



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Aug 14, 2017 – 05:48 PM EDT

PDB ID : 5VHF
EMDB ID: : EMD-8674
Title : Conformational Landscape of the p28-Bound Human Proteasome Regulatory Particle
Authors : Lu, Y.; Wu, J.; Dong, Y.; Chen, S.; Sun, S.; Ma, Y.B.; Ouyang, Q.; Finley, D.; Kirschner, M.W.; Mao, Y.
Deposited on : unknown
Resolution : 5.70 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

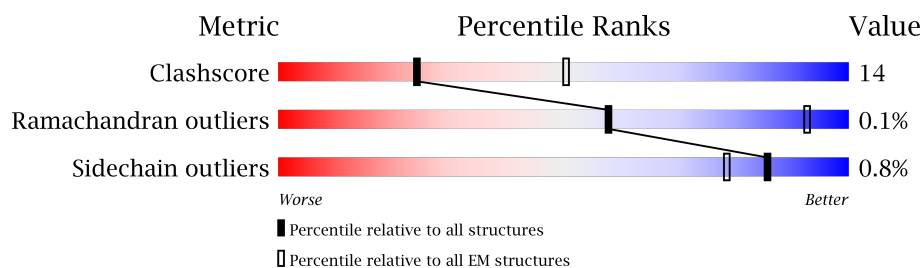
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.70 Å.

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







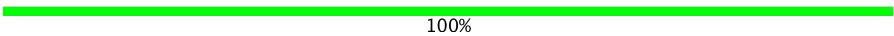
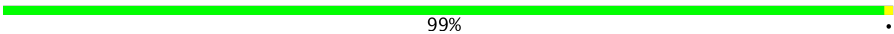
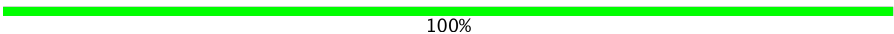

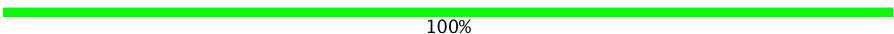

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	G	223	
2	A	352	
3	B	340	
4	C	385	
5	D	368	
6	E	379	
7	F	380	
8	U	841	
9	V	183	

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Mol	Chain	Length	Quality of chain
10	W	456	 73%26%
11	X	385	 82%18%
12	Y	378	 70%30%
13	Z	286	 75%25%
14	a	374	 100%
15	b	191	 99%.
16	c	287	 100%
17	d	136	 99%.
18	e	70	 100%
19	f	848	 79%.19%

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 51096 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 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	G	219	Total	C	N	O	S	0	0
			1662	1036	294	323	9		

- Molecule 2 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	341	Total	C	N	O	S	0	0
			2677	1690	473	497	17		

- Molecule 3 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	330	Total	C	N	O	S	0	0
			2579	1624	437	506	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	342	Total	C	N	O	S	0	0
			2709	1701	493	501	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	344	Total	C	N	O	S	0	0
			2751	1744	480	517	10		

- Molecule 6 is a protein called 26S proteasome regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	345	Total	C	N	O	S	0	0
			2736	1715	490	515	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	359	Total	C	N	O	S	0	0
			2808	1772	488	531	17		

- Molecule 8 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	U	751	Total	C	N	O	S	0	0
			5829	3696	1001	1088	44		

- Molecule 9 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	183	Total	C	N	O	S	0	0
			1480	949	260	265	6		

- Molecule 10 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	385	Total	C	N	O	S	0	0
			3048	1939	515	582	12		

- Molecule 12 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

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

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

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

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	a	374	Total	C	N	O	S	0	0
			3003	1915	511	562	15		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

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

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

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

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	d	136	Total	C	N	O	S	0	0
			1109	720	176	209	4		

- Molecule 18 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	e	70	Total	C	N	O	S	0	0
			583	357	89	135	2		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	f	686	Total	C	N	O	S	0	0
			5304	3335	901	1033	35		

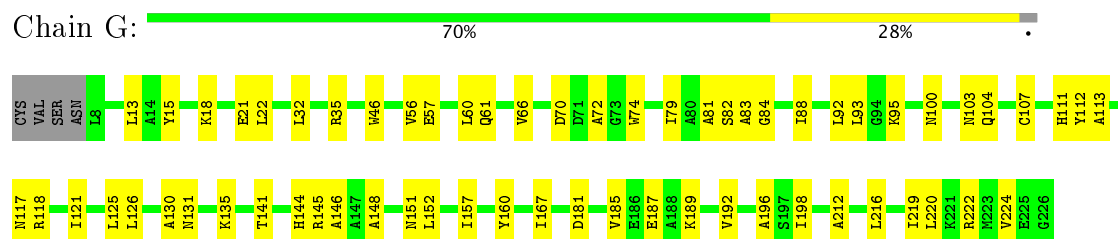
- Molecule 20 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

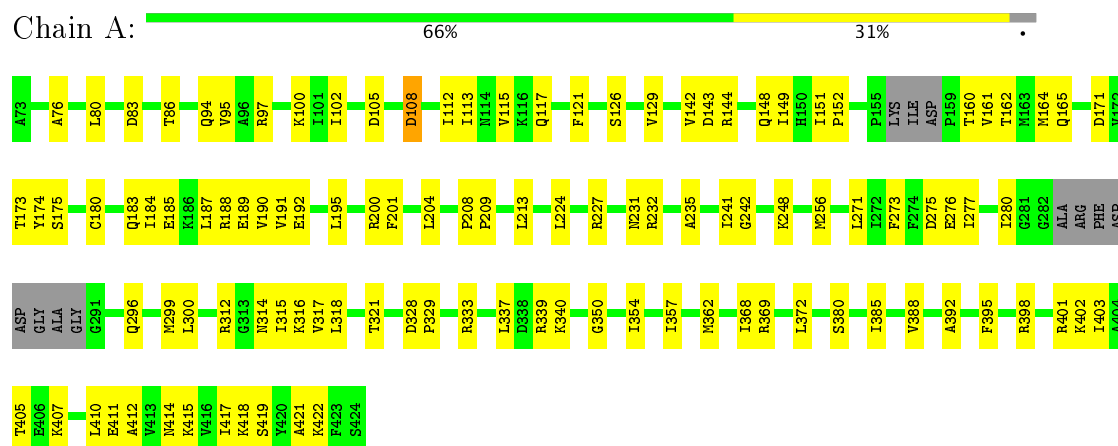
3 Residue-property plots

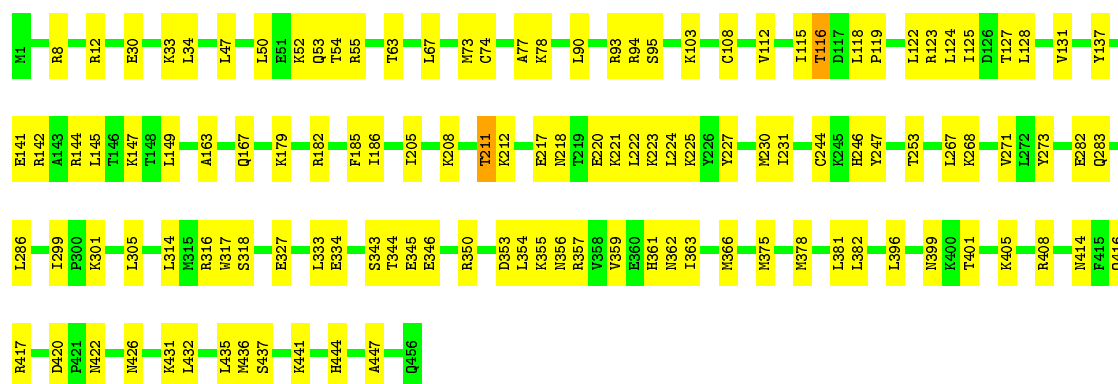
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

- Molecule 1: 26S proteasome non-ATPase regulatory subunit 10



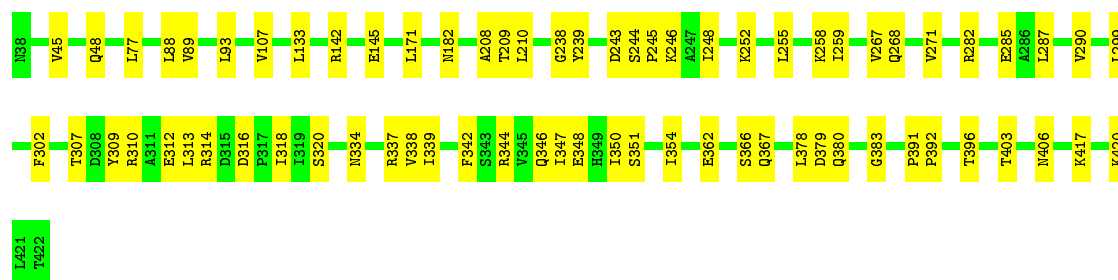
- Molecule 2: 26S proteasome regulatory subunit 7





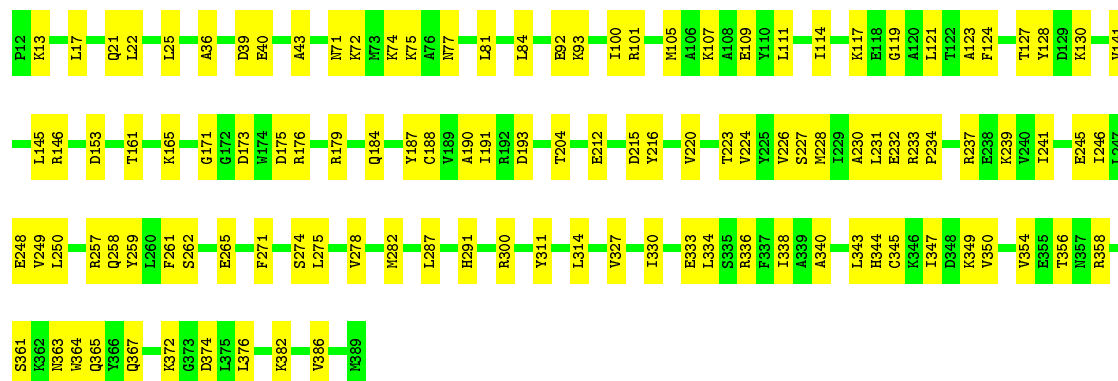
- Molecule 11: 26S proteasome non-ATPase regulatory subunit 11

Chain X: 82% 18%



- Molecule 12: 26S proteasome non-ATPase regulatory subunit 6

Chain Y: 70% 30%



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

Chain Z: 75% 25%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	39520	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	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

