	0.54
20:i:3:ARG:HH12	22:k:10:ARG:HH21	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:887:PHE:HE2	33:x:900:LEU:HD22	1.72	0.54
1:U:324:LYS:NZ	1:U:794:ASP:OD2	2.38	0.54
1:U:568:GLU:HG2	1:U:572:ARG:NH1	2.22	0.54
1:U:673:GLU:HB3	1:U:674:PRO:HD3	1.90	0.54
2:V:65:ARG:HG2	2:V:66:GLU:N	2.22	0.54
3:W:200:ILE:O	3:W:204:ILE:HG12	2.07	0.54
3:W:366:MET:HE1	3:W:415:PHE:CE1	2.43	0.54
5:Y:81:LEU:HD13	5:Y:107:LYS:HA	1.88	0.54
5:Y:111:LEU:O	5:Y:115:GLY:N	2.41	0.54
5:Y:315:THR:HA	5:Y:352:GLU:O	2.08	0.54
10:d:237:ILE:HG23	10:d:238:PRO:HD3	1.89	0.54
14:C:254:ILE:HD13	14:C:269:VAL:HG13	1.90	0.54
15:D:131:ALA:HB3	15:D:141:ASP:HB3	1.89	0.54
21:J:43:LEU:HD21	21:J:72:ALA:HB2	1.90	0.54
31:T:117:ASP:OD2	31:T:117:ASP:C	2.51	0.54
22:k:203:LYS:HD2	22:k:203:LYS:C	2.33	0.54
1:U:18:GLN:HA	1:U:21:GLU:OE2	2.08	0.53
2:V:153:LYS:NZ	2:V:202:ALA:HB1	2.23	0.53
3:W:43:VAL:HG13	3:W:48:LEU:HD11	1.89	0.53
3:W:104:MET:HG2	3:W:123:ARG:CZ	2.38	0.53
8:b:4:GLU:OE2	8:b:5:SER:N	2.41	0.53
8:b:108:ARG:HH22	8:b:139:ASP:HB2	1.72	0.53
8:b:188:ILE:HD12	8:b:189:LEU:N	2.23	0.53
13:B:251:VAL:HG13	14:C:278:ASN:ND2	2.23	0.53
16:E:261:LEU:HD11	16:E:264:MET:SD	2.48	0.53
17:F:251:LEU:HD22	17:F:256:LEU:HD21	1.90	0.53
22:K:133:MET:HE2	22:K:137:PHE:CE1	2.43	0.53
19:h:74:LEU:HD23	19:h:83:TYR:HE1	1.73	0.53
1:U:325:MET:HA	1:U:328:ILE:HG12	1.90	0.53
3:W:60:MET:SD	3:W:111:TYR:CD2	3.02	0.53
3:W:182:ARG:O	3:W:186:ILE:HG12	2.08	0.53
4:X:86:ALA:O	4:X:90:ARG:HG3	2.08	0.53
9:c:197:ASN:ND2	9:c:198:ARG:HD2	2.22	0.53
17:F:193:LYS:O	17:F:197:GLU:HG3	2.09	0.53
19:H:93:LEU:HD13	19:H:113:ARG:HB3	1.90	0.53
20:i:63:GLU:HG3	20:i:64:LYS:HG2	1.90	0.53
23:l:45:VAL:HG21	23:l:188:VAL:HG22	1.89	0.53
2:V:270:LEU:O	2:V:273:LYS:HG2	2.09	0.53
3:W:312:MET:HB3	3:W:365:ILE:HB	1.91	0.53
3:W:386:VAL:O	3:W:390:GLU:HG2	2.07	0.53
7:a:286:ALA:HA	7:a:289:ARG:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:53:THR:HG22	8:b:59:GLU:H	1.74	0.53
10:d:175:ARG:NH1	10:d:175:ARG:HA	2.23	0.53
14:C:138:MET:HE3	14:C:214:VAL:HA	1.90	0.53
15:D:389:GLU:OE1	15:D:391:ARG:HB2	2.08	0.53
16:E:23:ASP:O	16:E:27:LYS:HG2	2.08	0.53
26:O:37:ILE:HD11	26:O:56:THR:HG23	1.90	0.53
20:i:233:VAL:O	20:i:237:ILE:HG12	2.08	0.53
39:o:301:LDZ:C15	39:o:301:LDZ:O33	2.55	0.53
32:f:386:ARG:NH2	32:f:389:ARG:HH11	2.07	0.53
33:x:208:LEU:HA	33:x:211:ILE:HD11	1.90	0.53
1:U:544:ILE:HD12	1:U:545:LEU:H	1.73	0.53
2:V:336:GLU:OE2	2:V:342:ILE:HA	2.08	0.53
3:W:45:GLU:H	3:W:92:LYS:HD3	1.73	0.53
6:Z:36:VAL:HG13	6:Z:94:TRP:CE3	2.43	0.53
6:Z:143:GLU:HG2	6:Z:145:HIS:H	1.73	0.53
6:Z:235:ASN:ND2	7:a:352:ARG:HE	2.07	0.53
7:a:35:HIS:N	8:b:18:ASN:OD1	2.32	0.53
9:c:133:PHE:HA	9:c:136:LEU:HB3	1.91	0.53
9:c:251:LEU:HD21	9:c:284:LEU:HA	1.91	0.53
14:C:24:TYR:HB3	15:D:40:LEU:CD1	2.38	0.53
16:E:175:PRO:HD2	16:E:301:ILE:O	2.08	0.53
21:J:41:VAL:HG12	21:J:211:MET:HB2	1.90	0.53
21:J:241:LYS:HG3	21:J:242:LYS:N	2.23	0.53
24:M:19:ARG:NH2	24:M:24:GLU:OE1	2.40	0.53
33:x:71:TYR:HB3	33:x:72:ARG:NH2	2.23	0.53
1:U:99:THR:O	1:U:103:LYS:HG3	2.09	0.53
3:W:452:ILE:HG13	3:W:453:HIS:N	2.23	0.53
4:X:267:VAL:O	4:X:271:VAL:HG23	2.08	0.53
6:Z:95:TYR:HA	6:Z:122:VAL:O	2.08	0.53
6:Z:121:LEU:HD11	6:Z:138:TYR:HD2	1.72	0.53
8:b:7:MET:HE3	8:b:93:ALA:HA	1.90	0.53
12:A:213:LEU:HB2	12:A:337:LEU:HD13	1.90	0.53
16:E:335:SER:O	16:E:336:ASP:C	2.52	0.53
19:H:19:LEU:HD22	19:H:19:LEU:H	1.74	0.53
29:R:105:ASP:OD1	29:R:105:ASP:N	2.42	0.53
22:k:78:MET:HE3	22:k:85:ALA:CB	2.38	0.53
29:r:186:ARG:HB3	29:r:186:ARG:HH11	1.74	0.53
1:U:532:MET:HE1	1:U:551:GLY:HA3	1.91	0.53
3:W:208:LYS:O	3:W:211:THR:OG1	2.25	0.53
3:W:427:ASP:OD2	3:W:428:TRP:N	2.40	0.53
6:Z:78:MET:HA	6:Z:81:MET:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:275:LEU:HA	7:a:278:MET:HE3	1.90	0.53
13:B:71:TYR:CA	13:B:74:MET:HE1	2.35	0.53
14:C:372:ARG:HB3	14:C:373:GLU:OE1	2.07	0.53
15:D:115:ILE:HG22	15:D:139:LEU:HB3	1.88	0.53
15:D:377:SER:HB3	16:E:292:PRO:HD2	1.90	0.53
19:H:68:ILE:HD11	19:H:74:LEU:HD22	1.90	0.53
22:k:121:LEU:HD11	23:l:79:ALA:HA	1.90	0.53
24:m:228:PRO:HG2	24:m:232:ARG:NH2	2.24	0.53
1:U:247:GLN:OE1	1:U:247:GLN:CA	2.57	0.53
1:U:507:VAL:HG23	1:U:543:LYS:HE3	1.90	0.53
2:V:400:HIS:CD2	10:d:144:MET:HG3	2.44	0.53
4:X:385:LEU:CD2	4:X:387:ILE:CD1	2.86	0.53
5:Y:282:MET:HE3	5:Y:292:TYR:CD1	2.44	0.53
6:Z:68:TRP:CG	6:Z:104:ASN:HD21	2.27	0.53
6:Z:127:LYS:H	6:Z:128:PRO:HD2	1.74	0.53
13:B:429:LYS:NZ	14:C:308:PRO:HG3	2.24	0.53
14:C:11:LEU:HB3	14:C:14:GLY:HA3	1.89	0.53
16:E:196:LEU:HD23	16:E:232:MET:HE1	1.90	0.53
29:r:113:TYR:OH	29:r:115:ASP:OD2	2.26	0.53
33:x:230:CYS:SG	33:x:231:LEU:N	2.82	0.53
33:x:734:SER:HB2	33:x:768:LEU:CD2	2.38	0.53
3:W:124:LEU:HA	3:W:127:THR:HG22	1.89	0.53
7:a:234:ILE:HD12	7:a:235:ASP:H	1.71	0.53
8:b:147:GLU:CD	8:b:147:GLU:H	2.17	0.53
9:c:27:THR:C	9:c:29:GLU:H	2.16	0.53
10:d:104:LEU:HD23	10:d:166:PHE:HB2	1.91	0.53
12:A:158:ASP:HB3	12:A:161:VAL:HG22	1.90	0.53
14:C:273:MET:HE1	14:C:302:ASP:OD2	2.08	0.53
16:E:146:ARG:O	16:E:150:GLU:HB2	2.09	0.53
17:F:93:VAL:O	17:F:148:GLY:N	2.42	0.53
29:r:64:ARG:NH1	29:r:67:GLU:OE2	2.42	0.53
32:f:398:LEU:O	32:f:401:GLN:HG3	2.09	0.53
33:x:207:LEU:O	33:x:211:ILE:HG13	2.08	0.53
1:U:347:ASN:HB3	1:U:813:TYR:OH	2.08	0.53
1:U:761:VAL:O	1:U:765:VAL:HG12	2.09	0.53
2:V:209:LYS:HD2	2:V:210:CYS:N	2.23	0.53
2:V:372:LEU:HD23	2:V:372:LEU:H	1.73	0.53
2:V:416:ARG:HG2	2:V:459:GLN:HG2	1.90	0.53
3:W:9:ALA:O	3:W:13:ILE:HG23	2.09	0.53
3:W:56:THR:HA	3:W:59:ASP:HB2	1.90	0.53
3:W:167:GLN:OE1	3:W:168:GLU:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:250:ILE:HA	3:W:253:THR:OG1	2.09	0.53
3:W:375:MET:SD	3:W:376:LYS:N	2.82	0.53
5:Y:75:LYS:HD2	5:Y:75:LYS:C	2.34	0.53
5:Y:293:ARG:HD2	11:e:57:ARG:HD3	1.91	0.53
6:Z:134:PRO:HG2	6:Z:162:ILE:HG13	1.91	0.53
8:b:6:THR:HB	8:b:49:VAL:HG22	1.90	0.53
9:c:238:CYS:O	9:c:242:GLU:HG3	2.09	0.53
17:F:223:VAL:HB	17:F:329:ILE:HG22	1.91	0.53
23:l:22:ILE:O	23:l:26:MET:HG2	2.09	0.53
33:x:150:GLU:OE1	33:x:150:GLU:N	2.30	0.53
2:V:495:ARG:HB3	14:C:44:ARG:HG3	1.90	0.53
5:Y:226:VAL:HA	5:Y:229:ILE:HB	1.91	0.53
9:c:77:GLN:NE2	9:c:78:SER:O	2.42	0.53
11:e:6:GLN:N	11:e:7:PRO:CD	2.72	0.53
12:A:287:ASP:H	12:A:290:GLY:HA2	1.74	0.53
14:C:48:GLN:NE2	15:D:65:GLN:OE1	2.42	0.53
16:E:243:PHE:HB2	18:G:11:ARG:HH12	1.74	0.53
16:E:334:LEU:HD13	16:E:371:VAL:CG1	2.39	0.53
16:E:371:VAL:O	16:E:374:VAL:HG23	2.09	0.53
31:t:45:VAL:HB	31:t:49:THR:OG1	2.09	0.53
33:x:181:ARG:HA	33:x:184:LEU:HD21	1.90	0.53
33:x:253:LEU:CA	33:x:256:PHE:HD1	2.22	0.53
33:x:683:GLU:O	33:x:686:LEU:CD1	2.56	0.53
4:X:385:LEU:HD23	4:X:386:ILE:CA	2.39	0.52
6:Z:257:MET:HE1	6:Z:260:VAL:CG1	2.39	0.52
8:b:20:ASP:OD2	8:b:25:ARG:NH2	2.32	0.52
12:A:24:ALA:HA	13:B:410:ARG:CZ	2.38	0.52
12:A:394:MET:HE2	13:B:216:ILE:CD1	2.39	0.52
12:A:418:LYS:HA	12:A:422:LYS:HG3	1.91	0.52
16:E:102:MET:HE2	16:E:103:THR:HG23	1.91	0.52
21:j:224:GLU:OE1	21:j:224:GLU:N	2.40	0.52
33:x:263:PRO:O	33:x:267:ARG:HG2	2.08	0.52
33:x:560:LEU:CD2	33:x:801:VAL:HB	2.39	0.52
33:x:882:LEU:HD12	33:x:889:PRO:HD3	1.91	0.52
1:U:345:ASN:ND2	1:U:743:ASN:OD1	2.42	0.52
2:V:202:ALA:O	2:V:206:VAL:HG23	2.09	0.52
2:V:289:LEU:HD23	2:V:289:LEU:O	2.09	0.52
2:V:474:LEU:O	2:V:478:GLN:NE2	2.42	0.52
6:Z:43:TRP:NE1	6:Z:92:VAL:HG21	2.25	0.52
7:a:304:VAL:O	7:a:307:VAL:HG22	2.09	0.52
9:c:150:SER:OG	9:c:156:VAL:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:257:ASN:O	15:D:258:ALA:HB3	2.09	0.52
16:E:144:GLU:O	16:E:148:VAL:HG23	2.08	0.52
1:U:871:PRO:O	1:U:872:GLU:C	2.51	0.52
5:Y:88:LEU:CD2	5:Y:99:GLU:CD	2.76	0.52
6:Z:40:LEU:HB3	6:Z:89:GLU:HG2	1.92	0.52
12:A:303:ILE:HD11	12:A:331:LEU:HG	1.91	0.52
13:B:436:GLU:OE1	13:B:436:GLU:N	2.42	0.52
13:B:438:LEU:HD11	20:I:25:MET:HE1	1.90	0.52
15:D:79:VAL:O	15:D:82:ILE:HG22	2.09	0.52
16:E:5:ARG:O	16:E:9:LEU:N	2.41	0.52
16:E:83:CYS:SG	16:E:84:ARG:N	2.82	0.52
17:F:146:LYS:O	17:F:148:GLY:N	2.42	0.52
26:O:155:VAL:O	26:O:159:ILE:HG12	2.10	0.52
18:g:190:THR:O	18:g:194:THR:HG23	2.08	0.52
30:s:190:GLY:O	30:s:191:ASP:HB2	2.09	0.52
33:x:587:PHE:CD1	33:x:590:PHE:HB3	2.44	0.52
1:U:18:GLN:HG3	10:d:27:LYS:HZ2	1.75	0.52
1:U:631:GLU:O	1:U:634:PRO:HD2	2.09	0.52
2:V:82:LEU:HD23	2:V:82:LEU:H	1.74	0.52
3:W:24:VAL:O	3:W:28:LEU:HG	2.09	0.52
7:a:374:ILE:HG13	10:d:251:ARG:HA	1.90	0.52
10:d:137:VAL:O	10:d:141:GLN:HG2	2.09	0.52
15:D:57:GLN:O	15:D:61:ILE:HG12	2.10	0.52
15:D:264:ILE:CG2	15:D:267:ILE:CG2	2.79	0.52
15:D:271:ALA:HB1	15:D:317:LEU:HD13	1.90	0.52
18:G:231:THR:HG1	18:G:234:GLU:CD	2.17	0.52
26:O:159:ILE:O	26:O:163:ILE:HG13	2.10	0.52
24:m:108:LEU:HD23	24:m:147:GLN:HB2	1.92	0.52
27:p:135:ASP:OD1	27:p:135:ASP:N	2.38	0.52
33:x:105:LYS:O	33:x:108:GLU:HG3	2.09	0.52
33:x:776:LEU:HD21	33:x:825:MET:HB3	1.92	0.52
2:V:165:ALA:HB2	2:V:171:VAL:HG11	1.90	0.52
2:V:228:ARG:HD2	2:V:257:ASN:HB3	1.90	0.52
5:Y:229:ILE:HD11	5:Y:295:TYR:CD2	2.45	0.52
5:Y:326:GLY:HA3	5:Y:329:PHE:CE1	2.45	0.52
10:d:176:ASP:OD1	10:d:177:GLU:N	2.42	0.52
14:C:28:ILE:HG22	15:D:44:TYR:HB2	1.92	0.52
29:R:193:ALA:O	29:R:197:GLU:HG2	2.09	0.52
28:q:154:GLU:H	28:q:154:GLU:CD	2.14	0.52
34:v:11:UNK:C	34:v:13:UNK:N	2.73	0.52
1:U:174:PRO:HA	1:U:177:LEU:HD23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:415:HIS:HB3	1:U:419:ALA:HB2	1.90	0.52
1:U:576:PRO:HB3	1:U:611:ASN:HD22	1.75	0.52
1:U:620:GLU:OE2	1:U:651:GLY:HA2	2.10	0.52
2:V:29:PRO:HB2	2:V:33:GLN:HE21	1.75	0.52
2:V:224:LEU:HB3	2:V:257:ASN:ND2	2.25	0.52
2:V:476:PHE:CD2	6:Z:257:MET:HE1	2.44	0.52
3:W:79:GLU:HB2	3:W:130:MET:CE	2.40	0.52
5:Y:233:ARG:NH2	5:Y:264:TYR:O	2.43	0.52
8:b:134:GLU:O	8:b:135:LYS:HG2	2.09	0.52
9:c:266:THR:O	9:c:269:GLN:N	2.43	0.52
16:E:151:LEU:HB2	16:E:152:PRO:HD3	1.91	0.52
16:E:320:ILE:CG2	16:E:362:VAL:HG11	2.39	0.52
16:E:352:MET:C	16:E:354:ALA:H	2.17	0.52
16:E:364:GLN:HG2	16:E:365:GLU:N	2.23	0.52
32:f:386:ARG:HH22	32:f:389:ARG:HH11	1.57	0.52
1:U:108:TYR:HE1	1:U:157:THR:HG22	1.74	0.52
5:Y:187:TYR:CE2	5:Y:200:LEU:HD22	2.40	0.52
10:d:244:LYS:O	10:d:248:GLU:HG3	2.10	0.52
13:B:148:CYS:SG	13:B:149:SER:N	2.83	0.52
15:D:397:LYS:HG3	15:D:398:ASP:N	2.24	0.52
19:h:107:THR:HG21	19:h:138:GLY:HA3	1.92	0.52
21:j:36:ARG:HD3	21:j:157:LYS:HA	1.91	0.52
24:m:52:LEU:HA	24:m:209:PHE:HA	1.91	0.52
33:x:682:GLY:HA3	33:x:686:LEU:CD1	2.38	0.52
1:U:447:GLY:HA3	1:U:480:GLY:HA2	1.91	0.52
1:U:510:GLU:HA	1:U:547:GLY:HA3	1.91	0.52
1:U:788:VAL:HG12	1:U:909:GLY:HA2	1.92	0.52
3:W:98:LYS:HD3	3:W:135:LYS:HE3	1.91	0.52
9:c:57:MET:HA	9:c:72:VAL:HG12	1.92	0.52
9:c:191:ALA:O	9:c:196:LEU:N	2.42	0.52
11:e:6:GLN:N	11:e:7:PRO:HD3	2.25	0.52
14:C:57:ARG:O	14:C:61:GLU:HG2	2.09	0.52
18:G:103:TYR:O	26:O:81:ARG:NH1	2.43	0.52
20:I:14:PRO:O	20:I:15:GLU:HG2	2.10	0.52
29:R:187:VAL:O	29:R:188:SER:HB3	2.09	0.52
31:T:192:VAL:HG23	31:T:197:VAL:HG22	1.90	0.52
18:g:37:LEU:CD2	18:g:53:GLN:HG3	2.40	0.52
24:m:108:LEU:HD22	24:m:139:SER:HB3	1.92	0.52
32:f:386:ARG:CZ	32:f:386:ARG:HA	2.40	0.52
33:x:335:ARG:C	33:x:335:ARG:NE	2.66	0.52
2:V:354:LYS:HG3	2:V:358:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:371:ASN:HB3	2:V:374:LYS:HG2	1.92	0.52
6:Z:23:PHE:HB3	6:Z:126:VAL:HG21	1.92	0.52
10:d:120:GLU:HB3	10:d:121:ARG:NH2	2.25	0.52
10:d:191:PHE:HZ	10:d:202:THR:N	2.08	0.52
12:A:101:ILE:HG22	12:A:138:MET:O	2.09	0.52
13:B:99:VAL:HG12	13:B:138:PHE:CD2	2.44	0.52
15:D:130:VAL:HB	15:D:139:LEU:HD11	1.91	0.52
16:E:326:ILE:HG13	16:E:328:TYR:CZ	2.45	0.52
31:T:25:ASP:HA	31:T:187:PHE:HA	1.91	0.52
24:m:5:THR:O	24:m:5:THR:OG1	2.28	0.52
33:x:325:GLN:O	33:x:329:ASN:ND2	2.33	0.52
33:x:670:MET:O	33:x:670:MET:HE3	2.09	0.52
33:x:733:GLY:O	33:x:736:THR:OG1	2.28	0.52
33:x:734:SER:CB	33:x:768:LEU:HD22	2.38	0.52
1:U:225:ASP:OD1	1:U:225:ASP:O	2.28	0.52
1:U:811:PHE:HE2	1:U:885:MET:HG3	1.74	0.52
3:W:157:GLY:O	3:W:158:ASP:HB2	2.10	0.52
3:W:247:TYR:HA	3:W:250:ILE:HG12	1.92	0.52
4:X:70:LEU:HD22	4:X:92:LEU:HB3	1.91	0.52
4:X:394:ASP:N	4:X:394:ASP:OD1	2.43	0.52
5:Y:367:GLN:O	5:Y:371:LYS:HG2	2.10	0.52
6:Z:40:LEU:CD2	6:Z:91:ILE:HG12	2.39	0.52
16:E:178:THR:HG22	16:E:178:THR:O	2.10	0.52
21:J:76:LEU:H	21:J:129:ILE:HG22	1.75	0.52
26:o:200:GLY:O	26:o:201:ARG:NH1	2.42	0.52
30:s:176:LYS:HD3	30:s:208:VAL:HG21	1.91	0.52
30:s:184:GLU:OE2	30:s:211:ARG:NH1	2.43	0.52
1:U:590:TYR:CD2	1:U:598:ALA:HB2	2.45	0.51
1:U:632:GLN:O	1:U:633:CYS:C	2.54	0.51
5:Y:28:LEU:H	5:Y:28:LEU:HD22	1.74	0.51
10:d:188:LYS:H	10:d:188:LYS:CD	2.23	0.51
13:B:206:THR:O	33:x:740:ARG:NH1	2.43	0.51
15:D:138:ALA:HB3	15:D:140:VAL:HG13	1.92	0.51
15:D:368:ASP:HB2	15:D:370:ILE:CD1	2.40	0.51
22:K:24:VAL:O	22:K:28:ILE:HG12	2.10	0.51
28:Q:35:MET:HG2	28:Q:45:LEU:HG	1.91	0.51
24:m:8:ASP:O	24:m:22:GLN:NE2	2.43	0.51
26:o:135:MET:HE3	26:o:139:GLU:HG2	1.91	0.51
33:x:371:ASN:HB3	33:x:398:TRP:CH2	2.46	0.51
3:W:149:LEU:O	3:W:153:LYS:HG2	2.10	0.51
5:Y:162:GLU:HG3	5:Y:166:SER:OG	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:316:LEU:HA	5:Y:319:MET:HG2	1.93	0.51
6:Z:165:GLU:C	6:Z:166:GLU:O	2.52	0.51
9:c:123:SER:O	9:c:127:ILE:HG13	2.10	0.51
9:c:140:ALA:N	9:c:161:ARG:HH12	2.07	0.51
12:A:99:THR:OG1	12:A:140:VAL:O	2.24	0.51
13:B:398:ILE:HD12	13:B:423:LYS:HA	1.92	0.51
16:E:231:PHE:HE1	16:E:274:LYS:HE2	1.74	0.51
17:F:99:VAL:H	17:F:120:LYS:HD3	1.75	0.51
20:I:233:VAL:O	20:I:237:ILE:HG13	2.11	0.51
22:k:193:GLU:HA	22:k:196:LYS:HG2	1.92	0.51
26:o:19:ARG:HB3	26:o:169:SER:HA	1.93	0.51
33:x:62:ARG:O	33:x:65:GLU:HG2	2.10	0.51
33:x:131:MET:HE1	33:x:161:HIS:CB	2.39	0.51
33:x:688:ARG:NH2	33:x:720:GLU:OE1	2.44	0.51
1:U:8:ILE:HD11	1:U:27:LEU:HD12	1.91	0.51
2:V:196:SER:N	14:C:29:GLU:OE2	2.34	0.51
2:V:263:LEU:HD21	10:d:83:PHE:HE1	1.74	0.51
3:W:145:LEU:HD22	3:W:172:GLU:HG2	1.93	0.51
6:Z:69:PHE:CZ	8:b:95:LEU:HB3	2.45	0.51
19:H:107:THR:HG21	19:H:138:GLY:HA3	1.91	0.51
22:k:85:ALA:O	22:k:89:ILE:HG12	2.10	0.51
29:r:186:ARG:HB3	29:r:186:ARG:NH1	2.25	0.51
33:x:249:LEU:HD23	33:x:272:LEU:HB2	1.91	0.51
33:x:468:ASP:N	33:x:468:ASP:OD2	2.44	0.51
1:U:82:LEU:O	1:U:129:ARG:NH2	2.44	0.51
1:U:187:LEU:HD22	15:D:45:LYS:HG2	1.92	0.51
1:U:624:PHE:CE1	1:U:760:VAL:HG13	2.44	0.51
3:W:37:GLU:HG2	3:W:38:GLY:N	2.25	0.51
3:W:436:MET:O	3:W:439:VAL:HG12	2.11	0.51
5:Y:13:LYS:NZ	5:Y:112:CYS:SG	2.65	0.51
5:Y:72:LYS:HD3	5:Y:75:LYS:HE2	1.93	0.51
7:a:160:SER:O	7:a:163:TYR:HB3	2.10	0.51
7:a:215:GLU:CA	7:a:218:MET:SD	2.91	0.51
30:S:211:ARG:NE	30:S:213:ASP:OD2	2.44	0.51
33:x:557:TRP:N	33:x:557:TRP:CD1	2.78	0.51
33:x:562:LEU:HD11	33:x:576:ILE:HG21	1.92	0.51
1:U:140:ARG:HH21	1:U:144:ASP:HA	1.76	0.51
1:U:709:PHE:O	1:U:709:PHE:HD1	1.93	0.51
1:U:789:ILE:HB	1:U:911:ILE:HA	1.93	0.51
2:V:309:MET:CE	2:V:328:VAL:CG1	2.88	0.51
4:X:92:LEU:HA	4:X:95:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:68:TRP:CD1	6:Z:104:ASN:HD21	2.29	0.51
7:a:137:ASP:O	7:a:140:GLU:HG3	2.10	0.51
12:A:23:ARG:O	13:B:410:ARG:NH2	2.43	0.51
16:E:173:TYR:CE1	16:E:298:LYS:HB3	2.40	0.51
17:F:198:LEU:HD22	17:F:236:LEU:HD22	1.92	0.51
30:s:16:ALA:HB2	30:s:121:VAL:HG23	1.92	0.51
33:x:371:ASN:HB3	33:x:398:TRP:HH2	1.75	0.51
33:x:531:ASN:HB3	33:x:534:VAL:HB	1.93	0.51
1:U:195:ASN:OD1	1:U:196:LYS:N	2.42	0.51
1:U:847:GLU:O	1:U:851:GLU:HG3	2.11	0.51
4:X:334:ASN:HA	4:X:337:ARG:HB2	1.92	0.51
7:a:373:ASP:OD1	10:d:251:ARG:NH2	2.44	0.51
10:d:103:LEU:HD22	10:d:133:ILE:HG23	1.91	0.51
12:A:292:ASP:OD1	12:A:292:ASP:N	2.42	0.51
16:E:334:LEU:HB2	16:E:371:VAL:HG11	1.93	0.51
16:E:352:MET:HA	16:E:352:MET:HE3	1.91	0.51
22:k:201:ILE:O	22:k:205:VAL:HG23	2.10	0.51
33:x:670:MET:HE1	33:x:673:ARG:HD2	1.92	0.51
2:V:270:LEU:HG	2:V:295:ILE:HD11	1.92	0.51
2:V:416:ARG:HH12	5:Y:350:VAL:H	1.57	0.51
5:Y:159:ARG:O	5:Y:159:ARG:HG2	2.11	0.51
6:Z:250:TYR:HD2	6:Z:250:TYR:O	1.93	0.51
23:L:176:MET:HE3	24:M:57:LEU:HD23	1.93	0.51
24:M:191:LYS:HB3	24:M:238:TYR:CD2	2.46	0.51
24:M:230:ASP:OD1	24:M:231:ILE:N	2.43	0.51
20:i:140:ASP:OD2	20:i:146:GLN:NE2	2.32	0.51
24:m:77:VAL:HG21	24:m:84:ALA:HB1	1.92	0.51
33:x:291:GLN:HA	33:x:294:MET:HE1	1.93	0.51
1:U:353:LEU:HD11	1:U:376:MET:HE1	1.93	0.51
1:U:756:HIS:HB2	1:U:759:SER:HB3	1.93	0.51
2:V:152:GLY:O	2:V:156:SER:HB3	2.11	0.51
3:W:279:PHE:HA	3:W:283:GLN:HG2	1.91	0.51
3:W:370:TYR:OH	7:a:308:GLU:OE1	2.29	0.51
8:b:11:ASP:OD1	8:b:11:ASP:N	2.43	0.51
9:c:215:LYS:H	9:c:215:LYS:HZ1	1.58	0.51
10:d:191:PHE:HZ	10:d:202:THR:H	1.57	0.51
16:E:354:ALA:HA	16:E:358:ASP:OD1	2.11	0.51
17:F:48:LEU:HB3	17:F:52:ILE:HG23	1.93	0.51
18:G:17:SER:OG	18:G:19:GLU:OE2	2.20	0.51
19:h:12:THR:O	19:h:19:LEU:HD23	2.11	0.51
1:U:137:MET:HG3	14:C:20:LEU:HD21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:319:HIS:HB3	2:V:322:VAL:HB	1.92	0.51
5:Y:191:ILE:HG13	5:Y:290:PRO:HB2	1.93	0.51
7:a:169:HIS:CD2	7:a:206:LEU:HD23	2.45	0.51
9:c:291:LEU:O	9:c:295:ASN:ND2	2.44	0.51
12:A:258:ARG:HH12	17:F:255:GLN:HA	1.75	0.51
18:g:123:GLN:HE22	18:g:127:GLN:HB2	1.75	0.51
23:l:50:LYS:HG2	23:l:60:GLN:O	2.11	0.51
1:U:22:PHE:CE2	10:d:31:LEU:HG	2.45	0.51
1:U:247:GLN:HE21	1:U:912:ILE:HA	1.73	0.51
1:U:445:ALA:HA	1:U:448:LEU:HD12	1.93	0.51
2:V:79:VAL:HA	2:V:161:PRO:HB3	1.92	0.51
2:V:363:LEU:HB2	2:V:378:VAL:HG11	1.93	0.51
3:W:20:TYR:O	3:W:23:THR:HG22	2.11	0.51
4:X:147:LEU:HD13	4:X:176:THR:HG21	1.93	0.51
7:a:37:LEU:O	7:a:41:VAL:HG23	2.10	0.51
9:c:155:VAL:HG12	9:c:157:ILE:HG12	1.92	0.51
24:M:66:LEU:HD13	24:M:214:SER:HB2	1.93	0.51
27:p:25:ASP:OD1	27:p:41:LYS:NZ	2.44	0.51
33:x:388:ASP:OD1	33:x:389:LYS:N	2.44	0.51
33:x:559:PRO:CG	33:x:587:PHE:CZ	2.87	0.51
33:x:585:GLU:C	33:x:587:PHE:N	2.70	0.51
1:U:489:ALA:HA	1:U:520:MET:HE1	1.93	0.50
1:U:895:PRO:HG2	1:U:902:PRO:HD3	1.92	0.50
3:W:355:LYS:HE2	3:W:384:LEU:HD11	1.92	0.50
6:Z:260:VAL:HG13	6:Z:261:TYR:CD1	2.46	0.50
9:c:30:GLN:HA	9:c:204:THR:OG1	2.11	0.50
10:d:203:PRO:HG2	10:d:206:MET:N	2.23	0.50
13:B:193:GLN:OE1	13:B:193:GLN:N	2.44	0.50
15:D:115:ILE:O	15:D:115:ILE:CD1	2.42	0.50
18:G:113:MET:HE2	26:O:70:THR:HG22	1.94	0.50
24:M:229:LYS:O	24:M:233:GLU:HG2	2.11	0.50
26:O:104:ASP:OD2	26:O:104:ASP:N	2.45	0.50
33:x:59:LEU:HD11	33:x:77:GLU:HB3	1.92	0.50
1:U:115:ASN:HA	1:U:118:LEU:HD23	1.92	0.50
2:V:37:MET:C	2:V:37:MET:HE2	2.36	0.50
5:Y:192:ARG:CD	5:Y:194:PHE:HB3	2.40	0.50
6:Z:106:ILE:HG13	6:Z:153:LYS:HD2	1.93	0.50
7:a:68:GLU:O	7:a:69:HIS:ND1	2.44	0.50
9:c:232:GLN:HE21	9:c:237:HIS:HB2	1.76	0.50
10:d:12:LYS:C	10:d:12:LYS:HD3	2.36	0.50
13:B:82:GLN:HA	13:B:86:LYS:HZ3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:35:VAL:HG21	15:D:50:GLU:HB3	1.94	0.50
15:D:141:ASP:OD1	15:D:142:VAL:N	2.43	0.50
16:E:47:LEU:HD11	17:F:76:ASN:ND2	2.26	0.50
24:m:27:MET:HE1	24:m:152:ASP:OD1	2.12	0.50
33:x:782:HIS:HB2	33:x:895:GLU:OE2	2.12	0.50
1:U:215:ASN:OD1	1:U:216:VAL:N	2.41	0.50
2:V:132:LEU:HA	2:V:135:LEU:HG	1.93	0.50
2:V:165:ALA:C	2:V:167:LEU:H	2.18	0.50
2:V:182:LYS:O	2:V:186:LYS:HG3	2.11	0.50
2:V:267:ALA:HA	2:V:270:LEU:HD12	1.93	0.50
3:W:80:TRP:HZ3	18:G:242:LEU:C	2.19	0.50
3:W:89:LEU:C	3:W:91:SER:H	2.18	0.50
6:Z:129:LYS:HD2	6:Z:129:LYS:C	2.35	0.50
6:Z:192:THR:HG22	7:a:375:LEU:HD22	1.91	0.50
7:a:233:LEU:O	7:a:237:LEU:HG	2.11	0.50
7:a:290:GLN:HG2	7:a:330:ARG:HB3	1.94	0.50
17:F:38:THR:O	17:F:42:ILE:HB	2.10	0.50
18:G:211:LYS:HG2	18:G:212:PRO:HD2	1.93	0.50
1:U:140:ARG:HH21	1:U:144:ASP:CA	2.24	0.50
2:V:417:ILE:HA	5:Y:349:LYS:HB2	1.92	0.50
3:W:311:THR:C	3:W:313:GLU:H	2.19	0.50
5:Y:180:LEU:HD23	5:Y:183:TYR:HE2	1.77	0.50
6:Z:108:ILE:O	6:Z:111:LEU:HG	2.11	0.50
6:Z:263:ALA:HB1	9:c:288:VAL:HG13	1.93	0.50
7:a:93:ALA:O	7:a:97:LEU:HD22	2.12	0.50
7:a:177:LEU:HA	7:a:180:LEU:HG	1.92	0.50
9:c:78:SER:HB2	9:c:86:ALA:HA	1.93	0.50
10:d:1:MET:HE3	10:d:2:TYR:H	1.76	0.50
16:E:276:ILE:HD12	16:E:276:ILE:N	2.26	0.50
16:E:353:PHE:HD2	16:E:357:ALA:O	1.93	0.50
27:P:142:CYS:O	27:P:146:MET:HG3	2.10	0.50
28:q:43:LEU:HD12	28:q:183:ILE:HD11	1.92	0.50
33:x:263:PRO:O	33:x:267:ARG:NH1	2.44	0.50
3:W:317:TRP:HA	3:W:320:LEU:CD2	2.42	0.50
3:W:439:VAL:HB	6:Z:234:PHE:HZ	1.77	0.50
5:Y:80:GLU:O	5:Y:84:LEU:CD2	2.56	0.50
6:Z:256:GLN:HE22	6:Z:260:VAL:HG21	1.77	0.50
7:a:84:VAL:HG11	7:a:97:LEU:HD11	1.92	0.50
8:b:17:ARG:C	8:b:18:ASN:HD22	2.20	0.50
9:c:33:ILE:HG13	9:c:34:SER:H	1.75	0.50
13:B:85:MET:CE	33:x:619:HIS:CB	2.62	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:85:MET:C	13:B:87:PRO:HD3	2.36	0.50
16:E:36:LEU:O	16:E:39:GLN:HB2	2.12	0.50
24:M:8:ASP:O	24:M:22:GLN:NE2	2.43	0.50
18:g:174:GLU:OE1	18:g:174:GLU:N	2.44	0.50
23:l:171:TYR:CE2	23:l:193:ARG:HG2	2.47	0.50
1:U:602:LEU:HD21	1:U:618:ALA:HA	1.94	0.50
2:V:155:ALA:C	2:V:158:PRO:HD2	2.37	0.50
2:V:333:ILE:HD12	2:V:334:VAL:N	2.26	0.50
3:W:190:MET:HG2	3:W:205:ILE:HG13	1.94	0.50
3:W:251:TYR:HE1	3:W:267:LEU:HB2	1.76	0.50
3:W:361:HIS:O	3:W:365:ILE:HG13	2.11	0.50
9:c:54:MET:HE2	9:c:86:ALA:CB	2.38	0.50
18:g:213:SER:O	18:g:213:SER:OG	2.28	0.50
31:t:151:ARG:O	31:t:155:GLU:HG3	2.12	0.50
33:x:249:LEU:HD21	33:x:271:MET:HB2	1.92	0.50
33:x:373:ALA:HB2	33:x:760:PHE:CD1	2.45	0.50
33:x:680:ARG:NH1	33:x:681:TYR:OH	2.44	0.50
1:U:629:THR:HB	1:U:631:GLU:OE1	2.12	0.50
2:V:337:LEU:HD21	2:V:364:THR:HG23	1.94	0.50
3:W:230:MET:HE2	3:W:242:SER:OG	2.12	0.50
4:X:76:PHE:C	4:X:76:PHE:CD1	2.88	0.50
5:Y:160:ASN:C	5:Y:163:LYS:HB3	2.37	0.50
6:Z:53:SER:HB3	6:Z:95:TYR:CE2	2.47	0.50
8:b:107:MET:HB3	8:b:136:VAL:HG13	1.93	0.50
12:A:261:PHE:O	12:A:265:ARG:HG3	2.12	0.50
16:E:69:PHE:HE2	16:E:92:LEU:HD12	1.77	0.50
16:E:177:GLY:H	38:E:401:ADP:PB	2.35	0.50
17:F:304:ARG:O	17:F:308:ARG:HG2	2.12	0.50
18:g:211:LYS:HB3	18:g:212:PRO:HD2	1.93	0.50
33:x:615:ILE:HD11	33:x:649:HIS:CD2	2.41	0.50
1:U:160:LEU:HD23	1:U:200:VAL:HG21	1.94	0.50
2:V:153:LYS:HZ1	2:V:202:ALA:HB1	1.76	0.50
2:V:198:GLN:OE1	14:C:33:LEU:HD11	2.12	0.50
3:W:93:ARG:HD2	3:W:93:ARG:O	2.11	0.50
3:W:123:ARG:O	3:W:127:THR:HG22	2.12	0.50
3:W:169:LEU:O	3:W:182:ARG:NH1	2.37	0.50
4:X:93:LEU:O	4:X:97:LEU:HD12	2.11	0.50
4:X:379:ASP:O	4:X:383:GLY:N	2.45	0.50
5:Y:228:MET:HE1	5:Y:259:TYR:CE2	2.47	0.50
7:a:76:LEU:O	7:a:80:ILE:HG13	2.12	0.50
9:c:71:ASP:OD1	9:c:72:VAL:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:79:GLY:HA2	17:F:82:VAL:O	2.11	0.50
20:I:6:ASP:C	20:I:6:ASP:OD1	2.55	0.50
31:t:107:TRP:O	31:t:108:ASN:ND2	2.45	0.50
33:x:505:MET:SD	33:x:541:THR:OG1	2.67	0.50
33:x:705:ASN:N	33:x:705:ASN:OD1	2.45	0.50
2:V:90:GLU:OE1	2:V:90:GLU:N	2.45	0.50
2:V:128:ARG:NH1	2:V:165:ALA:HA	2.27	0.50
2:V:212:TYR:HB3	11:e:4:LYS:HZ3	1.76	0.50
3:W:366:MET:HE2	3:W:378:MET:SD	2.51	0.50
3:W:375:MET:HE2	3:W:411:GLY:HA3	1.94	0.50
5:Y:237:ARG:NE	5:Y:264:TYR:OH	2.45	0.50
8:b:56:ASN:N	8:b:83:LYS:O	2.45	0.50
15:D:270:ILE:HG22	15:D:285:VAL:HG13	1.94	0.50
15:D:281:ALA:HA	15:D:284:GLU:HB3	1.94	0.50
16:E:371:VAL:O	16:E:374:VAL:CG2	2.60	0.50
33:x:253:LEU:CA	33:x:256:PHE:CD1	2.94	0.50
33:x:431:LYS:HG3	33:x:432:TYR:CD1	2.46	0.50
1:U:132:GLY:HA2	1:U:135:ASN:OD1	2.12	0.49
1:U:692:ALA:HB2	1:U:733:ALA:HB1	1.93	0.49
1:U:796:LYS:NZ	1:U:916:ASP:OD2	2.39	0.49
2:V:212:TYR:HB3	11:e:4:LYS:NZ	2.26	0.49
2:V:250:LEU:HA	2:V:253:LEU:HD12	1.93	0.49
2:V:416:ARG:NH2	5:Y:350:VAL:HG22	2.27	0.49
5:Y:343:LEU:O	5:Y:345:CYS:N	2.45	0.49
6:Z:176:LEU:O	9:c:209:LYS:NZ	2.40	0.49
7:a:191:SER:O	7:a:194:GLN:HG2	2.11	0.49
8:b:16:MET:HA	8:b:25:ARG:HD2	1.92	0.49
12:A:44:GLN:O	12:A:48:VAL:HG23	2.12	0.49
14:C:343:ASN:HD22	14:C:346:LYS:HD3	1.77	0.49
15:D:64:GLU:OE1	15:D:67:ASN:ND2	2.45	0.49
15:D:151:ILE:HD12	15:D:151:ILE:O	2.11	0.49
17:F:134:LEU:HD12	17:F:134:LEU:O	2.12	0.49
29:R:1:THR:HG23	29:R:33:LYS:NZ	2.27	0.49
21:j:29:GLY:O	21:j:163:ARG:N	2.21	0.49
21:j:78:ALA:O	21:j:82:ILE:HG12	2.12	0.49
33:x:419:LEU:HD23	33:x:420:TRP:CG	2.47	0.49
33:x:659:LEU:HA	33:x:662:MET:SD	2.51	0.49
2:V:248:ALA:HB1	2:V:284:GLU:CD	2.37	0.49
3:W:49:SER:HA	3:W:52:LYS:HG2	1.93	0.49
5:Y:77:ASN:N	5:Y:77:ASN:ND2	2.59	0.49
6:Z:69:PHE:HZ	8:b:95:LEU:HB3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:38:THR:HG21	7:a:71:VAL:HG21	1.94	0.49
9:c:51:MET:HE3	9:c:51:MET:CA	2.15	0.49
10:d:206:MET:O	10:d:209:TYR:N	2.45	0.49
12:A:138:MET:HG2	12:A:139:ARG:N	2.25	0.49
12:A:351:ARG:NH1	12:A:378:PRO:O	2.45	0.49
16:E:6:ASP:OD1	16:E:7:LYS:N	2.45	0.49
16:E:324:GLY:O	16:E:326:ILE:N	2.45	0.49
27:p:122:CYS:SG	27:p:123:SER:N	2.84	0.49
33:x:288:VAL:HG12	33:x:292:LYS:HE3	1.94	0.49
33:x:301:HIS:HA	33:x:782:HIS:HE1	1.76	0.49
33:x:583:VAL:O	33:x:588:ARG:NH2	2.45	0.49
2:V:110:HIS:O	2:V:114:TYR:HB2	2.12	0.49
2:V:199:ASN:O	2:V:203:LEU:HG	2.12	0.49
2:V:476:PHE:HB3	6:Z:260:VAL:CG2	2.40	0.49
3:W:366:MET:O	3:W:370:TYR:HB2	2.11	0.49
3:W:373:ILE:HD13	3:W:378:MET:HE3	1.94	0.49
4:X:142:ARG:CZ	4:X:142:ARG:HA	2.42	0.49
4:X:171:LEU:O	4:X:175:LYS:HG3	2.11	0.49
4:X:302:PHE:CZ	4:X:327:TYR:HB2	2.47	0.49
5:Y:152:MET:O	5:Y:152:MET:HG3	2.10	0.49
6:Z:74:TYR:HE2	9:c:98:MET:HG2	1.76	0.49
6:Z:263:ALA:HB2	9:c:291:LEU:HD11	1.94	0.49
9:c:30:GLN:HG3	9:c:32:TYR:HE1	1.77	0.49
12:A:27:GLU:O	12:A:30:ILE:HG22	2.11	0.49
12:A:62:LEU:CD2	13:B:79:ILE:HD13	2.42	0.49
12:A:98:CYS:SG	13:B:122:ILE:HD11	2.52	0.49
24:M:191:LYS:HB3	24:M:238:TYR:HD2	1.77	0.49
33:x:112:ASN:OD1	33:x:113:MET:N	2.44	0.49
33:x:554:TYR:HD1	33:x:557:TRP:CH2	2.30	0.49
1:U:12:LEU:HD11	1:U:27:LEU:HD11	1.93	0.49
1:U:420:LEU:O	1:U:423:MET:SD	2.70	0.49
1:U:529:ILE:HD11	1:U:566:LEU:HD22	1.95	0.49
1:U:619:VAL:HG23	1:U:640:LEU:HD13	1.93	0.49
3:W:254:PRO:HA	3:W:257:GLN:HB2	1.94	0.49
3:W:366:MET:HE2	3:W:378:MET:CE	2.41	0.49
5:Y:50:MET:SD	5:Y:74:LYS:HD3	2.51	0.49
6:Z:206:LEU:O	6:Z:209:ARG:HG2	2.13	0.49
7:a:71:VAL:HA	8:b:17:ARG:HH12	1.77	0.49
7:a:96:PHE:O	7:a:100:THR:HG23	2.13	0.49
9:c:106:GLU:N	9:c:106:GLU:OE2	2.45	0.49
11:e:61:GLU:O	11:e:65:TYR:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:113:ARG:NH2	16:E:115:VAL:H	2.10	0.49
16:E:320:ILE:CG2	16:E:362:VAL:CG1	2.90	0.49
24:m:233:GLU:HA	24:m:236:GLU:CD	2.37	0.49
27:p:27:ARG:HB2	27:p:183:MET:HB2	1.93	0.49
33:x:559:PRO:CG	33:x:587:PHE:HZ	2.24	0.49
33:x:585:GLU:N	33:x:586:PRO:CD	2.74	0.49
2:V:309:MET:HE3	2:V:312:ALA:HB3	1.95	0.49
3:W:251:TYR:CE1	3:W:267:LEU:CA	2.96	0.49
5:Y:62:ASP:O	5:Y:63:TRP:HB2	2.13	0.49
6:Z:38:VAL:CG1	6:Z:54:PHE:CE1	2.95	0.49
12:A:244:GLU:OE2	12:A:244:GLU:HA	2.13	0.49
13:B:94:GLU:HB3	13:B:98:LYS:HD3	1.94	0.49
14:C:25:LEU:O	14:C:28:ILE:HG12	2.12	0.49
14:C:56:VAL:CG1	15:D:72:PHE:HD1	2.21	0.49
17:F:289:ASP:OD1	17:F:289:ASP:N	2.44	0.49
23:l:171:TYR:CD1	23:l:171:TYR:C	2.91	0.49
33:x:472:HIS:ND1	33:x:477:MET:SD	2.85	0.49
2:V:253:LEU:HB3	2:V:256:ARG:HH21	1.77	0.49
2:V:354:LYS:HG3	2:V:358:MET:CE	2.43	0.49
9:c:245:VAL:O	9:c:249:LEU:CD2	2.57	0.49
12:A:87:LEU:O	12:A:91:GLN:HB2	2.13	0.49
13:B:121:ALA:HB2	13:B:135:ILE:HD11	1.94	0.49
19:H:119:GLN:HG3	20:I:81:SER:HB3	1.93	0.49
18:g:206:LEU:HB3	18:g:208:ILE:HG13	1.95	0.49
33:x:460:ASP:OD2	33:x:494:ARG:NH1	2.46	0.49
33:x:719:PRO:O	33:x:723:TYR:HD1	1.95	0.49
33:x:727:PHE:CD1	33:x:761:MET:HE2	2.47	0.49
1:U:644:TYR:OH	14:C:57:ARG:HA	2.13	0.49
2:V:37:MET:HA	2:V:40:GLU:OE2	2.12	0.49
2:V:213:TYR:N	2:V:213:TYR:CD2	2.80	0.49
3:W:285:ASP:OD1	3:W:286:LEU:N	2.46	0.49
4:X:148:HIS:O	4:X:152:GLN:HG2	2.13	0.49
5:Y:157:ILE:HD13	5:Y:186:LEU:HG	1.93	0.49
6:Z:73:ASP:OD2	6:Z:74:TYR:N	2.45	0.49
6:Z:109:ASN:HB2	6:Z:153:LYS:HZ1	1.78	0.49
6:Z:202:ASN:OD1	6:Z:203:SER:N	2.46	0.49
7:a:17:GLY:O	7:a:21:VAL:HG22	2.13	0.49
9:c:36:LEU:HD11	9:c:40:LYS:HE2	1.94	0.49
16:E:346:VAL:HG13	16:E:370:ALA:HB1	1.93	0.49
19:H:219:ARG:NH2	19:H:225:GLU:OE1	2.46	0.49
23:L:128:TYR:O	23:L:149:PRO:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:T:96:MET:HE1	31:T:110:MET:CE	2.35	0.49
31:T:179:ARG:HD3	26:o:139:GLU:OE2	2.13	0.49
24:m:27:MET:HE2	24:m:153:PRO:HD2	1.93	0.49
31:t:207:THR:OG1	31:t:209:TRP:NE1	2.46	0.49
2:V:66:GLU:CG	2:V:205:LEU:HD22	2.42	0.49
2:V:66:GLU:HG2	2:V:205:LEU:HD22	1.94	0.49
2:V:218:TYR:HD2	2:V:224:LEU:HA	1.78	0.49
4:X:65:GLU:H	4:X:65:GLU:CD	2.21	0.49
5:Y:195:LYS:HB2	5:Y:199:GLU:OE1	2.12	0.49
6:Z:20:VAL:HA	6:Z:126:VAL:HG23	1.95	0.49
7:a:284:ARG:HA	7:a:284:ARG:NE	2.26	0.49
12:A:150:HIS:HB3	12:A:151:ILE:HD12	1.94	0.49
15:D:221:HIS:ND1	15:D:222:HIS:CE1	2.81	0.49
16:E:238:ILE:HD12	16:E:239:GLY:N	2.28	0.49
17:F:90:VAL:HA	17:F:152:GLY:HA2	1.95	0.49
20:I:118:LYS:NZ	20:I:150:SER:OG	2.46	0.49
31:t:63:LEU:HD13	31:t:110:MET:HE1	1.94	0.49
32:f:395:LEU:HD21	33:x:461:PRO:HB3	1.94	0.49
33:x:695:ALA:HB2	33:x:728:ALA:HA	1.93	0.49
1:U:96:TYR:CZ	1:U:100:ILE:HD13	2.48	0.49
2:V:199:ASN:C	2:V:203:LEU:HG	2.37	0.49
2:V:480:ILE:O	2:V:484:LEU:HG	2.12	0.49
3:W:413:ILE:HD12	3:W:415:PHE:CE1	2.48	0.49
14:C:370:ALA:HB1	14:C:375:ARG:O	2.12	0.49
16:E:277:MET:HE3	16:E:279:THR:HB	1.94	0.49
18:G:130:GLU:O	18:G:131:MET:CB	2.59	0.49
21:j:117:ARG:HH12	21:j:124:ARG:HH22	1.61	0.49
33:x:785:ARG:HH12	33:x:877:GLY:H	1.60	0.49
1:U:17:PRO:O	1:U:20:LYS:HB2	2.13	0.49
1:U:495:ASP:O	1:U:499:THR:HG23	2.13	0.49
2:V:25:GLU:HB3	2:V:26:PRO:HD3	1.94	0.49
2:V:157:THR:O	2:V:161:PRO:HD2	2.12	0.49
2:V:218:TYR:HE2	2:V:226:VAL:HB	1.77	0.49
2:V:292:THR:HA	2:V:295:ILE:HG22	1.94	0.49
3:W:167:GLN:OE1	3:W:168:GLU:N	2.46	0.49
3:W:317:TRP:HD1	3:W:358:VAL:HG21	1.77	0.49
5:Y:180:LEU:HA	5:Y:183:TYR:CD2	2.47	0.49
7:a:339:ARG:HH21	7:a:341:LEU:HD21	1.78	0.49
8:b:16:MET:O	8:b:25:ARG:HB2	2.13	0.49
13:B:360:THR:O	13:B:364:ILE:HG13	2.13	0.49
16:E:196:LEU:O	16:E:218:MET:HE2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:58:GLU:HA	17:F:61:ARG:HD2	1.94	0.49
19:h:75:VAL:HG12	19:h:135:LEU:HB2	1.94	0.49
33:x:184:LEU:HD23	33:x:184:LEU:H	1.78	0.49
1:U:532:MET:HE2	1:U:548:LEU:O	2.13	0.48
1:U:669:ILE:HG21	1:U:705:LYS:HG3	1.95	0.48
1:U:688:LEU:O	1:U:713:TYR:OH	2.31	0.48
2:V:228:ARG:O	2:V:232:HIS:ND1	2.46	0.48
2:V:242:HIS:CG	2:V:242:HIS:O	2.65	0.48
2:V:307:ARG:HG3	2:V:308:THR:N	2.28	0.48
2:V:309:MET:O	2:V:309:MET:CE	2.51	0.48
2:V:416:ARG:CG	2:V:459:GLN:HG2	2.43	0.48
3:W:142:ARG:H	3:W:142:ARG:CD	2.26	0.48
3:W:193:CYS:SG	3:W:198:ASP:HB3	2.53	0.48
7:a:76:LEU:O	7:a:79:ILE:HG22	2.13	0.48
8:b:29:GLN:O	8:b:33:VAL:HG13	2.13	0.48
8:b:141:ILE:HA	8:b:171:VAL:HB	1.95	0.48
9:c:278:GLN:C	9:c:280:PRO:HD2	2.37	0.48
13:B:137:SER:O	13:B:138:PHE:CD1	2.66	0.48
15:D:214:MET:HE2	38:D:501:ADP:H2'	1.95	0.48
16:E:287:PRO:O	16:E:291:ARG:HG2	2.13	0.48
19:H:182:LEU:HD13	19:H:186:ASP:HB2	1.94	0.48
26:O:24:MET:HE1	30:s:33:PHE:HE2	1.77	0.48
23:l:157:ARG:HH12	23:l:180:MET:HE1	1.78	0.48
33:x:837:LEU:HG	33:x:837:LEU:O	2.13	0.48
1:U:229:VAL:HA	1:U:232:ILE:HG12	1.93	0.48
1:U:544:ILE:HD12	1:U:545:LEU:N	2.28	0.48
2:V:37:MET:SD	2:V:38:LYS:N	2.86	0.48
3:W:268:LYS:O	3:W:336:PRO:HG2	2.13	0.48
3:W:365:ILE:HD12	3:W:366:MET:H	1.76	0.48
3:W:451:MET:HE3	6:Z:101:LEU:HB3	1.94	0.48
5:Y:37:VAL:HA	5:Y:40:GLU:HB3	1.94	0.48
5:Y:191:ILE:HD13	11:e:45:ASP:OD1	2.14	0.48
6:Z:69:PHE:HE1	8:b:92:VAL:HG13	1.78	0.48
6:Z:273:HIS:CD2	6:Z:277:ASN:OD1	2.66	0.48
8:b:35:ILE:HD12	8:b:36:VAL:N	2.28	0.48
10:d:12:LYS:NZ	10:d:14:PRO:CB	2.70	0.48
12:A:140:VAL:HB	12:A:149:ILE:HG23	1.95	0.48
14:C:52:LEU:HB2	15:D:68:LEU:HD13	1.94	0.48
14:C:337:ASN:HD21	14:C:376:VAL:HG12	1.77	0.48
16:E:329:GLU:HG3	16:E:333:LYS:HZ2	1.76	0.48
26:O:78:THR:O	26:O:82:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:g:52:THR:HG22	18:g:216:GLU:HG3	1.94	0.48
18:g:185:LYS:HD3	18:g:185:LYS:C	2.38	0.48
33:x:270:LEU:HD11	33:x:301:HIS:CE1	2.48	0.48
33:x:305:LEU:HB2	33:x:321:MET:HE1	1.96	0.48
1:U:427:LEU:HD13	1:U:430:ASP:HB2	1.94	0.48
3:W:50:LEU:HA	3:W:53:GLN:HG2	1.95	0.48
3:W:82:LEU:O	3:W:86:ASN:OD1	2.31	0.48
3:W:136:ILE:HG21	3:W:171:VAL:HG12	1.95	0.48
6:Z:35:VAL:O	6:Z:96:HIS:HD2	1.96	0.48
7:a:371:ALA:HB1	7:a:375:LEU:HB2	1.95	0.48
13:B:408:ARG:HH21	14:C:163:GLU:CD	2.21	0.48
14:C:38:LYS:NZ	15:D:58:GLU:HG3	2.28	0.48
30:S:151:ASN:OD1	27:p:173:ASN:ND2	2.46	0.48
18:g:71:LYS:O	18:g:95:ARG:NH1	2.45	0.48
21:j:116:GLN:HB2	21:j:151:GLY:HA3	1.93	0.48
33:x:184:LEU:HA	33:x:187:LEU:HD12	1.95	0.48
33:x:266:LEU:HB3	33:x:267:ARG:HH12	1.77	0.48
33:x:431:LYS:HA	33:x:434:TYR:CZ	2.48	0.48
33:x:736:THR:HB	33:x:738:ASN:HD21	1.77	0.48
33:x:807:ARG:O	33:x:811:LEU:HD22	2.13	0.48
1:U:475:HIS:NE2	1:U:507:VAL:O	2.46	0.48
1:U:619:VAL:HG13	1:U:651:GLY:HA3	1.96	0.48
3:W:56:THR:CG2	3:W:104:MET:CE	2.90	0.48
4:X:85:ALA:O	4:X:88:LEU:HG	2.12	0.48
8:b:5:SER:HB3	8:b:64:LEU:HD21	1.94	0.48
8:b:150:THR:O	8:b:154:THR:HG23	2.14	0.48
13:B:296:ASP:OD1	13:B:296:ASP:N	2.39	0.48
21:j:94:HIS:ND1	21:j:102:VAL:HG22	2.28	0.48
1:U:450:HIS:CD2	1:U:457:ILE:HD13	2.49	0.48
1:U:544:ILE:H	1:U:544:ILE:HG13	1.41	0.48
1:U:633:CYS:CB	1:U:659:CYS:SG	3.01	0.48
5:Y:57:LEU:HD11	5:Y:62:ASP:C	2.39	0.48
7:a:312:MET:O	7:a:316:SER:OG	2.23	0.48
8:b:116:PRO:HD3	8:b:145:GLU:OE2	2.14	0.48
11:e:41:ASP:C	11:e:43:TRP:H	2.20	0.48
12:A:73:ALA:O	12:A:78:TRP:NE1	2.46	0.48
26:O:24:MET:HE1	30:s:33:PHE:CE2	2.48	0.48
20:i:17:ARG:NH1	20:i:19:TYR:HA	2.27	0.48
20:i:216:LEU:HD12	20:i:225:ILE:HG12	1.95	0.48
22:k:88:LEU:HD23	22:k:119:LEU:HD23	1.95	0.48
39:o:301:LDZ:H2	27:p:126:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:q:3:TYR:OH	28:q:139:THR:HG21	2.12	0.48
28:q:19:ARG:HE	28:q:31:ASP:HA	1.78	0.48
2:V:161:PRO:HA	2:V:164:GLU:HB2	1.94	0.48
5:Y:63:TRP:CE2	5:Y:64:GLN:O	2.66	0.48
5:Y:180:LEU:HD22	5:Y:200:LEU:HD23	1.95	0.48
5:Y:268:TYR:HA	5:Y:271:PHE:HB3	1.95	0.48
6:Z:10:VAL:HG12	6:Z:49:ASP:HA	1.95	0.48
6:Z:108:ILE:HA	6:Z:111:LEU:HD23	1.96	0.48
6:Z:166:GLU:O	6:Z:167:ALA:HB3	2.13	0.48
13:B:405:MET:HG2	13:B:421:LYS:HE3	1.93	0.48
15:D:194:ILE:HG22	15:D:196:ILE:HG23	1.96	0.48
21:J:241:LYS:HG3	21:J:242:LYS:HG3	1.95	0.48
23:L:183:ASN:OD1	23:L:183:ASN:N	2.46	0.48
24:M:21:PHE:HA	24:M:24:GLU:HG3	1.96	0.48
25:N:188:VAL:HG12	25:N:190:LEU:HG	1.95	0.48
21:j:5:ARG:HD3	21:j:6:ALA:H	1.77	0.48
31:t:157:GLN:NE2	31:t:159:VAL:O	2.46	0.48
33:x:308:SER:O	33:x:311:VAL:HG12	2.14	0.48
33:x:605:ASN:O	33:x:609:VAL:HG23	2.13	0.48
33:x:727:PHE:C	33:x:731:MET:HE2	2.38	0.48
1:U:602:LEU:HD11	1:U:618:ALA:O	2.14	0.48
1:U:691:SER:HA	1:U:694:ILE:HG22	1.95	0.48
3:W:79:GLU:CB	3:W:130:MET:CE	2.92	0.48
3:W:316:ARG:HG3	3:W:383:ASP:OD2	2.14	0.48
4:X:202:CYS:O	4:X:204:PRO:HD3	2.14	0.48
7:a:9:GLN:NE2	7:a:12:GLN:OE1	2.46	0.48
10:d:198:LEU:HB3	10:d:205:LYS:NZ	2.29	0.48
15:D:54:LEU:O	15:D:58:GLU:HG2	2.13	0.48
15:D:384:MET:HE2	16:E:167:PRO:HB3	1.96	0.48
20:i:15:GLU:OE2	20:i:15:GLU:N	2.40	0.48
21:j:7:ILE:CD1	21:j:18:GLN:HB3	2.43	0.48
21:j:177:THR:OG1	21:j:178:ASP:N	2.47	0.48
23:l:65:HIS:O	23:l:89:ARG:NH1	2.46	0.48
33:x:584:SER:C	33:x:586:PRO:HD2	2.38	0.48
1:U:255:SER:O	1:U:757:MET:HE1	2.13	0.48
1:U:560:MET:HE2	1:U:590:TYR:HA	1.94	0.48
2:V:145:LEU:O	2:V:148:ARG:HD3	2.13	0.48
2:V:179:LYS:HE3	2:V:214:HIS:ND1	2.28	0.48
2:V:241:ARG:HD2	2:V:241:ARG:HA	1.65	0.48
3:W:89:LEU:O	3:W:90:LEU:HG	2.13	0.48
3:W:169:LEU:HD11	3:W:189:GLN:CD	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:432:LEU:HD21	9:c:309:PHE:CD1	2.49	0.48
4:X:281:GLY:O	4:X:285:GLU:HG2	2.14	0.48
9:c:26:ASP:N	9:c:174:PRO:HD2	2.21	0.48
10:d:175:ARG:NH2	10:d:198:LEU:HA	2.29	0.48
12:A:124:ASP:OD1	12:A:125:LEU:N	2.46	0.48
13:B:94:GLU:HB3	13:B:98:LYS:CD	2.44	0.48
13:B:329:MET:CE	13:B:347:ILE:CG2	2.92	0.48
14:C:207:THR:O	14:C:208:ASP:OD2	2.31	0.48
28:Q:43:LEU:HD12	28:Q:183:ILE:HD11	1.95	0.48
31:T:46:ASN:OD1	31:T:47:ASN:N	2.46	0.48
24:m:152:ASP:OD2	24:m:152:ASP:C	2.57	0.48
33:x:554:TYR:CD1	33:x:557:TRP:CZ2	3.01	0.48
1:U:261:LEU:HA	1:U:264:VAL:HG22	1.95	0.48
1:U:431:THR:OG1	1:U:438:GLN:HG2	2.13	0.48
2:V:451:ILE:HD12	2:V:452:ASN:H	1.79	0.48
3:W:377:ARG:O	3:W:381:LEU:HG	2.14	0.48
8:b:184:ILE:HA	8:b:188:ILE:HG13	1.95	0.48
9:c:161:ARG:CD	9:c:201:TYR:HE1	2.25	0.48
13:B:257:GLN:HE21	13:B:266:LEU:HD22	1.79	0.48
14:C:321:ASN:O	14:C:325:ARG:HB2	2.14	0.48
16:E:96:THR:HG21	16:E:110:TYR:CZ	2.49	0.48
16:E:258:MET:SD	16:E:262:ASN:ND2	2.87	0.48
16:E:264:MET:HG3	16:E:270:LEU:CD1	2.43	0.48
17:F:150:LEU:O	17:F:164:LEU:HB2	2.13	0.48
30:S:75:TYR:CD1	30:S:83:MET:HG2	2.49	0.48
24:m:99:ARG:NH1	24:m:105:ASN:OD1	2.46	0.48
33:x:333:LEU:HD12	33:x:829:MET:HG2	1.95	0.48
33:x:587:PHE:HD1	33:x:590:PHE:HB3	1.78	0.48
33:x:612:LEU:HD23	33:x:653:ALA:O	2.14	0.48
1:U:692:ALA:O	1:U:696:ILE:HG23	2.13	0.48
2:V:335:VAL:HA	2:V:338:LEU:HG	1.95	0.48
3:W:115:ILE:HG23	3:W:119:PRO:HB2	1.96	0.48
3:W:439:VAL:HB	6:Z:234:PHE:CZ	2.49	0.48
4:X:190:LEU:O	4:X:194:ARG:HG2	2.14	0.48
7:a:89:ASP:N	7:a:89:ASP:OD1	2.47	0.48
10:d:4:GLN:HB3	10:d:7:GLY:HA3	1.96	0.48
10:d:188:LYS:H	10:d:188:LYS:HD2	1.77	0.48
12:A:83:ASP:C	12:A:85:GLN:H	2.22	0.48
14:C:394:ASP:N	14:C:394:ASP:OD1	2.47	0.48
16:E:18:GLU:HG2	16:E:22:ILE:HG23	1.96	0.48
16:E:61:LEU:HB2	16:E:70:ILE:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:180:LYS:NZ	38:E:401:ADP:O1B	2.28	0.48
17:F:35:LYS:HB3	17:F:39:GLU:HG2	1.96	0.48
20:i:3:ARG:HH12	22:k:10:ARG:NH2	2.12	0.48
22:k:178:GLN:O	22:k:182:GLN:HG2	2.14	0.48
23:l:209:ASN:C	23:l:209:ASN:OD1	2.56	0.48
33:x:266:LEU:HB3	33:x:267:ARG:NH1	2.28	0.48
33:x:307:LEU:HB2	33:x:314:TYR:CE1	2.48	0.48
1:U:580:ARG:HG3	1:U:614:VAL:HA	1.95	0.47
1:U:889:LEU:HD23	1:U:889:LEU:H	1.79	0.47
2:V:309:MET:CE	2:V:312:ALA:HB3	2.44	0.47
2:V:364:THR:O	2:V:368:ARG:HG2	2.14	0.47
2:V:421:ASP:OD1	2:V:421:ASP:N	2.46	0.47
3:W:11:GLY:O	3:W:15:LYS:HG2	2.14	0.47
3:W:45:GLU:HG2	3:W:46:THR:N	2.28	0.47
4:X:283:GLN:OE1	4:X:283:GLN:HA	2.14	0.47
7:a:56:LEU:O	7:a:59:LEU:HG	2.14	0.47
9:c:254:ASN:ND2	9:c:279:ASP:OD2	2.47	0.47
10:d:107:LEU:HD22	10:d:170:LEU:HD11	1.96	0.47
13:B:48:LYS:O	13:B:49:LEU:CD2	2.62	0.47
13:B:149:SER:OG	13:B:163:LEU:HB3	2.14	0.47
15:D:115:ILE:CG2	15:D:139:LEU:CD2	2.80	0.47
15:D:370:ILE:N	15:D:370:ILE:HD12	2.30	0.47
25:N:89:ARG:HD2	25:N:90:TYR:CE2	2.49	0.47
27:P:159:ASP:OD1	27:P:159:ASP:N	2.31	0.47
33:x:405:HIS:ND1	33:x:813:LYS:HA	2.28	0.47
1:U:461:LEU:HA	1:U:464:GLN:HG2	1.95	0.47
3:W:101:VAL:HG21	3:W:135:LYS:CD	2.44	0.47
3:W:312:MET:N	3:W:312:MET:HE2	2.29	0.47
3:W:377:ARG:HD2	3:W:377:ARG:N	2.28	0.47
4:X:134:VAL:HG23	4:X:172:LEU:HD13	1.96	0.47
5:Y:194:PHE:CE1	5:Y:195:LYS:HB3	2.48	0.47
6:Z:12:HIS:ND1	6:Z:163:GLY:O	2.47	0.47
8:b:2:VAL:O	8:b:44:ASN:ND2	2.47	0.47
9:c:52:GLU:CD	9:c:82:VAL:HG13	2.39	0.47
9:c:57:MET:HB2	9:c:109:VAL:H	1.79	0.47
10:d:189:ILE:O	10:d:222:TYR:CD2	2.67	0.47
11:e:61:GLU:O	11:e:62:LYS:HD2	2.14	0.47
12:A:75:PRO:HA	12:A:78:TRP:NE1	2.28	0.47
14:C:48:GLN:O	14:C:51:GLU:HG3	2.14	0.47
