



Full wwPDB EM Validation Report ⓘ

Apr 6, 2026 – 03:44 AM UTC

PDB ID : 9MBP / pdb_00009mbp
EMDB ID : EMD-63776
Title : Substrate-engaged human 26S proteasome bound to midnolin with RPT1 at top of spiral staircase
Authors : Zhu, C.; Qin, L.; Liang, L.
Deposited on : 2025-03-17
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

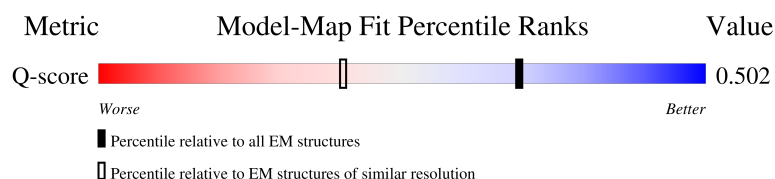
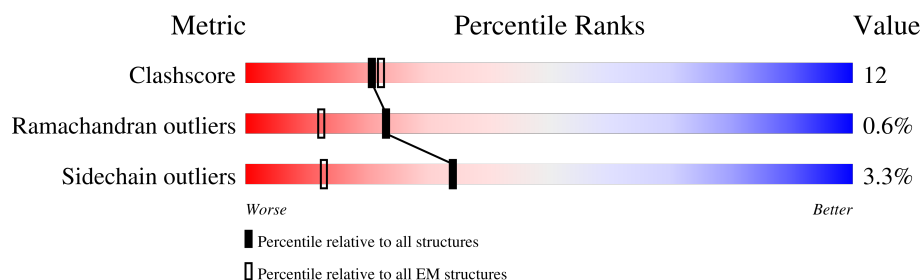
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 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.





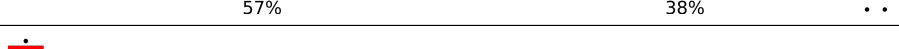
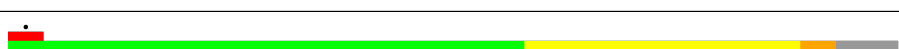
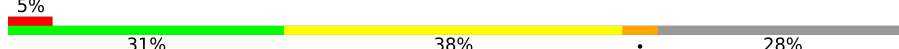


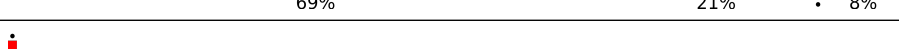



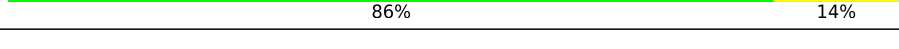

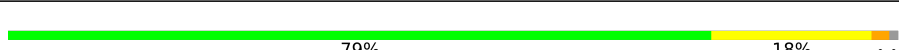


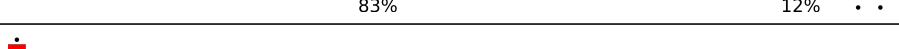







Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10570 (2.25 - 3.25)

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

Mol	Chain	Length	Quality of chain
1	U	953	
2	V	533	
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	309	
10	d	349	
11	e	70	
12	A	433	
13	B	440	
14	C	398	
15	D	418	
16	E	403	
17	F	439	
18	v	14	
19	G	245	
19	g	245	
20	H	233	
20	h	233	
21	I	260	
21	i	260	
22	J	247	
22	j	247	
23	K	240	
23	k	240	
24	L	268	

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Mol	Chain	Length	Quality of chain
24	l	268	
25	M	254	
25	m	254	
26	N	238	
26	n	238	
27	O	276	
27	o	276	
28	P	204	
28	p	204	
29	Q	201	
29	q	201	
30	R	262	
30	r	262	
31	S	240	
31	s	240	
32	T	263	
32	t	263	
33	f	468	
34	u	908	

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 105160 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	845	Total	C	N	O	S	0	0
			6595	4186	1120	1245	44		

- 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	452	Total	C	N	O	S	0	0
			3667	2314	631	697	25		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	b	191	Total	C	N	O	S	0	0
			1454	908	261	277	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	253	Total	C	N	O	S	0	0
			2078	1348	340	381	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
			3105	1954	558	576	17		

- 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 Proteasome 26S subunit, ATPase 6.

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 substrate peptide.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	H	231	Total	C	N	O	S	0	0
			1726	1097	293	331	5		
20	h	232	Total	C	N	O	S	0	0
			1727	1096	292	334	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	I	248	Total	C	N	O	S	0	0
			1895	1195	324	368	8		
21	i	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called Midnolin.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	f	39	Total	C	N	O	S	0	0
			331	196	80	54	1		

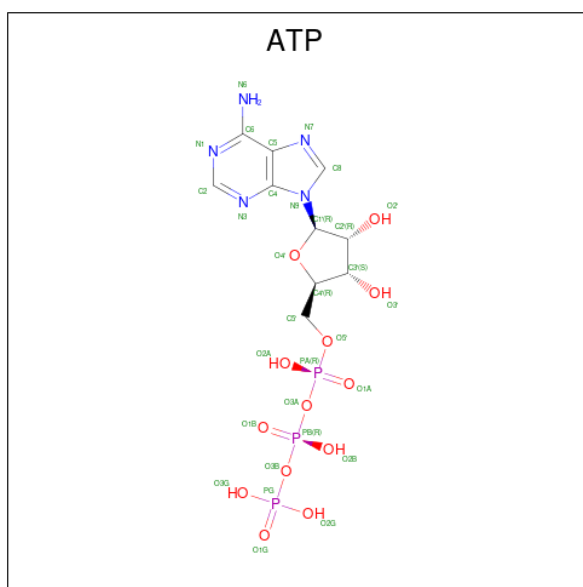
- Molecule 34 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	u	832	Total	C	N	O	S	0	0
			6439	4072	1090	1232	45		

- 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).

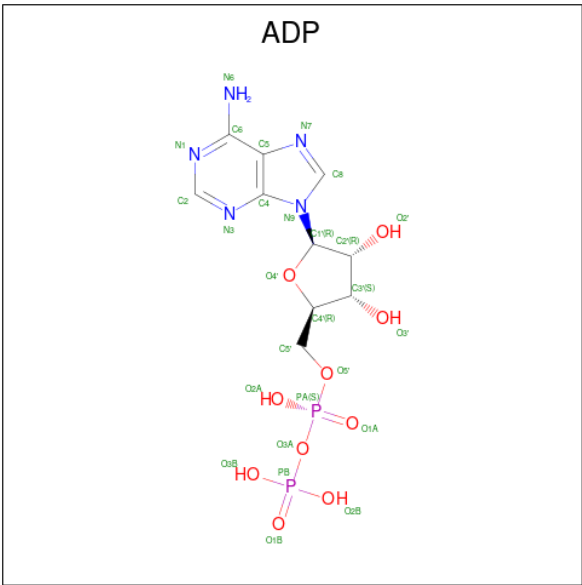


Mol	Chain	Residues	Atoms					AltConf
36	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	C	1	Total	C	N	O	P	0
			31	10	5	13	3	
36	F	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

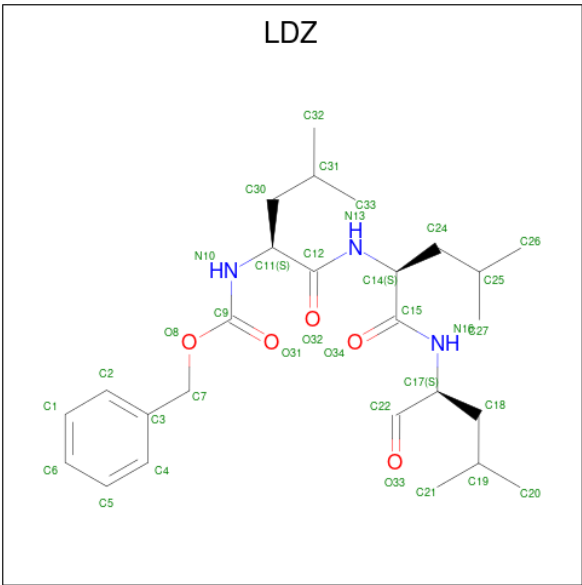
Mol	Chain	Residues	Atoms		AltConf
37	A	1	Total	Mg	0
			1	1	
37	B	1	Total	Mg	0
			1	1	
37	C	1	Total	Mg	0
			1	1	
37	D	1	Total	Mg	0
			1	1	
37	F	1	Total	Mg	0
			1	1	

- Molecule 38 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

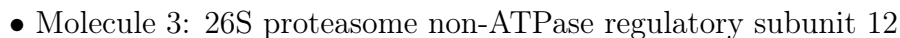
- Molecule 39 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(2S)-4-methyl-1-oxopentan-2-yl]-L-leucinamide (CCD ID: LDZ) (formula: C₂₆H₄₁N₃O₅) (labeled as "Ligand of Interest" by depositor).



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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	

Chain V:

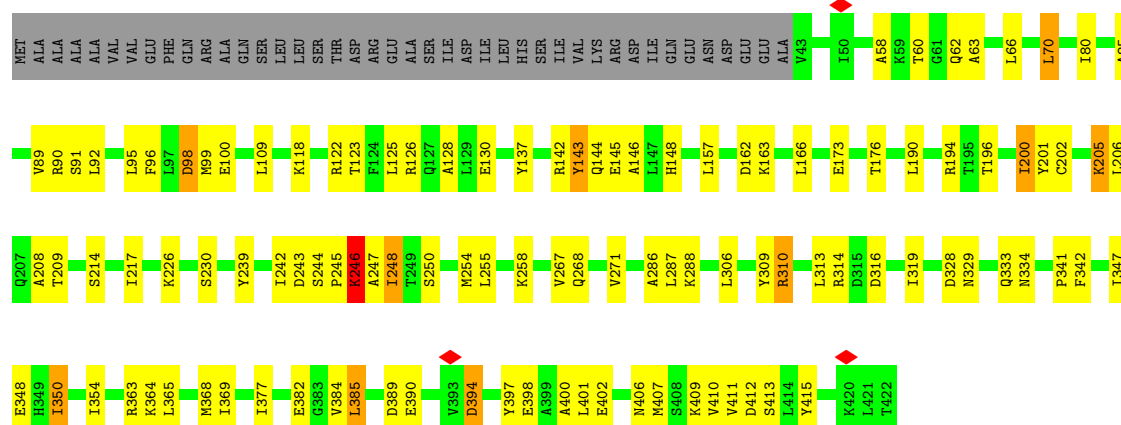


Chain W:

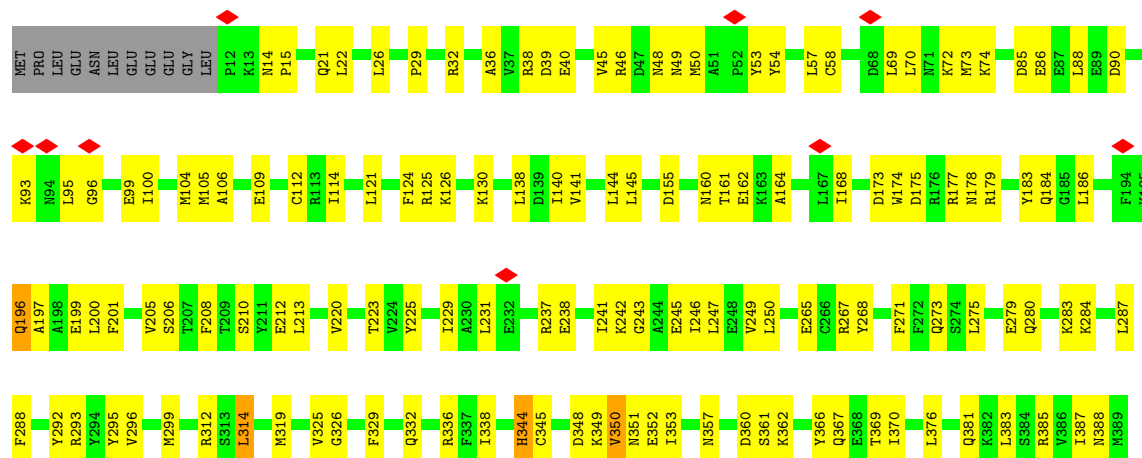




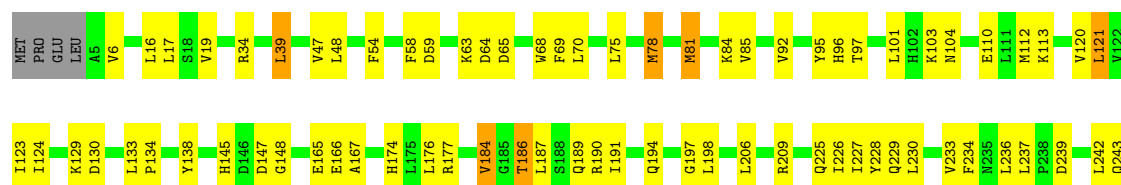
- Molecule 4: 26S proteasome non-ATPase regulatory subunit 11

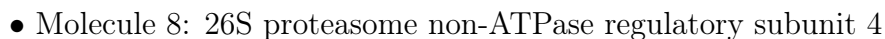


- Molecule 5: 26S proteasome non-ATPase regulatory subunit 6

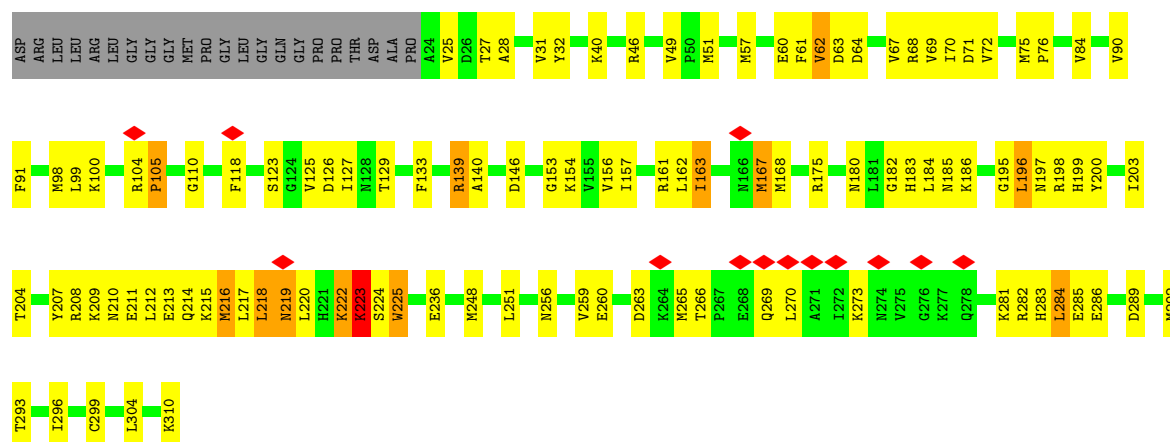


- Molecule 6: 26S proteasome non-ATPase regulatory subunit 7



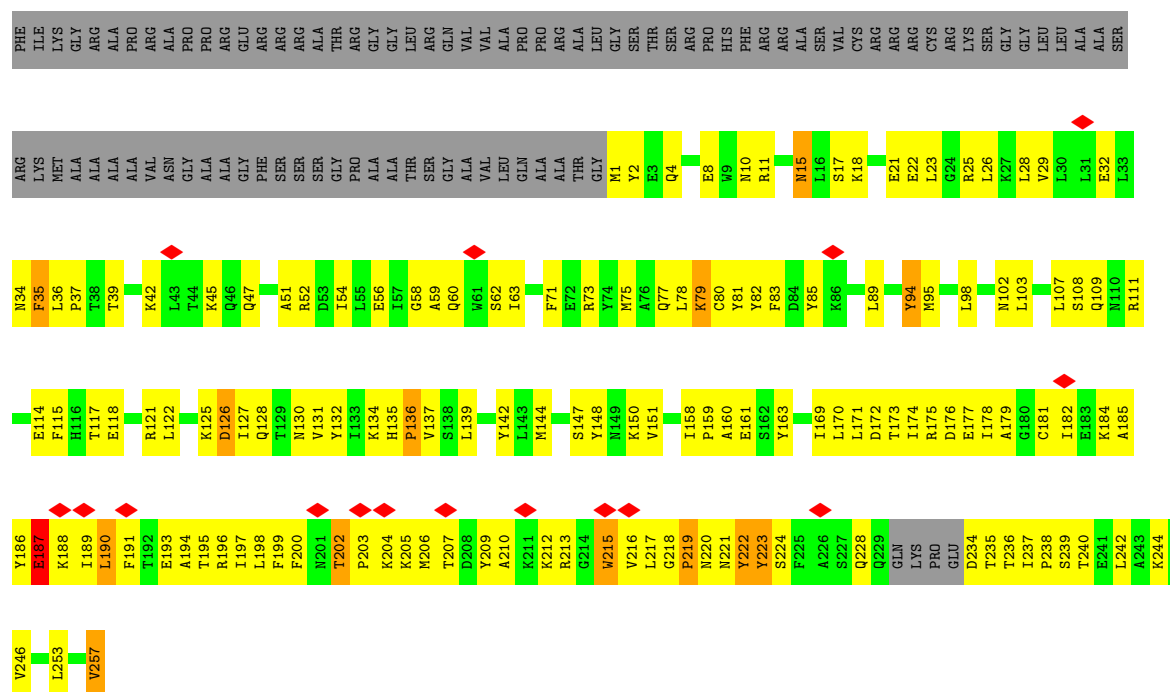


Chain c: 

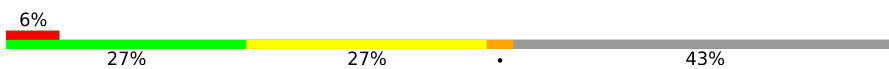


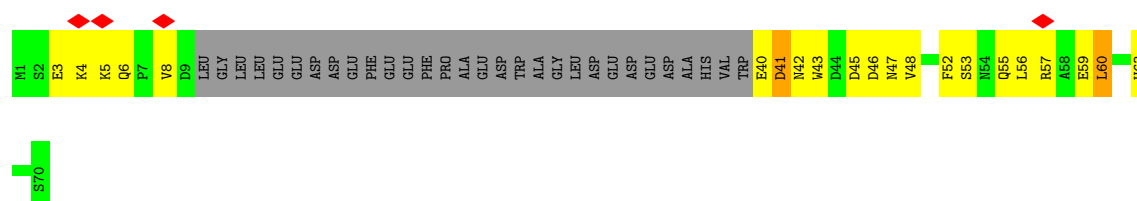
- Molecule 10: 26S proteasome non-ATPase regulatory subunit 8

Chain d: 

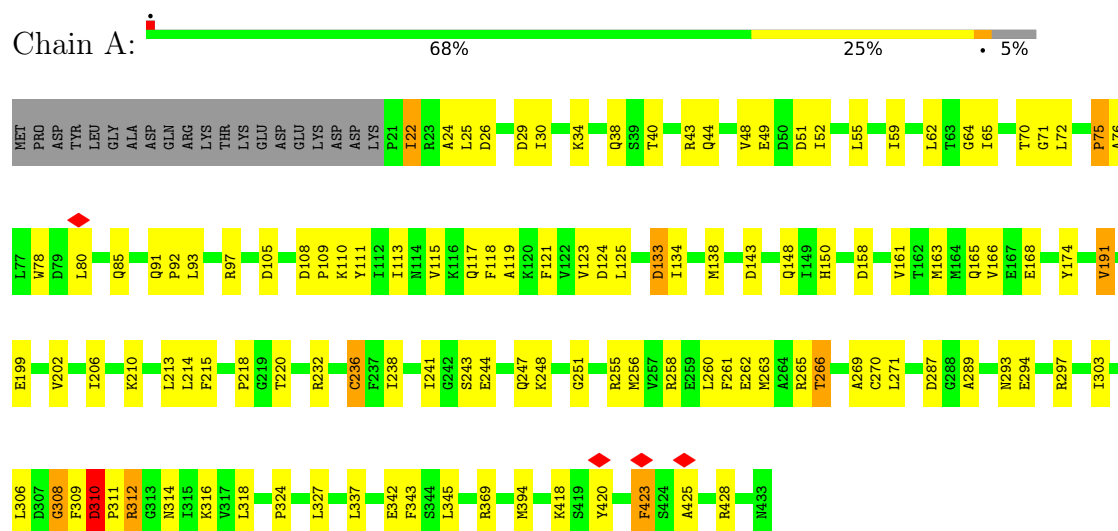


- Molecule 11: 26S proteasome complex subunit SEM1

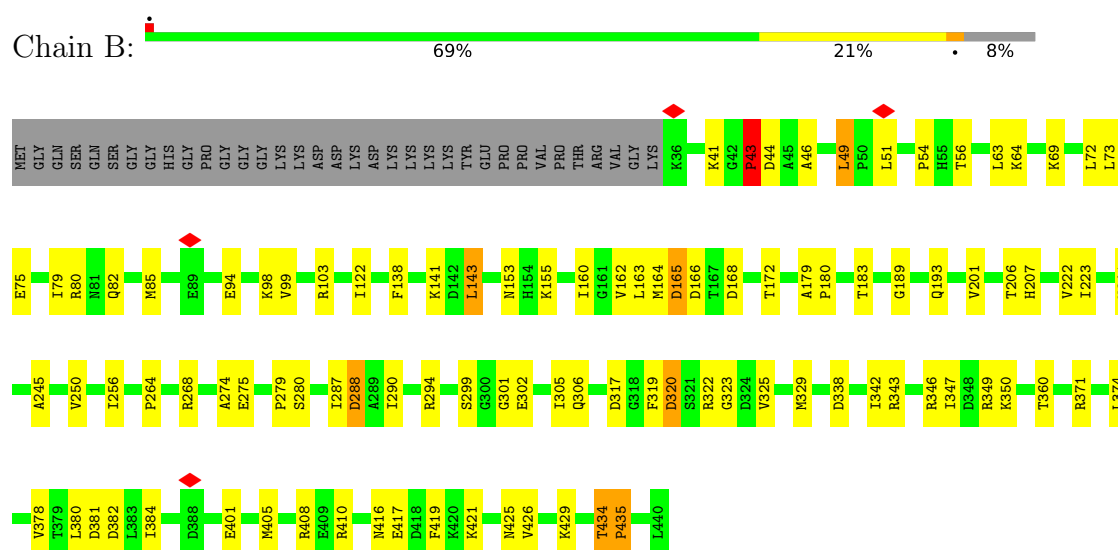
Chain e: 



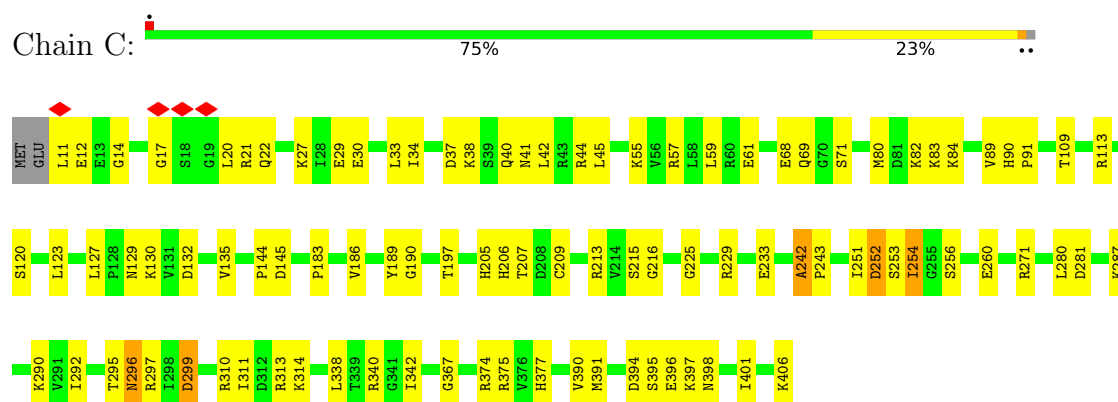
- Molecule 12: 26S proteasome regulatory subunit 7



- Molecule 13: 26S proteasome regulatory subunit 4

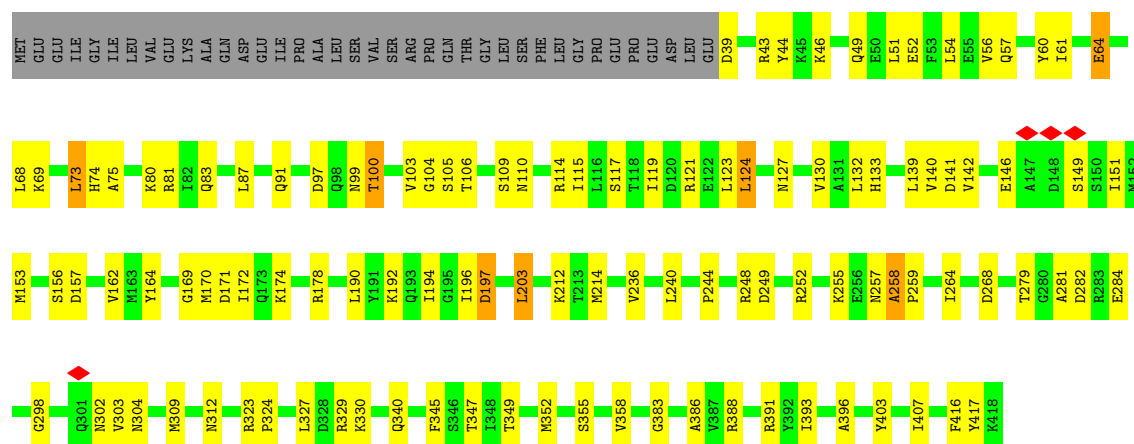


- Molecule 14: 26S proteasome regulatory subunit 8



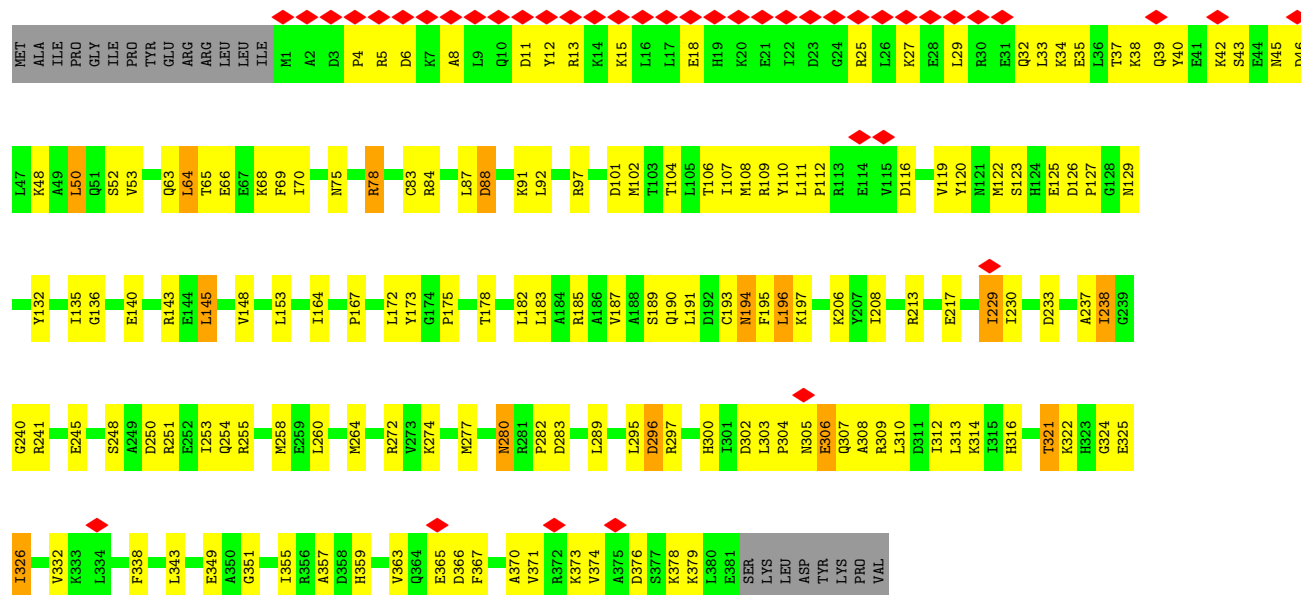
- Molecule 15: 26S proteasome regulatory subunit 6B

Chain D: 



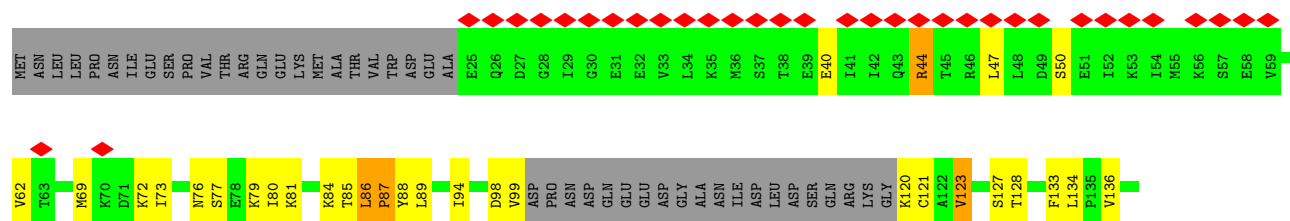
• Molecule 16: Proteasome 26S subunit, ATPase 6

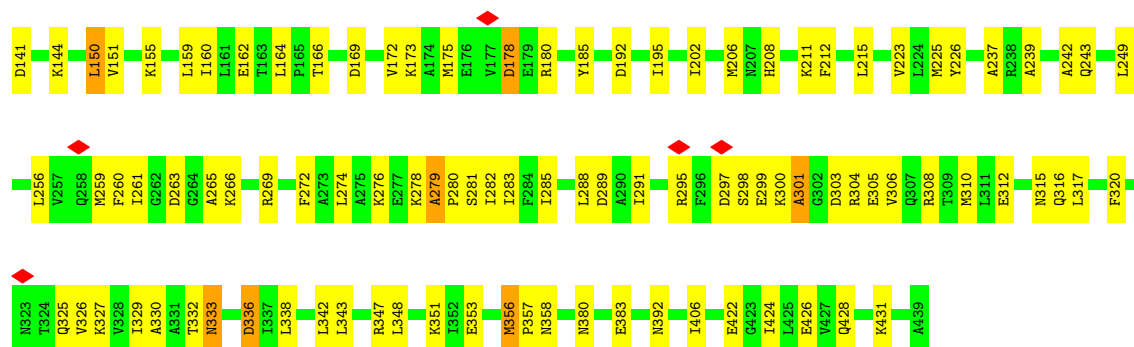
Chain E: 



• Molecule 17: 26S proteasome regulatory subunit 6A

Chain F: 





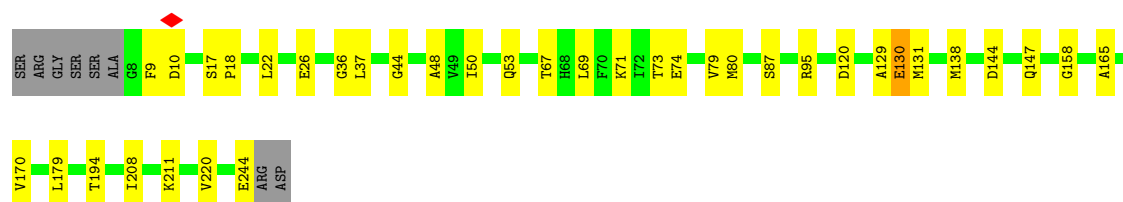
- Molecule 18: substrate peptide

Chain v: 86% 14%



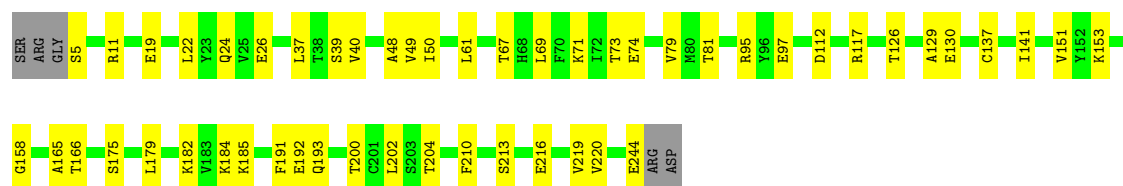
- Molecule 19: Proteasome subunit alpha type-6

Chain G: 82% 15%



- Molecule 19: Proteasome subunit alpha type-6

Chain g: 77% 21%




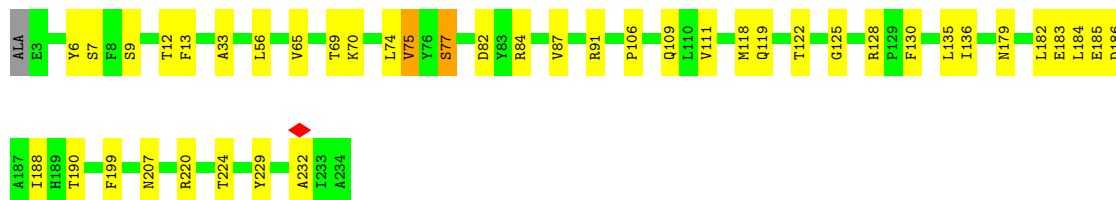
- Molecule 20: Proteasome subunit alpha type-2

Chain H: 79% 18%



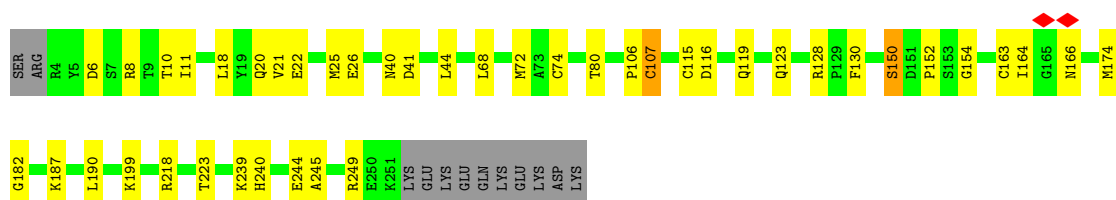
- Molecule 20: Proteasome subunit alpha type-2

Chain h:  82% 17%




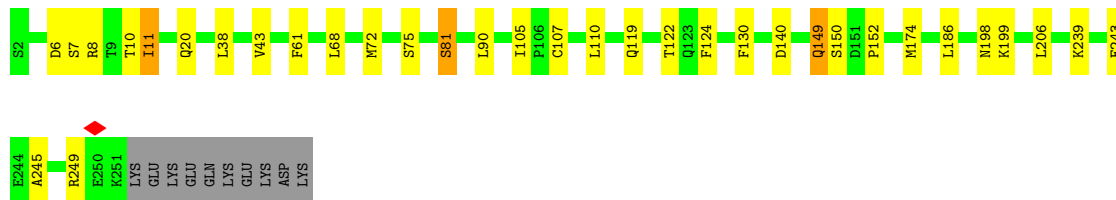
- Molecule 21: Proteasome subunit alpha type-4

Chain I:  79% 16% 5%




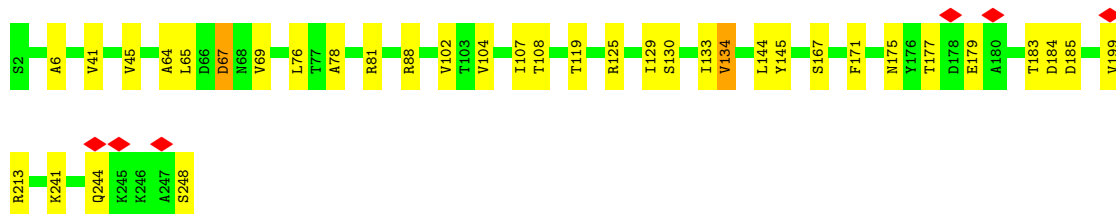
- Molecule 21: Proteasome subunit alpha type-4

Chain i:  83% 12%




- Molecule 22: Proteasome subunit alpha type-7

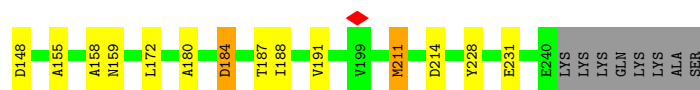
Chain J:  85% 14%



- Molecule 22: Proteasome subunit alpha type-7

Chain j:  77% 17%





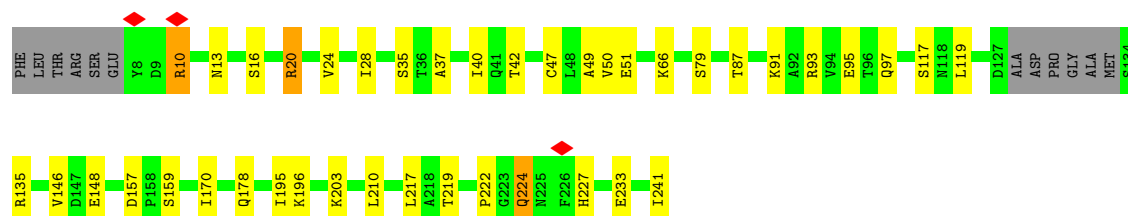
• Molecule 23: Proteasome subunit alpha type-5

Chain K: 82% 14%



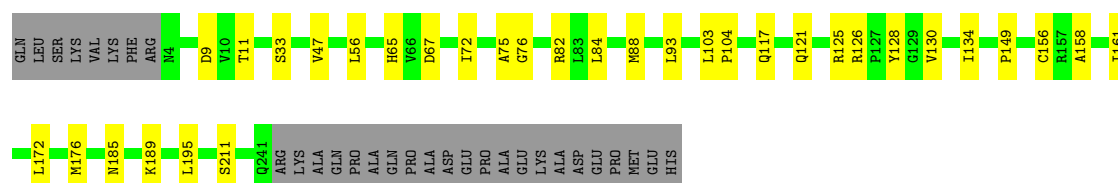
• Molecule 23: Proteasome subunit alpha type-5

Chain k: 78% 16% 5%



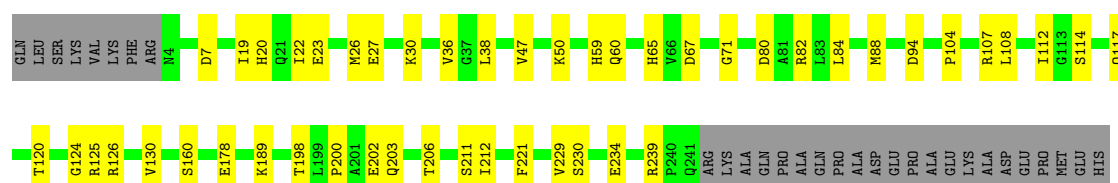
• Molecule 24: Isoform Long of Proteasome subunit alpha type-1

Chain L: 76% 12% 11%



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

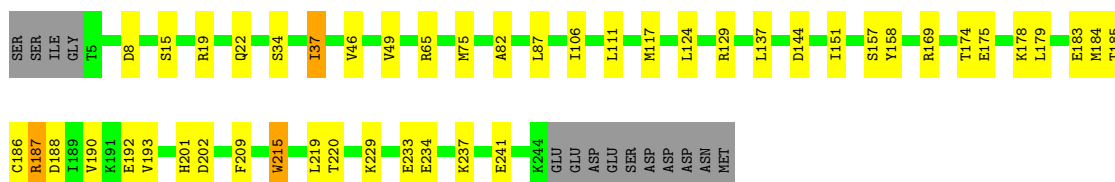
Chain l: 71% 18% 11%



• Molecule 25: Proteasome subunit alpha type-3

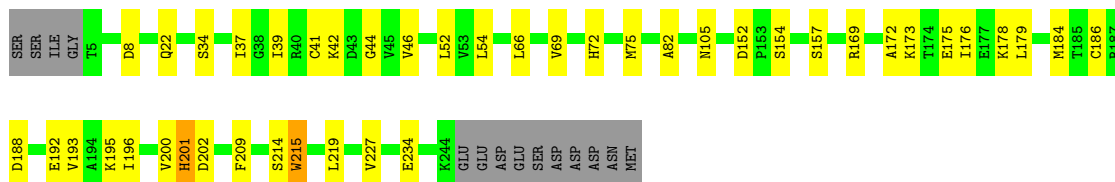
Chain M: 76% 17% 6%





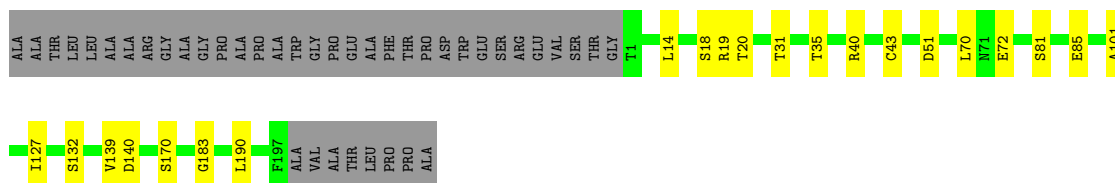
- Molecule 25: Proteasome subunit alpha type-3

Chain m: 78% 16% 6%



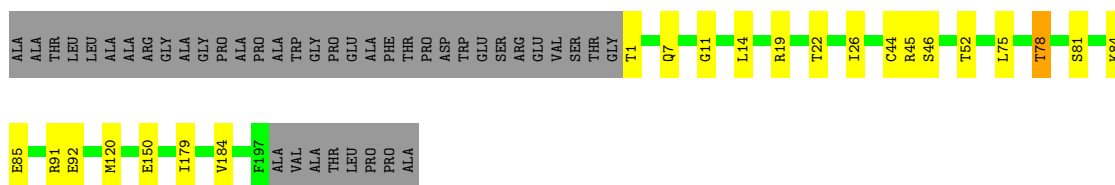
- Molecule 26: Proteasome subunit beta type-6

Chain N: 74% 9% 17%



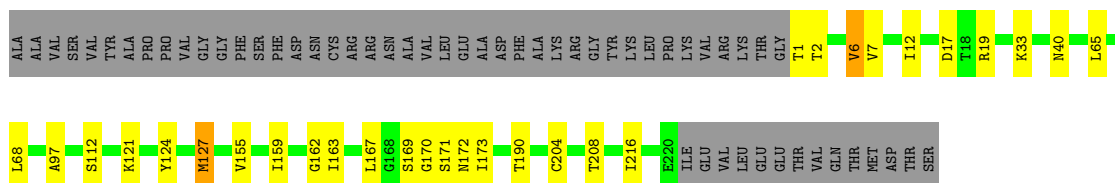
- Molecule 26: Proteasome subunit beta type-6

Chain n: 74% 9% 17%



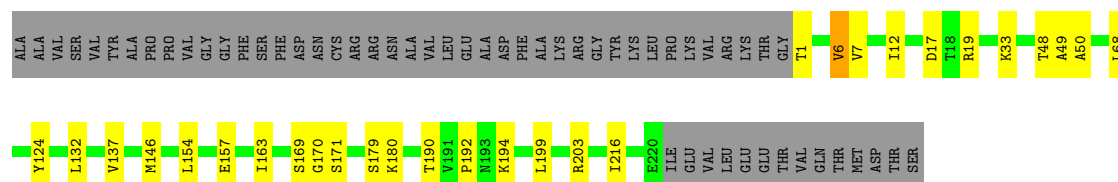
- Molecule 27: Proteasome subunit beta type-7

Chain O: 69% 10% 20%

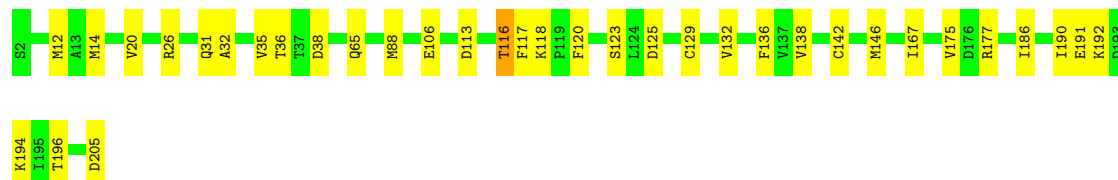
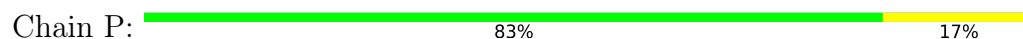


- Molecule 27: Proteasome subunit beta type-7

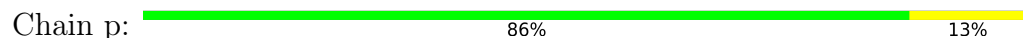
Chain o: 69% 10% 20%



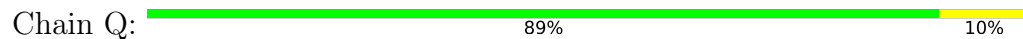
• Molecule 28: Proteasome subunit beta type-3



• Molecule 28: Proteasome subunit beta type-3



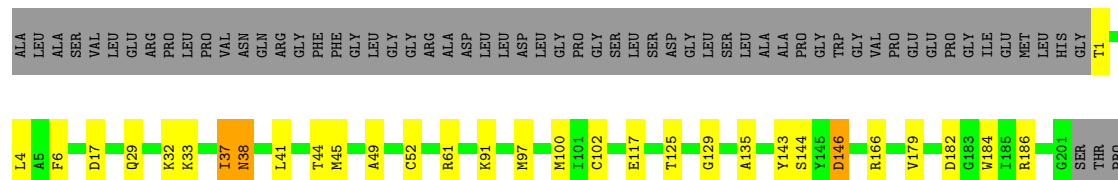
• Molecule 29: Proteasome subunit beta type-2



• Molecule 29: Proteasome subunit beta type-2

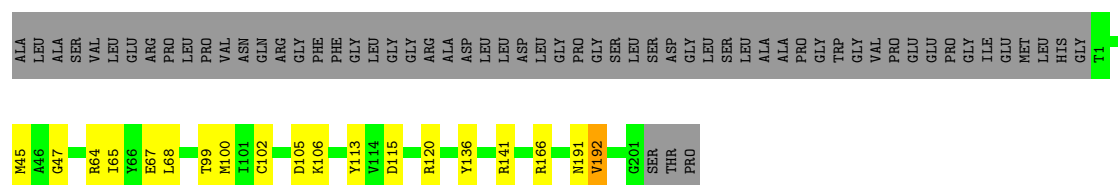


• Molecule 30: Proteasome subunit beta type-5




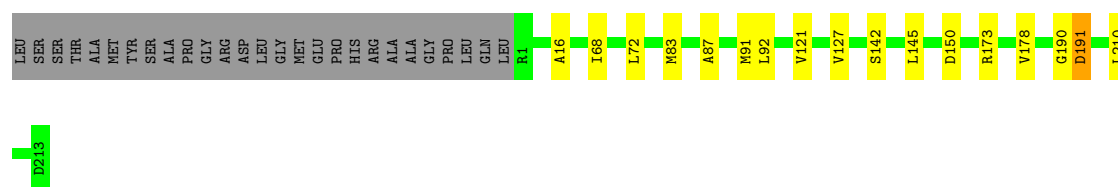
• Molecule 30: Proteasome subunit beta type-5