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 >2	RMSZ	# Z >2
1	G	0.23	0/1687	0.37	0/2279
10	W	0.23	0/3750	0.39	0/5039
11	X	0.23	0/3091	0.36	0/4165
12	Y	0.23	0/3173	0.37	0/4273
13	Z	0.23	0/2324	0.39	0/3150
14	a	0.23	0/3061	0.38	0/4144
15	b	0.23	0/1478	0.40	0/2001
16	c	0.23	0/2302	0.38	0/3110
17	d	0.24	0/1134	0.39	0/1534
18	e	0.23	0/596	0.40	0/805
19	f	0.24	0/5377	0.42	0/7248
2	A	0.23	0/2722	0.42	0/3673
3	B	0.23	0/2615	0.44	0/3530
4	C	0.23	0/2741	0.39	0/3681
5	D	0.24	0/2795	0.42	0/3773
6	E	0.32	2/2775 (0.1%)	0.47	3/3727 (0.1%)
7	F	0.24	0/2845	0.42	0/3832
8	U	0.23	0/5930	0.40	0/8021
9	V	0.24	0/1507	0.39	0/2029
All	All	0.24	2/51903 (0.0%)	0.40	3/70014 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	115	VAL	N-CA	8.47	1.63	1.46
6	E	115	VAL	CA-C	5.87	1.68	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	115	VAL	C-N-CA	-8.17	101.28	121.70
6	E	115	VAL	CA-C-N	7.58	133.87	117.20
6	E	115	VAL	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1662	0	1667	40	0
2	A	2677	0	2732	86	0
3	B	2579	0	2628	61	0
4	C	2709	0	2812	69	0
5	D	2751	0	2804	77	0
6	E	2736	0	2794	115	0
7	F	2808	0	2902	121	0
8	U	5829	0	5920	134	0
9	V	1480	0	1527	44	0
10	W	3703	0	3821	90	0
11	X	3048	0	3139	47	0
12	Y	3115	0	3120	79	0
13	Z	2281	0	2312	49	0
14	a	3003	0	3016	0	0
15	b	1458	0	1505	0	0
16	c	2260	0	2276	0	0
17	d	1109	0	1114	0	0
18	e	583	0	493	0	0
19	f	5304	0	5315	0	0
20	c	1	0	0	0	0
All	All	51096	0	51897	944	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (944) 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)
6:E:115:VAL:CG1	6:E:118:LEU:HB2	1.72	1.19
6:E:124:HIS:CD2	6:E:195:PHE:CE2	2.31	1.19
7:F:150:LEU:CB	7:F:166:THR:OG1	2.00	1.09
7:F:150:LEU:HB2	7:F:166:THR:OG1	1.52	1.08
6:E:124:HIS:CD2	6:E:195:PHE:CZ	2.43	1.05
7:F:167:GLU:HG2	7:F:173:LYS:CD	1.89	1.02
6:E:115:VAL:CG1	6:E:118:LEU:CB	2.36	1.02
8:U:339:LEU:O	8:U:343:ILE:HB	1.59	1.00
7:F:167:GLU:CB	7:F:173:LYS:HD3	1.91	1.00
4:C:278:ASN:O	4:C:282:GLY:HA3	1.62	0.97
4:C:361:GLY:O	4:C:365:GLU:HB2	1.65	0.97
7:F:167:GLU:OE1	7:F:168:TYR:N	1.98	0.96
8:U:338:HIS:O	8:U:342:LEU:HB2	1.66	0.96
7:F:74:LYS:O	7:F:78:GLU:HB2	1.65	0.95
6:E:216:ARG:O	6:E:220:ASN:HB2	1.66	0.95
12:Y:117:LYS:O	12:Y:121:LEU:HB2	1.69	0.91
6:E:124:HIS:HD2	6:E:195:PHE:CE2	1.90	0.90
5:D:177:VAL:O	5:D:181:VAL:HB	1.72	0.89
7:F:274:LEU:O	7:F:278:LYS:HB2	1.73	0.89
10:W:221:LYS:C	10:W:222:LEU:HD12	1.93	0.88
6:E:115:VAL:HG12	6:E:118:LEU:CB	2.02	0.87
3:B:198:LYS:O	3:B:202:GLU:HB2	1.74	0.87
9:V:473:GLN:O	9:V:477:HIS:HB2	1.75	0.86
12:Y:226:VAL:O	12:Y:230:ALA:HB3	1.77	0.85
7:F:168:TYR:CD1	7:F:169:ASP:N	2.45	0.85
4:C:277:LEU:O	4:C:281:ASP:HB3	1.75	0.85
12:Y:336:ARG:O	12:Y:340:ALA:HB3	1.77	0.85
6:E:115:VAL:HG13	6:E:118:LEU:CB	2.07	0.83
10:W:108:CYS:O	10:W:112:VAL:HB	1.79	0.82
10:W:350:ARG:O	10:W:354:LEU:HB2	1.81	0.81
6:E:182:LEU:O	6:E:186:ALA:HB2	1.81	0.81
6:E:188:ALA:HA	6:E:192:ASP:HB2	1.64	0.80
12:Y:17:LEU:O	12:Y:21:GLN:HB2	1.81	0.80
6:E:114:GLU:OE2	6:E:119:VAL:HG22	1.83	0.78
7:F:169:ASP:OD1	7:F:171:ARG:HG2	1.83	0.78
7:F:168:TYR:CE1	7:F:169:ASP:HB2	2.19	0.78
7:F:168:TYR:HD1	7:F:169:ASP:N	1.80	0.78
6:E:115:VAL:HG13	6:E:118:LEU:HB2	1.62	0.78
12:Y:124:PHE:O	12:Y:128:TYR:HB2	1.84	0.78
8:U:614:VAL:O	8:U:618:ALA:HB2	1.84	0.77
7:F:167:GLU:CG	7:F:173:LYS:HD3	2.13	0.77
7:F:150:LEU:HB3	7:F:166:THR:OG1	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:282:GLU:O	10:W:286:LEU:HB2	1.85	0.75
4:C:32:GLN:O	4:C:36:ASN:HB2	1.85	0.75
6:E:114:GLU:HG2	6:E:115:VAL:H	1.52	0.75
7:F:167:GLU:CG	7:F:173:LYS:CD	2.65	0.75
6:E:124:HIS:HD2	6:E:195:PHE:CZ	1.97	0.74
5:D:174:LYS:O	5:D:178:ARG:HB2	1.87	0.74
6:E:339:ASN:HB2	6:E:342:ASP:HB2	1.68	0.74
1:G:79:ILE:O	1:G:83:ALA:HB2	1.86	0.74
7:F:167:GLU:HG2	7:F:173:LYS:HD3	1.68	0.73
6:E:115:VAL:CG1	6:E:118:LEU:HB3	2.18	0.73
9:V:328:VAL:O	9:V:332:LEU:HB2	1.89	0.73
1:G:152:LEU:HD23	1:G:187:GLU:HG2	1.73	0.71
6:E:115:VAL:HG12	6:E:118:LEU:HB2	1.64	0.71
3:B:235:LEU:O	3:B:239:VAL:HB	1.90	0.71
13:Z:164:ALA:HB3	13:Z:169:GLU:HG3	1.73	0.71
10:W:405:LYS:HB3	10:W:414:ASN:HB2	1.71	0.71
7:F:167:GLU:HG2	7:F:173:LYS:CE	2.20	0.70
7:F:251:LEU:HB3	7:F:285:ILE:HG22	1.73	0.70
10:W:125:ILE:HD12	10:W:128:LEU:HD21	1.73	0.70
8:U:340:GLN:HE21	8:U:344:ARG:HH12	1.37	0.70
7:F:167:GLU:HB3	7:F:173:LYS:HD3	1.73	0.70
8:U:799:LYS:HB3	8:U:801:GLN:HE22	1.55	0.70
10:W:115:ILE:HG12	10:W:116:THR:HG22	1.73	0.70
6:E:115:VAL:HG12	6:E:118:LEU:HB3	1.73	0.69
10:W:8:ARG:O	10:W:12:ARG:HB2	1.92	0.69
8:U:436:ALA:HB1	8:U:472:ILE:HD13	1.74	0.69
12:Y:361:SER:O	12:Y:365:GLN:HB2	1.92	0.69
7:F:173:LYS:HB3	7:F:173:LYS:NZ	2.08	0.68
9:V:484:LEU:O	9:V:488:ASN:HB2	1.94	0.68
10:W:316:ARG:HG3	10:W:318:SER:H	1.58	0.68
8:U:506:ALA:HB1	8:U:543:LYS:HB2	1.73	0.68
5:D:289:LEU:O	5:D:293:LEU:HB2	1.93	0.68
1:G:103:ASN:HD21	1:G:107:CYS:HB2	1.59	0.68
6:E:213:ARG:O	6:E:217:GLU:HB2	1.94	0.67
4:C:201:ARG:O	4:C:205:HIS:HB2	1.94	0.67
5:D:179:GLU:HA	5:D:183:LEU:HD13	1.76	0.67
6:E:233:ASP:HA	6:E:278:ALA:HB3	1.77	0.67
2:A:224:LEU:HB3	2:A:227:ARG:HH11	1.58	0.67
5:D:337:ASP:HB3	5:D:340:GLN:HB2	1.76	0.67
5:D:85:ILE:HG21	6:E:68:LYS:HD2	1.75	0.67
6:E:204:VAL:HG21	7:F:308:ARG:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:184:GLN:O	12:Y:188:CYS:HB2	1.95	0.67
10:W:408:ARG:H	11:X:344:ARG:HE	1.43	0.66
12:Y:237:ARG:HA	12:Y:241:ILE:HB	1.77	0.66
6:E:204:VAL:HG11	7:F:308:ARG:HB2	1.76	0.66
2:A:76:ALA:O	2:A:80:LEU:HB2	1.96	0.66
13:Z:192:THR:O	13:Z:196:HIS:HB3	1.95	0.66
13:Z:202:ASN:O	13:Z:206:LEU:HB2	1.95	0.66
6:E:216:ARG:O	6:E:220:ASN:CB	2.43	0.65
7:F:167:GLU:HG2	7:F:173:LYS:HD2	1.75	0.65
8:U:223:LEU:HD12	8:U:225:ASP:H	1.60	0.65
3:B:403:GLY:O	3:B:407:LEU:HB2	1.96	0.65
4:C:34:ILE:HG22	4:C:38:LYS:HE2	1.77	0.65
8:U:418:GLU:O	8:U:422:LEU:HB2	1.97	0.65
9:V:384:GLU:O	9:V:388:ALA:CB	2.44	0.65
8:U:708:GLN:HA	8:U:711:GLN:HG2	1.78	0.65
7:F:150:LEU:CD2	7:F:166:THR:OG1	2.45	0.65
7:F:167:GLU:CD	7:F:168:TYR:H	2.00	0.65
2:A:102:ILE:HG22	2:A:113:ILE:HG12	1.79	0.65
7:F:291:ILE:HB	7:F:306:VAL:HG11	1.78	0.65
10:W:222:LEU:O	10:W:225:LYS:N	2.31	0.64
2:A:417:ILE:O	2:A:421:ALA:HB2	1.97	0.64
3:B:168:ASP:OD2	3:B:171:VAL:N	2.26	0.64
5:D:191:TYR:HB3	5:D:196:ILE:HD13	1.79	0.64
12:Y:261:PHE:O	12:Y:265:GLU:HB2	1.96	0.64
4:C:97:VAL:HG11	4:C:121:TYR:HB3	1.80	0.64
6:E:168:LYS:HD2	6:E:270:LEU:HB2	1.79	0.64