18:g:141:ILE:HG22	18:g:151:VAL:HG22	1.97	0.47
21:j:172:LEU:O	21:j:176:TYR:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:o:48:THR:H	39:o:301:LDZ:H32	1.78	0.47
27:p:205:ASP:C	27:p:205:ASP:OD1	2.57	0.47
33:x:206:ASP:OD1	33:x:207:LEU:N	2.47	0.47
1:U:70:HIS:CE1	2:V:236:ARG:HH22	2.32	0.47
3:W:68:VAL:O	3:W:72:LYS:HG2	2.14	0.47
5:Y:229:ILE:HD11	5:Y:295:TYR:HD2	1.78	0.47
6:Z:273:HIS:CD2	6:Z:273:HIS:C	2.92	0.47
7:a:21:VAL:HG23	7:a:22:TRP:CD1	2.49	0.47
7:a:89:ASP:OD2	7:a:92:VAL:HG13	2.14	0.47
9:c:56:LEU:HB2	9:c:73:PHE:CE1	2.49	0.47
9:c:148:ILE:HD12	9:c:148:ILE:O	2.13	0.47
10:d:96:HIS:HB3	10:d:130:ASN:ND2	2.29	0.47
12:A:190:VAL:HG11	12:A:212:VAL:HG23	1.97	0.47
13:B:54:PRO:O	13:B:55:HIS:CD2	2.68	0.47
15:D:315:ASP:OD1	15:D:315:ASP:N	2.45	0.47
15:D:409:LYS:O	15:D:411:GLU:OE1	2.31	0.47
17:F:228:PRO:CB	17:F:356:MET:HE2	2.34	0.47
21:J:183:THR:O	21:J:186:LEU:N	2.29	0.47
24:M:77:VAL:HG11	24:M:84:ALA:HB1	1.95	0.47
25:N:160:LEU:O	25:N:164:MET:HG3	2.14	0.47
19:h:49:GLU:HG3	19:h:199:PHE:CD2	2.49	0.47
25:n:112:TYR:CD1	25:n:120:MET:HE3	2.48	0.47
33:x:531:ASN:H	33:x:565:ASN:HD21	1.63	0.47
1:U:374:SER:HB3	1:U:407:SER:HB3	1.96	0.47
2:V:172:VAL:HG23	2:V:217:VAL:HG22	1.95	0.47
2:V:234:ARG:O	2:V:237:THR:HG22	2.13	0.47
2:V:238:ALA:C	2:V:240:LEU:H	2.22	0.47
2:V:266:GLN:HB3	2:V:299:GLN:NE2	2.28	0.47
2:V:407:VAL:HA	2:V:410:ILE:HD12	1.97	0.47
3:W:31:CYS:O	3:W:34:LEU:HB2	2.13	0.47
4:X:201:TYR:HA	19:H:176:LYS:O	2.15	0.47
5:Y:155:ASP:O	5:Y:159:ARG:N	2.48	0.47
6:Z:112:MET:HA	6:Z:115:TYR:HD2	1.79	0.47
8:b:62:THR:HG21	8:b:71:ILE:HG22	1.96	0.47
9:c:196:LEU:HA	9:c:200:TYR:CE1	2.50	0.47
12:A:110:LYS:NZ	17:F:165:PRO:HD3	2.30	0.47
13:B:245:ALA:HB1	13:B:279:PRO:O	2.15	0.47
13:B:278:ALA:HB1	13:B:279:PRO:CD	2.42	0.47
13:B:364:ILE:O	13:B:367:ILE:HG22	2.13	0.47
16:E:36:LEU:HD11	17:F:70:LYS:HG2	1.95	0.47
17:F:295:ARG:NH2	17:F:298:SER:HB2	2.19	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:G:65:THR:HG21	24:M:159:GLY:H	1.79	0.47
22:K:155:HIS:O	22:K:162:PHE:HA	2.15	0.47
31:T:153:VAL:HG21	31:T:168:LEU:HD11	1.97	0.47
33:x:110:TYR:CA	33:x:113:MET:HE1	2.40	0.47
33:x:251:CYS:O	33:x:255:VAL:HG13	2.15	0.47
1:U:132:GLY:O	1:U:135:ASN:ND2	2.47	0.47
1:U:898:CYS:SG	1:U:899:ARG:N	2.88	0.47
2:V:67:LEU:HD23	11:e:1:MET:HE3	1.95	0.47
3:W:360:GLU:O	3:W:364:ARG:HG2	2.15	0.47
3:W:370:TYR:HE1	7:a:326:GLU:HB3	1.79	0.47
3:W:448:LYS:O	3:W:452:ILE:HG23	2.14	0.47
4:X:96:PHE:CE1	4:X:106:GLU:HG2	2.50	0.47
5:Y:85:ASP:OD1	5:Y:85:ASP:N	2.46	0.47
5:Y:194:PHE:CG	5:Y:195:LYS:N	2.73	0.47
5:Y:293:ARG:HB3	5:Y:297:ARG:HH22	1.80	0.47
6:Z:36:VAL:HG13	6:Z:94:TRP:HE3	1.79	0.47
6:Z:209:ARG:HH22	7:a:354:GLU:HB2	1.79	0.47
7:a:319:LEU:O	7:a:337:GLN:OE1	2.32	0.47
10:d:101:LEU:HD22	10:d:166:PHE:CE2	2.49	0.47
12:A:306:LEU:HD21	12:A:317:VAL:HG21	1.96	0.47
13:B:121:ALA:HB1	13:B:123:VAL:HG13	1.97	0.47
15:D:61:ILE:O	15:D:65:GLN:HG2	2.15	0.47
16:E:363:VAL:HG11	16:E:365:GLU:OE2	2.14	0.47
18:G:10:ASP:OD1	18:G:10:ASP:N	2.47	0.47
21:j:93:SER:O	21:j:97:THR:HG23	2.14	0.47
30:s:162:GLU:OE2	30:s:162:GLU:HA	2.15	0.47
33:x:785:ARG:NH1	33:x:877:GLY:H	2.13	0.47
1:U:443:LEU:O	1:U:446:LEU:HG	2.14	0.47
1:U:506:ALA:HB1	1:U:541:HIS:CE1	2.50	0.47
2:V:416:ARG:O	2:V:416:ARG:HD2	2.15	0.47
4:X:80:ILE:HG12	4:X:81:SER:H	1.79	0.47
4:X:297:ARG:HD2	4:X:337:ARG:HH21	1.79	0.47
4:X:401:LEU:O	4:X:404:ILE:HG13	2.13	0.47
5:Y:236:LEU:O	5:Y:240:VAL:HG22	2.13	0.47
8:b:44:ASN:OD1	8:b:46:GLU:OE1	2.32	0.47
9:c:75:MET:SD	9:c:76:PRO:CD	3.02	0.47
12:A:103:ASN:C	12:A:103:ASN:OD1	2.58	0.47
13:B:65:LEU:HA	13:B:68:ILE:HG22	1.96	0.47
25:N:1:THR:HG21	39:N:301:LDZ:H14	1.96	0.47
18:g:117:ARG:HH21	18:g:121:ILE:HD11	1.79	0.47
33:x:862:ILE:HG13	33:x:881:GLU:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:602:LEU:O	1:U:605:VAL:HG12	2.15	0.47
1:U:634:PRO:O	1:U:635:SER:C	2.58	0.47
1:U:763:VAL:O	1:U:767:THR:HG23	2.14	0.47
1:U:873:PRO:C	1:U:875:PHE:N	2.65	0.47
2:V:247:GLN:O	2:V:251:LEU:HB2	2.15	0.47
2:V:394:LEU:O	2:V:398:LEU:HB2	2.14	0.47
3:W:82:LEU:O	3:W:86:ASN:HB2	2.14	0.47
3:W:340:VAL:CG1	3:W:341:PHE:CE2	2.96	0.47
4:X:47:GLU:OE1	4:X:76:PHE:CE1	2.67	0.47
4:X:130:GLU:O	4:X:134:VAL:HG13	2.14	0.47
4:X:359:ALA:O	4:X:363:ARG:HG3	2.15	0.47
6:Z:60:GLU:HA	6:Z:67:VAL:O	2.14	0.47
7:a:184:ASP:O	7:a:186:LYS:N	2.48	0.47
7:a:205:LEU:HD21	7:a:237:LEU:HD22	1.97	0.47
8:b:12:ASN:OD1	8:b:53:THR:OG1	2.33	0.47
9:c:173:GLU:N	9:c:174:PRO:HD3	2.29	0.47
10:d:181:CYS:O	10:d:186:TYR:CE2	2.67	0.47
12:A:23:ARG:HH12	33:x:44:GLU:H	1.62	0.47
13:B:198:LYS:HD3	13:B:202:GLU:OE1	2.13	0.47
13:B:299:SER:HB2	13:B:302:GLU:HG2	1.96	0.47
15:D:44:TYR:O	15:D:48:GLN:HG3	2.14	0.47
24:M:173:LYS:O	24:M:177:GLU:HG3	2.15	0.47
19:h:228:ASP:C	19:h:228:ASP:OD2	2.57	0.47
24:m:87:LEU:HD23	24:m:87:LEU:HA	1.78	0.47
25:n:14:LEU:HD23	25:n:44:CYS:SG	2.55	0.47
33:x:208:LEU:HD12	33:x:217:LEU:HD13	1.95	0.47
2:V:179:LYS:HE3	2:V:214:HIS:CE1	2.50	0.47
4:X:377:ILE:HG22	4:X:386:ILE:HG13	1.96	0.47
6:Z:38:VAL:HG12	6:Z:54:PHE:CE1	2.50	0.47
6:Z:94:TRP:HB3	6:Z:112:MET:CE	2.45	0.47
7:a:278:MET:HA	7:a:281:THR:CG2	2.42	0.47
9:c:33:ILE:HA	9:c:69:VAL:HB	1.97	0.47
14:C:90:HIS:CG	14:C:91:PRO:HD3	2.50	0.47
16:E:284:THR:C	16:E:285:LEU:HD12	2.40	0.47
16:E:288:ALA:O	16:E:294:ARG:NH1	2.48	0.47
17:F:69:MET:HE3	17:F:70:LYS:N	2.30	0.47
26:O:170:GLY:O	26:O:171:SER:HB2	2.15	0.47
30:S:191:ASP:H	30:S:210:LEU:HB2	1.80	0.47
23:l:234:GLU:OE1	23:l:235:GLY:N	2.48	0.47
33:x:521:ALA:N	33:x:524:MET:HE3	2.30	0.47
2:V:186:LYS:HG2	2:V:203:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:47:GLU:HA	4:X:50:ILE:HB	1.97	0.47
6:Z:101:LEU:HD13	6:Z:102:HIS:N	2.29	0.47
7:a:34:TRP:CZ2	7:a:64:ILE:HG23	2.50	0.47
7:a:68:GLU:HG3	7:a:71:VAL:HG23	1.95	0.47
10:d:78:LEU:CD1	10:d:98:LEU:HD11	2.45	0.47
10:d:115:PHE:CE2	10:d:119:LEU:HD11	2.50	0.47
16:E:338:PHE:HA	16:E:342:ASP:HB2	1.96	0.47
17:F:94:ILE:H	17:F:94:ILE:HD12	1.78	0.47
28:Q:118:MET:HE2	28:Q:124:LEU:HD13	1.96	0.47
29:R:1:THR:HG23	29:R:33:LYS:HZ3	1.80	0.47
33:x:218:GLU:HG3	33:x:255:VAL:HG12	1.95	0.47
2:V:169:LEU:HD12	2:V:170:LEU:N	2.29	0.47
3:W:369:TYR:CG	7:a:312:MET:HE1	2.50	0.47
4:X:201:TYR:CD2	19:H:177:ARG:HA	2.49	0.47
5:Y:88:LEU:O	5:Y:88:LEU:HD23	2.14	0.47
5:Y:131:THR:O	5:Y:131:THR:HG22	2.15	0.47
5:Y:241:ILE:O	5:Y:247:LEU:HD21	2.15	0.47
7:a:198:PHE:CE2	7:a:202:LEU:HD11	2.50	0.47
7:a:265:GLU:HA	7:a:268:LEU:HD21	1.97	0.47
8:b:56:ASN:HD22	8:b:82:GLY:HA2	1.79	0.47
16:E:296:ASP:C	16:E:296:ASP:OD1	2.58	0.47
23:L:47:VAL:HG11	23:L:192:LEU:HD12	1.96	0.47
18:g:93:ARG:HA	18:g:93:ARG:HD2	1.72	0.47
18:g:117:ARG:O	18:g:121:ILE:HG12	2.15	0.47
31:t:9:THR:OG1	31:t:10:SER:N	2.46	0.47
33:x:835:GLU:OE2	33:x:901:ARG:HG2	2.15	0.47
1:U:344:ARG:NH2	1:U:345:ASN:CB	2.77	0.46
1:U:510:GLU:HG3	1:U:543:LYS:HB3	1.96	0.46
1:U:803:LYS:HE2	1:U:877:LEU:HD21	1.96	0.46
1:U:880:ASN:HB2	1:U:881:PRO:HD3	1.97	0.46
2:V:137:GLU:O	2:V:141:THR:OG1	2.24	0.46
2:V:159:LEU:HB3	2:V:209:LYS:NZ	2.31	0.46
3:W:127:THR:O	3:W:131:VAL:HG23	2.14	0.46
3:W:251:TYR:CD1	3:W:266:ALA:HB3	2.48	0.46
5:Y:72:LYS:O	5:Y:75:LYS:HG3	2.15	0.46
7:a:217:LEU:HD21	7:a:238:TYR:HA	1.98	0.46
7:a:374:ILE:HG12	10:d:251:ARG:HA	1.97	0.46
8:b:86:PHE:HD2	8:b:86:PHE:O	1.97	0.46
8:b:90:ILE:HD11	8:b:127:LEU:HD13	1.97	0.46
18:G:73:THR:HG22	18:G:75:ASN:H	1.80	0.46
22:K:50:VAL:HB	22:K:67:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:P:58:THR:OG1	28:Q:121:LEU:O	2.28	0.46
22:k:15:PHE:CE2	23:l:126:ARG:HD2	2.49	0.46
26:o:6:VAL:HG23	26:o:124:TYR:HB3	1.96	0.46
26:o:55:THR:HG23	26:o:86:MET:HE2	1.98	0.46
28:q:118:MET:HE2	28:q:118:MET:HB2	1.77	0.46
33:x:612:LEU:HA	33:x:615:ILE:HG22	1.97	0.46
2:V:311:ASN:O	2:V:315:LYS:HB2	2.15	0.46
3:W:183:VAL:HG21	3:W:215:GLN:OE1	2.15	0.46
4:X:133:LEU:HD12	4:X:136:LEU:HD11	1.97	0.46
6:Z:109:ASN:HA	6:Z:112:MET:HG2	1.97	0.46
7:a:71:VAL:HA	8:b:17:ARG:NH1	2.31	0.46
13:B:391:SER:O	13:B:395:ILE:HG12	2.15	0.46
15:D:264:ILE:HG21	15:D:267:ILE:HG22	1.94	0.46
16:E:173:TYR:CB	16:E:282:PRO:HB3	2.45	0.46
16:E:189:SER:OG	16:E:190:GLN:NE2	2.44	0.46
17:F:375:VAL:HG23	17:F:415:LEU:HB2	1.97	0.46
26:O:143:ARG:NH1	26:O:150:GLU:OE1	2.27	0.46
31:T:124:TYR:HB2	31:T:137:LEU:HD13	1.98	0.46
28:q:154:GLU:OE2	28:q:154:GLU:N	2.27	0.46
30:s:65:THR:O	30:s:69:GLU:HG3	2.16	0.46
33:x:73:PRO:O	33:x:76:GLU:HG3	2.16	0.46
33:x:419:LEU:HD22	33:x:420:TRP:CD2	2.50	0.46
33:x:581:GLU:HG2	33:x:588:ARG:NH1	2.30	0.46
33:x:899:ILE:C	33:x:900:LEU:HD12	2.41	0.46
1:U:20:LYS:HD2	1:U:20:LYS:N	2.31	0.46
3:W:422:ASN:OD1	3:W:422:ASN:N	2.47	0.46
5:Y:97:GLU:CD	5:Y:97:GLU:N	2.70	0.46
14:C:27:LYS:O	14:C:31:LEU:HD23	2.15	0.46
16:E:91:LYS:HE2	16:E:110:TYR:CD1	2.50	0.46
17:F:146:LYS:HB3	17:F:149:ASP:OD1	2.14	0.46
17:F:151:VAL:HG12	17:F:163:THR:HA	1.97	0.46
29:r:113:TYR:CE2	29:r:115:ASP:OD2	2.68	0.46
31:t:63:LEU:CD1	31:t:110:MET:HE1	2.45	0.46
31:t:124:TYR:O	31:t:131:ALA:HA	2.13	0.46
1:U:12:LEU:HD13	1:U:44:LYS:HE3	1.97	0.46
2:V:468:SER:HA	6:Z:250:TYR:CE1	2.50	0.46
5:Y:96:GLY:O	5:Y:101:ARG:HB3	2.16	0.46
5:Y:101:ARG:NH1	5:Y:131:THR:HG23	2.29	0.46
5:Y:326:GLY:HA3	5:Y:329:PHE:CD1	2.50	0.46
7:a:143:ASN:CG	7:a:144:ASN:H	2.23	0.46
9:c:211:GLU:CD	9:c:212:LEU:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:265:ARG:HH12	12:A:312:ARG:HA	1.81	0.46
14:C:13:GLU:HG3	14:C:21:ARG:HH21	1.79	0.46
16:E:365:GLU:N	16:E:365:GLU:OE1	2.38	0.46
17:F:317:LEU:HD22	17:F:347:ARG:HG3	1.97	0.46
24:m:34:SER:HB2	24:m:65:ARG:HH12	1.80	0.46
25:n:1:THR:HG21	39:n:301:LDZ:H14	1.98	0.46
33:x:109:ILE:O	33:x:113:MET:CE	2.63	0.46
1:U:173:VAL:HG12	1:U:175:GLY:N	2.23	0.46
1:U:642:GLU:O	14:C:53:ASN:ND2	2.49	0.46
2:V:346:LEU:HA	2:V:357:LEU:HD13	1.97	0.46
3:W:425:LEU:HD23	3:W:428:TRP:HE3	1.80	0.46
4:X:53:LEU:HA	4:X:56:LEU:HG	1.98	0.46
4:X:358:LYS:HA	4:X:361:VAL:HG12	1.98	0.46
5:Y:28:LEU:HB2	5:Y:29:PRO:HD3	1.97	0.46
9:c:115:HIS:NE2	9:c:126:ASP:OD2	2.49	0.46
13:B:287:ILE:HG22	13:B:331:THR:HB	1.96	0.46
14:C:91:PRO:HG3	15:D:109:SER:HB2	1.97	0.46
16:E:261:LEU:O	16:E:264:MET:HB3	2.14	0.46
26:O:17:ASP:OD2	26:O:17:ASP:C	2.58	0.46
18:g:126:THR:HG22	19:h:128:ARG:HH12	1.79	0.46
19:h:166:ASN:OD1	19:h:166:ASN:O	2.34	0.46
23:l:199:LEU:HD23	23:l:199:LEU:HA	1.74	0.46
25:n:186:ARG:HE	25:n:186:ARG:HB3	1.65	0.46
33:x:445:LEU:HD12	33:x:445:LEU:HA	1.75	0.46
33:x:642:ALA:O	33:x:646:MET:HG2	2.15	0.46
33:x:695:ALA:HB1	33:x:731:MET:HB2	1.97	0.46
1:U:164:GLU:O	1:U:167:ILE:HG13	2.16	0.46
1:U:437:TYR:CD1	1:U:472:ILE:HD13	2.50	0.46
3:W:35:ALA:HB2	3:W:52:LYS:NZ	2.30	0.46
3:W:405:LYS:HG2	4:X:343:SER:HB3	1.98	0.46
5:Y:314:LEU:HD13	5:Y:315:THR:O	2.15	0.46
8:b:145:GLU:C	8:b:145:GLU:OE1	2.58	0.46
9:c:56:LEU:HD22	9:c:111:TRP:HB3	1.96	0.46
12:A:26:ASP:O	12:A:28:GLY:N	2.49	0.46
12:A:74:PRO:O	12:A:78:TRP:CD1	2.66	0.46
14:C:193:GLY:O	14:C:355:SER:HB2	2.15	0.46
15:D:153:MET:HE3	15:D:226:ALA:HB1	1.98	0.46
16:E:84:ARG:HH12	16:E:85:ARG:NH1	2.12	0.46
20:I:154:GLY:O	21:J:81:ARG:NH2	2.45	0.46
23:L:78:THR:O	23:L:82:ARG:HG2	2.15	0.46
25:N:75:LEU:O	25:N:78:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:j:171:PHE:CD1	21:j:171:PHE:C	2.94	0.46
28:q:35:MET:HG2	28:q:45:LEU:HG	1.98	0.46
33:x:719:PRO:HG2	33:x:720:GLU:OE2	2.16	0.46
1:U:351:MET:HB3	1:U:818:GLU:OE2	2.15	0.46
1:U:620:GLU:OE1	1:U:654:MET:HB3	2.16	0.46
1:U:723:ASP:OD1	1:U:725:MET:HE2	2.16	0.46
3:W:436:MET:HB3	9:c:226:MET:CG	2.39	0.46
5:Y:179:ARG:HB3	5:Y:183:TYR:CZ	2.51	0.46
5:Y:268:TYR:CZ	5:Y:307:LEU:HD13	2.50	0.46
5:Y:282:MET:SD	5:Y:292:TYR:HB3	2.55	0.46
6:Z:57:PRO:HD3	6:Z:74:TYR:HE1	1.73	0.46
7:a:226:ARG:HG2	7:a:229:ASP:O	2.16	0.46
7:a:303:THR:O	7:a:307:VAL:HG13	2.15	0.46
9:c:160:PHE:HB2	9:c:200:TYR:HB2	1.97	0.46
9:c:198:ARG:HD3	9:c:198:ARG:N	2.30	0.46
16:E:304:PRO:HA	16:E:308:ALA:HB3	1.97	0.46
23:l:171:TYR:CZ	23:l:193:ARG:HG2	2.50	0.46
30:s:199:THR:OG1	30:s:200:LYS:N	2.48	0.46
33:x:90:THR:HG22	33:x:92:VAL:H	1.81	0.46
33:x:181:ARG:HE	33:x:184:LEU:HD11	1.81	0.46
33:x:203:GLU:HA	33:x:206:ASP:OD2	2.16	0.46
33:x:818:LEU:O	33:x:821:LEU:HG	2.16	0.46
1:U:840:LYS:HA	1:U:840:LYS:HD3	1.65	0.46
2:V:88:GLY:O	2:V:91:PRO:HD2	2.15	0.46
2:V:106:ARG:O	2:V:110:HIS:ND1	2.49	0.46
2:V:415:SER:HB3	5:Y:346:LYS:HG2	1.97	0.46
3:W:273:TYR:CD2	3:W:340:VAL:HG21	2.51	0.46
4:X:96:PHE:CD1	4:X:106:GLU:HG2	2.51	0.46
4:X:201:TYR:CE2	19:H:177:ARG:HA	2.50	0.46
4:X:394:ASP:OD2	5:Y:365:GLN:NE2	2.48	0.46
5:Y:37:VAL:HA	5:Y:40:GLU:CB	2.46	0.46
6:Z:58:PHE:HA	6:Z:69:PHE:O	2.16	0.46
6:Z:120:VAL:HG23	6:Z:139:ILE:CD1	2.44	0.46
13:B:220:LYS:HB3	13:B:322:ARG:NH2	2.31	0.46
14:C:106:ASN:C	14:C:106:ASN:OD1	2.58	0.46
16:E:175:PRO:HG3	16:E:303:LEU:HB3	1.98	0.46
39:O:301:LDZ:H21	39:O:301:LDZ:H13	1.83	0.46
25:n:29:ARG:NH1	26:o:139:GLU:OE1	2.48	0.46
27:p:142:CYS:O	27:p:146:MET:HG3	2.16	0.46
31:t:122:LEU:HG	31:t:137:LEU:HD12	1.97	0.46
33:x:422:VAL:HG11	33:x:461:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:554:TYR:CD1	33:x:557:TRP:CH2	3.04	0.46
33:x:672:LEU:HD11	33:x:706:ILE:HD11	1.97	0.46
1:U:465:LEU:HD23	1:U:465:LEU:HA	1.80	0.46
1:U:557:TYR:HE1	1:U:760:VAL:HG11	1.80	0.46
2:V:365:GLN:O	2:V:369:THR:HG22	2.16	0.46
2:V:374:LYS:N	2:V:374:LYS:HE2	2.30	0.46
4:X:407:MET:HA	4:X:407:MET:CE	2.37	0.46
5:Y:117:LYS:HD2	5:Y:151:TYR:CD2	2.50	0.46
5:Y:328:GLU:HG2	5:Y:329:PHE:CD2	2.51	0.46
6:Z:14:LEU:HD23	9:c:43:LYS:HD3	1.98	0.46
9:c:246:LYS:C	9:c:249:LEU:CD2	2.89	0.46
26:O:84:LYS:HG3	26:O:85:GLN:N	2.31	0.46
27:P:88:MET:HE3	27:P:130:PRO:HB2	1.91	0.46
22:k:177:ALA:O	22:k:181:LEU:HB2	2.15	0.46
33:x:335:ARG:NH2	33:x:338:ASP:HB3	2.31	0.46
1:U:419:ALA:O	1:U:423:MET:HG3	2.16	0.46
3:W:223:LYS:HG3	3:W:224:LEU:HG	1.96	0.46
3:W:351:TRP:HA	3:W:351:TRP:CE3	2.51	0.46
4:X:46:LYS:HD3	4:X:50:ILE:HG12	1.97	0.46
4:X:172:LEU:HD23	4:X:172:LEU:HA	1.79	0.46
4:X:335:LEU:O	4:X:339:ILE:HB	2.16	0.46
6:Z:165:GLU:O	6:Z:169:GLU:HG2	2.15	0.46
6:Z:186:THR:HG22	9:c:293:THR:HB	1.98	0.46
7:a:72:ASN:ND2	7:a:74:LEU:HB2	2.31	0.46
7:a:109:GLU:HG3	7:a:151:VAL:HB	1.98	0.46
8:b:20:ASP:CG	8:b:25:ARG:HH21	2.22	0.46
8:b:137:ASN:HA	8:b:160:LEU:HD21	1.97	0.46
9:c:27:THR:HG22	9:c:28:ALA:H	1.81	0.46
9:c:246:LYS:C	9:c:249:LEU:HD23	2.40	0.46
10:d:124:ALA:HB1	10:d:128:GLN:NE2	2.31	0.46
14:C:167:LEU:HB3	14:C:168:PRO:HD3	1.98	0.46
16:E:121:ASN:O	16:E:121:ASN:ND2	2.49	0.46
27:P:12:MET:CE	27:P:171:MET:HG2	2.45	0.46
33:x:71:TYR:O	33:x:75:LEU:HG	2.16	0.46
33:x:193:PRO:O	33:x:196:MET:SD	2.73	0.46
1:U:780:SER:HA	1:U:783:TYR:CD2	2.50	0.45
2:V:198:GLN:NE2	14:C:29:GLU:OE1	2.49	0.45
2:V:391:THR:O	2:V:391:THR:OG1	2.31	0.45
3:W:48:LEU:HB3	3:W:52:LYS:HZ1	1.81	0.45
3:W:348:GLU:O	3:W:352:LYS:HG2	2.16	0.45
6:Z:22:HIS:C	6:Z:22:HIS:CD2	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:58:LEU:CG	9:c:106:GLU:HG3	2.44	0.45
9:c:196:LEU:O	9:c:198:ARG:N	2.49	0.45
9:c:232:GLN:NE2	9:c:237:HIS:HB2	2.31	0.45
12:A:348:LEU:O	12:A:352:THR:HG23	2.15	0.45
12:A:414:ASN:HA	12:A:418:LYS:HG3	1.98	0.45
13:B:75:GLU:O	13:B:79:ILE:HG13	2.16	0.45
13:B:164:MET:HE2	13:B:164:MET:HA	1.98	0.45
15:D:72:PHE:O	15:D:76:GLN:HG2	2.16	0.45
15:D:153:MET:HG3	15:D:153:MET:O	2.16	0.45
15:D:416:PHE:O	15:D:417:TYR:CD1	2.69	0.45
16:E:203:ILE:O	16:E:211:SER:OG	2.30	0.45
23:l:125:ARG:HD2	23:l:126:ARG:H	1.81	0.45
26:o:201:ARG:HD3	26:o:201:ARG:HA	1.73	0.45
29:r:167:ASP:OD1	29:r:168:ALA:N	2.49	0.45
33:x:419:LEU:HD23	33:x:420:TRP:N	2.30	0.45
33:x:646:MET:O	33:x:649:HIS:HE1	2.00	0.45
33:x:784:ASP:HA	33:x:879:ARG:NH1	2.30	0.45
2:V:205:LEU:HD12	2:V:206:VAL:N	2.30	0.45
2:V:484:LEU:HD13	10:d:252:GLN:CD	2.41	0.45
3:W:413:ILE:HD12	3:W:415:PHE:HE1	1.80	0.45
5:Y:313:SER:HB2	5:Y:353:ILE:HG23	1.99	0.45
7:a:35:HIS:CD2	8:b:18:ASN:ND2	2.85	0.45
15:D:282:ASP:O	15:D:286:GLN:HG3	2.16	0.45
16:E:168:LYS:HD3	16:E:168:LYS:HA	1.50	0.45
20:I:186:LEU:HD12	20:I:186:LEU:HA	1.83	0.45
21:j:107:ILE:HD12	21:j:107:ILE:HA	1.85	0.45
22:k:49:ALA:HB2	22:k:217:LEU:HD12	1.97	0.45
26:o:204:CYS:HB3	26:o:208:THR:HG21	1.98	0.45
26:o:219:LEU:HD11	27:p:195:ILE:HG13	1.97	0.45
30:s:39:ASP:OD2	30:s:39:ASP:C	2.59	0.45
33:x:587:PHE:CD1	33:x:587:PHE:O	2.68	0.45
33:x:718:ASP:HB3	33:x:721:VAL:HB	1.98	0.45
1:U:419:ALA:HB1	1:U:449:ILE:HD13	1.99	0.45
2:V:131:LEU:O	2:V:135:LEU:N	2.49	0.45
2:V:200:ARG:HH12	2:V:238:ALA:HA	1.82	0.45
3:W:346:GLU:O	3:W:349:LYS:HG2	2.16	0.45
4:X:201:TYR:CG	19:H:176:LYS:O	2.69	0.45
5:Y:282:MET:CE	5:Y:292:TYR:CD1	3.00	0.45
5:Y:282:MET:O	5:Y:285:ASP:HB3	2.16	0.45
6:Z:240:VAL:HG21	9:c:310:LYS:HG3	1.99	0.45
6:Z:243:GLN:O	6:Z:247:LYS:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:318:GLY:O	7:a:337:GLN:NE2	2.49	0.45
12:A:62:LEU:HD23	13:B:79:ILE:CD1	2.44	0.45
15:D:268:ASP:N	15:D:268:ASP:OD1	2.48	0.45
17:F:121:CYS:HB3	17:F:133:PHE:HE1	1.81	0.45
20:I:68:LEU:HD13	20:I:90:LEU:HD13	1.97	0.45
19:h:182:LEU:HD12	19:h:182:LEU:HA	1.80	0.45
22:k:199:LEU:HD23	22:k:199:LEU:HA	1.73	0.45
24:m:231:ILE:HD12	24:m:231:ILE:N	2.32	0.45
39:o:301:LDZ:C22	39:o:301:LDZ:H21	2.45	0.45
33:x:556:ARG:NH1	33:x:805:ASP:OD2	2.49	0.45
1:U:533:VAL:O	1:U:537:GLN:NE2	2.49	0.45
1:U:688:LEU:HD22	1:U:709:PHE:HZ	1.81	0.45
2:V:95:LEU:HD22	2:V:141:THR:HG21	1.99	0.45
2:V:323:GLY:HA2	2:V:326:GLN:OE1	2.16	0.45
3:W:37:GLU:HG2	3:W:38:GLY:H	1.81	0.45
3:W:408:ARG:H	4:X:344:ARG:NH1	2.13	0.45
5:Y:38:ARG:O	5:Y:42:MET:HE1	2.16	0.45
6:Z:177:ARG:HG3	6:Z:177:ARG:O	2.17	0.45
7:a:35:HIS:CE1	8:b:14:GLU:O	2.69	0.45
7:a:271:LYS:HA	7:a:271:LYS:HD2	1.74	0.45
9:c:58:LEU:HB3	9:c:71:ASP:O	2.17	0.45
9:c:96:LEU:O	9:c:100:LYS:HE2	2.16	0.45
9:c:229:LEU:HD13	9:c:229:LEU:HA	1.82	0.45
15:D:41:TYR:CD1	15:D:41:TYR:C	2.94	0.45
15:D:143:LEU:H	15:D:143:LEU:HD22	1.80	0.45
15:D:370:ILE:CG2	15:D:375:ILE:HG13	2.46	0.45
16:E:59:GLU:OE2	16:E:60:VAL:O	2.35	0.45
22:K:199:LEU:HD23	22:K:199:LEU:HA	1.82	0.45
30:S:91:MET:HE2	30:S:91:MET:HB3	1.85	0.45
18:g:22:LEU:O	18:g:26:GLU:HG3	2.17	0.45
33:x:131:MET:HE1	33:x:161:HIS:HB2	1.99	0.45
33:x:143:ARG:HH21	33:x:148:GLN:HA	1.82	0.45
33:x:884:THR:OG1	33:x:886:GLU:OE1	2.21	0.45
1:U:62:LEU:O	1:U:66:LYS:HG2	2.16	0.45
2:V:40:GLU:OE1	2:V:41:ALA:N	2.50	0.45
2:V:346:LEU:O	2:V:349:ARG:HD2	2.16	0.45
5:Y:23:ARG:NH1	5:Y:52:PRO:O	2.49	0.45
5:Y:81:LEU:HA	5:Y:84:LEU:HB2	1.97	0.45
5:Y:177:ARG:NH2	5:Y:178:ASN:HA	2.32	0.45
6:Z:175:LEU:O	9:c:209:LYS:NZ	2.39	0.45
10:d:61:TRP:CG	10:d:65:ARG:HH21	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:170:LEU:O	10:d:173:THR:HG22	2.16	0.45
10:d:237:ILE:O	10:d:239:SER:N	2.45	0.45
13:B:186:ASP:HA	13:B:367:ILE:HD11	1.98	0.45
13:B:335:GLU:OE1	13:B:335:GLU:N	2.49	0.45
16:E:149:ILE:HG12	16:E:153:LEU:HG	1.98	0.45
20:I:246:LYS:O	20:I:249:ARG:HB2	2.16	0.45
21:j:71:MET:SD	21:j:84:ILE:HG12	2.57	0.45
24:m:96:SER:OG	31:t:69:GLN:OE1	2.27	0.45
30:s:125:ASP:OD2	30:s:128:GLY:N	2.43	0.45
33:x:404:ASP:O	33:x:407:MET:SD	2.75	0.45
2:V:170:LEU:HG	2:V:174:PHE:CE2	2.52	0.45
2:V:179:LYS:NZ	2:V:210:CYS:O	2.50	0.45
2:V:310:THR:O	2:V:314:ARG:HG2	2.15	0.45
5:Y:77:ASN:N	5:Y:77:ASN:HD22	2.14	0.45
6:Z:157:HIS:C	6:Z:157:HIS:ND1	2.75	0.45
8:b:31:ASP:O	8:b:35:ILE:HG13	2.17	0.45
9:c:49:VAL:HG23	9:c:50:PRO:CD	2.45	0.45
10:d:63:ILE:HD11	10:d:165:PHE:HB2	1.99	0.45
13:B:133:VAL:HG11	13:B:158:ALA:HA	1.98	0.45
15:D:67:ASN:O	15:D:71:GLU:HG2	2.16	0.45
15:D:338:ARG:O	15:D:339:ARG:HB3	2.17	0.45
17:F:382:GLU:OE1	17:F:382:GLU:N	2.49	0.45
24:M:181:MET:O	24:M:181:MET:HG2	2.16	0.45
19:h:9:SER:HA	19:h:125:GLY:HA2	1.97	0.45
20:i:155:ASN:OD1	21:j:77:THR:OG1	2.30	0.45
21:j:68:ASN:HB2	21:j:137:ASP:HB2	1.98	0.45
26:o:113:ILE:HG23	26:o:119:THR:HG22	1.99	0.45
33:x:329:ASN:O	33:x:333:LEU:HG	2.17	0.45
34:v:11:UNK:O	34:v:12:UNK:C	2.65	0.45
1:U:144:ASP:OD2	14:C:21:ARG:NH2	2.50	0.45
1:U:520:MET:HB3	1:U:555:VAL:HG23	1.98	0.45
2:V:347:GLN:HG2	2:V:348:PHE:CD1	2.41	0.45
3:W:10:ASP:O	3:W:13:ILE:HG12	2.16	0.45
4:X:44:GLN:HA	4:X:47:GLU:HB3	1.99	0.45
7:a:112:ILE:O	7:a:116:THR:HG23	2.16	0.45
7:a:214:GLY:O	7:a:217:LEU:N	2.38	0.45
9:c:167:MET:HB3	9:c:170:LEU:O	2.17	0.45
10:d:189:ILE:O	10:d:222:TYR:HB2	2.17	0.45
10:d:189:ILE:HG12	10:d:215:TRP:CZ3	2.51	0.45
10:d:198:LEU:O	10:d:199:PHE:CB	2.57	0.45
12:A:56:LEU:HD22	13:B:48:LYS:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:35:VAL:HB	15:D:51:LEU:HD22	1.98	0.45
15:D:94:GLU:OE2	15:D:95:ALA:N	2.49	0.45
16:E:277:MET:O	16:E:277:MET:HG3	2.17	0.45
17:F:35:LYS:HB3	17:F:39:GLU:CG	2.46	0.45
17:F:171:ARG:HH11	17:F:267:LEU:HD11	1.81	0.45
19:H:25:ALA:O	19:H:29:VAL:HG23	2.17	0.45
23:L:159:MET:HG3	23:L:160:SER:N	2.32	0.45
29:R:35:ILE:HD12	29:R:56:GLU:HB2	1.98	0.45
31:T:144:TYR:HB2	26:o:132:LEU:HD23	1.98	0.45
20:i:28:ILE:HD11	20:i:131:GLY:C	2.42	0.45
28:q:136:ALA:HA	28:q:139:THR:HG22	1.98	0.45
33:x:830:LEU:HD22	33:x:874:LEU:HD11	1.98	0.45
1:U:846:LYS:NZ	33:x:571:GLU:OE1	2.34	0.45
2:V:36:GLU:OE2	2:V:89:LYS:HE2	2.17	0.45
2:V:199:ASN:O	2:V:202:ALA:N	2.48	0.45
3:W:340:VAL:HG12	3:W:341:PHE:CZ	2.51	0.45
3:W:425:LEU:HD23	3:W:428:TRP:CE3	2.52	0.45
5:Y:69:LEU:HB3	5:Y:73:MET:CE	2.46	0.45
5:Y:181:LYS:NZ	5:Y:219:PHE:CB	2.77	0.45
5:Y:291:HIS:HD2	5:Y:295:TYR:CD1	2.32	0.45
6:Z:45:LYS:HG2	6:Z:46:LYS:H	1.82	0.45
6:Z:252:LYS:NZ	9:c:303:MET:CE	2.77	0.45
12:A:376:LEU:O	12:A:378:PRO:HD3	2.16	0.45
14:C:20:LEU:O	14:C:23:TYR:CD2	2.70	0.45
15:D:107:THR:HG23	16:E:77:PRO:HG3	1.99	0.45
19:H:174:LEU:HD12	19:H:174:LEU:HA	1.77	0.45
18:g:129:ALA:C	18:g:130:GLU:OE1	2.60	0.45
18:g:236:ASP:OD1	18:g:236:ASP:O	2.34	0.45
19:h:118:MET:O	19:h:122:THR:HG23	2.16	0.45
24:m:234:GLU:OE1	24:m:234:GLU:N	2.50	0.45
1:U:596:ASN:OD1	15:D:52:GLU:HB3	2.16	0.45
2:V:228:ARG:HH21	2:V:231:LEU:HD23	1.82	0.45
3:W:2:ALA:HB3	3:W:47:LEU:HD13	1.99	0.45
5:Y:181:LYS:O	5:Y:184:GLN:HG3	2.17	0.45
5:Y:216:TYR:CD2	5:Y:217:LYS:HG3	2.52	0.45
6:Z:61:ASP:OD1	6:Z:63:LYS:HE2	2.16	0.45
9:c:52:GLU:OE2	9:c:113:HIS:ND1	2.46	0.45
11:e:52:PHE:CD2	11:e:55:GLN:HG3	2.52	0.45
16:E:18:GLU:O	16:E:22:ILE:HG12	2.17	0.45
17:F:69:MET:HE3	17:F:70:LYS:H	1.82	0.45
18:g:231:THR:HG22	18:g:232:GLU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:i:229:LYS:O	20:i:233:VAL:HG23	2.17	0.45
23:l:180:MET:HB3	23:l:181:GLU:OE1	2.16	0.45
31:t:27:LEU:HD11	31:t:34:ALA:HB1	1.99	0.45
33:x:692:LEU:H	33:x:692:LEU:HD22	1.82	0.45
33:x:720:GLU:OE2	33:x:807:ARG:NH2	2.50	0.45
2:V:350:GLN:HG3	2:V:351:PRO:HD2	1.99	0.45
3:W:124:LEU:C	3:W:128:LEU:HD23	2.42	0.45
3:W:374:THR:HG22	7:a:326:GLU:OE2	2.16	0.45
4:X:377:ILE:O	4:X:385:LEU:HA	2.16	0.45
5:Y:26:LEU:HG	5:Y:33:GLY:HA2	1.99	0.45
6:Z:39:LEU:HD12	6:Z:53:SER:OG	2.17	0.45
6:Z:209:ARG:NH2	7:a:354:GLU:OE1	2.50	0.45
6:Z:224:HIS:NE2	7:a:340:VAL:HG11	2.32	0.45
6:Z:236:LEU:O	7:a:289:ARG:NH2	2.50	0.45
7:a:41:VAL:HA	7:a:44:PHE:HB3	1.99	0.45
7:a:84:VAL:HA	7:a:87:MET:CG	2.44	0.45
10:d:12:LYS:HD3	10:d:14:PRO:HD3	1.98	0.45
10:d:52:ARG:HH11	10:d:53:ASP:HA	1.82	0.45
12:A:372:LEU:HD11	22:K:207:GLU:HB3	1.99	0.45
14:C:45:LEU:HD23	14:C:45:LEU:HA	1.83	0.45
15:D:121:ARG:NE	15:D:121:ARG:HA	2.31	0.45
15:D:340:GLN:O	15:D:344:ILE:HG13	2.17	0.45
16:E:252:GLU:O	16:E:256:THR:HG23	2.17	0.45
25:N:127:ILE:CG2	25:N:132:SER:HB2	2.48	0.45
26:o:1:THR:OG1	39:o:301:LDZ:C22	2.65	0.45
26:o:7:VAL:HG22	26:o:12:ILE:HD13	1.98	0.45
32:f:398:LEU:HD12	32:f:398:LEU:HA	1.79	0.45
33:x:429:ILE:HD13	33:x:447:ALA:HB1	1.99	0.45
33:x:679:LEU:HD21	33:x:690:VAL:HB	1.98	0.45
33:x:759:LEU:O	33:x:763:ARG:HG2	2.16	0.45
1:U:463:ASN:OD1	1:U:464:GLN:N	2.50	0.44
1:U:792:ASN:OD1	1:U:793:LYS:N	2.47	0.44
2:V:295:ILE:HD12	2:V:299:GLN:NE2	2.31	0.44
3:W:55:ARG:NH1	3:W:59:ASP:OD2	2.50	0.44
3:W:63:THR:O	3:W:111:TYR:OH	2.34	0.44
3:W:173:THR:HA	3:W:177:MET:HB3	2.00	0.44
5:Y:108:ALA:HA	5:Y:111:LEU:HG	1.99	0.44
5:Y:297:ARG:NH2	11:e:48:VAL:HG13	2.32	0.44
5:Y:380:VAL:O	5:Y:384:SER:OG	2.30	0.44
6:Z:38:VAL:HG22	6:Z:91:ILE:HG23	1.98	0.44
6:Z:175:LEU:O	6:Z:175:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:226:ILE:HD13	6:Z:226:ILE:HA	1.84	0.44
7:a:38:THR:HG21	7:a:71:VAL:HG11	1.99	0.44
7:a:295:GLU:OE2	7:a:299:SER:OG	2.27	0.44
8:b:33:VAL:HA	8:b:36:VAL:HG12	1.99	0.44
9:c:175:ARG:HB2	9:c:178:THR:HG22	1.99	0.44
9:c:203:ILE:HD12	9:c:203:ILE:HA	1.81	0.44
14:C:55:LYS:CG	15:D:72:PHE:CE1	3.01	0.44
15:D:205:TYR:CZ	15:D:332:GLU:HB2	2.52	0.44
16:E:264:MET:CE	16:E:270:LEU:HD12	2.42	0.44
21:j:116:GLN:HG3	22:k:83:ALA:HB1	1.99	0.44
28:q:88:LEU:HB3	28:q:122:ALA:HB2	1.98	0.44
33:x:737:ASN:O	33:x:737:ASN:ND2	2.50	0.44
33:x:870:THR:OG1	33:x:871:PRO:HD3	2.16	0.44
1:U:12:LEU:HA	1:U:20:LYS:NZ	2.32	0.44
1:U:177:LEU:HD22	1:U:177:LEU:H	1.81	0.44
1:U:503:GLN:OE1	1:U:505:ASP:CB	2.63	0.44
3:W:120:ILE:HD12	3:W:121:LYS:N	2.33	0.44
4:X:359:ALA:O	4:X:362:GLU:HG2	2.16	0.44
5:Y:308:LEU:HD23	5:Y:308:LEU:HA	1.79	0.44
12:A:52:ILE:CD1	13:B:72:LEU:HD22	2.47	0.44
12:A:197:HIS:HB3	12:A:200:ARG:HH11	1.82	0.44
15:D:132:LEU:HD23	15:D:137:ASN:O	2.17	0.44
16:E:50:LEU:HA	17:F:159:LEU:HD11	1.99	0.44
16:E:171:LEU:HD11	16:E:173:TYR:HB3	1.98	0.44
16:E:172:LEU:CG	16:E:276:ILE:HG23	2.42	0.44
16:E:194:ASN:OD1	16:E:230:ILE:HG23	2.17	0.44
17:F:43:GLN:HA	17:F:46:ARG:HB3	2.00	0.44
19:H:74:LEU:HD23	19:H:87:VAL:HG22	1.99	0.44
20:I:68:LEU:HD22	20:I:90:LEU:HB3	1.98	0.44
22:K:41:GLN:HA	22:K:46:VAL:HG22	1.98	0.44
20:i:60:PHE:C	20:i:62:SER:H	2.23	0.44
22:k:93:ARG:HG2	29:r:68:LEU:HD13	1.99	0.44
24:m:215:TRP:O	24:m:224:HIS:HD2	2.01	0.44
27:p:107:PRO:HG2	27:p:124:LEU:HB2	1.98	0.44
28:q:102:LEU:HD12	28:q:118:MET:HE3	1.99	0.44
33:x:116:GLY:H	33:x:120:ARG:NH1	2.15	0.44
33:x:414:LEU:H	33:x:414:LEU:HD22	1.81	0.44
33:x:736:THR:HG1	33:x:738:ASN:CG	2.19	0.44
1:U:341:PHE:CE1	1:U:344:ARG:NH2	2.86	0.44
1:U:505:ASP:HB3	1:U:508:THR:HG22	2.00	0.44
3:W:135:LYS:HB2	3:W:135:LYS:NZ	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:388:ASP:OD1	13:B:388:ASP:N	2.50	0.44
14:C:395:SER:OG	14:C:396:GLU:N	2.50	0.44
15:D:113:VAL:HG22	15:D:114:ARG:N	2.31	0.44
16:E:43:SER:OG	16:E:44:GLU:OE1	2.34	0.44
17:F:69:MET:CE	17:F:70:LYS:N	2.81	0.44
17:F:175:MET:CE	17:F:251:LEU:CD2	2.95	0.44
29:R:153:TYR:CE2	29:R:187:VAL:HG11	2.52	0.44
30:S:16:ALA:HB2	30:S:121:VAL:HG23	1.98	0.44
21:j:5:ARG:C	21:j:7:ILE:H	2.25	0.44
30:s:123:SER:O	30:s:130:TYR:HA	2.17	0.44
33:x:552:ASP:OD1	33:x:553:THR:N	2.50	0.44
33:x:585:GLU:O	33:x:586:PRO:C	2.59	0.44
1:U:118:LEU:HD12	1:U:122:GLU:HG3	1.98	0.44
2:V:269:LYS:NZ	2:V:295:ILE:HB	2.33	0.44
2:V:381:GLN:HG3	2:V:382:PHE:CD2	2.52	0.44
5:Y:141:VAL:HG12	5:Y:145:LEU:CD1	2.47	0.44
5:Y:258:GLN:NE2	5:Y:270:VAL:O	2.51	0.44
9:c:87:VAL:HG21	9:c:133:PHE:CE2	2.53	0.44
10:d:203:PRO:HB2	10:d:205:LYS:H	1.82	0.44
12:A:63:THR:HG22	13:B:79:ILE:HG12	2.00	0.44
14:C:194:THR:HG21	14:C:317:PHE:O	2.18	0.44
14:C:205:HIS:HD2	14:C:206:HIS:CE1	2.35	0.44
15:D:99:ASN:HB3	15:D:114:ARG:HH22	1.82	0.44
16:E:170:CYS:HB3	16:E:296:ASP:O	2.16	0.44
18:G:17:SER:HB3	18:G:21:ARG:H	1.82	0.44
20:I:44:LEU:HD22	20:I:190:LEU:HD23	1.99	0.44
25:N:84:LYS:HE2	25:N:84:LYS:HB3	1.81	0.44
27:P:41:LYS:HG2	27:P:53:LEU:O	2.17	0.44
21:j:120:GLN:HE22	22:k:137:PHE:HE1	1.65	0.44
23:l:104:PRO:HB2	23:l:107:ARG:HG2	1.97	0.44
33:x:95:PRO:O	33:x:99:LEU:CD1	2.65	0.44
33:x:587:PHE:CE1	33:x:590:PHE:CD1	3.03	0.44
1:U:149:GLN:HG3	14:C:24:TYR:CE2	2.53	0.44
1:U:341:PHE:HE1	1:U:344:ARG:NH2	2.15	0.44
1:U:634:PRO:O	1:U:637:VAL:N	2.50	0.44
1:U:696:ILE:HG22	1:U:737:LEU:HA	2.00	0.44
1:U:792:ASN:ND2	1:U:793:LYS:HZ2	2.16	0.44
2:V:18:PRO:HA	2:V:22:GLY:H	1.82	0.44
2:V:270:LEU:HD11	2:V:299:GLN:HG2	1.99	0.44
2:V:289:LEU:HD21	2:V:308:THR:O	2.17	0.44
3:W:450:GLU:HB2	6:Z:211:TYR:HE1	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:136:LEU:HD12	4:X:137:TYR:HD1	1.82	0.44
4:X:408:SER:O	4:X:411:VAL:HG12	2.17	0.44
5:Y:38:ARG:O	5:Y:42:MET:CE	2.66	0.44
6:Z:186:THR:O	6:Z:189:GLN:OE1	2.34	0.44
7:a:101:ARG:HG3	7:a:111:VAL:HA	1.99	0.44
7:a:222:LEU:O	7:a:224:SER:N	2.50	0.44
9:c:44:HIS:NE2	9:c:53:VAL:O	2.46	0.44
10:d:78:LEU:HD12	10:d:79:LYS:N	2.33	0.44
12:A:78:TRP:CD1	12:A:78:TRP:H	2.36	0.44
12:A:99:THR:O	12:A:139:ARG:HA	2.17	0.44
12:A:279:ALA:HB2	13:B:310:LEU:HD23	1.99	0.44
12:A:288:GLY:HA2	16:E:208:ILE:HG12	1.99	0.44
13:B:87:PRO:O	13:B:89:GLU:HG2	2.17	0.44
15:D:273:LYS:HG2	15:D:319:PRO:HD3	1.98	0.44
16:E:29:LEU:HD23	16:E:29:LEU:HA	1.76	0.44
16:E:85:ARG:HG3	16:E:86:GLN:HG2	2.00	0.44
16:E:198:VAL:CG2	16:E:218:MET:CE	2.95	0.44
16:E:243:PHE:CD1	16:E:243:PHE:N	2.85	0.44
17:F:122:ALA:HB3	17:F:134:LEU:CD1	2.47	0.44
17:F:175:MET:HE1	17:F:251:LEU:CD2	2.47	0.44
20:I:18:LEU:HD21	21:J:125:ARG:HD2	1.98	0.44
24:M:202:ASP:OD1	24:M:202:ASP:N	2.43	0.44
18:g:202:LEU:HA	18:g:202:LEU:HD23	1.80	0.44
21:j:109:ARG:HG2	21:j:153:TYR:CZ	2.53	0.44
24:m:81:LEU:O	24:m:85:ARG:HG3	2.17	0.44
29:r:197:GLU:OE1	29:r:198:LYS:N	2.51	0.44
33:x:72:ARG:CZ	33:x:118:ASN:HB3	2.48	0.44
33:x:102:HIS:O	33:x:106:LEU:HD12	2.18	0.44
33:x:457:ASN:HD22	33:x:461:PRO:HG3	1.82	0.44
33:x:861:THR:HG22	33:x:862:ILE:HD13	1.99	0.44
1:U:85:GLY:HA2	1:U:129:ARG:NH1	2.32	0.44
1:U:492:ASP:OD1	1:U:492:ASP:N	2.49	0.44
2:V:98:LEU:H	2:V:107:ARG:HG3	1.82	0.44
3:W:56:THR:HG21	3:W:104:MET:CE	2.47	0.44
3:W:225:LYS:HE2	3:W:226:TYR:HE1	1.82	0.44
3:W:229:LEU:O	3:W:233:LEU:CB	2.66	0.44
3:W:351:TRP:HA	3:W:351:TRP:HE3	1.83	0.44
5:Y:141:VAL:O	5:Y:145:LEU:CD1	2.65	0.44
6:Z:53:SER:HB3	6:Z:95:TYR:OH	2.18	0.44
6:Z:285:ALA:O	6:Z:289:GLU:HG2	2.17	0.44
8:b:68:THR:O	8:b:71:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:161:ASN:OD1	8:b:161:ASN:N	2.51	0.44
10:d:2:TYR:H	10:d:25:ARG:HH12	1.66	0.44
10:d:191:PHE:HZ	10:d:202:THR:CA	2.30	0.44
12:A:275:ASP:OD2	12:A:276:GLU:N	2.51	0.44
15:D:94:GLU:OE2	15:D:95:ALA:C	2.61	0.44
16:E:226:GLN:N	16:E:227:PRO:HD2	2.32	0.44
16:E:255:ARG:O	16:E:259:GLU:HB2	2.18	0.44
17:F:261:ILE:HG13	17:F:305:GLU:OE1	2.17	0.44
18:G:37:LEU:HG	18:G:53:GLN:HG3	2.00	0.44
21:J:38:ARG:HE	21:J:180:ALA:HB1	1.82	0.44
19:h:65:VAL:HG12	19:h:218:PHE:HZ	1.82	0.44
23:l:199:LEU:HD13	23:l:203:GLN:HG2	1.98	0.44
33:x:104:GLY:HA2	33:x:107:LYS:HE3	1.99	0.44
33:x:755:ASP:CG	33:x:758:ASN:HD22	2.25	0.44
34:v:11:UNK:C	34:v:13:UNK:H2	2.31	0.44
1:U:541:HIS:CD2	1:U:542:GLU:H	2.36	0.44
1:U:851:GLU:HG3	1:U:851:GLU:H	1.64	0.44
3:W:1:MET:SD	3:W:34:LEU:HG	2.58	0.44
3:W:172:GLU:HB2	3:W:182:ARG:HH11	1.82	0.44
3:W:442:THR:HA	3:W:445:LEU:CD2	2.48	0.44
4:X:140:THR:O	4:X:142:ARG:NH1	2.51	0.44
6:Z:167:ALA:O	9:c:42:LEU:HD21	2.18	0.44
7:a:180:LEU:HB3	7:a:196:ARG:NH2	2.32	0.44
9:c:233:ASP:OD2	9:c:235:SER:OG	2.35	0.44
14:C:25:LEU:CD1	15:D:40:LEU:HD22	2.48	0.44
15:D:125:LYS:NZ	15:D:126:PRO:O	2.46	0.44
16:E:352:MET:C	16:E:356:ARG:HG2	2.42	0.44
19:H:111:VAL:HG22	19:H:136:ILE:HD13	1.99	0.44
26:O:113:ILE:HG12	26:O:119:THR:HG22	2.00	0.44
18:g:25:VAL:HG21	18:g:126:THR:HG23	2.00	0.44
18:g:131:MET:HE2	18:g:131:MET:HB3	1.83	0.44
24:m:184:MET:H	24:m:184:MET:HG2	1.36	0.44
33:x:109:ILE:O	33:x:113:MET:HE3	2.18	0.44
33:x:253:LEU:HD23	33:x:268:LEU:HB2	2.00	0.44
33:x:407:MET:HE3	33:x:407:MET:HB3	1.89	0.44
1:U:366:HIS:NE2	1:U:395:ARG:NH1	2.64	0.44
2:V:133:PRO:HA	2:V:136:GLU:HG2	2.00	0.44
2:V:282:ASN:HB3	5:Y:385:ARG:HG3	1.99	0.44
3:W:117:ASP:O	3:W:120:ILE:HD12	2.18	0.44
3:W:121:LYS:HE3	3:W:121:LYS:HB2	1.79	0.44
3:W:251:TYR:CE1	3:W:267:LEU:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:310:THR:C	3:W:312:MET:H	2.25	0.44
6:Z:35:VAL:HG22	6:Z:97:THR:HG22	2.00	0.44
7:a:122:LYS:HD3	7:a:130:VAL:HB	2.00	0.44
9:c:189:ILE:HG13	9:c:190:GLN:NE2	2.32	0.44
10:d:68:ILE:HG23	10:d:105:PHE:CZ	2.53	0.44
12:A:90:GLU:O	12:A:90:GLU:HG2	2.17	0.44
13:B:71:TYR:O	13:B:75:GLU:HG3	2.17	0.44
13:B:365:PHE:HD2	13:B:384:ILE:HD11	1.83	0.44
27:P:134:ASP:OD1	27:P:134:ASP:N	2.51	0.44
21:j:92:GLN:HB3	28:q:62:LYS:HG3	2.00	0.44
22:k:114:GLN:HG3	22:k:162:PHE:CZ	2.53	0.44
26:o:194:LYS:NZ	26:o:195:LYS:O	2.44	0.44
33:x:619:HIS:O	33:x:620:PHE:HD1	2.01	0.44
33:x:803:PHE:CE2	33:x:806:VAL:HG11	2.53	0.44
1:U:108:TYR:OH	1:U:159:ARG:NH1	2.51	0.44
5:Y:32:ARG:HA	5:Y:32:ARG:HD3	1.86	0.44
5:Y:204:THR:O	5:Y:206:SER:N	2.51	0.44
7:a:69:HIS:ND1	7:a:70:ARG:HG2	2.33	0.44
8:b:4:GLU:OE1	8:b:6:THR:OG1	2.35	0.44
13:B:37:LYS:HA	13:B:37:LYS:HD2	1.79	0.44
15:D:97:ASP:OD1	15:D:97:ASP:C	2.61	0.44
15:D:99:ASN:CA	15:D:115:ILE:CD1	2.86	0.44
15:D:114:ARG:HB3	15:D:114:ARG:CZ	2.48	0.44
16:E:363:VAL:HG22	16:E:364:GLN:H	1.83	0.44
17:F:432:LYS:HE2	17:F:432:LYS:HB2	1.74	0.44
24:M:171:ALA:O	24:M:175:GLU:OE2	2.35	0.44
24:M:237:LYS:O	24:M:241:GLU:HG3	2.18	0.44
24:m:41:CYS:HB2	24:m:42:LYS:H	1.60	0.44
29:r:100:MET:HE3	29:r:100:MET:HB2	1.89	0.44
32:f:402:LYS:HB2	32:f:402:LYS:HE3	1.79	0.44
2:V:23:GLU:O	2:V:23:GLU:HG3	2.17	0.43
2:V:471:GLU:N	2:V:472:PRO:HD2	2.33	0.43
3:W:184:GLU:OE2	3:W:222:LEU:HG	2.18	0.43
4:X:71:LYS:H	4:X:71:LYS:HG2	1.64	0.43
5:Y:377:LEU:O	5:Y:381:GLN:HG3	2.18	0.43
7:a:69:HIS:O	7:a:70:ARG:HD2	2.18	0.43
14:C:16:ALA:HB3	14:C:21:ARG:NH2	2.33	0.43
15:D:237:GLN:OE1	16:E:213:ARG:NH2	2.51	0.43
16:E:231:PHE:CE1	16:E:274:LYS:HE2	2.53	0.43
16:E:311:ASP:HA	16:E:314:LYS:HG2	2.00	0.43
16:E:343:LEU:HA	16:E:343:LEU:HD23	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:363:VAL:HG22	16:E:364:GLN:N	2.33	0.43
20:I:230:GLN:O	20:I:234:GLU:HG3	2.18	0.43
22:K:157:ASP:OD1	22:K:157:ASP:C	2.61	0.43
31:T:96:MET:CE	31:T:110:MET:CE	2.94	0.43
21:j:3:TYR:N	21:j:3:TYR:CD1	2.86	0.43
21:j:7:ILE:HD11	21:j:19:VAL:HG23	2.00	0.43
22:k:12:VAL:HG11	22:k:22:PHE:HB2	2.00	0.43
33:x:170:TRP:CD1	33:x:211:ILE:HG22	2.52	0.43
33:x:211:ILE:O	33:x:213:GLN:NE2	2.51	0.43
33:x:343:LYS:N	33:x:343:LYS:HD3	2.33	0.43
33:x:838:ARG:NE	33:x:838:ARG:HA	2.33	0.43
1:U:749:GLN:HE21	1:U:749:GLN:HB3	1.64	0.43
2:V:131:LEU:O	2:V:135:LEU:HG	2.18	0.43
3:W:209:ILE:HD12	3:W:209:ILE:HA	1.86	0.43
3:W:229:LEU:O	3:W:233:LEU:HB2	2.17	0.43
3:W:240:TYR:O	3:W:243:ILE:HG12	2.19	0.43
3:W:378:MET:O	3:W:382:LEU:HG	2.18	0.43
4:X:363:ARG:CZ	4:X:363:ARG:HB3	2.47	0.43
5:Y:107:LYS:O	5:Y:111:LEU:HG	2.17	0.43
6:Z:7:GLN:HB2	6:Z:46:LYS:HG2	2.00	0.43
6:Z:59:ASP:O	6:Z:68:TRP:HA	2.18	0.43
8:b:100:ARG:NE	8:b:103:LYS:HA	2.32	0.43
9:c:183:HIS:N	9:c:183:HIS:ND1	2.66	0.43
12:A:42:SER:O	12:A:45:ILE:HG22	2.18	0.43
15:D:115:ILE:HG22	15:D:139:LEU:CG	2.47	0.43
15:D:155:THR:O	15:D:158:GLN:HB2	2.18	0.43
19:H:205:GLU:HG2	19:H:227:LYS:HA	1.99	0.43
21:J:241:LYS:HE3	21:J:242:LYS:HG3	2.00	0.43
33:x:181:ARG:HH22	33:x:213:GLN:NE2	2.15	0.43
1:U:387:ARG:HE	1:U:387:ARG:N	2.13	0.43
2:V:282:ASN:CB	5:Y:385:ARG:HG3	2.48	0.43
3:W:203:GLN:OE1	3:W:233:LEU:HD11	2.18	0.43
5:Y:71:ASN:HA	5:Y:74:LYS:HG2	1.99	0.43
7:a:157:ASP:O	7:a:161:LYS:HG2	2.18	0.43
7:a:173:TYR:O	7:a:177:LEU:HG	2.18	0.43
10:d:67:ASP:O	10:d:71:PHE:HB2	2.19	0.43
14:C:399:MET:HA	14:C:402:LYS:HB2	1.99	0.43
16:E:24:GLY:O	16:E:28:GLU:HG2	2.19	0.43
16:E:123:SER:C	16:E:124:HIS:CD2	2.96	0.43
24:M:215:TRP:HB2	24:M:227:VAL:HG12	1.99	0.43
33:x:655:LEU:HD21	33:x:800:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:187:LEU:HD13	15:D:45:LYS:HG2	2.00	0.43
2:V:243:ASP:OD1	2:V:246:GLY:N	2.49	0.43
2:V:344:ASP:HB2	11:e:46:ASP:CG	2.43	0.43
3:W:56:THR:HG22	3:W:104:MET:CE	2.48	0.43
3:W:91:SER:OG	3:W:92:LYS:N	2.49	0.43
4:X:379:ASP:OD1	5:Y:312:ARG:HB3	2.19	0.43
5:Y:297:ARG:HA	5:Y:300:ARG:HH21	1.84	0.43
6:Z:168:GLU:OE1	9:c:43:LYS:HB2	2.19	0.43
6:Z:284:ASP:HA	6:Z:287:LYS:HG2	1.99	0.43
7:a:319:LEU:HD23	7:a:319:LEU:N	2.31	0.43
9:c:122:LEU:HG	9:c:126:ASP:HB3	2.00	0.43
10:d:60:GLN:O	10:d:63:ILE:HG22	2.18	0.43
10:d:199:PHE:CD1	10:d:200:PHE:HD2	2.37	0.43
11:e:5:LYS:HB3	11:e:5:LYS:HE2	1.85	0.43
14:C:399:MET:O	14:C:399:MET:HG3	2.18	0.43
16:E:354:ALA:HA	16:E:358:ASP:CG	2.43	0.43
21:J:247:ALA:HA	33:x:907:ASP:C	2.43	0.43
25:N:40:ARG:NH1	25:N:183:GLY:HA2	2.33	0.43
20:i:174:MET:SD	20:i:199:LYS:HD3	2.59	0.43
22:k:67:ILE:CD1	22:k:216:GLU:HG3	2.49	0.43
23:l:200:PRO:HB2	23:l:202:GLU:OE2	2.18	0.43
30:s:28:ARG:NH2	30:s:191:ASP:OD1	2.50	0.43
33:x:192:VAL:O	33:x:196:MET:HG3	2.18	0.43
33:x:296:PHE:CE1	33:x:897:PHE:HD1	2.37	0.43
33:x:749:ALA:HB2	33:x:762:VAL:HG11	2.00	0.43
1:U:320:ASP:O	1:U:324:LYS:HG2	2.18	0.43
1:U:321:GLN:O	1:U:325:MET:CE	2.63	0.43
1:U:596:ASN:HA	1:U:599:ILE:HG12	2.01	0.43
1:U:639:LEU:HD21	14:C:49:ARG:HD2	2.01	0.43
3:W:147:LYS:O	3:W:151:THR:HG22	2.18	0.43
3:W:148:THR:O	3:W:152:ILE:CD1	2.65	0.43
3:W:428:TRP:CG	6:Z:245:PHE:HZ	2.37	0.43
5:Y:329:PHE:O	5:Y:333:GLU:HG3	2.18	0.43
7:a:275:LEU:HD23	7:a:278:MET:CE	2.43	0.43
7:a:277:LEU:HD11	7:a:310:LEU:HD13	2.01	0.43
7:a:311:VAL:O	7:a:315:LEU:CD1	2.50	0.43
9:c:186:LYS:O	9:c:188:SER:N	2.52	0.43
16:E:183:LEU:HD23	16:E:183:LEU:HA	1.76	0.43
17:F:63:THR:O	17:F:67:GLN:HB3	2.19	0.43
17:F:410:ARG:NH1	17:F:419:ASP:OD2	2.52	0.43
19:H:6:TYR:CD1	19:H:15:PRO:HD3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:H:10:LEU:HD12	19:H:10:LEU:HA	1.75	0.43
24:M:195:LYS:O	24:M:199:ILE:HG23	2.18	0.43
23:l:23:GLU:HA	23:l:26:MET:HG3	2.01	0.43
29:r:115:ASP:HB3	29:r:117:GLU:H	1.84	0.43
33:x:396:ASN:HB3	33:x:400:TYR:CE2	2.53	0.43
33:x:450:ILE:HD11	33:x:487:LEU:HD13	2.00	0.43
33:x:520:LEU:C	33:x:524:MET:CE	2.92	0.43
33:x:694:LEU:O	33:x:697:ILE:HG22	2.19	0.43
33:x:714:SER:OG	33:x:748:LEU:HD11	2.18	0.43
1:U:681:ASN:ND2	1:U:725:MET:CE	2.82	0.43
1:U:684:ARG:O	1:U:688:LEU:HG	2.17	0.43
2:V:107:ARG:HD3	2:V:107:ARG:HA	1.71	0.43
3:W:38:GLY:O	3:W:44:ILE:HG13	2.19	0.43
3:W:142:ARG:N	3:W:142:ARG:CD	2.81	0.43
4:X:204:PRO:O	4:X:206:LEU:N	2.52	0.43
4:X:410:VAL:C	4:X:414:LEU:HD23	2.43	0.43
6:Z:25:ARG:HH11	9:c:104:ARG:HG3	1.83	0.43
6:Z:79:TYR:CZ	6:Z:91:ILE:CG1	2.97	0.43
6:Z:81:MET:SD	6:Z:82:PHE:N	2.92	0.43
6:Z:274:ASN:OD1	6:Z:274:ASN:C	2.62	0.43
9:c:146:ASP:HB3	9:c:156:VAL:HG13	1.99	0.43
13:B:379:THR:O	13:B:379:THR:OG1	2.32	0.43
13:B:414:VAL:HG13	13:B:418:ASP:HB2	2.01	0.43
15:D:388:ARG:HH12	16:E:297:ARG:NE	2.16	0.43
17:F:143:GLU:OE2	17:F:143:GLU:N	2.45	0.43
17:F:314:LEU:HD21	17:F:347:ARG:HH21	1.83	0.43
27:P:34:MET:O	29:r:166:ARG:NH2	2.51	0.43
29:R:9:ARG:HG3	29:R:9:ARG:NH1	2.33	0.43
23:l:132:LEU:HB2	23:l:147:THR:HB	2.00	0.43
23:l:183:ASN:OD1	23:l:186:GLU:HB2	2.19	0.43
31:t:25:ASP:HA	31:t:187:PHE:HA	2.00	0.43
33:x:887:PHE:CE2	33:x:900:LEU:HB2	2.53	0.43
1:U:98:GLU:HA	1:U:101:ILE:HG12	1.99	0.43
1:U:757:MET:SD	1:U:757:MET:N	2.89	0.43
2:V:164:GLU:HA	2:V:166:TYR:CE1	2.53	0.43
4:X:212:MET:HE2	4:X:212:MET:HB3	1.78	0.43