Chain r:  69% 7% 23%




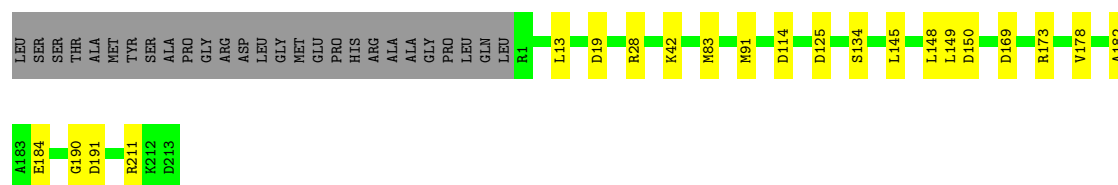
• Molecule 31: Proteasome subunit beta type-1

Chain S:  82% 7% 11%



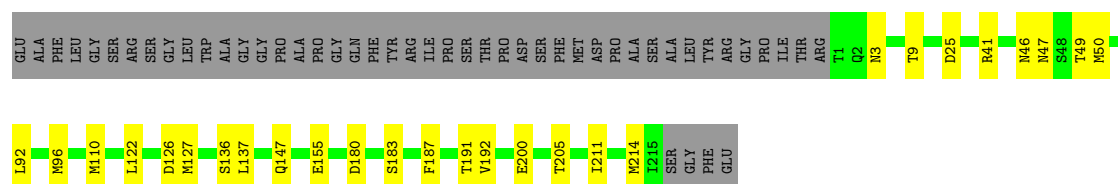
• Molecule 31: Proteasome subunit beta type-1

Chain s:  80% 9% 11%




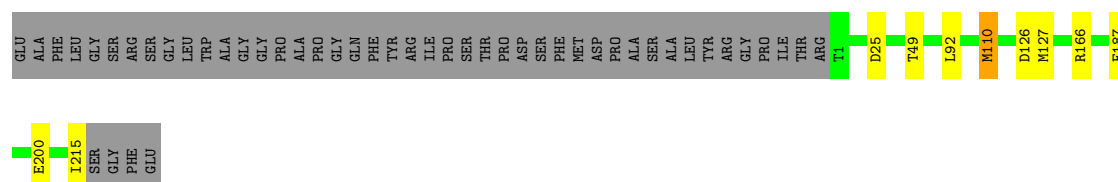
• Molecule 32: Proteasome subunit beta type-4

Chain T:  71% 10% 18%

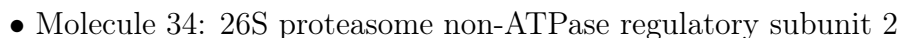


• Molecule 32: Proteasome subunit beta type-4

Chain t:  78% 18%



• Molecule 33: Midnolin





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40572	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)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.637	Depositor
Minimum map value	-16.829	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.997	Depositor
Recommended contour level	2	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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.24	0/6710	0.54	2/9074 (0.0%)
2	V	0.20	0/3929	0.56	1/5309 (0.0%)
3	W	0.26	0/3713	0.59	3/4988 (0.1%)
4	X	0.30	0/3053	0.50	1/4115 (0.0%)
5	Y	0.18	0/3173	0.48	0/4273
6	Z	0.19	0/2324	0.51	0/3150
7	a	0.23	0/3053	0.52	1/4133 (0.0%)
8	b	0.32	0/1474	0.59	2/1996 (0.1%)
9	c	0.33	0/2302	0.63	3/3110 (0.1%)
10	d	0.28	0/2122	0.64	2/2864 (0.1%)
11	e	0.21	0/338	0.66	0/450
12	A	0.26	0/3283	0.51	1/4433 (0.0%)
13	B	0.18	0/3208	0.46	2/4327 (0.0%)
14	C	0.19	0/3146	0.44	3/4226 (0.1%)
15	D	0.17	0/3090	0.42	0/4168
16	E	0.15	0/3077	0.42	0/4141
17	F	0.22	0/3137	0.47	0/4223
18	v	1.10	0/69	1.52	0/95
19	G	0.18	0/1842	0.41	1/2500 (0.0%)
19	g	0.15	0/1863	0.34	0/2527
20	H	0.27	0/1762	0.47	0/2394
20	h	0.15	0/1764	0.31	0/2399
21	I	0.29	0/1925	0.46	1/2606 (0.0%)
21	i	0.16	0/1942	0.37	0/2628
22	J	0.16	0/1869	0.37	0/2531
22	j	0.15	0/1728	0.37	0/2358
23	K	0.17	0/1772	0.33	0/2397
23	k	0.15	0/1747	0.33	0/2364
24	L	0.16	0/1885	0.33	0/2552
24	l	0.15	0/1885	0.34	0/2552
25	M	0.27	0/1891	0.47	0/2552
25	m	0.19	0/1897	0.41	0/2559

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
26	N	0.17	0/1508	0.34	0/2040
26	n	0.18	0/1508	0.35	0/2040
27	O	0.19	0/1670	0.39	0/2265
27	o	0.17	0/1670	0.41	0/2265
28	P	0.18	0/1620	0.36	0/2184
28	p	0.17	0/1620	0.35	0/2184
29	Q	0.17	0/1603	0.35	0/2174
29	q	0.17	0/1607	0.37	0/2178
30	R	0.18	0/1579	0.36	0/2134
30	r	0.16	0/1579	0.31	0/2134
31	S	0.17	0/1671	0.35	0/2253
31	s	0.17	0/1671	0.33	0/2253
32	T	0.18	0/1700	0.36	0/2305
32	t	0.17	0/1706	0.33	0/2312
33	f	0.12	0/331	0.31	0/436
34	u	0.15	0/6548	0.39	0/8864
All	All	0.21	0/106564	0.45	23/144015 (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
3	W	0	1
12	A	0	1
25	M	0	2
All	All	0	4

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	43	PRO	CA-N-CD	-10.43	97.39	112.00
1	U	119	PRO	CA-N-CD	-10.40	97.43	112.00
13	B	435	PRO	CA-N-CD	-9.68	98.45	112.00
12	A	75	PRO	CA-N-CD	-9.07	99.31	112.00
4	X	341	PRO	CA-N-CD	-8.35	100.31	112.00
1	U	174	PRO	N-CA-C	-6.93	104.83	113.84
9	c	139	ARG	CA-CB-CG	6.56	127.23	114.10
7	a	164	GLN	N-CA-C	-6.38	104.33	111.28
9	c	167	MET	CB-CG-SD	6.35	131.75	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	I	128	ARG	N-CA-C	-6.03	101.77	110.40
9	c	105	PRO	CA-N-CD	-5.96	103.66	112.00
8	b	177	PRO	N-CA-CB	-5.59	97.38	103.25
3	W	63	THR	N-CA-C	-5.49	106.28	112.87
14	C	252	ASP	N-CA-C	-5.41	105.28	111.07
2	V	133	PRO	CA-N-CD	-5.40	104.44	112.00
10	d	136	PRO	CA-N-CD	-5.24	104.67	112.00
19	G	211	LYS	N-CA-C	-5.20	102.60	110.50
14	C	296	ASN	CA-C-N	5.18	131.44	121.54
14	C	296	ASN	C-N-CA	5.18	131.44	121.54
8	b	181	ASP	N-CA-C	-5.15	105.64	112.34
3	W	64	SER	N-CA-C	-5.11	105.69	112.34
10	d	190	LEU	N-CA-C	5.09	121.64	110.80
3	W	59	ASP	N-CA-C	-5.08	107.15	113.19

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	A	312	ARG	Sidechain
25	M	183	GLU	Mainchain
25	M	187	ARG	Sidechain
3	W	65	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	U	6595	0	6648	239	0
2	V	3852	0	3893	182	0
3	W	3667	0	3786	218	0
4	X	3009	0	3113	92	0
5	Y	3115	0	3120	107	0
6	Z	2281	0	2312	93	0
7	a	2995	0	3012	125	0
8	b	1454	0	1501	83	0
9	c	2260	0	2276	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	d	2078	0	2107	169	0
11	e	334	0	294	19	0
12	A	3229	0	3263	89	0
13	B	3162	0	3224	78	0
14	C	3105	0	3219	70	0
15	D	3040	0	3076	81	0
16	E	3031	0	3103	117	0
17	F	3098	0	3187	111	0
18	v	70	0	69	1	0
19	G	1809	0	1781	22	0
19	g	1830	0	1807	30	0
20	H	1726	0	1646	33	0
20	h	1727	0	1619	25	0
21	I	1895	0	1833	28	0
21	i	1912	0	1851	23	0
22	J	1844	0	1747	19	0
22	j	1704	0	1517	31	0
23	K	1746	0	1695	19	0
23	k	1722	0	1673	24	0
24	L	1850	0	1822	18	0
24	l	1850	0	1822	29	0
25	M	1856	0	1816	28	0
25	m	1862	0	1827	25	0
26	N	1482	0	1450	10	0
26	n	1482	0	1450	12	0
27	O	1643	0	1644	22	0
27	o	1643	0	1644	20	0
28	P	1591	0	1609	21	0
28	p	1591	0	1609	16	0
29	Q	1570	0	1547	13	0
29	q	1574	0	1558	17	0
30	R	1548	0	1499	20	0
30	r	1548	0	1499	13	0
31	S	1641	0	1618	10	0
31	s	1641	0	1618	13	0
32	T	1667	0	1628	14	0
32	t	1673	0	1639	5	0
33	f	331	0	361	12	0
34	u	6439	0	6456	161	0
35	c	1	0	0	0	0
36	A	31	0	12	0	0
36	B	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	D	1	0	0	0	0
37	F	1	0	0	0	0
38	D	27	0	12	2	0
38	E	27	0	12	1	0
39	N	34	0	41	1	0
39	O	34	0	41	3	0
39	R	34	0	41	4	0
39	n	34	0	41	3	0
39	o	34	0	41	3	0
39	r	34	0	41	4	0
All	All	105160	0	104806	2526	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 12.