6:E:366:ASP:O	6:E:370:ALA:HB3	1.96	0.64
7:F:167:GLU:HG2	7:F:173:LYS:HE3	1.79	0.64
9:V:383:GLY:O	9:V:387:GLN:NE2	2.31	0.64
8:U:212:ASP:OD2	8:U:215:ASN:ND2	2.31	0.64
11:X:310:ARG:HA	11:X:313:LEU:HB2	1.80	0.64
6:E:115:VAL:HG11	6:E:118:LEU:HB2	1.75	0.64
1:G:57:GLU:O	1:G:61:GLN:HB2	1.98	0.64
10:W:220:GLU:HB3	10:W:223:LYS:HD2	1.80	0.64
13:Z:12:HIS:ND1	13:Z:50:VAL:O	2.30	0.64
3:B:231:GLY:O	3:B:235:LEU:HB3	1.97	0.64
10:W:299:ILE:HG22	10:W:301:LYS:H	1.62	0.64
3:B:115:ILE:HD11	3:B:144:LEU:HD23	1.79	0.63
7:F:170:SER:HA	7:F:173:LYS:NZ	2.13	0.63
7:F:181:PRO:HG2	7:F:242:ALA:HB2	1.79	0.63
8:U:842:LYS:O	8:U:880:ASN:N	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:789:ILE:HD12	8:U:911:ILE:HG12	1.80	0.63
4:C:66:LEU:HD23	5:D:136:SER:HB3	1.80	0.63
10:W:220:GLU:HB3	10:W:223:LYS:CD	2.29	0.63
7:F:357:PRO:O	7:F:362:ARG:NH1	2.30	0.63
10:W:417:ARG:NH2	10:W:420:ASP:OD2	2.31	0.63
9:V:377:GLN:O	9:V:381:GLN:HB2	1.98	0.63
4:C:158:ILE:HA	4:C:161:ILE:HG22	1.81	0.63
8:U:493:VAL:O	8:U:497:LEU:HB2	1.99	0.63
2:A:312:ARG:HG2	2:A:315:ILE:HG23	1.81	0.63
12:Y:361:SER:O	12:Y:365:GLN:CB	2.46	0.62
8:U:415:HIS:HD2	8:U:935:ILE:HG23	1.62	0.62
4:C:38:LYS:O	4:C:42:LEU:HB2	1.99	0.62
1:G:82:SER:HB2	1:G:112:TYR:HB3	1.82	0.62
7:F:166:THR:HG22	7:F:167:GLU:N	2.15	0.62
3:B:248:LEU:HD23	3:B:282:VAL:HG22	1.81	0.62
8:U:342:LEU:HD23	8:U:345:ASN:HD21	1.64	0.62
6:E:204:VAL:O	7:F:304:ARG:NH1	2.33	0.62
10:W:408:ARG:O	11:X:346:GLN:NE2	2.32	0.62
11:X:406:ASN:HD22	13:Z:265:LEU:HD23	1.64	0.62
5:D:103:VAL:HG11	5:D:132:LEU:HD11	1.82	0.62
8:U:155:LEU:O	8:U:158:ARG:NH1	2.32	0.62
2:A:115:VAL:HG13	2:A:117:GLN:H	1.65	0.61
4:C:301:LEU:O	4:C:305:LEU:HB2	1.99	0.61
6:E:50:LEU:HG	7:F:137:ILE:HD12	1.81	0.61
9:V:410:ILE:HD12	9:V:422:ILE:HD11	1.81	0.61
11:X:182:ASN:ND2	12:Y:248:GLU:OE2	2.33	0.61
9:V:468:SER:HA	12:Y:363:ASN:HD22	1.65	0.61
2:A:213:LEU:HB3	2:A:340:LYS:HA	1.81	0.61
3:B:125:THR:HG22	3:B:129:SER:H	1.66	0.61
6:E:265:ASP:HB2	6:E:294:ARG:HH21	1.65	0.61
2:A:180:CYS:HB3	2:A:183:GLN:HB2	1.82	0.61
6:E:114:GLU:HG2	6:E:115:VAL:N	2.15	0.61
2:A:329:PRO:O	2:A:333:ARG:HB3	2.01	0.61
1:G:72:ALA:HB1	1:G:104:GLN:HB2	1.83	0.61
1:G:60:LEU:HD22	1:G:95:LYS:HG3	1.81	0.61
10:W:222:LEU:HD12	10:W:222:LEU:N	2.16	0.61
11:X:310:ARG:O	11:X:314:ARG:HB2	1.99	0.61
12:Y:124:PHE:O	12:Y:128:TYR:CB	2.48	0.61
3:B:398:ILE:HA	3:B:401:GLU:HG2	1.81	0.61
2:A:414:ASN:O	2:A:418:LYS:HB2	2.00	0.61
10:W:224:LEU:HD22	10:W:253:THR:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:333:LEU:HD12	10:W:334:GLU:HG2	1.82	0.61
2:A:398:ARG:HA	3:B:199:GLU:HG2	1.82	0.61
4:C:11:LEU:O	8:U:140:ARG:NH1	2.34	0.61
10:W:179:LYS:O	10:W:218:ASN:ND2	2.34	0.61
11:X:362:GLU:OE2	11:X:380:GLN:NE2	2.33	0.61
12:Y:278:VAL:O	12:Y:282:MET:HB2	2.01	0.61
9:V:350:GLN:HE21	9:V:353:LEU:HD13	1.65	0.61
10:W:222:LEU:HD23	10:W:225:LYS:HD2	1.82	0.61
3:B:231:GLY:O	3:B:235:LEU:CB	2.49	0.60
8:U:127:ASP:OD2	8:U:129:ARG:NH1	2.34	0.60
7:F:266:LYS:O	7:F:270:ASP:HB2	2.02	0.60
5:D:181:VAL:O	5:D:306:LYS:NZ	2.33	0.60
11:X:171:LEU:HD13	11:X:210:LEU:HD23	1.83	0.60
10:W:408:ARG:HB2	11:X:344:ARG:HG2	1.83	0.60
4:C:154:LEU:N	4:C:327:ASP:OD2	2.35	0.60
6:E:235:ILE:HG22	6:E:279:THR:HB	1.84	0.60
3:B:313:LEU:HD22	3:B:341:LEU:HD23	1.83	0.60
4:C:200:ALA:O	4:C:204:ALA:HB3	2.02	0.60
7:F:141:ASP:HB3	7:F:144:LYS:HB2	1.83	0.60
11:X:307:THR:HA	11:X:310:ARG:HE	1.66	0.60
8:U:457:ILE:HG22	8:U:460:TYR:HB3	1.84	0.59
3:B:190:LEU:HB2	3:B:193:GLN:HB3	1.84	0.59
10:W:205:ILE:O	10:W:208:LYS:N	2.35	0.59
10:W:422:ASN:OD1	10:W:426:ASN:ND2	2.34	0.59
1:G:81:ALA:HB1	1:G:113:ALA:HB2	1.83	0.59
4:C:43:ARG:HB2	8:U:639:LEU:HD11	1.84	0.59
7:F:167:GLU:HB2	7:F:173:LYS:HD3	1.78	0.59
11:X:309:TYR:O	11:X:312:GLU:N	2.35	0.59
5:D:244:PRO:HD3	5:D:288:ILE:HD13	1.85	0.59
6:E:180:LYS:NZ	6:E:279:THR:O	2.35	0.59
7:F:150:LEU:HD22	7:F:166:THR:OG1	2.03	0.59
7:F:168:TYR:HD1	7:F:169:ASP:H	1.46	0.59
10:W:408:ARG:NH1	11:X:383:GLY:O	2.36	0.59
4:C:71:SER:HB2	4:C:117:ARG:HA	1.85	0.59
5:D:173:GLN:NE2	5:D:204:MET:SD	2.75	0.59
10:W:8:ARG:O	10:W:12:ARG:CB	2.51	0.59
6:E:37:THR:HG21	7:F:66:LEU:HD22	1.83	0.59
4:C:362:VAL:O	4:C:366:ALA:HB2	2.03	0.58
8:U:792:ASN:HB3	8:U:914:LEU:HB3	1.84	0.58
11:X:252:LYS:HG3	11:X:287:LEU:HD11	1.84	0.58
8:U:421:GLN:O	8:U:425:THR:OG1	2.20	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:238:ARG:HH11	7:F:250:LYS:HD2	1.68	0.58
4:C:371:LEU:O	4:C:374:ARG:NH2	2.36	0.58
2:A:208:PRO:HD2	2:A:314:ASN:HD21	1.68	0.58
10:W:182:ARG:O	10:W:186:ILE:HB	2.02	0.58
10:W:314:LEU:HD11	10:W:382:LEU:HD21	1.86	0.58
2:A:184:ILE:O	2:A:188:ARG:HB2	2.04	0.58
2:A:97:ARG:HB3	2:A:142:VAL:HG13	1.86	0.58
10:W:230:MET:HG3	10:W:231:ILE:HG12	1.85	0.58
1:G:157:ILE:HA	1:G:160:TYR:HD2	1.68	0.58
5:D:267:ILE:O	5:D:271:ALA:HB3	2.04	0.58
7:F:121:CYS:HA	7:F:135:PRO:HA	1.86	0.58
6:E:115:VAL:HG13	6:E:118:LEU:H	1.68	0.57
12:Y:330:ILE:HA	12:Y:333:GLU:HB2	1.86	0.57
9:V:479:ARG:NH1	12:Y:374:ASP:OD1	2.36	0.57
7:F:169:ASP:OD2	7:F:266:LYS:NZ	2.37	0.57
10:W:431:LYS:O	10:W:435:LEU:HB2	2.04	0.57
12:Y:271:PHE:O	12:Y:275:LEU:HB2	2.03	0.57
3:B:217:LYS:O	3:B:219:PRO:HD3	2.03	0.57
4:C:57:ARG:NH1	8:U:644:TYR:OH	2.36	0.57
5:D:89:ILE:HD11	6:E:80:VAL:HG13	1.85	0.57
1:G:84:GLY:HA2	1:G:118:ARG:HG3	1.87	0.57
4:C:13:GLU:HB2	8:U:140:ARG:HH12	1.69	0.57
10:W:220:GLU:O	10:W:221:LYS:HB3	2.03	0.57
6:E:81:VAL:HG12	6:E:105:LEU:HB3	1.85	0.57
8:U:392:TRP:O	8:U:395:ARG:NH1	2.37	0.57
13:Z:18:SER:O	13:Z:22:HIS:ND1	2.30	0.57
6:E:209:GLY:O	6:E:255:ARG:NH1	2.35	0.57
7:F:224:LEU:HD13	7:F:348:LEU:HD13	1.86	0.57
1:G:181:ASP:OD2	5:D:338:ARG:NH1	2.37	0.57
10:W:73:MET:O	10:W:77:ALA:CB	2.52	0.57
13:Z:133:LEU:HD23	13:Z:135:THR:H	1.69	0.57
2:A:126:SER:HB3	2:A:148:GLN:HB2	1.87	0.57
8:U:600:ARG:O	8:U:604:HIS:HB2	2.05	0.57
2:A:401:ARG:NH1	2:A:403:ILE:O	2.38	0.56
1:G:212:ALA:HB1	1:G:216:LEU:HB3	1.87	0.56
13:Z:21:ASP:OD2	13:Z:25:ARG:NH2	2.36	0.56
1:G:185:VAL:HG12	1:G:189:LYS:HE2	1.85	0.56
8:U:474:ARG:NH2	8:U:500:ASN:O	2.33	0.56
2:A:95:VAL:HB	2:A:143:ASP:HA	1.85	0.56
5:D:285:VAL:HA	5:D:288:ILE:HD12	1.88	0.56
6:E:177:GLY:HA2	6:E:339:ASN:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:227:SER:HA	12:Y:231:LEU:HD13	1.86	0.56
5:D:184:PRO:HA	5:D:190:LEU:HD23	1.88	0.56
1:G:100:ASN:HD21	1:G:131:ASN:H	1.51	0.56
12:Y:232:GLU:HG3	12:Y:234:PRO:HD2	1.87	0.56