5:Y:217:LYS:O	5:Y:221:THR:HG23	2.19	0.43
6:Z:108:ILE:O	6:Z:112:MET:HG2	2.18	0.43
8:b:20:ASP:OD1	8:b:21:PHE:N	2.50	0.43
8:b:143:PHE:HA	8:b:173:VAL:HG11	1.99	0.43
10:d:25:ARG:NH2	10:d:50:LEU:HD23	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:151:ILE:HD12	12:A:151:ILE:N	2.33	0.43
12:A:418:LYS:C	12:A:423:PHE:HB2	2.44	0.43
16:E:287:PRO:HA	16:E:290:LEU:HB2	2.00	0.43
21:J:65:LEU:HB2	21:J:69:VAL:HG23	2.01	0.43
26:O:63:LEU:HD13	26:O:82:MET:HE2	2.01	0.43
39:O:301:LDZ:H15	39:O:301:LDZ:H11	2.00	0.43
27:P:80:ARG:H	27:P:80:ARG:HG2	1.66	0.43
1:U:344:ARG:CZ	1:U:345:ASN:HB2	2.48	0.43
1:U:353:LEU:HD22	1:U:353:LEU:H	1.83	0.43
1:U:366:HIS:CD2	1:U:395:ARG:HH11	2.36	0.43
1:U:452:ASN:O	1:U:453:HIS:ND1	2.49	0.43
1:U:636:VAL:HG13	1:U:637:VAL:HG23	2.01	0.43
1:U:803:LYS:HG2	1:U:875:PHE:C	2.43	0.43
1:U:823:LYS:HD2	1:U:824:GLU:N	2.34	0.43
2:V:65:ARG:HH22	2:V:205:LEU:HD21	1.81	0.43
2:V:159:LEU:O	2:V:162:GLU:HB2	2.18	0.43
2:V:454:GLU:HG2	10:d:187:GLU:CD	2.43	0.43
3:W:82:LEU:CD1	3:W:86:ASN:OD1	2.66	0.43
6:Z:39:LEU:HD21	6:Z:50:VAL:HG11	2.01	0.43
6:Z:165:GLU:HG3	6:Z:166:GLU:O	2.18	0.43
9:c:183:HIS:C	9:c:184:LEU:HD12	2.44	0.43
12:A:53:GLN:OE1	12:A:53:GLN:HA	2.18	0.43
12:A:317:VAL:HG11	12:A:319:MET:HE2	2.00	0.43
15:D:368:ASP:O	15:D:370:ILE:CD1	2.62	0.43
15:D:387:VAL:HG21	16:E:159:PHE:HE1	1.83	0.43
16:E:200:SER:HB2	16:E:235:ILE:HA	2.00	0.43
18:G:143:ILE:HD13	18:G:149:PRO:HA	2.01	0.43
19:H:99:LEU:HD23	19:H:99:LEU:HA	1.85	0.43
22:k:35:SER:HB3	22:k:51:GLU:HG3	2.01	0.43
23:l:18:ARG:NH2	23:l:23:GLU:OE2	2.52	0.43
27:p:83:LYS:HB2	27:p:83:LYS:HE2	1.82	0.43
31:t:15:LYS:HD2	31:t:135:PRO:HA	2.01	0.43
33:x:196:MET:SD	33:x:197:ALA:N	2.91	0.43
33:x:516:GLY:HA2	33:x:558:LEU:HD23	2.00	0.43
2:V:153:LYS:N	2:V:153:LYS:HD3	2.32	0.43
2:V:209:LYS:HD2	2:V:209:LYS:C	2.43	0.43
2:V:234:ARG:HG2	2:V:250:LEU:CD1	2.48	0.43
3:W:86:ASN:C	3:W:87:ILE:HD13	2.43	0.43
3:W:420:ASP:HB3	3:W:422:ASN:OD1	2.19	0.43
4:X:57:LEU:HD23	4:X:66:LEU:N	2.34	0.43
4:X:90:ARG:HE	4:X:128:ALA:HB1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:99:MET:HE2	4:X:99:MET:HB2	1.96	0.43
4:X:255:LEU:O	4:X:259:ILE:HD12	2.18	0.43
4:X:270:LEU:CD1	4:X:270:LEU:N	2.82	0.43
6:Z:26:ILE:CG1	6:Z:35:VAL:HG11	2.49	0.43
6:Z:198:LEU:HD13	7:a:364:GLU:HA	2.00	0.43
6:Z:228:TYR:CD1	7:a:340:VAL:HG23	2.54	0.43
7:a:229:ASP:HB3	7:a:230:ARG:HE	1.84	0.43
7:a:235:ASP:HB3	7:a:249:GLN:OE1	2.19	0.43
8:b:91:ARG:O	8:b:94:HIS:ND1	2.51	0.43
9:c:130:GLN:O	9:c:134:GLU:HG2	2.18	0.43
11:e:45:ASP:HB3	11:e:48:VAL:HB	1.99	0.43
12:A:217:PRO:O	12:A:220:THR:OG1	2.36	0.43
12:A:225:CYS:O	12:A:229:VAL:HG13	2.19	0.43
15:D:94:GLU:HB3	15:D:102:ILE:HG22	2.01	0.43
15:D:189:GLU:HG2	15:D:190:LEU:N	2.34	0.43
15:D:388:ARG:NH2	16:E:297:ARG:HG2	2.20	0.43
16:E:121:ASN:ND2	16:E:121:ASN:C	2.77	0.43
23:L:88:MET:HE3	23:L:112:ILE:HD11	2.00	0.43
23:l:43:HIS:CD2	23:l:216:GLY:HA3	2.54	0.43
24:m:233:GLU:C	24:m:236:GLU:OE1	2.62	0.43
33:x:184:LEU:O	33:x:188:VAL:HG23	2.19	0.43
33:x:670:MET:CE	33:x:673:ARG:HD2	2.49	0.43
33:x:784:ASP:H	33:x:879:ARG:HH22	1.67	0.43
33:x:828:ARG:C	33:x:829:MET:SD	3.01	0.43
33:x:889:PRO:CB	33:x:900:LEU:HD23	2.49	0.43
1:U:666:LYS:HE2	1:U:666:LYS:HB2	1.79	0.43
1:U:808:PRO:HD2	1:U:809:SER:N	2.34	0.43
1:U:811:PHE:CE2	1:U:885:MET:HG3	2.54	0.43
2:V:280:ALA:HB1	2:V:284:GLU:HB3	2.00	0.43
3:W:366:MET:HE2	3:W:378:MET:HE3	2.01	0.43
4:X:47:GLU:CD	4:X:76:PHE:CZ	2.97	0.43
4:X:105:GLN:HA	4:X:108:GLU:CD	2.44	0.43
5:Y:268:TYR:CE2	5:Y:307:LEU:HD13	2.54	0.43
9:c:279:ASP:O	9:c:280:PRO:C	2.61	0.43
9:c:306:THR:HA	9:c:309:PHE:CE2	2.53	0.43
10:d:190:LEU:HD13	10:d:192:THR:H	1.84	0.43
12:A:187:LEU:HD11	12:A:318:LEU:HD11	2.01	0.43
15:D:73:LEU:O	15:D:76:GLN:HG3	2.19	0.43
15:D:370:ILE:CD1	15:D:370:ILE:N	2.82	0.43
16:E:26:LEU:HG	16:E:30:ARG:HD2	2.00	0.43
21:J:102:VAL:HG12	21:J:103:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:K:97:GLN:HG3	29:R:65:ILE:HG13	2.01	0.43
28:Q:184:ASP:N	28:Q:184:ASP:OD1	2.49	0.43
18:g:206:LEU:HD23	18:g:208:ILE:HD11	2.00	0.43
20:i:41:ASP:OD1	20:i:41:ASP:N	2.43	0.43
23:l:201:ALA:N	23:l:202:GLU:OE2	2.52	0.43
25:n:116:MET:HE3	25:n:116:MET:HB3	1.80	0.43
30:s:27:THR:O	30:s:27:THR:OG1	2.34	0.43
1:U:185:MET:HB3	1:U:218:GLN:OE1	2.19	0.42
1:U:870:GLU:HG3	1:U:871:PRO:HD3	2.00	0.42
2:V:250:LEU:HA	2:V:253:LEU:HD13	2.01	0.42
2:V:296:LYS:HE3	2:V:304:GLU:HG2	2.01	0.42
2:V:309:MET:HE2	2:V:328:VAL:HG12	1.99	0.42
3:W:136:ILE:O	3:W:136:ILE:HG22	2.19	0.42
3:W:141:GLU:OE1	3:W:142:ARG:HA	2.18	0.42
5:Y:16:ASP:O	5:Y:19:ILE:HG12	2.18	0.42
10:d:63:ILE:HD12	10:d:63:ILE:HA	1.86	0.42
10:d:200:PHE:HB3	10:d:203:PRO:CB	2.46	0.42
10:d:246:VAL:HA	10:d:249:TYR:CD2	2.53	0.42
14:C:208:ASP:OD2	14:C:208:ASP:C	2.62	0.42
14:C:215:SER:HB2	14:C:218:GLU:HB2	2.00	0.42
15:D:89:ILE:HG22	16:E:78:ARG:O	2.19	0.42
16:E:364:GLN:O	16:E:367:PHE:N	2.52	0.42
23:L:62:LYS:NZ	23:L:74:ILE:O	2.50	0.42
28:Q:118:MET:HE3	28:Q:118:MET:HB2	1.84	0.42
29:R:44:THR:HG21	29:R:100:MET:HE3	1.99	0.42
18:g:116:LYS:HE3	18:g:116:LYS:HB3	1.75	0.42
21:j:184:ASP:OD1	21:j:184:ASP:N	2.51	0.42
21:j:187:THR:O	21:j:191:VAL:HG23	2.19	0.42
24:m:66:LEU:HD13	24:m:214:SER:OG	2.19	0.42
28:q:13:VAL:HG23	28:q:113:PRO:HB2	2.01	0.42
28:q:101:ASN:HB3	28:q:132:HIS:CD2	2.54	0.42
33:x:398:TRP:CE3	33:x:398:TRP:O	2.72	0.42
33:x:731:MET:SD	33:x:768:LEU:HD13	2.59	0.42
1:U:867:LYS:HB3	1:U:867:LYS:HE2	1.71	0.42
2:V:454:GLU:HG2	10:d:187:GLU:CG	2.48	0.42
3:W:79:GLU:HG2	3:W:130:MET:CE	2.49	0.42
3:W:229:LEU:HD12	3:W:232:GLN:HB2	2.02	0.42
3:W:377:ARG:HA	3:W:380:GLN:HG2	2.00	0.42
4:X:130:GLU:HB3	4:X:153:LEU:HD22	2.01	0.42
4:X:302:PHE:CD1	4:X:302:PHE:C	2.96	0.42
7:a:35:HIS:NE2	8:b:14:GLU:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:31:VAL:HG23	9:c:67:VAL:HG13	2.01	0.42
9:c:125:VAL:HA	9:c:128:ASN:HD21	1.82	0.42
9:c:241:ASN:O	9:c:245:VAL:HG23	2.19	0.42
10:d:54:ILE:O	10:d:57:ILE:HG22	2.20	0.42
10:d:184:LYS:HB2	10:d:186:TYR:CE2	2.54	0.42
12:A:24:ALA:O	12:A:25:LEU:HD13	2.19	0.42
12:A:428:ARG:NH2	21:J:20:GLU:O	2.46	0.42
15:D:384:MET:SD	16:E:164:ILE:HG21	2.59	0.42
16:E:64:LEU:HD21	16:E:70:ILE:HB	2.00	0.42
16:E:122:MET:O	16:E:196:LEU:HA	2.19	0.42
16:E:238:ILE:HA	16:E:241:ARG:HD3	2.01	0.42
17:F:43:GLN:HG2	17:F:46:ARG:NH2	2.34	0.42
17:F:66:LEU:HD23	17:F:66:LEU:C	2.43	0.42
17:F:154:ASN:HB3	17:F:159:LEU:H	1.84	0.42
22:K:201:ILE:O	22:K:205:VAL:HG22	2.19	0.42
20:i:38:LEU:HD23	20:i:160:LYS:HG3	2.00	0.42
22:k:175:GLU:OE1	22:k:176:GLY:N	2.52	0.42
33:x:353:LEU:H	33:x:353:LEU:HD12	1.84	0.42
1:U:377:HIS:CE1	1:U:384:GLN:HE22	2.37	0.42
1:U:443:LEU:HD23	1:U:477:GLY:HA2	2.01	0.42
1:U:772:TRP:HD1	1:U:775:LEU:HG	1.84	0.42
1:U:842:LYS:NZ	33:x:243:PRO:HD3	2.34	0.42
3:W:33:LYS:HA	3:W:36:LYS:HG3	2.00	0.42
3:W:312:MET:HE2	3:W:312:MET:H	1.85	0.42
4:X:43:VAL:O	4:X:47:GLU:HB2	2.19	0.42
4:X:317:PRO:C	4:X:319:ILE:H	2.26	0.42
4:X:345:VAL:HG22	4:X:349:HIS:CE1	2.54	0.42
4:X:380:GLN:OE1	5:Y:314:LEU:CD2	2.68	0.42
5:Y:125:ARG:NH2	5:Y:156:LEU:HD11	2.34	0.42
7:a:61:GLU:OE1	7:a:79:ILE:HD13	2.20	0.42
7:a:74:LEU:HD13	7:a:74:LEU:HA	1.79	0.42
7:a:194:GLN:HB3	7:a:225:LEU:HD12	2.02	0.42
7:a:231:GLN:O	7:a:234:ILE:CD1	2.67	0.42
7:a:363:MET:HE1	9:c:304:LEU:HA	2.00	0.42
9:c:196:LEU:C	9:c:196:LEU:HD13	2.43	0.42
13:B:103:ARG:NH2	13:B:160:ILE:O	2.52	0.42
16:E:356:ARG:HB2	16:E:357:ALA:H	1.72	0.42
17:F:383:GLU:HA	17:F:386:ARG:HG2	2.01	0.42
18:G:131:MET:HG3	24:M:124:LEU:HB3	2.01	0.42
20:I:4:ARG:NE	20:I:4:ARG:HA	2.34	0.42
21:J:244:GLN:HA	21:J:248:SER:C	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:N:14:LEU:HD23	25:N:44:CYS:SG	2.59	0.42
19:h:166:ASN:ND2	19:h:198:SER:OG	2.52	0.42
32:f:411:ASP:OD1	32:f:411:ASP:N	2.50	0.42
1:U:615:ARG:O	1:U:619:VAL:HG12	2.19	0.42
1:U:751:ARG:N	1:U:751:ARG:HD2	2.35	0.42
2:V:68:ASP:O	2:V:72:LEU:N	2.52	0.42
2:V:391:THR:OG1	2:V:397:ARG:NH2	2.51	0.42
2:V:452:ASN:HB3	2:V:457:TYR:HB2	2.00	0.42
3:W:186:ILE:HD13	3:W:189:GLN:NE2	2.34	0.42
3:W:431:LYS:HZ1	3:W:432:LEU:N	2.17	0.42
4:X:136:LEU:HD12	4:X:137:TYR:N	2.35	0.42
5:Y:78:GLU:O	5:Y:82:LYS:HB2	2.18	0.42
5:Y:121:LEU:HB3	5:Y:125:ARG:HH12	1.84	0.42
8:b:56:ASN:OD1	8:b:56:ASN:C	2.63	0.42
8:b:124:LEU:HD13	8:b:156:PHE:HB2	2.00	0.42
11:e:59:GLU:O	11:e:63:HIS:HB2	2.20	0.42
13:B:105:THR:HG22	13:B:106:PRO:HD3	2.01	0.42
13:B:193:GLN:HG3	13:B:351:ILE:CG2	2.50	0.42
15:D:132:LEU:HA	15:D:138:ALA:O	2.19	0.42
16:E:180:LYS:HD3	16:E:278:ALA:O	2.20	0.42
16:E:283:ASP:O	16:E:285:LEU:CD1	2.68	0.42
16:E:362:VAL:CG1	16:E:367:PHE:HZ	2.32	0.42
25:n:30:VAL:HG23	25:n:30:VAL:O	2.18	0.42
25:n:184:VAL:C	25:n:185:GLU:OE2	2.60	0.42
31:t:86:ARG:HE	31:t:86:ARG:HB2	1.70	0.42
1:U:188:MET:SD	1:U:188:MET:C	3.03	0.42
1:U:247:GLN:HG2	1:U:913:ILE:HG13	2.01	0.42
1:U:901:GLN:O	1:U:915:LYS:HB2	2.19	0.42
2:V:32:PRO:O	2:V:36:GLU:HG3	2.20	0.42
4:X:73:VAL:O	4:X:77:LEU:HD23	2.20	0.42
4:X:266:ASP:O	4:X:269:ALA:N	2.45	0.42
5:Y:124:PHE:HA	5:Y:127:THR:HG22	2.01	0.42
13:B:95:GLU:O	13:B:99:VAL:HG22	2.19	0.42
13:B:356:PRO:HB3	13:B:360:THR:HG23	2.01	0.42
14:C:214:VAL:HG21	14:C:248:MET:HE3	2.01	0.42
15:D:133:HIS:CD2	15:D:134:LYS:H	2.38	0.42
16:E:285:LEU:HD12	16:E:285:LEU:N	2.34	0.42
16:E:329:GLU:CG	16:E:333:LYS:NZ	2.76	0.42
20:I:174:MET:HE1	20:I:199:LYS:HG2	2.00	0.42
39:O:301:LDZ:O34	39:O:301:LDZ:H27	2.19	0.42
27:P:26:ARG:HD3	27:P:186:ILE:HB	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:S:169:ASP:OD2	30:S:173:ARG:NH1	2.51	0.42
23:l:119:PRO:HB3	23:l:125:ARG:HG3	2.00	0.42
27:p:47:ASP:OD2	27:p:47:ASP:N	2.51	0.42
28:q:74:GLU:HG2	28:q:75:LEU:N	2.35	0.42
33:x:727:PHE:O	33:x:731:MET:HG2	2.19	0.42
1:U:260:PHE:O	1:U:264:VAL:HG13	2.19	0.42
1:U:623:GLY:O	1:U:627:PHE:HB3	2.20	0.42
2:V:224:LEU:HB3	2:V:257:ASN:CG	2.44	0.42
3:W:35:ALA:HB2	3:W:52:LYS:HZ1	1.83	0.42
3:W:112:VAL:HA	3:W:115:ILE:HB	2.02	0.42
3:W:166:LEU:HD11	3:W:201:ARG:HD2	2.00	0.42
4:X:131:ALA:O	4:X:134:VAL:HG22	2.20	0.42
4:X:267:VAL:HG21	4:X:291:ALA:HB1	2.02	0.42
5:Y:328:GLU:H	5:Y:328:GLU:CD	2.27	0.42
7:a:291:LEU:HD12	7:a:295:GLU:OE1	2.18	0.42
10:d:12:LYS:HZ2	10:d:14:PRO:HB3	1.75	0.42
13:B:78:PHE:C	13:B:78:PHE:HD2	2.25	0.42
15:D:410:ASP:O	15:D:412:GLN:N	2.52	0.42
16:E:182:LEU:HD11	38:E:401:ADP:H3'	2.02	0.42
16:E:371:VAL:O	16:E:372:ARG:C	2.62	0.42
17:F:97:LEU:HD22	17:F:98:ASP:N	2.35	0.42
17:F:294:LYS:HE2	17:F:294:LYS:HB2	1.82	0.42
28:q:19:ARG:HB2	28:q:177:THR:HG23	2.01	0.42
33:x:419:LEU:CD2	33:x:420:TRP:CD2	3.03	0.42
33:x:594:LEU:HD12	33:x:595:VAL:N	2.34	0.42
1:U:439:GLU:HG3	1:U:440:GLY:N	2.34	0.42
2:V:66:GLU:HB2	2:V:205:LEU:HD22	2.00	0.42
2:V:338:LEU:HD22	2:V:397:ARG:HB2	2.02	0.42
4:X:233:TYR:O	4:X:237:GLU:HG3	2.20	0.42
8:b:147:GLU:O	8:b:150:THR:HG23	2.20	0.42
9:c:75:MET:HE3	9:c:88:ASP:H	1.80	0.42
13:B:222:VAL:HG22	13:B:349:ARG:HB2	2.01	0.42
14:C:149:GLU:H	14:C:149:GLU:HG3	1.72	0.42
15:D:153:MET:O	15:D:154:LEU:C	2.62	0.42
16:E:226:GLN:HG3	16:E:273:VAL:HG23	2.01	0.42
16:E:230:ILE:HG12	16:E:273:VAL:HG22	2.02	0.42
19:H:29:VAL:HG11	19:H:133:SER:HB3	2.01	0.42
19:H:182:LEU:HD13	19:H:186:ASP:CB	2.50	0.42
20:I:95:GLN:HG3	27:P:73:LEU:HG	2.01	0.42
28:Q:101:ASN:HB3	28:Q:132:HIS:CE1	2.55	0.42
39:R:301:LDZ:H33	39:R:301:LDZ:H11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:g:209:ASP:OD2	18:g:209:ASP:C	2.63	0.42
21:j:11:SER:O	21:j:14:GLY:N	2.49	0.42
22:k:121:LEU:HD11	23:l:79:ALA:CA	2.49	0.42
31:t:177:TYR:HE2	31:t:207:THR:HG21	1.85	0.42
33:x:394:ASP:OD1	33:x:394:ASP:N	2.53	0.42
33:x:899:ILE:C	33:x:900:LEU:HG	2.45	0.42
1:U:14:GLU:HB3	1:U:19:LEU:HD11	2.02	0.42
2:V:421:ASP:HA	2:V:424:GLN:OE1	2.19	0.42
2:V:484:LEU:HD13	10:d:252:GLN:HG2	2.02	0.42
3:W:231:ILE:C	3:W:233:LEU:H	2.28	0.42
5:Y:88:LEU:HD23	5:Y:99:GLU:OE2	2.19	0.42
6:Z:120:VAL:HA	6:Z:139:ILE:CD1	2.50	0.42
6:Z:219:LYS:HD3	6:Z:220:LEU:HD23	2.00	0.42
7:a:41:VAL:HG12	7:a:79:ILE:HD11	2.01	0.42
7:a:280:MET:O	7:a:283:THR:HG22	2.19	0.42
7:a:321:LYS:HE3	7:a:336:VAL:HG21	2.02	0.42
12:A:110:LYS:HZ2	17:F:165:PRO:HD3	1.85	0.42
13:B:165:ASP:HB3	13:B:166:ASP:H	1.69	0.42
13:B:342:ILE:H	13:B:342:ILE:HG13	1.72	0.42
15:D:215:LEU:O	15:D:219:VAL:HG23	2.19	0.42
25:N:148:THR:OG1	25:N:151:GLU:HG3	2.20	0.42
26:O:163:ILE:HG12	26:O:169:SER:CB	2.49	0.42
25:n:98:ILE:H	25:n:98:ILE:HG12	1.70	0.42
26:o:19:ARG:CB	26:o:169:SER:HA	2.50	0.42
30:s:28:ARG:NE	30:s:191:ASP:OD1	2.50	0.42
31:t:59:ASP:HB3	31:t:106:LEU:HD22	2.01	0.42
33:x:70:LEU:C	33:x:73:PRO:HD2	2.44	0.42
1:U:500:ASN:O	1:U:503:GLN:CG	2.67	0.42
1:U:794:ASP:OD1	1:U:794:ASP:N	2.51	0.42
2:V:212:TYR:HB3	11:e:4:LYS:CE	2.50	0.42
2:V:243:ASP:OD2	2:V:247:GLN:HB3	2.20	0.42
2:V:269:LYS:CE	2:V:295:ILE:HB	2.50	0.42
2:V:336:GLU:CD	2:V:341:GLU:O	2.63	0.42
3:W:87:ILE:HB	3:W:91:SER:HB3	2.02	0.42
3:W:134:GLY:C	3:W:136:ILE:H	2.28	0.42
3:W:251:TYR:CZ	3:W:267:LEU:HD23	2.54	0.42
3:W:322:GLU:H	3:W:322:GLU:HG2	1.56	0.42
5:Y:228:MET:HE1	5:Y:259:TYR:CE1	2.54	0.42
7:a:82:HIS:O	7:a:85:ARG:HG2	2.20	0.42
7:a:169:HIS:HA	7:a:172:TYR:HB3	2.01	0.42
8:b:76:HIS:CE1	17:F:61:ARG:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:41:MET:HG2	9:c:112:TYR:CD2	2.54	0.42
10:d:97:GLN:O	10:d:101:LEU:HG	2.20	0.42
10:d:205:LYS:CB	10:d:209:TYR:CD2	2.94	0.42
10:d:217:LEU:HD11	10:d:220:ASN:HA	2.00	0.42
12:A:125:LEU:HD13	12:A:129:VAL:O	2.20	0.42
12:A:339:ARG:HH22	17:F:405:MET:CE	2.33	0.42
13:B:85:MET:HE1	33:x:619:HIS:CA	2.45	0.42
14:C:84:LYS:HD3	14:C:84:LYS:HA	1.79	0.42
14:C:273:MET:HE2	14:C:277:LEU:HD11	2.02	0.42
15:D:45:LYS:O	15:D:49:GLN:HG3	2.18	0.42
39:N:301:LDZ:H19	39:N:301:LDZ:H13	1.76	0.42
30:s:1:ARG:HB2	30:s:2:PHE:H	1.63	0.42
33:x:181:ARG:NH2	33:x:213:GLN:HE22	2.16	0.42
1:U:688:LEU:HD22	1:U:709:PHE:CZ	2.55	0.42
1:U:900:TYR:HB3	1:U:914:LEU:HD21	2.02	0.42
2:V:162:GLU:HG2	2:V:171:VAL:HG22	2.02	0.42
2:V:385:LYS:HD2	2:V:385:LYS:HA	1.81	0.42
2:V:403:ILE:HD12	2:V:404:LYS:N	2.35	0.42
2:V:430:SER:HB2	2:V:433:ASP:CG	2.45	0.42
3:W:297:GLU:HA	3:W:302:TYR:HD2	1.85	0.42
3:W:406:VAL:HG23	3:W:413:ILE:HG22	2.02	0.42
4:X:103:THR:HG22	4:X:107:VAL:HG13	2.02	0.42
4:X:338:VAL:HG11	4:X:353:LEU:HD13	2.02	0.42
4:X:344:ARG:HB3	4:X:386:ILE:HG22	2.01	0.42
5:Y:143:TYR:HA	5:Y:146:ARG:CD	2.50	0.42
5:Y:203:ASP:OD2	5:Y:203:ASP:N	2.53	0.42
6:Z:53:SER:HB3	6:Z:95:TYR:CZ	2.55	0.42
9:c:137:SER:C	9:c:139:ARG:H	2.27	0.42
10:d:142:TYR:CD1	10:d:142:TYR:N	2.88	0.42
13:B:189:GLY:HA3	13:B:360:THR:OG1	2.20	0.42
15:D:384:MET:HE1	16:E:159:PHE:CZ	2.55	0.42
16:E:13:ARG:NH1	17:F:29:ILE:HG12	2.34	0.42
16:E:165:ILE:H	16:E:165:ILE:HG13	1.66	0.42
17:F:333:ASN:OD1	17:F:333:ASN:N	2.42	0.42
19:h:106:PRO:HG2	19:h:109:GLN:HG2	2.02	0.42
19:h:148:GLN:O	19:h:155:TYR:HA	2.19	0.42
30:s:169:ASP:OD1	30:s:173:ARG:NH1	2.53	0.42
31:t:92:LEU:HD21	31:t:110:MET:SD	2.60	0.42
32:f:417:HIS:CE1	32:f:418:TRP:HE3	2.38	0.42
33:x:335:ARG:CB	33:x:340:MET:HE2	2.40	0.42
33:x:618:GLU:OE2	33:x:620:PHE:CE2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:182:LYS:HA	1:U:185:MET:HG3	2.01	0.41
2:V:35:VAL:HA	2:V:38:LYS:HE2	2.02	0.41
2:V:231:LEU:HD12	2:V:231:LEU:HA	1.83	0.41
3:W:22:ALA:O	3:W:26:GLN:HB2	2.19	0.41
3:W:220:GLU:HG2	3:W:256:ILE:HG22	2.02	0.41
3:W:251:TYR:CE1	3:W:267:LEU:HA	2.54	0.41
3:W:279:PHE:HB3	3:W:364:ARG:HH12	1.85	0.41
3:W:326:MET:H	3:W:326:MET:HG3	1.73	0.41
3:W:409:LEU:HB3	4:X:344:ARG:CD	2.50	0.41
5:Y:49:ASN:OD1	5:Y:52:PRO:HD2	2.20	0.41
5:Y:250:LEU:HD13	5:Y:250:LEU:HA	1.71	0.41
6:Z:67:VAL:HG22	8:b:92:VAL:CG2	2.46	0.41
7:a:310:LEU:HD12	7:a:311:VAL:N	2.35	0.41
9:c:309:PHE:O	9:c:309:PHE:CD2	2.67	0.41
10:d:141:GLN:HA	10:d:144:MET:HG2	2.02	0.41
13:B:69:LYS:HE3	13:B:73:LEU:HD21	2.02	0.41
14:C:72:TYR:O	14:C:115:ALA:HA	2.19	0.41
14:C:138:MET:CE	14:C:214:VAL:HG22	2.50	0.41
14:C:142:LYS:HB3	14:C:142:LYS:HE2	1.91	0.41
16:E:158:LEU:O	16:E:161:ARG:NE	2.53	0.41
17:F:279:ALA:HB1	17:F:280:PRO:HD2	2.02	0.41
19:H:107:THR:O	19:H:111:VAL:HG23	2.20	0.41
19:H:182:LEU:HD23	19:H:182:LEU:HA	1.72	0.41
23:L:88:MET:HG2	23:L:112:ILE:HD11	2.02	0.41
21:j:100:ASP:OD1	29:r:107:ARG:NH2	2.43	0.41
25:n:19:ARG:HE	25:n:19:ARG:HB2	1.67	0.41
39:n:301:LDZ:H26	39:n:301:LDZ:N10	2.35	0.41
2:V:193:GLN:HG2	14:C:26:SER:HA	2.01	0.41
2:V:211:TYR:HD1	2:V:211:TYR:HA	1.65	0.41
3:W:46:THR:O	3:W:50:LEU:HD22	2.20	0.41
3:W:82:LEU:HD22	3:W:86:ASN:OD1	2.20	0.41
3:W:142:ARG:CZ	3:W:146:THR:HG21	2.48	0.41
3:W:406:VAL:HA	3:W:413:ILE:HG22	2.02	0.41
4:X:105:GLN:HG3	4:X:108:GLU:CG	2.50	0.41
4:X:363:ARG:HB3	4:X:363:ARG:NH1	2.35	0.41
4:X:408:SER:OG	5:Y:376:LEU:HD11	2.20	0.41
5:Y:173:ASP:C	5:Y:175:ASP:H	2.28	0.41
6:Z:201:LEU:O	6:Z:205:LEU:HD12	2.20	0.41
7:a:310:LEU:HD12	7:a:311:VAL:HG13	2.02	0.41
10:d:8:GLU:HG2	10:d:18:LYS:HE3	2.02	0.41
14:C:92:GLU:OE2	14:C:92:GLU:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:145:LEU:HD12	16:E:145:LEU:O	2.20	0.41
16:E:313:LEU:HD13	16:E:328:TYR:HD1	1.84	0.41
17:F:169:ASP:OD1	17:F:170:SER:N	2.53	0.41
25:N:190:LEU:HD12	25:N:190:LEU:N	2.35	0.41
26:O:24:MET:HG2	30:s:188:TYR:HE2	1.85	0.41
18:g:73:THR:HG22	18:g:74:GLU:N	2.35	0.41
20:i:241:GLU:O	20:i:244:GLU:HG2	2.20	0.41
33:x:180:GLN:O	33:x:183:PRO:HD2	2.19	0.41
33:x:258:LYS:HB3	33:x:258:LYS:HE2	1.81	0.41
33:x:472:HIS:O	33:x:478:ARG:NE	2.24	0.41
33:x:740:ARG:HD2	33:x:741:LEU:N	2.32	0.41
33:x:766:GLN:O	33:x:769:THR:OG1	2.38	0.41
1:U:469:SER:HB3	1:U:473:VAL:HG21	2.02	0.41
1:U:529:ILE:O	1:U:533:VAL:HG22	2.20	0.41
1:U:643:SER:OG	1:U:648:VAL:HB	2.20	0.41
2:V:295:ILE:CD1	2:V:299:GLN:NE2	2.84	0.41
2:V:419:LEU:HD21	2:V:456:GLY:HA2	2.02	0.41
2:V:433:ASP:OD1	2:V:434:ALA:N	2.52	0.41
2:V:476:PHE:HD2	6:Z:256:GLN:NE2	2.18	0.41
3:W:89:LEU:O	3:W:91:SER:N	2.53	0.41
5:Y:88:LEU:HD21	5:Y:99:GLU:OE2	2.10	0.41
6:Z:136:GLU:OE1	6:Z:137:ALA:N	2.53	0.41
6:Z:186:THR:HG22	9:c:293:THR:CB	2.51	0.41
6:Z:194:GLN:NE2	9:c:301:ALA:HB2	2.35	0.41
8:b:124:LEU:HD21	8:b:152:LYS:HB2	2.01	0.41
9:c:30:GLN:HG3	9:c:32:TYR:CE1	2.54	0.41
10:d:190:LEU:CD1	10:d:193:GLU:H	2.32	0.41
12:A:303:ILE:HD13	12:A:303:ILE:HA	1.87	0.41
12:A:337:LEU:HD23	12:A:337:LEU:HA	1.90	0.41
13:B:211:TYR:CD2	13:B:211:TYR:N	2.88	0.41
14:C:43:ARG:O	14:C:46:GLN:HG3	2.20	0.41
14:C:187:LEU:HD23	14:C:314:LYS:HG2	2.03	0.41
15:D:170:MET:HB2	15:D:174:LYS:HG3	2.01	0.41
16:E:143:ARG:NH2	16:E:146:ARG:HD2	2.36	0.41
17:F:146:LYS:N	17:F:149:ASP:OD2	2.53	0.41
19:H:69:THR:HG23	19:H:71:HIS:H	1.85	0.41
24:M:88:ALA:O	24:M:92:ARG:HG3	2.19	0.41
24:M:202:ASP:HB2	24:M:209:PHE:CE2	2.56	0.41
19:h:74:LEU:HD23	19:h:83:TYR:CE1	2.52	0.41
20:i:49:ARG:NH1	20:i:58:GLU:OE1	2.53	0.41
23:l:14:SER:HB3	23:l:18:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:o:301:LDZ:O33	39:o:301:LDZ:H33	2.21	0.41
33:x:50:LYS:HD2	33:x:50:LYS:HA	1.85	0.41
33:x:593:THR:HA	33:x:596:ASP:OD2	2.21	0.41
2:V:73:GLU:O	2:V:77:GLU:HG3	2.21	0.41
2:V:148:ARG:HG2	2:V:149:PRO:HD3	2.02	0.41
2:V:159:LEU:CB	2:V:209:LYS:NZ	2.82	0.41
2:V:186:LYS:NZ	2:V:207:ALA:HB2	2.35	0.41
2:V:326:GLN:HA	2:V:329:HIS:ND1	2.36	0.41
3:W:131:VAL:O	3:W:133:GLU:N	2.47	0.41
3:W:442:THR:HA	3:W:445:LEU:HD23	2.02	0.41
4:X:399:ALA:HB1	9:c:245:VAL:HG12	2.02	0.41
6:Z:26:ILE:HD12	6:Z:30:GLY:HA2	2.03	0.41
6:Z:121:LEU:HG	6:Z:138:TYR:HB2	2.02	0.41
6:Z:185:GLY:O	6:Z:186:THR:CB	2.67	0.41
7:a:280:MET:HA	7:a:283:THR:HG22	2.02	0.41
7:a:333:MET:HE2	7:a:335:TRP:N	2.35	0.41
9:c:52:GLU:HG3	9:c:114:SER:O	2.20	0.41
10:d:55:LEU:HD12	10:d:81:TYR:CE2	2.55	0.41
10:d:203:PRO:HG2	10:d:206:MET:HB2	2.02	0.41
10:d:242:LEU:HA	10:d:245:GLN:OE1	2.19	0.41
14:C:32:GLN:CD	15:D:47:LEU:HD21	2.45	0.41
14:C:143:VAL:HG13	14:C:144:PRO:O	2.21	0.41
15:D:172:ILE:H	15:D:172:ILE:HG13	1.66	0.41
16:E:40:TYR:O	16:E:43:SER:OG	2.38	0.41
16:E:261:LEU:CD1	16:E:264:MET:SD	3.08	0.41
16:E:263:GLN:O	16:E:268:ASP:HB2	2.20	0.41
23:L:74:ILE:HG22	23:L:132:LEU:HD23	2.03	0.41
20:i:65:ILE:HG13	20:i:212:GLU:OE2	2.20	0.41
21:j:177:THR:CG2	21:j:179:GLU:HG2	2.39	0.41
24:m:229:LYS:NZ	24:m:236:GLU:OE2	2.54	0.41
26:o:190:THR:HG22	26:o:192:PRO:HD3	2.02	0.41
33:x:230:CYS:HB2	33:x:256:PHE:HE2	1.85	0.41
33:x:485:LEU:HD12	33:x:501:LEU:HD21	2.02	0.41
33:x:576:ILE:H	33:x:576:ILE:HD12	1.85	0.41
1:U:567:ILE:HG22	1:U:601:ARG:NH2	2.36	0.41
1:U:619:VAL:HA	1:U:622:LEU:CD1	2.51	0.41
1:U:724:VAL:HA	1:U:727:LYS:HG2	2.02	0.41
1:U:758:PRO:HB3	1:U:781:LEU:HD11	2.02	0.41
1:U:862:LYS:O	1:U:863:GLU:HG2	2.21	0.41
2:V:215:ALA:HA	2:V:224:LEU:HD13	2.02	0.41
2:V:259:LEU:HD21	2:V:294:ARG:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:56:THR:HG22	3:W:104:MET:HE2	2.03	0.41
3:W:326:MET:HB2	3:W:330:LYS:O	2.21	0.41
3:W:366:MET:SD	3:W:366:MET:C	3.04	0.41
5:Y:51:ALA:HA	5:Y:54:TYR:CE2	2.56	0.41
7:a:249:GLN:O	7:a:253:THR:OG1	2.28	0.41
7:a:314:ALA:HB1	7:a:319:LEU:HD21	2.02	0.41
9:c:305:ASP:HA	9:c:308:VAL:HG12	2.01	0.41
12:A:339:ARG:HH22	17:F:405:MET:HE3	1.85	0.41
14:C:21:ARG:O	14:C:24:TYR:HB2	2.20	0.41
15:D:84:SER:C	15:D:85:ILE:HG12	2.44	0.41
15:D:231:VAL:HG23	15:D:234:GLU:HB2	2.00	0.41
15:D:280:GLY:C	15:D:282:ASP:H	2.28	0.41
16:E:113:ARG:NH2	16:E:115:VAL:O	2.47	0.41
17:F:314:LEU:HD21	17:F:347:ARG:NH2	2.35	0.41
19:H:106:PRO:HG2	19:H:109:GLN:HG3	2.02	0.41
26:O:112:SER:O	26:O:119:THR:HA	2.20	0.41
30:S:13:LEU:HD11	30:S:149:LEU:HD11	2.01	0.41
19:h:103:GLU:HG2	19:h:104:PRO:HD2	2.03	0.41
19:h:199:PHE:CE1	19:h:203:MET:HG2	2.56	0.41
22:k:10:ARG:HD3	23:l:124:GLY:O	2.21	0.41
22:k:72:ALA:HB1	22:k:225:ASN:ND2	2.34	0.41
28:q:161:ARG:HB3	28:q:161:ARG:HH11	1.84	0.41
30:s:83:MET:HE3	30:s:87:ALA:HB1	2.02	0.41
33:x:372:LEU:HD11	33:x:409:SER:HB2	2.02	0.41
33:x:776:LEU:HD12	33:x:776:LEU:HA	1.88	0.41
1:U:460:TYR:HA	1:U:463:ASN:ND2	2.35	0.41
1:U:848:LYS:HA	1:U:851:GLU:OE2	2.21	0.41
2:V:65:ARG:HE	2:V:153:LYS:HE3	1.86	0.41
3:W:68:VAL:O	3:W:71:VAL:HG12	2.21	0.41
3:W:264:GLN:O	3:W:268:LYS:NZ	2.53	0.41
3:W:453:HIS:NE2	6:Z:221:PRO:HD2	2.36	0.41
4:X:122:ARG:HD2	4:X:122:ARG:HA	1.73	0.41
4:X:133:LEU:CD1	4:X:136:LEU:HD11	2.50	0.41
4:X:230:SER:HB2	15:D:339:ARG:HG3	2.02	0.41
5:Y:221:THR:O	5:Y:224:VAL:HG12	2.20	0.41
5:Y:374:ASP:HA	5:Y:377:LEU:HB2	2.02	0.41
6:Z:54:PHE:CD1	6:Z:54:PHE:C	2.99	0.41
7:a:328:ASP:O	7:a:329:LYS:HB2	2.19	0.41
12:A:78:TRP:CE3	13:B:138:PHE:HB3	2.55	0.41
12:A:83:ASP:C	12:A:85:GLN:N	2.79	0.41
12:A:213:LEU:HD11	12:A:321:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:422:LYS:HE3	12:A:422:LYS:HB2	1.89	0.41
13:B:153:ASN:HD21	13:B:156:VAL:H	1.68	0.41
13:B:214:MET:HE2	13:B:214:MET:HB2	1.84	0.41
16:E:152:PRO:HG2	16:E:167:PRO:CD	2.50	0.41
16:E:159:PHE:CE2	16:E:167:PRO:HD3	2.50	0.41
16:E:362:VAL:HG12	16:E:367:PHE:CZ	2.56	0.41
16:E:363:VAL:CG1	16:E:365:GLU:CD	2.93	0.41
19:H:59:GLU:H	19:H:59:GLU:HG2	1.67	0.41
21:J:96:LEU:HA	21:J:96:LEU:HD12	1.85	0.41
25:N:140:ASP:OD1	25:n:166:ARG:NH1	2.54	0.41
26:O:18:THR:OG1	26:O:172:ASN:HB2	2.20	0.41
29:R:37:ILE:O	29:R:38:ASN:O	2.38	0.41
31:T:92:LEU:HD23	31:T:92:LEU:HA	1.90	0.41
18:g:182:LYS:HD2	18:g:182:LYS:HA	1.76	0.41
21:j:48:LYS:H	21:j:205:ASN:HB3	1.85	0.41
22:k:63:SER:O	22:k:63:SER:OG	2.35	0.41
25:n:71:ASN:O	25:n:71:ASN:ND2	2.54	0.41
39:n:301:LDZ:H22	39:n:301:LDZ:H13	1.90	0.41
33:x:63:LEU:CD1	33:x:109:ILE:HG21	2.51	0.41
33:x:535:THR:O	33:x:538:ILE:HG13	2.21	0.41
33:x:704:LEU:HD23	33:x:704:LEU:HA	1.91	0.41
33:x:768:LEU:O	33:x:768:LEU:HD23	2.20	0.41
1:U:7:GLY:HA3	10:d:80:CYS:SG	2.60	0.41
1:U:500:ASN:O	1:U:503:GLN:HG2	2.21	0.41
1:U:666:LYS:HA	1:U:669:ILE:HG13	2.03	0.41
1:U:804:SER:OG	1:U:805:ASN:N	2.53	0.41
2:V:89:LYS:HA	2:V:89:LYS:HD3	1.91	0.41
2:V:343:PRO:O	2:V:345:ARG:NH1	2.54	0.41
3:W:203:GLN:CD	3:W:233:LEU:HD21	2.46	0.41
3:W:215:GLN:HE22	3:W:222:LEU:HD12	1.86	0.41
3:W:268:LYS:HG2	3:W:299:ILE:HG21	2.02	0.41
3:W:338:THR:HA	3:W:341:PHE:O	2.20	0.41
4:X:297:ARG:HE	4:X:297:ARG:HB2	1.81	0.41
5:Y:55:GLU:OE1	5:Y:55:GLU:N	2.33	0.41
6:Z:39:LEU:HB2	6:Z:95:TYR:CD2	2.53	0.41
6:Z:125:ASP:HB3	6:Z:128:PRO:HD2	2.02	0.41
7:a:108:ASP:O	7:a:111:VAL:HG12	2.20	0.41
9:c:173:GLU:OE1	9:c:201:TYR:HB2	2.20	0.41
9:c:192:LEU:HA	9:c:196:LEU:HB3	2.03	0.41
12:A:114:ASN:CB	12:A:120:LYS:HG2	2.45	0.41
13:B:319:PHE:O	13:B:320:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:251:ILE:HD12	14:C:251:ILE:HA	1.91	0.41
16:E:168:LYS:HD2	16:E:264:MET:CE	2.48	0.41
16:E:235:ILE:O	16:E:277:MET:CE	2.69	0.41
16:E:252:GLU:HG3	16:E:255:ARG:NH2	2.36	0.41
20:I:62:SER:OG	20:I:65:ILE:O	2.39	0.41
26:O:159:ILE:HG21	26:O:173:ILE:HG23	2.02	0.41
30:S:211:ARG:HH21	26:o:193:ASN:HB3	1.85	0.41
19:h:177:ARG:O	19:h:177:ARG:HG3	2.20	0.41
20:i:161:ALA:HB1	20:i:175:LEU:HD13	2.03	0.41
24:m:62:SER:O	24:m:63:ASN:C	2.63	0.41
24:m:90:ILE:HD13	24:m:90:ILE:HA	1.83	0.41
30:s:57:PHE:HD2	30:s:60:ASP:OD1	2.04	0.41
30:s:145:LEU:HD22	30:s:178:VAL:HB	2.02	0.41
33:x:783:SER:HB3	33:x:787:LEU:HD23	2.02	0.41
1:U:142:LEU:HA	1:U:147:TYR:OH	2.19	0.41
1:U:572:ARG:HH22	1:U:601:ARG:HH21	1.68	0.41
1:U:697:GLN:OE1	1:U:742:HIS:HA	2.21	0.41
2:V:65:ARG:CZ	2:V:205:LEU:HD21	2.51	0.41
2:V:266:GLN:HB3	2:V:299:GLN:HE22	1.84	0.41
2:V:339:LEU:HD23	2:V:339:LEU:HA	1.89	0.41
2:V:438:VAL:HG12	2:V:442:ILE:HD11	2.03	0.41
3:W:48:LEU:HB3	3:W:52:LYS:NZ	2.35	0.41
3:W:52:LYS:HD3	3:W:52:LYS:N	2.35	0.41
3:W:65:ARG:H	3:W:65:ARG:HG2	1.59	0.41
3:W:210:ASN:OD1	3:W:210:ASN:N	2.53	0.41
3:W:432:LEU:HB3	3:W:436:MET:CE	2.45	0.41
4:X:258:LYS:HD2	4:X:258:LYS:HA	1.91	0.41
5:Y:12:PRO:C	5:Y:13:LYS:HD2	2.46	0.41
7:a:320:VAL:CG2	7:a:333:MET:HB2	2.49	0.41
9:c:75:MET:HG2	9:c:87:VAL:HA	2.02	0.41
9:c:184:LEU:O	9:c:186:LYS:HD2	2.21	0.41
10:d:52:ARG:C	10:d:52:ARG:CD	2.90	0.41
10:d:174:ILE:O	10:d:178:ILE:HG12	2.20	0.41
12:A:56:LEU:HD22	13:B:48:LYS:HZ1	1.83	0.41
12:A:116:LYS:HA	12:A:116:LYS:CE	2.49	0.41
12:A:256:MET:HE2	12:A:256:MET:HB3	1.76	0.41
12:A:258:ARG:NH1	12:A:301:GLU:OE2	2.54	0.41
14:C:132:ASP:HB2	14:C:233:GLU:OE1	2.20	0.41
14:C:391:MET:HE3	14:C:391:MET:HB3	1.77	0.41
15:D:387:VAL:HG21	16:E:159:PHE:CE1	2.55	0.41
16:E:320:ILE:CG1	16:E:347:CYS:SG	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:356:ARG:NH2	17:F:200:GLU:OE1	2.54	0.41
21:J:7:ILE:HD11	21:J:121:SER:O	2.21	0.41
22:K:159:SER:OG	22:K:161:THR:HG23	2.20	0.41
26:O:35:HIS:HB2	26:O:56:THR:HG21	2.03	0.41
26:O:162:GLY:O	26:O:165:ASN:ND2	2.54	0.41
30:S:187:VAL:CG2	26:o:24:MET:SD	3.08	0.41
23:l:49:LEU:HB2	23:l:195:LEU:HD21	2.03	0.41
33:x:211:ILE:HG13	33:x:211:ILE:H	1.78	0.41
33:x:502:LEU:HD23	33:x:502:LEU:HA	1.93	0.41
1:U:44:LYS:HE2	1:U:44:LYS:HB3	1.88	0.41
1:U:231:ASP:HA	1:U:234:GLU:OE1	2.21	0.41
1:U:392:TRP:CD1	1:U:392:TRP:C	2.99	0.41
1:U:450:HIS:CG	1:U:457:ILE:HD13	2.56	0.41
1:U:680:VAL:O	1:U:684:ARG:NH1	2.54	0.41
1:U:727:LYS:O	1:U:731:ILE:HG22	2.21	0.41
1:U:789:ILE:HG22	1:U:791:LEU:HG	2.01	0.41
2:V:89:LYS:HB3	2:V:93:PHE:CD2	2.56	0.41
2:V:443:ARG:NH1	10:d:184:LYS:HZ1	2.19	0.41
3:W:314:LEU:HD21	3:W:381:LEU:HD13	2.03	0.41
3:W:373:ILE:HD13	3:W:378:MET:HG2	2.03	0.41
3:W:392:PHE:O	3:W:396:LEU:HG	2.20	0.41
3:W:433:ASN:OD1	3:W:433:ASN:N	2.53	0.41
5:Y:66:ASP:O	5:Y:70:LEU:HG	2.21	0.41
5:Y:137:ARG:O	5:Y:141:VAL:HG23	2.21	0.41
5:Y:156:LEU:C	5:Y:159:ARG:H	2.28	0.41
6:Z:38:VAL:CG2	6:Z:91:ILE:HG23	2.50	0.41
6:Z:79:TYR:CE2	6:Z:91:ILE:HG13	2.55	0.41
6:Z:206:LEU:HA	6:Z:209:ARG:HG2	2.03	0.41
7:a:142:LEU:HD11	7:a:152:HIS:ND1	2.36	0.41
7:a:182:CYS:SG	7:a:183:VAL:HG22	2.61	0.41
7:a:205:LEU:HD22	7:a:240:PHE:CE2	2.56	0.41
10:d:108:SER:HB3	10:d:169:ILE:HG23	2.02	0.41
10:d:191:PHE:CZ	10:d:202:THR:N	2.82	0.41
10:d:199:PHE:HD1	10:d:200:PHE:HD2	1.68	0.41
10:d:201:ASN:N	10:d:201:ASN:OD1	2.53	0.41
12:A:143:ASP:HB3	12:A:148:GLN:N	2.33	0.41
13:B:112:LEU:HD22	13:B:145:GLU:O	2.20	0.41
13:B:153:ASN:ND2	13:B:156:VAL:H	2.18	0.41
14:C:383:PHE:O	14:C:387:VAL:HG12	2.20	0.41
16:E:30:ARG:NH2	17:F:58:GLU:OE2	2.53	0.41
16:E:62:LYS:HG2	16:E:63:GLN:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:194:ASN:ND2	16:E:230:ILE:HD12	2.36	0.41
16:E:309:ARG:O	16:E:312:ILE:HG22	2.21	0.41
19:H:6:TYR:OH	20:I:6:ASP:OD2	2.38	0.41
24:M:243:LEU:HD12	24:M:244:LYS:N	2.35	0.41
25:N:35:THR:OG1	25:N:43:CYS:SG	2.78	0.41
29:R:4:LEU:HD11	29:R:135:ALA:CB	2.49	0.41
19:h:49:GLU:HG3	19:h:199:PHE:CE2	2.56	0.41
21:j:80:ALA:O	21:j:84:ILE:HG13	2.21	0.41
25:n:70:LEU:HD23	25:n:70:LEU:HA	1.82	0.41
26:o:124:TYR:CE2	26:o:135:MET:HE1	2.55	0.41
27:p:12:MET:HE2	27:p:12:MET:HB2	1.94	0.41
27:p:131:MET:HE3	27:p:131:MET:HB3	1.85	0.41
31:t:25:ASP:OD2	31:t:25:ASP:C	2.64	0.41
33:x:252:ALA:O	33:x:255:VAL:HG22	2.21	0.41
33:x:618:GLU:CD	33:x:620:PHE:CZ	2.99	0.41
33:x:777:THR:HG22	33:x:826:GLN:O	2.21	0.41
33:x:809:ILE:HG23	33:x:814:SER:HB2	2.03	0.41
33:x:865:PHE:CD1	33:x:865:PHE:C	2.96	0.41
1:U:549:ALA:HB1	1:U:581:SER:HB2	2.02	0.41
1:U:791:LEU:O	1:U:913:ILE:HA	2.21	0.41
1:U:811:PHE:HE2	1:U:885:MET:CG	2.33	0.41
2:V:328:VAL:O	2:V:331:LEU:HG	2.21	0.41
2:V:340:GLY:HA2	2:V:405:THR:HG23	2.03	0.41
3:W:136:ILE:HA	3:W:141:GLU:O	2.21	0.41
4:X:108:GLU:OE2	4:X:108:GLU:N	2.54	0.41
5:Y:69:LEU:O	5:Y:73:MET:CE	2.58	0.41
5:Y:72:LYS:HD3	5:Y:72:LYS:HA	1.95	0.41
5:Y:94:ASN:O	5:Y:100:ILE:HG21	2.21	0.41
6:Z:94:TRP:CB	6:Z:112:MET:HE1	2.48	0.41
6:Z:278:ASN:OD1	6:Z:279:LYS:N	2.53	0.41
7:a:300:ALA:O	7:a:301:LYS:HG2	2.20	0.41
8:b:62:THR:OG1	8:b:70:ARG:HD2	2.21	0.41
10:d:1:MET:HE3	10:d:25:ARG:HH12	1.86	0.41
12:A:348:LEU:HD22	22:K:175:GLU:HG2	2.03	0.41
12:A:417:ILE:HG22	12:A:422:LYS:HG2	2.01	0.41
13:B:383:LEU:HD12	13:B:383:LEU:H	1.85	0.41
14:C:135:VAL:O	14:C:237:MET:HE1	2.19	0.41
14:C:191:PRO:O	14:C:194:THR:OG1	2.39	0.41
14:C:230:MET:HE2	14:C:230:MET:HB3	1.84	0.41
15:D:188:PHE:CE1	15:D:192:LYS:HG2	2.56	0.41
15:D:411:GLU:HB2	15:D:412:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:75:ASN:OD1	17:F:130:GLN:HG2	2.21	0.41
20:I:106:PRO:O	20:I:107:CYS:SG	2.79	0.41
21:J:13:ASP:OD1	21:J:13:ASP:N	2.47	0.41
21:J:221:ASN:HB2	21:J:224:GLU:OE1	2.21	0.41
18:g:191:PHE:HE1	18:g:219:VAL:HG21	1.86	0.41
23:l:180:MET:C	23:l:181:GLU:OE1	2.64	0.41
1:U:105:ILE:HD13	1:U:130:LEU:HD11	2.03	0.40
1:U:696:ILE:HA	1:U:737:LEU:HD12	2.03	0.40
2:V:55:THR:HB	14:C:36:ASN:ND2	2.36	0.40
2:V:148:ARG:HD3	2:V:148:ARG:H	1.86	0.40
2:V:160:LEU:HD12	2:V:160:LEU:HA	1.95	0.40
2:V:348:PHE:CD1	2:V:348:PHE:N	2.89	0.40
3:W:186:ILE:HA	3:W:189:GLN:NE2	2.36	0.40
3:W:297:GLU:HA	3:W:302:TYR:CD2	2.56	0.40
3:W:317:TRP:O	3:W:321:VAL:HG12	2.20	0.40
5:Y:82:LYS:HA	5:Y:82:LYS:HD3	1.85	0.40
5:Y:183:TYR:HA	5:Y:186:LEU:HD13	2.03	0.40
5:Y:347:ILE:HG13	5:Y:354:VAL:HG22	2.02	0.40
6:Z:21:ASP:O	6:Z:25:ARG:HG3	2.21	0.40
6:Z:139:ILE:HG23	6:Z:141:VAL:HG13	2.02	0.40
9:c:32:TYR:O	9:c:68:ARG:HA	2.22	0.40
9:c:120:CYS:SG	9:c:158:ASP:HB2	2.61	0.40
9:c:195:GLY:O	9:c:196:LEU:C	2.62	0.40
10:d:147:SER:OG	10:d:150:LYS:HB2	2.22	0.40
13:B:381:ASP:HA	13:B:384:ILE:HB	2.03	0.40
15:D:115:ILE:HA	15:D:139:LEU:HB3	2.03	0.40
16:E:286:ASP:HA	16:E:287:PRO:HD3	1.96	0.40
17:F:66:LEU:O	17:F:70:LYS:HB2	2.20	0.40
17:F:76:ASN:C	17:F:76:ASN:HD22	2.28	0.40
17:F:84:LYS:HE3	17:F:84:LYS:HB3	1.85	0.40
20:I:41:ASP:OD1	20:I:41:ASP:N	2.48	0.40
24:M:215:TRP:CZ2	24:M:219:LEU:HD11	2.55	0.40
20:i:246:LYS:HD2	20:i:246:LYS:O	2.21	0.40
23:l:36:VAL:HG22	23:l:160:SER:HB2	2.01	0.40
33:x:271:MET:HG2	33:x:787:LEU:HD13	2.03	0.40
33:x:296:PHE:CZ	33:x:837:LEU:CD1	3.01	0.40
33:x:556:ARG:HA	33:x:587:PHE:CE2	2.56	0.40
1:U:532:MET:CE	1:U:552:ILE:N	2.82	0.40
1:U:628:ARG:HA	1:U:749:GLN:OE1	2.21	0.40
2:V:29:PRO:N	2:V:30:PRO:HD2	2.36	0.40
4:X:76:PHE:CD1	4:X:76:PHE:O	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:50:MET:HA	5:Y:70:LEU:HD13	2.03	0.40
7:a:101:ARG:HD2	7:a:111:VAL:HG23	2.03	0.40
11:e:61:GLU:HA	11:e:65:TYR:HD2	1.85	0.40
12:A:286:ASP:OD1	17:F:294:LYS:HB3	2.21	0.40
15:D:264:ILE:HG22	15:D:267:ILE:HG23	1.99	0.40
15:D:372:GLY:HA3	38:D:501:ADP:C8	2.55	0.40
16:E:171:LEU:CD1	16:E:173:TYR:HB3	2.51	0.40
16:E:250:ASP:HA	16:E:253:ILE:HG12	2.04	0.40
21:J:243:LYS:HD2	21:J:246:LYS:HB3	2.02	0.40
22:K:84:ASP:HB3	22:K:137:PHE:HD1	1.85	0.40
22:K:142:LEU:HD21	22:K:168:ARG:HG2	2.03	0.40
29:R:5:ALA:HA	29:R:13:ILE:O	2.22	0.40
33:x:376:PHE:CD2	33:x:376:PHE:C	3.00	0.40
33:x:583:VAL:HG12	33:x:584:SER:O	2.21	0.40
33:x:680:ARG:HD3	33:x:681:TYR:CZ	2.56	0.40
1:U:20:LYS:HE3	1:U:20:LYS:HA	2.04	0.40
1:U:619:VAL:C	1:U:622:LEU:HD13	2.44	0.40
2:V:347:GLN:OE1	2:V:347:GLN:N	2.54	0.40
2:V:437:ILE:HD11	10:d:146:GLY:HA3	2.02	0.40
3:W:60:MET:SD	3:W:111:TYR:HD2	2.44	0.40
3:W:75:TYR:OH	3:W:100:ALA:HB3	2.21	0.40
3:W:343:SER:HB2	3:W:347:GLY:N	2.24	0.40
5:Y:21:GLN:OE1	5:Y:286:TRP:HB2	2.21	0.40
5:Y:97:GLU:OE2	5:Y:97:GLU:N	2.52	0.40
5:Y:181:LYS:HD2	5:Y:219:PHE:CE1	2.57	0.40
5:Y:288:PHE:HA	5:Y:291:HIS:HB2	2.03	0.40
6:Z:96:HIS:CE1	6:Z:102:HIS:HE1	2.40	0.40
6:Z:177:ARG:HH11	6:Z:177:ARG:C	2.29	0.40
10:d:9:TRP:HB2	10:d:57:ILE:HD11	2.02	0.40
10:d:203:PRO:C	10:d:205:LYS:N	2.78	0.40
14:C:61:GLU:HA	14:C:64:GLN:OE1	2.21	0.40
14:C:213:ARG:HD3	15:D:299:PHE:CD2	2.56	0.40
15:D:61:ILE:HG22	15:D:65:GLN:NE2	2.36	0.40
15:D:146:GLU:HG3	15:D:147:ALA:H	1.86	0.40
16:E:229:ILE:HG12	16:E:272:ARG:HG2	2.04	0.40
16:E:253:ILE:O	16:E:256:THR:OG1	2.39	0.40
16:E:353:PHE:CB	16:E:357:ALA:H	2.34	0.40
17:F:167:GLU:HG2	17:F:168:TYR:H	1.86	0.40
28:Q:108:ASP:OD1	28:Q:111:GLU:N	2.47	0.40
28:Q:197:PRO:HA	28:q:199:GLN:H	1.85	0.40
31:T:70:MET:HE3	31:T:70:MET:HB3	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:x:137:ARG:HE	33:x:169:GLU:HG2	1.86	0.40
33:x:162:LEU:O	33:x:166:VAL:HG13	2.21	0.40
1:U:579:ARG:NH1	1:U:609:ASP:OD1	2.54	0.40
2:V:334:VAL:O	2:V:338:LEU:HG	2.22	0.40
2:V:442:ILE:HD12	2:V:442:ILE:H	1.85	0.40
3:W:82:LEU:HD11	3:W:96:GLN:NE2	2.36	0.40
3:W:87:ILE:HG22	3:W:88:MET:N	2.31	0.40
3:W:87:ILE:HB	3:W:91:SER:CB	2.52	0.40
3:W:192:LEU:HD13	3:W:192:LEU:HA	1.93	0.40
4:X:113:CYS:SG	4:X:129:LEU:HD13	2.61	0.40
5:Y:359:PRO:HB2	5:Y:364:TRP:HB2	2.03	0.40
6:Z:81:MET:HE2	6:Z:81:MET:HB2	1.91	0.40
7:a:82:HIS:HA	7:a:85:ARG:HG2	2.03	0.40
8:b:61:LEU:HD12	8:b:61:LEU:H	1.86	0.40
9:c:189:ILE:HA	9:c:192:LEU:HB3	2.04	0.40
10:d:203:PRO:HB2	10:d:205:LYS:HB2	2.04	0.40
11:e:66:LYS:HD3	11:e:66:LYS:H	1.86	0.40
14:C:34:ILE:HG22	15:D:51:LEU:HD11	2.03	0.40
14:C:65:LEU:HD13	14:C:65:LEU:C	2.46	0.40
14:C:397:LYS:HE2	14:C:397:LYS:HB2	1.79	0.40
15:D:238:LYS:HE2	15:D:238:LYS:HB2	1.96	0.40
19:H:186:ASP:O	19:H:190:THR:HG22	2.21	0.40
25:N:33:LYS:HE2	39:N:301:LDZ:H16	2.03	0.40
27:P:31:GLN:HB3	27:P:32:ALA:H	1.65	0.40
31:T:117:ASP:OD2	31:T:117:ASP:O	2.39	0.40
24:m:195:LYS:HD3	24:m:238:TYR:CE2	2.57	0.40
26:o:104:ASP:OD1	26:o:104:ASP:C	2.64	0.40
33:x:838:ARG:HE	33:x:839:PRO:HD3	1.85	0.40
1:U:153:ILE:O	1:U:156:GLU:HG2	2.20	0.40
1:U:583:MET:HE3	1:U:583:MET:N	2.37	0.40
1:U:597:LYS:H	1:U:597:LYS:CD	2.34	0.40
1:U:622:LEU:N	1:U:622:LEU:HD12	2.36	0.40
2:V:263:LEU:HD21	10:d:83:PHE:CE1	2.55	0.40
2:V:395:ILE:HB	2:V:399:ARG:HH21	1.87	0.40
2:V:407:VAL:HA	2:V:410:ILE:CD1	2.51	0.40
3:W:251:TYR:CE1	3:W:267:LEU:N	2.90	0.40
4:X:55:SER:O	4:X:59:LYS:HB2	2.20	0.40
4:X:70:LEU:CD2	4:X:92:LEU:HB3	2.51	0.40
4:X:77:LEU:O	4:X:80:ILE:HG22	2.22	0.40
4:X:351:SER:HB2	4:X:356:LEU:O	2.22	0.40
6:Z:278:ASN:OD1	6:Z:278:ASN:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:c:141:VAL:HA	9:c:161:ARG:HA	2.02	0.40
9:c:211:GLU:O	9:c:212:LEU:HB2	2.20	0.40
13:B:94:GLU:O	13:B:98:LYS:HD3	2.21	0.40
13:B:113:GLU:HB3	13:B:122:ILE:CG2	2.50	0.40
15:D:352:MET:HE2	16:E:164:ILE:HD11	2.04	0.40
16:E:353:PHE:HB3	16:E:357:ALA:C	2.47	0.40
19:H:64:LYS:HB3	19:H:64:LYS:HE3	1.75	0.40
20:I:175:LEU:O	20:I:179:TYR:HB2	2.22	0.40
25:N:107:GLU:HB2	25:N:110:GLN:NE2	2.36	0.40
26:O:68:LEU:HD12	26:O:68:LEU:HA	1.96	0.40
18:g:161:CYS:SG	18:g:162:GLY:N	2.94	0.40
20:i:237:ILE:HG12	20:i:237:ILE:H	1.77	0.40
33:x:870:THR:O	33:x:872:VAL:N	2.55	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	U	868/921 (94%)	783 (90%)	83 (10%)	2 (0%)	43	71
2	V	478/480 (100%)	417 (87%)	61 (13%)	0	100	100
3	W	449/456 (98%)	382 (85%)	61 (14%)	6 (1%)	9	33
4	X	378/422 (90%)	347 (92%)	26 (7%)	5 (1%)	9	33
5	Y	376/389 (97%)	327 (87%)	44 (12%)	5 (1%)	9	33
6	Z	284/324 (88%)	244 (86%)	36 (13%)	4 (1%)	9	31
7	a	371/376 (99%)	325 (88%)	43 (12%)	3 (1%)	16	44
8	b	189/377 (50%)	168 (89%)	21 (11%)	0	100	100
9	c	285/310 (92%)	233 (82%)	46 (16%)	6 (2%)	5	22
10	d	255/350 (73%)	212 (83%)	41 (16%)	2 (1%)	16	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	e	36/70 (51%)	25 (69%)	10 (28%)	1 (3%)	4	18
12	A	411/433 (95%)	372 (90%)	37 (9%)	2 (0%)	24	54
13	B	403/440 (92%)	361 (90%)	41 (10%)	1 (0%)	43	71
14	C	394/406 (97%)	362 (92%)	28 (7%)	4 (1%)	12	39
15	D	378/418 (90%)	341 (90%)	32 (8%)	5 (1%)	9	33
16	E	379/389 (97%)	296 (78%)	76 (20%)	7 (2%)	6	26
17	F	391/439 (89%)	351 (90%)	37 (10%)	3 (1%)	16	44
18	G	235/245 (96%)	222 (94%)	10 (4%)	3 (1%)	9	33
18	g	238/245 (97%)	228 (96%)	10 (4%)	0	100	100
19	H	229/233 (98%)	217 (95%)	12 (5%)	0	100	100
19	h	227/233 (97%)	219 (96%)	7 (3%)	1 (0%)	30	58
20	I	246/260 (95%)	234 (95%)	11 (4%)	1 (0%)	30	58
20	i	248/260 (95%)	231 (93%)	15 (6%)	2 (1%)	16	44
21	J	245/247 (99%)	226 (92%)	15 (6%)	4 (2%)	7	28
21	j	237/247 (96%)	207 (87%)	29 (12%)	1 (0%)	30	58
22	K	226/240 (94%)	219 (97%)	7 (3%)	0	100	100
22	k	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
23	L	236/268 (88%)	228 (97%)	8 (3%)	0	100	100
23	l	236/268 (88%)	226 (96%)	10 (4%)	0	100	100
24	M	238/254 (94%)	229 (96%)	8 (3%)	1 (0%)	30	58
24	m	238/254 (94%)	221 (93%)	15 (6%)	2 (1%)	16	44
25	N	195/238 (82%)	184 (94%)	10 (5%)	1 (0%)	24	54
25	n	195/238 (82%)	189 (97%)	6 (3%)	0	100	100
26	O	218/276 (79%)	207 (95%)	10 (5%)	1 (0%)	24	54
26	o	218/276 (79%)	201 (92%)	17 (8%)	0	100	100
27	P	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
27	p	202/204 (99%)	188 (93%)	14 (7%)	0	100	100
28	Q	197/201 (98%)	184 (93%)	13 (7%)	0	100	100
28	q	197/201 (98%)	189 (96%)	8 (4%)	0	100	100
29	R	199/262 (76%)	191 (96%)	7 (4%)	1 (0%)	24	54
29	r	199/262 (76%)	193 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	S	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	24	54
30	s	211/240 (88%)	205 (97%)	5 (2%)	1 (0%)	24	54
31	T	213/263 (81%)	205 (96%)	8 (4%)	0	100	100
31	t	213/263 (81%)	204 (96%)	9 (4%)	0	100	100
32	f	40/468 (8%)	39 (98%)	1 (2%)	0	100	100
33	x	865/908 (95%)	817 (94%)	47 (5%)	1 (0%)	48	76
All	All	13403/15238 (88%)	12262 (92%)	1064 (8%)	77 (1%)	23	49