All (2526) 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)
10:d:218:GLY:CA	10:d:222:TYR:HA	1.64	1.25
6:Z:16:LEU:HD13	9:c:216:MET:CE	1.73	1.16
10:d:218:GLY:HA3	10:d:222:TYR:HA	1.22	1.16
10:d:186:TYR:HB2	10:d:221:ASN:HB2	1.36	1.07
6:Z:16:LEU:CD1	9:c:216:MET:HE2	1.85	1.05
8:b:22:LEU:HD23	8:b:177:PRO:HB2	1.38	1.05
2:V:148:ARG:HD2	2:V:149:PRO:HD3	1.43	0.98
12:A:75:PRO:HD2	12:A:76:ALA:H	1.31	0.96
10:d:189:ILE:H	10:d:220:ASN:N	1.63	0.96
9:c:219:ASN:HB2	9:c:223:LYS:HD3	1.49	0.94
16:E:303:LEU:HD12	16:E:304:PRO:HD2	1.50	0.94
14:C:17:GLY:HA2	14:C:21:ARG:HB3	1.51	0.93
1:U:147:TYR:HE2	1:U:169:GLU:HA	1.33	0.92
6:Z:16:LEU:HD13	9:c:216:MET:HE2	1.45	0.92
10:d:190:LEU:HA	10:d:219:PRO:HA	1.51	0.92
6:Z:16:LEU:CD1	9:c:216:MET:CE	2.46	0.90
1:U:147:TYR:CE2	1:U:169:GLU:HA	2.06	0.90
8:b:35:ILE:HG21	8:b:184:ILE:HG22	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:22:LEU:CD2	8:b:177:PRO:HB2	2.03	0.89
3:W:152:ILE:HG13	3:W:161:GLU:HB3	1.55	0.88
13:B:43:PRO:HD2	13:B:44:ASP:H	1.36	0.88
3:W:5:GLY:HA2	3:W:8:ARG:HD3	1.55	0.87
22:j:7:ILE:HD11	22:j:126:PRO:HD3	1.58	0.86
30:R:45:MET:HG2	30:R:52:CYS:HB3	1.59	0.85
3:W:78:LYS:HA	3:W:78:LYS:HE3	1.56	0.85
3:W:384:LEU:HD12	3:W:388:GLU:HB3	1.59	0.84
27:O:2:THR:HG21	27:O:162:GLY:HA3	1.60	0.83
1:U:596:ASN:HD21	15:D:52:GLU:HB2	1.43	0.82
3:W:95:SER:HA	3:W:98:LYS:HB3	1.62	0.82
10:d:189:ILE:HG12	10:d:220:ASN:HA	1.59	0.82
7:a:222:LEU:HB2	7:a:226:ARG:HH12	1.43	0.81
7:a:247:ARG:HD2	7:a:247:ARG:H	1.45	0.81
16:E:127:PRO:HG2	16:E:185:ARG:HE	1.45	0.81
3:W:66:ILE:H	3:W:66:ILE:HD12	1.46	0.80
2:V:248:ALA:HB1	2:V:284:GLU:HG3	1.61	0.80
10:d:188:LYS:H	10:d:220:ASN:HB2	1.45	0.80
2:V:355:ARG:HA	2:V:358:MET:HE3	1.61	0.80
10:d:218:GLY:HA2	10:d:222:TYR:HA	1.58	0.80
17:F:208:HIS:HB3	17:F:211:LYS:HB3	1.63	0.80
12:A:425:ALA:HB1	12:A:428:ARG:HB2	1.64	0.80
8:b:22:LEU:HG	8:b:23:PRO:HD3	1.64	0.79
27:o:163:ILE:HG12	27:o:169:SER:HB3	1.64	0.79
14:C:367:GLY:HA3	15:D:196:ILE:HG21	1.63	0.79
12:A:75:PRO:HD2	12:A:76:ALA:N	1.96	0.78
2:V:79:VAL:HA	2:V:161:PRO:HB3	1.65	0.78
5:Y:105:MET:HE1	5:Y:140:ILE:HD11	1.65	0.78
6:Z:242:LEU:HD13	10:d:235:THR:HG21	1.65	0.78
10:d:142:TYR:HB3	10:d:147:SER:HB2	1.65	0.78
10:d:219:PRO:HD2	10:d:223:TYR:N	1.99	0.77
2:V:182:LYS:O	2:V:182:LYS:NZ	2.16	0.77
3:W:311:THR:HG23	7:a:316:SER:HB2	1.65	0.77
2:V:91:PRO:HA	2:V:94:VAL:HG12	1.65	0.77
2:V:263:LEU:HG	10:d:121:ARG:HH21	1.49	0.77
10:d:147:SER:HB3	10:d:150:LYS:HB2	1.66	0.76
26:N:127:ILE:HD12	26:N:132:SER:HB2	1.67	0.76
10:d:34:ASN:OD1	10:d:35:PHE:N	2.19	0.76
6:Z:16:LEU:HD12	9:c:216:MET:HE2	1.68	0.76
8:b:27:GLN:OE1	8:b:27:GLN:N	2.18	0.76
3:W:320:LEU:O	3:W:324:TYR:HB3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:451:MET:HE3	6:Z:101:LEU:HB2	1.69	0.75
7:a:112:ILE:HD11	7:a:138:VAL:HA	1.67	0.75
8:b:138:VAL:HB	8:b:160:LEU:HD11	1.68	0.75
3:W:142:ARG:HG3	3:W:145:LEU:HB3	1.69	0.75
14:C:45:LEU:HB3	15:D:61:ILE:HG21	1.68	0.75
8:b:110:ILE:HG22	8:b:139:ASP:HB2	1.68	0.75
10:d:218:GLY:HA3	10:d:222:TYR:CD1	2.21	0.75
10:d:219:PRO:HD2	10:d:223:TYR:H	1.51	0.75
8:b:3:LEU:HD23	8:b:44:ASN:HD21	1.51	0.75
9:c:139:ARG:O	9:c:139:ARG:HD3	1.87	0.74
34:u:664:GLU:HG2	34:u:667:GLY:H	1.51	0.74
8:b:7:MET:HB3	8:b:109:ILE:HD13	1.69	0.74
13:B:43:PRO:HD2	13:B:44:ASP:N	1.97	0.74
17:F:282:ILE:HG22	17:F:327:LYS:HB2	1.68	0.74
1:U:147:TYR:HE2	1:U:169:GLU:CA	2.00	0.74
8:b:186:SER:HB3	8:b:187:PRO:HD2	1.69	0.74
2:V:443:ARG:NH1	10:d:181:CYS:SG	2.60	0.74
10:d:187:GLU:HB3	10:d:223:TYR:HA	1.69	0.74
1:U:7:GLY:N	10:d:80:CYS:HG	1.85	0.74
1:U:142:LEU:HD11	1:U:165:LYS:HG3	1.68	0.74
24:l:212:ILE:HD11	24:l:229:VAL:HG13	1.69	0.74
31:S:72:LEU:HD23	31:S:83:MET:HE3	1.68	0.74
13:B:165:ASP:OD1	13:B:166:ASP:N	2.21	0.73
12:A:165:GLN:NE2	12:A:236:CYS:SG	2.61	0.73
1:U:104:CYS:HA	1:U:107:HIS:HB3	1.70	0.73
10:d:210:ALA:HB1	10:d:216:VAL:HG22	1.70	0.73
17:F:86:LEU:HD12	17:F:87:PRO:HD3	1.68	0.73
10:d:32:GLU:OE1	10:d:47:GLN:NE2	2.21	0.73
10:d:189:ILE:H	10:d:220:ASN:H	1.37	0.73
17:F:121:CYS:HB3	17:F:133:PHE:HE1	1.54	0.73
3:W:27:ARG:NH1	3:W:31:CYS:SG	2.62	0.73
21:I:119:GLN:HG3	22:J:78:ALA:HB1	1.69	0.73
2:V:139:MET:HA	2:V:143:ALA:HB2	1.71	0.72
1:U:162:VAL:O	1:U:165:LYS:HG2	1.89	0.72
2:V:33:GLN:NE2	2:V:83:GLU:O	2.22	0.72
6:Z:246:VAL:HG22	10:d:236:THR:HG23	1.70	0.72
1:U:105:ILE:HG12	1:U:134:VAL:HG22	1.71	0.72
1:U:145:HIS:ND1	1:U:170:SER:HB2	2.03	0.72
10:d:206:MET:HE2	10:d:206:MET:HA	1.70	0.72
2:V:146:GLN:HA	2:V:148:ARG:HH21	1.54	0.72
2:V:194:LYS:HD2	2:V:198:GLN:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:112:ILE:HA	7:a:115:LYS:HE2	1.71	0.72
7:a:166:ILE:H	7:a:166:ILE:HD12	1.55	0.72
9:c:184:LEU:HD22	9:c:185:ASN:H	1.54	0.72
10:d:218:GLY:HA3	10:d:222:TYR:CA	2.10	0.72
33:f:410:ARG:HH22	34:u:838:ARG:HH21	1.36	0.72
17:F:40:GLU:O	17:F:44:ARG:NH1	2.23	0.72
23:k:91:LYS:HG3	23:k:119:LEU:HD13	1.71	0.72
26:n:19:ARG:HD3	26:n:26:ILE:HG12	1.72	0.72
3:W:93:ARG:H	3:W:96:GLN:HE21	1.38	0.71
12:A:65:ILE:HD12	12:A:65:ILE:H	1.55	0.71
11:e:45:ASP:O	11:e:47:ASN:N	2.24	0.71
3:W:59:ASP:HA	3:W:63:THR:CG2	2.20	0.71
9:c:167:MET:HE2	9:c:167:MET:O	1.91	0.71
34:u:441:LYS:HB3	34:u:477:MET:HE1	1.73	0.71
10:d:4:GLN:O	10:d:25:ARG:NH1	2.24	0.71
16:E:8:ALA:O	17:F:44:ARG:NH2	2.23	0.71
16:E:313:LEU:HG	16:E:343:LEU:HD23	1.71	0.71
8:b:61:LEU:HG	8:b:74:LYS:HD3	1.72	0.71
3:W:366:MET:O	3:W:370:TYR:HB2	1.90	0.71
6:Z:75:LEU:HD11	6:Z:112:MET:HE1	1.72	0.71
8:b:6:THR:HB	8:b:49:VAL:HG12	1.72	0.71
2:V:342:ILE:HD12	2:V:343:PRO:HD2	1.72	0.71
34:u:182:GLU:HA	34:u:185:LEU:HD12	1.72	0.70
1:U:325:MET:HA	1:U:328:ILE:HG12	1.71	0.70
1:U:185:MET:HE1	1:U:198:LEU:HD11	1.72	0.70
8:b:171:VAL:HG22	8:b:187:PRO:HG2	1.72	0.70
32:t:126:ASP:OD2	32:t:127:MET:N	2.24	0.70
1:U:173:VAL:HG22	1:U:175:GLY:H	1.54	0.70
22:j:4:ASP:OD1	23:k:10:ARG:NH2	2.22	0.70
2:V:81:GLN:H	2:V:86:VAL:HB	1.56	0.70
15:D:212:LYS:NZ	15:D:312:ASN:OD1	2.25	0.70
2:V:133:PRO:HD2	2:V:134:PHE:H	1.57	0.70
5:Y:184:GLN:HG3	5:Y:197:ALA:HA	1.73	0.70
22:j:5:ARG:HG3	22:j:6:ALA:H	1.57	0.70
9:c:211:GLU:OE2	9:c:215:LYS:HG3	1.92	0.70
3:W:172:GLU:OE1	3:W:172:GLU:N	2.23	0.70
21:I:218:ARG:NH1	21:I:223:THR:OG1	2.24	0.70
32:T:126:ASP:OD1	32:T:127:MET:N	2.24	0.70
24:l:200:PRO:O	24:l:239:ARG:NH2	2.25	0.70
1:U:765:VAL:HG11	1:U:778:PHE:CD2	2.27	0.70
14:C:83:LYS:HE2	14:C:83:LYS:N	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:Q:118:MET:HE2	29:Q:124:LEU:HD13	1.73	0.70
10:d:136:PRO:HD2	10:d:137:VAL:H	1.56	0.69
8:b:1:MET:N	8:b:1:MET:SD	2.64	0.69
21:I:187:LYS:H	21:I:187:LYS:HE2	1.55	0.69
6:Z:84:LYS:HZ1	9:c:76:PRO:HB3	1.56	0.69
9:c:236:GLU:N	9:c:236:GLU:OE2	2.25	0.69
10:d:200:PHE:CD2	10:d:205:LYS:HD3	2.28	0.69
14:C:375:ARG:HG2	14:C:377:HIS:H	1.57	0.69
8:b:107:MET:HB3	8:b:136:VAL:HG23	1.75	0.69
26:N:81:SER:O	26:N:85:GLU:HG2	1.93	0.69
1:U:742:HIS:O	1:U:883:ARG:NH1	2.26	0.69
2:V:30:PRO:HA	2:V:33:GLN:HB2	1.75	0.69
14:C:83:LYS:HE2	14:C:83:LYS:H	1.58	0.69
17:F:85:THR:HG22	17:F:87:PRO:HD2	1.73	0.69
8:b:16:MET:HB2	8:b:25:ARG:HG3	1.75	0.69
10:d:188:LYS:N	10:d:220:ASN:H	1.91	0.69
2:V:313:LEU:O	2:V:317:PRO:HG3	1.93	0.68
10:d:200:PHE:O	10:d:202:THR:N	2.26	0.68
15:D:87:LEU:HG	15:D:140:VAL:HG21	1.74	0.68
1:U:799:LYS:H	1:U:923:GLU:HG2	1.58	0.68
3:W:79:GLU:HG2	3:W:130:MET:HG3	1.75	0.68
16:E:127:PRO:HB2	16:E:185:ARG:HH21	1.59	0.68
32:T:25:ASP:OD1	32:T:41:ARG:NH1	2.25	0.68
34:u:75:LEU:HD12	34:u:121:PHE:HB3	1.74	0.68
5:Y:349:LYS:O	5:Y:352:GLU:N	2.21	0.68
6:Z:65:ASP:HB3	6:Z:103:LYS:HE2	1.75	0.68
4:X:244:SER:HB3	4:X:245:PRO:HD2	1.75	0.68
4:X:90:ARG:HH12	4:X:128:ALA:HB1	1.57	0.68
10:d:26:LEU:HA	10:d:29:VAL:HG12	1.74	0.68
17:F:300:LYS:O	17:F:304:ARG:NH1	2.27	0.68
2:V:247:GLN:OE1	2:V:247:GLN:N	2.22	0.68
3:W:157:GLY:HA2	3:W:161:GLU:OE1	1.94	0.68
1:U:798:PRO:O	1:U:880:ASN:ND2	2.27	0.68
3:W:136:ILE:HG22	3:W:143:ALA:HB3	1.76	0.67
6:Z:96:HIS:HE2	6:Z:123:ILE:HG12	1.58	0.67
12:A:210:LYS:HE2	12:A:309:PHE:CZ	2.29	0.67
21:I:163:CYS:SG	21:I:164:ILE:N	2.68	0.67
5:Y:177:ARG:NH2	5:Y:205:VAL:O	2.28	0.67
13:B:49:LEU:HD13	13:B:51:LEU:H	1.59	0.67
23:k:35:SER:HB3	23:k:51:GLU:HG2	1.77	0.67
23:k:117:SER:OG	24:l:82:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:397:TYR:CZ	6:Z:257:MET:HG3	2.30	0.67
22:j:23:GLN:NE2	22:j:148:ASP:OD2	2.28	0.67
3:W:107:GLN:N	3:W:107:GLN:OE1	2.25	0.67
3:W:107:GLN:O	3:W:111:TYR:HB2	1.95	0.67
10:d:204:LYS:HE2	10:d:204:LYS:HA	1.77	0.67
23:K:117:SER:OG	24:L:82:ARG:NH2	2.26	0.67
30:R:49:ALA:HA	39:R:301:LDZ:H22	1.75	0.67
31:s:184:GLU:OE2	31:s:211:ARG:NH1	2.26	0.67
2:V:81:GLN:HB2	2:V:85:ALA:HB3	1.77	0.67
8:b:109:ILE:HB	8:b:138:VAL:HG22	1.77	0.67
26:n:75:LEU:HB2	26:n:78:THR:HG22	1.76	0.67
1:U:82:LEU:HB3	1:U:129:ARG:HH21	1.58	0.67
1:U:167:ILE:C	1:U:169:GLU:H	2.02	0.67
13:B:153:ASN:HB2	13:B:160:ILE:HD11	1.77	0.67
13:B:317:ASP:OD2	13:B:343:ARG:NH2	2.28	0.67
1:U:158:ARG:HD3	1:U:193:PHE:CD1	2.30	0.67
3:W:50:LEU:HD12	3:W:53:GLN:HE21	1.58	0.67
10:d:204:LYS:HG3	10:d:207:THR:HG22	1.76	0.67
1:U:509:GLY:HA3	1:U:544:ILE:HD12	1.76	0.67
3:W:440:ASN:HD22	9:c:225:TRP:HZ3	1.42	0.67
19:g:97:GLU:HG2	19:g:117:ARG:HG2	1.77	0.67
1:U:405:THR:HG23	1:U:441:GLY:HA3	1.77	0.66
10:d:1:MET:HE2	10:d:1:MET:HA	1.77	0.66
1:U:321:GLN:HA	1:U:324:LYS:HD2	1.77	0.66
2:V:111:TYR:OH	2:V:150:ARG:NH2	2.24	0.66
5:Y:220:VAL:HG21	5:Y:249:VAL:HG21	1.75	0.66
8:b:181:ASP:C	8:b:183:LEU:H	2.02	0.66
1:U:168:LEU:O	1:U:169:GLU:C	2.39	0.66
10:d:188:LYS:H	10:d:220:ASN:CB	2.08	0.66
1:U:40:GLU:O	1:U:41:SER:OG	2.07	0.66
12:A:158:ASP:OD2	12:A:255:ARG:NH2	2.29	0.66
19:G:80:MET:HE1	19:G:138:MET:HE3	1.76	0.66
32:T:96:MET:HE2	32:T:110:MET:HE1	1.76	0.66
25:m:42:LYS:HB2	25:m:184:MET:O	1.96	0.66
34:u:585:GLU:HA	34:u:588:ARG:HG2	1.78	0.66
12:A:30:ILE:HG22	12:A:34:LYS:HZ2	1.60	0.66
10:d:75:MET:HE3	10:d:102:ASN:HB2	1.77	0.66
34:u:853:VAL:HG12	34:u:855:GLN:HG2	1.78	0.66
3:W:188:GLU:HA	3:W:191:ARG:HH21	1.59	0.66
17:F:297:ASP:C	17:F:299:GLU:H	2.03	0.66
1:U:397:THR:OG1	1:U:401:LYS:NZ	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:186:TYR:HB2	10:d:221:ASN:CB	2.21	0.66
17:F:304:ARG:O	17:F:308:ARG:HG2	1.96	0.66
1:U:226:PRO:HB2	1:U:267:ASN:HD21	1.61	0.66
1:U:903:PHE:HB2	1:U:915:LYS:HB2	1.77	0.66
7:a:341:LEU:HD13	7:a:345:GLN:HB2	1.77	0.66
9:c:223:LYS:HG2	9:c:224:SER:N	2.11	0.66
7:a:365:MET:HE2	7:a:365:MET:HA	1.78	0.65
8:b:22:LEU:HD23	8:b:177:PRO:CB	2.22	0.65
13:B:342:ILE:HG22	13:B:347:ILE:HD12	1.79	0.65
24:l:36:VAL:HG22	24:l:160:SER:HB2	1.77	0.65
2:V:211:TYR:OH	2:V:234:ARG:NH1	2.28	0.65
2:V:246:GLY:O	2:V:250:LEU:HG	1.97	0.65
5:Y:245:GLU:OE1	5:Y:245:GLU:N	2.22	0.65
1:U:246:TYR:OH	1:U:324:LYS:HE3	1.97	0.65
10:d:75:MET:HE1	10:d:98:LEU:HG	1.77	0.65
10:d:188:LYS:H	10:d:220:ASN:H	1.45	0.65
26:n:150:GLU:OE2	26:n:150:GLU:N	2.28	0.65
1:U:807:LYS:HB2	1:U:808:PRO:HD3	1.77	0.65
10:d:36:LEU:HB3	10:d:37:PRO:HD3	1.79	0.65
10:d:219:PRO:CD	10:d:223:TYR:H	2.10	0.65
3:W:152:ILE:HG21	3:W:165:ILE:HD11	1.79	0.65
3:W:446:ILE:HD13	6:Z:227:ILE:HD12	1.79	0.65
6:Z:184:VAL:HG22	6:Z:186:THR:H	1.62	0.65
34:u:797:LEU:O	34:u:801:VAL:HG22	1.96	0.65
2:V:245:ASP:H	2:V:247:GLN:HE22	1.43	0.65
4:X:306:LEU:HD21	4:X:314:ARG:HH12	1.62	0.65
3:W:169:LEU:HD21	3:W:189:GLN:HG2	1.77	0.65
4:X:245:PRO:HG2	4:X:246:LYS:HD2	1.79	0.65
5:Y:74:LYS:HZ3	5:Y:114:ILE:HG13	1.62	0.65
5:Y:175:ASP:HA	14:C:340:ARG:HH21	1.62	0.65
9:c:125:VAL:O	9:c:129:THR:HG22	1.96	0.65
10:d:128:GLN:O	10:d:134:LYS:NZ	2.30	0.65
13:B:163:LEU:HD11	14:C:80:MET:HE1	1.78	0.65
30:R:4:LEU:HD21	30:R:135:ALA:HB1	1.78	0.65
23:k:203:LYS:HB2	23:k:210:LEU:HD22	1.79	0.65
1:U:172:ASP:O	1:U:173:VAL:HB	1.97	0.64
34:u:136:GLU:OE1	34:u:137:ARG:N	2.29	0.64
1:U:95:GLU:HG2	1:U:96:TYR:HD1	1.63	0.64
10:d:234:ASP:HB2	10:d:237:ILE:HD11	1.78	0.64
15:D:146:GLU:OE1	15:D:146:GLU:N	2.31	0.64
16:E:135:ILE:HG23	16:E:182:LEU:HD23	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:a:68:GLU:HG3	7:a:71:VAL:HB	1.79	0.64
14:C:242:ALA:HB1	14:C:243:PRO:HD2	1.79	0.64
34:u:168:LYS:O	34:u:168:LYS:NZ	2.30	0.64
5:Y:184:GLN:NE2	5:Y:200:LEU:HD13	2.12	0.64
1:U:245:ALA:HB1	1:U:325:MET:HE1	1.80	0.64
10:d:187:GLU:C	10:d:219:PRO:HB2	2.22	0.64
14:C:253:SER:O	14:C:254:ILE:HG22	1.97	0.64
34:u:99:LEU:HB3	34:u:129:LEU:HD21	1.79	0.64
2:V:137:GLU:HG2	2:V:138:PRO:HD3	1.80	0.64
3:W:439:VAL:HB	6:Z:234:PHE:HZ	1.63	0.64
4:X:328:ASP:OD2	4:X:364:LYS:NZ	2.30	0.64
6:Z:103:LYS:H	6:Z:103:LYS:HD3	1.62	0.64
20:H:179:ASN:O	20:H:180:GLU:HB2	1.95	0.64
28:P:177:ARG:NH2	31:s:150:ASP:OD2	2.29	0.64
10:d:238:PRO:HB2	10:d:242:LEU:HG	1.79	0.64
27:O:204:CYS:HB2	27:O:208:THR:HG21	1.80	0.64
32:T:9:THR:O	32:T:41:ARG:NH2	2.31	0.64
34:u:466:LEU:HD23	34:u:481:SER:HA	1.80	0.64
25:M:8:ASP:O	25:M:22:GLN:NE2	2.30	0.64
31:S:150:ASP:OD2	28:p:177:ARG:NH2	2.29	0.64
34:u:49:ASP:OD1	34:u:50:LYS:N	2.31	0.64
6:Z:68:TRP:CG	6:Z:104:ASN:HD21	2.16	0.63
7:a:290:GLN:HB3	7:a:330:ARG:HH21	1.63	0.63
9:c:223:LYS:HG2	9:c:224:SER:H	1.63	0.63
17:F:206:MET:HA	17:F:206:MET:HE2	1.78	0.63
2:V:337:LEU:HD11	2:V:367:VAL:HG21	1.81	0.63
2:V:452:ASN:HB3	2:V:457:TYR:HB2	1.80	0.63
9:c:139:ARG:HA	9:c:161:ARG:HH22	1.62	0.63
1:U:137:MET:HA	1:U:137:MET:HE3	1.81	0.63
1:U:423:MET:HA	1:U:423:MET:HE3	1.79	0.63
2:V:480:ILE:HD11	6:Z:260:VAL:HG22	1.81	0.63
3:W:142:ARG:HH12	3:W:185:PHE:HB2	1.64	0.63
28:p:2:SER:OG	28:p:3:ILE:N	2.30	0.63
1:U:149:GLN:HG2	14:C:20:LEU:HD13	1.80	0.63
1:U:410:VAL:HG23	1:U:448:LEU:HD13	1.79	0.63
3:W:58:SER:O	3:W:63:THR:HG23	1.99	0.63
33:f:402:LYS:HG3	33:f:405:ARG:HH22	1.63	0.63
34:u:591:ALA:O	34:u:595:VAL:HG22	1.97	0.63
2:V:63:SER:O	2:V:67:LEU:HD12	1.98	0.63
3:W:273:TYR:HB2	3:W:276:LEU:HB2	1.81	0.63
16:E:229:ILE:HG12	16:E:272:ARG:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:348:GLU:OE1	4:X:348:GLU:N	2.31	0.63
6:Z:225:GLN:HG3	6:Z:226:ILE:HG13	1.79	0.63
15:D:49:GLN:O	15:D:52:GLU:HG3	1.99	0.63
34:u:372:LEU:HD21	34:u:409:SER:HB2	1.81	0.63
7:a:172:TYR:HE1	7:a:200:LEU:HA	1.63	0.63
22:J:64:ALA:O	22:J:88:ARG:NH1	2.31	0.63
33:f:409:ARG:NH2	34:u:319:GLU:OE1	2.32	0.63
1:U:814:PRO:HB2	1:U:816:PRO:HD3	1.80	0.63
17:F:212:PHE:HA	17:F:215:LEU:HB2	1.80	0.63
34:u:531:ASN:HB3	34:u:534:VAL:HG22	1.78	0.63
2:V:482:PHE:HZ	5:Y:381:GLN:HG3	1.63	0.62
3:W:223:LYS:HG3	3:W:224:LEU:HD22	1.80	0.62
5:Y:293:ARG:HH12	11:e:57:ARG:HB3	1.64	0.62
6:Z:129:LYS:HE3	9:c:215:LYS:HE3	1.81	0.62
9:c:68:ARG:HH22	9:c:208:ARG:HH22	1.47	0.62
9:c:219:ASN:CB	9:c:223:LYS:HD3	2.28	0.62
12:A:166:VAL:HG12	12:A:168:GLU:H	1.63	0.62
3:W:2:ALA:HB2	3:W:47:LEU:HD22	1.79	0.62
4:X:255:LEU:HD22	4:X:267:VAL:HG13	1.82	0.62
12:A:64:GLY:O	34:u:680:ARG:NH2	2.32	0.62
17:F:141:ASP:OD2	17:F:144:LYS:NZ	2.30	0.62
3:W:224:LEU:HD12	3:W:250:ILE:HG22	1.80	0.62
6:Z:19:VAL:HG21	6:Z:124:ILE:HD12	1.81	0.62
8:b:32:ALA:HB1	8:b:183:LEU:HD12	1.82	0.62
1:U:159:ARG:O	1:U:160:LEU:HB2	1.99	0.62
7:a:341:LEU:HD11	7:a:346:ILE:HD13	1.82	0.62
13:B:180:PRO:O	13:B:241:ASN:ND2	2.29	0.62
19:g:158:GLY:O	20:h:84:ARG:NH2	2.33	0.62
27:o:17:ASP:HB2	27:o:169:SER:HB2	1.80	0.62
2:V:94:VAL:HA	2:V:138:PRO:HG3	1.81	0.62
3:W:15:LYS:HB2	3:W:19:ASP:HB3	1.81	0.62
15:D:169:GLY:O	15:D:340:GLN:NE2	2.33	0.62
34:u:761:MET:HE2	34:u:761:MET:HA	1.82	0.62
2:V:29:PRO:HB3	2:V:85:ALA:HB2	1.81	0.62
7:a:119:GLY:HA2	7:a:122:LYS:HZ2	1.64	0.62
8:b:155:ALA:O	8:b:159:THR:HG22	1.99	0.62
14:C:11:LEU:HD22	14:C:14:GLY:HA3	1.81	0.62
19:g:71:LYS:O	19:g:95:ARG:NH1	2.33	0.62
34:u:182:GLU:OE1	34:u:182:GLU:N	2.33	0.62
1:U:96:TYR:CD2	1:U:97:VAL:HG23	2.35	0.62
3:W:88:MET:HE2	19:G:208:ILE:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:263:SER:O	1:U:267:ASN:ND2	2.33	0.62
1:U:269:ARG:HD2	1:U:270:THR:N	2.14	0.62
2:V:350:GLN:H	2:V:353:LEU:HB3	1.64	0.62
3:W:267:LEU:O	3:W:271:VAL:HG12	2.00	0.62
16:E:135:ILE:HD13	16:E:183:LEU:HD23	1.81	0.62
17:F:86:LEU:O	17:F:88:TYR:N	2.32	0.62
1:U:16:GLU:HB3	1:U:19:LEU:HD23	1.82	0.61
6:Z:177:ARG:O	6:Z:177:ARG:NE	2.33	0.61
14:C:390:VAL:HG12	14:C:391:MET:HG2	1.80	0.61
34:u:425:GLY:O	34:u:429:ILE:HG13	1.99	0.61
34:u:851:ASP:HB2	34:u:860:LYS:HG2	1.81	0.61
3:W:12:ARG:HD2	3:W:24:VAL:HG22	1.82	0.61
6:Z:252:LYS:HE2	6:Z:252:LYS:HA	1.81	0.61
27:O:159:ILE:O	27:O:163:ILE:HG12	2.01	0.61
19:g:126:THR:HG22	20:h:128:ARG:HH21	1.65	0.61
4:X:255:LEU:HB2	4:X:287:LEU:HD13	1.81	0.61
5:Y:125:ARG:HH11	5:Y:125:ARG:HG3	1.65	0.61
12:A:251:GLY:N	12:A:294:GLU:OE2	2.29	0.61
3:W:30:GLU:HA	3:W:33:LYS:HD2	1.82	0.61
15:D:323:ARG:NH1	15:D:324:PRO:O	2.33	0.61
39:n:301:LDZ:H26	39:n:301:LDZ:H8	1.66	0.61
6:Z:165:GLU:OE1	6:Z:165:GLU:N	2.33	0.61
9:c:51:MET:HA	9:c:51:MET:HE3	1.80	0.61
13:B:94:GLU:HB3	13:B:98:LYS:HE3	1.82	0.61
1:U:151:ILE:HD11	1:U:163:PHE:CD2	2.35	0.61
7:a:276:CYS:O	7:a:279:GLU:HG3	2.00	0.61
8:b:141:ILE:HA	8:b:171:VAL:HB	1.82	0.61
23:k:97:GLN:HG3	30:r:65:ILE:HG13	1.83	0.61
6:Z:236:LEU:HD21	7:a:335:TRP:HB3	1.81	0.61
7:a:119:GLY:HA2	7:a:122:LYS:NZ	2.15	0.61
16:E:109:ARG:HH21	16:E:110:TYR:HD2	1.47	0.61
2:V:29:PRO:HA	2:V:32:PRO:HG2	1.83	0.61
4:X:99:MET:HE3	4:X:100:GLU:HB3	1.81	0.61
12:A:133:ASP:N	12:A:133:ASP:OD1	2.32	0.61
34:u:486:GLY:HA2	34:u:525:ILE:HD11	1.82	0.61
17:F:259:MET:SD	17:F:260:PHE:HB2	2.41	0.61
31:s:169:ASP:O	31:s:173:ARG:HG3	2.01	0.61
10:d:171:LEU:HB3	10:d:175:ARG:HH12	1.66	0.60
13:B:103:ARG:HB3	13:B:160:ILE:HG21	1.83	0.60
2:V:463:MET:HA	2:V:463:MET:HE2	1.82	0.60
3:W:120:ILE:O	3:W:124:LEU:HD23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:381:GLN:OE1	5:Y:385:ARG:NH1	2.34	0.60
6:Z:59:ASP:HB3	6:Z:69:PHE:CZ	2.36	0.60
25:M:117:MET:HE2	25:M:117:MET:HA	1.82	0.60
20:h:69:THR:HG22	20:h:70:LYS:H	1.65	0.60
34:u:144:LEU:O	34:u:148:GLN:NE2	2.33	0.60
2:V:96:ARG:HB2	2:V:150:ARG:HH12	1.66	0.60
6:Z:16:LEU:HD13	9:c:216:MET:HE1	1.77	0.60
34:u:282:PHE:HA	34:u:294:MET:HE1	1.81	0.60
2:V:346:LEU:HD12	2:V:357:LEU:HD11	1.82	0.60
2:V:496:PHE:CE1	14:C:40:GLN:HB3	2.36	0.60
3:W:130:MET:SD	3:W:130:MET:N	2.63	0.60
4:X:62:GLN:N	4:X:62:GLN:OE1	2.35	0.60
6:Z:34:ARG:HA	6:Z:97:THR:O	2.01	0.60
8:b:35:ILE:CG2	8:b:184:ILE:HG22	2.29	0.60
15:D:153:MET:SD	15:D:257:ASN:ND2	2.74	0.60
31:S:173:ARG:HG2	27:o:199:LEU:HB3	1.82	0.60
13:B:382:ASP:N	13:B:382:ASP:OD1	2.34	0.60
25:M:229:LYS:O	25:M:233:GLU:HG2	2.01	0.60
33:f:381:ARG:NH2	34:u:435:SER:O	2.34	0.60
6:Z:103:LYS:H	6:Z:103:LYS:CD	2.15	0.60
34:u:256:PHE:HD1	34:u:261:ARG:HB2	1.65	0.60
3:W:75:TYR:O	3:W:79:GLU:HG3	2.02	0.60
4:X:63:ALA:HB2	4:X:99:MET:HE1	1.83	0.60
9:c:163:ILE:N	9:c:199:HIS:O	2.35	0.60
26:n:91:ARG:HG3	26:n:92:GLU:HG2	1.83	0.60
34:u:60:VAL:HG11	34:u:102:HIS:CD2	2.37	0.60
3:W:259:GLU:O	3:W:263:TRP:HB2	2.01	0.60
27:o:190:THR:HG22	27:o:192:PRO:HD3	1.83	0.60
9:c:219:ASN:O	9:c:220:LEU:C	2.45	0.60
22:j:41:VAL:HG23	22:j:211:MET:HB2	1.83	0.60
1:U:158:ARG:HD3	1:U:193:PHE:CE1	2.36	0.60
7:a:286:ALA:HB1	7:a:289:ARG:CZ	2.32	0.60
10:d:56:GLU:O	10:d:60:GLN:HG2	2.02	0.60
13:B:82:GLN:NE2	34:u:681:TYR:O	2.34	0.60
17:F:225:MET:HE1	17:F:237:ALA:HB2	1.84	0.60
19:g:191:PHE:HE1	19:g:219:VAL:HG21	1.66	0.60
10:d:188:LYS:HB3	10:d:220:ASN:CG	2.27	0.59
24:L:185:ASN:OD1	24:L:189:LYS:NZ	2.34	0.59
2:V:264:TYR:HE1	10:d:118:GLU:HA	1.68	0.59
9:c:289:ASP:O	9:c:293:THR:HG23	2.02	0.59
9:c:32:TYR:HB2	9:c:68:ARG:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:309:ARG:H	16:E:312:ILE:HG13	1.66	0.59
17:F:175:MET:HE1	17:F:249:LEU:HD23	1.84	0.59
17:F:301:ALA:HB3	17:F:304:ARG:HH12	1.66	0.59
28:P:88:MET:HE1	28:P:132:VAL:HG22	1.83	0.59
23:k:146:VAL:HG21	23:k:222:PRO:HA	1.83	0.59
3:W:146:THR:HG23	3:W:147:LYS:HD2	1.84	0.59
21:I:8:ARG:HH21	21:I:11:ILE:HD11	1.67	0.59
4:X:90:ARG:HH22	4:X:128:ALA:C	2.10	0.59
28:P:191:GLU:OE1	28:P:194:LYS:NZ	2.35	0.59
31:S:190:GLY:O	31:S:191:ASP:HB2	2.01	0.59
3:W:120:ILE:HG23	3:W:123:ARG:HH21	1.67	0.59
5:Y:246:ILE:HG12	5:Y:250:LEU:HD23	1.85	0.59
13:B:371:ARG:NH1	13:B:371:ARG:HB2	2.17	0.59
27:o:179:SER:OG	27:o:180:LYS:N	2.36	0.59
1:U:97:VAL:HA	1:U:100:ILE:HG22	1.83	0.59
1:U:374:SER:OG	1:U:407:SER:HB2	2.03	0.59
2:V:256:ARG:NH2	11:e:4:LYS:O	2.35	0.59
3:W:299:ILE:HG22	3:W:301:LYS:H	1.67	0.59
14:C:229:ARG:O	14:C:233:GLU:HG3	2.02	0.59
16:E:132:TYR:CE1	16:E:190:GLN:HG3	2.36	0.59
2:V:144:ASP:HB3	2:V:147:PHE:HB2	1.85	0.59
3:W:104:MET:HE1	3:W:123:ARG:HD3	1.85	0.59
8:b:58:CYS:HB3	8:b:92:VAL:HG11	1.84	0.59
12:A:44:GLN:O	12:A:48:VAL:HG23	2.03	0.59
22:j:184:ASP:O	22:j:188:ILE:HG13	2.03	0.59
3:W:69:ALA:O	3:W:72:LYS:HG2	2.03	0.59
3:W:189:GLN:NE2	3:W:190:MET:SD	2.76	0.59
7:a:134:THR:O	7:a:138:VAL:HG23	2.03	0.59
10:d:8:GLU:CD	10:d:18:LYS:HE2	2.28	0.59
20:h:65:VAL:O	20:h:220:ARG:NH1	2.36	0.59
1:U:470:ASN:OD1	1:U:474:ARG:NH2	2.32	0.59
1:U:609:ASP:O	1:U:615:ARG:NH1	2.36	0.59
4:X:268:GLN:OE1	4:X:288:LYS:NZ	2.36	0.59
8:b:29:GLN:O	8:b:33:VAL:HG13	2.03	0.59
10:d:218:GLY:HA2	10:d:223:TYR:H	1.68	0.59
13:B:49:LEU:HG	34:u:666:ILE:HG23	1.85	0.59
16:E:367:PHE:HA	16:E:370:ALA:HB3	1.85	0.59
34:u:478:ARG:O	34:u:482:ILE:HG22	2.03	0.59
2:V:176:MET:HA	2:V:179:LYS:HB3	1.85	0.58
4:X:91:SER:O	4:X:95:LEU:HD23	2.02	0.58
15:D:103:VAL:HG21	15:D:132:LEU:HD21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:L:84:LEU:O	24:L:88:MET:HG3	2.03	0.58
29:Q:39:SER:OG	29:Q:40:GLU:N	2.36	0.58
22:j:8:THR:HG23	23:k:135:ARG:HB3	1.84	0.58
1:U:421:GLN:O	1:U:425:THR:HG23	2.03	0.58
7:a:180:LEU:HD11	7:a:221:VAL:HG11	1.84	0.58
10:d:171:LEU:HB3	10:d:175:ARG:NH1	2.17	0.58
10:d:240:THR:O	10:d:244:LYS:HG2	2.03	0.58
13:B:322:ARG:NH1	13:B:325:VAL:O	2.36	0.58
15:D:81:ARG:HG2	15:D:81:ARG:HH11	1.68	0.58
16:E:305:ASN:H	16:E:308:ALA:HB3	1.67	0.58
20:H:191:ALA:HA	20:H:194:THR:HG22	1.83	0.58
28:P:65:GLN:OE1	29:Q:86:ARG:NH2	2.37	0.58
21:i:6:ASP:OD2	21:i:7:SER:N	2.35	0.58
26:n:84:LYS:HD3	26:n:120:MET:HE2	1.83	0.58
1:U:765:VAL:HG11	1:U:778:PHE:HD2	1.68	0.58
2:V:93:PHE:HB3	2:V:96:ARG:HH22	1.68	0.58
2:V:212:TYR:HE1	2:V:253:LEU:HD21	1.67	0.58
3:W:312:MET:HB3	3:W:365:ILE:HG12	1.85	0.58
6:Z:134:PRO:HG3	9:c:220:LEU:HD22	1.84	0.58
9:c:211:GLU:HG3	9:c:212:LEU:H	1.68	0.58
12:A:119:ALA:HB2	17:F:128:THR:HG23	1.85	0.58
13:B:374:LEU:HD22	13:B:378:VAL:HG11	1.86	0.58
2:V:68:ASP:O	2:V:73:GLU:N	2.36	0.58
14:C:406:LYS:HG2	21:I:80:THR:HB	1.85	0.58
17:F:86:LEU:N	17:F:87:PRO:HD2	2.19	0.58
17:F:285:ILE:O	17:F:330:ALA:HA	2.03	0.58
24:L:125:ARG:NH1	24:L:126:ARG:O	2.36	0.58
28:P:26:ARG:HD3	28:P:186:ILE:HB	1.86	0.58
1:U:619:VAL:HG21	1:U:648:VAL:HG13	1.84	0.58
3:W:182:ARG:O	3:W:186:ILE:HG23	2.02	0.58
13:B:222:VAL:HG22	13:B:349:ARG:HB2	1.86	0.58
27:O:112:SER:HB2	27:O:127:MET:HE3	1.84	0.58
3:W:374:THR:O	3:W:376:LYS:N	2.36	0.58
15:D:141:ASP:OD1	15:D:142:VAL:N	2.37	0.58
34:u:266:LEU:HD22	34:u:294:MET:HB2	1.86	0.58
3:W:166:LEU:HA	3:W:169:LEU:HD23	1.84	0.58
6:Z:252:LYS:NZ	9:c:299:CYS:HB3	2.18	0.58
12:A:55:LEU:O	12:A:59:ILE:HG22	2.04	0.58
15:D:255:LYS:HD3	15:D:302:ASN:HA	1.86	0.58
16:E:37:THR:HA	17:F:69:MET:HE1	1.85	0.58
29:Q:49:GLU:HG3	29:Q:99:HIS:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:68:PHE:HD2	1:U:76:GLU:HB2	1.69	0.58
6:Z:186:THR:O	6:Z:190:ARG:HG2	2.04	0.58
13:B:103:ARG:HH21	13:B:160:ILE:HG22	1.69	0.58
16:E:254:GLN:O	16:E:258:MET:HG3	2.04	0.58
25:M:237:LYS:O	25:M:241:GLU:HG2	2.04	0.58
6:Z:48:LEU:HD11	6:Z:92:VAL:HG21	1.84	0.58
12:A:124:ASP:HB3	17:F:86:LEU:HD22	1.86	0.58
19:G:120:ASP:OD1	20:H:84:ARG:NH1	2.37	0.58
9:c:139:ARG:C	9:c:161:ARG:HH12	2.12	0.57
16:E:322:LYS:HD2	16:E:326:ILE:HG13	1.85	0.57
19:G:71:LYS:O	19:G:95:ARG:NH1	2.37	0.57
23:k:13:ASN:HB3	24:l:126:ARG:HB3	1.86	0.57
23:k:79:SER:HB2	23:k:170:ILE:HD12	1.86	0.57
3:W:144:ARG:HH22	3:W:172:GLU:HG3	1.69	0.57
7:a:112:ILE:O	7:a:116:THR:HG23	2.04	0.57
8:b:179:LEU:C	8:b:181:ASP:H	2.12	0.57
34:u:143:ARG:HH21	34:u:148:GLN:HA	1.69	0.57
1:U:874:ASN:ND2	1:U:874:ASN:H	2.00	0.57
4:X:205:LYS:O	4:X:206:LEU:C	2.45	0.57
4:X:245:PRO:C	4:X:247:ALA:H	2.12	0.57
6:Z:78:MET:HE1	9:c:98:MET:HE2	1.86	0.57
7:a:236:THR:OG1	7:a:249:GLN:NE2	2.26	0.57
9:c:168:MET:HE2	9:c:168:MET:N	2.19	0.57
12:A:24:ALA:HA	13:B:410:ARG:NH2	2.20	0.57
12:A:247:GLN:HG3	12:A:256:MET:HE1	1.86	0.57
25:M:188:ASP:OD1	25:M:188:ASP:N	2.37	0.57
25:M:234:GLU:HA	25:M:237:LYS:HG2	1.86	0.57
19:g:67:THR:HG22	19:g:69:LEU:H	1.68	0.57
1:U:31:VAL:HG22	1:U:35:TRP:CD1	2.39	0.57
14:C:215:SER:OG	14:C:216:GLY:N	2.33	0.57
16:E:120:TYR:O	16:E:122:MET:HE2	2.04	0.57
1:U:109:THR:OG1	1:U:157:THR:HG23	2.05	0.57
9:c:270:LEU:HA	9:c:273:LYS:HG2	1.86	0.57
19:G:158:GLY:O	20:H:84:ARG:NH2	2.37	0.57
25:M:151:ILE:HG13	25:M:157:SER:HB2	1.86	0.57
2:V:417:ILE:HA	5:Y:349:LYS:HG2	1.85	0.57
5:Y:96:GLY:O	5:Y:130:LYS:NZ	2.37	0.57
5:Y:220:VAL:HA	5:Y:223:THR:HG22	1.85	0.57
7:a:45:VAL:HG11	7:a:79:ILE:HG22	1.86	0.57
10:d:190:LEU:CA	10:d:219:PRO:HA	2.29	0.57
10:d:218:GLY:HA3	10:d:222:TYR:CG	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:324:PRO:HA	12:A:327:LEU:HD23	1.87	0.57
27:O:17:ASP:OD1	27:O:33:LYS:NZ	2.25	0.57
24:l:230:SER:O	24:l:234:GLU:HG2	2.03	0.57
34:u:761:MET:HE2	34:u:764:LEU:HD23	1.86	0.57
2:V:349:ARG:NH2	11:e:40:GLU:OE1	2.37	0.57
4:X:202:CYS:CB	4:X:206:LEU:HD23	2.35	0.57
12:A:174:TYR:HD2	12:A:232:ARG:HH21	1.53	0.57
15:D:264:ILE:HD12	15:D:309:MET:HE2	1.86	0.57
15:D:281:ALA:HB1	16:E:208:ILE:HD12	1.86	0.57
1:U:17:PRO:O	1:U:21:GLU:HG3	2.05	0.57
1:U:545:LEU:HB3	1:U:577:ILE:HG21	1.86	0.57
5:Y:104:MET:HE2	5:Y:126:LYS:HZ1	1.70	0.57
10:d:114:GLU:HA	10:d:117:THR:HG22	1.85	0.57
15:D:417:TYR:HA	20:H:79:MET:HA	1.87	0.57
26:n:81:SER:O	26:n:85:GLU:HG2	2.05	0.57
32:t:166:ARG:NH2	32:t:200:GLU:OE2	2.37	0.57
1:U:902:PRO:HB3	1:U:914:LEU:HD23	1.87	0.57
3:W:439:VAL:HB	6:Z:234:PHE:CZ	2.40	0.57
7:a:8:LEU:HD23	7:a:8:LEU:H	1.69	0.57
9:c:266:THR:HB	9:c:269:GLN:HB2	1.87	0.57
11:e:53:SER:N	11:e:55:GLN:OE1	2.38	0.57
24:L:158:ALA:HB1	24:L:172:LEU:HD13	1.86	0.57
28:P:35:VAL:HG12	28:P:36:THR:HG23	1.87	0.57
1:U:465:LEU:HD11	1:U:477:GLY:HA3	1.87	0.57
3:W:44:ILE:O	3:W:46:THR:N	2.38	0.57
3:W:125:ILE:O	3:W:129:ARG:NE	2.34	0.57
3:W:173:THR:HG23	3:W:182:ARG:HH21	1.70	0.57
4:X:400:ALA:HB1	6:Z:262:LEU:HD21	1.87	0.57
8:b:25:ARG:NH2	8:b:144:GLY:HA3	2.20	0.57
8:b:184:ILE:HG13	8:b:185:SER:N	2.19	0.57
14:C:145:ASP:OD1	14:C:145:ASP:N	2.35	0.57
24:L:72:ILE:HG22	24:L:134:ILE:HG12	1.87	0.57
23:k:227:HIS:NE2	23:k:233:GLU:OE1	2.32	0.57
3:W:311:THR:O	3:W:312:MET:HG3	2.05	0.56
12:A:49:GLU:O	12:A:52:ILE:HG13	2.05	0.56
15:D:162:VAL:HG11	15:D:214:MET:HG3	1.87	0.56
16:E:309:ARG:HD2	16:E:332:VAL:HG13	1.87	0.56
39:O:301:LDZ:H15	39:O:301:LDZ:H11	1.86	0.56
19:g:129:ALA:O	19:g:130:GLU:HG3	2.06	0.56
27:o:48:THR:O	27:o:50:ALA:N	2.37	0.56
6:Z:58:PHE:HB2	6:Z:70:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:191:PHE:HA	10:d:194:ALA:HB3	1.88	0.56
21:I:21:VAL:O	21:I:25:MET:HG3	2.05	0.56
22:j:5:ARG:HG3	22:j:6:ALA:N	2.20	0.56
25:m:200:VAL:O	25:m:201:HIS:HB3	2.04	0.56
34:u:524:MET:HA	34:u:527:VAL:HG13	1.87	0.56
34:u:662:MET:HG3	34:u:781:TYR:CE1	2.40	0.56
1:U:835:ILE:HA	1:U:838:LYS:HZ3	1.71	0.56
4:X:334:ASN:HB3	4:X:354:ILE:HD11	1.86	0.56
4:X:402:GLU:O	4:X:406:ASN:ND2	2.35	0.56
5:Y:325:VAL:HG12	5:Y:326:GLY:H	1.69	0.56
6:Z:174:HIS:HB2	9:c:153:GLY:HA2	1.87	0.56
16:E:238:ILE:H	16:E:241:ARG:HG2	1.71	0.56
17:F:263:ASP:HA	17:F:266:LYS:HD2	1.87	0.56
24:L:103:LEU:HD12	24:L:104:PRO:HD2	1.87	0.56
28:p:20:VAL:HG12	28:p:190:ILE:HB	1.86	0.56
34:u:573:ILE:HD12	34:u:576:ILE:HD13	1.87	0.56
34:u:692:LEU:HB3	34:u:800:LEU:HD12	1.87	0.56
2:V:345:ARG:HE	2:V:360:TYR:HB2	1.70	0.56
3:W:159:VAL:HG22	3:W:196:VAL:HG12	1.88	0.56
3:W:267:LEU:HD11	3:W:296:LEU:HD13	1.87	0.56
4:X:314:ARG:HG3	4:X:314:ARG:O	2.04	0.56
5:Y:70:LEU:HA	5:Y:73:MET:HG2	1.87	0.56
7:a:216:LEU:HD13	7:a:222:LEU:HD21	1.88	0.56
27:o:146:MET:HE1	27:o:154:LEU:HD22	1.87	0.56
3:W:95:SER:O	3:W:99:GLN:HG3	2.05	0.56
5:Y:212:GLU:HG3	5:Y:213:LEU:HG	1.87	0.56
6:Z:256:GLN:O	6:Z:260:VAL:HG23	2.06	0.56
9:c:222:LYS:O	9:c:223:LYS:HB2	2.06	0.56
32:T:136:SER:HG	32:T:147:GLN:HE22	1.54	0.56
4:X:137:TYR:HB3	4:X:146:ALA:HB2	1.87	0.56
7:a:350:LYS:O	7:a:354:GLU:HG2	2.05	0.56
17:F:206:MET:O	17:F:325:GLN:NE2	2.39	0.56
25:M:185:THR:HG23	25:M:187:ARG:H	1.69	0.56
21:i:245:ALA:O	21:i:249:ARG:HG2	2.05	0.56
1:U:233:LEU:HD11	1:U:325:MET:SD	2.46	0.56
2:V:309:MET:HB2	2:V:332:LEU:HD13	1.88	0.56
3:W:276:LEU:HD11	3:W:341:PHE:HE2	1.70	0.56
12:A:24:ALA:H	12:A:25:LEU:HD22	1.71	0.56
15:D:259:PRO:HG3	15:D:304:ASN:HD22	1.71	0.56
4:X:398:GLU:HA	4:X:401:LEU:HD12	1.87	0.56
7:a:211:PHE:HD1	7:a:213:PHE:HD1	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:51:LEU:HD23	8:b:71:ILE:HG23	1.88	0.56
24:L:9:ASP:OD2	24:L:11:THR:OG1	2.23	0.56
27:o:19:ARG:HB2	27:o:170:GLY:H	1.70	0.56
28:p:48:ARG:NH1	28:p:192:LYS:O	2.39	0.56
1:U:713:TYR:O	1:U:717:ILE:HG22	2.06	0.56
5:Y:265:GLU:OE1	5:Y:267:ARG:NH1	2.39	0.56
9:c:57:MET:HA	9:c:72:VAL:HG12	1.87	0.56
12:A:236:CYS:HB3	12:A:270:CYS:SG	2.46	0.56
15:D:249:ASP:OD1	15:D:252:ARG:NH1	2.39	0.56
15:D:281:ALA:HA	15:D:284:GLU:HB3	1.87	0.56
28:P:88:MET:HE3	28:P:120:PHE:HZ	1.69	0.56
19:g:5:SER:O	19:g:11:ARG:NH1	2.39	0.56
22:j:104:VAL:HG11	22:j:143:ARG:HB2	1.87	0.56
24:l:36:VAL:HB	24:l:47:VAL:HG12	1.87	0.56
8:b:27:GLN:HA	8:b:30:GLN:HG3	1.87	0.56
16:E:173:TYR:HB2	16:E:282:PRO:HG3	1.87	0.56
1:U:583:MET:HE3	1:U:618:ALA:HB2	1.87	0.55
3:W:370:TYR:OH	7:a:308:GLU:OE2	2.24	0.55
14:C:37:ASP:OD1	14:C:38:LYS:N	2.39	0.55
20:H:29:VAL:HG11	20:H:133:SER:HB2	1.87	0.55
26:n:179:ILE:HG12	26:n:184:VAL:HG22	1.87	0.55
34:u:466:LEU:HB2	34:u:485:LEU:HD13	1.88	0.55
2:V:228:ARG:HG3	2:V:257:ASN:HD21	1.72	0.55
10:d:189:ILE:N	10:d:220:ASN:N	2.44	0.55
14:C:186:VAL:HG12	14:C:313:ARG:HB2	1.88	0.55
16:E:83:CYS:SG	16:E:84:ARG:N	2.78	0.55
21:I:68:LEU:HD11	21:I:74:CYS:HB3	1.87	0.55
22:j:228:TYR:HA	22:j:231:GLU:OE1	2.06	0.55
1:U:159:ARG:HE	1:U:162:VAL:HG13	1.71	0.55
2:V:265:ASP:O	2:V:269:LYS:HG3	2.06	0.55
3:W:173:THR:HG23	3:W:182:ARG:HE	1.71	0.55
10:d:122:LEU:HB3	10:d:125:LYS:HG3	1.88	0.55
13:B:49:LEU:HD11	34:u:666:ILE:HG12	1.88	0.55
16:E:45:ASN:OD1	16:E:48:LYS:NZ	2.35	0.55
23:K:108:THR:HG1	23:K:111:SER:HG	1.55	0.55
21:i:174:MET:HE1	21:i:199:LYS:HG2	1.87	0.55
7:a:286:ALA:O	7:a:289:ARG:NH1	2.40	0.55
9:c:211:GLU:CG	9:c:212:LEU:H	2.20	0.55
11:e:41:ASP:HB2	11:e:43:TRP:CD1	2.41	0.55
14:C:41:ASN:OD1	14:C:44:ARG:NH2	2.40	0.55
26:N:20:THR:HG23	39:N:301:LDZ:H13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:g:11:ARG:O	19:g:24:GLN:NE2	2.36	0.55
22:j:214:ASP:OD1	22:j:214:ASP:N	2.39	0.55
27:o:1:THR:OG1	39:o:301:LDZ:O33	2.22	0.55
2:V:203:LEU:HA	2:V:206:VAL:HG22	1.88	0.55
3:W:20:TYR:HD2	3:W:22:ALA:H	1.54	0.55
9:c:223:LYS:NZ	9:c:223:LYS:HB3	2.20	0.55
10:d:187:GLU:CB	10:d:223:TYR:HA	2.36	0.55
15:D:383:GLY:HA3	16:E:164:ILE:HG21	1.88	0.55
24:l:27:GLU:OE2	24:l:30:LYS:NZ	2.36	0.55
2:V:106:ARG:O	2:V:110:HIS:ND1	2.39	0.55
3:W:268:LYS:O	3:W:272:LEU:HB2	2.06	0.55
5:Y:38:ARG:NH1	5:Y:39:ASP:HA	2.22	0.55
1:U:108:TYR:HD1	1:U:126:ILE:HG13	1.72	0.55
5:Y:293:ARG:HH12	11:e:57:ARG:HD2	1.71	0.55
5:Y:387:ILE:HG13	6:Z:276:ILE:HD11	1.89	0.55
9:c:110:GLY:HA2	9:c:140:ALA:HB1	1.88	0.55
14:C:30:GLU:O	14:C:34:ILE:HG12	2.07	0.55
25:M:202:ASP:OD1	25:M:202:ASP:N	2.35	0.55
32:t:92:LEU:HD22	32:t:110:MET:HE1	1.88	0.55
1:U:357:LYS:HE3	1:U:392:TRP:CD1	2.41	0.55
2:V:182:LYS:NZ	2:V:186:LYS:HB3	2.22	0.55
4:X:390:GLU:N	4:X:390:GLU:OE2	2.39	0.55
5:Y:292:TYR:CZ	5:Y:293:ARG:HD3	2.42	0.55
9:c:218:LEU:O	9:c:219:ASN:C	2.49	0.55
2:V:182:LYS:HZ1	2:V:186:LYS:HB3	1.71	0.55
10:d:186:TYR:CB	10:d:221:ASN:HB2	2.24	0.55
12:A:310:ASP:HB2	12:A:311:PRO:HD3	1.89	0.55
21:i:8:ARG:HB3	21:i:11:ILE:HD12	1.89	0.55
3:W:144:ARG:NH1	3:W:145:LEU:HB2	2.21	0.55
9:c:263:ASP:HB2	9:c:265:MET:HE1	1.88	0.55
9:c:296:ILE:HD11	10:d:246:VAL:HG13	1.87	0.55
10:d:189:ILE:O	10:d:219:PRO:C	2.50	0.55
22:j:132:LEU:HD21	22:j:159:ASN:HB3	1.89	0.55
1:U:160:LEU:O	1:U:163:PHE:HB3	2.07	0.54
1:U:325:MET:HG2	1:U:328:ILE:HD11	1.88	0.54
3:W:68:VAL:HA	3:W:71:VAL:CG2	2.37	0.54
5:Y:161:THR:HG23	5:Y:183:TYR:OH	2.07	0.54
8:b:22:LEU:HD23	8:b:177:PRO:O	2.07	0.54
9:c:214:GLN:O	9:c:218:LEU:HB2	2.06	0.54
9:c:219:ASN:HB2	9:c:223:LYS:CD	2.30	0.54
10:d:59:ALA:O	10:d:63:ILE:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:71:GLY:HA2	13:B:162:VAL:HG12	1.89	0.54
15:D:64:GLU:O	15:D:68:LEU:HD12	2.07	0.54
15:D:97:ASP:OD1	15:D:97:ASP:N	2.40	0.54
22:J:177:THR:HG22	22:J:179:GLU:H	1.72	0.54
27:O:19:ARG:HB2	27:O:170:GLY:N	2.22	0.54
1:U:160:LEU:O	1:U:161:ASP:C	2.50	0.54
3:W:19:ASP:OD2	3:W:23:THR:OG1	2.20	0.54
3:W:45:GLU:O	3:W:49:SER:N	2.31	0.54
3:W:173:THR:HG23	3:W:182:ARG:NH2	2.22	0.54
5:Y:90:ASP:O	5:Y:93:LYS:NZ	2.38	0.54
9:c:259:VAL:HG13	9:c:260:GLU:OE1	2.07	0.54
12:A:105:ASP:HB2	12:A:110:LYS:HD3	1.89	0.54
1:U:401:LYS:O	1:U:405:THR:HG22	2.07	0.54
2:V:306:ARG:HD2	2:V:306:ARG:C	2.32	0.54
3:W:68:VAL:HA	3:W:71:VAL:HG23	1.87	0.54
4:X:194:ARG:NH1	4:X:214:SER:OG	2.40	0.54
5:Y:74:LYS:NZ	5:Y:114:ILE:HG13	2.22	0.54
7:a:284:ARG:HH11	7:a:286:ALA:HA	1.72	0.54
8:b:24:THR:HG22	8:b:26:LEU:H	1.72	0.54
17:F:150:LEU:HD21	17:F:166:THR:HA	1.90	0.54
20:H:182:LEU:H	20:H:182:LEU:HD23	1.72	0.54
33:f:402:LYS:O	33:f:406:ARG:HG2	2.07	0.54
3:W:286:LEU:O	3:W:290:ILE:HG22	2.07	0.54
6:Z:16:LEU:HD13	9:c:216:MET:HE3	1.82	0.54
8:b:25:ARG:HH22	8:b:145:GLU:H	1.55	0.54
23:k:50:VAL:HG11	23:k:66:LYS:HB2	1.89	0.54
3:W:80:TRP:NE1	19:G:244:GLU:OE1	2.40	0.54
3:W:101:VAL:O	3:W:105:VAL:HG13	2.08	0.54
7:a:77:VAL:O	7:a:81:LEU:HD22	2.08	0.54
10:d:83:PHE:HD2	10:d:121:ARG:HH11	1.55	0.54
10:d:188:LYS:N	10:d:219:PRO:HB2	2.22	0.54
13:B:429:LYS:H	13:B:429:LYS:HD3	1.72	0.54
21:I:116:ASP:OD1	22:J:81:ARG:NH1	2.41	0.54
22:j:158:ALA:HB1	22:j:172:LEU:HD23	1.89	0.54
34:u:479:LEU:HG	34:u:514:VAL:HG12	1.89	0.54
3:W:108:CYS:HA	3:W:123:ARG:NH2	2.23	0.54
12:A:311:PRO:HB2	12:A:314:ASN:ND2	2.23	0.54
13:B:301:GLY:O	13:B:305:ILE:HG12	2.06	0.54
34:u:574:GLU:N	34:u:574:GLU:OE1	2.40	0.54
1:U:628:ARG:HG3	1:U:749:GLN:HE22	1.73	0.54
2:V:65:ARG:O	2:V:69:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Z:148:GLY:HA2	7:a:181:GLY:HA3	1.90	0.54
6:Z:197:GLY:HA2	9:c:225:TRP:HD1	1.73	0.54
7:a:247:ARG:O	7:a:251:LEU:HG	2.08	0.54
8:b:93:ALA:HB1	8:b:109:ILE:HD11	1.89	0.54
16:E:167:PRO:O	16:E:274:LYS:NZ	2.40	0.54
2:V:200:ARG:HB3	2:V:201:ARG:HH21	1.73	0.54
3:W:144:ARG:O	3:W:148:THR:HG23	2.07	0.54
3:W:406:VAL:HG13	3:W:413:ILE:HG22	1.90	0.54
5:Y:138:LEU:HD13	5:Y:168:ILE:HG21	1.90	0.54
7:a:150:SER:OG	7:a:154:ARG:NH1	2.41	0.54
12:A:62:LEU:HD11	13:B:80:ARG:HD2	1.90	0.54
15:D:74:HIS:C	15:D:74:HIS:CD2	2.86	0.54
22:J:65:LEU:HB2	22:J:69:VAL:HG23	1.90	0.54
30:R:166:ARG:NH1	29:q:144:ASP:OD2	2.41	0.54
32:T:136:SER:OG	32:T:147:GLN:NE2	2.41	0.54
1:U:233:LEU:O	1:U:237:VAL:HG12	2.08	0.54
4:X:389:ASP:OD1	4:X:389:ASP:N	2.40	0.54
5:Y:314:LEU:HD21	5:Y:319:MET:HE1	1.88	0.54
9:c:223:LYS:HB3	9:c:223:LYS:HZ2	1.73	0.54
16:E:125:GLU:OE1	16:E:125:GLU:N	2.40	0.54
20:H:187:ALA:HA	20:H:190:THR:HG22	1.89	0.54
3:W:267:LEU:HD12	3:W:299:ILE:HD13	1.90	0.54
5:Y:85:ASP:OD1	5:Y:86:GLU:N	2.41	0.54
7:a:260:ASP:HA	7:a:263:ALA:HB3	1.90	0.54
8:b:33:VAL:HA	8:b:36:VAL:HG22	1.90	0.54
12:A:210:LYS:HE2	12:A:309:PHE:CE2	2.42	0.54
15:D:388:ARG:HB2	15:D:388:ARG:NH1	2.23	0.54
1:U:744:VAL:HA	1:U:785:PRO:HA	1.88	0.53
1:U:813:TYR:CG	1:U:813:TYR:O	2.61	0.53
8:b:100:ARG:NH1	8:b:105:HIS:O	2.40	0.53
9:c:256:ASN:HA	9:c:259:VAL:HG12	1.89	0.53
10:d:161:GLU:HG3	10:d:163:TYR:CE1	2.43	0.53
10:d:184:LYS:HB3	10:d:228:GLN:OE1	2.08	0.53
13:B:153:ASN:HD21	13:B:155:LYS:HE3	1.71	0.53
14:C:229:ARG:NH2	14:C:233:GLU:OE2	2.40	0.53
19:g:49:VAL:HG22	19:g:219:VAL:HG23	1.90	0.53
22:j:5:ARG:HD3	22:j:8:THR:HB	1.89	0.53
34:u:524:MET:HB2	34:u:564:LEU:HD21	1.90	0.53
7:a:68:GLU:O	7:a:69:HIS:ND1	2.41	0.53
7:a:144:ASN:HB3	7:a:145:LEU:HD22	1.90	0.53
10:d:188:LYS:HB3	10:d:220:ASN:ND2	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:215:TRP:CZ3	10:d:224:SER:HB3	2.44	0.53
12:A:80:LEU:O	12:A:85:GLN:NE2	2.42	0.53
15:D:119:ILE:O	15:D:121:ARG:NH1	2.37	0.53
19:G:67:THR:HG22	19:G:69:LEU:H	1.72	0.53
34:u:115:PRO:HA	34:u:119:LYS:HD2	1.91	0.53
1:U:122:GLU:HG3	1:U:123:LYS:H	1.72	0.53
15:D:203:LEU:HB2	15:D:327:LEU:HD13	1.91	0.53
17:F:332:THR:HG21	17:F:338:LEU:HD11	1.90	0.53
24:L:76:GLY:HA3	24:L:130:VAL:HA	1.90	0.53
3:W:117:ASP:OD1	3:W:118:LEU:N	2.42	0.53
5:Y:49:ASN:C	5:Y:50:MET:HE2	2.34	0.53
10:d:21:GLU:O	10:d:25:ARG:HG3	2.09	0.53
14:C:119:ASP:OD1	14:C:120:SER:N	2.42	0.53
14:C:280:LEU:HD23	14:C:310:ARG:HG3	1.91	0.53
14:C:394:ASP:O	14:C:397:LYS:NZ	2.41	0.53
28:P:205:ASP:HB3	30:r:192:VAL:HG11	1.89	0.53
1:U:101:ILE:HA	1:U:104:CYS:HB2	1.90	0.53
1:U:243:LEU:HG	1:U:913:ILE:HG21	1.89	0.53
3:W:65:ARG:O	3:W:68:VAL:HG13	2.07	0.53
8:b:21:PHE:CD2	8:b:178:SER:O	2.61	0.53
9:c:211:GLU:O	9:c:213:GLU:N	2.37	0.53
17:F:424:ILE:O	17:F:428:GLN:HG3	2.09	0.53
32:T:46:ASN:OD1	32:T:47:ASN:N	2.42	0.53
19:g:73:THR:HG22	19:g:74:GLU:H	1.73	0.53
29:q:68:LYS:HG3	29:q:74:GLU:HG3	1.89	0.53
1:U:269:ARG:HD2	1:U:270:THR:H	1.72	0.53
2:V:37:MET:HA	2:V:40:GLU:OE2	2.08	0.53
2:V:213:TYR:O	2:V:217:VAL:HG23	2.09	0.53
3:W:172:GLU:HB2	3:W:182:ARG:NH1	2.24	0.53
5:Y:73:MET:N	5:Y:73:MET:SD	2.82	0.53
7:a:223:GLU:OE1	7:a:234:ILE:HB	2.09	0.53
15:D:130:VAL:HG21	15:D:139:LEU:HD12	1.91	0.53
34:u:662:MET:HG3	34:u:781:TYR:HE1	1.72	0.53
1:U:196:LYS:O	1:U:199:ARG:HG2	2.09	0.53
1:U:836:THR:HG22	34:u:607:LEU:HD21	1.90	0.53
5:Y:348:ASP:OD1	5:Y:349:LYS:N	2.42	0.53
8:b:26:LEU:O	8:b:29:GLN:HG2	2.07	0.53
11:e:6:GLN:O	11:e:8:VAL:N	2.42	0.53
17:F:300:LYS:O	17:F:301:ALA:HB3	2.09	0.53
20:h:75:VAL:HG12	20:h:135:LEU:HB2	1.91	0.53
29:q:182:ILE:HG22	29:q:189:HIS:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:505:ASP:HB3	1:U:508:THR:HG22	1.90	0.53
1:U:748:LEU:HD23	1:U:760:VAL:HG22	1.90	0.53
1:U:874:ASN:O	1:U:875:PHE:CB	2.57	0.53
3:W:338:THR:HA	3:W:342:GLY:HA3	1.90	0.53
7:a:54:ASP:HA	7:a:57:ILE:HG22	1.91	0.53
7:a:307:VAL:O	7:a:311:VAL:HG23	2.08	0.53
10:d:212:LYS:HG3	10:d:213:ARG:HG3	1.91	0.53
16:E:119:VAL:HA	16:E:123:SER:HB3	1.90	0.53
34:u:581:GLU:OE1	34:u:581:GLU:N	2.40	0.53
34:u:760:PHE:O	34:u:764:LEU:HD22	2.09	0.53
2:V:28:PRO:O	2:V:32:PRO:HD2	2.09	0.53
4:X:95:LEU:HA	4:X:98:ASP:OD1	2.09	0.53
5:Y:49:ASN:O	5:Y:50:MET:HE2	2.09	0.53
19:G:129:ALA:O	19:G:130:GLU:HG3	2.09	0.53
27:O:163:ILE:HG23	27:O:169:SER:CB	2.39	0.53
29:Q:2:GLU:HG2	29:Q:34:LYS:HE2	1.90	0.53
1:U:162:VAL:HA	1:U:165:LYS:HD2	1.90	0.53
1:U:837:ALA:O	1:U:840:LYS:HG2	2.09	0.53
1:U:903:PHE:HB2	1:U:915:LYS:HE3	1.90	0.53
16:E:300:HIS:NE2	16:E:302:ASP:OD1	2.42	0.53
17:F:239:ALA:O	17:F:243:GLN:HG2	2.09	0.53
17:F:291:ILE:HG22	17:F:306:VAL:HG13	1.90	0.53
23:k:24:VAL:O	23:k:28:ILE:HG12	2.08	0.53
34:u:275:MET:H	34:u:275:MET:CE	2.22	0.53
1:U:140:ARG:HG2	1:U:140:ARG:HH11	1.74	0.52
3:W:144:ARG:H	3:W:144:ARG:HD3	1.74	0.52
17:F:279:ALA:O	17:F:325:GLN:HB3	2.09	0.52
17:F:336:ASP:OD1	17:F:336:ASP:N	2.39	0.52
22:J:67:ASP:OD1	22:J:67:ASP:N	2.41	0.52
25:m:186:CYS:HB3	25:m:219:LEU:HD11	1.90	0.52
34:u:48:GLU:HA	34:u:51:GLN:HG2	1.90	0.52
1:U:169:GLU:O	1:U:171:ASN:N	2.42	0.52
1:U:571:CYS:HB3	1:U:601:ARG:HH22	1.74	0.52
9:c:68:ARG:NH2	9:c:208:ARG:HH22	2.07	0.52
9:c:282:ARG:O	9:c:286:GLU:HG2	2.09	0.52
10:d:71:PHE:O	10:d:75:MET:HB2	2.10	0.52
21:I:154:GLY:O	22:J:81:ARG:NH2	2.39	0.52
25:m:46:VAL:HG22	25:m:215:TRP:CD1	2.44	0.52
33:f:394:ARG:O	33:f:398:LEU:HG	2.08	0.52
1:U:45:ILE:HG21	1:U:64:ALA:HB2	1.90	0.52
4:X:122:ARG:HD2	4:X:125:LEU:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:336:ARG:HH22	11:e:52:PHE:HZ	1.57	0.52
9:c:292:MET:HE3	10:d:253:LEU:HD11	1.92	0.52
12:A:289:ALA:HA	17:F:301:ALA:HB2	1.90	0.52
14:C:183:PRO:O	14:C:290:LYS:NZ	2.42	0.52
16:E:4:PRO:O	16:E:5:ARG:HG3	2.10	0.52
1:U:68:PHE:CD2	1:U:76:GLU:HB2	2.45	0.52
26:n:1:THR:HG21	26:n:46:SER:HB2	1.92	0.52
1:U:793:LYS:HB2	1:U:796:LYS:HB2	1.91	0.52
3:W:386:VAL:O	3:W:390:GLU:HG2	2.09	0.52
4:X:126:ARG:O	4:X:130:GLU:HG2	2.10	0.52
5:Y:88:LEU:HG	5:Y:100:ILE:HG13	1.91	0.52
5:Y:279:GLU:HG3	5:Y:296:VAL:HG21	1.91	0.52
10:d:189:ILE:N	10:d:220:ASN:H	2.06	0.52
15:D:74:HIS:HD2	15:D:74:HIS:O	1.93	0.52
16:E:308:ALA:O	16:E:309:ARG:HB3	2.09	0.52
17:F:261:ILE:HD13	17:F:305:GLU:HA	1.91	0.52
5:Y:283:LYS:HD3	5:Y:288:PHE:HE2	1.74	0.52
7:a:214:GLY:O	7:a:216:LEU:N	2.43	0.52
7:a:244:ASN:HD21	7:a:246:GLU:HG2	1.72	0.52
9:c:195:GLY:O	9:c:196:LEU:C	2.51	0.52
19:G:22:LEU:O	19:G:26:GLU:HG3	2.09	0.52
34:u:422:VAL:O	34:u:426:LEU:HD12	2.10	0.52
1:U:239:GLU:OE1	1:U:241:ASN:HB2	2.09	0.52
3:W:219:THR:HG21	3:W:222:LEU:HD22	1.90	0.52
12:A:238:ILE:HG21	12:A:260:LEU:HD11	1.91	0.52
13:B:380:LEU:O	13:B:384:ILE:HD12	2.10	0.52
17:F:297:ASP:C	17:F:299:GLU:N	2.68	0.52
34:u:83:ARG:HB2	34:u:154:TRP:HZ3	1.74	0.52
2:V:252:ASN:HD21	2:V:284:GLU:HG2	1.75	0.52
4:X:245:PRO:O	4:X:248:ILE:HD12	2.09	0.52
4:X:365:LEU:O	4:X:369:ILE:HG12	2.10	0.52
8:b:95:LEU:HA	8:b:98:LYS:HG3	1.91	0.52
9:c:40:LYS:HZ2	9:c:72:VAL:HG23	1.73	0.52
10:d:144:MET:HA	10:d:144:MET:HE3	1.92	0.52
16:E:65:THR:OG1	16:E:66:GLU:OE1	2.26	0.52
24:l:50:LYS:HB3	24:l:59:HIS:HB3	1.92	0.52
3:W:148:THR:O	3:W:152:ILE:HD13	2.08	0.52
5:Y:112:CYS:HG	5:Y:124:PHE:HE2	1.56	0.52
5:Y:284:LYS:HD3	5:Y:284:LYS:N	2.25	0.52
7:a:127:ASP:OD1	7:a:127:ASP:N	2.37	0.52
7:a:240:PHE:HZ	7:a:268:LEU:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:274:ALA:O	13:B:280:SER:OG	2.24	0.52
16:E:6:ASP:OD1	16:E:6:ASP:N	2.43	0.52
16:E:145:LEU:HD21	16:E:187:VAL:HG21	1.92	0.52
22:j:121:SER:HB3	22:j:124:ARG:HE	1.74	0.52
1:U:364:VAL:O	1:U:364:VAL:HG12	2.10	0.52
3:W:33:LYS:HA	3:W:36:LYS:HD2	1.91	0.52
3:W:188:GLU:HA	3:W:191:ARG:NH2	2.25	0.52
3:W:294:LYS:HD2	3:W:295:LYS:N	2.25	0.52
7:a:12:GLN:HG2	7:a:18:GLN:NE2	2.25	0.52
10:d:188:LYS:N	10:d:220:ASN:HB2	2.19	0.52
13:B:46:ALA:HB3	13:B:179:ALA:H	1.75	0.52
13:B:434:THR:OG1	13:B:435:PRO:HD2	2.10	0.52
15:D:99:ASN:HA	15:D:115:ILE:HG12	1.92	0.52
15:D:214:MET:HE1	38:D:501:ADP:C4	2.45	0.52
16:E:29:LEU:O	16:E:32:GLN:HG3	2.10	0.52
22:J:108:THR:HG21	22:J:145:TYR:HB2	1.90	0.52
24:l:178:GLU:OE1	24:l:178:GLU:N	2.40	0.52
28:p:107:PRO:HG2	28:p:124:LEU:HB2	1.91	0.52
34:u:275:MET:H	34:u:275:MET:HE3	1.74	0.52
2:V:165:ALA:O	2:V:167:LEU:N	2.41	0.51
4:X:244:SER:HB3	4:X:245:PRO:CD	2.39	0.51
7:a:112:ILE:HG23	7:a:151:VAL:HG21	1.91	0.51
7:a:320:VAL:HG12	7:a:335:TRP:CD1	2.45	0.51
13:B:122:ILE:HG22	13:B:122:ILE:O	2.11	0.51
20:H:19:LEU:HD22	20:H:19:LEU:H	1.75	0.51
19:g:200:THR:O	19:g:204:THR:HG23	2.09	0.51
24:l:65:HIS:NE2	24:l:67:ASP:O	2.43	0.51
34:u:53:GLN:NE2	34:u:57:GLU:OE2	2.42	0.51
34:u:394:ASP:HB3	34:u:397:LYS:HG2	1.91	0.51
1:U:661:ALA:HB1	1:U:746:ILE:HD12	1.92	0.51
2:V:332:LEU:HA	2:V:335:VAL:HG22	1.93	0.51
6:Z:209:ARG:HH21	7:a:354:GLU:HA	1.75	0.51
7:a:31:LYS:O	7:a:32:LYS:HG3	2.09	0.51
8:b:180:ALA:C	8:b:182:ALA:N	2.66	0.51
14:C:260:GLU:H	14:C:260:GLU:CD	2.18	0.51
17:F:85:THR:O	17:F:88:TYR:CE1	2.63	0.51
17:F:281:SER:O	17:F:326:VAL:HA	2.11	0.51
27:O:33:LYS:HE2	39:O:301:LDZ:H22	1.91	0.51
1:U:529:ILE:O	1:U:533:VAL:HG12	2.11	0.51
3:W:145:LEU:HD22	3:W:148:THR:OG1	2.10	0.51
3:W:372:ARG:HH12	7:a:327:VAL:HG11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:190:LEU:HD22	4:X:217:ILE:HD12	1.92	0.51
13:B:374:LEU:HD21	13:B:419:PHE:HE2	1.75	0.51
17:F:343:LEU:HD13	17:F:351:LYS:HD3	1.92	0.51
27:O:1:THR:HG23	39:O:301:LDZ:C22	2.40	0.51
26:n:11:GLY:HA3	26:n:179:ILE:O	2.11	0.51
34:u:179:VAL:HG13	34:u:180:GLN:HG3	1.93	0.51
34:u:705:ASN:N	34:u:705:ASN:OD1	2.44	0.51
34:u:865:PHE:HD1	34:u:865:PHE:H	1.59	0.51
1:U:157:THR:HG22	1:U:157:THR:O	2.11	0.51
1:U:901:GLN:HG2	1:U:902:PRO:HD2	1.92	0.51
4:X:406:ASN:O	4:X:409:LYS:HG3	2.11	0.51
7:a:77:VAL:HG21	7:a:110:ALA:HB1	1.93	0.51
9:c:225:TRP:CD1	9:c:225:TRP:O	2.64	0.51
10:d:217:LEU:O	10:d:219:PRO:HD3	2.10	0.51
10:d:222:TYR:C	10:d:224:SER:N	2.67	0.51
10:d:222:TYR:O	10:d:224:SER:N	2.42	0.51
13:B:206:THR:HG22	13:B:207:HIS:CD2	2.45	0.51
14:C:398:ASN:ND2	14:C:401:ILE:HD13	2.26	0.51
20:h:91:ARG:HD3	27:o:68:LEU:HD23	1.91	0.51
3:W:4:GLY:O	3:W:7:GLU:HG3	2.11	0.51
3:W:395:ASN:OD1	3:W:396:LEU:N	2.42	0.51
6:Z:17:LEU:HD12	9:c:217:LEU:HD21	1.93	0.51
7:a:42:LEU:HD11	7:a:78:GLU:HG3	1.91	0.51
25:M:219:LEU:HD12	25:M:220:THR:HG23	1.91	0.51
22:j:104:VAL:O	22:j:108:THR:OG1	2.28	0.51
1:U:764:LEU:O	1:U:765:VAL:C	2.53	0.51
5:Y:50:MET:HE1	5:Y:70:LEU:HD23	1.92	0.51
13:B:189:GLY:HA3	13:B:360:THR:HG23	1.93	0.51
27:O:97:ALA:HB1	27:O:127:MET:SD	2.51	0.51
34:u:834:ASP:N	34:u:838:ARG:O	2.37	0.51
7:a:7:PHE:HE2	7:a:60:TYR:HB2	1.75	0.51
9:c:210:ASN:OD1	9:c:211:GLU:N	2.40	0.51
13:B:41:LYS:HD2	13:B:41:LYS:N	2.25	0.51
16:E:148:VAL:HG21	16:E:297:ARG:HG2	1.93	0.51
27:O:155:VAL:O	27:O:159:ILE:HG12	2.11	0.51
25:m:175:GLU:HA	25:m:178:LYS:HD3	1.92	0.51
34:u:420:TRP:HD1	34:u:455:VAL:HG13	1.76	0.51
1:U:587:ALA:HB2	1:U:621:SER:HB3	1.92	0.51
1:U:793:LYS:HA	1:U:793:LYS:HE2	1.93	0.51
2:V:193:GLN:HB3	2:V:241:ARG:NH2	2.26	0.51
3:W:403:PHE:HE2	3:W:417:ARG:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:347:ILE:HD13	4:X:350:ILE:HD11	1.93	0.51
7:a:37:LEU:O	7:a:41:VAL:HG12	2.11	0.51
7:a:247:ARG:HD2	7:a:247:ARG:N	2.21	0.51
9:c:27:THR:OG1	9:c:28:ALA:N	2.40	0.51
9:c:70:ILE:HD12	9:c:104:ARG:HH22	1.75	0.51
9:c:139:ARG:HA	9:c:161:ARG:NH2	2.26	0.51
10:d:189:ILE:H	10:d:220:ASN:CA	2.23	0.51
17:F:295:ARG:HH12	17:F:304:ARG:HH22	1.56	0.51
3:W:220:GLU:OE2	3:W:257:GLN:NE2	2.44	0.51
15:D:91:GLN:NE2	15:D:127:ASN:OD1	2.43	0.51
17:F:180:ARG:NH1	17:F:242:ALA:HA	2.26	0.51
23:K:25:GLU:O	23:K:29:GLU:HG2	2.11	0.51
23:k:16:SER:OG	23:k:20:ARG:O	2.24	0.51
34:u:55:GLU:HA	34:u:58:MET:HG3	1.92	0.51
1:U:898:CYS:SG	1:U:899:ARG:N	2.84	0.51
2:V:148:ARG:HD2	2:V:149:PRO:CD	2.28	0.51
2:V:165:ALA:HB2	2:V:171:VAL:HG11	1.92	0.51
2:V:170:LEU:O	2:V:173:ILE:HG22	2.10	0.51
3:W:58:SER:C	3:W:60:MET:H	2.19	0.51
5:Y:22:LEU:HD23	5:Y:40:GLU:HB2	1.91	0.51
9:c:123:SER:H	9:c:126:ASP:HB2	1.76	0.51
12:A:241:ILE:HD12	12:A:244:GLU:HG3	1.93	0.51
14:C:251:ILE:HG22	14:C:295:THR:HB	1.93	0.51
31:S:16:ALA:HB2	31:S:121:VAL:HG23	1.93	0.51
20:h:179:ASN:HB3	20:h:182:LEU:HD13	1.93	0.51
31:s:28:ARG:O	31:s:42:LYS:NZ	2.43	0.51
31:s:145:LEU:HD21	31:s:182:ALA:HB2	1.92	0.51
1:U:695:MET:HE1	1:U:709:PHE:HD2	1.76	0.50
2:V:189:ASP:HA	2:V:192:MET:SD	2.51	0.50
2:V:318:GLN:O	2:V:319:HIS:ND1	2.44	0.50
2:V:346:LEU:HA	2:V:357:LEU:HD22	1.92	0.50
3:W:62:SER:C	3:W:64:SER:N	2.68	0.50
3:W:320:LEU:O	3:W:324:TYR:CB	2.57	0.50
3:W:451:MET:HE1	6:Z:138:TYR:HE2	1.76	0.50
5:Y:69:LEU:O	5:Y:72:LYS:HG2	2.11	0.50
5:Y:349:LYS:O	5:Y:351:ASN:N	2.44	0.50
16:E:8:ALA:C	17:F:44:ARG:HH21	2.19	0.50
19:g:185:LYS:HE2	19:g:185:LYS:N	2.26	0.50
34:u:656:GLY:O	34:u:660:ILE:HG13	2.10	0.50
2:V:255:LEU:O	2:V:259:LEU:HD23	2.11	0.50
3:W:243:ILE:HG13	3:W:273:TYR:HE2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:199:GLU:OE2	5:Y:200:LEU:HG	2.11	0.50
10:d:215:TRP:HA	10:d:215:TRP:CE3	2.46	0.50
19:G:80:MET:HG2	19:G:87:SER:HB3	1.94	0.50
23:K:121:LEU:HD12	23:K:160:GLY:HA3	1.94	0.50
23:k:49:ALA:HB2	23:k:217:LEU:HD12	1.93	0.50
25:m:192:GLU:O	25:m:196:ILE:HG13	2.12	0.50
34:u:868:HIS:CE1	34:u:872:VAL:HG21	2.46	0.50
3:W:435:LEU:HG	6:Z:234:PHE:HE1	1.77	0.50
4:X:245:PRO:O	4:X:247:ALA:N	2.41	0.50
5:Y:29:PRO:HB2	5:Y:32:ARG:HB2	1.93	0.50
17:F:297:ASP:O	17:F:299:GLU:N	2.44	0.50
24:L:47:VAL:HG12	24:L:195:LEU:HD22	1.94	0.50
1:U:475:HIS:ND1	1:U:511:ALA:HB2	2.26	0.50
1:U:815:ALA:N	1:U:816:PRO:HD3	2.27	0.50
2:V:440:LYS:HE2	10:d:148:TYR:CZ	2.46	0.50
3:W:340:VAL:HG12	3:W:341:PHE:CD2	2.47	0.50
4:X:306:LEU:HD21	4:X:314:ARG:HH22	1.76	0.50
8:b:150:THR:O	8:b:154:THR:HG23	2.11	0.50
12:A:143:ASP:HB3	12:A:148:GLN:H	1.75	0.50
13:B:425:ASN:C	13:B:425:ASN:HD22	2.18	0.50
25:M:75:MET:HB2	25:M:137:LEU:HD23	1.93	0.50
28:P:117:PHE:CE2	28:P:192:LYS:HE2	2.46	0.50
4:X:162:ASP:O	4:X:166:LEU:HD13	2.11	0.50
10:d:77:GLN:O	10:d:81:TYR:HD1	1.94	0.50
10:d:172:ASP:HA	10:d:175:ARG:HD2	1.93	0.50
13:B:75:GLU:O	13:B:79:ILE:HG22	2.11	0.50
17:F:159:LEU:HD12	17:F:160:ILE:N	2.26	0.50
21:I:18:LEU:O	21:I:22:GLU:HG2	2.11	0.50
2:V:77:GLU:HB2	2:V:86:VAL:HG21	1.94	0.50
2:V:176:MET:O	2:V:180:ARG:HG2	2.12	0.50
2:V:231:LEU:HD11	2:V:250:LEU:O	2.11	0.50
10:d:22:GLU:HA	10:d:25:ARG:HG3	1.94	0.50
10:d:215:TRP:HZ3	10:d:224:SER:HB3	1.74	0.50
16:E:42:LYS:NZ	16:E:46:ASP:OD1	2.44	0.50
17:F:202:ILE:O	17:F:206:MET:HB2	2.12	0.50
17:F:249:LEU:HD13	17:F:283:ILE:HG13	1.92	0.50
25:m:42:LYS:CB	25:m:184:MET:O	2.59	0.50
1:U:803:LYS:HA	1:U:876:GLN:O	2.12	0.50
2:V:91:PRO:HB2	2:V:114:TYR:CE1	2.46	0.50
2:V:482:PHE:CZ	5:Y:381:GLN:HG3	2.46	0.50
2:V:495:ARG:O	2:V:496:PHE:CD1	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:52:LYS:HA	3:W:55:ARG:CD	2.41	0.50
4:X:142:ARG:HB3	4:X:145:GLU:HG2	1.93	0.50
5:Y:388:ASN:ND2	5:Y:388:ASN:O	2.39	0.50
13:B:85:MET:SD	13:B:85:MET:N	2.84	0.50
14:C:395:SER:OG	14:C:397:LYS:NZ	2.45	0.50
17:F:274:LEU:O	17:F:278:LYS:HG2	2.12	0.50
21:I:187:LYS:H	21:I:187:LYS:CE	2.23	0.50
23:K:171:GLY:O	23:K:174:SER:OG	2.24	0.50
27:O:216:ILE:HG12	28:P:196:THR:HG23	1.93	0.50
30:R:91:LYS:NZ	30:R:117:GLU:O	2.44	0.50
19:g:165:ALA:HB3	20:h:56:LEU:HD22	1.94	0.50
22:j:99:GLU:OE2	30:r:120:ARG:NH2	2.44	0.50
27:o:49:ALA:HB2	39:o:301:LDZ:H15	1.93	0.50
29:q:49:GLU:HG3	29:q:99:HIS:HB3	1.93	0.50
1:U:115:ASN:HB3	1:U:123:LYS:HG2	1.93	0.50
1:U:796:LYS:HG2	1:U:924:LEU:HD23	1.93	0.50
1:U:874:ASN:O	1:U:875:PHE:HB3	2.12	0.50
3:W:125:ILE:HG23	3:W:129:ARG:HH21	1.77	0.50
7:a:21:VAL:HG23	7:a:22:TRP:CD1	2.47	0.50
8:b:142:ASN:HB3	8:b:146:GLU:OE2	2.11	0.50
10:d:73:ARG:HG3	10:d:77:GLN:HE22	1.76	0.50
10:d:169:ILE:O	10:d:173:THR:HG23	2.12	0.50
17:F:192:ASP:HA	17:F:195:ILE:HD12	1.94	0.50
32:t:25:ASP:HA	32:t:187:PHE:HA	1.93	0.50
3:W:58:SER:O	3:W:61:VAL:HG22	2.12	0.50
7:a:132:LYS:O	7:a:135:ILE:HG22	2.12	0.50
10:d:222:TYR:C	10:d:224:SER:H	2.20	0.50
15:D:46:LYS:HE2	15:D:46:LYS:HA	1.94	0.50
16:E:140:GLU:OE2	16:E:140:GLU:N	2.23	0.50
17:F:185:TYR:CE2	17:F:243:GLN:HG3	2.47	0.50
25:M:202:ASP:HB2	25:M:209:PHE:CE1	2.46	0.50
34:u:291:GLN:HA	34:u:294:MET:HE2	1.94	0.50
2:V:78:HIS:HB3	2:V:164:GLU:OE1	2.12	0.49
3:W:248:ARG:HG2	3:W:270:VAL:HG21	1.94	0.49
6:Z:81:MET:HE1	9:c:91:PHE:HZ	1.77	0.49
12:A:72:LEU:HD13	13:B:138:PHE:HB2	1.94	0.49
13:B:153:ASN:ND2	13:B:155:LYS:HE3	2.27	0.49
16:E:145:LEU:HD12	16:E:172:LEU:HD21	1.94	0.49
33:f:410:ARG:NH1	33:f:415:PRO:HG2	2.26	0.49
3:W:11:GLY:O	3:W:15:LYS:HG2	2.12	0.49
3:W:50:LEU:O	3:W:54:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:96:PHE:CE2	4:X:109:LEU:HD22	2.47	0.49
7:a:162:TYR:C	7:a:164:GLN:H	2.20	0.49
10:d:52:ARG:HH22	10:d:89:LEU:HD13	1.77	0.49
10:d:176:ASP:OD1	10:d:177:GLU:N	2.45	0.49
10:d:218:GLY:C	10:d:222:TYR:HA	2.35	0.49
16:E:42:LYS:HA	16:E:45:ASN:HD22	1.77	0.49
16:E:245:GLU:HB3	19:G:18:PRO:HG2	1.94	0.49
1:U:145:HIS:CE1	1:U:170:SER:HB2	2.47	0.49
1:U:717:ILE:HD13	1:U:731:ILE:HD11	1.93	0.49
1:U:792:ASN:HD22	1:U:916:ASP:HB2	1.77	0.49
3:W:3:ASP:OD1	3:W:3:ASP:N	2.43	0.49
3:W:148:THR:HA	3:W:151:THR:HG22	1.94	0.49
3:W:187:LEU:HD13	3:W:226:TYR:CG	2.48	0.49
7:a:91:ASN:OD1	7:a:91:ASN:N	2.41	0.49
8:b:24:THR:HB	8:b:27:GLN:OE1	2.11	0.49
16:E:136:GLY:HA2	16:E:312:ILE:HG12	1.93	0.49
26:N:14:LEU:HD21	26:N:101:ALA:HB3	1.95	0.49
23:k:10:ARG:HB3	24:l:124:GLY:O	2.13	0.49
3:W:88:MET:HG2	3:W:89:LEU:H	1.77	0.49
3:W:186:ILE:O	3:W:190:MET:HG2	2.13	0.49
5:Y:360:ASP:O	5:Y:362:LYS:N	2.44	0.49
8:b:161:ASN:CG	8:b:167:GLY:H	2.20	0.49
10:d:174:ILE:O	10:d:178:ILE:HG23	2.12	0.49
13:B:287:ILE:HG12	13:B:329:MET:HE3	1.94	0.49
20:H:95:GLN:HG3	27:O:65:LEU:HG	1.95	0.49
30:R:37:ILE:O	30:R:41:LEU:HB2	2.13	0.49
1:U:803:LYS:HG2	1:U:893:THR:HB	1.95	0.49
1:U:842:LYS:HA	1:U:845:GLU:HG2	1.94	0.49
4:X:377:ILE:HG21	5:Y:312:ARG:HB3	1.93	0.49
5:Y:54:TYR:O	5:Y:57:LEU:HG	2.12	0.49
7:a:326:GLU:N	7:a:326:GLU:OE1	2.45	0.49
8:b:186:SER:HB3	8:b:187:PRO:CD	2.42	0.49
10:d:75:MET:SD	10:d:79:LYS:NZ	2.85	0.49
10:d:195:THR:HG23	10:d:205:LYS:HG2	1.93	0.49
15:D:69:LYS:HD3	15:D:73:LEU:HD23	1.93	0.49
16:E:376:ASP:HA	16:E:379:LYS:HG2	1.95	0.49
21:I:115:CYS:SG	21:I:150:SER:OG	2.69	0.49
29:Q:197:PRO:HA	29:q:199:GLN:H	1.77	0.49
24:l:125:ARG:HD3	24:l:126:ARG:H	1.77	0.49
3:W:228:ASN:HA	3:W:246:HIS:HE1	1.77	0.49
16:E:108:MET:HE2	16:E:108:MET:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:r:45:MET:HE3	39:r:301:LDZ:H17	1.94	0.49
34:u:349:TYR:HE1	34:u:763:ARG:HD2	1.77	0.49
34:u:505:MET:HE2	34:u:505:MET:HA	1.94	0.49
1:U:641:SER:O	1:U:641:SER:OG	2.31	0.49
2:V:479:ARG:HD2	6:Z:261:TYR:OH	2.13	0.49
5:Y:178:ASN:ND2	5:Y:212:GLU:OE1	2.45	0.49
6:Z:39:LEU:HD13	6:Z:95:TYR:HB3	1.95	0.49
7:a:246:GLU:O	7:a:250:THR:OG1	2.20	0.49
8:b:9:CYS:SG	8:b:54:LEU:HD22	2.53	0.49
9:c:265:MET:N	9:c:265:MET:SD	2.85	0.49
17:F:223:VAL:O	17:F:329:ILE:HA	2.13	0.49
24:L:128:TYR:O	24:L:149:PRO:HB3	2.12	0.49
19:g:129:ALA:C	19:g:130:GLU:HG3	2.37	0.49
20:h:119:GLN:HG3	21:i:81:SER:HB2	1.94	0.49
34:u:560:LEU:O	34:u:564:LEU:HB3	2.13	0.49
1:U:142:LEU:HD12	1:U:165:LYS:HE2	1.95	0.49
1:U:144:ASP:HB2	14:C:12:GLU:O	2.13	0.49
1:U:418:GLU:HA	1:U:421:GLN:OE1	2.12	0.49
2:V:172:VAL:O	2:V:175:MET:HB2	2.13	0.49
2:V:337:LEU:O	2:V:401:ASN:ND2	2.45	0.49
4:X:143:TYR:CE2	4:X:144:GLN:HG2	2.48	0.49
8:b:16:MET:HG3	8:b:26:LEU:HD12	1.95	0.49
9:c:60:GLU:HB3	9:c:68:ARG:HD3	1.95	0.49
20:H:107:THR:O	20:H:111:VAL:HG23	2.13	0.49
19:g:192:GLU:OE1	19:g:192:GLU:N	2.42	0.49
1:U:697:GLN:NE2	1:U:744:VAL:O	2.46	0.49
3:W:173:THR:HG23	3:W:182:ARG:NE	2.28	0.49
4:X:413:SER:OG	9:c:260:GLU:OE2	2.31	0.49
8:b:181:ASP:C	8:b:183:LEU:N	2.68	0.49
20:H:10:LEU:HD13	20:H:21:GLN:HB2	1.95	0.49
29:q:2:GLU:HB2	29:q:47:VAL:HG21	1.95	0.49
31:s:19:ASP:N	31:s:19:ASP:OD1	2.43	0.49
34:u:308:SER:OG	34:u:310:ASP:OD1	2.30	0.49
1:U:372:ALA:O	1:U:376:MET:HG2	2.13	0.49
13:B:405:MET:HA	13:B:408:ARG:HD2	1.94	0.49
15:D:258:ALA:HB1	15:D:259:PRO:CD	2.42	0.49
20:H:91:ARG:HD3	27:O:68:LEU:HD23	1.95	0.49
20:h:186:ASP:O	20:h:190:THR:HG22	2.13	0.49
25:m:8:ASP:O	25:m:22:GLN:NE2	2.45	0.49
34:u:313:GLU:O	34:u:317:LEU:HG	2.13	0.49
1:U:450:HIS:CG	1:U:457:ILE:HD13	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:567:ILE:HG12	1:U:586:VAL:HG23	1.95	0.48
2:V:392:TYR:O	2:V:395:ILE:HG22	2.12	0.48
3:W:317:TRP:CD1	3:W:358:VAL:HG21	2.48	0.48
7:a:136:GLU:O	7:a:140:GLU:HB2	2.13	0.48
10:d:82:TYR:CZ	10:d:95:MET:HB3	2.48	0.48
14:C:34:ILE:HG22	15:D:51:LEU:HD11	1.95	0.48
14:C:299:ASP:OD1	14:C:299:ASP:N	2.45	0.48
30:R:182:ASP:OD1	30:R:182:ASP:N	2.44	0.48
33:f:393:GLU:HG3	33:f:394:ARG:NH2	2.28	0.48
34:u:62:ARG:HD3	34:u:70:LEU:HD23	1.95	0.48
1:U:22:PHE:O	1:U:26:LYS:HB3	2.13	0.48
1:U:602:LEU:HD11	1:U:621:SER:HB2	1.96	0.48
3:W:42:GLU:N	3:W:42:GLU:OE1	2.46	0.48
3:W:52:LYS:O	3:W:55:ARG:HD3	2.12	0.48
6:Z:101:LEU:HD13	6:Z:123:ILE:HD11	1.94	0.48
7:a:269:LEU:HD12	7:a:272:ILE:HD11	1.95	0.48
16:E:238:ILE:HA	16:E:241:ARG:HE	1.78	0.48
20:h:199:PHE:HZ	20:h:207:ASN:HD22	1.61	0.48
24:l:117:GLN:O	24:l:120:THR:OG1	2.30	0.48
2:V:256:ARG:HH12	11:e:5:LYS:HB2	1.79	0.48
4:X:394:ASP:OD1	4:X:394:ASP:N	2.35	0.48
6:Z:17:LEU:CD1	9:c:217:LEU:HD21	2.42	0.48
7:a:172:TYR:O	7:a:173:TYR:C	2.57	0.48
10:d:189:ILE:HG23	10:d:220:ASN:OD1	2.14	0.48
14:C:89:VAL:HG12	14:C:91:PRO:HD2	1.95	0.48
16:E:363:VAL:HG13	16:E:365:GLU:H	1.78	0.48
22:J:183:THR:O	22:J:185:ASP:N	2.46	0.48
24:l:7:ASP:OD1	24:l:20:HIS:ND1	2.47	0.48
1:U:418:GLU:HG2	1:U:418:GLU:O	2.12	0.48
2:V:224:LEU:HD23	2:V:257:ASN:HB3	1.95	0.48
4:X:407:MET:HA	4:X:410:VAL:HG12	1.95	0.48
6:Z:257:MET:HE3	6:Z:257:MET:C	2.37	0.48
10:d:219:PRO:O	10:d:220:ASN:C	2.56	0.48
12:A:108:ASP:HB3	12:A:110:LYS:HD2	1.94	0.48
12:A:258:ARG:O	12:A:262:GLU:HG2	2.13	0.48
16:E:312:ILE:HG22	16:E:316:HIS:CE1	2.48	0.48
17:F:175:MET:SD	17:F:249:LEU:HB3	2.53	0.48
20:H:182:LEU:HD23	20:H:182:LEU:N	2.29	0.48
34:u:208:LEU:HB3	34:u:214:VAL:HA	1.96	0.48
3:W:65:ARG:HG3	3:W:67:LEU:HB3	1.96	0.48
3:W:310:THR:C	3:W:312:MET:H	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:d:179:ALA:O	10:d:182:ILE:HG22	2.14	0.48
15:D:258:ALA:HB1	15:D:259:PRO:HD2	1.94	0.48
15:D:268:ASP:N	15:D:268:ASP:OD1	2.47	0.48
19:g:22:LEU:O	19:g:26:GLU:HG3	2.13	0.48
25:m:172:ALA:O	25:m:176:ILE:HG13	2.12	0.48
29:q:31:ASP:N	29:q:31:ASP:OD1	2.47	0.48
1:U:919:GLU:HG3	1:U:920:ASP:H	1.79	0.48
2:V:306:ARG:O	2:V:310:THR:HG23	2.13	0.48
3:W:71:VAL:O	3:W:74:CYS:HB3	2.14	0.48
4:X:202:CYS:HB2	4:X:206:LEU:HD23	1.95	0.48
4:X:286:ALA:HB2	4:X:309:TYR:CD2	2.48	0.48
16:E:101:ASP:OD1	16:E:102:MET:N	2.46	0.48
16:E:194:ASN:HB2	16:E:230:ILE:HD13	1.95	0.48
16:E:321:THR:OG1	16:E:322:LYS:N	2.47	0.48
17:F:94:ILE:HG22	17:F:123:VAL:HG13	1.94	0.48
23:K:233:GLU:O	23:K:237:VAL:HG23	2.14	0.48
25:M:188:ASP:O	25:M:192:GLU:HG2	2.13	0.48
20:h:69:THR:HG22	20:h:70:LYS:N	2.29	0.48
34:u:292:LYS:O	34:u:296:PHE:HD1	1.96	0.48
1:U:167:ILE:C	1:U:169:GLU:N	2.66	0.48
2:V:88:GLY:HA2	2:V:118:GLN:OE1	2.14	0.48
2:V:245:ASP:H	2:V:247:GLN:NE2	2.10	0.48
2:V:419:LEU:H	2:V:419:LEU:HD23	1.79	0.48
3:W:59:ASP:HA	3:W:63:THR:HG23	1.93	0.48
5:Y:220:VAL:HG11	5:Y:249:VAL:HG23	1.95	0.48
10:d:170:LEU:O	10:d:174:ILE:HG13	2.13	0.48
12:A:158:ASP:HB3	12:A:161:VAL:HB	1.95	0.48
12:A:213:LEU:HB2	12:A:337:LEU:HD13	1.96	0.48
15:D:60:TYR:CE1	15:D:64:GLU:HG3	2.48	0.48
17:F:85:THR:C	17:F:87:PRO:HD2	2.37	0.48
19:G:50:ILE:HG21	19:G:79:VAL:HB	1.95	0.48
21:I:130:PHE:O	21:I:152:PRO:HB3	2.14	0.48
24:L:75:ALA:HB3	24:L:161:ILE:HD12	1.96	0.48
20:h:7:SER:O	22:j:2:SER:OG	2.26	0.48
1:U:148:LYS:O	1:U:151:ILE:HG22	2.14	0.48
2:V:40:GLU:O	2:V:43:THR:OG1	2.26	0.48
3:W:59:ASP:HA	3:W:63:THR:OG1	2.13	0.48
7:a:130:VAL:O	7:a:134:THR:HG23	2.12	0.48
8:b:98:LYS:HD2	8:b:98:LYS:C	2.37	0.48
10:d:42:LYS:HA	10:d:45:LYS:HG3	1.96	0.48
14:C:197:THR:HG21	15:D:298:GLY:HA2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:417:TYR:HB3	20:H:79:MET:HG3	1.96	0.48
28:P:113:ASP:HB3	28:P:116:THR:O	2.12	0.48