4:C:14:GLY:HA2	4:C:18:SER:HB3	1.86	0.56
6:E:178:THR:HG22	6:E:339:ASN:HB3	1.86	0.56
6:E:368:MET:O	6:E:372:ARG:HB2	2.05	0.56
7:F:381:TYR:O	7:F:385:ALA:HB2	2.06	0.56
8:U:374:SER:HB3	8:U:407:SER:HB3	1.87	0.56
8:U:498:LYS:HD3	8:U:501:LEU:HD21	1.87	0.56
9:V:491:VAL:HA	9:V:494:MET:HG2	1.87	0.56
7:F:151:VAL:HG12	7:F:163:THR:HG23	1.88	0.56
11:X:338:VAL:HG23	11:X:339:ILE:HD12	1.86	0.56
12:Y:109:GLU:HG2	12:Y:146:ARG:HH22	1.70	0.56
8:U:100:ILE:O	8:U:104:CYS:HB2	2.05	0.56
8:U:604:HIS:O	8:U:608:SER:HB2	2.06	0.56
8:U:889:LEU:HD13	8:U:909:GLY:H	1.71	0.56
9:V:384:GLU:O	9:V:388:ALA:HB2	2.05	0.56
10:W:124:LEU:HD13	10:W:149:LEU:HD13	1.86	0.56
10:W:416:GLN:HG3	10:W:417:ARG:H	1.71	0.56
4:C:71:SER:OG	5:D:112:TYR:O	2.22	0.56
7:F:167:GLU:CD	7:F:173:LYS:HE3	2.25	0.56
8:U:799:LYS:NZ	8:U:926:GLU:OE2	2.37	0.56
8:U:141:CYS:HB3	8:U:149:GLN:HE21	1.71	0.56
3:B:395:ILE:HA	3:B:398:ILE:HG12	1.88	0.56
1:G:103:ASN:OD1	1:G:107:CYS:N	2.38	0.56
5:D:261:ILE:HG12	5:D:306:LYS:HB2	1.89	0.55
7:F:422:GLU:O	7:F:426:GLU:HB2	2.07	0.55
10:W:52:LYS:HE3	10:W:55:ARG:HH21	1.70	0.55
8:U:257:SER:HB3	8:U:260:PHE:HB3	1.88	0.55
8:U:261:LEU:HA	8:U:264:VAL:HG12	1.87	0.55
9:V:396:ILE:HD12	9:V:399:ARG:HD3	1.89	0.55
10:W:74:CYS:HB3	10:W:78:LYS:HE2	1.88	0.55
12:Y:161:THR:O	12:Y:165:LYS:HB2	2.05	0.55
6:E:261:LEU:HA	6:E:294:ARG:HH22	1.70	0.55
7:F:169:ASP:OD2	7:F:266:LYS:HE3	2.07	0.55
7:F:167:GLU:CG	7:F:173:LYS:HE3	2.35	0.55
11:X:282:ARG:NH1	11:X:285:GLU:OE1	2.39	0.55
7:F:192:ASP:HA	7:F:195:ILE:HG22	1.87	0.55
8:U:259:GLN:NE2	8:U:521:LEU:O	2.39	0.55
10:W:147:LYS:HB3	10:W:185:PHE:HE1	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:179:ARG:NH1	12:Y:212:GLU:OE1	2.38	0.55
6:E:371:VAL:O	6:E:375:ALA:CB	2.54	0.55
12:Y:101:ARG:O	12:Y:105:MET:CB	2.54	0.55
13:Z:278:ASN:O	13:Z:282:ASN:ND2	2.40	0.55
2:A:388:VAL:O	2:A:392:ALA:HB3	2.06	0.55
3:B:273:VAL:O	3:B:277:HIS:HB2	2.07	0.55
4:C:168:PRO:HG3	4:C:290:LYS:HD2	1.88	0.55
7:F:170:SER:HA	7:F:173:LYS:HZ3	1.72	0.55
7:F:69:MET:HA	7:F:72:LYS:HG2	1.89	0.55
3:B:120:HIS:HB2	3:B:132:TYR:HB2	1.88	0.55
3:B:192:ASN:HA	3:B:195:GLN:HG2	1.89	0.55
6:E:11:ASP:HA	6:E:14:LYS:HE3	1.87	0.55
6:E:115:VAL:HG22	6:E:116:ASP:N	2.22	0.54
13:Z:228:TYR:O	13:Z:232:ASP:HB2	2.07	0.54
4:C:89:VAL:HG12	4:C:90:HIS:H	1.73	0.54
5:D:366:ARG:HG2	5:D:370:ILE:HD11	1.89	0.54
7:F:273:ALA:O	7:F:277:GLU:HB3	2.07	0.54
2:A:190:VAL:HG23	2:A:209:PRO:HG2	1.88	0.54
9:V:442:ILE:HA	9:V:447:ILE:HD11	1.89	0.54
12:Y:124:PHE:HA	12:Y:127:THR:HG22	1.90	0.54
12:Y:300:ARG:NH2	12:Y:333:GLU:OE2	2.40	0.54
12:Y:344:HIS:HD2	12:Y:358:ARG:HG3	1.73	0.54
4:C:84:LYS:HG2	4:C:96:VAL:HG22	1.90	0.54
7:F:173:LYS:HB3	7:F:173:LYS:HZ3	1.70	0.54
8:U:749:GLN:HA	8:U:755:THR:HA	1.89	0.54
8:U:841:LYS:NZ	8:U:882:ALA:O	2.40	0.54
8:U:799:LYS:HG2	8:U:843:GLU:HA	1.89	0.54
10:W:316:ARG:NH2	10:W:381:LEU:O	2.41	0.54
2:A:143:ASP:OD1	2:A:144:ARG:N	2.40	0.54
4:C:200:ALA:O	4:C:204:ALA:CB	2.56	0.54
7:F:252:ALA:HB3	7:F:255:GLN:HG2	1.89	0.54
11:X:396:THR:HG21	12:Y:365:GLN:HG2	1.89	0.54
6:E:129:ASN:ND2	6:E:190:GLN:OE1	2.40	0.54
1:G:148:ALA:O	5:D:342:ARG:NH2	2.40	0.54
7:F:269:ARG:O	7:F:273:ALA:HB2	2.08	0.54
7:F:60:LEU:O	7:F:64:HIS:ND1	2.31	0.54
7:F:84:LYS:HG3	7:F:161:LEU:HB2	1.89	0.54
10:W:268:LYS:NZ	10:W:327:GLU:OE2	2.41	0.54
11:X:259:ILE:HD13	11:X:267:VAL:HG21	1.90	0.54
6:E:206:LYS:HG2	7:F:305:GLU:HG2	1.89	0.54
2:A:417:ILE:O	2:A:421:ALA:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:295:ARG:HH21	7:F:301:ALA:HB1	1.73	0.53
4:C:42:LEU:HD22	13:Z:167:ALA:HB1	41.99	0.53
10:W:163:ALA:O	10:W:167:GLN:CB	2.56	0.53
12:Y:191:ILE:HG23	12:Y:193:ASP:H	1.72	0.53
7:F:272:PHE:O	7:F:276:LYS:CB	2.56	0.53
8:U:458:ILE:HG23	8:U:481:LEU:HD11	1.90	0.53
8:U:474:ARG:O	8:U:478:SER:CB	2.57	0.53
11:X:107:VAL:HG23	11:X:133:LEU:HD11	1.89	0.53
6:E:346:VAL:HG12	6:E:371:VAL:HG22	1.90	0.53
8:U:265:ILE:HG13	8:U:329:LEU:HD22	1.90	0.53
8:U:894:MET:SD	8:U:901:GLN:NE2	2.81	0.53
10:W:163:ALA:O	10:W:167:GLN:HB2	2.07	0.53
4:C:202:ALA:O	4:C:206:HIS:ND1	2.41	0.53
5:D:202:VAL:HA	5:D:329:ARG:HB2	1.90	0.53
8:U:543:LYS:HA	8:U:546:ARG:HG2	1.89	0.53
3:B:398:ILE:HG21	3:B:426:VAL:HG23	1.90	0.53
11:X:45:VAL:HA	11:X:48:GLN:HG2	1.91	0.53
12:Y:101:ARG:O	12:Y:105:MET:HB2	2.07	0.53
9:V:498:PRO:HG3	13:Z:274:ASN:HB3	1.91	0.53
2:A:402:LYS:HD3	3:B:210:TYR:HE1	1.73	0.53
5:D:200:ARG:NH2	5:D:300:ASP:OD1	2.41	0.53
7:F:306:VAL:O	7:F:310:MET:CB	2.56	0.53
7:F:307:GLN:O	7:F:311:LEU:HB2	2.09	0.53
1:G:70:ASP:OD1	1:G:74:TRP:N	2.35	0.53
8:U:361:ARG:N	8:U:365:CYS:SG	2.80	0.53
8:U:681:ASN:HA	8:U:684:ARG:HE	1.73	0.53
2:A:200:ARG:O	2:A:204:LEU:HB3	2.07	0.53
3:B:187:ILE:HD11	3:B:194:ILE:HD12	1.89	0.53
8:U:634:PRO:O	8:U:638:SER:HB3	2.09	0.53
10:W:344:THR:HG23	10:W:345:GLU:HG2	1.91	0.53
5:D:176:GLU:O	5:D:180:ALA:HB3	2.07	0.53
5:D:289:LEU:HD12	5:D:292:LEU:HD11	1.90	0.53
6:E:59:GLU:O	6:E:72:LYS:N	2.40	0.53
12:Y:345:CYS:SG	12:Y:356:THR:OG1	2.63	0.53
7:F:167:GLU:CG	7:F:173:LYS:CE	2.87	0.52
7:F:221:LYS:HD3	7:F:327:LYS:HG3	1.90	0.52
1:G:146:ALA:HB1	1:G:151:ASN:HB2	1.90	0.52
2:A:201:PHE:HA	7:F:408:LEU:HD11	1.90	0.52
5:D:244:PRO:O	5:D:248:ARG:CB	2.57	0.52
13:Z:131:LEU:HD21	13:Z:199:LYS:HG2	1.92	0.52
13:Z:186:THR:OG1	13:Z:190:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:398:ILE:O	3:B:402:ALA:CB	2.58	0.52
7:F:272:PHE:O	7:F:276:LYS:HB3	2.10	0.52
8:U:505:ASP:HB2	8:U:508:THR:HG22	1.92	0.52
2:A:362:MET:H	3:B:216:ILE:HD11	1.74	0.52
5:D:353:ASN:HB3	5:D:393:ILE:HG23	1.91	0.52
6:E:124:HIS:CD2	6:E:195:PHE:CD2	2.96	0.52
13:Z:106:ILE:O	13:Z:110:GLU:HB2	2.08	0.52
2:A:162:THR:HG22	2:A:256:MET:HG3	1.90	0.52
2:A:312:ARG:HG3	2:A:314:ASN:H	1.73	0.52
5:D:274:ARG:O	5:D:283:ARG:NH2	2.43	0.52
6:E:292:PRO:HG3	10:W:90:LEU:HD23	1.92	0.52
7:F:173:LYS:NZ	7:F:173:LYS:CB	2.73	0.52
8:U:580:ARG:HD3	8:U:613:ASP:HB3	1.91	0.52
9:V:384:GLU:O	9:V:388:ALA:HB3	2.09	0.52
3:B:202:GLU:O	3:B:206:THR:OG1	2.24	0.52
7:F:121:CYS:SG	7:F:122:ALA:N	2.83	0.52
7:F:166:THR:CG2	7:F:167:GLU:N	2.73	0.52
1:G:141:THR:H	1:G:144:HIS:HD2	1.57	0.52
2:A:184:ILE:HD12	2:A:187:LEU:HD11	1.90	0.52
2:A:195:LEU:HD22	2:A:232:ARG:HH11	1.73	0.52
7:F:341:ALA:O	7:F:347:ARG:NH2	2.41	0.52
8:U:413:LYS:HG3	8:U:449:ILE:HA	1.92	0.52
8:U:414:GLY:HA2	8:U:453:HIS:HE1	1.75	0.52
8:U:772:TRP:HD1	8:U:775:LEU:HG	1.75	0.52