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	W	41	GLN
3	W	329	ARG
3	W	335	SER
4	X	267	VAL
4	X	318	ILE
7	a	185	ILE
9	c	28	ALA
9	c	197	ASN
9	c	280	PRO
10	d	199	PHE
10	d	206	MET
11	e	46	ASP
12	A	27	GLU
13	B	278	ALA
14	C	90	HIS
14	C	242	ALA
14	C	254	ILE
15	D	258	ALA
15	D	411	GLU
16	E	229	ILE
16	E	309	ARG
16	E	326	ILE
16	E	336	ASP
17	F	86	LEU
18	G	129	ALA
18	G	146	GLU
20	I	107	CYS
21	J	199	VAL
30	S	191	ASP

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Mol	Chain	Res	Type
20	i	19	TYR
20	i	107	CYS
21	j	239	ASN
3	W	91	SER
4	X	205	LYS
5	Y	165	LYS
5	Y	361	SER
15	D	259	PRO
16	E	372	ARG
21	J	213	ARG
24	M	201	HIS
30	s	191	ASP
3	W	158	ASP
5	Y	161	THR
5	Y	163	LYS
6	Z	127	LYS
6	Z	166	GLU
6	Z	185	GLY
9	c	233	ASP
15	D	303	VAL
18	G	131	MET
25	N	19	ARG
26	O	172	ASN
33	x	586	PRO
1	U	173	VAL
1	U	874	ASN
3	W	332	SER
9	c	25	VAL
17	F	40	GLU
17	F	180	ARG
24	m	184	MET
24	m	201	HIS
7	a	35	HIS
9	c	184	LEU
12	A	66	LYS
14	C	373	GLU
15	D	109	SER
16	E	234	GLU
19	h	232	ALA
4	X	143	TYR
5	Y	205	VAL
6	Z	243	GLN