25:m:41:CYS:HB2	25:m:44:GLY:C	2.38	0.48
1:U:259:GLN:HA	1:U:262:SER:HB3	1.94	0.48
2:V:205:LEU:H	2:V:205:LEU:HD12	1.78	0.48
2:V:495:ARG:HG2	2:V:497:PRO:HD3	1.95	0.48
4:X:92:LEU:HA	4:X:95:LEU:CD2	2.43	0.48
5:Y:49:ASN:HA	5:Y:114:ILE:HD12	1.94	0.48
7:a:123:LEU:HD22	7:a:127:ASP:OD2	2.13	0.48
13:B:294:ARG:NH1	13:B:338:ASP:OD2	2.46	0.48
14:C:20:LEU:HD12	14:C:21:ARG:N	2.29	0.48
23:K:178:GLN:O	23:K:182:GLN:HG3	2.13	0.48
19:g:213:SER:O	19:g:213:SER:OG	2.30	0.48
2:V:292:THR:O	2:V:295:ILE:HG13	2.14	0.48
3:W:178:GLU:O	3:W:182:ARG:HB2	2.14	0.48
6:Z:239:ASP:OD1	6:Z:239:ASP:N	2.46	0.48
7:a:101:ARG:HA	7:a:104:VAL:HG12	1.96	0.48
8:b:126:LYS:O	8:b:130:ARG:HG2	2.13	0.48
12:A:218:PRO:HB2	13:B:343:ARG:HD3	1.96	0.48
19:G:144:ASP:OD1	19:G:147:GLN:HG3	2.14	0.48
20:H:107:THR:HG21	20:H:138:GLY:HA3	1.96	0.48
24:L:121:GLN:HG3	25:M:129:ARG:HG2	1.95	0.48
24:L:172:LEU:O	24:L:176:MET:HB3	2.14	0.48
25:M:179:LEU:HB3	25:M:184:MET:HE1	1.95	0.48
30:R:1:THR:O	30:R:129:GLY:HA3	2.14	0.48
34:u:339:ILE:HG22	34:u:773:LYS:HD3	1.95	0.48
34:u:378:ASN:OD1	34:u:382:ASN:ND2	2.47	0.48
34:u:902:LYS:HZ1	34:u:906:TYR:HB3	1.78	0.48
2:V:418:SER:O	2:V:422:ILE:HG13	2.14	0.47
6:Z:176:LEU:HA	6:Z:176:LEU:HD23	1.73	0.47
6:Z:186:THR:OG1	6:Z:187:LEU:N	2.42	0.47
7:a:216:LEU:HB2	7:a:222:LEU:HD21	1.96	0.47
7:a:226:ARG:O	7:a:226:ARG:HG2	2.14	0.47
1:U:146:LYS:HE2	1:U:148:LYS:HG3	1.95	0.47
4:X:200:ILE:HG12	4:X:201:TYR:N	2.29	0.47
10:d:75:MET:SD	10:d:78:LEU:HD11	2.53	0.47
16:E:97:ARG:HE	16:E:111:LEU:HB3	1.79	0.47
16:E:303:LEU:HD11	16:E:338:PHE:O	2.13	0.47
17:F:299:GLU:O	17:F:300:LYS:HB2	2.14	0.47
20:H:68:ILE:HG21	20:H:110:LEU:HD21	1.96	0.47
20:H:179:ASN:OD1	20:H:180:GLU:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:N:35:THR:HG1	26:N:43:CYS:HG	1.60	0.47
1:U:142:LEU:HD23	1:U:142:LEU:HA	1.65	0.47
2:V:200:ARG:HA	2:V:203:LEU:HB3	1.95	0.47
2:V:467:TYR:HH	4:X:397:TYR:HH	1.52	0.47
3:W:180:LYS:O	3:W:184:GLU:HG3	2.14	0.47
8:b:94:HIS:NE2	8:b:134:GLU:HG3	2.29	0.47
8:b:95:LEU:HD12	8:b:96:ALA:N	2.29	0.47
12:A:143:ASP:HB2	12:A:150:HIS:NE2	2.30	0.47
16:E:104:THR:HG22	16:E:106:THR:HG23	1.97	0.47
28:P:106:GLU:HG2	28:P:125:ASP:HA	1.95	0.47
28:p:135:ASP:OD1	28:p:135:ASP:N	2.46	0.47
34:u:385:PHE:CZ	34:u:773:LYS:HD2	2.50	0.47
34:u:784:ASP:CG	34:u:879:ARG:HE	2.22	0.47
1:U:353:LEU:HA	1:U:356:THR:HG22	1.96	0.47
2:V:259:LEU:HD22	2:V:269:LYS:HE2	1.95	0.47
3:W:91:SER:OG	3:W:96:GLN:NE2	2.35	0.47
7:a:136:GLU:HA	7:a:139:GLU:HG2	1.97	0.47
10:d:107:LEU:HD12	10:d:115:PHE:CE2	2.49	0.47
10:d:132:TYR:CE1	10:d:160:ALA:HB2	2.49	0.47
15:D:81:ARG:HG2	15:D:81:ARG:NH1	2.29	0.47
16:E:122:MET:HB3	16:E:196:LEU:HB2	1.95	0.47
17:F:212:PHE:O	17:F:215:LEU:C	2.58	0.47
21:I:26:GLU:OE2	21:I:166:ASN:ND2	2.47	0.47
22:j:145:TYR:CE2	22:j:155:ALA:HB2	2.49	0.47
1:U:11:LEU:HG	10:d:73:ARG:HH21	1.80	0.47
1:U:320:ASP:O	1:U:324:LYS:HB2	2.14	0.47
3:W:52:LYS:HA	3:W:55:ARG:NE	2.30	0.47
3:W:340:VAL:HA	3:W:350:ARG:CZ	2.43	0.47
4:X:58:ALA:CB	4:X:95:LEU:HD12	2.45	0.47
5:Y:206:SER:HB3	5:Y:213:LEU:HD13	1.97	0.47
10:d:196:ARG:HB3	10:d:196:ARG:NH1	2.30	0.47
12:A:115:VAL:O	12:A:118:PHE:N	2.47	0.47
12:A:293:ASN:HB3	12:A:297:ARG:NH1	2.29	0.47
19:G:10:ASP:OD1	19:G:17:SER:HB2	2.14	0.47
21:I:41:ASP:OD1	21:I:41:ASP:N	2.48	0.47
22:j:4:ASP:O	22:j:123:GLY:N	2.47	0.47
1:U:628:ARG:HG3	1:U:749:GLN:NE2	2.30	0.47
5:Y:104:MET:HG3	5:Y:126:LYS:NZ	2.29	0.47
7:a:65:SER:HB2	7:a:76:LEU:HD21	1.97	0.47
10:d:139:LEU:HD12	10:d:151:VAL:HG12	1.95	0.47
12:A:117:GLN:NE2	12:A:118:PHE:HD1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:260:LEU:O	16:E:264:MET:HB2	2.15	0.47
20:h:12:THR:OG1	21:i:20:GLN:OE1	2.32	0.47
34:u:472:HIS:CD2	34:u:474:SER:HB3	2.50	0.47
1:U:332:GLU:OE1	1:U:332:GLU:N	2.46	0.47
1:U:801:GLN:HB3	1:U:877:LEU:HD22	1.96	0.47
2:V:69:THR:HA	2:V:73:GLU:HB2	1.96	0.47
2:V:324:PHE:HZ	11:e:3:GLU:H	1.63	0.47
3:W:395:ASN:HA	3:W:398:VAL:HG22	1.97	0.47
3:W:441:LYS:NZ	6:Z:230:LEU:HD11	2.29	0.47
5:Y:293:ARG:NH1	11:e:57:ARG:HB3	2.30	0.47
6:Z:92:VAL:HG23	6:Z:92:VAL:O	2.15	0.47
6:Z:129:LYS:HE2	6:Z:129:LYS:HB2	1.65	0.47
7:a:138:VAL:O	7:a:142:LEU:HB2	2.14	0.47
7:a:197:ALA:HB3	7:a:226:ARG:HH22	1.78	0.47
8:b:52:ILE:HD12	8:b:59:GLU:O	2.15	0.47
8:b:157:VAL:HG21	8:b:170:LEU:HB2	1.97	0.47
9:c:175:ARG:HE	9:c:182:GLY:N	2.11	0.47
13:B:381:ASP:HA	13:B:384:ILE:HD12	1.97	0.47
14:C:55:LYS:HB3	14:C:55:LYS:HE2	1.63	0.47
15:D:391:ARG:NH1	15:D:393:ILE:O	2.48	0.47
16:E:194:ASN:N	16:E:194:ASN:OD1	2.48	0.47
17:F:86:LEU:HD12	17:F:87:PRO:CD	2.41	0.47
17:F:266:LYS:HA	17:F:269:ARG:HG2	1.97	0.47
30:R:44:THR:HG21	30:R:100:MET:HE3	1.95	0.47
24:l:84:LEU:O	24:l:88:MET:HG3	2.14	0.47
26:n:14:LEU:HD23	26:n:44:CYS:SG	2.55	0.47
1:U:96:TYR:CE2	1:U:97:VAL:HG23	2.50	0.47
1:U:452:ASN:O	1:U:453:HIS:ND1	2.26	0.47
7:a:33:LEU:HD11	7:a:36:GLN:HB2	1.95	0.47
8:b:179:LEU:C	8:b:181:ASP:N	2.73	0.47
9:c:175:ARG:HE	9:c:182:GLY:H	1.63	0.47
9:c:208:ARG:O	9:c:208:ARG:HG2	2.14	0.47
10:d:181:CYS:HA	10:d:184:LYS:NZ	2.29	0.47
12:A:271:LEU:CD2	12:A:316:LYS:HB2	2.44	0.47
15:D:52:GLU:O	15:D:56:VAL:HG23	2.15	0.47
15:D:69:LYS:HE3	15:D:69:LYS:HA	1.96	0.47
15:D:212:LYS:N	38:D:501:ADP:O1B	2.47	0.47
24:L:65:HIS:NE2	24:L:67:ASP:O	2.48	0.47
19:g:184:LYS:HB3	19:g:185:LYS:HE2	1.96	0.47
20:h:118:MET:O	20:h:122:THR:HG23	2.14	0.47
28:p:25:ASP:OD1	28:p:41:LYS:NZ	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:f:389:ARG:HG2	34:u:434:TYR:CZ	2.49	0.47
2:V:130:PHE:O	2:V:133:PRO:HD2	2.14	0.47
2:V:238:ALA:C	2:V:240:LEU:H	2.22	0.47
3:W:324:TYR:O	3:W:324:TYR:CG	2.67	0.47
5:Y:280:GLN:OE1	5:Y:280:GLN:HA	2.13	0.47
7:a:133:GLU:HA	7:a:136:GLU:HG3	1.97	0.47
9:c:218:LEU:O	9:c:220:LEU:N	2.48	0.47
15:D:106:THR:HG21	16:E:78:ARG:HD3	1.96	0.47
15:D:259:PRO:HG3	15:D:304:ASN:ND2	2.30	0.47
16:E:213:ARG:O	16:E:217:GLU:HG2	2.14	0.47
17:F:265:ALA:HB1	17:F:269:ARG:HH21	1.79	0.47
20:h:82:ASP:HB3	20:h:130:PHE:HD1	1.80	0.47
29:q:102:LEU:HD12	29:q:118:MET:HE3	1.95	0.47
34:u:869:THR:HG22	34:u:871:PRO:HD2	1.97	0.47
1:U:213:PHE:HB2	1:U:248:ILE:HG22	1.96	0.47
2:V:38:LYS:HD2	2:V:38:LYS:O	2.15	0.47
2:V:366:ALA:HB2	2:V:374:LYS:HE3	1.97	0.47
2:V:374:LYS:O	2:V:378:VAL:HG23	2.14	0.47
3:W:16:MET:HE3	3:W:61:VAL:HG21	1.97	0.47
3:W:50:LEU:O	3:W:53:GLN:HG3	2.15	0.47
4:X:205:LYS:O	4:X:208:ALA:N	2.48	0.47
7:a:122:LYS:HE2	7:a:130:VAL:HB	1.96	0.47
8:b:44:ASN:HB3	8:b:47:ASN:ND2	2.29	0.47
8:b:110:ILE:HD12	8:b:110:ILE:O	2.15	0.47
10:d:182:ILE:HG12	10:d:215:TRP:CZ2	2.50	0.47
13:B:99:VAL:O	13:B:103:ARG:HG2	2.15	0.47
15:D:121:ARG:HA	15:D:124:LEU:HD23	1.97	0.47
17:F:282:ILE:HD12	17:F:282:ILE:O	2.15	0.47
20:H:64:LYS:HG2	20:H:76:TYR:HE1	1.80	0.47
25:m:41:CYS:SG	25:m:186:CYS:HA	2.55	0.47
34:u:139:CYS:SG	34:u:158:TYR:HE1	2.38	0.47
1:U:54:PHE:HA	1:U:55:ARG:NH1	2.30	0.46
2:V:32:PRO:HB2	2:V:85:ALA:HB1	1.97	0.46
2:V:243:ASP:HB2	2:V:247:GLN:OE1	2.15	0.46
3:W:98:LYS:HD2	3:W:98:LYS:C	2.40	0.46
13:B:275:GLU:OE2	13:B:323:GLY:HA3	2.14	0.46
14:C:27:LYS:HE3	14:C:27:LYS:HB3	1.79	0.46
14:C:225:GLY:O	14:C:229:ARG:HG2	2.15	0.46
16:E:296:ASP:OD1	16:E:296:ASP:N	2.48	0.46
17:F:256:LEU:HD21	17:F:285:ILE:HD11	1.96	0.46
17:F:272:PHE:O	17:F:276:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:I:239:LYS:O	21:I:239:LYS:HD3	2.14	0.46
1:U:333:MET:O	1:U:336:GLU:HG3	2.15	0.46
1:U:799:LYS:HE2	1:U:925:VAL:HB	1.97	0.46
1:U:874:ASN:O	1:U:875:PHE:CG	2.69	0.46
3:W:66:ILE:HG13	3:W:115:ILE:HD11	1.98	0.46
3:W:324:TYR:CE1	3:W:327:GLU:HB3	2.51	0.46
9:c:68:ARG:NH2	9:c:208:ARG:HH12	2.13	0.46
10:d:51:ALA:O	10:d:54:ILE:HG12	2.15	0.46
10:d:136:PRO:HD2	10:d:137:VAL:N	2.28	0.46
16:E:33:LEU:HD11	17:F:62:VAL:HG13	1.97	0.46
20:H:93:LEU:HD13	20:H:113:ARG:HB3	1.96	0.46
20:H:204:THR:HG22	20:H:206:ASP:H	1.80	0.46
28:P:142:CYS:O	28:P:146:MET:HG3	2.15	0.46
20:h:185:GLU:OE2	20:h:229:TYR:OH	2.24	0.46
1:U:142:LEU:CD1	1:U:165:LYS:HG3	2.41	0.46
2:V:90:GLU:HA	2:V:134:PHE:CE1	2.51	0.46
5:Y:376:LEU:HD12	6:Z:265:LEU:HD21	1.98	0.46
7:a:109:GLU:OE1	7:a:109:GLU:N	2.43	0.46
8:b:169:HIS:CE1	8:b:191:GLY:C	2.93	0.46
9:c:61:PHE:HZ	9:c:139:ARG:HB3	1.80	0.46
12:A:93:LEU:HD12	12:A:93:LEU:HA	1.80	0.46
12:A:394:MET:HG2	13:B:349:ARG:HH21	1.80	0.46
13:B:256:ILE:HD13	13:B:305:ILE:HD12	1.98	0.46
18:v:21:ALA:O	18:v:22:ALA:HB3	2.15	0.46
22:J:134:VAL:HG23	22:J:144:LEU:HD13	1.97	0.46
34:u:567:LEU:HD23	34:u:790:GLN:HG2	1.97	0.46
1:U:230:SER:HB2	1:U:267:ASN:OD1	2.15	0.46
2:V:93:PHE:HB3	2:V:96:ARG:NH2	2.30	0.46
2:V:261:TYR:HB2	2:V:265:ASP:OD2	2.15	0.46
2:V:426:LEU:O	2:V:427:GLN:HG2	2.16	0.46
3:W:96:GLN:HG3	3:W:97:LEU:H	1.81	0.46
3:W:280:ASP:OD1	3:W:281:ASN:N	2.47	0.46
5:Y:70:LEU:O	5:Y:74:LYS:HG2	2.16	0.46
5:Y:106:ALA:HA	5:Y:109:GLU:HG3	1.96	0.46
8:b:187:PRO:C	8:b:188:ILE:HG22	2.40	0.46
13:B:302:GLU:O	13:B:306:GLN:HG3	2.16	0.46
16:E:88:ASP:HB2	16:E:91:LYS:HD3	1.98	0.46
16:E:310:LEU:O	16:E:314:LYS:HG2	2.14	0.46
29:Q:144:ASP:OD2	30:r:166:ARG:NH1	2.45	0.46
19:g:50:ILE:HG21	19:g:79:VAL:HB	1.97	0.46
21:i:174:MET:HE2	21:i:174:MET:HB2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:j:187:THR:O	22:j:191:VAL:HG23	2.16	0.46
27:o:19:ARG:HB3	27:o:169:SER:HA	1.98	0.46
34:u:113:MET:HE1	34:u:118:ASN:HB2	1.98	0.46
1:U:95:GLU:O	1:U:97:VAL:N	2.48	0.46
1:U:141:CYS:HA	1:U:144:ASP:HB3	1.98	0.46
1:U:258:GLN:C	1:U:260:PHE:H	2.24	0.46
3:W:89:LEU:HD13	16:E:307:GLN:HG3	1.97	0.46
3:W:107:GLN:HA	3:W:110:THR:HG22	1.97	0.46
5:Y:14:ASN:HB2	5:Y:15:PRO:HD3	1.98	0.46
5:Y:293:ARG:HD2	5:Y:293:ARG:HA	1.61	0.46
7:a:247:ARG:H	7:a:247:ARG:CD	2.24	0.46
25:m:152:ASP:OD1	25:m:154:SER:OG	2.29	0.46
31:s:148:LEU:HD23	31:s:178:VAL:HG12	1.97	0.46
4:X:90:ARG:NH1	4:X:128:ALA:HB1	2.28	0.46
7:a:214:GLY:O	7:a:217:LEU:N	2.35	0.46
7:a:274:LEU:HD11	7:a:319:LEU:HD12	1.97	0.46
8:b:48:ASN:OD1	8:b:48:ASN:N	2.46	0.46
10:d:1:MET:HB3	10:d:2:TYR:H	1.63	0.46
10:d:108:SER:O	10:d:173:THR:HG21	2.16	0.46
10:d:132:TYR:HD1	10:d:159:PRO:HB2	1.80	0.46
10:d:194:ALA:O	10:d:197:ILE:HG22	2.16	0.46
11:e:6:GLN:HA	11:e:6:GLN:OE1	2.16	0.46
12:A:124:ASP:HB3	17:F:86:LEU:CD2	2.44	0.46
12:A:243:SER:OG	13:B:268:ARG:NH2	2.39	0.46
15:D:358:VAL:HB	15:D:396:ALA:HB2	1.96	0.46
16:E:84:ARG:H	16:E:87:LEU:HD12	1.80	0.46
16:E:363:VAL:HG12	16:E:366:ASP:OD2	2.15	0.46
17:F:162:GLU:HG2	17:F:164:LEU:HD23	1.97	0.46
24:l:88:MET:HE2	24:l:108:LEU:HD21	1.97	0.46
28:p:12:MET:HG3	28:p:138:VAL:HG12	1.98	0.46
34:u:62:ARG:HG3	34:u:62:ARG:HH11	1.80	0.46
1:U:885:MET:HB3	1:U:885:MET:HE2	1.72	0.46
3:W:63:THR:C	3:W:65:ARG:N	2.72	0.46
3:W:70:VAL:O	3:W:74:CYS:N	2.45	0.46
3:W:144:ARG:HH12	3:W:172:GLU:HG3	1.80	0.46
7:a:7:PHE:CE2	7:a:60:TYR:HB2	2.51	0.46
10:d:237:ILE:N	10:d:238:PRO:HD3	2.30	0.46
12:A:43:ARG:HA	12:A:43:ARG:NE	2.31	0.46
16:E:191:LEU:HD22	16:E:193:CYS:SG	2.55	0.46
21:I:174:MET:HE1	21:I:199:LYS:HB3	1.97	0.46
24:L:93:LEU:HD23	24:L:93:LEU:HA	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:P:125:ASP:OD1	28:P:129:CYS:HB3	2.16	0.46
30:R:6:PHE:HB2	30:R:125:THR:HG22	1.97	0.46
1:U:117:ASP:O	1:U:119:PRO:HD2	2.15	0.46
2:V:34:ASP:HA	2:V:37:MET:HE3	1.97	0.46
2:V:189:ASP:OD1	2:V:194:LYS:HG2	2.16	0.46
2:V:373:ALA:O	2:V:377:GLN:HG2	2.16	0.46
3:W:56:THR:OG1	3:W:103:LYS:NZ	2.35	0.46
6:Z:121:LEU:HD21	6:Z:138:TYR:HB2	1.98	0.46
8:b:32:ALA:HB1	8:b:183:LEU:CD1	2.45	0.46
10:d:135:HIS:O	10:d:139:LEU:HD22	2.14	0.46
13:B:193:GLN:OE1	13:B:193:GLN:N	2.48	0.46
16:E:38:LYS:HA	16:E:38:LYS:HD2	1.68	0.46
17:F:282:ILE:HA	17:F:327:LYS:O	2.15	0.46
20:H:69:THR:HG23	20:H:71:HIS:H	1.79	0.46
28:p:49:LEU:C	28:p:50:TYR:HD1	2.24	0.46
28:p:149:MET:HE2	28:p:173:ASN:HB2	1.98	0.46
29:q:37:LYS:O	29:q:61:GLN:NE2	2.48	0.46
33:f:410:ARG:HH12	33:f:415:PRO:HG2	1.80	0.46
1:U:58:GLN:HB3	1:U:87:LEU:HD23	1.98	0.46
3:W:344:THR:HG23	3:W:345:GLU:N	2.30	0.46
7:a:176:ALA:HB3	7:a:200:LEU:HD12	1.97	0.46
8:b:23:PRO:O	8:b:24:THR:OG1	2.31	0.46
9:c:216:MET:O	9:c:220:LEU:HB2	2.16	0.46
10:d:125:LYS:HB3	10:d:130:ASN:ND2	2.31	0.46
12:A:119:ALA:HB1	17:F:127:SER:OG	2.16	0.46
12:A:369:ARG:H	12:A:369:ARG:HG2	1.64	0.46
15:D:259:PRO:HA	15:D:304:ASN:O	2.16	0.46
16:E:97:ARG:NH2	16:E:112:PRO:O	2.49	0.46
19:g:81:THR:HG23	19:g:137:CYS:HB3	1.98	0.46
28:p:142:CYS:O	28:p:146:MET:HG3	2.15	0.46
3:W:222:LEU:O	3:W:226:TYR:HB2	2.15	0.46
7:a:61:GLU:O	7:a:64:ILE:HG22	2.16	0.46
7:a:173:TYR:C	7:a:173:TYR:CD2	2.93	0.46
14:C:190:GLY:O	14:C:296:ASN:HB2	2.16	0.46
17:F:72:LYS:HE2	17:F:72:LYS:HB2	1.77	0.46
29:Q:198:LYS:H	29:q:197:PRO:HA	1.81	0.46
19:g:153:LYS:HD3	19:g:166:THR:HG21	1.97	0.46
3:W:122:LEU:O	3:W:125:ILE:HG22	2.16	0.45
3:W:192:LEU:O	3:W:196:VAL:HG13	2.15	0.45
7:a:370:GLN:HG3	10:d:244:LYS:HE3	1.97	0.45
16:E:43:SER:HB3	17:F:73:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p:13:ALA:HB3	28:p:137:VAL:HG23	1.98	0.45
3:W:126:ASP:O	3:W:129:ARG:HG2	2.16	0.45
4:X:202:CYS:HB3	4:X:206:LEU:HD23	1.97	0.45
4:X:409:LYS:HA	4:X:412:ASP:OD2	2.15	0.45
5:Y:243:GLY:O	5:Y:247:LEU:HB2	2.16	0.45
5:Y:275:LEU:HD21	5:Y:296:VAL:HG13	1.98	0.45
6:Z:189:GLN:OE1	6:Z:189:GLN:HA	2.16	0.45
8:b:184:ILE:CG1	8:b:185:SER:N	2.79	0.45
16:E:69:PHE:CE2	16:E:83:CYS:HB2	2.51	0.45
17:F:178:ASP:OD1	17:F:178:ASP:N	2.35	0.45
20:H:222:THR:OG1	20:H:225:GLU:HG3	2.16	0.45
29:Q:170:ARG:NH1	29:q:27:GLN:O	2.48	0.45
30:R:186:ARG:HE	30:R:186:ARG:HB2	1.61	0.45
29:q:38:MET:O	29:q:65:GLN:NE2	2.50	0.45
31:s:190:GLY:O	31:s:191:ASP:HB2	2.16	0.45
1:U:101:ILE:O	1:U:105:ILE:HG13	2.15	0.45
2:V:73:GLU:O	2:V:77:GLU:HG3	2.16	0.45
2:V:169:LEU:C	2:V:171:VAL:H	2.23	0.45
3:W:142:ARG:O	3:W:146:THR:HG22	2.16	0.45
5:Y:344:HIS:ND1	5:Y:344:HIS:N	2.63	0.45
7:a:135:ILE:HD12	7:a:135:ILE:HA	1.88	0.45
8:b:145:GLU:C	8:b:146:GLU:HG2	2.41	0.45
9:c:218:LEU:HG	9:c:219:ASN:H	1.80	0.45
10:d:60:GLN:O	10:d:63:ILE:HG12	2.17	0.45
16:E:15:LYS:HA	16:E:18:GLU:HG2	1.97	0.45
16:E:297:ARG:HD3	16:E:297:ARG:HA	1.63	0.45
17:F:44:ARG:HH11	17:F:44:ARG:H	1.64	0.45
17:F:185:TYR:CZ	17:F:243:GLN:HG3	2.51	0.45
17:F:303:ASP:HB2	17:F:304:ARG:NH2	2.31	0.45
19:G:48:ALA:HB3	19:G:220:VAL:HG12	1.98	0.45
23:K:42:THR:HG22	23:K:43:SER:H	1.81	0.45
21:i:124:PHE:HB3	22:j:124:ARG:HG3	1.99	0.45
23:k:224:GLN:HE21	23:k:224:GLN:C	2.25	0.45
34:u:409:SER:O	34:u:819:TYR:OH	2.28	0.45
2:V:238:ALA:HB1	2:V:243:ASP:HB3	1.98	0.45
3:W:93:ARG:H	3:W:96:GLN:NE2	2.09	0.45
3:W:174:TYR:HE1	16:E:143:ARG:HG2	1.81	0.45
12:A:261:PHE:O	12:A:265:ARG:HG3	2.16	0.45
21:I:106:PRO:O	21:I:107:CYS:SG	2.74	0.45
34:u:540:GLN:HA	34:u:543:MET:HE3	1.98	0.45
1:U:678:ASP:OD1	1:U:679:PRO:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:799:LYS:O	1:U:801:GLN:NE2	2.50	0.45
2:V:183:GLU:HA	2:V:186:LYS:HG3	1.97	0.45
2:V:392:TYR:O	2:V:392:TYR:HD2	1.99	0.45
3:W:12:ARG:HE	3:W:27:ARG:HE	1.62	0.45
3:W:92:LYS:HB3	3:W:94:ARG:H	1.81	0.45
6:Z:237:LEU:HD23	6:Z:237:LEU:O	2.17	0.45
12:A:306:LEU:C	12:A:308:GLY:H	2.24	0.45
16:E:27:LYS:HD3	16:E:27:LYS:HA	1.75	0.45
16:E:349:GLU:OE1	16:E:373:LYS:NZ	2.38	0.45
20:H:111:VAL:HG22	20:H:136:ILE:HD12	1.98	0.45
32:T:110:MET:HE3	32:T:110:MET:HB2	1.82	0.45
19:g:19:GLU:OE1	19:g:19:GLU:N	2.50	0.45
19:g:165:ALA:HB1	19:g:179:LEU:HD13	1.99	0.45
25:m:37:ILE:HD11	25:m:193:VAL:HG13	1.99	0.45
30:r:47:GLY:H	39:r:301:LDZ:H15	1.82	0.45
1:U:106:ASP:HA	1:U:109:THR:HB	1.98	0.45
1:U:483:LEU:HD22	1:U:778:PHE:HE1	1.82	0.45
2:V:160:LEU:HA	2:V:163:VAL:HG23	1.99	0.45
3:W:88:MET:O	3:W:89:LEU:HG	2.16	0.45
5:Y:237:ARG:H	5:Y:237:ARG:HD3	1.81	0.45
10:d:188:LYS:H	10:d:220:ASN:N	2.12	0.45
12:A:163:MET:HE3	12:A:163:MET:O	2.17	0.45
36:B:501:ATP:O2G	14:C:310:ARG:NH2	2.50	0.45
17:F:320:PHE:CD1	17:F:320:PHE:C	2.94	0.45
25:M:175:GLU:HA	25:M:178:LYS:HG3	1.99	0.45
25:m:169:ARG:O	25:m:173:LYS:HG2	2.15	0.45
34:u:805:ASP:OD2	34:u:808:ASN:ND2	2.49	0.45
3:W:10:ASP:HA	3:W:13:ILE:HG22	1.98	0.45
3:W:60:MET:HA	3:W:64:SER:OG	2.16	0.45
3:W:81:ASP:O	3:W:85:GLU:HG3	2.16	0.45
4:X:250:SER:O	4:X:254:MET:HG3	2.16	0.45
4:X:306:LEU:HD21	4:X:314:ARG:NH1	2.29	0.45
7:a:76:LEU:HD12	7:a:76:LEU:HA	1.88	0.45
7:a:269:LEU:O	7:a:272:ILE:HG13	2.16	0.45
10:d:15:ASN:OD1	10:d:17:SER:N	2.50	0.45
14:C:17:GLY:O	14:C:22:GLN:HG2	2.17	0.45
16:E:378:LYS:HA	16:E:378:LYS:HD3	1.74	0.45
19:g:48:ALA:HB3	19:g:220:VAL:HG12	1.97	0.45
29:q:61:GLN:O	29:q:65:GLN:HG2	2.17	0.45
2:V:231:LEU:HD12	2:V:254:LEU:HB2	1.99	0.45
2:V:264:TYR:HB2	10:d:121:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:111:TYR:HB2	3:W:123:ARG:HH22	1.81	0.45
3:W:136:ILE:CG2	3:W:144:ARG:HD2	2.46	0.45
3:W:268:LYS:HE2	3:W:268:LYS:HB3	1.88	0.45
4:X:58:ALA:HB3	4:X:95:LEU:HD12	1.97	0.45
4:X:196:THR:O	4:X:196:THR:HG22	2.16	0.45
4:X:271:VAL:HG21	4:X:288:LYS:HD2	1.99	0.45
4:X:329:ASN:O	4:X:333:GLN:HG2	2.16	0.45
13:B:63:LEU:HD13	34:u:239:TYR:HB2	1.99	0.45
13:B:401:GLU:OE2	14:C:313:ARG:NH2	2.45	0.45
21:I:40:ASN:ND2	21:I:182:GLY:O	2.50	0.45
25:M:34:SER:OG	25:M:65:ARG:NH1	2.49	0.45
25:M:46:VAL:HG22	25:M:215:TRP:CD1	2.51	0.45
20:h:111:VAL:HG22	20:h:136:ILE:HD13	1.99	0.45
21:i:119:GLN:HG3	22:j:78:ALA:HB1	1.99	0.45
30:r:64:ARG:NH1	30:r:67:GLU:OE1	2.50	0.45
34:u:749:ALA:HB2	34:u:762:VAL:HG11	1.99	0.45
34:u:907:ASP:OD1	34:u:907:ASP:N	2.50	0.45
1:U:49:TYR:CE1	1:U:61:ALA:HB2	2.52	0.45
1:U:151:ILE:HD11	1:U:163:PHE:CE2	2.52	0.45
2:V:65:ARG:HB2	2:V:65:ARG:CZ	2.46	0.45
2:V:212:TYR:O	2:V:216:ARG:HG2	2.16	0.45
3:W:58:SER:C	3:W:60:MET:N	2.74	0.45
5:Y:283:LYS:HD3	5:Y:288:PHE:CE2	2.51	0.45
9:c:146:ASP:HB3	9:c:156:VAL:CG2	2.47	0.45
10:d:185:ALA:C	10:d:186:TYR:CD1	2.95	0.45
10:d:218:GLY:HA2	10:d:223:TYR:N	2.32	0.45
11:e:41:ASP:O	11:e:42:ASN:ND2	2.50	0.45
12:A:255:ARG:HG2	12:A:255:ARG:HH11	1.81	0.45
13:B:72:LEU:HD23	13:B:72:LEU:HA	1.83	0.45
14:C:91:PRO:HG3	15:D:109:SER:HB3	1.98	0.45
20:H:39:LYS:HE2	20:H:39:LYS:HB3	1.80	0.45
20:H:189:HIS:O	20:H:193:LEU:HD12	2.17	0.45
1:U:261:LEU:O	1:U:264:VAL:HG12	2.17	0.45
1:U:580:ARG:HH11	1:U:584:TYR:HE2	1.65	0.45
2:V:131:LEU:HA	2:V:134:PHE:HB3	1.99	0.45
5:Y:161:THR:HG23	5:Y:183:TYR:CZ	2.52	0.45
6:Z:63:LYS:HD3	6:Z:63:LYS:HA	1.74	0.45
7:a:225:LEU:HD22	7:a:225:LEU:H	1.82	0.45
13:B:245:ALA:HB1	13:B:279:PRO:O	2.17	0.45
14:C:144:PRO:O	14:C:205:HIS:ND1	2.47	0.45
14:C:338:LEU:HD23	14:C:342:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:374:ARG:HD2	14:C:374:ARG:HA	1.76	0.45
15:D:80:LYS:HA	15:D:83:GLN:NE2	2.32	0.45
17:F:87:PRO:HB2	17:F:155:LYS:HD3	1.98	0.45
21:I:44:LEU:HD22	21:I:190:LEU:HD23	1.99	0.45
32:T:25:ASP:HA	32:T:187:PHE:HA	1.98	0.45
27:o:33:LYS:HG2	39:o:301:LDZ:H20	1.99	0.45
1:U:645:ASN:OD1	1:U:645:ASN:N	2.47	0.44
1:U:797:MET:N	1:U:797:MET:HE3	2.32	0.44
3:W:43:VAL:HG23	3:W:47:LEU:HD12	1.99	0.44
3:W:142:ARG:HG2	3:W:146:THR:HB	1.99	0.44
3:W:298:GLU:OE1	3:W:299:ILE:HG13	2.17	0.44
5:Y:126:LYS:HD2	5:Y:126:LYS:C	2.42	0.44
5:Y:144:LEU:HB3	5:Y:160:ASN:HD22	1.83	0.44
7:a:216:LEU:HA	7:a:219:HIS:HB2	1.98	0.44
20:H:183:GLU:OE1	20:H:183:GLU:HA	2.17	0.44
22:J:69:VAL:HG12	22:J:104:VAL:HG22	1.99	0.44
23:K:146:VAL:HG11	23:K:222:PRO:HA	1.98	0.44
26:N:51:ASP:OD1	26:N:51:ASP:N	2.51	0.44
1:U:98:GLU:O	1:U:101:ILE:HG22	2.17	0.44
4:X:310:ARG:HA	4:X:310:ARG:HD2	1.67	0.44
5:Y:367:GLN:HA	5:Y:370:ILE:HG22	1.99	0.44
10:d:195:THR:CG2	10:d:205:LYS:HG2	2.47	0.44
13:B:319:PHE:O	13:B:320:ASP:HB2	2.17	0.44
15:D:244:PRO:O	15:D:248:ARG:HG3	2.18	0.44
16:E:40:TYR:HD1	17:F:73:ILE:HB	1.82	0.44
16:E:116:ASP:N	16:E:116:ASP:OD1	2.50	0.44
23:K:137:PHE:O	23:K:158:PRO:HB3	2.16	0.44
23:K:181:LEU:HD23	23:K:181:LEU:HA	1.83	0.44
23:k:157:ASP:OD1	23:k:159:SER:OG	2.32	0.44
27:o:194:LYS:HE2	27:o:194:LYS:HB2	1.74	0.44
1:U:128:GLN:HA	1:U:131:GLU:CD	2.43	0.44
1:U:145:HIS:CE1	1:U:172:ASP:OD1	2.70	0.44
1:U:539:THR:OG1	1:U:544:ILE:HG21	2.18	0.44
1:U:612:ASP:HB3	1:U:647:HIS:CG	2.52	0.44
3:W:435:LEU:HG	6:Z:234:PHE:CE1	2.52	0.44
5:Y:162:GLU:OE1	5:Y:162:GLU:N	2.50	0.44
6:Z:282:ASN:OD1	6:Z:283:ARG:N	2.51	0.44
7:a:231:GLN:HA	7:a:234:ILE:HG12	1.98	0.44
9:c:75:MET:HG3	9:c:76:PRO:HD2	1.99	0.44
10:d:37:PRO:HB2	10:d:39:THR:HG23	2.00	0.44
10:d:215:TRP:CD1	10:d:222:TYR:CE2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:29:LEU:O	16:E:33:LEU:HG	2.16	0.44
17:F:44:ARG:NH1	17:F:44:ARG:HB3	2.33	0.44
25:M:15:SER:OG	25:M:19:ARG:HG2	2.17	0.44
26:N:40:ARG:NH2	26:N:183:GLY:HA2	2.33	0.44
27:O:6:VAL:HG23	27:O:124:TYR:HB3	1.98	0.44
27:O:7:VAL:HG22	27:O:12:ILE:HD13	1.99	0.44
1:U:525:ASN:O	1:U:529:ILE:HG22	2.17	0.44
1:U:589:ALA:C	1:U:590:TYR:HD1	2.26	0.44
2:V:156:SER:O	2:V:159:LEU:HB3	2.17	0.44
2:V:209:LYS:HB3	2:V:209:LYS:HE2	1.78	0.44
2:V:218:TYR:HD1	2:V:224:LEU:HA	1.82	0.44
2:V:244:ALA:C	2:V:246:GLY:H	2.24	0.44
3:W:65:ARG:C	3:W:67:LEU:N	2.76	0.44
3:W:127:THR:HG21	3:W:147:LYS:NZ	2.32	0.44
3:W:162:ALA:O	3:W:166:LEU:HD12	2.18	0.44
5:Y:46:ARG:C	5:Y:48:ASN:H	2.26	0.44
7:a:109:GLU:H	7:a:109:GLU:CD	2.23	0.44
12:A:420:TYR:CZ	13:B:350:LYS:HE3	2.53	0.44
14:C:311:ILE:HG22	14:C:314:LYS:HE3	1.99	0.44
27:O:40:ASN:OD1	27:O:40:ASN:N	2.50	0.44
31:S:91:MET:HE2	31:S:91:MET:HB3	1.85	0.44
20:h:9:SER:HA	20:h:125:GLY:HA2	1.99	0.44
21:i:122:THR:O	22:j:125:ARG:NH1	2.51	0.44
25:m:46:VAL:HG22	25:m:215:TRP:HD1	1.81	0.44
34:u:48:GLU:OE1	34:u:48:GLU:N	2.39	0.44
1:U:696:ILE:HD11	1:U:745:THR:HA	2.00	0.44
2:V:79:VAL:HG22	2:V:80:LYS:H	1.81	0.44
2:V:254:LEU:HD23	2:V:255:LEU:HD12	1.99	0.44
3:W:265:GLN:OE1	3:W:335:SER:HB3	2.17	0.44
4:X:226:LYS:HE2	4:X:226:LYS:HB2	1.72	0.44
7:a:12:GLN:HG2	7:a:18:GLN:HE21	1.82	0.44
16:E:280:ASN:OD1	16:E:280:ASN:N	2.51	0.44
16:E:324:GLY:O	16:E:325:GLU:HG2	2.18	0.44
17:F:317:LEU:HD13	17:F:347:ARG:HB2	1.99	0.44
21:I:245:ALA:O	21:I:249:ARG:HG2	2.17	0.44
23:K:157:ASP:OD2	23:K:157:ASP:C	2.60	0.44
29:Q:101:ASN:HB3	29:Q:132:HIS:CE1	2.52	0.44
21:i:119:GLN:NE2	22:j:79:ASP:OD1	2.50	0.44
1:U:874:ASN:ND2	1:U:874:ASN:N	2.66	0.44
3:W:52:LYS:N	3:W:52:LYS:HD3	2.32	0.44
3:W:144:ARG:HH11	3:W:145:LEU:HB2	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:258:LYS:HD3	4:X:258:LYS:HA	1.73	0.44
5:Y:21:GLN:OE1	5:Y:21:GLN:C	2.61	0.44
6:Z:228:TYR:OH	7:a:340:VAL:HA	2.18	0.44
7:a:17:GLY:O	7:a:21:VAL:HG22	2.17	0.44
7:a:79:ILE:HD12	7:a:80:ILE:N	2.33	0.44
8:b:21:PHE:CE2	8:b:178:SER:O	2.71	0.44
8:b:180:ALA:O	8:b:183:LEU:HB2	2.17	0.44
12:A:345:LEU:H	12:A:345:LEU:HD22	1.83	0.44
13:B:417:GLU:O	13:B:421:LYS:HG2	2.18	0.44
17:F:278:LYS:O	17:F:280:PRO:HD2	2.17	0.44
17:F:342:LEU:HD13	17:F:348:LEU:HD12	1.99	0.44
17:F:356:MET:HE3	17:F:392:ASN:HB3	1.99	0.44
22:J:108:THR:HG22	22:J:133:ILE:HD13	1.99	0.44
22:J:244:GLN:HA	22:J:248:SER:C	2.42	0.44
29:Q:162:LYS:HE3	29:Q:162:LYS:HB2	1.61	0.44
1:U:170:SER:C	1:U:172:ASP:N	2.74	0.44
1:U:265:ILE:HD12	1:U:326:ILE:HD13	2.00	0.44
2:V:326:GLN:OE1	2:V:326:GLN:N	2.49	0.44
5:Y:208:PHE:CD2	5:Y:210:SER:HB2	2.53	0.44
6:Z:84:LYS:NZ	9:c:76:PRO:HB3	2.30	0.44
7:a:122:LYS:NZ	7:a:131:THR:HA	2.33	0.44
9:c:185:ASN:OD1	9:c:186:LYS:N	2.51	0.44
10:d:189:ILE:HG13	10:d:193:GLU:OE2	2.18	0.44
10:d:220:ASN:O	10:d:221:ASN:ND2	2.46	0.44
12:A:263:MET:O	12:A:266:THR:HG22	2.17	0.44
14:C:207:THR:HG23	14:C:209:CYS:H	1.81	0.44
27:O:121:LYS:HD3	32:t:215:ILE:HG21	2.00	0.44
28:P:12:MET:HG3	28:P:138:VAL:HG12	1.99	0.44
20:h:106:PRO:HG2	20:h:109:GLN:HG2	2.00	0.44
29:q:54:VAL:O	29:q:58:GLU:HG3	2.18	0.44
34:u:580:LEU:O	34:u:580:LEU:HD13	2.18	0.44
2:V:25:GLU:HB2	2:V:26:PRO:HD3	2.00	0.44
3:W:76:GLU:HA	3:W:79:GLU:OE2	2.18	0.44
3:W:191:ARG:NH1	3:W:191:ARG:HB3	2.32	0.44
3:W:369:TYR:CB	7:a:312:MET:HE1	2.48	0.44
8:b:37:CYS:SG	8:b:38:HIS:N	2.91	0.44
15:D:386:ALA:HA	15:D:391:ARG:NH2	2.33	0.44
16:E:125:GLU:HB2	16:E:195:PHE:HB3	2.00	0.44
16:E:289:LEU:O	16:E:295:LEU:HB2	2.17	0.44
16:E:357:ALA:O	16:E:359:HIS:ND1	2.51	0.44
17:F:316:GLN:HA	17:F:316:GLN:HE21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:O:17:ASP:OD1	27:O:17:ASP:C	2.61	0.44
21:i:239:LYS:O	21:i:243:GLU:HG2	2.17	0.44
24:l:19:ILE:HB	24:l:22:ILE:HD12	2.00	0.44
31:s:145:LEU:HD22	31:s:178:VAL:HB	2.00	0.44
34:u:178:LYS:HA	34:u:178:LYS:HD2	1.70	0.44
1:U:335:ILE:HD12	1:U:335:ILE:HA	1.83	0.44
1:U:427:LEU:HD13	1:U:430:ASP:HB2	1.99	0.44
5:Y:179:ARG:HD3	5:Y:179:ARG:HA	1.72	0.44
8:b:83:LYS:HA	8:b:83:LYS:HD3	1.80	0.44
12:A:248:LYS:HE2	12:A:248:LYS:HB3	1.69	0.44
14:C:186:VAL:HG23	14:C:292:ILE:HG23	1.99	0.44
22:J:41:VAL:HB	22:J:134:VAL:HG13	2.00	0.44
25:M:87:LEU:HD23	25:M:87:LEU:HA	1.88	0.44
26:N:140:ASP:C	26:N:140:ASP:OD2	2.60	0.44
25:m:202:ASP:HB2	25:m:209:PHE:CD1	2.53	0.44
34:u:275:MET:SD	34:u:275:MET:N	2.88	0.44
34:u:574:GLU:HA	34:u:577:LEU:CD2	2.48	0.44
1:U:26:LYS:HE2	10:d:36:LEU:HD12	2.00	0.43
1:U:114:GLU:O	1:U:118:LEU:HG	2.18	0.43
1:U:244:MET:HE2	1:U:244:MET:HA	1.98	0.43
1:U:695:MET:HE2	1:U:695:MET:HB2	1.93	0.43
1:U:756:HIS:ND1	1:U:758:PRO:HD2	2.33	0.43
2:V:43:THR:HG23	2:V:65:ARG:HH11	1.83	0.43
4:X:80:ILE:HG23	4:X:85:ALA:HB2	1.99	0.43
6:Z:103:LYS:HD3	6:Z:103:LYS:N	2.32	0.43
7:a:60:TYR:HA	7:a:63:PHE:CE1	2.53	0.43
10:d:95:MET:HE1	10:d:125:LYS:NZ	2.33	0.43
10:d:238:PRO:O	10:d:239:SER:C	2.61	0.43
14:C:42:LEU:HD21	15:D:57:GLN:OE1	2.17	0.43
16:E:136:GLY:N	38:E:401:ADP:N1	2.66	0.43
20:H:193:LEU:HD11	20:H:234:ALA:O	2.18	0.43
22:J:241:LYS:HA	22:J:241:LYS:HD2	1.81	0.43
33:f:410:ARG:HH21	34:u:837:LEU:HD12	1.82	0.43
34:u:58:MET:HA	34:u:61:GLU:CD	2.43	0.43
2:V:362:LEU:HG	2:V:374:LYS:HZ1	1.83	0.43
2:V:495:ARG:HB2	6:Z:278:ASN:HD21	1.82	0.43
3:W:65:ARG:HG3	3:W:67:LEU:CB	2.48	0.43
4:X:415:TYR:CD1	5:Y:383:LEU:HD23	2.53	0.43
5:Y:349:LYS:HD2	5:Y:349:LYS:HA	1.70	0.43
6:Z:229:GLN:HG2	7:a:338:PRO:HB2	2.00	0.43
12:A:287:ASP:O	17:F:295:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:D:164:TYR:HD1	15:D:174:LYS:HD3	1.83	0.43
16:E:83:CYS:SG	16:E:87:LEU:HD12	2.58	0.43
17:F:288:LEU:HD23	17:F:288:LEU:HA	1.88	0.43
23:K:24:VAL:O	23:K:28:ILE:HG12	2.18	0.43
34:u:236:CYS:HA	34:u:239:TYR:HD2	1.82	0.43
34:u:376:PHE:HE1	34:u:819:TYR:CZ	2.36	0.43
34:u:511:SER:O	34:u:514:VAL:HG22	2.18	0.43
1:U:437:TYR:CE1	1:U:472:ILE:HD13	2.54	0.43
2:V:43:THR:CG2	2:V:65:ARG:HH11	2.31	0.43
2:V:75:ILE:HA	2:V:78:HIS:NE2	2.33	0.43
2:V:148:ARG:HE	2:V:148:ARG:H	1.67	0.43
2:V:296:LYS:HZ2	2:V:296:LYS:HG2	1.76	0.43
3:W:39:ARG:HD2	3:W:42:GLU:HB2	2.00	0.43
3:W:111:TYR:HA	3:W:114:GLU:HG3	2.00	0.43
3:W:228:ASN:HA	3:W:246:HIS:CE1	2.53	0.43
5:Y:268:TYR:HA	5:Y:271:PHE:HB3	2.00	0.43
6:Z:96:HIS:NE2	6:Z:123:ILE:HG12	2.28	0.43
9:c:281:LYS:O	9:c:285:GLU:HG2	2.18	0.43
11:e:56:LEU:HD12	11:e:63:HIS:CE1	2.53	0.43
14:C:29:GLU:O	14:C:33:LEU:HD23	2.19	0.43
14:C:281:ASP:OD1	14:C:281:ASP:O	2.37	0.43
16:E:237:ALA:O	16:E:238:ILE:HG22	2.18	0.43
23:k:40:ILE:HB	23:k:47:CYS:SG	2.58	0.43
25:m:39:ILE:HD12	25:m:193:VAL:HG22	1.99	0.43
39:n:301:LDZ:H26	39:n:301:LDZ:N10	2.31	0.43
34:u:58:MET:SD	34:u:59:LEU:N	2.92	0.43
34:u:446:LEU:HD11	34:u:483:PHE:HB3	1.99	0.43
1:U:173:VAL:C	1:U:175:GLY:N	2.72	0.43
3:W:5:GLY:O	3:W:8:ARG:HG2	2.18	0.43
3:W:220:GLU:OE2	3:W:253:THR:HG23	2.18	0.43
3:W:442:THR:O	3:W:446:ILE:HG12	2.17	0.43
6:Z:78:MET:HE1	9:c:98:MET:CE	2.47	0.43
9:c:105:PRO:HD2	9:c:105:PRO:O	2.18	0.43
13:B:143:LEU:HD13	13:B:162:VAL:HG11	1.99	0.43
13:B:317:ASP:HB3	13:B:346:ARG:HG2	2.01	0.43
17:F:226:TYR:CZ	17:F:353:GLU:HB3	2.53	0.43
20:h:74:LEU:HD23	20:h:87:VAL:HG22	2.00	0.43
21:i:72:MET:HE2	21:i:72:MET:HB3	1.68	0.43
30:r:100:MET:HE3	30:r:100:MET:HB2	1.87	0.43
39:r:301:LDZ:H33	39:r:301:LDZ:H11	1.87	0.43
1:U:145:HIS:ND1	1:U:170:SER:CB	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:214:ILE:O	1:U:218:GLN:HB2	2.18	0.43
1:U:602:LEU:HD21	1:U:618:ALA:O	2.18	0.43
2:V:341:GLU:OE1	2:V:341:GLU:N	2.50	0.43
3:W:39:ARG:HB3	3:W:40:LEU:H	1.57	0.43
5:Y:99:GLU:OE1	5:Y:99:GLU:N	2.47	0.43
5:Y:173:ASP:OD1	5:Y:174:TRP:N	2.51	0.43
6:Z:64:ASP:OD2	6:Z:64:ASP:N	2.52	0.43
6:Z:209:ARG:NH2	7:a:354:GLU:OE1	2.52	0.43
10:d:103:LEU:HD21	10:d:118:GLU:HG3	2.00	0.43
12:A:91:GLN:HB2	12:A:92:PRO:HD3	2.00	0.43
13:B:329:MET:HE2	13:B:329:MET:HB2	1.83	0.43
15:D:203:LEU:HD23	15:D:309:MET:HB2	1.99	0.43
16:E:12:TYR:HD2	16:E:13:ARG:HE	1.65	0.43
16:E:65:THR:HG21	16:E:68:LYS:HE3	2.00	0.43
17:F:169:ASP:O	17:F:173:LYS:HG2	2.18	0.43
32:T:96:MET:HE2	32:T:110:MET:CE	2.44	0.43
19:g:184:LYS:HB2	19:g:184:LYS:HE3	1.82	0.43
22:j:69:VAL:HG13	22:j:104:VAL:HG23	2.00	0.43
24:l:104:PRO:HB2	24:l:107:ARG:HG2	2.00	0.43
34:u:349:TYR:CE1	34:u:763:ARG:HD2	2.53	0.43
1:U:763:VAL:O	1:U:767:THR:HG23	2.19	0.43
2:V:393:THR:O	2:V:396:ILE:HG22	2.19	0.43
4:X:316:ASP:CB	4:X:319:ILE:HD12	2.49	0.43
5:Y:237:ARG:HA	5:Y:241:ILE:HB	2.01	0.43
5:Y:238:GLU:HA	5:Y:242:LYS:HB2	2.01	0.43
5:Y:299:MET:HA	5:Y:299:MET:HE3	1.99	0.43
5:Y:329:PHE:HA	5:Y:332:GLN:OE1	2.17	0.43
8:b:7:MET:HB2	8:b:97:LEU:HD21	2.01	0.43
8:b:8:VAL:HG12	8:b:50:GLY:O	2.19	0.43
9:c:32:TYR:HB2	9:c:68:ARG:CB	2.48	0.43
9:c:183:HIS:O	9:c:184:LEU:HB3	2.18	0.43
12:A:97:ARG:CB	12:A:97:ARG:HH11	2.31	0.43
15:D:203:LEU:HB3	15:D:330:LYS:HG3	2.00	0.43
16:E:306:GLU:HB3	16:E:307:GLN:OE1	2.18	0.43
19:G:36:GLY:HA2	19:G:170:VAL:HG21	2.00	0.43
28:P:38:ASP:OD1	28:P:38:ASP:N	2.50	0.43
21:i:186:LEU:HD23	21:i:186:LEU:HA	1.80	0.43
34:u:124:ASP:O	34:u:128:VAL:HG23	2.19	0.43
1:U:38:ILE:HD12	1:U:38:ILE:N	2.34	0.43
1:U:213:PHE:CD1	1:U:213:PHE:C	2.96	0.43
1:U:636:VAL:HG13	1:U:637:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:838:LYS:HA	1:U:841:LYS:HB2	2.01	0.43
2:V:159:LEU:HA	2:V:162:GLU:OE1	2.19	0.43
3:W:102:ALA:HA	3:W:105:VAL:HG22	1.99	0.43
6:Z:54:PHE:CD1	6:Z:78:MET:HG3	2.54	0.43
7:a:52:GLN:C	7:a:54:ASP:H	2.27	0.43
9:c:216:MET:HE3	9:c:220:LEU:HD12	2.01	0.43
11:e:55:GLN:OE1	11:e:55:GLN:N	2.49	0.43
12:A:22:ILE:HD12	12:A:22:ILE:O	2.19	0.43
13:B:168:ASP:O	13:B:172:THR:HG23	2.18	0.43
16:E:197:LYS:HB3	16:E:197:LYS:HE3	1.70	0.43
17:F:81:LYS:HA	17:F:84:LYS:HG2	2.00	0.43
17:F:312:GLU:HA	17:F:315:ASN:ND2	2.34	0.43
21:I:72:MET:HE2	21:I:72:MET:HB3	1.93	0.43
23:K:104:ASN:O	23:K:104:ASN:ND2	2.52	0.43
21:i:130:PHE:O	21:i:152:PRO:HB3	2.19	0.43
25:m:234:GLU:H	25:m:234:GLU:HG3	1.62	0.43
34:u:57:GLU:HA	34:u:60:VAL:HG12	2.01	0.43
34:u:366:ASP:HB2	34:u:370:MET:HE2	2.01	0.43
34:u:560:LEU:HD22	34:u:594:LEU:HD21	2.01	0.43
34:u:686:LEU:HD23	34:u:686:LEU:HA	1.89	0.43
1:U:509:GLY:CA	1:U:544:ILE:HD12	2.47	0.43
3:W:296:LEU:HG	3:W:302:TYR:CD1	2.54	0.43
7:a:168:ASN:O	7:a:169:HIS:C	2.62	0.43
12:A:51:ASP:OD1	12:A:52:ILE:N	2.52	0.43
31:S:145:LEU:HD22	31:S:178:VAL:HB	2.00	0.43
34:u:238:ASN:N	34:u:238:ASN:OD1	2.51	0.43
34:u:588:ARG:HG3	34:u:589:SER:N	2.33	0.43
1:U:427:LEU:HB2	1:U:430:ASP:HB2	2.00	0.43
1:U:765:VAL:O	1:U:766:PHE:C	2.61	0.43
2:V:263:LEU:HG	10:d:121:ARG:NH2	2.25	0.43
3:W:219:THR:HG21	3:W:222:LEU:HB2	2.01	0.43
5:Y:141:VAL:HG11	5:Y:164:ALA:HB2	2.00	0.43
6:Z:227:ILE:HD13	6:Z:227:ILE:HA	1.86	0.43
7:a:157:ASP:O	7:a:161:LYS:HG2	2.19	0.43
10:d:122:LEU:HD12	10:d:122:LEU:H	1.82	0.43
12:A:30:ILE:HG22	12:A:34:LYS:NZ	2.30	0.43
12:A:85:GLN:H	12:A:85:GLN:CD	2.26	0.43
12:A:111:TYR:CE2	12:A:125:LEU:HD22	2.53	0.43
13:B:264:PRO:O	13:B:268:ARG:HG3	2.18	0.43
13:B:416:ASN:ND2	13:B:416:ASN:O	2.52	0.43
14:C:59:LEU:HD23	15:D:75:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:F:310:MET:HE2	17:F:310:MET:HB3	1.80	0.43
25:M:49:VAL:HG11	25:M:65:ARG:HB2	2.01	0.43
30:R:37:ILE:O	30:R:38:ASN:HB2	2.19	0.43
19:g:244:GLU:OE1	19:g:244:GLU:N	2.51	0.43
24:l:71:GLY:HA3	24:l:221:PHE:CZ	2.53	0.43
24:l:88:MET:HE3	24:l:112:ILE:HD11	2.00	0.43
34:u:244:GLU:O	34:u:248:LEU:HD22	2.19	0.43
5:Y:121:LEU:HG	5:Y:125:ARG:HH12	1.84	0.43
8:b:182:ALA:O	8:b:186:SER:OG	2.32	0.43
9:c:64:ASP:OD1	9:c:64:ASP:N	2.40	0.43
10:d:58:GLY:O	10:d:62:SER:OG	2.25	0.43
12:A:97:ARG:NH1	12:A:97:ARG:HB3	2.34	0.43
13:B:288:ASP:OD1	13:B:288:ASP:N	2.37	0.43
15:D:39:ASP:O	15:D:43:ARG:HG3	2.18	0.43
16:E:11:ASP:O	16:E:15:LYS:HG2	2.19	0.43
17:F:84:LYS:HG3	17:F:84:LYS:O	2.18	0.43
17:F:333:ASN:OD1	17:F:333:ASN:N	2.48	0.43
19:G:73:THR:HG22	19:G:74:GLU:N	2.33	0.43
20:H:86:LEU:HD13	20:H:134:LEU:HD11	2.01	0.43
31:s:114:ASP:C	31:s:114:ASP:OD1	2.62	0.43
34:u:225:ALA:O	34:u:229:VAL:HG22	2.19	0.43
34:u:707:LEU:HD23	34:u:707:LEU:HA	1.88	0.43
1:U:18:GLN:OE1	1:U:18:GLN:N	2.49	0.42
1:U:216:VAL:HG11	1:U:248:ILE:HB	2.01	0.42
2:V:337:LEU:HD11	2:V:367:VAL:HG11	2.00	0.42
3:W:17:GLU:HG2	3:W:18:VAL:N	2.33	0.42
3:W:169:LEU:HA	3:W:185:PHE:HZ	1.83	0.42
5:Y:184:GLN:HE21	5:Y:200:LEU:HD13	1.83	0.42
5:Y:273:GLN:H	5:Y:273:GLN:HG2	1.62	0.42
9:c:62:VAL:HG13	9:c:63:ASP:H	1.84	0.42
14:C:38:LYS:HB2	15:D:54:LEU:HD13	2.00	0.42
16:E:37:THR:HA	17:F:69:MET:CE	2.49	0.42
17:F:98:ASP:OD1	17:F:120:LYS:HG3	2.19	0.42
20:H:189:HIS:NE2	20:H:234:ALA:O	2.52	0.42
25:M:169:ARG:H	25:M:169:ARG:HG3	1.63	0.42
26:N:18:SER:HB3	26:N:31:THR:H	1.84	0.42
22:j:80:ALA:HA	22:j:129:ILE:HD13	2.00	0.42
34:u:213:GLN:O	34:u:216:MET:HE3	2.19	0.42
34:u:437:GLU:OE1	34:u:439:TYR:HB2	2.19	0.42
34:u:885:GLU:CD	34:u:885:GLU:N	2.77	0.42
1:U:160:LEU:O	1:U:163:PHE:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:405:THR:CG2	1:U:441:GLY:HA3	2.47	0.42
4:X:60:THR:OG1	4:X:62:GLN:OE1	2.22	0.42
4:X:313:LEU:HD23	4:X:319:ILE:HG21	2.00	0.42
4:X:363:ARG:HA	4:X:363:ARG:HD2	1.83	0.42
4:X:365:LEU:HD23	4:X:385:LEU:HD13	2.01	0.42
5:Y:45:VAL:HG23	5:Y:46:ARG:HH12	1.83	0.42
9:c:75:MET:HE3	9:c:75:MET:HB2	1.70	0.42
9:c:139:ARG:HH12	9:c:203:ILE:HD11	1.84	0.42
9:c:219:ASN:O	9:c:222:LYS:N	2.52	0.42
9:c:266:THR:O	9:c:269:GLN:N	2.53	0.42
10:d:23:LEU:HD12	10:d:26:LEU:HD11	2.00	0.42
12:A:310:ASP:CB	12:A:311:PRO:HD3	2.48	0.42
13:B:64:LYS:HE3	34:u:239:TYR:OH	2.19	0.42
13:B:223:ILE:HB	13:B:347:ILE:HD13	2.01	0.42
30:R:146:ASP:OD1	30:R:146:ASP:N	2.53	0.42
21:i:38:LEU:HD12	21:i:43:VAL:HB	2.01	0.42
21:i:198:ASN:HA	21:i:206:LEU:HD22	2.00	0.42
1:U:52:GLU:HA	1:U:57:ARG:HD2	2.02	0.42
1:U:462:LEU:HD11	1:U:493:VAL:HG22	2.01	0.42
1:U:874:ASN:C	1:U:875:PHE:CD2	2.97	0.42
2:V:91:PRO:HA	2:V:94:VAL:CG1	2.42	0.42
2:V:128:ARG:NH1	2:V:165:ALA:HA	2.34	0.42
3:W:51:GLU:O	3:W:54:THR:OG1	2.25	0.42
4:X:89:VAL:HG11	4:X:125:LEU:HD21	2.00	0.42
4:X:92:LEU:HA	4:X:95:LEU:HD21	2.00	0.42
7:a:191:SER:O	7:a:194:GLN:HG2	2.19	0.42
8:b:109:ILE:HG22	8:b:138:VAL:HG13	2.02	0.42
9:c:100:LYS:HE2	9:c:100:LYS:HB3	1.85	0.42
12:A:26:ASP:HB2	12:A:29:ASP:HB2	2.01	0.42
12:A:191:VAL:HG21	12:A:318:LEU:HD21	2.00	0.42
14:C:189:TYR:HA	14:C:295:THR:O	2.19	0.42
15:D:164:TYR:CZ	15:D:178:ARG:HD3	2.53	0.42
16:E:35:GLU:O	16:E:39:GLN:HG2	2.19	0.42
17:F:79:LYS:HD2	17:F:80:ILE:N	2.34	0.42
17:F:342:LEU:HD12	17:F:343:LEU:HD23	2.01	0.42
23:K:98:ASN:OD1	30:R:61:ARG:NH1	2.52	0.42
26:n:1:THR:HB	39:n:301:LDZ:O33	2.18	0.42
28:p:158:MET:HE2	28:p:158:MET:HB2	1.89	0.42
30:r:113:TYR:O	30:r:120:ARG:HA	2.19	0.42
34:u:82:ILE:O	34:u:86:THR:HG23	2.18	0.42
34:u:467:SER:HB2	34:u:500:LEU:HD11	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:u:902:LYS:NZ	34:u:906:TYR:HB3	2.34	0.42
1:U:245:ALA:CB	1:U:325:MET:HE1	2.46	0.42
1:U:707:ASN:N	1:U:707:ASN:OD1	2.51	0.42
1:U:766:PHE:O	1:U:767:THR:C	2.61	0.42
2:V:217:VAL:O	2:V:221:LEU:HD12	2.19	0.42
2:V:322:VAL:HG22	2:V:324:PHE:H	1.84	0.42
3:W:62:SER:C	3:W:64:SER:H	2.27	0.42
5:Y:26:LEU:HD21	5:Y:36:ALA:HB3	2.01	0.42
6:Z:147:ASP:OD1	6:Z:148:GLY:N	2.46	0.42
7:a:27:GLU:HG3	7:a:31:LYS:HD2	2.01	0.42
10:d:182:ILE:CD1	10:d:198:LEU:HD11	2.49	0.42
11:e:59:GLU:O	11:e:60:LEU:HD23	2.19	0.42
12:A:111:TYR:HE2	12:A:125:LEU:HD22	1.84	0.42
12:A:134:ILE:HA	12:A:138:MET:HE1	2.02	0.42
12:A:214:LEU:HD23	12:A:343:PHE:CE1	2.55	0.42
15:D:279:THR:HB	15:D:282:ASP:HB2	2.00	0.42
16:E:251:ARG:O	16:E:255:ARG:HG3	2.18	0.42
17:F:44:ARG:HH11	17:F:44:ARG:N	2.17	0.42
19:G:165:ALA:HB1	19:G:179:LEU:HD13	2.02	0.42
21:I:123:GLN:O	21:I:123:GLN:CG	2.67	0.42
25:m:69:VAL:HG21	25:m:75:MET:HE3	2.01	0.42
27:o:137:VAL:HG11	27:o:157:GLU:HG2	2.01	0.42
33:f:414:GLY:N	33:f:415:PRO:HD3	2.34	0.42
34:u:271:MET:CE	34:u:786:GLN:HB3	2.49	0.42
1:U:563:ALA:O	1:U:567:ILE:HD12	2.20	0.42
1:U:769:PHE:O	1:U:770:TRP:C	2.62	0.42
1:U:841:LYS:O	1:U:845:GLU:HG2	2.19	0.42
3:W:375:MET:SD	3:W:376:LYS:N	2.93	0.42
4:X:123:THR:HA	4:X:126:ARG:HG2	2.01	0.42
4:X:157:LEU:HB3	4:X:166:LEU:CD1	2.50	0.42
5:Y:196:GLN:HG3	5:Y:200:LEU:CD1	2.49	0.42
9:c:31:VAL:HG23	9:c:67:VAL:HG13	2.00	0.42
10:d:172:ASP:O	10:d:175:ARG:HB2	2.19	0.42
12:A:55:LEU:HD12	12:A:55:LEU:HA	1.80	0.42
12:A:65:ILE:H	12:A:65:ILE:CD1	2.30	0.42
23:K:182:GLN:HA	24:L:56:LEU:HD11	2.01	0.42
28:P:14:MET:HE2	28:P:167:ILE:HB	2.02	0.42
23:k:91:LYS:NZ	23:k:95:GLU:OE2	2.43	0.42
24:l:50:LYS:HG2	24:l:60:GLN:O	2.19	0.42
25:m:54:LEU:HD23	25:m:54:LEU:HA	1.85	0.42
27:o:216:ILE:HD13	28:p:196:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:r:113:TYR:CZ	30:r:115:ASP:OD2	2.72	0.42
34:u:331:LEU:HD22	34:u:340:MET:HE1	2.01	0.42
34:u:585:GLU:HG3	34:u:586:PRO:HD3	2.00	0.42
34:u:870:THR:OG1	34:u:871:PRO:HD3	2.20	0.42
34:u:884:THR:OG1	34:u:885:GLU:N	2.53	0.42
1:U:158:ARG:HB3	1:U:159:ARG:H	1.65	0.42
2:V:212:TYR:CE1	2:V:253:LEU:HD21	2.50	0.42
7:a:7:PHE:CE1	7:a:56:LEU:HD13	2.54	0.42
7:a:219:HIS:ND1	7:a:220:PRO:HD2	2.35	0.42
9:c:71:ASP:OD1	9:c:72:VAL:N	2.51	0.42
9:c:196:LEU:HA	9:c:196:LEU:HD23	1.82	0.42
10:d:29:VAL:HA	10:d:32:GLU:HG3	2.01	0.42
10:d:200:PHE:CE2	10:d:209:TYR:HD2	2.37	0.42
14:C:68:GLU:CD	14:C:69:GLN:H	2.26	0.42
14:C:287:LYS:HE2	14:C:287:LYS:HB2	1.89	0.42
15:D:190:LEU:O	15:D:194:ILE:HG13	2.20	0.42
16:E:277:MET:HG3	16:E:295:LEU:HD11	2.02	0.42
28:P:20:VAL:HG12	28:P:190:ILE:HB	2.01	0.42
19:g:130:GLU:HG2	20:h:6:TYR:CE1	2.54	0.42
21:i:174:MET:HE1	21:i:199:LYS:CG	2.49	0.42
29:q:41:LYS:O	29:q:106:GLY:HA2	2.20	0.42
1:U:19:LEU:H	1:U:19:LEU:HD22	1.85	0.42
2:V:171:VAL:O	2:V:175:MET:HG2	2.20	0.42
3:W:55:ARG:HH11	3:W:56:THR:HG23	1.84	0.42
3:W:187:LEU:HD13	3:W:226:TYR:CD1	2.55	0.42
4:X:118:LYS:HD2	4:X:118:LYS:HA	1.73	0.42
7:a:26:GLU:O	7:a:30:THR:HG23	2.19	0.42
7:a:206:LEU:HD21	7:a:261:LEU:HD12	2.00	0.42
8:b:132:LYS:HD2	8:b:159:THR:O	2.19	0.42
10:d:115:PHE:CD1	10:d:115:PHE:C	2.98	0.42
10:d:125:LYS:HA	10:d:128:GLN:HG2	2.02	0.42
10:d:126:ASP:O	10:d:134:LYS:NZ	2.47	0.42
13:B:54:PRO:O	13:B:56:THR:HG23	2.19	0.42
13:B:256:ILE:HD12	14:C:271:ARG:HD3	2.02	0.42
13:B:290:ILE:HD12	13:B:290:ILE:HA	1.90	0.42
14:C:27:LYS:HZ1	15:D:44:TYR:HB2	1.84	0.42
15:D:388:ARG:HB2	15:D:388:ARG:HH11	1.85	0.42
25:M:144:ASP:OD1	25:M:144:ASP:N	2.53	0.42
24:l:80:ASP:HB2	24:l:130:VAL:HG13	2.02	0.42
34:u:688:ARG:O	34:u:724:ASN:ND2	2.51	0.42
34:u:846:VAL:O	34:u:865:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:15:ASP:HA	1:U:20:LYS:HE3	2.02	0.42
2:V:40:GLU:HA	2:V:43:THR:OG1	2.20	0.42
3:W:69:ALA:HA	3:W:72:LYS:CD	2.50	0.42
3:W:452:ILE:HD12	3:W:452:ILE:HA	1.95	0.42
5:Y:145:LEU:HD13	5:Y:179:ARG:HH11	1.85	0.42
6:Z:110:GLU:HA	6:Z:113:LYS:HD3	2.02	0.42
7:a:122:LYS:HZ1	7:a:131:THR:HA	1.84	0.42
7:a:368:GLU:OE1	7:a:368:GLU:HA	2.18	0.42
8:b:110:ILE:HD12	8:b:110:ILE:C	2.45	0.42
9:c:154:LYS:HE3	9:c:154:LYS:HB3	1.87	0.42
13:B:405:MET:HE3	13:B:421:LYS:HE2	2.01	0.42
15:D:100:THR:HA	15:D:114:ARG:HA	2.01	0.42
16:E:25:ARG:O	16:E:29:LEU:HG	2.20	0.42
16:E:153:LEU:HD22	16:E:229:ILE:HG13	2.02	0.42
17:F:77:SER:HA	17:F:80:ILE:HG22	2.01	0.42
17:F:269:ARG:NH2	17:F:312:GLU:OE2	2.53	0.42
20:H:75:VAL:HG12	20:H:135:LEU:HB2	2.01	0.42
32:T:180:ASP:O	32:T:183:SER:OG	2.38	0.42
24:l:80:ASP:OD1	24:l:80:ASP:N	2.51	0.42
34:u:737:ASN:OD1	34:u:737:ASN:N	2.52	0.42
34:u:777:THR:HB	34:u:828:ARG:HD3	2.01	0.42
1:U:191:LYS:HE2	1:U:194:ARG:NH2	2.35	0.42
1:U:572:ARG:NH1	1:U:572:ARG:HB3	2.34	0.42
2:V:80:LYS:HD3	2:V:126:ALA:HB3	2.02	0.42
2:V:181:TYR:O	2:V:185:GLN:NE2	2.53	0.42
2:V:372:LEU:HD23	2:V:399:ARG:NH2	2.35	0.42
3:W:221:LYS:HA	3:W:221:LYS:HD2	1.95	0.42
3:W:252:ASP:O	3:W:256:ILE:HG13	2.20	0.42
3:W:324:TYR:HE2	3:W:351:TRP:CZ3	2.37	0.42
4:X:206:LEU:O	4:X:209:THR:N	2.53	0.42
4:X:382:GLU:OE1	4:X:382:GLU:N	2.53	0.42
7:a:186:LYS:O	7:a:188:LEU:HG	2.20	0.42
8:b:12:ASN:OD1	8:b:12:ASN:N	2.50	0.42
8:b:128:ALA:HB2	8:b:156:PHE:CD1	2.55	0.42
10:d:78:LEU:HD22	10:d:98:LEU:HD21	2.02	0.42
10:d:127:ILE:HD12	10:d:127:ILE:HA	1.90	0.42
12:A:418:LYS:HB3	12:A:423:PHE:CD2	2.54	0.42
14:C:57:ARG:O	14:C:61:GLU:HG3	2.20	0.42
16:E:370:ALA:O	16:E:374:VAL:HG23	2.19	0.42
19:G:44:GLY:HA3	19:G:194:THR:HG21	2.02	0.42
39:R:301:LDZ:H9	39:R:301:LDZ:H39	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:37:ALA:HB2	23:k:50:VAL:HG23	2.01	0.42
39:r:301:LDZ:H42	39:r:301:LDZ:H9	1.79	0.42
34:u:137:ARG:NH2	34:u:172:GLU:OE2	2.53	0.42
34:u:311:VAL:HG23	34:u:314:TYR:HB2	2.02	0.42
1:U:653:ALA:HB2	1:U:675:MET:CE	2.50	0.42
3:W:243:ILE:HG13	3:W:273:TYR:CE2	2.55	0.42
4:X:173:GLU:HA	4:X:176:THR:HG22	2.01	0.42
10:d:111:ARG:NH1	10:d:114:GLU:OE1	2.53	0.42
10:d:175:ARG:HG2	10:d:200:PHE:HE1	1.84	0.42
12:A:123:VAL:HA	17:F:86:LEU:HD13	2.01	0.42
12:A:215:PHE:CZ	12:A:342:GLU:HB2	2.54	0.42
16:E:351:GLY:O	16:E:355:ILE:HG13	2.20	0.42
22:J:171:PHE:O	22:J:175:ASN:HB2	2.19	0.42
28:P:31:GLN:HB3	28:P:32:ALA:H	1.59	0.42
22:j:107:ILE:HD12	22:j:107:ILE:HA	1.92	0.42
34:u:869:THR:HG22	34:u:871:PRO:CD	2.50	0.42
1:U:38:ILE:HD12	1:U:38:ILE:H	1.84	0.41
1:U:162:VAL:HA	1:U:165:LYS:CD	2.50	0.41
1:U:703:CYS:HA	1:U:704:PRO:HD3	1.86	0.41
1:U:766:PHE:O	1:U:768:GLN:N	2.53	0.41
1:U:789:ILE:HG22	1:U:791:LEU:H	1.85	0.41
2:V:291:TYR:O	2:V:295:ILE:HG23	2.20	0.41
3:W:147:LYS:HD2	3:W:147:LYS:N	2.35	0.41
4:X:239:TYR:O	4:X:242:ILE:HG12	2.20	0.41
7:a:69:HIS:ND1	7:a:70:ARG:HG2	2.35	0.41
12:A:241:ILE:C	12:A:243:SER:H	2.28	0.41
16:E:325:GLU:CG	16:E:326:ILE:H	2.33	0.41
21:I:240:HIS:NE2	21:I:244:GLU:OE2	2.52	0.41
30:R:17:ASP:OD1	30:R:33:LYS:NZ	2.47	0.41
34:u:535:THR:HG23	34:u:562:LEU:HD11	2.01	0.41
1:U:460:TYR:HD2	1:U:461:LEU:HD12	1.84	0.41
2:V:96:ARG:HB2	2:V:150:ARG:NH1	2.33	0.41
3:W:151:THR:O	3:W:154:GLU:HB2	2.20	0.41
6:Z:272:LEU:HD12	6:Z:272:LEU:HA	1.83	0.41
7:a:180:LEU:HD23	7:a:180:LEU:HA	1.86	0.41
7:a:198:PHE:CD1	7:a:233:LEU:HD22	2.54	0.41
16:E:63:GLN:HG3	16:E:69:PHE:HD1	1.85	0.41
17:F:356:MET:HG3	17:F:357:PRO:HD2	2.02	0.41
20:H:184:LEU:HD23	20:H:184:LEU:HA	1.69	0.41
26:N:70:LEU:HD23	26:N:70:LEU:HA	1.90	0.41
19:g:141:ILE:HG22	19:g:151:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:k:93:ARG:HG2	30:r:68:LEU:HD13	2.02	0.41
34:u:220:ASP:N	34:u:220:ASP:OD1	2.53	0.41
34:u:338:ASP:O	34:u:339:ILE:HD13	2.21	0.41
34:u:420:TRP:CD1	34:u:455:VAL:HG13	2.55	0.41
34:u:487:LEU:HA	34:u:524:MET:HE1	2.03	0.41
34:u:558:LEU:H	34:u:558:LEU:HD22	1.84	0.41
1:U:611:ASN:HB3	1:U:614:VAL:HG12	2.02	0.41
2:V:207:ALA:HB1	2:V:211:TYR:CZ	2.55	0.41
2:V:310:THR:HG22	2:V:332:LEU:HD21	2.01	0.41
2:V:394:LEU:HA	2:V:397:ARG:HE	1.84	0.41
4:X:66:LEU:HD23	4:X:96:PHE:HA	2.02	0.41
5:Y:338:ILE:HD11	5:Y:345:CYS:SG	2.60	0.41
6:Z:259:VAL:HG23	9:c:292:MET:SD	2.60	0.41
6:Z:266:ILE:HG21	9:c:284:LEU:HD11	2.02	0.41
7:a:300:ALA:O	7:a:301:LYS:HG2	2.20	0.41
8:b:146:GLU:HB2	8:b:148:VAL:HG12	2.03	0.41
10:d:186:TYR:HB3	10:d:220:ASN:HB3	2.02	0.41
13:B:69:LYS:O	13:B:73:LEU:HG	2.21	0.41
17:F:76:ASN:O	17:F:79:LYS:HG3	2.21	0.41
24:L:117:GLN:HG3	25:M:82:ALA:HB1	2.01	0.41
31:S:83:MET:HG2	31:S:87:ALA:HB3	2.02	0.41
21:i:8:ARG:C	21:i:10:THR:H	2.29	0.41
25:m:52:LEU:HA	25:m:209:PHE:HA	2.02	0.41
30:r:105:ASP:OD1	30:r:106:LYS:N	2.45	0.41
34:u:838:ARG:HD3	34:u:839:PRO:HD2	2.02	0.41
2:V:417:ILE:HD12	2:V:418:SER:H	1.85	0.41
3:W:136:ILE:HG21	3:W:144:ARG:HD2	2.03	0.41
3:W:144:ARG:H	3:W:144:ARG:CD	2.32	0.41
4:X:162:ASP:O	4:X:163:LYS:HD2	2.19	0.41
5:Y:225:TYR:O	5:Y:295:TYR:OH	2.22	0.41
6:Z:194:GLN:O	6:Z:198:LEU:HD12	2.20	0.41
6:Z:261:TYR:O	6:Z:265:LEU:HB2	2.21	0.41
7:a:12:GLN:HG3	7:a:22:TRP:CD1	2.56	0.41
7:a:34:TRP:O	7:a:35:HIS:C	2.64	0.41
7:a:304:VAL:O	7:a:307:VAL:HG22	2.20	0.41
10:d:125:LYS:O	10:d:130:ASN:ND2	2.48	0.41
10:d:209:TYR:CE1	10:d:213:ARG:HG3	2.54	0.41
12:A:123:VAL:C	17:F:86:LEU:HD13	2.46	0.41
13:B:75:GLU:OE2	34:u:673:ARG:NH1	2.53	0.41
14:C:84:LYS:HB2	14:C:84:LYS:HE3	1.70	0.41
14:C:132:ASP:HB3	14:C:135:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:252:ASP:OD1	14:C:295:THR:OG1	2.38	0.41
16:E:349:GLU:HB3	16:E:373:LYS:HE3	2.02	0.41
17:F:86:LEU:H	17:F:86:LEU:HG	1.68	0.41
17:F:172:VAL:O	17:F:175:MET:HB3	2.20	0.41
17:F:269:ARG:HA	17:F:316:GLN:OE1	2.20	0.41
19:G:37:LEU:HD22	19:G:53:GLN:HG3	2.02	0.41
19:G:131:MET:HE3	25:M:124:LEU:HD13	2.01	0.41
27:O:163:ILE:HG23	27:O:169:SER:OG	2.20	0.41
28:P:14:MET:HG3	28:P:136:PHE:HB3	2.03	0.41
31:S:191:ASP:H	31:S:210:LEU:HB2	1.85	0.41
32:T:122:LEU:HG	32:T:137:LEU:HD12	2.01	0.41
19:g:40:VAL:HG23	19:g:202:LEU:HD13	2.03	0.41
21:i:149:GLN:HG3	21:i:150:SER:N	2.34	0.41
22:j:38:ARG:HH12	22:j:180:ALA:HB1	1.84	0.41
22:j:66:ASP:HB2	22:j:91:CYS:SG	2.60	0.41
1:U:145:HIS:O	1:U:145:HIS:CG	2.73	0.41
1:U:155:LEU:HD23	1:U:155:LEU:HA	1.90	0.41
1:U:388:ASP:OD1	1:U:389:ASN:N	2.54	0.41
1:U:801:GLN:HB3	1:U:877:LEU:HB3	2.02	0.41
2:V:91:PRO:HB2	2:V:114:TYR:CD1	2.55	0.41
4:X:157:LEU:HD23	4:X:157:LEU:HA	1.85	0.41
6:Z:288:LYS:O	6:Z:288:LYS:HD2	2.20	0.41
7:a:211:PHE:O	7:a:211:PHE:CG	2.73	0.41
8:b:14:GLU:HB2	8:b:17:ARG:HE	1.85	0.41
8:b:161:ASN:CG	8:b:161:ASN:O	2.63	0.41
16:E:175:PRO:HD2	16:E:178:THR:HG21	2.03	0.41
20:H:184:LEU:O	20:H:188:ILE:HG13	2.20	0.41
27:O:173:ILE:HB	27:O:190:THR:HG22	2.01	0.41
20:h:33:ALA:O	20:h:77:SER:OG	2.38	0.41
22:j:51:ALA:O	22:j:52:LYS:HB2	2.21	0.41
27:o:17:ASP:HB2	27:o:169:SER:CB	2.47	0.41
1:U:176:MET:HE2	1:U:176:MET:HA	2.03	0.41
1:U:184:CYS:SG	1:U:197:VAL:HG11	2.61	0.41
2:V:90:GLU:HB3	2:V:124:ASN:HB3	2.01	0.41
2:V:173:ILE:HA	2:V:176:MET:SD	2.60	0.41
3:W:97:LEU:HD23	3:W:97:LEU:HA	1.84	0.41
3:W:206:SER:O	3:W:209:ILE:HG22	2.21	0.41
5:Y:357:ASN:OD1	5:Y:357:ASN:N	2.54	0.41
5:Y:366:TYR:HA	5:Y:369:THR:HG22	2.03	0.41
9:c:207:TYR:N	9:c:207:TYR:CD1	2.87	0.41
10:d:215:TRP:HA	10:d:215:TRP:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:C:113:ARG:NH2	14:C:129:ASN:O	2.54	0.41
15:D:104:GLY:HA2	15:D:110:ASN:HA	2.02	0.41
16:E:50:LEU:HD22	16:E:50:LEU:HA	1.94	0.41
16:E:324:GLY:O	16:E:326:ILE:HG12	2.20	0.41
30:R:32:LYS:HD3	30:R:32:LYS:HA	1.90	0.41
25:m:66:LEU:HD13	25:m:214:SER:OG	2.21	0.41
25:m:195:LYS:HE3	25:m:195:LYS:HB3	1.89	0.41
1:U:102:ALA:O	1:U:105:ILE:HB	2.21	0.41
2:V:364:THR:HA	2:V:367:VAL:HG12	2.02	0.41
9:c:197:ASN:N	9:c:200:TYR:O	2.44	0.41
12:A:121:PHE:CE1	17:F:89:LEU:HB3	2.56	0.41
15:D:240:LEU:HD23	15:D:240:LEU:HA	1.87	0.41
16:E:126:ASP:N	16:E:127:PRO:HD3	2.36	0.41
17:F:380:ASN:HB3	17:F:383:GLU:HB2	2.03	0.41
21:I:6:ASP:O	21:I:20:GLN:NE2	2.54	0.41
21:I:10:THR:O	22:J:125:ARG:HG3	2.20	0.41
23:K:88:LEU:HD13	23:K:156:MET:HE1	2.03	0.41
25:M:106:ILE:HG12	25:M:111:LEU:HB2	2.02	0.41
29:Q:30:ASP:OD1	29:Q:30:ASP:N	2.52	0.41
32:T:211:ILE:HG22	32:T:214:MET:HE3	2.03	0.41
27:o:163:ILE:HG21	27:o:171:SER:OG	2.21	0.41
29:q:118:MET:HE2	29:q:118:MET:HB2	1.85	0.41
34:u:120:ARG:HB3	34:u:147:SER:HA	2.02	0.41
34:u:426:LEU:HA	34:u:429:ILE:HD11	2.02	0.41
1:U:791:LEU:O	1:U:913:ILE:HD13	2.21	0.41
1:U:904:LYS:HZ2	1:U:904:LYS:HG2	1.65	0.41
2:V:236:ARG:NE	2:V:236:ARG:O	2.54	0.41
2:V:491:VAL:HG11	10:d:257:VAL:HG11	2.02	0.41
3:W:260:SER:HA	3:W:263:TRP:HB3	2.02	0.41
3:W:405:LYS:HD2	3:W:405:LYS:HA	1.79	0.41
4:X:242:ILE:O	4:X:243:ASP:HB2	2.21	0.41
4:X:415:TYR:CE1	5:Y:383:LEU:HD23	2.56	0.41
6:Z:130:ASP:OD1	6:Z:130:ASP:C	2.64	0.41
8:b:22:LEU:HD22	8:b:177:PRO:HB2	1.96	0.41
12:A:191:VAL:CG2	12:A:318:LEU:HD21	2.51	0.41
15:D:327:LEU:HD23	15:D:327:LEU:HA	1.92	0.41
19:G:36:GLY:O	19:G:37:LEU:HD23	2.21	0.41
27:O:170:GLY:O	27:O:171:SER:HB2	2.20	0.41
30:R:1:THR:OG1	39:R:301:LDZ:C22	2.69	0.41
31:S:68:ILE:HD11	31:S:92:LEU:HD13	2.03	0.41
21:i:105:ILE:HG12	21:i:110:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:l:202:GLU:HG2	24:l:203:GLN:HG2	2.03	0.41
29:q:108:ASP:OD2	29:q:111:GLU:HG2	2.21	0.41
31:s:83:MET:HE1	31:s:91:MET:SD	2.60	0.41
1:U:54:PHE:CE2	1:U:56:SER:HB2	2.55	0.41
1:U:483:LEU:HD11	1:U:781:LEU:HD11	2.02	0.41
1:U:732:LEU:HD23	1:U:732:LEU:HA	1.76	0.41
2:V:37:MET:SD	2:V:38:LYS:N	2.94	0.41
2:V:86:VAL:O	2:V:89:LYS:HG2	2.21	0.41
2:V:133:PRO:HD2	2:V:134:PHE:N	2.28	0.41
2:V:169:LEU:HD12	2:V:169:LEU:HA	1.82	0.41
2:V:209:LYS:HA	2:V:212:TYR:CD2	2.55	0.41
2:V:348:PHE:HB2	2:V:353:LEU:HD23	2.02	0.41
3:W:371:THR:HG22	3:W:372:ARG:HG3	2.02	0.41
3:W:436:MET:O	3:W:439:VAL:HG12	2.20	0.41
4:X:163:LYS:HB3	4:X:200:ILE:HD12	2.03	0.41
5:Y:95:LEU:HD13	5:Y:95:LEU:HA	1.97	0.41
7:a:32:LYS:O	7:a:32:LYS:HD2	2.21	0.41
7:a:132:LYS:HB2	7:a:132:LYS:HE2	1.94	0.41
7:a:172:TYR:CD1	7:a:172:TYR:C	2.99	0.41
9:c:251:LEU:HD21	9:c:283:HIS:HB2	2.03	0.41
9:c:304:LEU:HD12	9:c:304:LEU:HA	1.94	0.41
10:d:29:VAL:HA	10:d:32:GLU:CG	2.51	0.41
10:d:109:GLN:OE1	10:d:109:GLN:HA	2.20	0.41
10:d:187:GLU:H	10:d:220:ASN:HB2	1.86	0.41
10:d:216:VAL:O	10:d:217:LEU:C	2.63	0.41
12:A:199:GLU:HA	12:A:202:VAL:HG22	2.03	0.41
13:B:43:PRO:CD	13:B:44:ASP:N	2.76	0.41
14:C:82:LYS:HA	14:C:82:LYS:HD3	1.88	0.41
14:C:129:ASN:OD1	14:C:130:LYS:N	2.53	0.41
14:C:394:ASP:O	14:C:395:SER:OG	2.38	0.41
15:D:74:HIS:CD2	15:D:74:HIS:O	2.72	0.41
15:D:403:TYR:O	15:D:407:ILE:HG12	2.21	0.41
15:D:416:PHE:O	15:D:417:TYR:CD1	2.74	0.41
16:E:34:LYS:HE2	16:E:34:LYS:HB3	1.87	0.41
16:E:129:ASN:HA	16:E:189:SER:OG	2.21	0.41
17:F:47:LEU:HD12	17:F:50:SER:HB2	2.02	0.41
17:F:99:VAL:HG13	17:F:120:LYS:HD2	2.03	0.41
22:J:107:ILE:HD12	22:J:107:ILE:HA	1.88	0.41
25:M:37:ILE:HD11	25:M:193:VAL:HG13	2.02	0.41
28:P:118:LYS:HE3	28:P:118:LYS:HB2	1.79	0.41
29:Q:155:ARG:HA	29:Q:155:ARG:HD3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:h:12:THR:OG1	20:h:13:PHE:N	2.54	0.41
23:k:196:LYS:HG3	23:k:241:ILE:HG21	2.03	0.41
24:l:23:GLU:HA	24:l:26:MET:HG3	2.03	0.41
24:l:189:LYS:NZ	24:l:234:GLU:O	2.47	0.41
25:m:72:HIS:CE1	25:m:105:ASN:HB3	2.56	0.41
34:u:83:ARG:HB2	34:u:154:TRP:CZ3	2.56	0.41
34:u:209:MET:HE3	34:u:209:MET:HB3	1.84	0.41
34:u:585:GLU:N	34:u:586:PRO:HD2	2.36	0.41
2:V:33:GLN:HG3	2:V:85:ALA:HA	2.03	0.41
2:V:95:LEU:HB3	2:V:107:ARG:CZ	2.51	0.41
2:V:354:LYS:HA	2:V:357:LEU:CD2	2.50	0.41
3:W:374:THR:C	3:W:375:MET:HG3	2.46	0.41
4:X:70:LEU:HD23	4:X:92:LEU:HD23	2.03	0.41
4:X:364:LYS:O	4:X:368:MET:HG2	2.19	0.41
5:Y:114:ILE:HD13	5:Y:114:ILE:HA	1.83	0.41
5:Y:124:PHE:CD1	5:Y:140:ILE:HD12	2.56	0.41
5:Y:140:ILE:HD13	5:Y:140:ILE:HA	1.77	0.41
6:Z:191:ILE:HD13	6:Z:191:ILE:HA	1.96	0.41
7:a:122:LYS:HE3	7:a:134:THR:HG21	2.03	0.41
9:c:46:ARG:HA	9:c:49:VAL:HG23	2.02	0.41
9:c:218:LEU:CG	9:c:219:ASN:H	2.34	0.41
10:d:73:ARG:HG3	10:d:77:GLN:NE2	2.35	0.41
10:d:131:VAL:HG22	10:d:159:PRO:HB3	2.01	0.41
10:d:178:ILE:HD11	10:d:198:LEU:HD23	2.03	0.41
12:A:113:ILE:HD12	12:A:113:ILE:O	2.21	0.41
15:D:156:SER:O	15:D:157:ASP:HB3	2.20	0.41
15:D:170:MET:O	15:D:172:ILE:N	2.53	0.41
15:D:349:THR:HG22	15:D:352:MET:SD	2.61	0.41
30:R:33:LYS:HG2	39:R:301:LDZ:H19	2.03	0.41
20:h:184:LEU:O	20:h:188:ILE:HG13	2.21	0.41
24:l:94:ASP:N	24:l:94:ASP:OD1	2.54	0.41
24:l:117:GLN:HG3	25:m:82:ALA:HB1	2.03	0.41
30:r:141:ARG:HD3	30:r:141:ARG:HA	1.87	0.41
31:s:13:LEU:HD11	31:s:149:LEU:HD11	2.02	0.41
31:s:125:ASP:OD1	31:s:125:ASP:C	2.64	0.41
34:u:50:LYS:HD2	34:u:50:LYS:HA	1.87	0.41
34:u:689:ALA:HA	34:u:692:LEU:HD23	2.03	0.41
34:u:887:PHE:HD1	34:u:900:LEU:HD13	1.86	0.41
3:W:96:GLN:O	3:W:99:GLN:NE2	2.54	0.40
3:W:444:HIS:NE2	6:Z:133:LEU:HD13	2.36	0.40
4:X:60:THR:HG1	4:X:62:GLN:CD	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:143:TYR:CG	4:X:144:GLN:N	2.86	0.40
6:Z:206:LEU:HD23	6:Z:206:LEU:HA	1.79	0.40
9:c:163:ILE:HD12	9:c:163:ILE:HA	1.85	0.40
15:D:87:LEU:HD12	15:D:133:HIS:HA	2.03	0.40
15:D:355:SER:O	15:D:355:SER:OG	2.34	0.40
16:E:84:ARG:HB2	16:E:87:LEU:HG	2.03	0.40
30:R:52:CYS:SG	30:R:97:MET:HG3	2.60	0.40
32:T:50:MET:CE	32:T:192:VAL:HG23	2.50	0.40
26:n:45:ARG:HD2	26:n:52:THR:HB	2.03	0.40
28:p:73:LEU:HA	28:p:73:LEU:HD23	1.81	0.40
34:u:497:VAL:HG12	34:u:501:LEU:HD13	2.04	0.40
34:u:740:ARG:O	34:u:744:MET:HG3	2.20	0.40
34:u:881:GLU:HA	34:u:894:LEU:HD22	2.03	0.40
2:V:137:GLU:HA	2:V:140:ASP:OD2	2.20	0.40
3:W:327:GLU:O	3:W:337:ALA:HB1	2.21	0.40
6:Z:69:PHE:CZ	8:b:95:LEU:HD13	2.55	0.40
8:b:31:ASP:O	8:b:35:ILE:HG12	2.21	0.40
10:d:181:CYS:HA	10:d:184:LYS:HZ3	1.86	0.40
10:d:182:ILE:HD13	10:d:198:LEU:HD11	2.04	0.40
17:F:406:ILE:HD13	17:F:422:GLU:HG2	2.03	0.40
23:K:59:MET:HE2	23:K:64:ILE:HD11	2.04	0.40
25:M:186:CYS:O	25:M:190:VAL:HG23	2.21	0.40
34:u:154:TRP:HA	34:u:154:TRP:CE3	2.56	0.40
34:u:339:ILE:HG22	34:u:339:ILE:O	2.21	0.40
34:u:486:GLY:HA3	34:u:521:ALA:HB1	2.02	0.40
34:u:885:GLU:N	34:u:885:GLU:OE1	2.55	0.40
1:U:162:VAL:O	1:U:163:PHE:C	2.64	0.40
1:U:665:ASN:C	1:U:667:GLU:H	2.30	0.40
1:U:796:LYS:C	1:U:797:MET:HE3	2.47	0.40
2:V:91:PRO:O	2:V:94:VAL:HG12	2.22	0.40
3:W:282:GLU:HA	3:W:285:ASP:OD2	2.22	0.40
3:W:412:ILE:N	3:W:412:ILE:HD12	2.36	0.40
4:X:66:LEU:HD12	4:X:66:LEU:HA	1.89	0.40
5:Y:104:MET:HG3	5:Y:126:LYS:HZ1	1.87	0.40
6:Z:145:HIS:O	6:Z:145:HIS:ND1	2.54	0.40
6:Z:166:GLU:OE1	9:c:46:ARG:NH2	2.55	0.40
7:a:227:ASN:O	7:a:231:GLN:NE2	2.48	0.40
9:c:139:ARG:HA	9:c:161:ARG:HH12	1.86	0.40
10:d:25:ARG:O	10:d:28:LEU:HG	2.21	0.40
10:d:75:MET:CE	10:d:102:ASN:HB2	2.48	0.40
11:e:45:ASP:HB3	11:e:48:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:75:PRO:HA	12:A:78:TRP:NE1	2.36	0.40
13:B:63:LEU:HA	13:B:63:LEU:HD23	1.84	0.40
13:B:141:LYS:HB3	13:B:141:LYS:HE2	1.82	0.40
16:E:52:SER:OG	17:F:136:VAL:HB	2.21	0.40
16:E:107:ILE:O	16:E:108:MET:HE2	2.20	0.40
16:E:206:LYS:HB3	16:E:206:LYS:HE3	1.85	0.40
16:E:253:ILE:HD13	16:E:253:ILE:HA	1.92	0.40
21:I:8:ARG:HG2	21:I:10:THR:H	1.86	0.40
30:R:179:VAL:HG22	30:R:184:TRP:HB3	2.03	0.40
27:o:7:VAL:HG22	27:o:12:ILE:HD13	2.03	0.40
34:u:315:GLU:OE1	34:u:315:GLU:N	2.46	0.40
34:u:373:ALA:HB2	34:u:760:PHE:CD1	2.55	0.40
34:u:662:MET:C	34:u:664:GLU:H	2.29	0.40
1:U:510:GLU:HA	1:U:547:GLY:HA3	2.02	0.40
1:U:766:PHE:C	1:U:768:GLN:N	2.76	0.40
2:V:31:ALA:O	2:V:35:VAL:HB	2.21	0.40
2:V:68:ASP:O	2:V:72:LEU:N	2.54	0.40
2:V:264:TYR:CE1	10:d:118:GLU:HA	2.50	0.40
8:b:122:LYS:O	8:b:125:VAL:HG12	2.21	0.40
9:c:175:ARG:NH1	9:c:175:ARG:HB3	2.36	0.40
10:d:78:LEU:HD12	10:d:79:LYS:N	2.36	0.40
12:A:38:GLN:OE1	12:A:40:THR:N	2.54	0.40
14:C:396:GLU:OE2	14:C:398:ASN:ND2	2.55	0.40
16:E:197:LYS:HB2	16:E:233:ASP:HB3	2.03	0.40
17:F:206:MET:SD	17:F:325:GLN:HG2	2.61	0.40
23:K:108:THR:OG1	23:K:111:SER:OG	2.28	0.40
27:o:6:VAL:HG23	27:o:124:TYR:HB3	2.03	0.40
28:p:204:MET:HE3	28:p:204:MET:HB3	1.91	0.40
34:u:785:ARG:O	34:u:785:ARG:HD2	2.22	0.40
1:U:361:ARG:HD3	1:U:361:ARG:HA	1.83	0.40
2:V:159:LEU:HD23	2:V:160:LEU:HD23	2.03	0.40
2:V:410:ILE:HD11	2:V:425:LYS:HB3	2.03	0.40
3:W:44:ILE:HG23	3:W:45:GLU:CD	2.46	0.40
3:W:417:ARG:HA	3:W:417:ARG:HD3	1.92	0.40
5:Y:155:ASP:N	5:Y:155:ASP:OD1	2.54	0.40
9:c:216:MET:C	9:c:218:LEU:N	2.79	0.40
10:d:193:GLU:HA	10:d:196:ARG:HB2	2.03	0.40
11:e:4:LYS:HE3	11:e:4:LYS:HB3	1.92	0.40
12:A:70:THR:HG21	13:B:164:MET:H	1.85	0.40
15:D:196:ILE:O	15:D:197:ASP:HB2	2.22	0.40
16:E:64:LEU:H	16:E:69:PHE:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:E:193:CYS:HB3	16:E:229:ILE:O	2.21	0.40
22:J:76:LEU:H	22:J:129:ILE:HG22	1.86	0.40
21:i:68:LEU:HD22	21:i:90:LEU:HD13	2.02	0.40
21:i:140:ASP:OD1	21:i:140:ASP:C	2.65	0.40
23:k:195:ILE:HD11	23:k:219:THR:HG21	2.03	0.40
34:u:208:LEU:HD22	34:u:213:GLN:O	2.21	0.40
34:u:790:GLN:HA	34:u:793:VAL:HG12	2.03	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	839/953 (88%)	745 (89%)	86 (10%)	8 (1%)	12	24
2	V	478/533 (90%)	421 (88%)	56 (12%)	1 (0%)	43	64
3	W	448/456 (98%)	407 (91%)	39 (9%)	2 (0%)	30	50
4	X	378/422 (90%)	358 (95%)	16 (4%)	4 (1%)	11	22
5	Y	376/389 (97%)	334 (89%)	40 (11%)	2 (0%)	24	43
6	Z	284/324 (88%)	250 (88%)	31 (11%)	3 (1%)	11	22
7	a	371/376 (99%)	326 (88%)	41 (11%)	4 (1%)	11	22
8	b	189/377 (50%)	166 (88%)	20 (11%)	3 (2%)	7	14
9	c	285/309 (92%)	238 (84%)	43 (15%)	4 (1%)	9	17
10	d	249/349 (71%)	194 (78%)	48 (19%)	7 (3%)	4	6
11	e	36/70 (51%)	26 (72%)	8 (22%)	2 (6%)	1	2
12	A	411/433 (95%)	365 (89%)	41 (10%)	5 (1%)	10	20
13	B	403/440 (92%)	359 (89%)	40 (10%)	4 (1%)	12	24
14	C	394/398 (99%)	361 (92%)	29 (7%)	4 (1%)	12	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	D	378/418 (90%)	345 (91%)	28 (7%)	5 (1%)	9	18
16	E	379/403 (94%)	330 (87%)	44 (12%)	5 (1%)	9	18
17	F	391/439 (89%)	352 (90%)	35 (9%)	4 (1%)	12	24
18	v	12/14 (86%)	10 (83%)	2 (17%)	0	100	100
19	G	235/245 (96%)	226 (96%)	7 (3%)	2 (1%)	14	28
19	g	238/245 (97%)	227 (95%)	11 (5%)	0	100	100
20	H	229/233 (98%)	216 (94%)	12 (5%)	1 (0%)	30	50
20	h	230/233 (99%)	224 (97%)	5 (2%)	1 (0%)	30	50
21	I	246/260 (95%)	228 (93%)	17 (7%)	1 (0%)	30	50
21	i	248/260 (95%)	230 (93%)	17 (7%)	1 (0%)	30	50
22	J	245/247 (99%)	230 (94%)	11 (4%)	4 (2%)	7	14
22	j	237/247 (96%)	213 (90%)	23 (10%)	1 (0%)	30	50
23	K	226/240 (94%)	219 (97%)	7 (3%)	0	100	100
23	k	224/240 (93%)	212 (95%)	12 (5%)	0	100	100
24	L	236/268 (88%)	231 (98%)	5 (2%)	0	100	100
24	l	236/268 (88%)	227 (96%)	9 (4%)	0	100	100
25	M	238/254 (94%)	230 (97%)	7 (3%)	1 (0%)	30	50
25	m	238/254 (94%)	223 (94%)	14 (6%)	1 (0%)	30	50
26	N	195/238 (82%)	189 (97%)	5 (3%)	1 (0%)	24	43
26	n	195/238 (82%)	187 (96%)	8 (4%)	0	100	100
27	O	218/276 (79%)	212 (97%)	5 (2%)	1 (0%)	24	43
27	o	218/276 (79%)	201 (92%)	17 (8%)	0	100	100
28	P	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
28	p	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
29	Q	197/201 (98%)	184 (93%)	13 (7%)	0	100	100
29	q	197/201 (98%)	187 (95%)	10 (5%)	0	100	100
30	R	199/262 (76%)	196 (98%)	1 (0%)	2 (1%)	12	24
30	r	199/262 (76%)	195 (98%)	4 (2%)	0	100	100
31	S	211/240 (88%)	207 (98%)	3 (1%)	1 (0%)	24	43
31	s	211/240 (88%)	206 (98%)	5 (2%)	0	100	100
32	T	213/263 (81%)	206 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	t	213/263 (81%)	205 (96%)	8 (4%)	0	100	100
33	f	37/468 (8%)	37 (100%)	0	0	100	100
34	u	826/908 (91%)	803 (97%)	23 (3%)	0	100	100
All	All	13340/15341 (87%)	12323 (92%)	932 (7%)	85 (1%)	23	38