4:C:186:VAL:HG21	4:C:315:ILE:HD12	1.92	0.52
8:U:247:GLN:HE21	8:U:913:ILE:H	1.58	0.52
8:U:564:ASP:OD1	8:U:590:TYR:OH	2.27	0.52
5:D:171:ASP:O	5:D:175:GLN:HB2	2.09	0.52
6:E:371:VAL:O	6:E:375:ALA:HB3	2.09	0.52
2:A:121:PHE:HA	7:F:89:LEU:HA	1.92	0.52
2:A:191:VAL:HG13	2:A:192:GLU:HG3	1.92	0.52
2:A:339:ARG:NH1	13:Z:225:GLN:OE1	122.59	0.52
5:D:355:SER:HB3	5:D:358:VAL:HG23	1.91	0.52
8:U:885:MET:HB3	8:U:888:GLN:HG3	1.92	0.52
9:V:410:ILE:HG13	9:V:426:LEU:HD11	1.91	0.52
6:E:213:ARG:O	6:E:217:GLU:CB	2.58	0.51
1:G:145:ARG:HB3	5:D:361:GLU:HB3	1.92	0.51
5:D:43:ARG:O	5:D:47:LEU:HB2	2.11	0.51
6:E:201:SER:HB2	7:F:308:ARG:HA	1.92	0.51
6:E:242:ARG:NH1	6:E:254:GLN:OE1	2.41	0.51
7:F:362:ARG:NH2	7:F:388:THR:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:246:ILE:HA	12:Y:249:VAL:HG22	1.91	0.51
7:F:381:TYR:O	7:F:385:ALA:CB	2.58	0.51
7:F:169:ASP:OD2	7:F:266:LYS:CE	2.59	0.51
10:W:144:ARG:HD3	10:W:147:LYS:HZ3	1.75	0.51
12:Y:72:LYS:HA	12:Y:75:LYS:HE3	1.92	0.51
9:V:501:TYR:HA	13:Z:282:ASN:HD21	1.76	0.51
2:A:317:VAL:HB	2:A:337:LEU:HG	1.93	0.51
12:Y:364:TRP:HA	12:Y:367:GLN:HB2	1.93	0.51
13:Z:202:ASN:O	13:Z:206:LEU:CB	2.58	0.51
5:D:391:ARG:HH12	5:D:397:LYS:HB2	1.75	0.51
1:G:32:LEU:HD23	1:G:35:ARG:HD2	1.92	0.51
10:W:137:TYR:HE2	10:W:141:GLU:H	1.59	0.51
12:Y:117:LYS:O	12:Y:121:LEU:CB	2.52	0.51
6:E:15:LYS:O	6:E:19:HIS:ND1	2.34	0.51
2:A:296:GLN:O	2:A:300:LEU:HB2	2.11	0.51
10:W:63:THR:HG22	10:W:67:LEU:HD13	1.91	0.51
2:A:271:LEU:HD23	2:A:316:LYS:HD2	1.91	0.51
8:U:683:VAL:O	8:U:687:ALA:HB2	2.11	0.51
8:U:688:LEU:HD11	8:U:715:LYS:HE2	1.93	0.51
12:Y:231:LEU:HD21	12:Y:239:LYS:HD2	1.92	0.51
6:E:51:GLN:O	13:Z:88:ARG:NH2	2.44	0.50
7:F:325:GLN:HG2	7:F:326:VAL:H	1.74	0.50
11:X:367:GLN:HG3	12:Y:233:ARG:HH22	1.76	0.50
13:Z:240:VAL:HG12	13:Z:242:LEU:H	1.76	0.50
4:C:169:VAL:HG22	4:C:207:THR:HG23	1.93	0.50
4:C:276:LEU:O	4:C:280:LEU:HB2	2.11	0.50
4:C:295:THR:HG22	4:C:300:ILE:HG12	1.93	0.50
10:W:267:LEU:HD23	10:W:299:ILE:HD11	1.91	0.50
3:B:268:ARG:HA	3:B:315:GLN:HE22	1.77	0.50
6:E:124:HIS:HD2	6:E:195:PHE:CD2	2.29	0.50
7:F:150:LEU:HB3	7:F:166:THR:HG1	1.73	0.50
7:F:168:TYR:CD1	7:F:169:ASP:HB2	2.47	0.50
10:W:179:LYS:HD2	10:W:217:GLU:HB2	1.93	0.50
11:X:417:LYS:HA	11:X:420:LYS:HG2	1.92	0.50
11:X:77:LEU:HD21	11:X:88:LEU:HD23	1.93	0.50
6:E:366:ASP:O	6:E:370:ALA:CB	2.59	0.50
1:G:198:ILE:HD13	1:G:224:VAL:HG21	1.93	0.50
10:W:118:LEU:HB3	10:W:119:PRO:HD3	1.94	0.50
7:F:175:MET:HG3	7:F:176:GLU:H	1.76	0.50
8:U:127:ASP:HB3	8:U:130:LEU:HD13	1.93	0.50
8:U:586:VAL:HG21	8:U:601:ARG:HH12	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:442:ILE:HG21	9:V:451:ILE:HD11	1.93	0.50
3:B:187:ILE:HG22	3:B:367:ILE:HD13	1.92	0.50
3:B:398:ILE:O	3:B:402:ALA:HB2	2.12	0.50
6:E:50:LEU:HD11	7:F:138:GLY:H	1.76	0.50
11:X:417:LYS:HA	11:X:420:LYS:HE3	1.93	0.50
4:C:362:VAL:O	4:C:366:ALA:CB	2.59	0.50
11:X:255:LEU:O	11:X:259:ILE:HB	2.11	0.50
8:U:581:SER:O	8:U:585:THR:OG1	2.19	0.49
8:U:680:VAL:HG12	8:U:682:TYR:H	1.77	0.49
10:W:124:LEU:HA	10:W:127:THR:HG22	1.93	0.49
13:Z:164:ALA:HB1	13:Z:168:GLU:HB3	1.94	0.49
6:E:124:HIS:NE2	6:E:195:PHE:CZ	2.80	0.49
7:F:168:TYR:CD1	7:F:168:TYR:C	2.85	0.49
7:F:246:ALA:HB1	7:F:281:SER:HA	1.94	0.49
8:U:196:LYS:HA	8:U:199:ARG:HG2	1.94	0.49
8:U:545:LEU:HB3	8:U:577:ILE:HG21	1.93	0.49
10:W:34:LEU:HD11	10:W:47:LEU:HD11	1.94	0.49
12:Y:347:ILE:HD11	12:Y:354:VAL:HG22	1.94	0.49
8:U:765:VAL:HG11	8:U:778:PHE:HD2	1.78	0.49
12:Y:184:GLN:HA	12:Y:187:TYR:CE1	2.46	0.49
6:E:172:LEU:HD22	6:E:301:ILE:HD11	1.95	0.49
10:W:211:THR:HG23	10:W:212:LYS:H	1.78	0.49
5:D:173:GLN:HG3	5:D:331:ILE:HD13	1.94	0.49
12:Y:175:ASP:O	12:Y:179:ARG:HB2	2.11	0.49
2:A:185:GLU:OE1	2:A:188:ARG:NH2	2.41	0.49
5:D:116:LEU:HD23	5:D:118:THR:H	1.78	0.49
6:E:312:ILE:HG13	6:E:316:HIS:CD2	2.48	0.49
6:E:63:GLN:HG3	6:E:69:PHE:HB3	1.93	0.49
1:G:135:LYS:HE2	1:G:167:ILE:HG23	1.95	0.49
11:X:316:ASP:OD2	11:X:320:SER:OG	2.26	0.49
13:Z:39:LEU:H	13:Z:94:TRP:HA	1.78	0.49
6:E:168:LYS:NZ	6:E:293:GLY:O	2.45	0.49
6:E:31:GLU:HG3	6:E:34:LYS:HE3	1.94	0.49
2:A:108:ASP:OD1	2:A:108:ASP:N	2.26	0.49
4:C:198:LEU:O	4:C:202:ALA:CB	2.60	0.49
7:F:228:PRO:HG2	7:F:356:MET:HG3	1.94	0.49
6:E:185:ARG:HA	6:E:188:ALA:HB3	1.95	0.48
6:E:50:LEU:HD23	7:F:159:LEU:HD13	1.95	0.48
7:F:318:ASP:OD1	7:F:344:ARG:NE	2.45	0.48
12:Y:190:ALA:O	12:Y:291:HIS:NE2	2.46	0.48
2:A:200:ARG:O	2:A:204:LEU:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:218:PRO:O	3:B:326:LYS:NZ	2.46	0.48
7:F:73:ILE:O	7:F:77:SER:OG	2.19	0.48
9:V:351:PRO:HB2	9:V:355:ARG:HH22	1.79	0.48
10:W:73:MET:O	10:W:77:ALA:HB3	2.11	0.48
4:C:25:LEU:HD11	5:D:47:LEU:HD23	1.95	0.48
13:Z:96:HIS:CE1	13:Z:123:ILE:HG12	2.48	0.48
2:A:100:LYS:HG2	2:A:142:VAL:HG11	1.95	0.48
2:A:415:LYS:O	2:A:419:SER:OG	2.16	0.48
12:Y:100:ILE:HG22	12:Y:130:LYS:HE3	1.95	0.48
13:Z:201:LEU:O	13:Z:205:LEU:HB3	2.13	0.48
13:Z:39:LEU:HB2	13:Z:95:TYR:HD1	1.78	0.48
4:C:327:ASP:OD1	4:C:328:ILE:N	2.47	0.48
5:D:123:LEU:HD23	5:D:142:VAL:HG13	1.96	0.48
7:F:288:LEU:HB3	7:F:332:THR:HG22	1.95	0.48
1:G:81:ALA:HA	1:G:121:ILE:HG21	1.96	0.48
8:U:340:GLN:O	8:U:343:ILE:HG22	2.13	0.48
8:U:376:MET:HA	8:U:740:GLY:H	1.77	0.48
10:W:432:LEU:O	10:W:436:MET:CB	2.62	0.48
12:Y:171:GLY:O	12:Y:176:ARG:NH2	2.46	0.48
6:E:98:VAL:HA	6:E:110:TYR:HA	1.96	0.48
8:U:496:LEU:HA	8:U:499:THR:HG22	1.95	0.48
7:F:152:GLY:N	7:F:162:GLU:O	2.47	0.48
12:Y:250:LEU:HD13	12:Y:257:ARG:HD3	1.96	0.48
2:A:188:ARG:HA	2:A:191:VAL:HG12	1.95	0.48
7:F:176:GLU:HG3	7:F:250:LYS:HB2	1.96	0.48
7:F:204:LEU:HG	7:F:205:PRO:HD3	1.94	0.48
1:G:46:TRP:HH2	5:D:391:ARG:HA	1.79	0.48
8:U:473:VAL:O	8:U:477:GLY:HA3	2.14	0.48
8:U:482:GLY:HA3	8:U:515:ALA:HB1	1.96	0.48
8:U:497:LEU:HD23	8:U:501:LEU:HD23	1.95	0.48
2:A:388:VAL:O	2:A:392:ALA:CB	2.61	0.47
3:B:234:LEU:HD13	3:B:330:ALA:HB1	1.95	0.47
6:E:215:ILE:O	6:E:219:PHE:HB2	2.13	0.47
8:U:135:ASN:HA	8:U:138:PHE:HB3	1.96	0.47
10:W:356:ASN:HA	10:W:359:VAL:HG12	1.96	0.47
11:X:258:LYS:HZ1	11:X:267:VAL:N	2.11	0.47
13:Z:197:GLY:O	13:Z:201:LEU:HB2	2.13	0.47
1:G:107:CYS:SG	1:G:145:ARG:NH2	2.83	0.47
8:U:266:GLN:HA	8:U:269:ARG:HB3	1.96	0.47
12:Y:261:PHE:O	12:Y:265:GLU:CB	2.62	0.47
4:C:300:ILE:O	4:C:304:ALA:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:326:LEU:HD21	4:C:345:ARG:HD3	1.94	0.47
6:E:240:GLY:O	6:E:254:GLN:NE2	2.46	0.47
8:U:397:THR:HA	8:U:401:LYS:HE2	1.97	0.47