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Mol	Chain	Res	Type
7	a	144	ASN
16	E	306	GLU
21	J	6	ALA
21	J	184	ASP
29	R	38	ASN
4	X	204	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	748/789 (95%)	721 (96%)	27 (4%)	31	58
2	V	414/414 (100%)	400 (97%)	14 (3%)	32	60
3	W	413/416 (99%)	394 (95%)	19 (5%)	24	53
4	X	327/362 (90%)	318 (97%)	9 (3%)	38	63
5	Y	333/344 (97%)	320 (96%)	13 (4%)	28	57
6	Z	257/295 (87%)	245 (95%)	12 (5%)	23	52
7	a	333/336 (99%)	317 (95%)	16 (5%)	23	51
8	b	167/312 (54%)	164 (98%)	3 (2%)	51	70
9	c	252/268 (94%)	238 (94%)	14 (6%)	19	46
10	d	231/294 (79%)	218 (94%)	13 (6%)	19	46
11	e	38/63 (60%)	38 (100%)	0	100	100
12	A	348/372 (94%)	335 (96%)	13 (4%)	30	58
13	B	352/385 (91%)	343 (97%)	9 (3%)	40	65
14	C	341/352 (97%)	332 (97%)	9 (3%)	40	65
15	D	333/366 (91%)	321 (96%)	12 (4%)	31	58
16	E	333/341 (98%)	322 (97%)	11 (3%)	33	60
17	F	340/379 (90%)	328 (96%)	12 (4%)	32	59
18	G	191/209 (91%)	187 (98%)	4 (2%)	47	68
18	g	194/209 (93%)	187 (96%)	7 (4%)	31	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	H	166/190 (87%)	159 (96%)	7 (4%)	26	55
19	h	165/190 (87%)	162 (98%)	3 (2%)	51	70
20	I	191/220 (87%)	184 (96%)	7 (4%)	30	58
20	i	193/220 (88%)	190 (98%)	3 (2%)	55	72
21	J	179/210 (85%)	169 (94%)	10 (6%)	19	46
21	j	152/210 (72%)	147 (97%)	5 (3%)	33	60
22	K	189/202 (94%)	183 (97%)	6 (3%)	34	61
22	k	186/202 (92%)	179 (96%)	7 (4%)	29	57
23	L	198/229 (86%)	191 (96%)	7 (4%)	32	59
23	l	198/229 (86%)	195 (98%)	3 (2%)	57	73
24	M	192/211 (91%)	189 (98%)	3 (2%)	55	72
24	m	193/211 (92%)	182 (94%)	11 (6%)	18	46
25	N	154/180 (86%)	147 (96%)	7 (4%)	24	53
25	n	154/180 (86%)	153 (99%)	1 (1%)	78	81
26	O	177/227 (78%)	176 (99%)	1 (1%)	78	81
26	o	177/227 (78%)	176 (99%)	1 (1%)	78	81
27	P	173/173 (100%)	168 (97%)	5 (3%)	37	63
27	p	173/173 (100%)	167 (96%)	6 (4%)	32	59
28	Q	164/171 (96%)	159 (97%)	5 (3%)	36	62
28	q	165/171 (96%)	164 (99%)	1 (1%)	78	81
29	R	153/201 (76%)	150 (98%)	3 (2%)	48	69
29	r	153/201 (76%)	150 (98%)	3 (2%)	48	69
30	S	174/198 (88%)	173 (99%)	1 (1%)	78	81
30	s	174/198 (88%)	171 (98%)	3 (2%)	53	71
31	T	175/214 (82%)	170 (97%)	5 (3%)	37	63
31	t	176/214 (82%)	174 (99%)	2 (1%)	65	76
32	f	37/377 (10%)	36 (97%)	1 (3%)	39	64
33	x	733/763 (96%)	710 (97%)	23 (3%)	35	61
All	All	11259/12898 (87%)	10902 (97%)	357 (3%)	35	61