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	U	41	SER
1	U	173	VAL
1	U	875	PHE
3	W	45	GLU
3	W	375	MET
4	X	310	ARG
5	Y	361	SER
6	Z	167	ALA
7	a	215	GLU
10	d	187	GLU
10	d	219	PRO
11	e	46	ASP
12	A	423	PHE
14	C	90	HIS
14	C	254	ILE
14	C	297	ARG
15	D	258	ALA
16	E	238	ILE
17	F	87	PRO
17	F	279	ALA
20	H	180	GLU
21	I	107	CYS
22	J	199	VAL
31	S	191	ASP
21	i	107	CYS
22	j	52	LYS
1	U	96	TYR
4	X	205	LYS
4	X	246	LYS
8	b	188	ILE
9	c	218	LEU
9	c	219	ASN
9	c	223	LYS

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Mol	Chain	Res	Type
10	d	94	TYR
11	e	60	LEU
12	A	109	PRO
13	B	165	ASP
15	D	149	SER
16	E	248	SER
16	E	306	GLU
17	F	298	SER
19	G	130	GLU
22	J	184	ASP
22	J	213	ARG
25	M	201	HIS
1	U	168	LEU
2	V	465	ASP
6	Z	186	THR
10	d	199	PHE
10	d	223	TYR
12	A	269	ALA
12	A	310	ASP
13	B	434	THR
14	C	242	ALA
15	D	303	VAL
16	E	326	ILE
1	U	159	ARG
1	U	169	GLU
4	X	143	TYR
6	Z	243	GLN
8	b	182	ALA
15	D	171	ASP
15	D	197	ASP
17	F	301	ALA
19	G	9	PHE
26	N	19	ARG
27	O	172	ASN
1	U	876	GLN
7	a	144	ASN
9	c	25	VAL
10	d	222	TYR
13	B	320	ASP
22	J	6	ALA
30	R	143	TYR
7	a	166	ILE