8:U:793:LYS:HB3	8:U:796:LYS:HB2	1.96	0.47
10:W:271:VAL:HG23	10:W:305:LEU:HD13	1.95	0.47
11:X:142:ARG:NE	11:X:145:GLU:OE2	2.39	0.47
11:X:243:ASP:HB3	11:X:246:LYS:HB2	1.96	0.47
2:A:204:LEU:HD12	7:F:413:THR:HB	1.96	0.47
3:B:116:ILE:HG22	3:B:118:ASP:H	1.78	0.47
5:D:323:ARG:NH1	5:D:324:PRO:O	2.48	0.47
6:E:62:LYS:HE3	6:E:64:LEU:HD11	1.97	0.47
8:U:112:CYS:O	8:U:116:ALA:HB2	2.13	0.47
8:U:374:SER:HB2	8:U:410:VAL:HB	1.96	0.47
13:Z:73:ASP:OD1	13:Z:77:ASN:ND2	2.47	0.47
6:E:367:PHE:O	6:E:371:VAL:HB	2.15	0.47
6:E:378:LYS:O	6:E:382:SER:HB3	2.14	0.47
7:F:80:ILE:O	7:F:84:LYS:HB2	2.14	0.47
8:U:368:ALA:HA	8:U:371:ILE:HG22	1.97	0.47
10:W:408:ARG:HH12	11:X:347:ILE:HG23	1.79	0.47
3:B:201:VAL:HG11	3:B:328:ILE:HD11	1.95	0.47
8:U:474:ARG:O	8:U:478:SER:HB2	2.15	0.47
13:Z:123:ILE:HD12	13:Z:138:TYR:HE2	1.79	0.47
6:E:261:LEU:HD23	6:E:294:ARG:HH12	1.80	0.47
7:F:168:TYR:O	7:F:169:ASP:C	2.52	0.47
8:U:740:GLY:HA3	8:U:744:VAL:HG22	1.96	0.47
12:Y:173:ASP:HB2	12:Y:176:ARG:HB3	1.96	0.47
3:B:381:ASP:O	3:B:385:MET:HB2	2.14	0.47
4:C:277:LEU:O	4:C:281:ASP:CB	2.58	0.47
7:F:229:PRO:HG3	7:F:333:ASN:HB3	1.96	0.47
1:G:93:LEU:HD11	1:G:125:LEU:HD23	1.97	0.47
3:B:282:VAL:HB	3:B:327:VAL:HA	1.95	0.47
6:E:338:PHE:HE1	6:E:379:LYS:HD3	1.79	0.47
9:V:372:LEU:O	9:V:376:ASN:HB2	2.14	0.47
10:W:432:LEU:O	10:W:436:MET:HB2	2.15	0.47
12:Y:13:LYS:HB2	12:Y:212:GLU:HG2	1.97	0.47
9:V:414:TYR:CD1	12:Y:349:LYS:HB2	2.50	0.47
3:B:264:PRO:HG3	3:B:311:GLU:HG2	1.97	0.47
8:U:255:SER:OG	8:U:256:ALA:N	2.48	0.47
9:V:337:LEU:HB3	9:V:342:ILE:HD13	1.96	0.47
9:V:345:ARG:NH2	9:V:348:PHE:O	2.39	0.47
10:W:220:GLU:CB	10:W:223:LYS:CD	2.93	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:139:ILE:HG12	13:Z:141:VAL:HG13	1.96	0.47
6:E:175:PRO:O	6:E:177:GLY:N	2.44	0.46
6:E:23:ASP:HB3	7:F:56:LYS:HE2	1.96	0.46
6:E:344:ARG:HH22	7:F:218:GLN:HB2	1.80	0.46
8:U:154:ALA:HB1	8:U:163:PHE:HB3	1.97	0.46
11:X:209:THR:OG1	11:X:239:TYR:OH	2.28	0.46
11:X:268:GLN:HA	11:X:271:VAL:HG22	1.97	0.46
6:E:254:GLN:O	6:E:258:MET:HG2	2.16	0.46
8:U:344:ARG:HD2	8:U:880:ASN:HB3	1.97	0.46
10:W:227:TYR:HA	10:W:230:MET:HG2	1.96	0.46
10:W:247:TYR:HB2	10:W:273:TYR:HB3	1.98	0.46
12:Y:92:GLU:HG2	12:Y:93:LYS:HD2	1.98	0.46
3:B:313:LEU:HD21	3:B:344:PRO:HG2	1.97	0.46
1:G:15:TYR:HE1	5:D:393:ILE:HD11	1.81	0.46
6:E:102:MET:HG3	6:E:103:THR:HG23	1.98	0.46
6:E:303:LEU:HD23	6:E:309:ARG:HG3	1.96	0.46
2:A:76:ALA:O	2:A:80:LEU:CB	2.63	0.46
4:C:43:ARG:HB2	8:U:639:LEU:HD21	1.97	0.46
8:U:414:GLY:H	8:U:449:ILE:HG23	1.81	0.46
2:A:277:ILE:HG13	2:A:280:ILE:HD11	1.97	0.46
1:G:111:HIS:HE2	1:G:141:THR:HA	1.80	0.46
8:U:338:HIS:HA	8:U:341:PHE:CE1	2.50	0.46
2:A:173:THR:HG23	2:A:175:SER:H	1.79	0.46
4:C:198:LEU:O	4:C:202:ALA:HB2	2.15	0.46
6:E:253:ILE:O	6:E:256:THR:OG1	2.27	0.46
7:F:375:VAL:HA	7:F:415:LEU:HB3	1.98	0.46
8:U:510:GLU:HA	8:U:547:GLY:HA3	1.96	0.46
8:U:712:LEU:HD21	8:U:734:GLN:HG2	1.98	0.46
10:W:220:GLU:HG3	10:W:220:GLU:O	2.15	0.46
4:C:371:LEU:HD11	5:D:190:LEU:HD21	1.97	0.46
7:F:306:VAL:O	7:F:310:MET:HB2	2.15	0.46
2:A:160:THR:O	2:A:164:MET:HB2	2.16	0.46
5:D:207:PRO:HG2	5:D:208:PRO:HD3	1.98	0.46
12:Y:224:VAL:O	12:Y:228:MET:CB	2.64	0.46
13:Z:261:TYR:O	13:Z:265:LEU:HB2	2.16	0.46
13:Z:284:ASP:HA	13:Z:287:LYS:HG2	1.98	0.46
2:A:100:LYS:HB3	2:A:115:VAL:HG23	1.98	0.46
2:A:411:GLU:O	2:A:415:LYS:HB2	2.16	0.46
7:F:169:ASP:OD1	7:F:171:ARG:CG	2.61	0.46
8:U:250:PHE:O	8:U:254:GLU:HB2	2.16	0.46
10:W:222:LEU:O	10:W:223:LYS:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:354:ILE:O	2:A:357:ILE:HG22	2.16	0.45
2:A:407:LYS:HA	2:A:410:LEU:HD23	1.98	0.45
6:E:188:ALA:HB2	6:E:231:PHE:HE2	1.80	0.45
8:U:546:ARG:HE	8:U:771:PHE:HD2	1.64	0.45
10:W:12:ARG:NH1	10:W:30:GLU:OE1	2.48	0.45
12:Y:188:CYS:HA	12:Y:191:ILE:HG22	1.97	0.45
3:B:140:ASP:O	3:B:141:LYS:HG2	2.17	0.45
5:D:359:ASP:OD1	5:D:360:LEU:N	2.50	0.45
8:U:229:VAL:HG23	8:U:232:ILE:HD11	1.98	0.45
8:U:613:ASP:O	8:U:616:ARG:HD2	2.16	0.45
12:Y:220:VAL:HA	12:Y:223:THR:HG22	1.97	0.45
4:C:300:ILE:O	4:C:304:ALA:CB	2.64	0.45
5:D:145:PRO:HB3	5:D:245:ARG:HB3	1.98	0.45
5:D:244:PRO:O	5:D:248:ARG:HB2	2.17	0.45
5:D:297:ASP:OD2	5:D:326:ARG:NH2	2.45	0.45
5:D:62:LYS:HD3	5:D:65:GLN:NE2	2.32	0.45
6:E:286:ASP:O	6:E:289:LEU:N	2.48	0.45
6:E:312:ILE:HG13	6:E:316:HIS:HD2	1.80	0.45
8:U:612:ASP:OD1	8:U:645:ASN:ND2	2.49	0.45
3:B:197:ILE:HD11	3:B:328:ILE:HD13	1.98	0.45
4:C:339:THR:HB	4:C:377:HIS:CD2	2.52	0.45
5:D:171:ASP:O	5:D:175:GLN:CB	2.65	0.45
13:Z:48:LEU:HD11	13:Z:92:VAL:HG21	1.97	0.45
5:D:197:ASP:C	5:D:199:PRO:HD3	2.36	0.45
7:F:381:TYR:HD1	7:F:384:LEU:HD11	1.82	0.45
12:Y:36:ALA:O	12:Y:40:GLU:HB2	2.16	0.45
7:F:293:THR:HA	7:F:337:ILE:HG21	1.98	0.45
8:U:418:GLU:O	8:U:422:LEU:CB	2.62	0.45
8:U:696:ILE:HG22	8:U:737:LEU:HA	1.98	0.45
12:Y:215:ASP:OD1	12:Y:216:TYR:N	2.50	0.45
2:A:414:ASN:HA	2:A:417:ILE:HG12	1.98	0.45
3:B:269:GLU:HA	3:B:272:ARG:HG2	1.99	0.45
7:F:167:GLU:O	7:F:168:TYR:CD2	2.70	0.45
8:U:247:GLN:HE21	8:U:913:ILE:HG13	1.81	0.45
10:W:405:LYS:N	10:W:414:ASN:O	2.50	0.45
12:Y:84:LEU:HD13	12:Y:107:LYS:HA	1.98	0.45
2:A:105:ASP:N	2:A:105:ASP:OD1	2.49	0.45
2:A:362:MET:HG3	3:B:214:MET:HB3	1.98	0.45
4:C:168:PRO:HB2	4:C:288:ASN:HD22	1.81	0.45
4:C:325:ARG:O	4:C:329:LEU:HB2	2.17	0.45
5:D:267:ILE:O	5:D:271:ALA:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:221:ILE:HG22	8:U:256:ALA:HB2	1.99	0.45
8:U:685:GLN:HG3	8:U:729:GLY:HA3	1.99	0.45
9:V:420:ALA:O	9:V:424:GLN:HB3	2.17	0.45
10:W:343:SER:HB2	10:W:346:GLU:HB3	1.98	0.45
12:Y:22:LEU:HD22	12:Y:25:LEU:HD21	1.98	0.45
3:B:110:GLY:HA3	3:B:152:LEU:HD13	1.98	0.45
4:C:229:ARG:HG2	4:C:231:VAL:HG22	1.99	0.45
4:C:263:SER:O	4:C:267:SER:HB2	2.16	0.45
5:D:282:ASP:HA	5:D:285:VAL:HG22	1.98	0.45
1:G:219:ILE:HA	1:G:222:ARG:HB3	1.99	0.45
1:G:79:ILE:O	1:G:83:ALA:CB	2.59	0.45
8:U:142:LEU:HD21	8:U:166:THR:HG22	1.98	0.45
12:Y:36:ALA:O	12:Y:40:GLU:CB	2.65	0.45
2:A:171:ASP:OD1	2:A:171:ASP:N	2.50	0.45
4:C:184:LYS:HE3	4:C:281:ASP:HA	1.98	0.45
6:E:81:VAL:HG11	6:E:100:LEU:HD22	1.98	0.45
12:Y:204:THR:HG23	12:Y:245:GLU:HG2	1.99	0.45
6:E:65:THR:HG22	6:E:67:GLU:H	1.82	0.44
8:U:472:ILE:HG13	8:U:473:VAL:H	1.82	0.44
10:W:244:CYS:HA	10:W:273:TYR:HB2	1.99	0.44
13:Z:213:GLU:O	13:Z:217:THR:OG1	2.26	0.44
2:A:83:ASP:O	2:A:86:THR:OG1	2.29	0.44
6:E:182:LEU:O	6:E:186:ALA:CB	2.58	0.44