All (357) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	27	LEU
1	U	135	ASN
1	U	259	GLN
1	U	263	SER
1	U	339	LEU
1	U	348	THR
1	U	362	ASN
1	U	364	VAL
1	U	386	LEU
1	U	399	TRP
1	U	415	HIS
1	U	462	LEU
1	U	470	ASN
1	U	472	ILE
1	U	492	ASP
1	U	493	VAL
1	U	544	ILE
1	U	552	ILE
1	U	555	VAL
1	U	607	VAL
1	U	631	GLU
1	U	736	ILE
1	U	776	SER
1	U	780	SER
1	U	800	VAL
1	U	826	GLU
1	U	828	VAL
2	V	82	LEU
2	V	94	VAL
2	V	214	HIS
2	V	265	ASP
2	V	342	ILE
2	V	391	THR
2	V	412	LEU
2	V	417	ILE
2	V	421	ASP
2	V	428	LEU
2	V	446	VAL
2	V	465	ASP
2	V	467	TYR
2	V	477	HIS
3	W	14	VAL
3	W	135	LYS

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Mol	Chain	Res	Type
3	W	160	LYS
3	W	184	GLU
3	W	192	LEU
3	W	203	GLN
3	W	213	PHE
3	W	236	HIS
3	W	294	LYS
3	W	322	GLU
3	W	344	THR
3	W	351	TRP
3	W	369	TYR
3	W	401	THR
3	W	406	VAL
3	W	415	PHE
3	W	425	LEU
3	W	438	LEU
3	W	450	GLU
4	X	78	ASN
4	X	80	ILE
4	X	93	LEU
4	X	155	ARG
4	X	167	VAL
4	X	176	THR
4	X	185	LYS
4	X	256	LEU
4	X	388	PHE
5	Y	77	ASN
5	Y	100	ILE
5	Y	132	VAL
5	Y	155	ASP
5	Y	201	PHE
5	Y	207	THR
5	Y	209	THR
5	Y	250	LEU
5	Y	256	VAL
5	Y	271	PHE
5	Y	272	PHE
5	Y	353	ILE
5	Y	367	GLN
6	Z	15	VAL
6	Z	56	VAL
6	Z	124	ILE

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Mol	Chain	Res	Type
6	Z	157	HIS
6	Z	175	LEU
6	Z	186	THR
6	Z	196	HIS
6	Z	211	TYR
6	Z	224	HIS
6	Z	240	VAL
6	Z	260	VAL
6	Z	282	ASN
7	a	23	HIS
7	a	37	LEU
7	a	38	THR
7	a	71	VAL
7	a	92	VAL
7	a	112	ILE
7	a	125	ILE
7	a	159	SER
7	a	166	ILE
7	a	183	VAL
7	a	200	LEU
7	a	236	THR
7	a	334	THR
7	a	336	VAL
7	a	343	LEU
7	a	376	THR
8	b	12	ASN
8	b	48	ASN
8	b	71	ILE
9	c	65	TYR
9	c	67	VAL
9	c	109	VAL
9	c	125	VAL
9	c	156	VAL
9	c	160	PHE
9	c	166	ASN
9	c	183	HIS
9	c	212	LEU
9	c	215	LYS
9	c	229	LEU
9	c	237	HIS
9	c	240	HIS
9	c	259	VAL

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Mol	Chain	Res	Type
10	d	13	SER
10	d	44	THR
10	d	61	TRP
10	d	62	SER
10	d	127	ILE
10	d	138	SER
10	d	187	GLU
10	d	188	LYS
10	d	201	ASN
10	d	207	THR
10	d	224	SER
10	d	235	THR
10	d	237	ILE
12	A	32	LEU
12	A	59	ILE
12	A	133	ASP
12	A	134	ILE
12	A	140	VAL
12	A	142	VAL
12	A	191	VAL
12	A	220	THR
12	A	234	ASP
12	A	250	VAL
12	A	312	ARG
12	A	371	GLU
12	A	403	ILE
13	B	51	LEU
13	B	73	LEU
13	B	133	VAL
13	B	149	SER
13	B	156	VAL
13	B	192	ASN
13	B	201	VAL
13	B	288	ASP
13	B	416	ASN
14	C	58	LEU
14	C	71	SER
14	C	116	LEU
14	C	123	LEU
14	C	143	VAL
14	C	292	ILE
14	C	300	ILE

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Mol	Chain	Res	Type
14	C	337	ASN
14	C	397	LYS
15	D	59	GLU
15	D	85	ILE
15	D	100	THR
15	D	107	THR
15	D	143	LEU
15	D	154	LEU
15	D	175	GLN
15	D	231	VAL
15	D	236	VAL
15	D	259	PRO
15	D	279	THR
15	D	407	ILE
16	E	67	GLU
16	E	105	LEU
16	E	121	ASN
16	E	155	ASN
16	E	162	VAL
16	E	170	CYS
16	E	224	ASP
16	E	335	SER
16	E	359	HIS
16	E	366	ASP
16	E	380	LEU
17	F	97	LEU
17	F	124	ILE
17	F	131	THR
17	F	136	VAL
17	F	140	VAL
17	F	183	GLU
17	F	289	ASP
17	F	320	PHE
17	F	338	LEU
17	F	375	VAL
17	F	416	THR
17	F	435	LEU
18	G	10	ASP
18	G	73	THR
18	G	112	ASP
18	G	115	CYS
19	H	19	LEU

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Mol	Chain	Res	Type
19	H	56	LEU
19	H	75	VAL
19	H	174	LEU
19	H	180	GLU
19	H	181	ASP
19	H	182	LEU
20	I	28	ILE
20	I	43	VAL
20	I	44	LEU
20	I	85	VAL
20	I	168	SER
20	I	186	LEU
20	I	200	THR
21	J	4	ASP
21	J	35	VAL
21	J	58	THR
21	J	68	ASN
21	J	70	CYS
21	J	134	VAL
21	J	139	ASP
21	J	146	GLN
21	J	175	ASN
21	J	184	ASP
22	K	7	GLU
22	K	36	THR
22	K	47	CYS
22	K	50	VAL
22	K	63	SER
22	K	204	GLN
23	L	33	SER
23	L	53	GLN
23	L	93	LEU
23	L	178	GLU
23	L	182	CYS
23	L	190	HIS
23	L	226	ASP
24	M	169	ARG
24	M	183	GLU
24	M	200	VAL
25	N	1	THR
25	N	6	VAL
25	N	21	THR

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Mol	Chain	Res	Type
25	N	46	SER
25	N	127	ILE
25	N	144	ARG
25	N	190	LEU
26	O	167	LEU
27	P	3	ILE
27	P	83	LYS
27	P	135	ASP
27	P	159	ASP
27	P	175	VAL
28	Q	5	ILE
28	Q	132	HIS
28	Q	148	THR
28	Q	160	LEU
28	Q	192	ASP
29	R	29	GLN
29	R	133	VAL
29	R	192	VAL
30	S	127	VAL
31	T	49	THR
31	T	82	SER
31	T	163	THR
31	T	191	THR
31	T	206	GLU
18	g	19	GLU
18	g	166	THR
18	g	177	SER
18	g	207	SER
18	g	210	PHE
18	g	211	LYS
18	g	213	SER
19	h	20	VAL
19	h	75	VAL
19	h	172	THR
20	i	30	HIS
20	i	92	LEU
20	i	234	GLU
21	j	13	ASP
21	j	58	THR
21	j	119	THR
21	j	200	GLN
21	j	214	ASP

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Mol	Chain	Res	Type
22	k	24	VAL
22	k	31	ILE
22	k	33	LEU
22	k	54	ILE
22	k	139	VAL
22	k	188	SER
22	k	190	THR
23	l	83	LEU
23	l	114	SER
23	l	147	THR
24	m	33	SER
24	m	34	SER
24	m	37	ILE
24	m	55	SER
24	m	77	VAL
24	m	175	GLU
24	m	184	MET
24	m	188	ASP
24	m	189	ILE
24	m	216	VAL
24	m	220	THR
25	n	22	THR
26	o	6	VAL
27	p	49	LEU
27	p	58	THR
27	p	116	THR
27	p	122	CYS
27	p	123	SER
27	p	193	ASP
28	q	195	SER
29	r	29	GLN
29	r	75	SER
29	r	102	CYS
30	s	123	SER
30	s	131	GLN
30	s	199	THR
31	t	20	VAL
31	t	21	VAL
32	f	392	VAL
33	x	69	SER
33	x	85	SER
33	x	87	THR

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Mol	Chain	Res	Type
33	x	92	VAL
33	x	96	LEU
33	x	112	ASN
33	x	175	ASP
33	x	240	VAL
33	x	258	LYS
33	x	273	ASN
33	x	405	HIS
33	x	583	VAL
33	x	586	PRO
33	x	613	LEU
33	x	615	ILE
33	x	659	LEU
33	x	672	LEU
33	x	766	GLN
33	x	796	LEU
33	x	810	ILE
33	x	830	LEU
33	x	842	VAL
33	x	900	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) such sidechains are listed below:

Mol	Chain	Res	Type
1	U	111	GLN
1	U	340	GLN
1	U	345	ASN
1	U	384	GLN
1	U	421	GLN
2	V	33	GLN
2	V	257	ASN
2	V	282	ASN
2	V	401	ASN
2	V	478	GLN
3	W	189	GLN
3	W	228	ASN
3	W	361	HIS
4	X	333	GLN
4	X	349	HIS
5	Y	160	ASN
5	Y	258	GLN
6	Z	24	ASN

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Mol	Chain	Res	Type
6	Z	102	HIS
6	Z	174	HIS
6	Z	225	GLN
6	Z	235	ASN
6	Z	256	GLN
6	Z	273	HIS
7	a	9	GLN
8	b	44	ASN
9	c	115	HIS
9	c	190	GLN
9	c	197	ASN
9	c	232	GLN
9	c	298	GLN
12	A	314	ASN
12	A	322	ASN
12	A	433	ASN
13	B	82	GLN
13	B	257	GLN
13	B	315	GLN
13	B	368	HIS
13	B	416	ASN
14	C	36	ASN
14	C	41	ASN
14	C	53	ASN
14	C	206	HIS
14	C	221	GLN
14	C	278	ASN
14	C	332	HIS
15	D	67	ASN
15	D	222	HIS
15	D	286	GLN
15	D	301	GLN
15	D	414	HIS
16	E	45	ASN
16	E	124	HIS
16	E	190	GLN
16	E	262	ASN
16	E	345	ASN
17	F	64	HIS
17	F	76	ASN
17	F	92	ASN
17	F	255	GLN

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Mol	Chain	Res	Type
17	F	315	ASN
17	F	316	GLN
18	G	12	HIS
20	I	95	GLN
20	I	167	ASN
21	J	15	HIS
21	J	68	ASN
21	J	122	ASN
21	J	215	GLN
22	K	182	GLN
23	L	5	GLN
23	L	152	ASN
23	L	175	HIS
23	L	185	ASN
24	M	221	ASN
25	N	158	ASN
26	O	62	ASN
28	Q	27	GLN
28	Q	87	ASN
28	Q	101	ASN
29	R	38	ASN
29	R	70	ASN
29	R	162	GLN
30	S	108	ASN
31	T	2	GLN
31	T	108	ASN
31	T	213	HIS
18	g	123	GLN
18	g	127	GLN
19	h	166	ASN
20	i	53	HIS
20	i	84	ASN
20	i	88	ASN
20	i	95	GLN
20	i	167	ASN
21	j	23	GLN
22	k	97	GLN
24	m	147	GLN
25	n	53	GLN
25	n	77	HIS
25	n	187	GLN
27	p	169	GLN

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Mol	Chain	Res	Type
28	q	87	ASN
28	q	101	ASN
28	q	110	HIS
29	r	162	GLN
29	r	191	ASN
30	s	8	ASN
30	s	108	ASN
30	s	157	ASN
31	t	89	HIS
33	x	213	GLN
33	x	301	HIS
33	x	327	ASN
33	x	355	ASN
33	x	452	ASN
33	x	457	ASN
33	x	715	HIS
33	x	738	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 5 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	LDZ	o	301	-	33,34,34	0.18	0	42,44,44	0.45	1 (2%)
39	LDZ	r	301	-	33,34,34	0.50	0	42,44,44	0.75	1 (2%)
39	LDZ	n	301	-	33,34,34	0.49	1 (3%)	42,44,44	1.70	5 (11%)
38	ADP	D	501	-	28,29,29	1.43	4 (14%)	43,45,45	1.90	8 (18%)
38	ADP	E	401	-	28,29,29	1.45	5 (17%)	43,45,45	1.83	9 (20%)
39	LDZ	N	301	-	33,34,34	0.43	0	42,44,44	0.66	0
39	LDZ	R	301	-	33,34,34	0.50	1 (3%)	42,44,44	0.92	3 (7%)
36	ATP	B	501	37	32,33,33	0.35	0	48,52,52	0.34	0
36	ATP	A	501	37	32,33,33	0.30	0	48,52,52	0.27	0
39	LDZ	O	301	-	33,34,34	0.41	0	42,44,44	1.57	5 (11%)
36	ATP	C	501	37	32,33,33	0.33	0	48,52,52	0.31	0
36	ATP	F	501	37	32,33,33	0.47	0	48,52,52	0.33	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
39	LDZ	o	301	-	-	23/38/39/39	0/1/1/1
39	LDZ	r	301	-	-	10/38/39/39	0/1/1/1
39	LDZ	n	301	-	-	26/38/39/39	0/1/1/1
38	ADP	D	501	-	-	0/16/32/32	0/3/3/3
38	ADP	E	401	-	-	6/16/32/32	0/3/3/3
39	LDZ	N	301	-	-	9/38/39/39	0/1/1/1
39	LDZ	R	301	-	-	9/38/39/39	0/1/1/1
36	ATP	B	501	37	-	7/22/38/38	0/3/3/3
36	ATP	A	501	37	-	4/22/38/38	0/3/3/3
39	LDZ	O	301	-	-	20/38/39/39	0/1/1/1
36	ATP	C	501	37	-	6/22/38/38	0/3/3/3
36	ATP	F	501	37	-	5/22/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	D	501	ADP	C5-C4	4.80	1.47	1.39
38	E	401	ADP	C5-C4	4.69	1.47	1.39
38	D	501	ADP	C5-C6	2.67	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	401	ADP	C5-C6	2.66	1.48	1.41
38	D	501	ADP	C5-N7	-2.46	1.34	1.39
38	E	401	ADP	C5-N7	-2.40	1.34	1.39
38	E	401	ADP	PA-O3A	2.38	1.62	1.59
38	E	401	ADP	C8-N7	2.26	1.36	1.31
38	D	501	ADP	C8-N7	2.24	1.36	1.31
39	R	301	LDZ	C17-N16	-2.16	1.43	1.46
39	n	301	LDZ	C17-N16	-2.04	1.43	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	301	LDZ	C14-N13-C12	7.69	138.18	121.65
39	O	301	LDZ	C18-C17-N16	7.33	121.75	110.69
38	D	501	ADP	C5-C4-N3	-6.26	118.10	126.72
38	E	401	ADP	C5-C4-N3	-5.87	118.64	126.72
38	D	501	ADP	N3-C4-N9	4.96	135.61	127.17
38	E	401	ADP	N3-C4-N9	4.68	135.13	127.17
39	n	301	LDZ	C24-C14-N13	4.61	120.99	110.58
38	E	401	ADP	C2-N3-C4	3.65	120.75	111.83
38	D	501	ADP	C2-N3-C4	3.65	120.74	111.83
38	D	501	ADP	C4-C5-N7	-3.53	106.55	110.58
38	E	401	ADP	C4-C5-N7	-3.33	106.78	110.58
39	R	301	LDZ	C18-C17-N16	-3.19	105.87	110.69
38	E	401	ADP	N3-C2-N1	-3.09	123.90	128.58
39	n	301	LDZ	C12-C11-N10	-3.00	102.99	111.11
39	O	301	LDZ	C18-C17-C22	-2.89	106.55	110.99
38	D	501	ADP	N3-C2-N1	-2.85	124.26	128.58
38	D	501	ADP	C3'-C2'-C1'	2.82	106.79	101.46
38	E	401	ADP	C3'-C2'-C1'	2.65	106.48	101.46
39	O	301	LDZ	C14-N13-C12	2.56	127.16	121.65
38	D	501	ADP	C5-N7-C8	2.55	107.45	103.45
39	r	301	LDZ	C14-N13-C12	2.52	127.06	121.65
39	O	301	LDZ	C14-C15-N16	2.50	121.97	116.63
38	E	401	ADP	C4-N9-C8	2.50	108.36	105.74
38	D	501	ADP	C4-N9-C8	2.49	108.36	105.74
39	R	301	LDZ	C18-C17-C22	2.46	114.78	110.99
38	E	401	ADP	C5-N7-C8	2.39	107.21	103.45
39	O	301	LDZ	O34-C15-N16	-2.38	118.70	122.96
39	n	301	LDZ	C11-C12-N13	2.36	121.66	116.63
39	o	301	LDZ	C22-C17-N16	2.28	113.90	109.50
39	R	301	LDZ	C15-C14-N13	-2.17	105.24	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	n	301	LDZ	C15-C14-N13	-2.08	105.48	111.11
38	E	401	ADP	C2'-C1'-N9	-2.01	108.31	113.30

There are no chirality outliers.