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Mol	Chain	Res	Type
10	d	203	PRO
12	A	308	GLY
16	E	240	GLY
30	R	38	ASN
20	h	232	ALA
25	m	201	HIS
5	Y	350	VAL
8	b	23	PRO
13	B	43	PRO
7	a	185	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	722/816 (88%)	694 (96%)	28 (4%)	28	51
2	V	414/459 (90%)	401 (97%)	13 (3%)	35	59
3	W	412/416 (99%)	392 (95%)	20 (5%)	22	43
4	X	327/362 (90%)	314 (96%)	13 (4%)	28	50
5	Y	334/344 (97%)	322 (96%)	12 (4%)	31	55
6	Z	257/295 (87%)	246 (96%)	11 (4%)	26	47
7	a	333/336 (99%)	313 (94%)	20 (6%)	17	32
8	b	166/312 (53%)	157 (95%)	9 (5%)	20	38
9	c	252/267 (94%)	229 (91%)	23 (9%)	9	17
10	d	226/293 (77%)	213 (94%)	13 (6%)	18	34
11	e	38/63 (60%)	37 (97%)	1 (3%)	40	63
12	A	348/372 (94%)	338 (97%)	10 (3%)	37	61
13	B	352/385 (91%)	344 (98%)	8 (2%)	44	66
14	C	340/346 (98%)	332 (98%)	8 (2%)	43	65
15	D	333/366 (91%)	319 (96%)	14 (4%)	26	49
16	E	333/353 (94%)	315 (95%)	18 (5%)	20	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	F	340/379 (90%)	326 (96%)	14 (4%)	27	49
19	G	191/209 (91%)	191 (100%)	0	100	100
19	g	194/209 (93%)	185 (95%)	9 (5%)	24	45
20	H	169/190 (89%)	161 (95%)	8 (5%)	23	45
20	h	167/190 (88%)	163 (98%)	4 (2%)	43	65
21	I	191/220 (87%)	190 (100%)	1 (0%)	81	89
21	i	193/220 (88%)	188 (97%)	5 (3%)	40	63
22	J	179/210 (85%)	172 (96%)	7 (4%)	28	51
22	j	152/210 (72%)	140 (92%)	12 (8%)	11	21
23	K	189/202 (94%)	185 (98%)	4 (2%)	47	67
23	k	186/202 (92%)	179 (96%)	7 (4%)	29	52
24	L	198/229 (86%)	195 (98%)	3 (2%)	57	74
24	l	198/229 (86%)	193 (98%)	5 (2%)	42	64
25	M	192/211 (91%)	188 (98%)	4 (2%)	47	67
25	m	193/211 (92%)	187 (97%)	6 (3%)	35	59
26	N	154/180 (86%)	150 (97%)	4 (3%)	40	63
26	n	154/180 (86%)	151 (98%)	3 (2%)	50	70
27	O	177/227 (78%)	174 (98%)	3 (2%)	53	71
27	o	177/227 (78%)	174 (98%)	3 (2%)	53	71
28	P	173/173 (100%)	170 (98%)	3 (2%)	53	71
28	p	173/173 (100%)	168 (97%)	5 (3%)	37	61
29	Q	164/171 (96%)	160 (98%)	4 (2%)	43	65
29	q	165/171 (96%)	163 (99%)	2 (1%)	63	78
30	R	153/201 (76%)	148 (97%)	5 (3%)	33	57
30	r	153/201 (76%)	148 (97%)	5 (3%)	33	57
31	S	174/198 (88%)	172 (99%)	2 (1%)	65	79
31	s	174/198 (88%)	173 (99%)	1 (1%)	78	88
32	T	175/214 (82%)	168 (96%)	7 (4%)	28	50
32	t	176/214 (82%)	174 (99%)	2 (1%)	65	79
33	f	34/377 (9%)	34 (100%)	0	100	100
34	u	702/763 (92%)	690 (98%)	12 (2%)	53	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	11197/12974 (86%)	10826 (97%)	371 (3%)	34 57

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	U	35	TRP
1	U	62	LEU
1	U	69	TYR
1	U	78	LEU
1	U	107	HIS
1	U	126	ILE
1	U	144	ASP
1	U	161	ASP
1	U	169	GLU
1	U	172	ASP
1	U	353	LEU
1	U	408	LEU
1	U	453	HIS
1	U	472	ILE
1	U	554	LEU
1	U	666	LYS
1	U	701	ILE
1	U	707	ASN
1	U	756	HIS
1	U	764	LEU
1	U	770	TRP
1	U	813	TYR
1	U	873	PRO
1	U	874	ASN
1	U	875	PHE
1	U	876	GLN
1	U	921	ILE
1	U	925	VAL
2	V	71	THR
2	V	103	SER
2	V	159	LEU
2	V	231	LEU
2	V	235	LEU
2	V	242	HIS
2	V	265	ASP
2	V	285	TRP
2	V	322	VAL

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Mol	Chain	Res	Type
2	V	337	LEU
2	V	418	SER
2	V	430	SER
2	V	469	THR
3	W	47	LEU
3	W	63	THR
3	W	67	LEU
3	W	73	MET
3	W	145	LEU
3	W	169	LEU
3	W	205	ILE
3	W	227	TYR
3	W	253	THR
3	W	255	CYS
3	W	282	GLU
3	W	286	LEU
3	W	288	HIS
3	W	338	THR
3	W	365	ILE
3	W	381	LEU
3	W	387	ASP
3	W	406	VAL
3	W	434	SER
3	W	443	THR
4	X	70	LEU
4	X	98	ASP
4	X	148	HIS
4	X	200	ILE
4	X	230	SER
4	X	246	LYS
4	X	248	ILE
4	X	342	PHE
4	X	350	ILE
4	X	384	VAL
4	X	385	LEU
4	X	394	ASP
4	X	411	VAL
5	Y	53	TYR
5	Y	58	CYS
5	Y	186	LEU
5	Y	196	GLN
5	Y	201	PHE