7:F:74:LYS:O	7:F:78:GLU:CB	2.53	0.44
13:Z:208:ILE:HA	13:Z:211:TYR:HB3	1.99	0.44
2:A:248:LYS:HB3	3:B:307:ARG:HH21	1.82	0.44
5:D:218:ALA:O	5:D:222:HIS:ND1	2.35	0.44
2:A:242:GLY:H	2:A:276:GLU:HB2	1.82	0.44
7:F:87:PRO:HB3	7:F:152:GLY:HA2	1.99	0.44
7:F:192:ASP:O	7:F:196:GLN:HB2	2.17	0.44
9:V:483:CYS:O	9:V:487:HIS:ND1	2.37	0.44
10:W:127:THR:HG23	10:W:145:LEU:HD13	1.99	0.44
11:X:342:PHE:HD2	11:X:350:ILE:HD12	1.83	0.44
12:Y:226:VAL:O	12:Y:230:ALA:CB	2.58	0.44
12:Y:190:ALA:HB2	12:Y:287:LEU:HD21	1.98	0.44
3:B:313:LEU:HD11	3:B:344:PRO:HB2	2.00	0.44
3:B:312:LEU:O	3:B:316:LEU:HB2	2.18	0.44
3:B:223:ILE:HD12	3:B:346:ARG:HB2	2.00	0.44
4:C:273:MET:HG3	4:C:307:ARG:HH12	1.82	0.44
5:D:106:THR:HG21	6:E:77:PRO:HA	1.97	0.44
5:D:187:HIS:HB2	5:D:190:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:353:ASP:O	10:W:357:ARG:HB2	2.18	0.44
2:A:112:ILE:HG13	2:A:112:ILE:H	4.34	0.44
2:A:129:VAL:HG21	2:A:149:ILE:HG22	2.00	0.44
4:C:278:ASN:O	4:C:282:GLY:CA	2.49	0.44
7:F:153:VAL:HG23	7:F:158:TYR:HA	1.99	0.44
7:F:87:PRO:HB3	7:F:153:VAL:H	1.82	0.44
8:U:394:ALA:HA	8:U:401:LYS:HD3	1.99	0.44
9:V:326:GLN:O	9:V:330:LYS:HB2	2.17	0.44
4:C:298:ILE:H	4:C:298:ILE:HD12	1.83	0.44
1:G:192:VAL:HA	1:G:196:ALA:HB3	2.00	0.44
11:X:366:SER:HB3	11:X:378:LEU:HD12	2.00	0.44
3:B:198:LYS:HD2	3:B:202:GLU:HG3	1.99	0.44
8:U:159:ARG:HB3	8:U:162:VAL:HB	1.99	0.44
12:Y:153:ASP:OD1	12:Y:153:ASP:N	2.50	0.44
2:A:339:ARG:HD2	13:Z:225:GLN:HE22	122.40	0.44
2:A:350:GLY:O	2:A:354:ILE:HD12	2.17	0.44
2:A:369:ARG:HH11	2:A:372:LEU:HD22	1.83	0.44
8:U:362:ASN:HA	8:U:395:ARG:HH21	1.83	0.44
9:V:484:LEU:HD21	13:Z:260:VAL:HG22	1.99	0.44
11:X:245:PRO:HA	11:X:248:ILE:HG22	2.00	0.44
2:A:380:SER:HB3	2:A:385:ILE:HG23	2.00	0.43
4:C:329:LEU:O	4:C:333:SER:CB	2.66	0.43
4:C:344:LEU:HA	4:C:347:ILE:HG22	2.00	0.43
6:E:63:GLN:HE21	6:E:66:GLU:HA	1.82	0.43
8:U:506:ALA:O	8:U:510:GLU:HB2	2.18	0.43
8:U:701:ILE:HD13	8:U:810:THR:HG22	2.00	0.43
11:X:420:LYS:HZ3	13:Z:276:ILE:HG23	1.83	0.43
2:A:161:VAL:HA	2:A:164:MET:HB3	2.00	0.43
3:B:103:ARG:HD3	4:C:84:LYS:HZ1	1.82	0.43
8:U:601:ARG:HA	8:U:604:HIS:HB3	1.99	0.43
4:C:162:LYS:HG2	4:C:166:GLU:HG3	2.00	0.43
1:G:13:LEU:HD23	1:G:22:LEU:HA	1.99	0.43
1:G:216:LEU:HD23	1:G:220:LEU:HG	2.00	0.43
10:W:122:LEU:HA	10:W:125:ILE:HG22	1.99	0.43
12:Y:258:GLN:O	12:Y:262:SER:OG	2.24	0.43
12:Y:327:VAL:HA	12:Y:330:ILE:HG12	1.99	0.43
2:A:315:ILE:HG13	2:A:316:LYS:H	1.83	0.43
2:A:94:GLN:O	2:A:144:ARG:NH1	2.38	0.43
4:C:299:ASP:OD1	4:C:299:ASP:N	2.50	0.43
6:E:115:VAL:HG13	6:E:118:LEU:HB3	1.89	0.43
7:F:228:PRO:O	7:F:233:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:903:PHE:HB3	8:U:915:LYS:HD2	2.00	0.43
2:A:113:ILE:O	2:A:121:PHE:N	2.44	0.43
7:F:100:ASP:HB3	7:F:101:PRO:HD3	2.00	0.43
9:V:393:THR:O	9:V:396:ILE:HG22	2.18	0.43
12:Y:259:TYR:OH	12:Y:274:SER:O	2.23	0.43
6:E:352:MET:HA	6:E:355:ILE:HG22	2.01	0.43
1:G:66:VAL:HG23	1:G:92:LEU:HD22	2.01	0.43
8:U:219:CYS:SG	8:U:220:LEU:N	2.91	0.43
2:A:232:ARG:HD2	2:A:235:ALA:O	2.18	0.43
4:C:329:LEU:O	4:C:333:SER:OG	2.23	0.43
8:U:139:GLN:HA	8:U:142:LEU:HB2	2.00	0.43
9:V:360:TYR:CZ	9:V:363:LEU:HD11	2.54	0.43
9:V:420:ALA:O	9:V:424:GLN:CB	2.66	0.43
10:W:218:ASN:O	10:W:223:LYS:NZ	2.41	0.43
2:A:277:ILE:HG22	2:A:321:THR:HB	2.00	0.43
5:D:244:PRO:O	5:D:248:ARG:HB3	2.19	0.43
5:D:93:LEU:HD23	5:D:94:GLU:HG3	2.00	0.43
7:F:84:LYS:HG3	7:F:161:LEU:HD13	1.99	0.43
8:U:456:ASP:HB3	8:U:458:ILE:HG13	2.00	0.43
8:U:683:VAL:O	8:U:687:ALA:CB	2.66	0.43
3:B:343:ARG:HB2	3:B:344:PRO:HD3	2.00	0.43
6:E:191:LEU:HG	6:E:193:CYS:H	1.83	0.43
6:E:368:MET:O	6:E:372:ARG:CB	2.67	0.43
7:F:289:ASP:OD2	7:F:334:ARG:N	2.52	0.43
11:X:348:GLU:HA	11:X:351:SER:HG	1.83	0.43
4:C:158:ILE:O	4:C:162:LYS:HG3	2.19	0.43
5:D:401:LYS:HA	5:D:404:LYS:HG2	2.01	0.43
11:X:255:LEU:HB2	11:X:287:LEU:HD13	2.01	0.43
2:A:328:ASP:HB3	2:A:329:PRO:HD3	2.00	0.42
2:A:411:GLU:O	2:A:415:LYS:CB	2.67	0.42
3:B:223:ILE:HG12	3:B:329:MET:HB2	2.01	0.42
3:B:392:GLY:HA2	3:B:395:ILE:HG22	2.00	0.42
5:D:283:ARG:HA	5:D:286:GLN:HG2	2.00	0.42
5:D:397:LYS:O	5:D:401:LYS:CB	2.67	0.42
8:U:142:LEU:HG	8:U:145:HIS:ND1	2.33	0.42
8:U:247:GLN:HG2	8:U:912:ILE:HA	2.00	0.42
8:U:633:CYS:HB2	8:U:634:PRO:HD3	2.01	0.42
8:U:98:GLU:HA	8:U:101:ILE:HG12	2.01	0.42
9:V:361:PHE:HA	9:V:364:THR:HG22	2.01	0.42
9:V:363:LEU:O	9:V:367:VAL:HG23	2.19	0.42
10:W:93:ARG:HG2	10:W:95:SER:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:155:LYS:C	3:B:157:HIS:H	2.22	0.42
3:B:346:ARG:HH21	3:B:350:LYS:H	1.66	0.42
6:E:191:LEU:C	6:E:193:CYS:H	2.23	0.42
5:D:398:ASP:O	5:D:402:ALA:CB	2.68	0.42
8:U:772:TRP:CD1	8:U:775:LEU:HG	2.53	0.42
9:V:414:TYR:CG	12:Y:349:LYS:HE3	2.54	0.42
3:B:196:GLU:O	3:B:200:SER:HB2	2.20	0.42
4:C:370:ALA:HB2	4:C:378:VAL:HG22	2.00	0.42
10:W:437:SER:O	10:W:441:LYS:CB	2.67	0.42
10:W:444:HIS:HA	10:W:447:ALA:HB3	2.00	0.42
5:D:99:ASN:HA	5:D:115:ILE:HD11	2.02	0.42
6:E:171:LEU:HB2	6:E:295:LEU:HD22	2.02	0.42
7:F:306:VAL:O	7:F:310:MET:HB3	2.19	0.42
8:U:373:ASN:HA	8:U:376:MET:HG2	2.02	0.42
8:U:530:GLU:HA	8:U:533:VAL:HG12	2.02	0.42
10:W:396:LEU:HB3	10:W:401:THR:HB	2.02	0.42
12:Y:141:VAL:O	12:Y:145:LEU:HG	2.20	0.42
3:B:251:VAL:HG22	3:B:285:ASP:HB3	2.00	0.42
5:D:198:PRO:O	5:D:200:ARG:N	2.44	0.42
5:D:366:ARG:HB3	5:D:367:PRO:HD3	2.02	0.42
5:D:391:ARG:HH21	5:D:395:LEU:H	1.67	0.42
6:E:327:ASP:N	6:E:364:GLN:OE1	2.53	0.42
8:U:545:LEU:O	8:U:549:ALA:HB2	2.20	0.42
11:X:208:ALA:HB2	11:X:238:GLY:HA3	2.02	0.42
3:B:387:LYS:HA	3:B:430:LYS:HZ2	1.85	0.42
5:D:283:ARG:HG3	5:D:286:GLN:HE21	1.84	0.42
6:E:114:GLU:OE2	6:E:119:VAL:CG2	2.63	0.42
6:E:42:LYS:HA	6:E:45:ASN:HD22	1.85	0.42
9:V:354:LYS:O	9:V:358:MET:HG3	2.19	0.42
9:V:360:TYR:CE1	9:V:363:LEU:HD11	2.54	0.42
10:W:108:CYS:SG	10:W:123:ARG:HD2	2.60	0.42
10:W:375:MET:HA	10:W:378:MET:HB3	2.01	0.42
3:B:152:LEU:HD23	3:B:157:HIS:HD2	1.85	0.42
3:B:204:PRO:HB3	3:B:211:TYR:CZ	2.55	0.42
3:B:260:LEU:HD13	3:B:261:GLY:N	2.35	0.42
6:E:247:THR:HG23	6:E:249:ALA:H	1.84	0.42
6:E:291:ARG:HD2	6:E:292:PRO:HD2	2.00	0.42
8:U:712:LEU:O	8:U:734:GLN:NE2	2.48	0.42
11:X:391:PRO:HG2	11:X:392:PRO:HD3	2.02	0.42
13:Z:278:ASN:OD1	13:Z:279:LYS:N	2.53	0.42
2:A:273:PHE:HE1	2:A:318:LEU:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:201:ARG:O	4:C:205:HIS:CB	2.65	0.42
5:D:293:LEU:O	5:D:326:ARG:NH1	2.50	0.42
9:V:328:VAL:O	9:V:332:LEU:CB	2.64	0.42