All (125) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	501	ATP	C5'-O5'-PA-O1A
36	A	501	ATP	C5'-O5'-PA-O3A
36	B	501	ATP	C5'-O5'-PA-O1A
36	B	501	ATP	C5'-O5'-PA-O2A
36	B	501	ATP	C5'-O5'-PA-O3A
36	B	501	ATP	O4'-C4'-C5'-O5'
36	C	501	ATP	C5'-O5'-PA-O2A
36	C	501	ATP	C5'-O5'-PA-O3A
36	C	501	ATP	O4'-C4'-C5'-O5'
36	F	501	ATP	C5'-O5'-PA-O1A
38	E	401	ADP	PA-O3A-PB-O3B
38	E	401	ADP	C5'-O5'-PA-O1A
38	E	401	ADP	C5'-O5'-PA-O2A
38	E	401	ADP	C5'-O5'-PA-O3A
39	N	301	LDZ	N10-C11-C30-C31
39	N	301	LDZ	C22-C17-C18-C19
39	O	301	LDZ	O8-C9-N10-C11
39	O	301	LDZ	O31-C9-N10-C11
39	O	301	LDZ	C18-C17-N16-C15
39	O	301	LDZ	C22-C17-C18-C19
39	R	301	LDZ	O31-C9-O8-C7
39	R	301	LDZ	N10-C9-O8-C7
39	R	301	LDZ	C22-C17-C18-C19
39	n	301	LDZ	O8-C9-N10-C11
39	n	301	LDZ	O31-C9-N10-C11
39	n	301	LDZ	C30-C11-N10-C9
39	n	301	LDZ	C24-C14-N13-C12
39	n	301	LDZ	C22-C17-C18-C19
39	o	301	LDZ	C14-C15-N16-C17
39	o	301	LDZ	O34-C15-N16-C17
39	o	301	LDZ	C22-C17-N16-C15
39	n	301	LDZ	O31-C9-O8-C7
39	O	301	LDZ	N10-C9-O8-C7
39	O	301	LDZ	C15-C14-C24-C25
39	o	301	LDZ	O8-C9-N10-C11

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Mol	Chain	Res	Type	Atoms
39	O	301	LDZ	O31-C9-O8-C7
39	n	301	LDZ	N10-C9-O8-C7
39	n	301	LDZ	C15-C14-C24-C25
39	o	301	LDZ	O31-C9-N10-C11
39	N	301	LDZ	N16-C17-C18-C19
39	O	301	LDZ	N10-C11-C30-C31
36	B	501	ATP	C3'-C4'-C5'-O5'
36	C	501	ATP	C3'-C4'-C5'-O5'
39	O	301	LDZ	N16-C17-C18-C19
39	R	301	LDZ	N13-C14-C24-C25
39	n	301	LDZ	N13-C14-C24-C25
39	O	301	LDZ	C12-C11-C30-C31
39	R	301	LDZ	N10-C11-C30-C31
39	n	301	LDZ	N10-C11-C30-C31
39	O	301	LDZ	C17-C18-C19-C21
39	R	301	LDZ	C12-C11-C30-C31
39	R	301	LDZ	C15-C14-C24-C25
39	n	301	LDZ	C12-C11-C30-C31
39	R	301	LDZ	C14-C24-C25-C26
39	n	301	LDZ	C17-C18-C19-C21
39	n	301	LDZ	N16-C17-C18-C19
39	n	301	LDZ	C11-C30-C31-C33
39	n	301	LDZ	C17-C18-C19-C20
39	O	301	LDZ	C14-C15-N16-C17
39	R	301	LDZ	C14-C24-C25-C27
39	o	301	LDZ	C14-C24-C25-C26
39	o	301	LDZ	C14-C24-C25-C27
39	O	301	LDZ	C14-C24-C25-C27
39	n	301	LDZ	C11-C30-C31-C32
39	O	301	LDZ	C17-C18-C19-C20
39	O	301	LDZ	O34-C15-N16-C17
39	n	301	LDZ	O32-C12-N13-C14
39	O	301	LDZ	C14-C24-C25-C26
39	N	301	LDZ	C14-C24-C25-C26
39	N	301	LDZ	C14-C24-C25-C27
39	n	301	LDZ	C11-C12-N13-C14
39	o	301	LDZ	C11-C30-C31-C33
39	N	301	LDZ	C12-C11-C30-C31
39	o	301	LDZ	C30-C11-C12-N13
39	o	301	LDZ	C30-C11-C12-O32
39	o	301	LDZ	C15-C14-N13-C12
39	O	301	LDZ	C15-C14-N13-C12

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Mol	Chain	Res	Type	Atoms
39	N	301	LDZ	C17-C18-C19-C20
39	r	301	LDZ	C15-C14-C24-C25
39	n	301	LDZ	N10-C11-C12-O32
39	o	301	LDZ	C17-C18-C19-C20
39	r	301	LDZ	N13-C14-C24-C25
39	o	301	LDZ	N10-C9-O8-C7
39	n	301	LDZ	C22-C17-N16-C15
39	r	301	LDZ	C22-C17-N16-C15
39	n	301	LDZ	N10-C11-C12-N13
39	o	301	LDZ	C17-C18-C19-C21
39	r	301	LDZ	C14-C24-C25-C27
39	n	301	LDZ	N13-C14-C15-O34
39	r	301	LDZ	C12-C11-C30-C31
39	n	301	LDZ	N13-C14-C15-N16
39	o	301	LDZ	C11-C30-C31-C32
39	n	301	LDZ	C18-C17-N16-C15
39	r	301	LDZ	C18-C17-N16-C15
39	o	301	LDZ	N10-C11-C12-O32
39	r	301	LDZ	N10-C11-C30-C31
36	C	501	ATP	PG-O3B-PB-O2B
39	O	301	LDZ	C24-C14-N13-C12
36	A	501	ATP	C5'-O5'-PA-O2A
36	F	501	ATP	C5'-O5'-PA-O3A
39	o	301	LDZ	O31-C9-O8-C7
39	O	301	LDZ	N13-C14-C24-C25
36	F	501	ATP	C3'-C4'-C5'-O5'
39	o	301	LDZ	C15-C14-C24-C25
39	o	301	LDZ	N13-C14-C24-C25
39	r	301	LDZ	C14-C24-C25-C26
39	o	301	LDZ	N10-C11-C12-N13
39	N	301	LDZ	C22-C17-N16-C15
39	r	301	LDZ	N13-C14-C15-O34
39	o	301	LDZ	C22-C17-C18-C19
39	o	301	LDZ	C24-C14-N13-C12
38	E	401	ADP	PA-O3A-PB-O1B
39	o	301	LDZ	C24-C14-C15-O34
39	r	301	LDZ	N13-C14-C15-N16
39	N	301	LDZ	C18-C17-N16-C15
36	B	501	ATP	PG-O3B-PB-O1B
36	B	501	ATP	PG-O3B-PB-O2B
36	F	501	ATP	PA-O3A-PB-O1B
36	F	501	ATP	PA-O3A-PB-O2B

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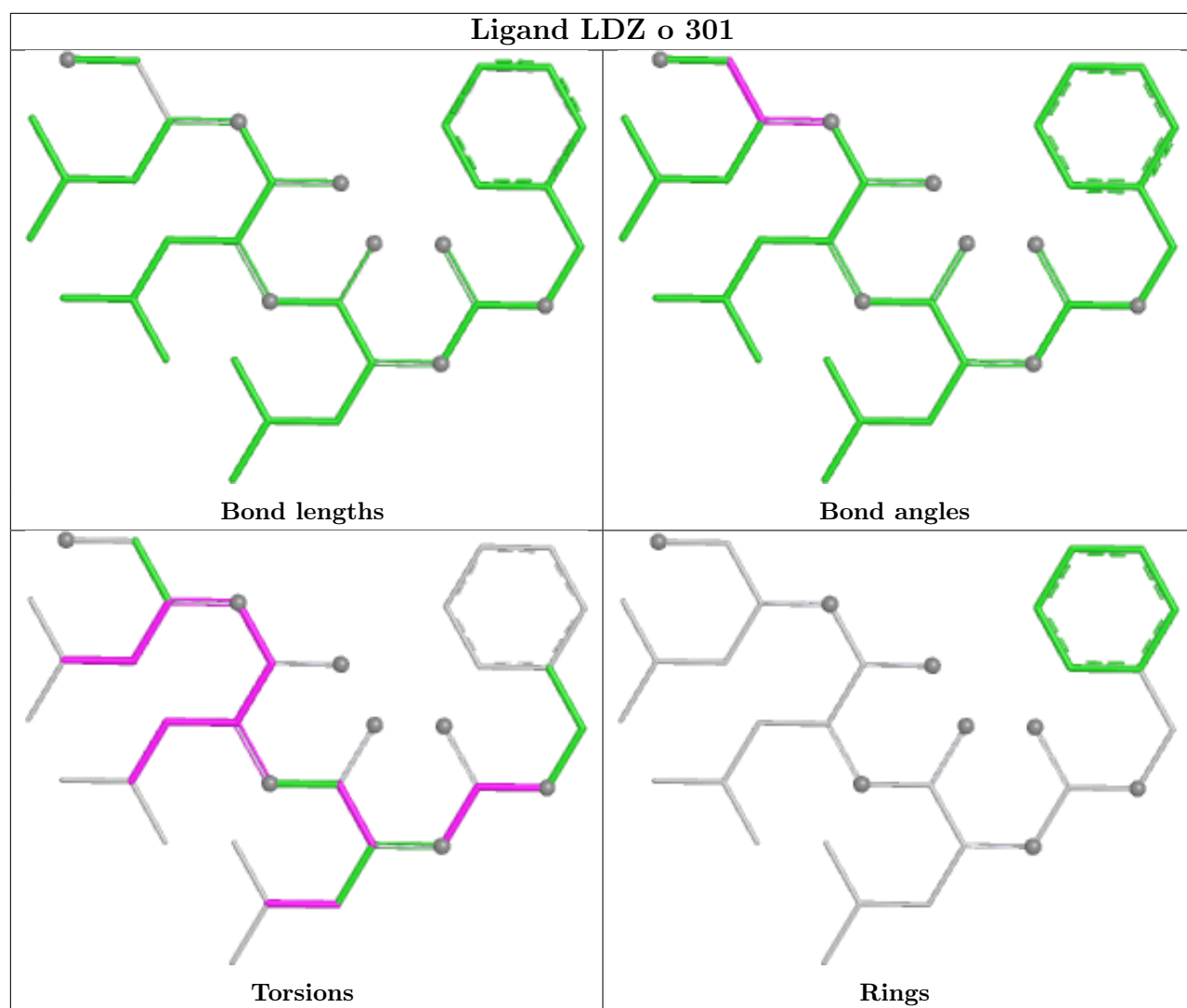
Mol	Chain	Res	Type	Atoms
39	O	301	LDZ	C3-C7-O8-C9
39	n	301	LDZ	C30-C11-C12-O32
39	n	301	LDZ	C24-C14-C15-O34
36	A	501	ATP	PG-O3B-PB-O2B
36	C	501	ATP	PG-O3B-PB-O1B
38	E	401	ADP	PB-O3A-PA-O2A

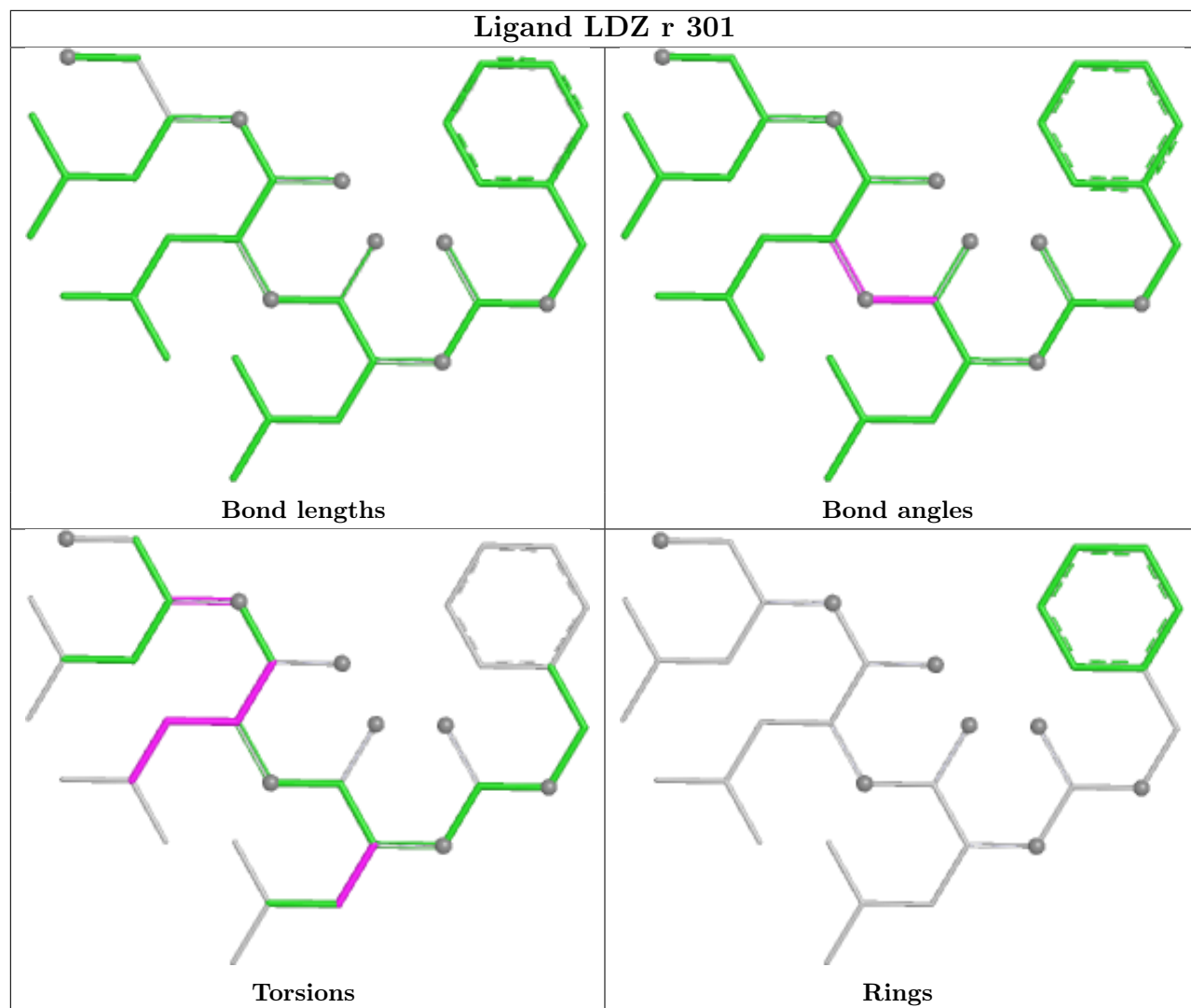
There are no ring outliers.

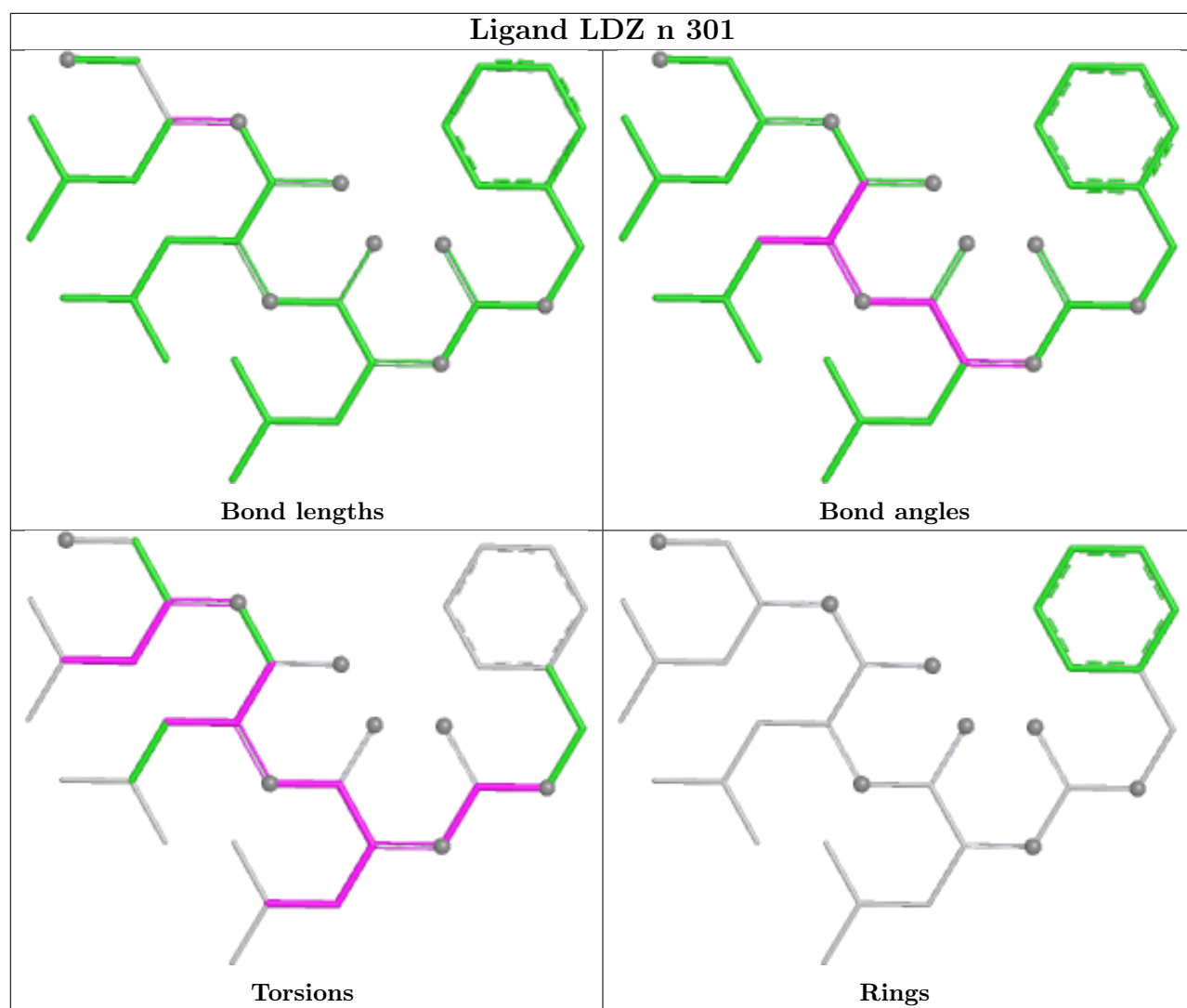
9 monomers are involved in 27 short contacts:

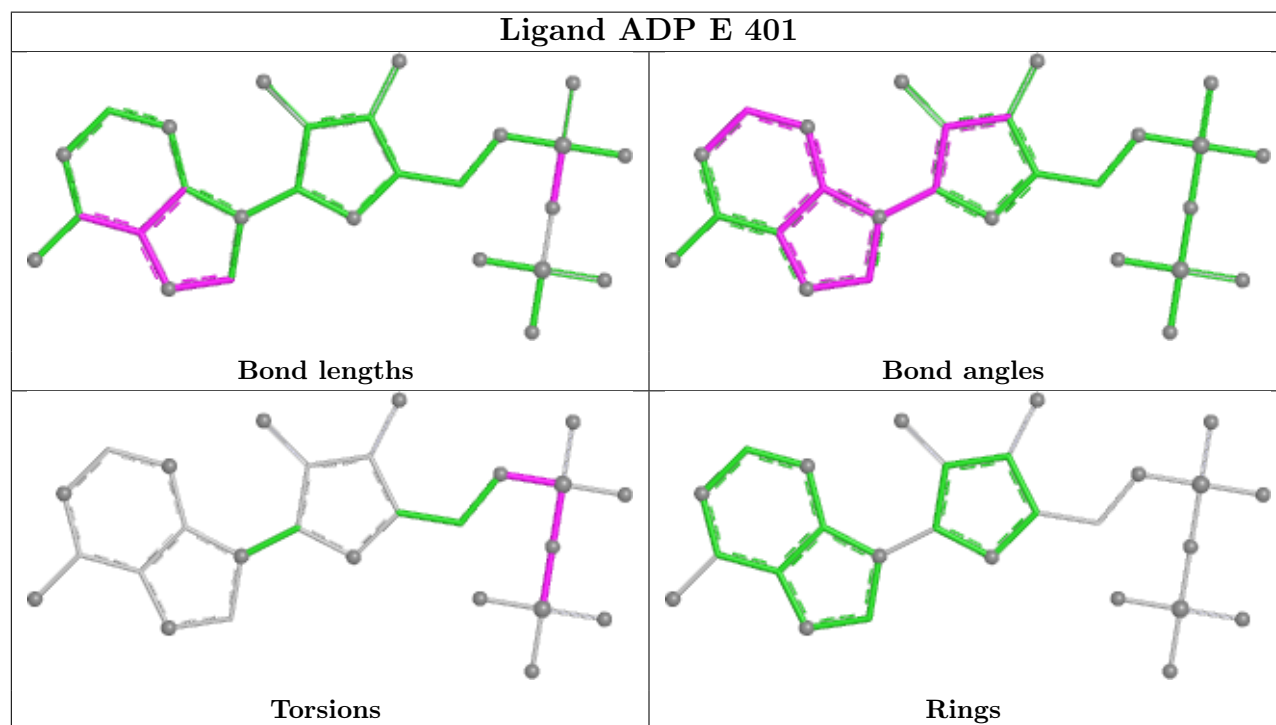
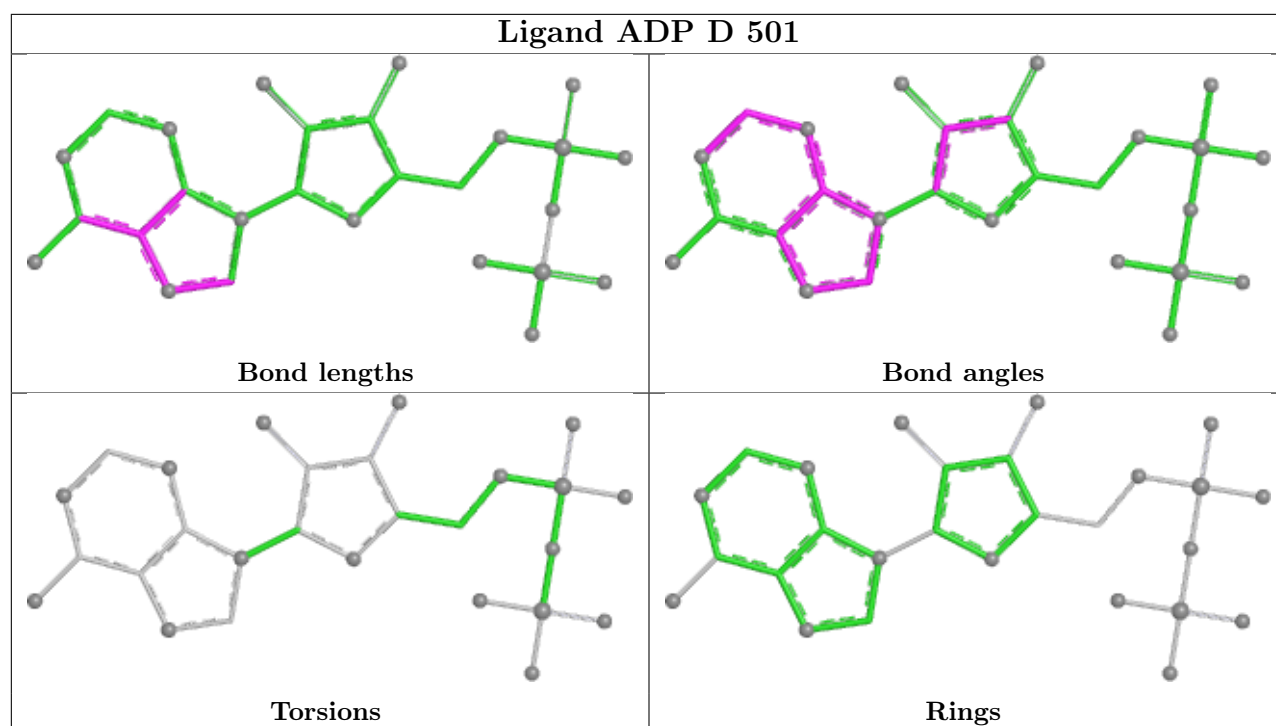
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	o	301	LDZ	7	0
39	n	301	LDZ	3	0
38	D	501	ADP	2	0
38	E	401	ADP	3	0
39	N	301	LDZ	3	0
39	R	301	LDZ	3	0
36	B	501	ATP	1	0
36	A	501	ATP	1	0
39	O	301	LDZ	4	0

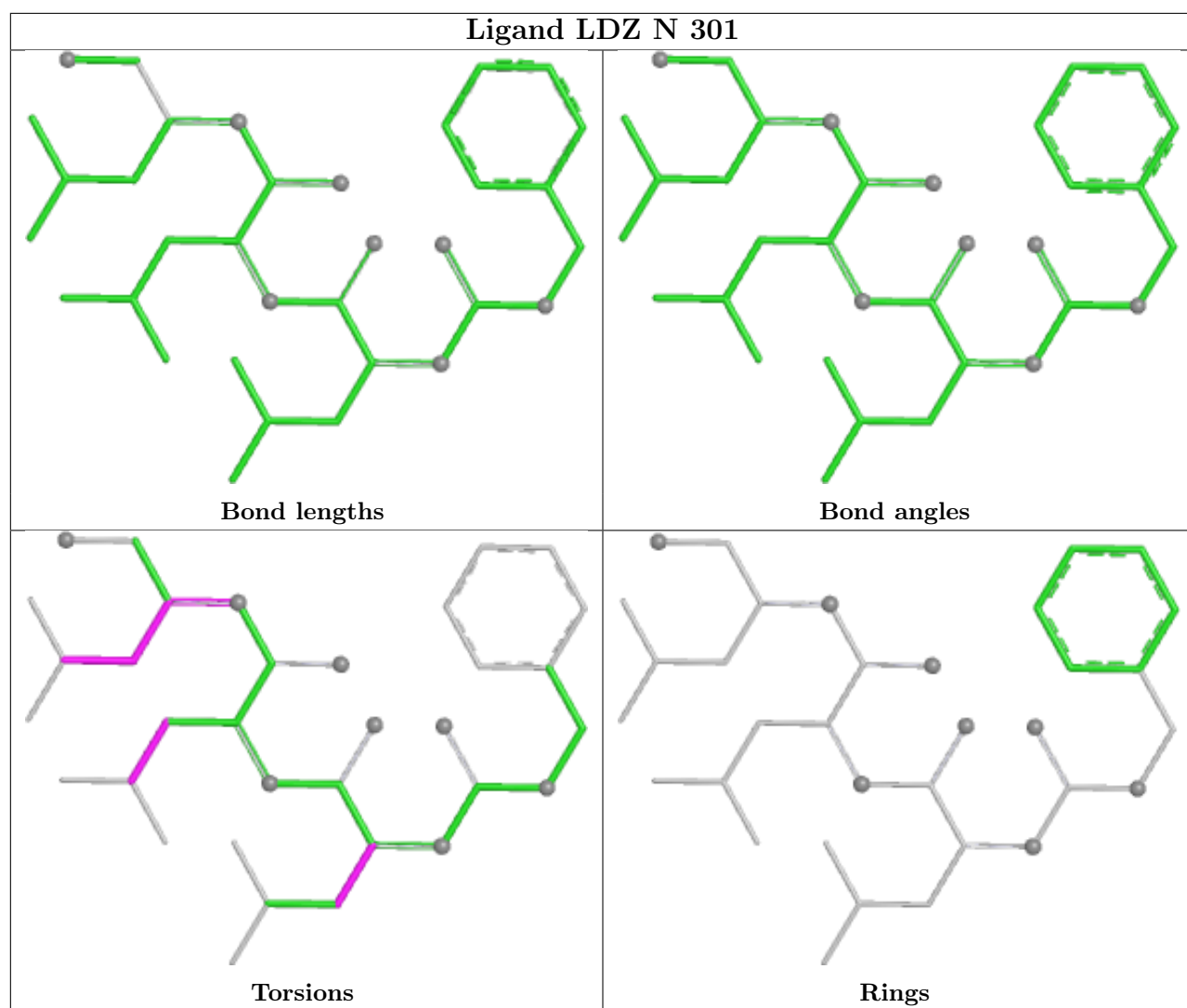
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