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Mol	Chain	Res	Type
5	Y	229	ILE
5	Y	231	LEU
5	Y	287	LEU
5	Y	314	LEU
5	Y	344	HIS
5	Y	350	VAL
5	Y	353	ILE
6	Z	6	VAL
6	Z	39	LEU
6	Z	47	VAL
6	Z	78	MET
6	Z	81	MET
6	Z	85	VAL
6	Z	120	VAL
6	Z	121	LEU
6	Z	184	VAL
6	Z	233	VAL
6	Z	262	LEU
7	a	32	LYS
7	a	65	SER
7	a	81	LEU
7	a	153	SER
7	a	165	THR
7	a	166	ILE
7	a	169	HIS
7	a	188	LEU
7	a	211	PHE
7	a	236	THR
7	a	237	LEU
7	a	250	THR
7	a	264	ASN
7	a	292	THR
7	a	304	VAL
7	a	316	SER
7	a	324	ILE
7	a	333	MET
7	a	346	ILE
7	a	358	THR
8	b	63	THR
8	b	109	ILE
8	b	113	VAL
8	b	166	THR

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Mol	Chain	Res	Type
8	b	177	PRO
8	b	179	LEU
8	b	181	ASP
8	b	183	LEU
8	b	188	ILE
9	c	62	VAL
9	c	69	VAL
9	c	84	VAL
9	c	90	VAL
9	c	99	LEU
9	c	118	PHE
9	c	127	ILE
9	c	133	PHE
9	c	157	ILE
9	c	162	LEU
9	c	163	ILE
9	c	180	ASN
9	c	196	LEU
9	c	198	ARG
9	c	204	THR
9	c	209	LYS
9	c	216	MET
9	c	222	LYS
9	c	223	LYS
9	c	225	TRP
9	c	248	MET
9	c	284	LEU
9	c	310	LYS
10	d	10	ASN
10	d	11	ARG
10	d	15	ASN
10	d	35	PHE
10	d	79	LYS
10	d	85	TYR
10	d	94	TYR
10	d	126	ASP
10	d	158	ILE
10	d	187	GLU
10	d	202	THR
10	d	215	TRP
10	d	257	VAL
11	e	41	ASP

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Mol	Chain	Res	Type
12	A	22	ILE
12	A	133	ASP
12	A	191	VAL
12	A	206	ILE
12	A	220	THR
12	A	236	CYS
12	A	266	THR
12	A	303	ILE
12	A	310	ASP
12	A	312	ARG
13	B	49	LEU
13	B	143	LEU
13	B	183	THR
13	B	201	VAL
13	B	250	VAL
13	B	288	ASP
13	B	299	SER
13	B	426	VAL
14	C	71	SER
14	C	109	THR
14	C	123	LEU
14	C	127	LEU
14	C	206	HIS
14	C	213	ARG
14	C	256	SER
14	C	299	ASP
15	D	64	GLU
15	D	73	LEU
15	D	100	THR
15	D	105	SER
15	D	117	SER
15	D	123	LEU
15	D	124	LEU
15	D	151	ILE
15	D	192	LYS
15	D	203	LEU
15	D	236	VAL
15	D	329	ARG
15	D	345	PHE
15	D	347	THR
16	E	50	LEU
16	E	53	VAL

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Mol	Chain	Res	Type
16	E	64	LEU
16	E	70	ILE
16	E	75	ASN
16	E	78	ARG
16	E	88	ASP
16	E	92	LEU
16	E	145	LEU
16	E	194	ASN
16	E	196	LEU
16	E	229	ILE
16	E	250	ASP
16	E	280	ASN
16	E	283	ASP
16	E	296	ASP
16	E	321	THR
16	E	371	VAL
17	F	44	ARG
17	F	86	LEU
17	F	123	VAL
17	F	134	LEU
17	F	150	LEU
17	F	151	VAL
17	F	178	ASP
17	F	289	ASP
17	F	333	ASN
17	F	336	ASP
17	F	356	MET
17	F	358	ASN
17	F	426	GLU
17	F	431	LYS
20	H	10	LEU
20	H	19	LEU
20	H	77	SER
20	H	133	SER
20	H	168	VAL
20	H	184	LEU
20	H	192	ILE
20	H	198	SER
21	I	150	SER
22	J	45	VAL
22	J	67	ASP
22	J	102	VAL

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Mol	Chain	Res	Type
22	J	119	THR
22	J	130	SER
22	J	134	VAL
22	J	167	SER
23	K	12	VAL
23	K	214	ASN
23	K	217	LEU
23	K	238	ILE
24	L	33	SER
24	L	156	CYS
24	L	211	SER
25	M	37	ILE
25	M	158	TYR
25	M	174	THR
25	M	215	TRP
26	N	72	GLU
26	N	139	VAL
26	N	170	SER
26	N	190	LEU
27	O	6	VAL
27	O	127	MET
27	O	167	LEU
28	P	116	THR
28	P	123	SER
28	P	175	VAL
29	Q	31	ASP
29	Q	39	SER
29	Q	181	ARG
29	Q	195	SER
30	R	29	GLN
30	R	37	ILE
30	R	102	CYS
30	R	144	SER
30	R	146	ASP
31	S	127	VAL
31	S	142	SER
32	T	3	ASN
32	T	49	THR
32	T	92	LEU
32	T	155	GLU
32	T	191	THR
32	T	200	GLU

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Mol	Chain	Res	Type
32	T	205	THR
19	g	37	LEU
19	g	39	SER
19	g	61	LEU
19	g	112	ASP
19	g	175	SER
19	g	182	LYS
19	g	193	GLN
19	g	210	PHE
19	g	216	GLU
20	h	75	VAL
20	h	77	SER
20	h	183	GLU
20	h	224	THR
21	i	11	ILE
21	i	61	PHE
21	i	75	SER
21	i	81	SER
21	i	149	GLN
22	j	5	ARG
22	j	13	ASP
22	j	26	VAL
22	j	35	VAL
22	j	41	VAL
22	j	68	ASN
22	j	102	VAL
22	j	108	THR
22	j	121	SER
22	j	134	VAL
22	j	184	ASP
22	j	211	MET
23	k	10	ARG
23	k	20	ARG
23	k	42	THR
23	k	87	THR
23	k	148	GLU
23	k	178	GLN
23	k	224	GLN
24	l	38	LEU
24	l	114	SER
24	l	198	THR
24	l	206	THR

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Mol	Chain	Res	Type
24	l	211	SER
25	m	34	SER
25	m	157	SER
25	m	179	LEU
25	m	188	ASP
25	m	215	TRP
25	m	227	VAL
26	n	7	GLN
26	n	22	THR
26	n	78	THR
27	o	6	VAL
27	o	132	LEU
27	o	203	ARG
28	p	116	THR
28	p	122	CYS
28	p	126	LEU
28	p	137	VAL
28	p	158	MET
29	q	47	VAL
29	q	94	SER
30	r	99	THR
30	r	102	CYS
30	r	136	TYR
30	r	191	ASN
30	r	192	VAL
31	s	134	SER
32	t	49	THR
32	t	110	MET
34	u	129	LEU
34	u	136	GLU
34	u	229	VAL
34	u	248	LEU
34	u	376	PHE
34	u	459	CYS
34	u	655	LEU
34	u	737	ASN
34	u	748	LEU
34	u	817	VAL
34	u	850	VAL
34	u	891	THR

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

Mol	Chain	Res	Type
1	U	89	ASN
1	U	149	GLN
1	U	171	ASN
1	U	189	GLN
1	U	207	ASN
1	U	267	ASN
1	U	412	HIS
1	U	467	ASN
1	U	540	GLN
1	U	596	ASN
1	U	611	ASN
1	U	742	HIS
1	U	874	ASN
2	V	33	GLN
2	V	177	ASN
2	V	365	GLN
3	W	96	GLN
3	W	257	GLN
4	X	296	ASN
5	Y	71	ASN
5	Y	178	ASN
6	Z	277	ASN
7	a	12	GLN
7	a	18	GLN
7	a	168	ASN
8	b	169	HIS
9	c	172	HIS
9	c	197	ASN
10	d	88	GLN
10	d	128	GLN
10	d	135	HIS
10	d	221	ASN
12	A	60	ASN
12	A	148	GLN
12	A	165	GLN
12	A	322	ASN
13	B	84	GLN
13	B	153	ASN
13	B	207	HIS
13	B	332	ASN
14	C	40	GLN
14	C	53	ASN
14	C	67	GLN

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Mol	Chain	Res	Type
14	C	90	HIS
15	D	175	GLN
15	D	222	HIS
15	D	278	GLN
15	D	304	ASN
16	E	39	GLN
16	E	220	ASN
16	E	263	GLN
16	E	271	HIS
17	F	83	ASN
17	F	208	HIS
17	F	258	GLN
17	F	316	GLN
17	F	367	GLN
17	F	434	ASN
19	G	53	GLN
21	I	84	ASN
21	I	95	GLN
22	J	15	HIS
22	J	85	ASN
22	J	122	ASN
23	K	186	HIS
24	L	143	HIS
27	O	66	HIS
28	P	7	ASN
28	P	81	GLN
28	P	93	ASN
28	P	169	GLN
29	Q	24	ASN
29	Q	87	ASN
30	R	162	GLN
30	R	175	ASN
31	S	36	HIS
31	S	108	ASN
31	S	131	GLN
31	S	151	ASN
31	S	152	GLN
31	S	163	HIS
32	T	3	ASN
32	T	108	ASN
32	T	147	GLN
21	i	109	GLN

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Mol	Chain	Res	Type
21	i	155	ASN
22	j	15	HIS
22	j	54	GLN
22	j	122	ASN
23	k	13	ASN
23	k	97	GLN
25	m	97	ASN
26	n	7	GLN
26	n	154	GLN
27	o	62	ASN
27	o	66	HIS
27	o	80	ASN
28	p	7	ASN
29	q	71	ASN
29	q	101	ASN
30	r	162	GLN
31	s	8	ASN
31	s	79	ASN
31	s	108	ASN
32	t	46	ASN
32	t	47	ASN
32	t	208	ASN
33	f	385	ASN
34	u	51	GLN
34	u	53	GLN
34	u	118	ASN
34	u	213	GLN
34	u	371	ASN
34	u	472	HIS
34	u	475	ASN
34	u	808	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 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
36	ATP	A	501	37	32,33,33	0.37	0	48,52,52	0.27	0
36	ATP	B	501	37	32,33,33	0.41	0	48,52,52	0.30	0
36	ATP	C	501	37	32,33,33	0.43	0	48,52,52	0.32	0
39	LDZ	R	301	-	33,34,34	0.20	0	42,44,44	0.41	1 (2%)
39	LDZ	n	301	-	33,34,34	0.53	1 (3%)	42,44,44	1.60	4 (9%)
36	ATP	F	501	37	32,33,33	0.32	0	48,52,52	0.33	0
39	LDZ	N	301	-	33,34,34	0.43	0	42,44,44	0.72	1 (2%)
39	LDZ	o	301	-	33,34,34	0.49	0	42,44,44	0.84	2 (4%)
38	ADP	E	401	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (18%)
39	LDZ	r	301	-	33,34,34	0.50	0	42,44,44	0.67	1 (2%)
38	ADP	D	501	37	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
39	LDZ	O	301	-	33,34,34	0.37	0	42,44,44	1.55	3 (7%)

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
36	ATP	A	501	37	-	4/22/38/38	0/3/3/3
36	ATP	B	501	37	-	5/22/38/38	0/3/3/3
36	ATP	C	501	37	-	3/22/38/38	0/3/3/3
39	LDZ	R	301	-	-	10/38/39/39	0/1/1/1
39	LDZ	n	301	-	-	22/38/39/39	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	F	501	37	-	5/22/38/38	0/3/3/3
39	LDZ	N	301	-	-	6/38/39/39	0/1/1/1
39	LDZ	o	301	-	-	17/38/39/39	0/1/1/1
38	ADP	E	401	-	-	5/16/32/32	0/3/3/3
39	LDZ	r	301	-	-	8/38/39/39	0/1/1/1
38	ADP	D	501	37	-	0/16/32/32	0/3/3/3
39	LDZ	O	301	-	-	17/38/39/39	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	E	401	ADP	C5-C4	4.73	1.47	1.39
38	D	501	ADP	C5-C4	4.51	1.47	1.39
38	E	401	ADP	C5-C6	2.69	1.48	1.41
38	D	501	ADP	C5-C6	2.57	1.48	1.41
38	D	501	ADP	C5-N7	-2.43	1.34	1.39
38	E	401	ADP	C5-N7	-2.39	1.34	1.39
38	E	401	ADP	C8-N7	2.27	1.36	1.31
39	n	301	LDZ	C17-N16	-2.22	1.43	1.46
38	D	501	ADP	C8-N7	2.14	1.35	1.31

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	O	301	LDZ	C18-C17-N16	7.84	122.51	110.69
39	n	301	LDZ	C14-N13-C12	7.80	138.41	121.65
38	E	401	ADP	C5-C4-N3	-6.10	118.32	126.72
38	D	501	ADP	C5-C4-N3	-5.82	118.71	126.72
38	E	401	ADP	N3-C4-N9	4.90	135.50	127.17
38	D	501	ADP	N3-C4-N9	4.69	135.14	127.17
38	E	401	ADP	C2-N3-C4	3.80	121.11	111.83
38	D	501	ADP	C2-N3-C4	3.69	120.85	111.83
39	n	301	LDZ	C24-C14-N13	3.39	118.22	110.58
38	D	501	ADP	C4-C5-N7	-3.31	106.79	110.58
38	D	501	ADP	N3-C2-N1	-3.30	123.59	128.58
38	E	401	ADP	C4-C5-N7	-3.28	106.83	110.58
38	E	401	ADP	N3-C2-N1	-3.23	123.69	128.58
39	O	301	LDZ	C14-C15-N16	3.06	123.16	116.63
38	E	401	ADP	C3'-C2'-C1'	2.79	106.74	101.46
39	O	301	LDZ	C18-C17-C22	-2.71	106.81	110.99
38	D	501	ADP	C3'-C2'-C1'	2.69	106.56	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	D	501	ADP	C4-N9-C8	2.68	108.56	105.74
39	o	301	LDZ	C14-N13-C12	2.67	127.39	121.65
39	n	301	LDZ	C11-C12-N13	2.57	122.11	116.63
38	E	401	ADP	C5-N7-C8	2.47	107.33	103.45
38	D	501	ADP	C5-N7-C8	2.44	107.29	103.45
38	E	401	ADP	C4-N9-C8	2.38	108.24	105.74
39	r	301	LDZ	C14-N13-C12	2.25	126.47	121.65
39	o	301	LDZ	C15-C14-N13	-2.21	105.13	111.11
39	n	301	LDZ	C18-C17-C22	-2.13	107.72	110.99
39	R	301	LDZ	O33-C22-C17	-2.11	119.35	124.77
39	N	301	LDZ	C14-N13-C12	2.02	125.99	121.65

There are no chirality outliers.

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	A	501	ATP	PB-O3B-PG-O3G
36	A	501	ATP	C5'-O5'-PA-O1A
36	B	501	ATP	C5'-O5'-PA-O2A
36	B	501	ATP	C5'-O5'-PA-O3A
36	C	501	ATP	C5'-O5'-PA-O2A
36	C	501	ATP	C5'-O5'-PA-O3A
36	F	501	ATP	C5'-O5'-PA-O1A
36	F	501	ATP	C5'-O5'-PA-O3A
38	E	401	ADP	C5'-O5'-PA-O1A
38	E	401	ADP	C5'-O5'-PA-O2A
38	E	401	ADP	C5'-O5'-PA-O3A
38	E	401	ADP	O4'-C4'-C5'-O5'
39	O	301	LDZ	O31-C9-O8-C7
39	O	301	LDZ	N10-C9-O8-C7
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	C18-C17-C22-O33
39	R	301	LDZ	C22-C17-C18-C19
39	n	301	LDZ	C30-C11-N10-C9
39	n	301	LDZ	O31-C9-N10-C11
39	n	301	LDZ	O8-C9-N10-C11
39	n	301	LDZ	C24-C14-N13-C12
39	N	301	LDZ	N10-C11-C30-C31
39	O	301	LDZ	N16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
39	R	301	LDZ	N13-C14-C24-C25
39	n	301	LDZ	N13-C14-C24-C25
39	r	301	LDZ	N13-C14-C24-C25
39	O	301	LDZ	C17-C18-C19-C21
39	R	301	LDZ	N16-C17-C18-C19
39	r	301	LDZ	C15-C14-C24-C25
39	n	301	LDZ	C17-C18-C19-C21
39	o	301	LDZ	C30-C11-C12-O32
39	R	301	LDZ	C12-C11-C30-C31
39	R	301	LDZ	C15-C14-C24-C25
39	n	301	LDZ	C15-C14-C24-C25
39	O	301	LDZ	C14-C24-C25-C26
39	o	301	LDZ	C30-C11-C12-N13
38	E	401	ADP	C3'-C4'-C5'-O5'
39	o	301	LDZ	C15-C14-C24-C25
39	n	301	LDZ	C11-C30-C31-C32
39	n	301	LDZ	C11-C30-C31-C33
39	O	301	LDZ	C14-C15-N16-C17
39	O	301	LDZ	C14-C24-C25-C27
39	O	301	LDZ	O34-C15-N16-C17
39	O	301	LDZ	C17-C18-C19-C20
39	n	301	LDZ	C17-C18-C19-C20
39	o	301	LDZ	C17-C18-C19-C20
39	n	301	LDZ	O32-C12-N13-C14
39	o	301	LDZ	C14-C24-C25-C26
39	n	301	LDZ	C11-C12-N13-C14
39	o	301	LDZ	C17-C18-C19-C21
39	O	301	LDZ	C12-C11-N10-C9
39	R	301	LDZ	N10-C11-C30-C31
39	o	301	LDZ	C14-C24-C25-C27
39	O	301	LDZ	N13-C14-C24-C25
39	o	301	LDZ	N13-C14-C24-C25
39	o	301	LDZ	C24-C14-N13-C12
39	R	301	LDZ	C11-C30-C31-C32
39	N	301	LDZ	C14-C24-C25-C27
39	n	301	LDZ	N16-C17-C18-C19
39	n	301	LDZ	N13-C14-C15-N16
39	n	301	LDZ	N10-C11-C12-O32
39	n	301	LDZ	N13-C14-C15-O34
39	o	301	LDZ	N13-C14-C15-O34
39	n	301	LDZ	N10-C11-C12-N13
39	o	301	LDZ	N13-C14-C15-N16

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Mol	Chain	Res	Type	Atoms
39	n	301	LDZ	C22-C17-C18-C19
36	B	501	ATP	PB-O3B-PG-O1G
39	o	301	LDZ	C18-C17-N16-C15
36	F	501	ATP	PB-O3A-PA-O2A
39	N	301	LDZ	C14-C24-C25-C26
39	o	301	LDZ	C15-C14-N13-C12
36	A	501	ATP	C5'-O5'-PA-O3A
36	F	501	ATP	C5'-O5'-PA-O2A
39	r	301	LDZ	C14-C24-C25-C27
36	C	501	ATP	PG-O3B-PB-O2B
39	r	301	LDZ	N10-C11-C30-C31
39	n	301	LDZ	N10-C9-O8-C7
39	r	301	LDZ	C12-C11-C30-C31
39	o	301	LDZ	C3-C7-O8-C9
39	O	301	LDZ	C12-C11-C30-C31
39	N	301	LDZ	C22-C17-N16-C15
39	o	301	LDZ	C22-C17-N16-C15
39	O	301	LDZ	C15-C14-C24-C25
36	A	501	ATP	PB-O3B-PG-O1G
39	r	301	LDZ	N10-C9-O8-C7
36	B	501	ATP	PB-O3B-PG-O2G
36	B	501	ATP	PB-O3B-PG-O3G
39	N	301	LDZ	C18-C17-N16-C15
39	n	301	LDZ	C18-C17-N16-C15
39	r	301	LDZ	C18-C17-N16-C15
36	F	501	ATP	PB-O3A-PA-O1A
39	N	301	LDZ	C12-C11-C30-C31
39	n	301	LDZ	O31-C9-O8-C7
39	O	301	LDZ	C30-C11-N10-C9
39	o	301	LDZ	C24-C14-C15-O34
39	n	301	LDZ	C30-C11-C12-O32
39	r	301	LDZ	O31-C9-O8-C7
39	o	301	LDZ	C24-C14-C15-N16
39	O	301	LDZ	N10-C11-C30-C31

There are no ring outliers.

9 monomers are involved in 22 short contacts:

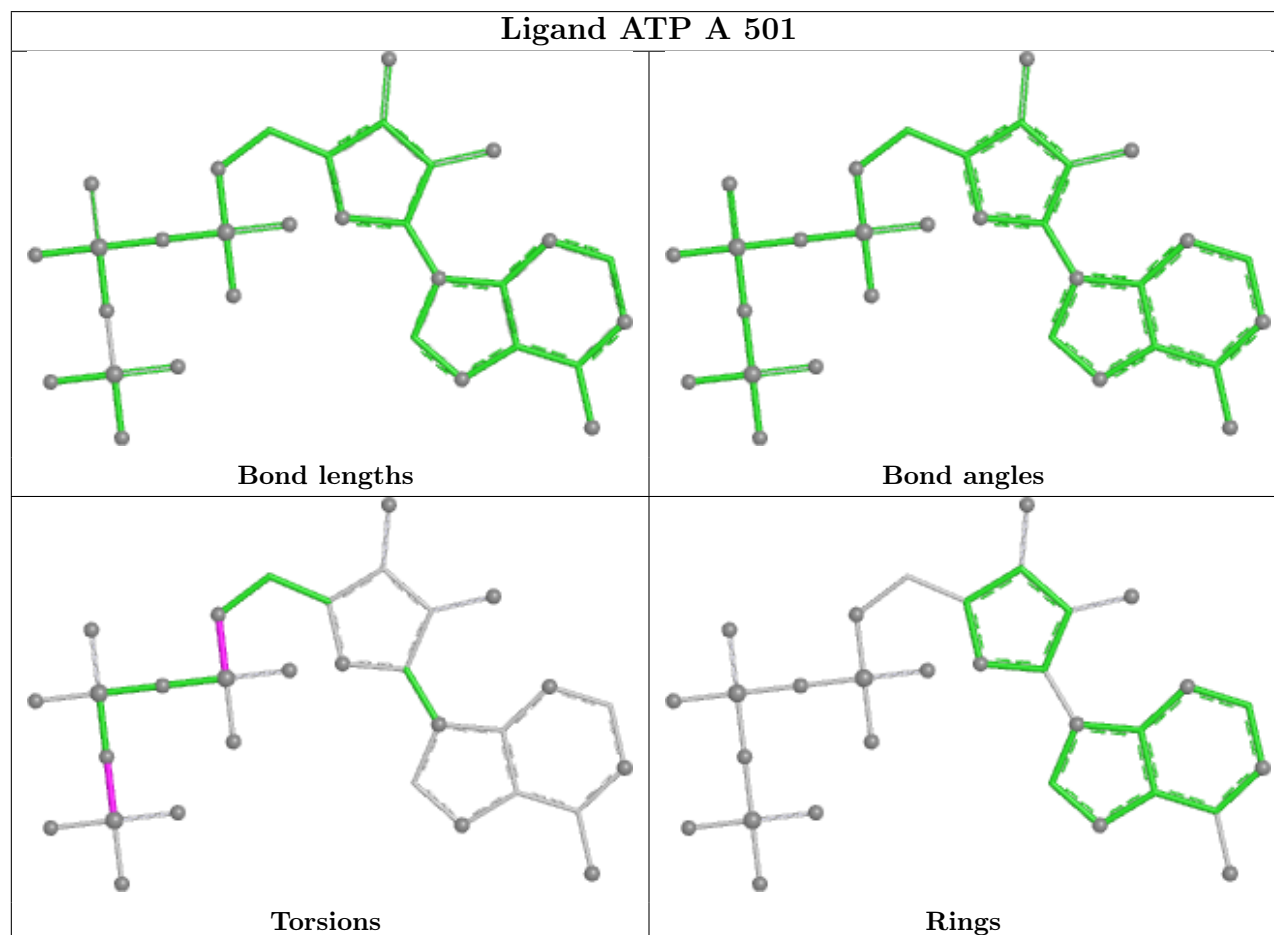
Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	B	501	ATP	1	0
39	R	301	LDZ	4	0
39	n	301	LDZ	3	0

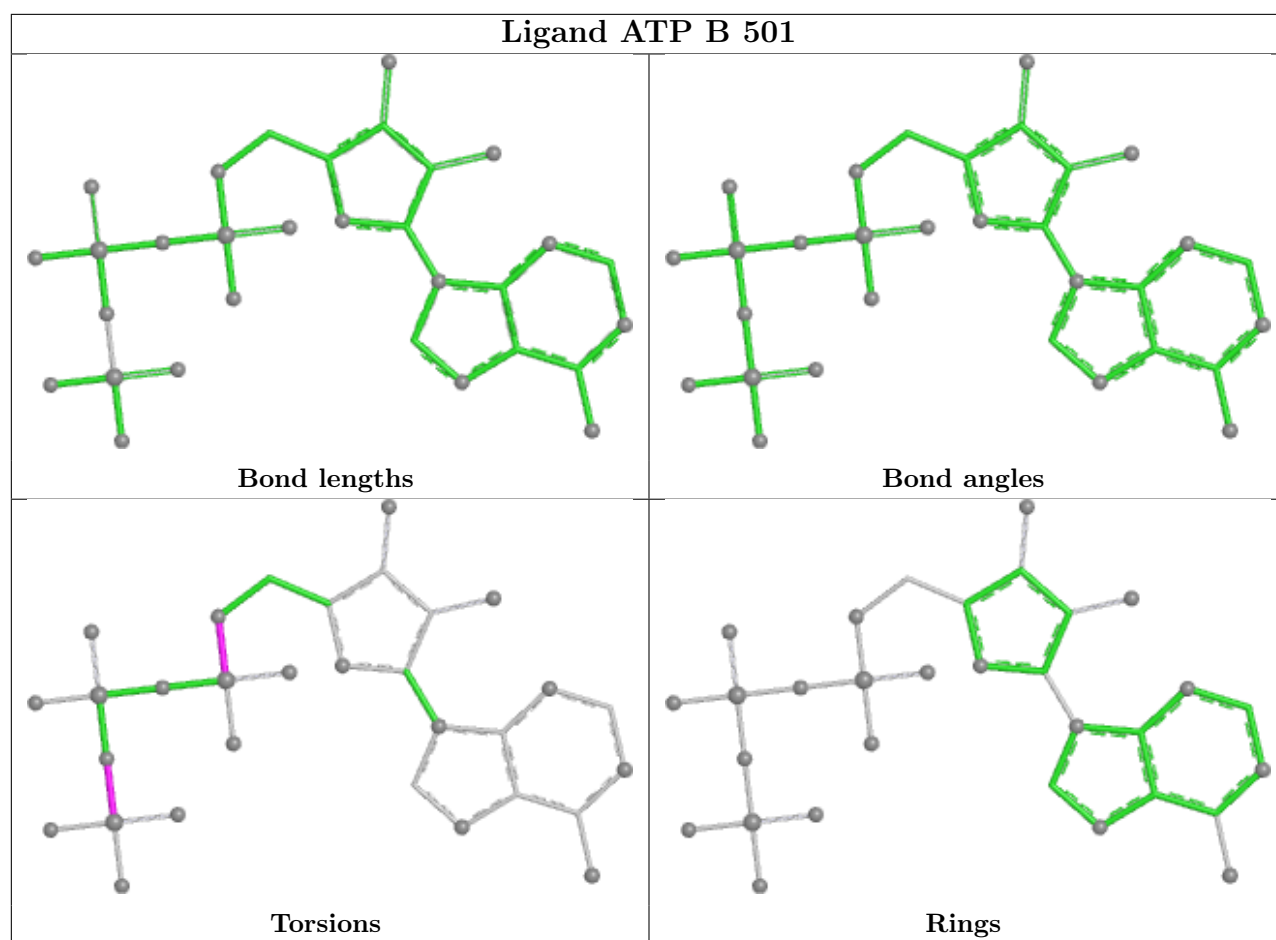
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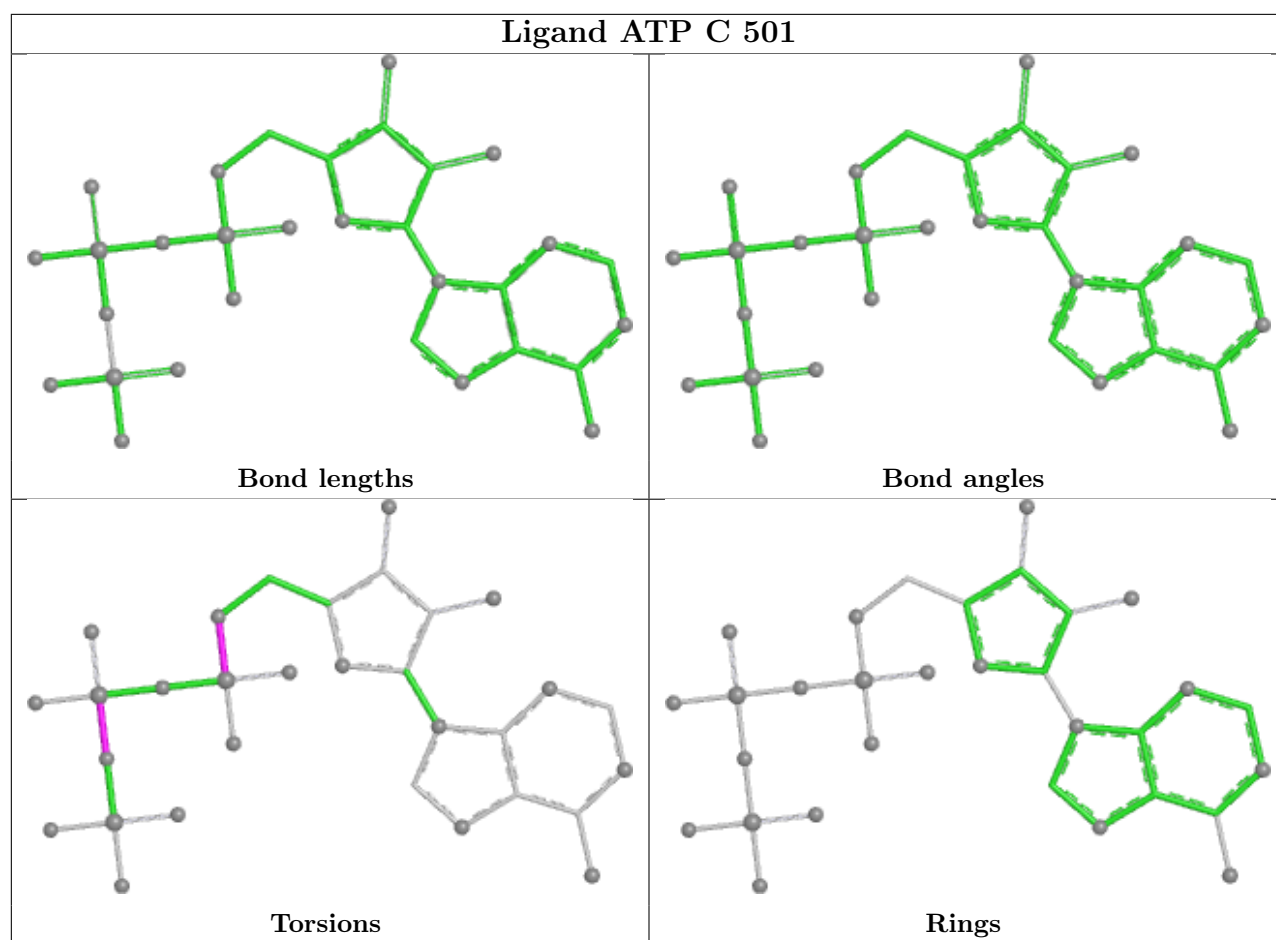
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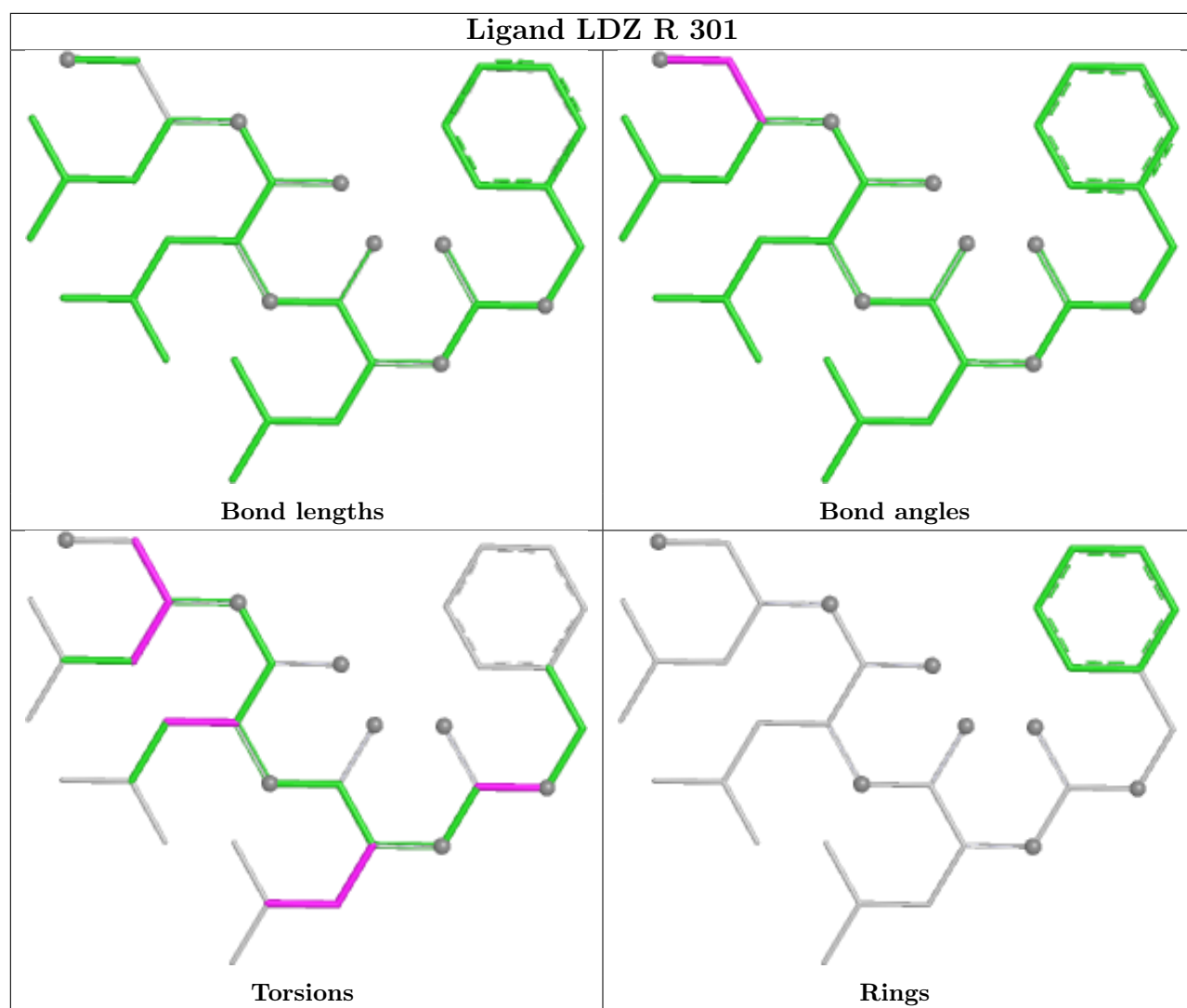
Mol	Chain	Res	Type	Clashes	Symm-Clashes
39	N	301	LDZ	1	0
39	o	301	LDZ	3	0
38	E	401	ADP	1	0
39	r	301	LDZ	4	0
38	D	501	ADP	2	0
39	O	301	LDZ	3	0

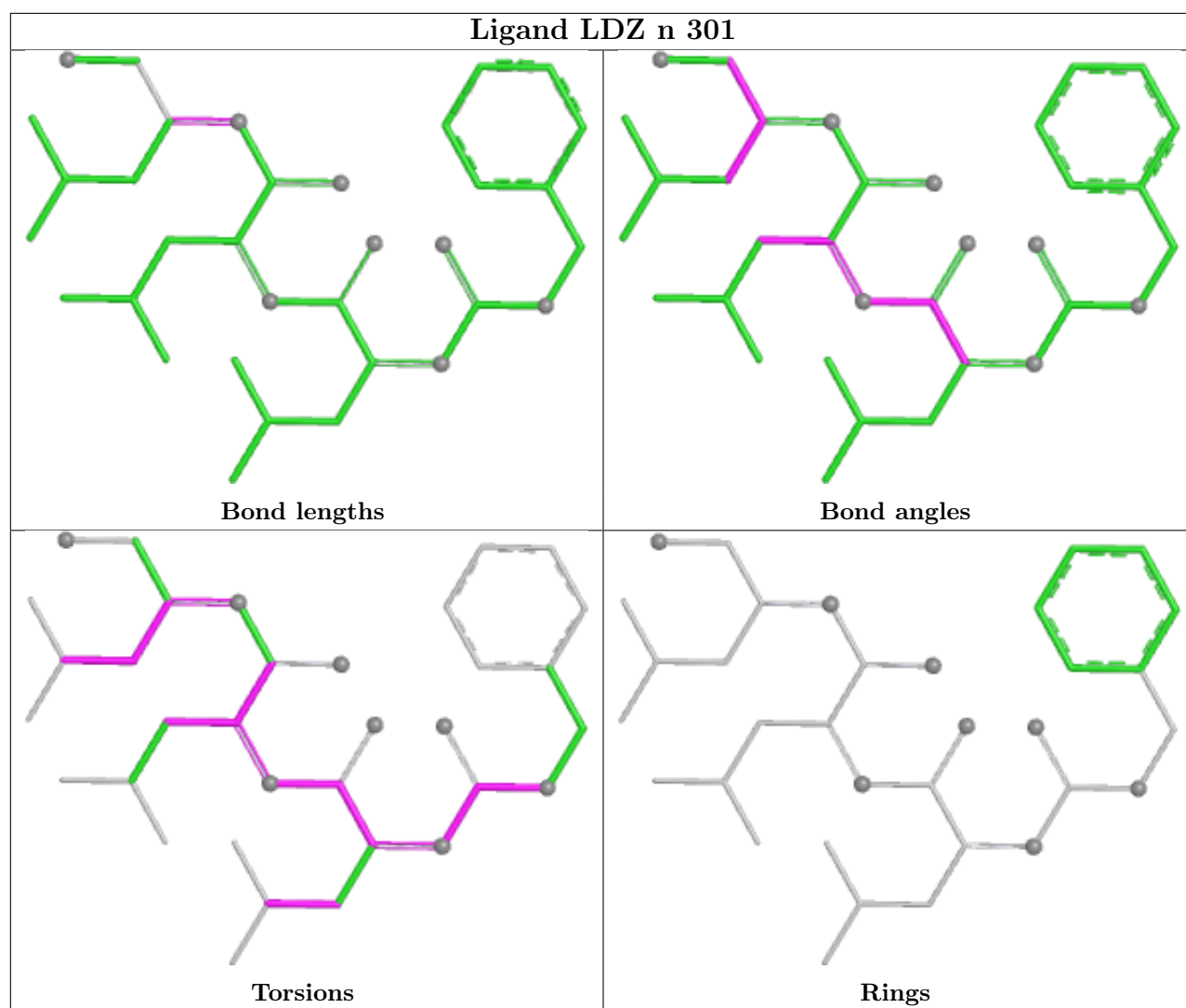
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

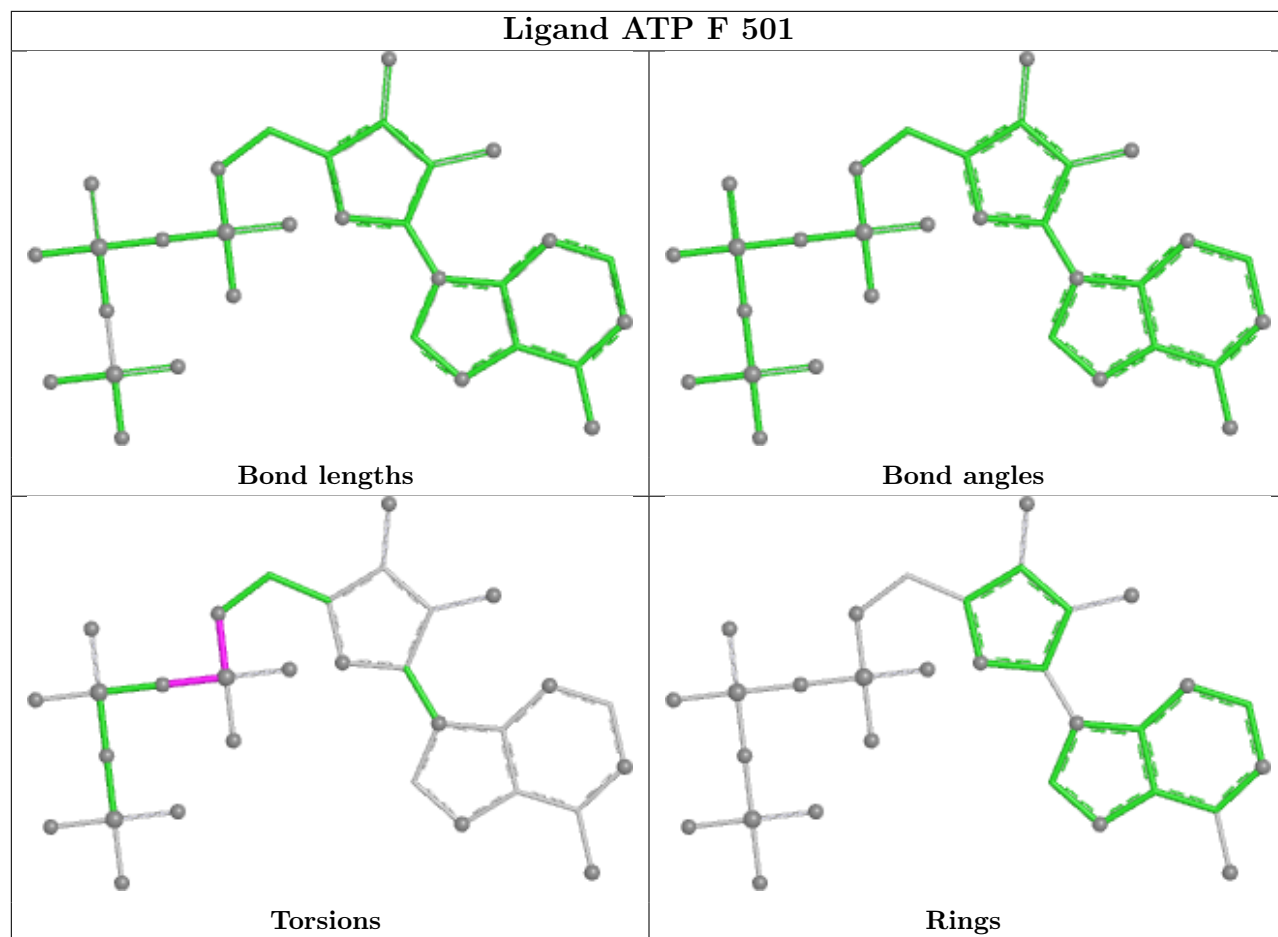


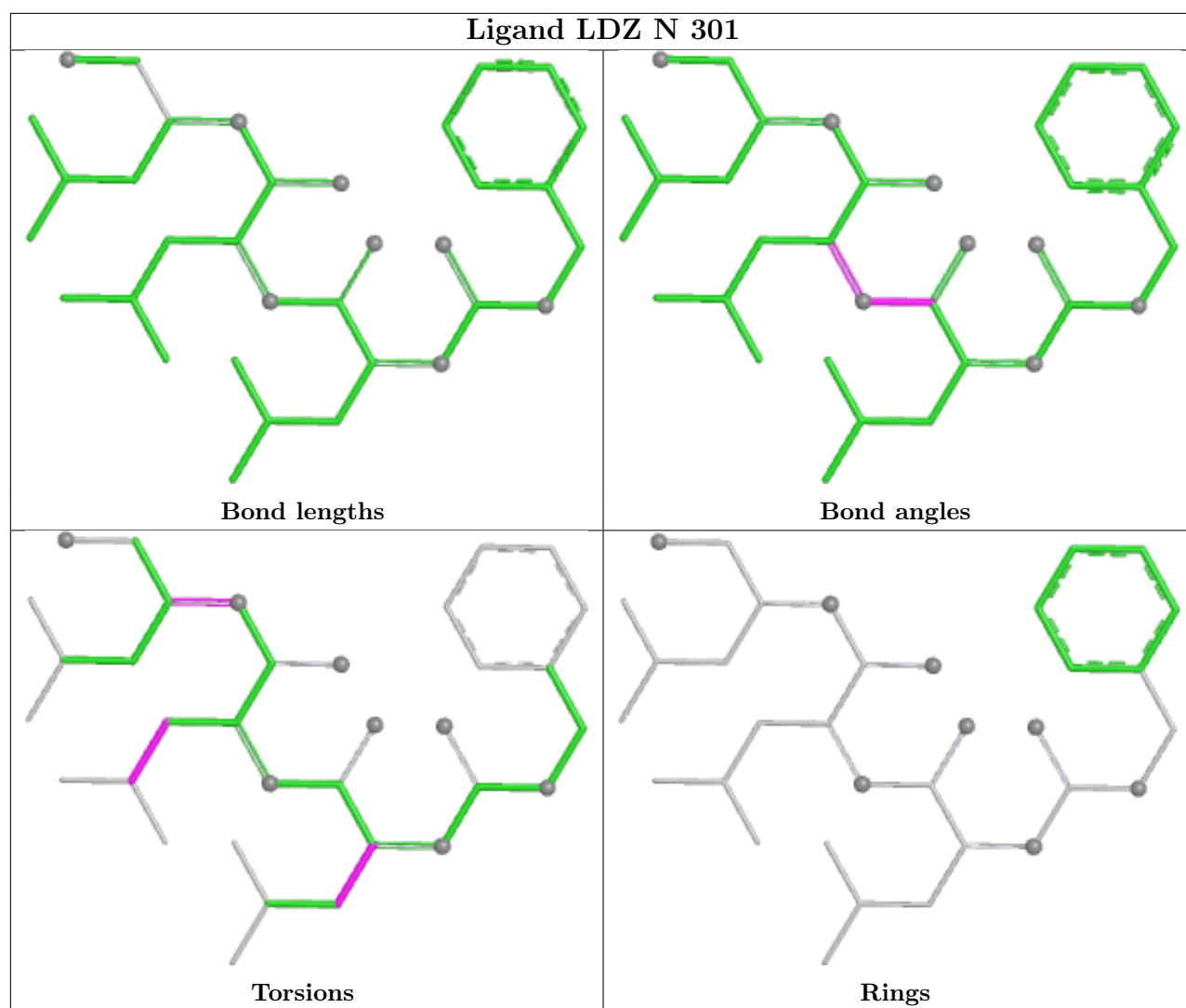


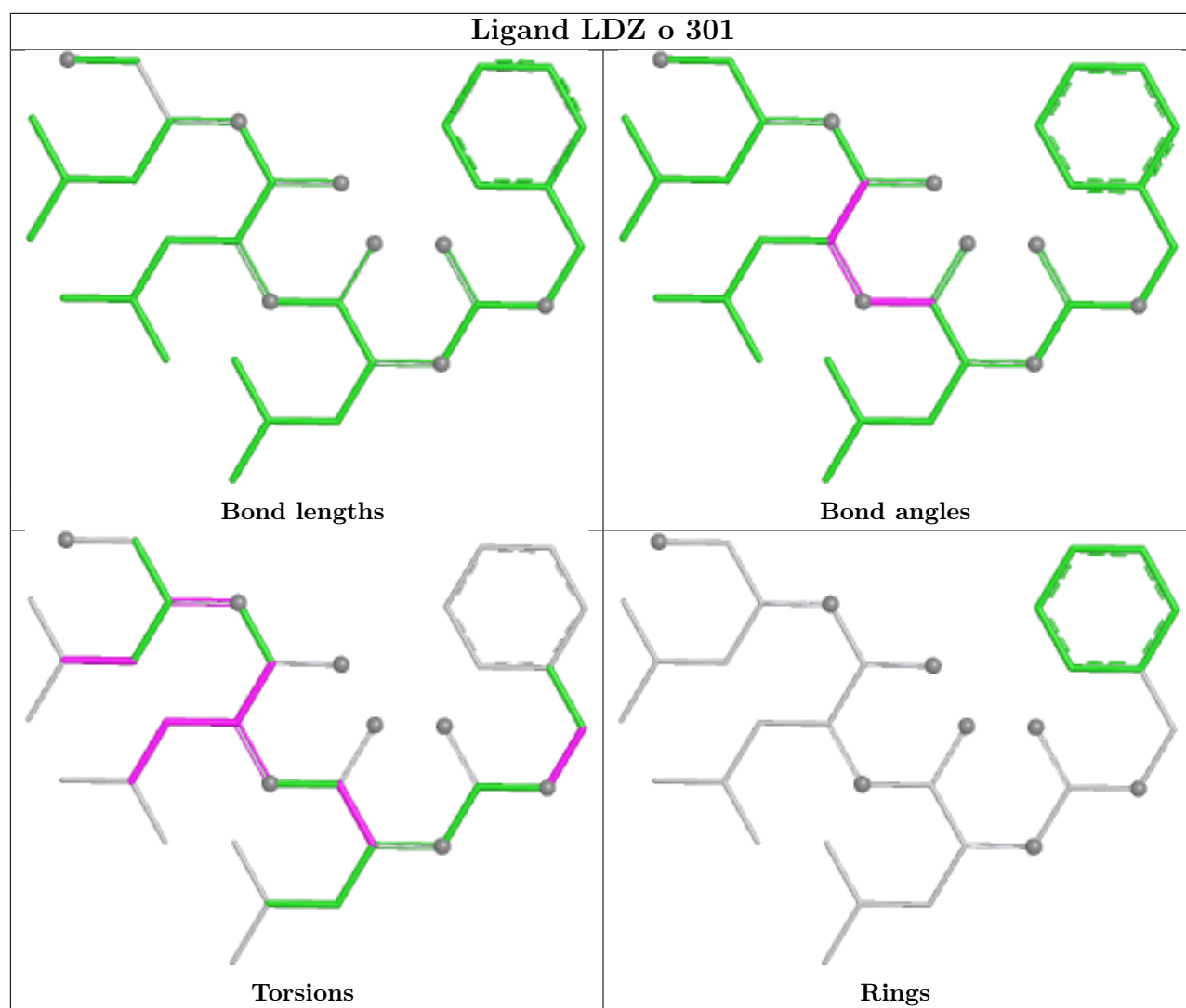


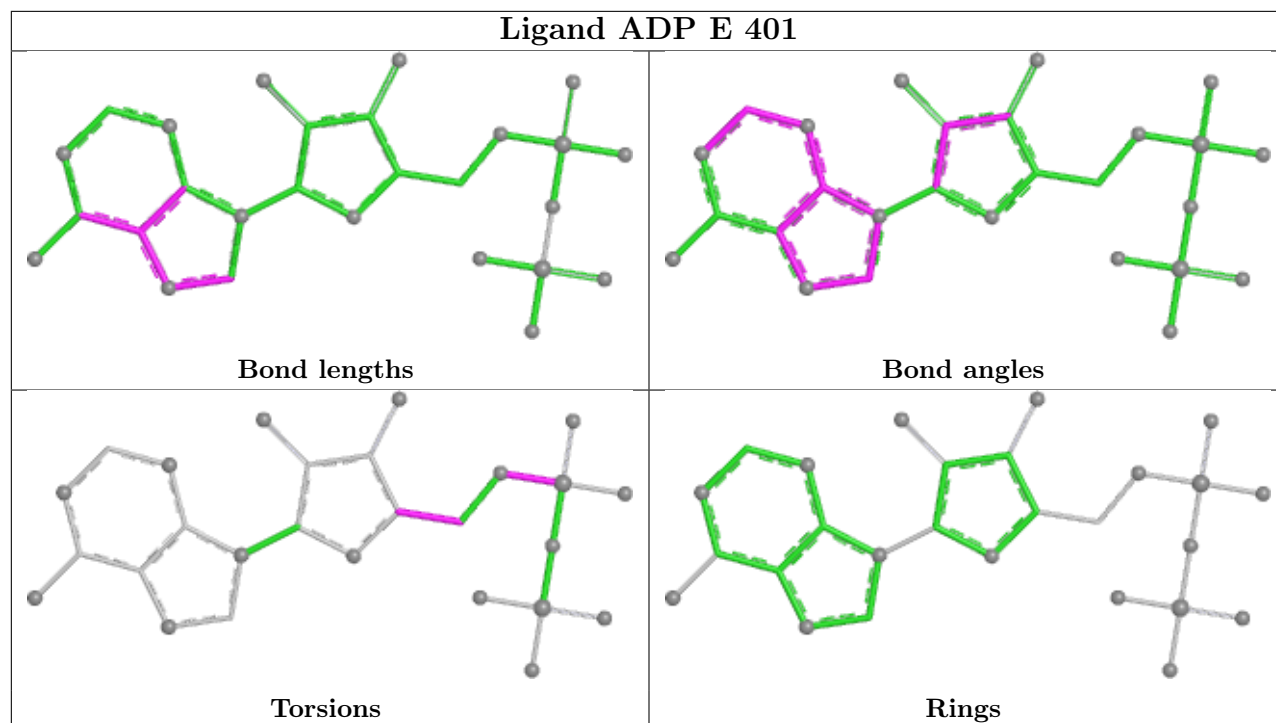


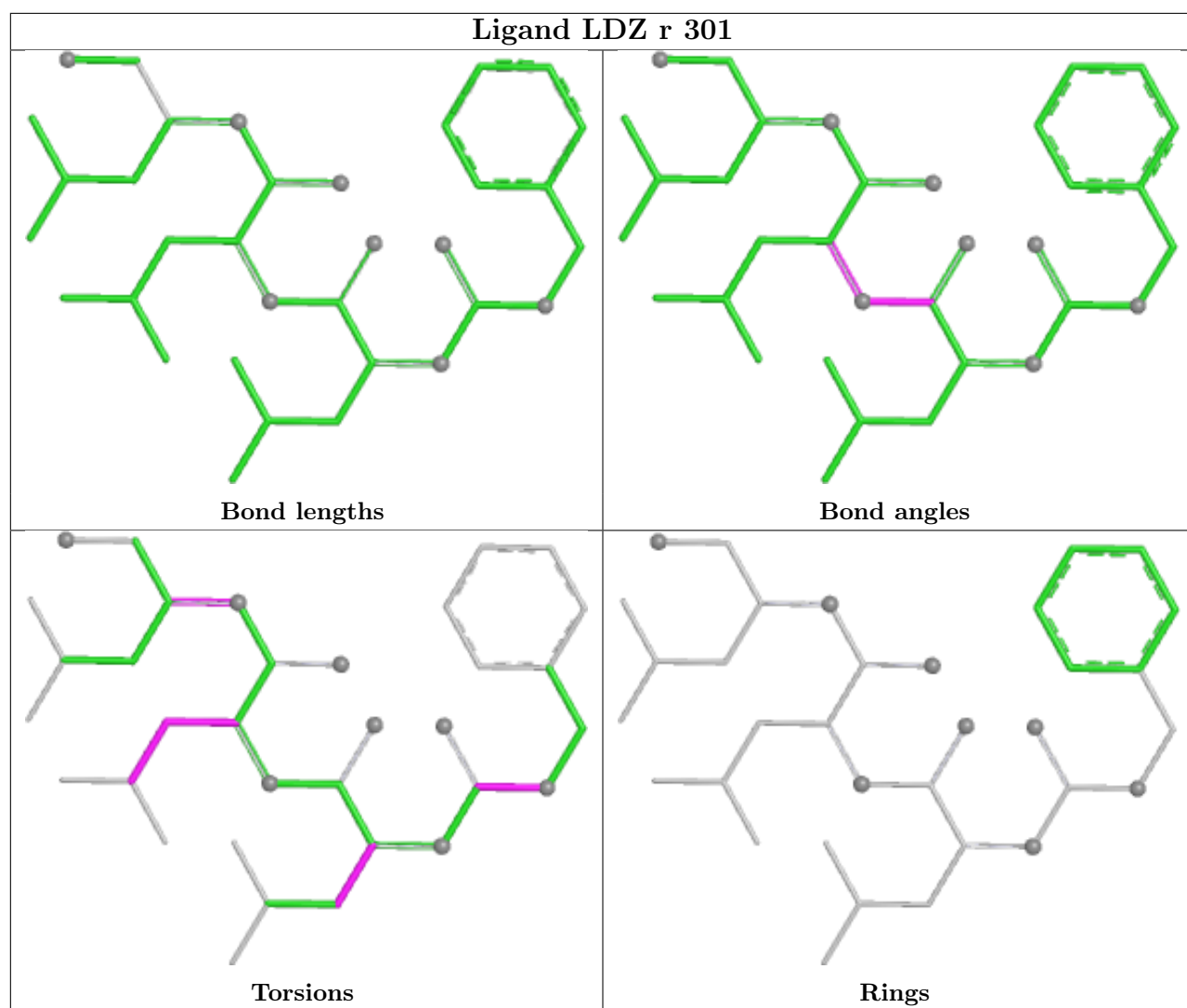


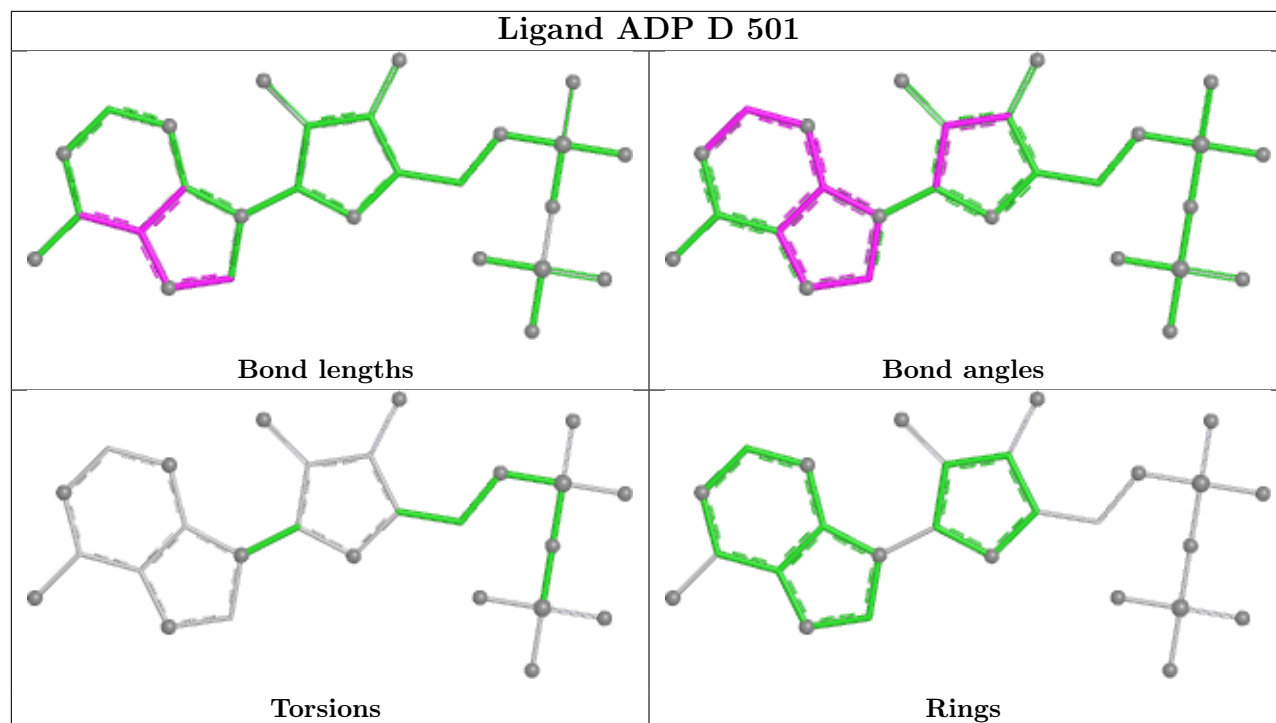


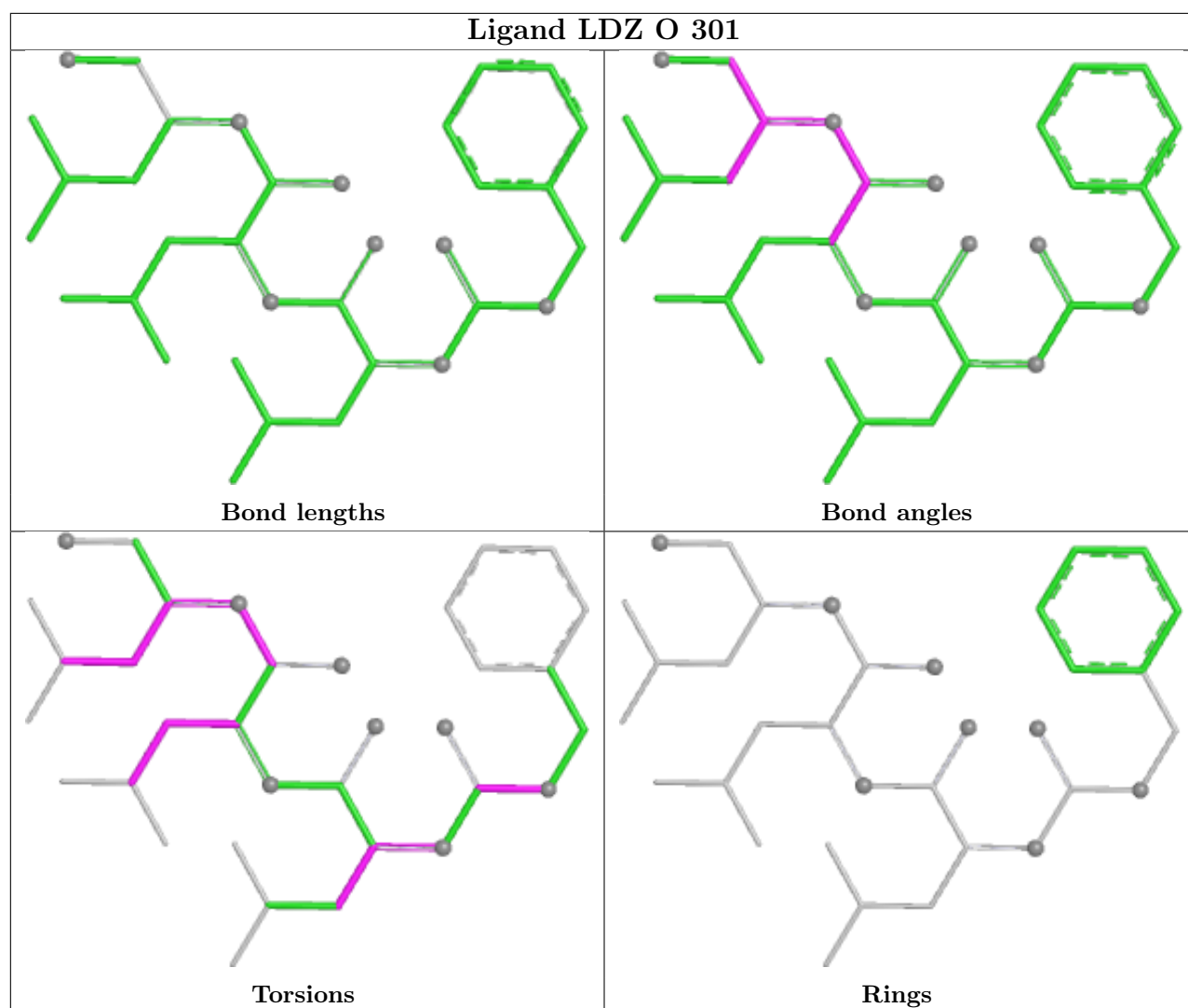












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

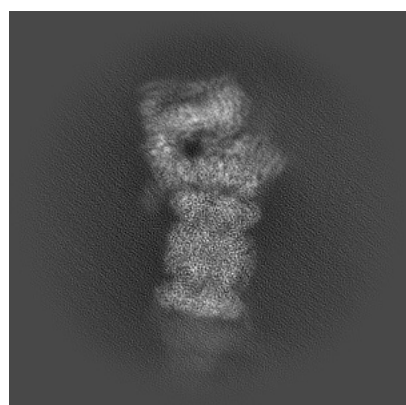
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-63776. These allow visual inspection of the internal detail of the map and identification of artifacts.

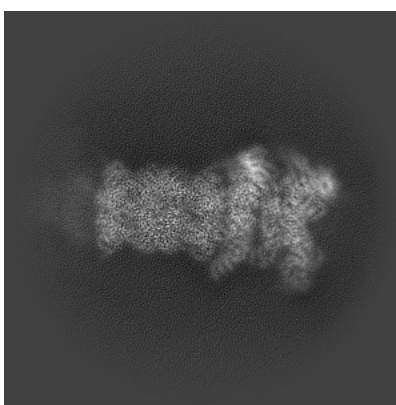
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

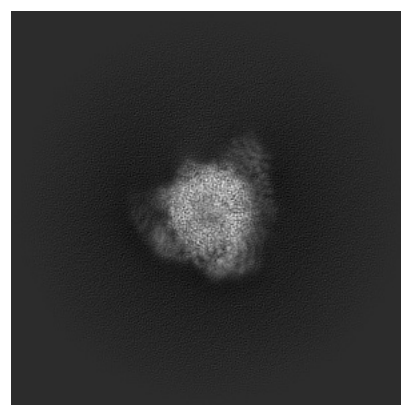
6.1.1 Primary map



X



Y

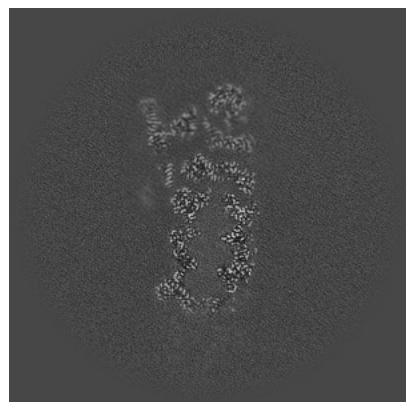


Z

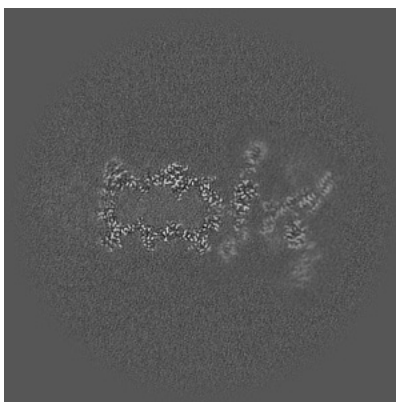
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

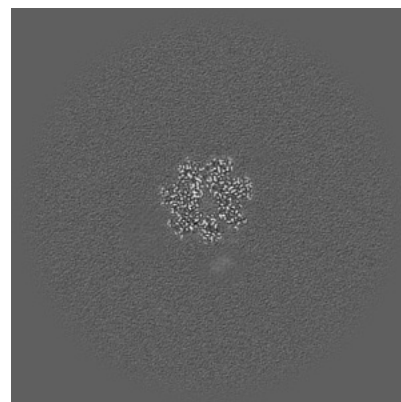
6.2.1 Primary map



X Index: 300



Y Index: 300

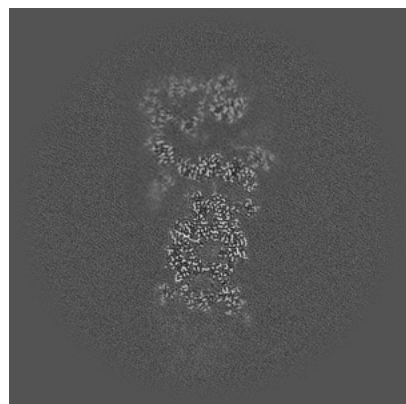


Z Index: 300

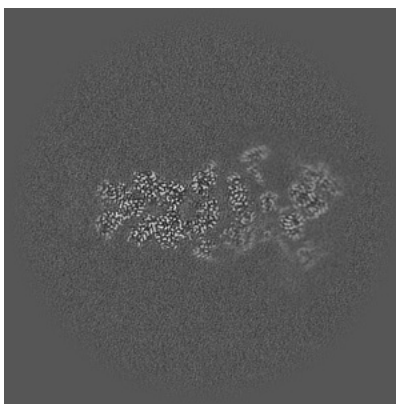
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

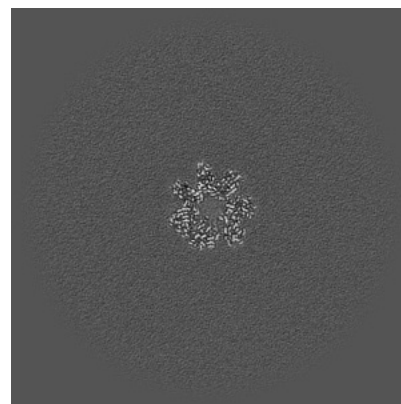
6.3.1 Primary map



X Index: 327



Y Index: 330

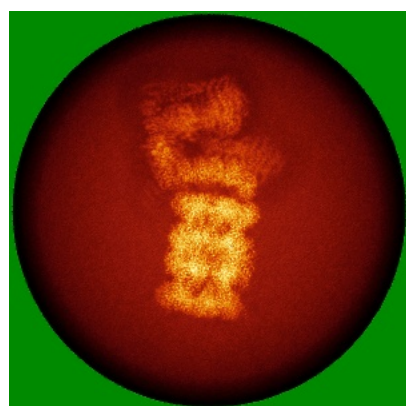


Z Index: 255

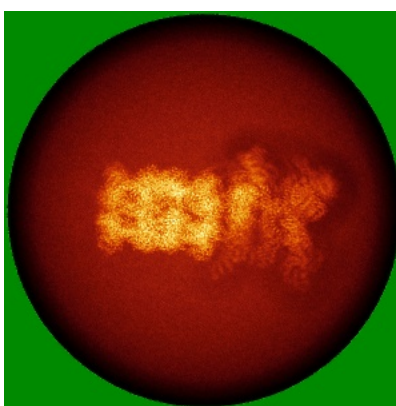
The images above show the largest variance slices of the map in three orthogonal directions.

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

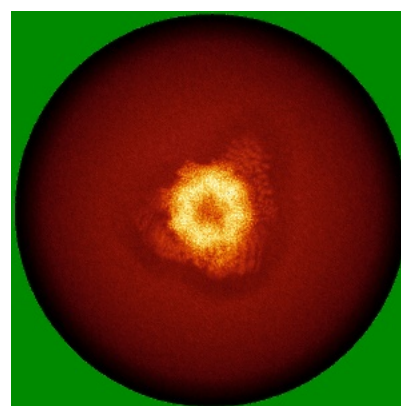
6.4.1 Primary map



X



Y

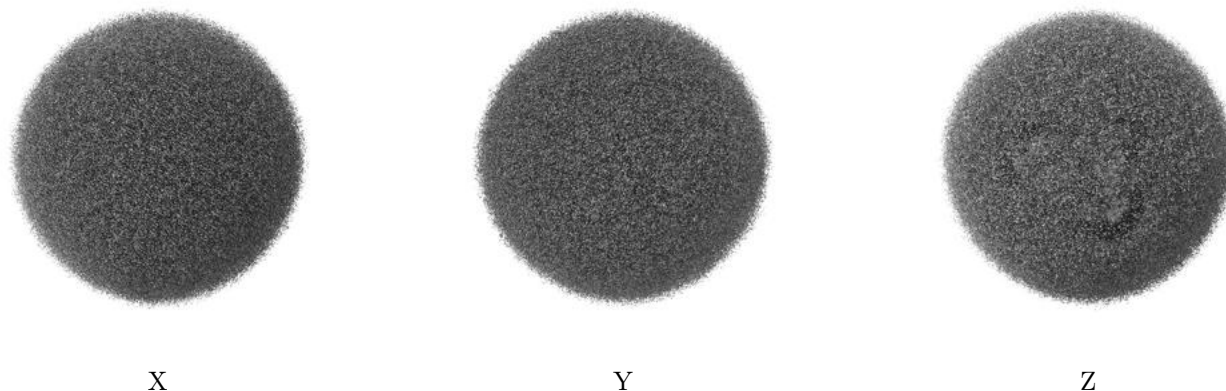


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

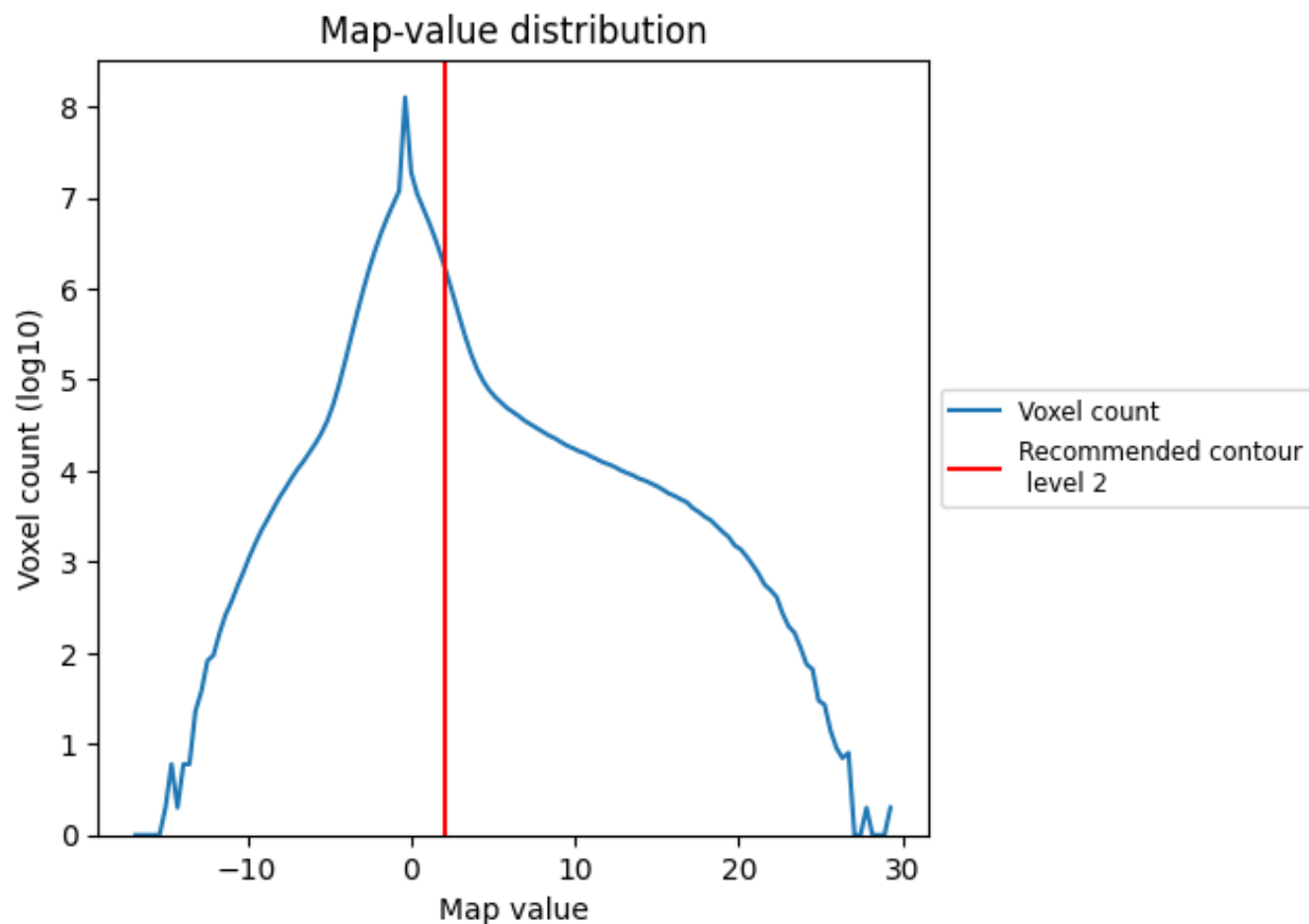
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

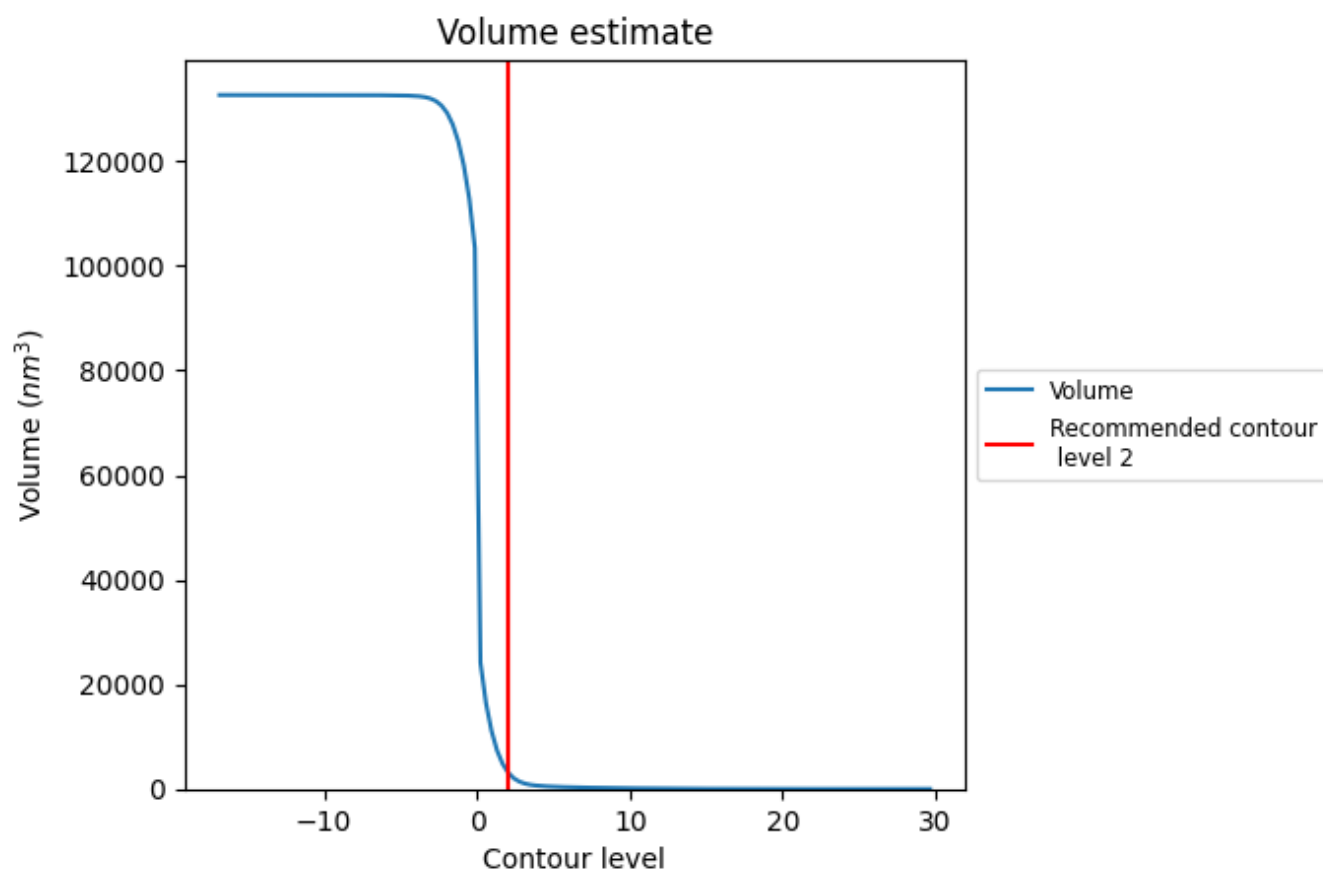
This section contains the results of statistical analysis of the map.

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.

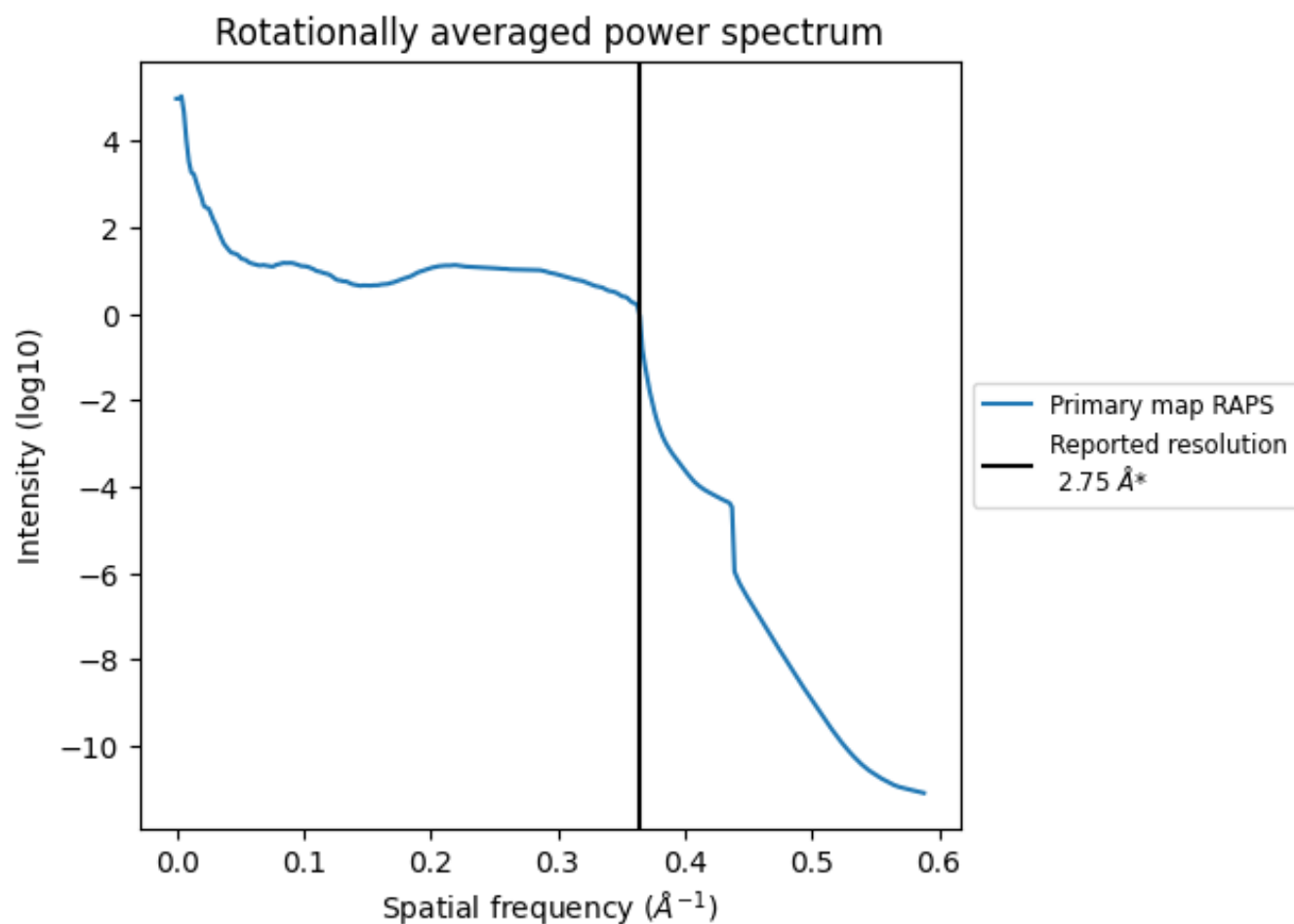
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3329 nm³; this corresponds to an approximate mass of 3007 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 0.364 Å⁻¹

8 Fourier-Shell correlation

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

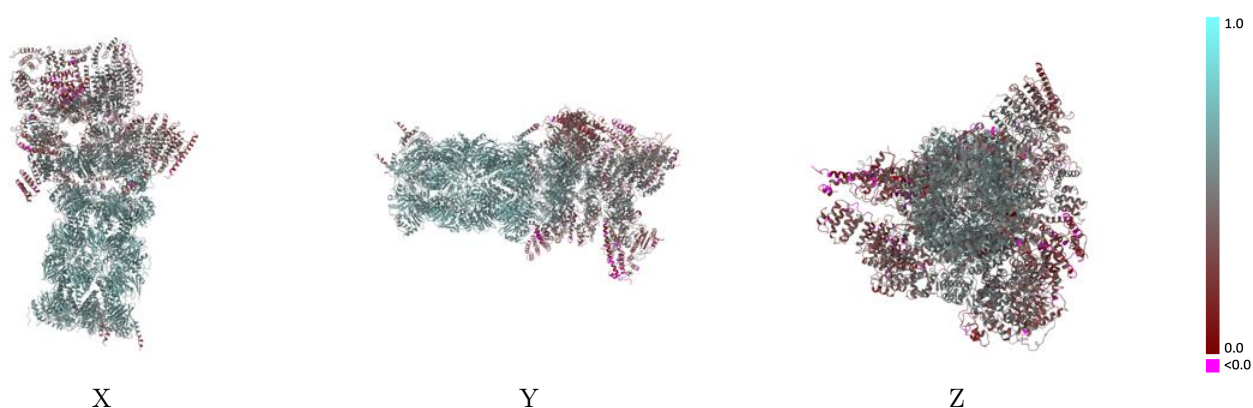
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63776 and PDB model 9MBP. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)

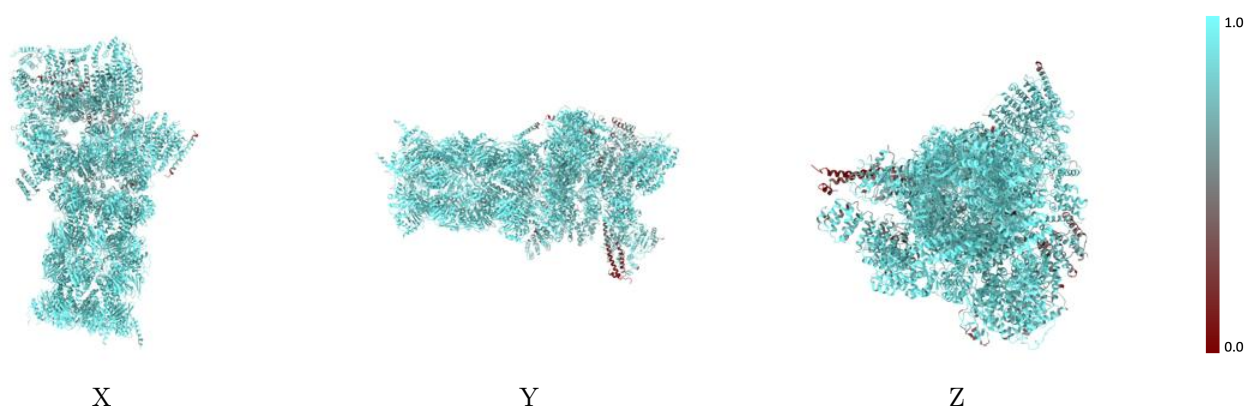
This section was not generated.

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



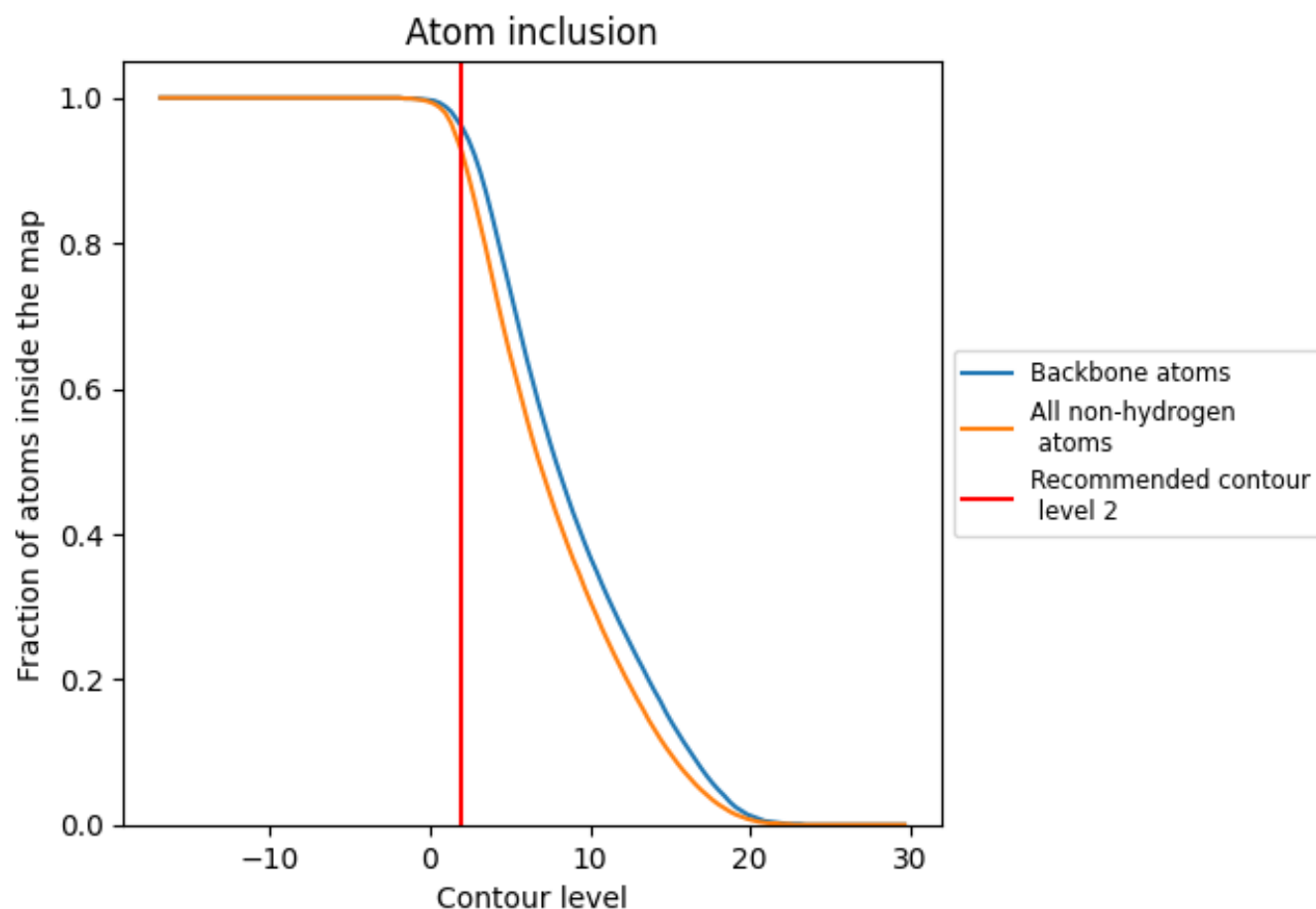
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.5020
A	 0.9250	 0.5040
B	 0.9260	 0.5200
C	 0.9450	 0.5380
D	 0.9410	 0.5300
E	 0.7980	 0.3780
F	 0.8250	 0.4170
G	 0.9790	 0.6080
H	 0.9840	 0.6210
I	 0.9740	 0.5930
J	 0.9470	 0.5760
K	 0.9840	 0.6210
L	 0.9910	 0.6320
M	 0.9820	 0.6150
N	 0.9890	 0.6380
O	 0.9850	 0.6250
P	 0.9910	 0.6320
Q	 0.9940	 0.6360
R	 0.9940	 0.6410
S	 0.9940	 0.6400
T	 0.9930	 0.6390
U	 0.9090	 0.4150
V	 0.7530	 0.2940
W	 0.8310	 0.3150
X	 0.9060	 0.4260
Y	 0.9000	 0.4040
Z	 0.9190	 0.4360
a	 0.8600	 0.3410
b	 0.7700	 0.2930
c	 0.8980	 0.4320
d	 0.8230	 0.3520
e	 0.7700	 0.2610
f	 0.5890	 0.1430
g	 0.9900	 0.6020
h	 0.9810	 0.6000



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Chain	Atom inclusion	Q-score
i	 0.9680	 0.5600
j	 0.9500	 0.5200
k	 0.9650	 0.5660
l	 0.9880	 0.5980
m	 0.9780	 0.5950
n	 0.9930	 0.6320
o	 0.9820	 0.6160
p	 0.9920	 0.6360
q	 0.9900	 0.6310
r	 0.9930	 0.6320
s	 0.9950	 0.6380
t	 0.9910	 0.6330
u	 0.9120	 0.3900
v	 0.9430	 0.5640