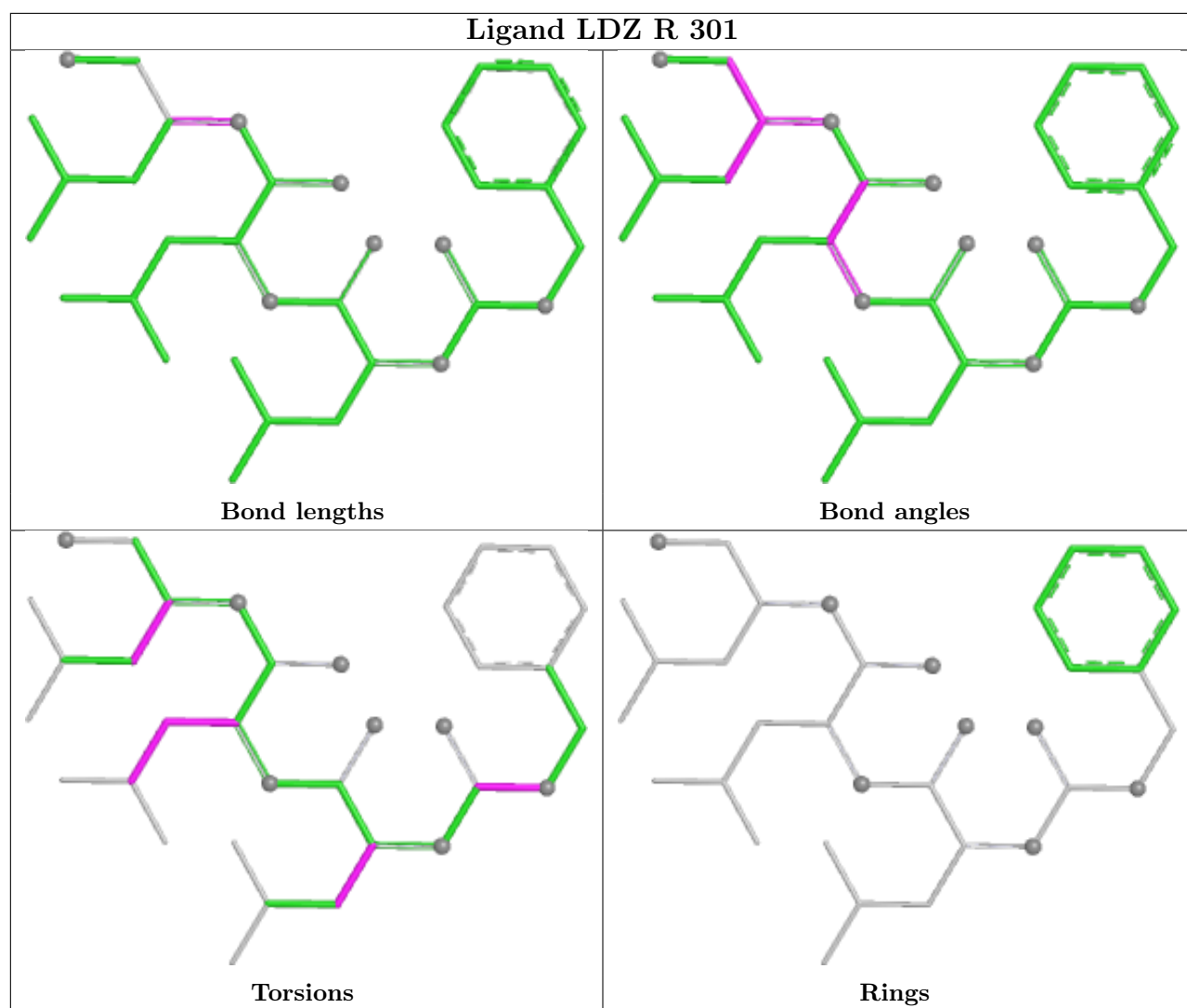


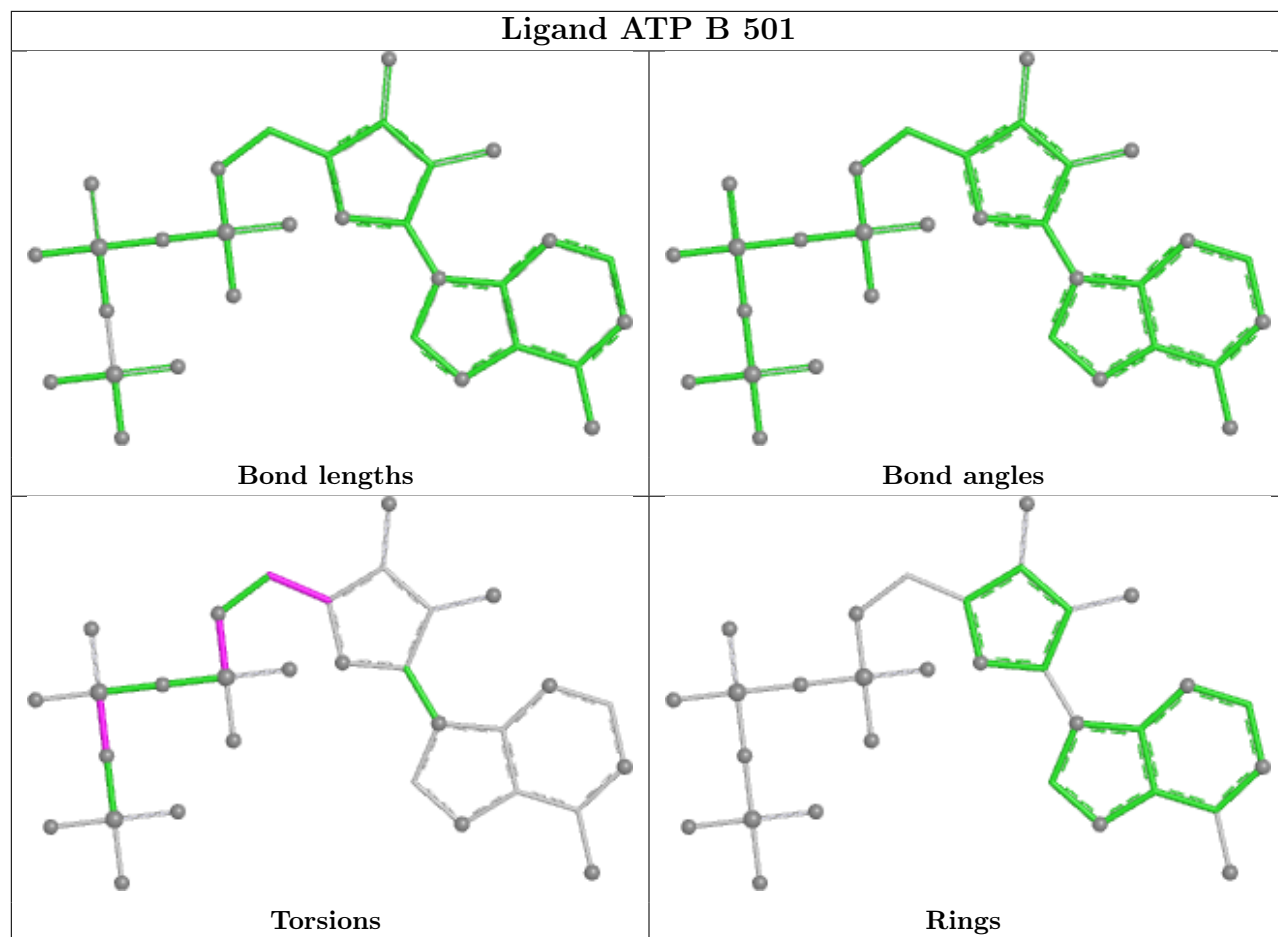


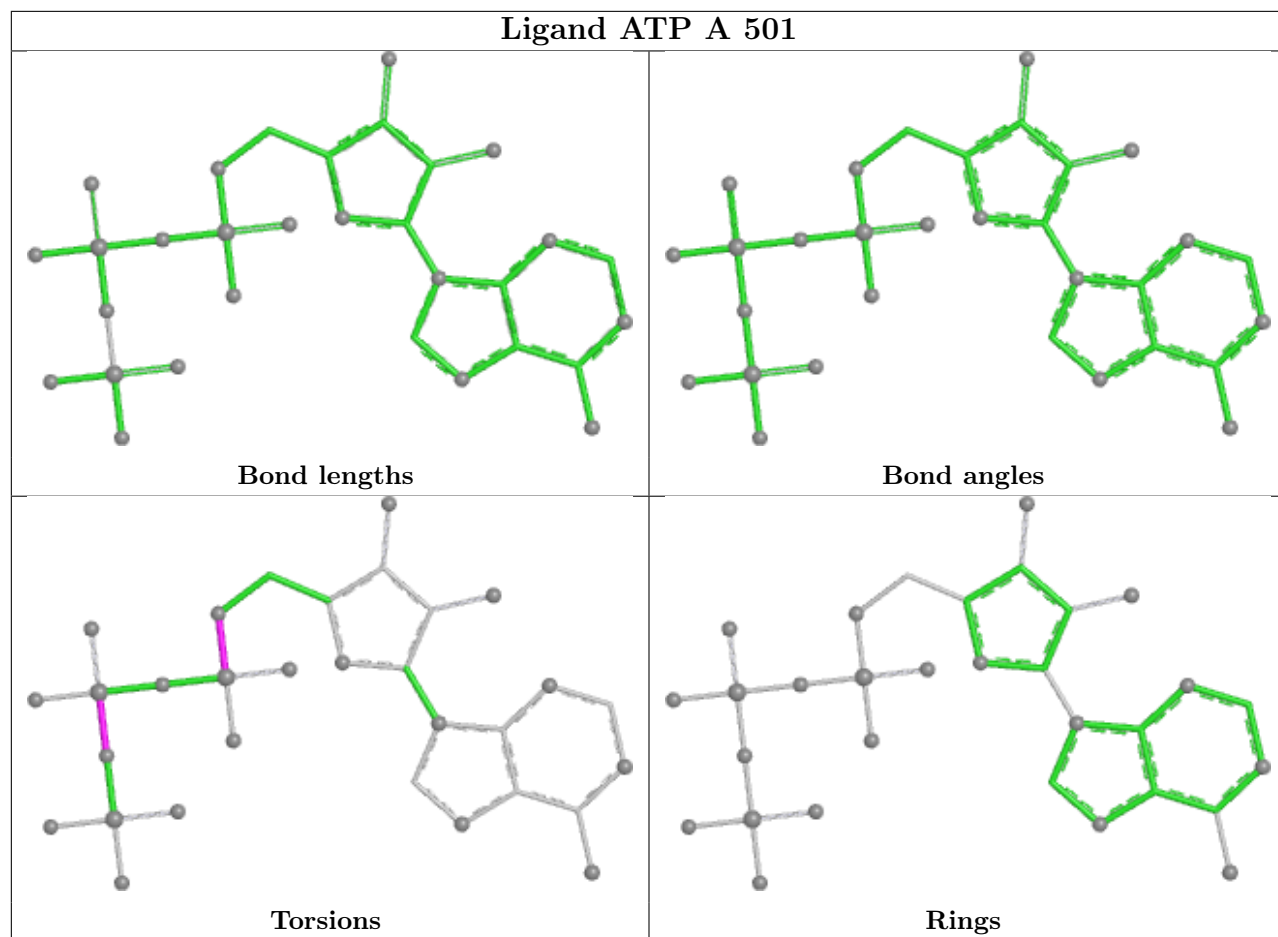


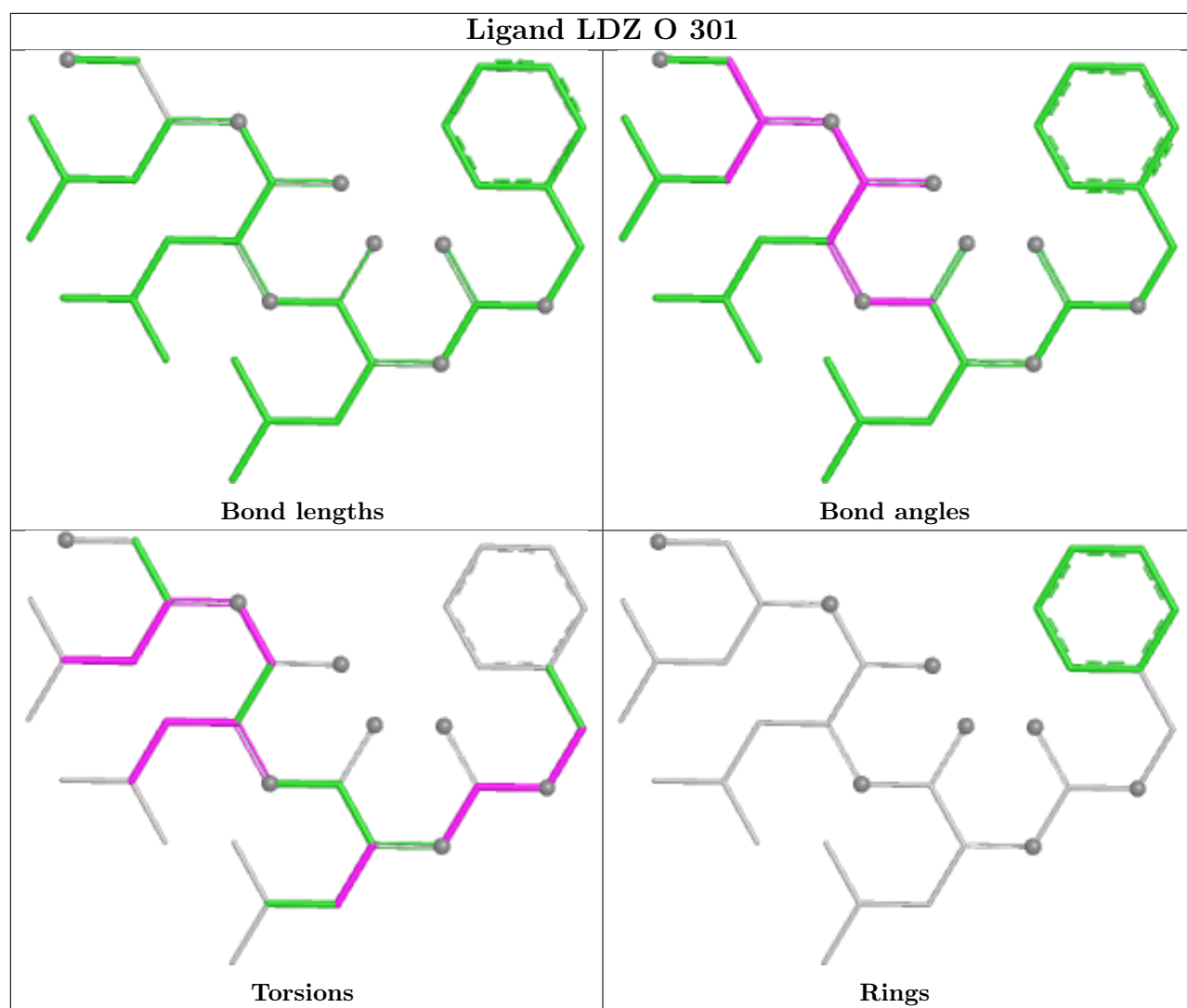


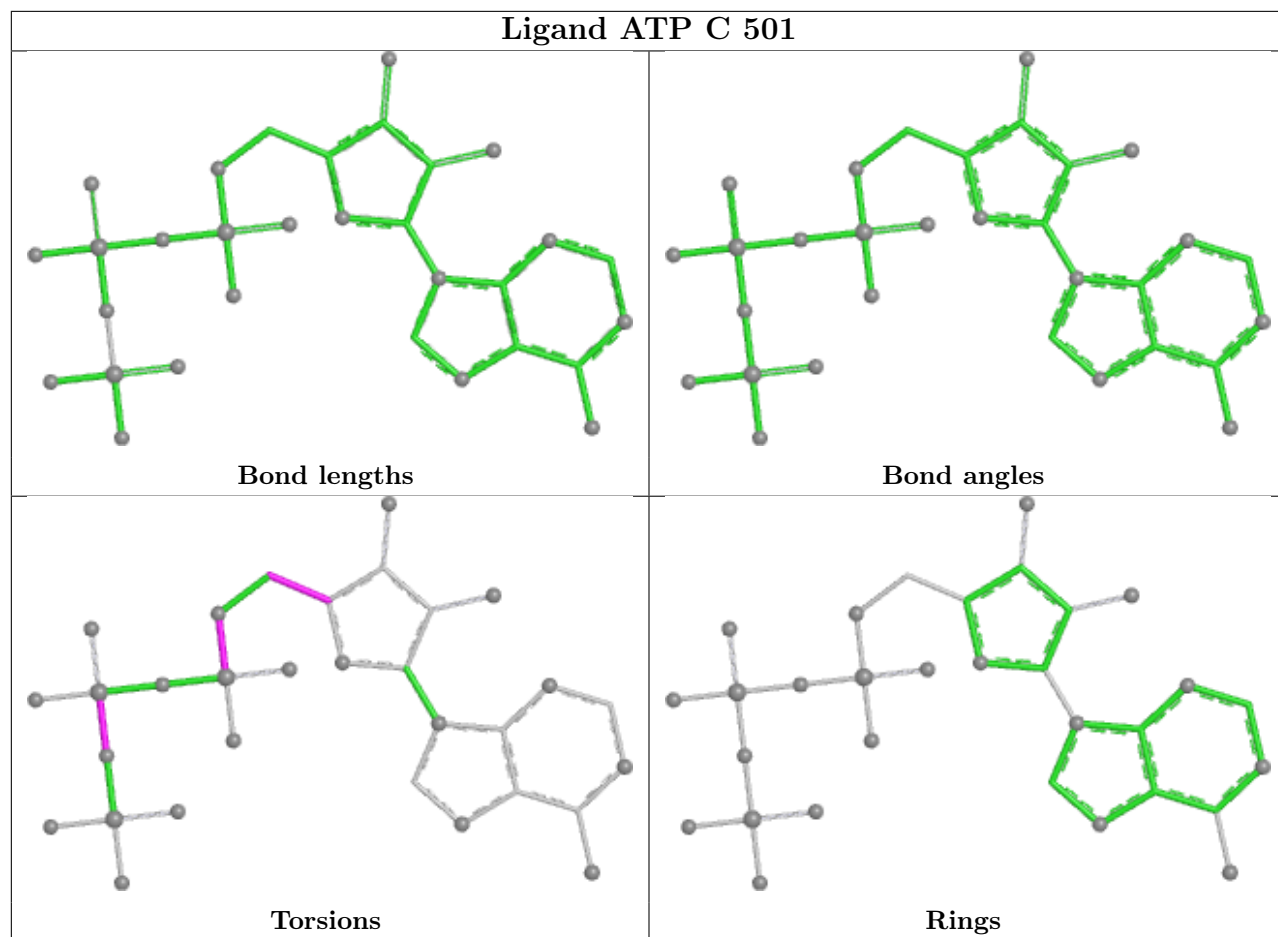


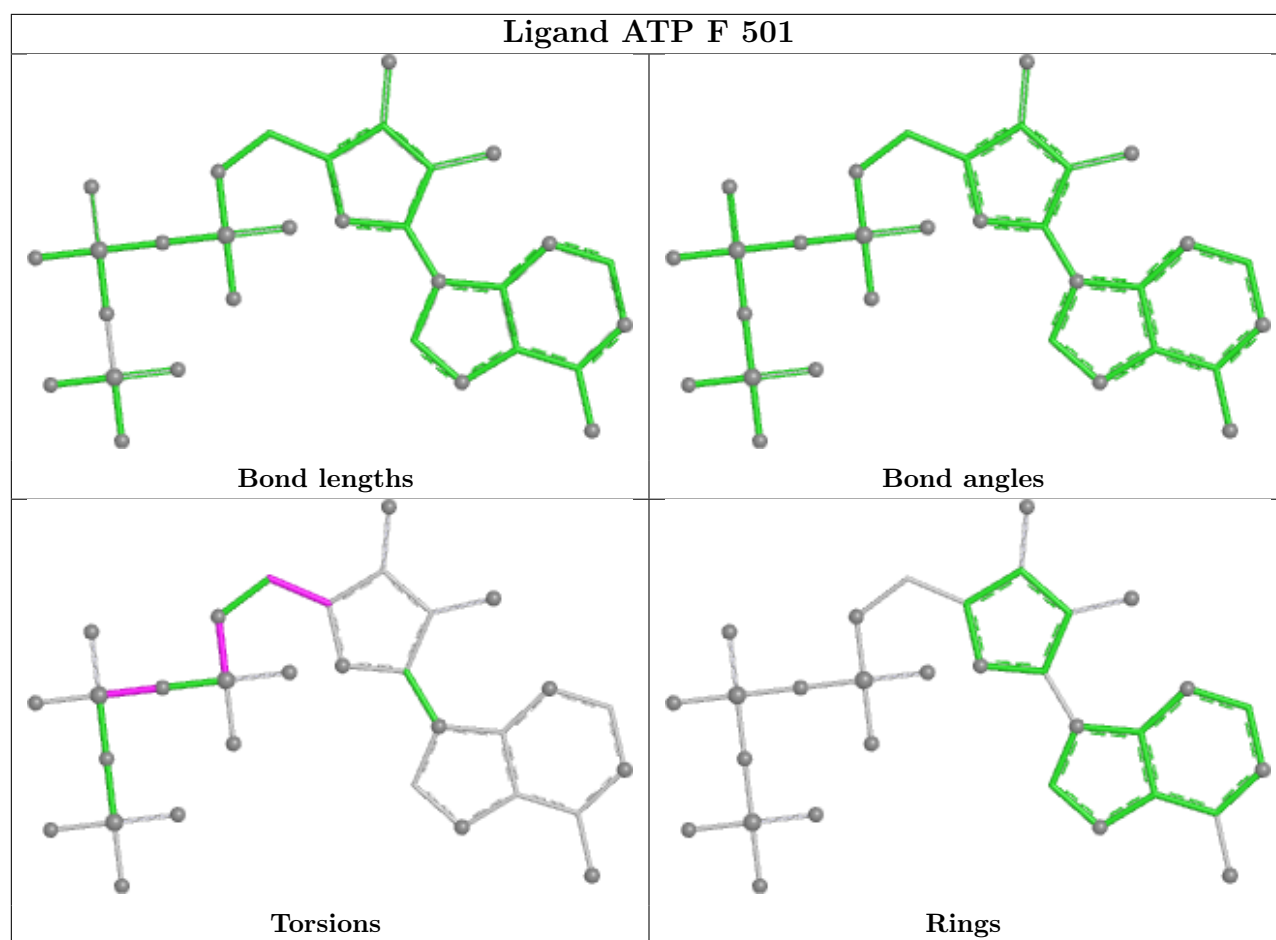












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

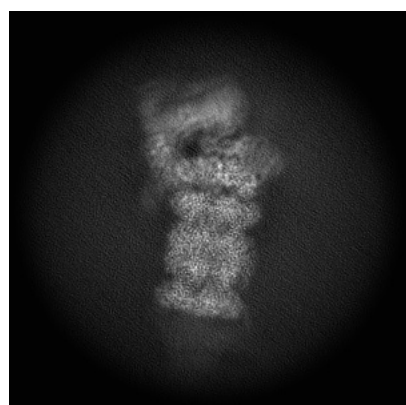
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63777. These allow visual inspection of the internal detail of the map and identification of artifacts.

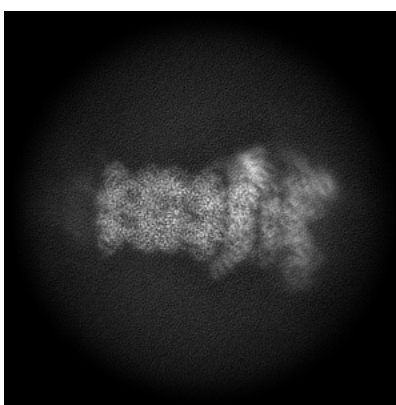
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

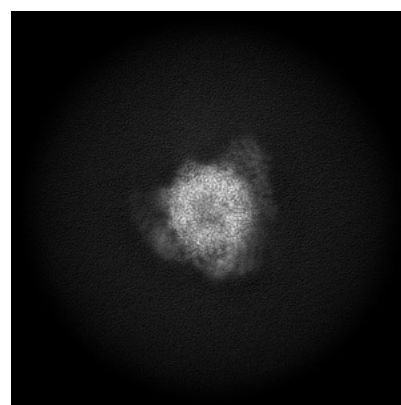
6.1.1 Primary map



X



Y

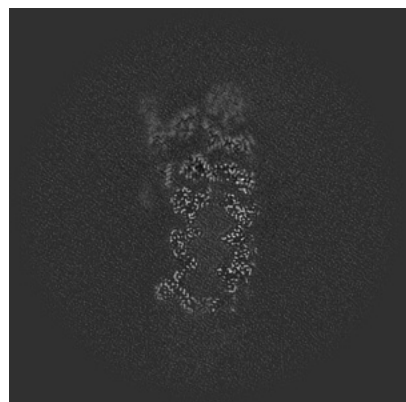


Z

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

6.2 Central slices [i](#)

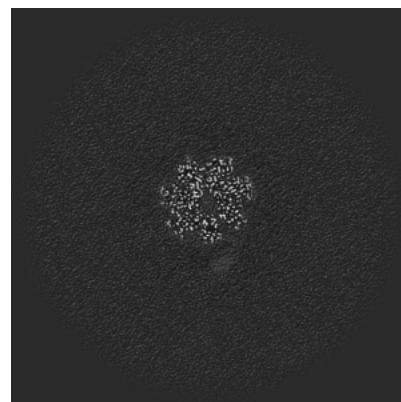
6.2.1 Primary map



X Index: 300



Y Index: 300

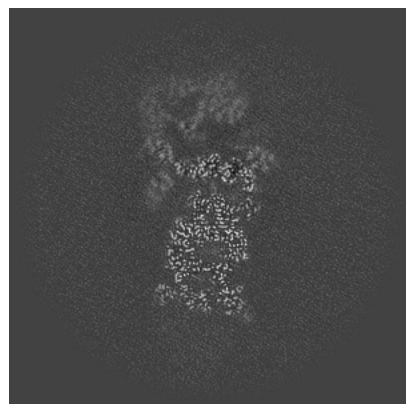


Z Index: 300

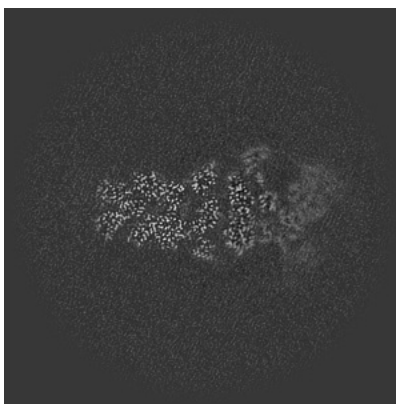
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

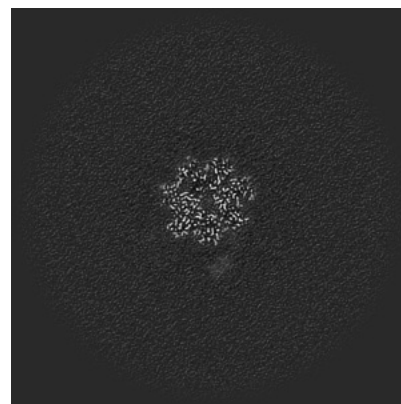
6.3.1 Primary map



X Index: 326



Y Index: 330

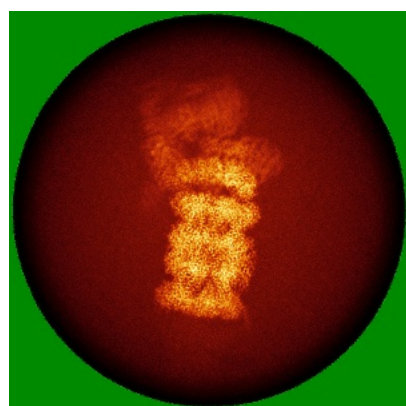


Z Index: 303

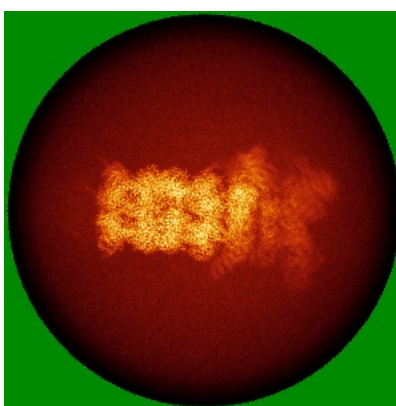
The images above show the largest variance slices of the map in three orthogonal directions.

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

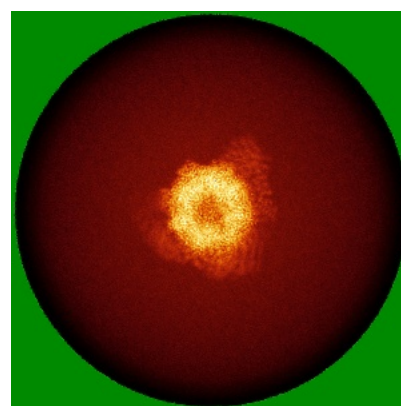
6.4.1 Primary map



X



Y



Z

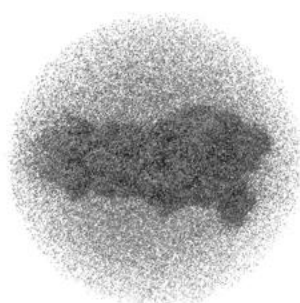
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

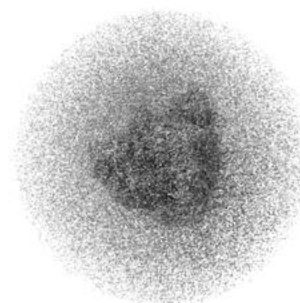
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.42. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

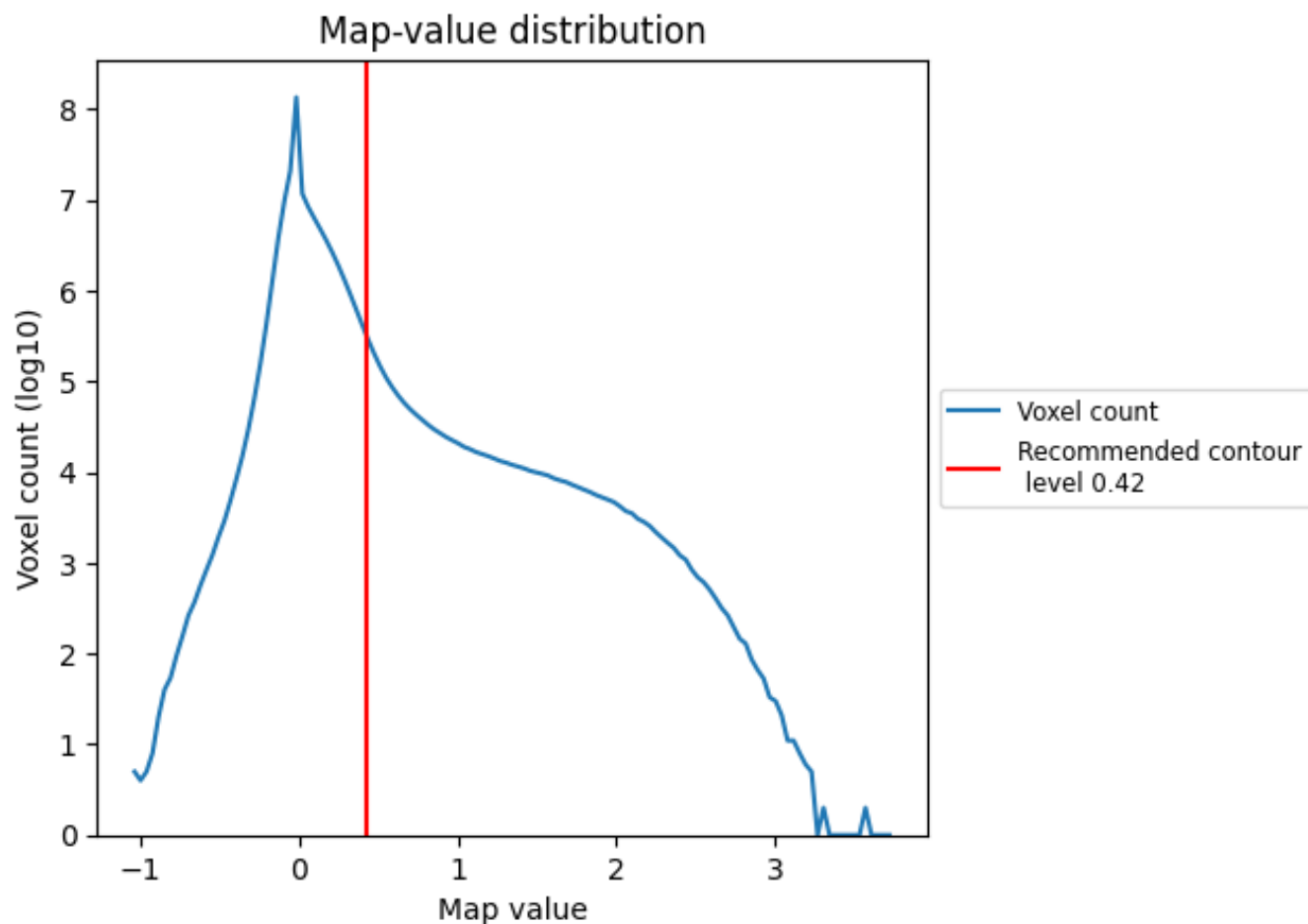
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

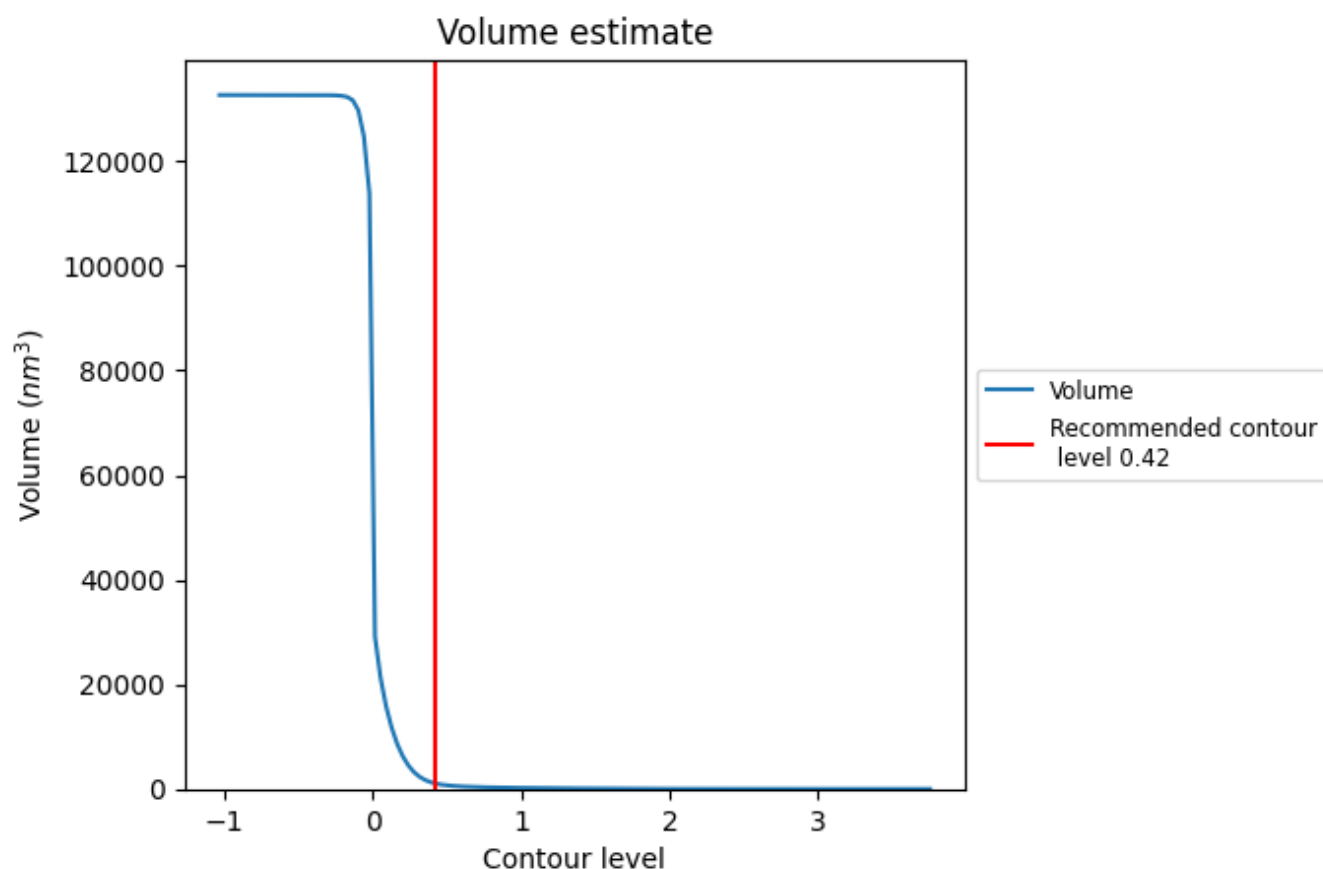
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

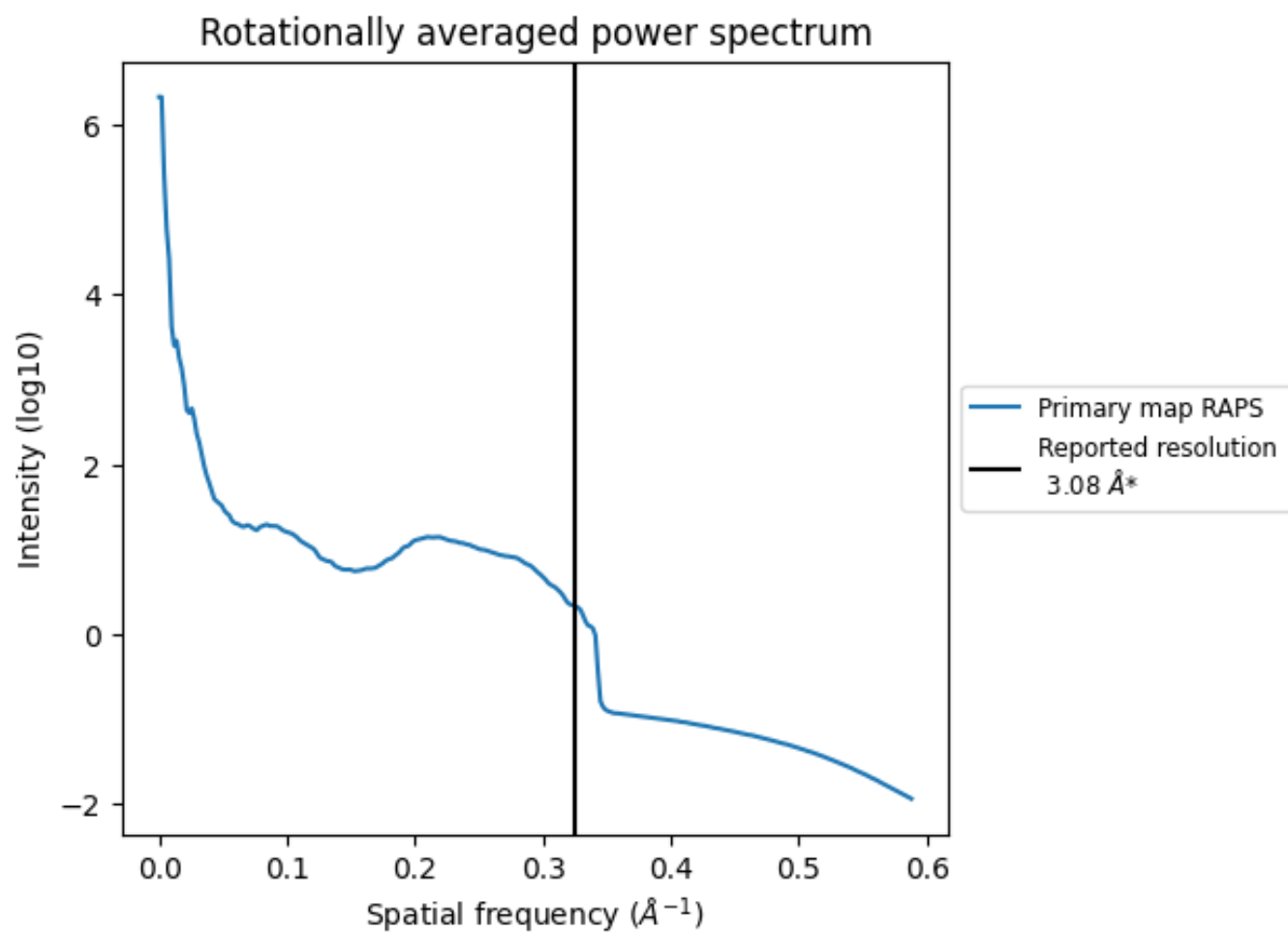
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1067 nm^3 ; this corresponds to an approximate mass of 964 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

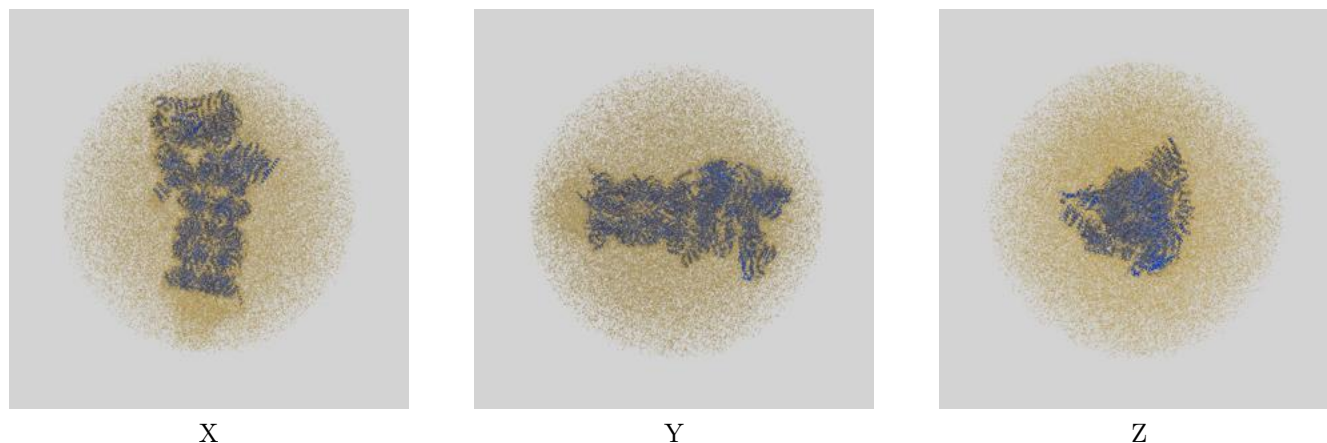
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

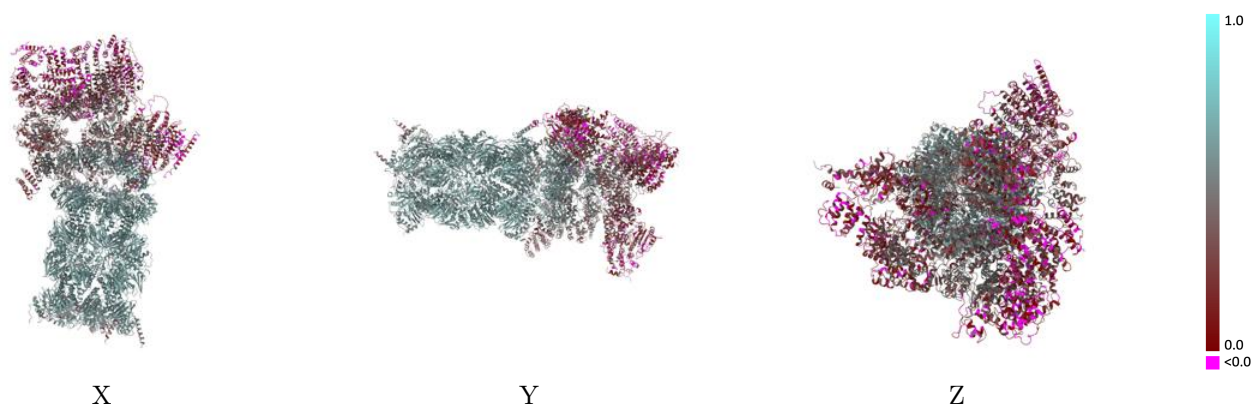
This section contains information regarding the fit between EMDB map EMD-63777 and PDB model 9MBQ. Per-residue inclusion information can be found in section [3](#) on page [14](#).

9.1 Map-model overlay [i](#)



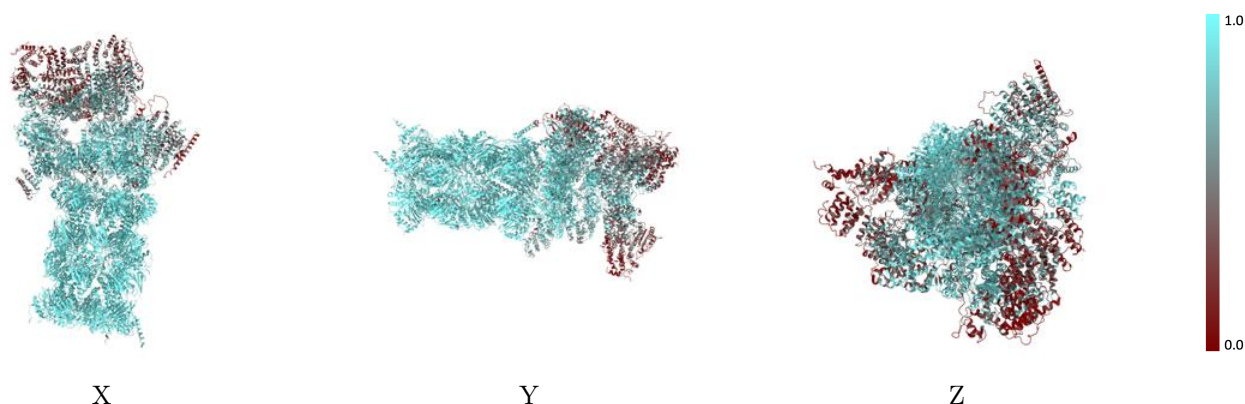
The images above show the 3D surface view of the map at the recommended contour level 0.42 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



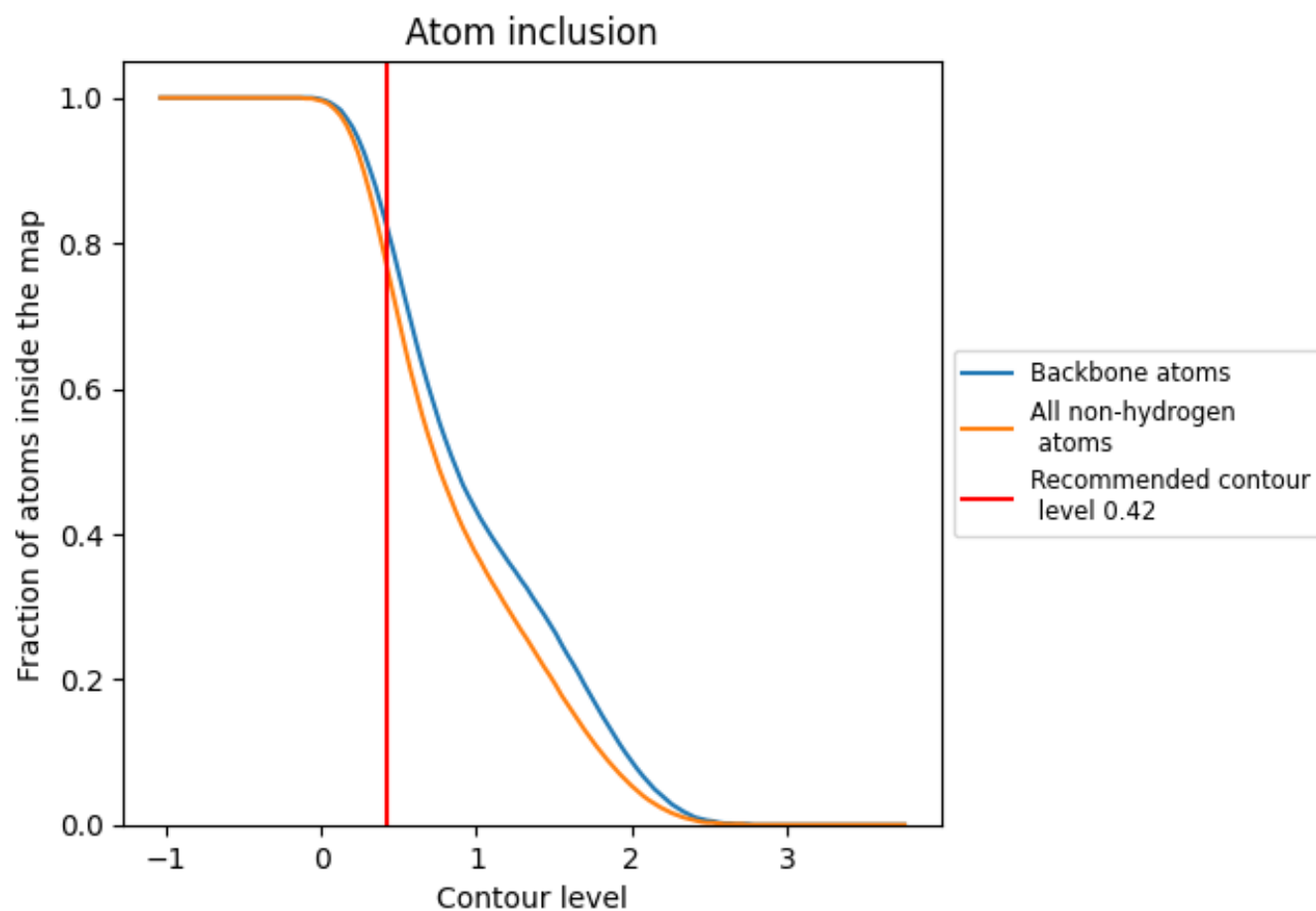
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.42).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.42) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7720	 0.4450
A	 0.8920	 0.5200
B	 0.8930	 0.5210
C	 0.8840	 0.5140
D	 0.8620	 0.4950
E	 0.6140	 0.3340
F	 0.8130	 0.4810
G	 0.9550	 0.5960
H	 0.9620	 0.6010
I	 0.9390	 0.5830
J	 0.9080	 0.5590
K	 0.9490	 0.6010
L	 0.9610	 0.6060
M	 0.9480	 0.5920
N	 0.9710	 0.6180
O	 0.9560	 0.5970
P	 0.9730	 0.6120
Q	 0.9680	 0.6130
R	 0.9690	 0.6160
S	 0.9650	 0.6160
T	 0.9700	 0.6150
U	 0.4140	 0.1930
V	 0.3610	 0.1790
W	 0.6520	 0.3420
X	 0.7200	 0.3930
Y	 0.7590	 0.3820
Z	 0.5910	 0.2270
a	 0.3770	 0.1750
b	 0.3200	 0.1820
c	 0.6810	 0.3490
d	 0.2300	 0.1290
e	 0.6030	 0.2760
f	 0.1750	 0.0870
g	 0.9480	 0.5800
h	 0.9550	 0.5820



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Chain	Atom inclusion	Q-score
i	 0.9080	 0.5620
j	 0.8930	 0.5240
k	 0.8870	 0.5360
l	 0.9300	 0.5650
m	 0.9290	 0.5720
n	 0.9700	 0.6160
o	 0.9620	 0.6000
p	 0.9710	 0.6120
q	 0.9640	 0.6070
r	 0.9600	 0.6080
s	 0.9700	 0.6110
t	 0.9640	 0.6100
v	 0.9710	 0.5650
x	 0.6300	 0.2350