9:V:357:LEU:HD23	9:V:361:PHE:HB2	2.02	0.42
10:W:317:TRP:HD1	10:W:355:LYS:HZ2	1.66	0.42
11:X:244:SER:HB2	11:X:245:PRO:HD3	2.02	0.42
5:D:134:LYS:HG3	5:D:135:HIS:ND1	2.35	0.41
6:E:241:ARG:HD2	6:E:284:THR:HA	2.01	0.41
7:F:221:LYS:HE3	7:F:324:THR:HA	2.02	0.41
9:V:333:ILE:HB	9:V:342:ILE:HD11	2.02	0.41
10:W:50:LEU:O	10:W:54:THR:HG23	2.19	0.41
10:W:73:MET:O	10:W:77:ALA:HB2	2.19	0.41
12:Y:77:ASN:O	12:Y:81:LEU:HB2	2.20	0.41
6:E:199:VAL:HG12	6:E:201:SER:H	1.85	0.41
6:E:370:ALA:O	6:E:374:VAL:HB	2.20	0.41
6:E:97:ARG:HE	6:E:111:LEU:HD23	1.85	0.41
1:G:13:LEU:HD21	1:G:21:GLU:HG2	2.02	0.41
8:U:134:VAL:O	8:U:138:PHE:HB2	2.19	0.41
8:U:493:VAL:HA	8:U:496:LEU:HG	2.03	0.41
10:W:222:LEU:HB3	10:W:225:LYS:HB2	2.01	0.41
6:E:296:ASP:HB3	10:W:94:ARG:HH22	1.86	0.41
13:Z:285:ALA:O	13:Z:289:GLU:HB2	2.20	0.41
13:Z:75:LEU:O	13:Z:79:TYR:HB3	2.20	0.41
4:C:100:ASP:OD1	4:C:100:ASP:N	2.54	0.41
4:C:286:THR:O	4:C:289:ILE:HG12	2.20	0.41
7:F:289:ASP:HB3	7:F:332:THR:HB	2.01	0.41
7:F:427:VAL:HG23	7:F:428:GLN:HG3	2.02	0.41
8:U:198:LEU:HD23	8:U:219:CYS:HA	2.01	0.41
8:U:472:ILE:HG13	8:U:473:VAL:N	2.35	0.41
9:V:375:PHE:HA	9:V:378:VAL:HB	2.02	0.41
6:E:171:LEU:HB2	6:E:295:LEU:HD13	2.01	0.41
1:G:126:LEU:HD23	1:G:130:ALA:HB3	2.01	0.41
8:U:436:ALA:HB1	8:U:472:ILE:HG21	2.02	0.41
8:U:592:GLY:HA2	8:U:628:ARG:HE	1.85	0.41
4:C:37:ASP:HB2	9:V:503:LYS:HB2	2.02	0.41
10:W:363:ILE:HA	10:W:366:MET:HG2	2.02	0.41
9:V:416:ARG:NH2	12:Y:350:VAL:O	2.53	0.41
2:A:201:PHE:HD2	2:A:208:PRO:HB3	1.85	0.41
2:A:241:ILE:HA	2:A:275:ASP:HB3	2.02	0.41
6:E:309:ARG:HD2	6:E:332:VAL:HG13	2.01	0.41
6:E:309:ARG:HD3	6:E:335:SER:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:334:ASN:OD1	11:X:337:ARG:NH2	2.53	0.41
11:X:379:ASP:OD1	11:X:380:GLN:N	2.54	0.41
12:Y:372:LYS:O	12:Y:376:LEU:HB2	2.21	0.41
4:C:211:PHE:HE2	4:C:213:ARG:HH11	1.68	0.41
6:E:114:GLU:HG3	6:E:118:LEU:HD23	2.02	0.41
8:U:150:ALA:O	8:U:154:ALA:CB	2.69	0.41
4:C:50:ASN:HD21	8:U:643:SER:HA	1.85	0.41
8:U:792:ASN:OD1	8:U:793:LYS:N	2.50	0.41
12:Y:39:ASP:O	12:Y:43:ALA:HB3	2.21	0.41
13:Z:101:LEU:HD13	13:Z:123:ILE:HD11	2.01	0.41
11:X:403:THR:HG22	13:Z:265:LEU:HD21	2.02	0.41
13:Z:277:ASN:HA	13:Z:280:ILE:HG13	2.02	0.41
13:Z:40:LEU:HB2	13:Z:52:ASN:O	2.21	0.41
2:A:165:GLN:HE21	2:A:241:ILE:H	1.68	0.41
5:D:39:ASP:N	8:U:179:TYR:HH	2.19	0.41
6:E:192:ASP:C	6:E:194:ASN:H	2.23	0.41
11:X:318:ILE:HD12	11:X:318:ILE:H	1.85	0.41
2:A:174:TYR:HB2	2:A:231:ASN:HD21	1.86	0.41
2:A:232:ARG:NH2	2:A:271:LEU:HB2	2.36	0.41
5:D:72:PHE:O	5:D:76:GLN:HB2	2.21	0.41
11:X:89:VAL:O	11:X:93:LEU:HB2	2.20	0.41
12:Y:119:GLY:O	12:Y:123:ALA:HB2	2.21	0.41
12:Y:382:LYS:O	12:Y:386:VAL:HG23	2.21	0.41
2:A:275:ASP:OD1	2:A:276:GLU:N	2.54	0.41
3:B:270:LEU:HA	3:B:273:VAL:HG12	2.02	0.41
4:C:275:GLU:HA	4:C:278:ASN:HB2	2.02	0.41
5:D:133:HIS:HB2	5:D:137:ASN:N	2.36	0.41
7:F:85:THR:HG23	7:F:86:LEU:H	1.86	0.41
1:G:56:VAL:HG21	1:G:88:ILE:HD12	2.03	0.41
12:Y:311:TYR:CD2	12:Y:314:LEU:HD21	2.56	0.41
2:A:395:PHE:HD2	2:A:412:ALA:HB2	1.85	0.41
5:D:115:ILE:HG22	5:D:139:LEU:HD21	2.02	0.41
7:F:294:LYS:HA	7:F:307:GLN:HE21	1.85	0.41
9:V:496:PHE:HB3	9:V:497:PRO:HD3	2.03	0.41
10:W:53:GLN:HG3	10:W:103:LYS:HE2	2.03	0.41
10:W:396:LEU:HA	10:W:399:ASN:HB3	2.02	0.41
13:Z:98:GLY:HA2	13:Z:99:PRO:HD3	1.91	0.41
10:W:131:VAL:HA	10:W:142:ARG:HD2	2.01	0.41
2:A:273:PHE:CE2	2:A:275:ASP:HB2	2.56	0.40
3:B:100:ASP:HA	3:B:103:ARG:HG2	2.02	0.40
5:D:267:ILE:HD13	5:D:309:MET:SD	2.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:LYS:HB3	1:G:21:GLU:HB3	2.04	0.40
8:U:600:ARG:O	8:U:604:HIS:CB	2.69	0.40
12:Y:334:LEU:O	12:Y:338:ILE:HG12	2.20	0.40
12:Y:361:SER:O	12:Y:365:GLN:HB3	2.22	0.40
2:A:151:ILE:HD12	2:A:152:PRO:HD2	2.02	0.40
2:A:296:GLN:HA	2:A:299:MET:HG2	2.03	0.40
5:D:346:SER:O	5:D:350:SER:OG	2.34	0.40
6:E:124:HIS:CG	6:E:195:PHE:CE2	3.01	0.40
1:G:185:VAL:HG22	1:G:216:LEU:HD11	2.02	0.40
10:W:222:LEU:CD1	10:W:222:LEU:N	2.83	0.40
2:A:418:LYS:O	2:A:422:LYS:HG3	2.22	0.40
3:B:220:LYS:HZ2	3:B:316:LEU:HD23	1.87	0.40
4:C:319:PRO:HA	4:C:320:PRO:HD3	1.99	0.40
6:E:74:THR:HG1	6:E:97:ARG:HH12	1.67	0.40
7:F:204:LEU:N	7:F:205:PRO:HD2	2.36	0.40
7:F:276:LYS:HD2	7:F:325:GLN:OE1	2.21	0.40
2:A:189:GLU:OE2	7:F:409:ARG:NE	2.54	0.40
12:Y:111:LEU:HA	12:Y:114:ILE:HG22	2.02	0.40
12:Y:233:ARG:HB2	12:Y:234:PRO:HD3	2.03	0.40
12:Y:258:GLN:O	12:Y:262:SER:CB	2.69	0.40
13:Z:183:THR:OG1	13:Z:188:SER:OG	2.33	0.40
13:Z:211:TYR:O	13:Z:215:VAL:HG23	2.21	0.40
2:A:368:ILE:HD11	2:A:405:THR:HA	2.04	0.40
4:C:267:SER:HA	4:C:270:GLN:HB2	2.04	0.40
5:D:340:GLN:O	5:D:344:ILE:HB	2.22	0.40
5:D:53:PHE:CE2	8:U:632:GLN:HB3	2.56	0.40
10:W:231:ILE:HG21	10:W:246:HIS:HB2	2.04	0.40
10:W:283:GLN:HE22	10:W:361:HIS:CE1	2.40	0.40
10:W:362:ASN:OD1	10:W:363:ILE:N	2.55	0.40
11:X:299:LEU:HB3	11:X:354:ILE:HD11	2.02	0.40
12:Y:71:ASN:HA	12:Y:74:LYS:HE3	2.03	0.40
3:B:232:LYS:HG3	3:B:392:GLY:HA3	2.04	0.40
5:D:133:HIS:HD2	5:D:138:ALA:HB3	1.87	0.40
5:D:267:ILE:HG12	5:D:311:THR:HB	2.04	0.40
6:E:185:ARG:O	6:E:189:SER:HB3	2.21	0.40
7:F:73:ILE:O	7:F:77:SER:CB	2.69	0.40
8:U:159:ARG:HH21	8:U:162:VAL:HA	1.86	0.40
9:V:501:TYR:CD1	13:Z:278:ASN:HA	2.56	0.40
11:X:290:VAL:HG13	11:X:302:PHE:HE1	1.86	0.40
12:Y:224:VAL:O	12:Y:228:MET:HB2	2.22	0.40
13:Z:201:LEU:O	13:Z:205:LEU:CB	2.70	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	G	217/223 (97%)	214 (99%)	3 (1%)	0	100	100
2	A	335/352 (95%)	301 (90%)	34 (10%)	0	100	100
3	B	326/340 (96%)	294 (90%)	30 (9%)	2 (1%)	28	70
4	C	334/385 (87%)	313 (94%)	21 (6%)	0	100	100
5	D	340/368 (92%)	317 (93%)	23 (7%)	0	100	100
6	E	341/379 (90%)	311 (91%)	28 (8%)	2 (1%)	28	70
7	F	353/380 (93%)	329 (93%)	23 (6%)	1 (0%)	44	81
8	U	743/841 (88%)	714 (96%)	29 (4%)	0	100	100
9	V	181/183 (99%)	170 (94%)	11 (6%)	0	100	100
10	W	452/456 (99%)	414 (92%)	38 (8%)	0	100	100
11	X	381/385 (99%)	375 (98%)	6 (2%)	0	100	100
12	Y	376/378 (100%)	357 (95%)	19 (5%)	0	100	100
13	Z	284/286 (99%)	267 (94%)	17 (6%)	0	100	100
14	a	372/374 (100%)	351 (94%)	21 (6%)	0	100	100
15	b	189/191 (99%)	174 (92%)	15 (8%)	0	100	100
16	c	285/287 (99%)	271 (95%)	14 (5%)	0	100	100
17	d	134/136 (98%)	123 (92%)	11 (8%)	0	100	100
18	e	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
19	f	664/848 (78%)	597 (90%)	67 (10%)	0	100	100
All	All	6375/6862 (93%)	5956 (93%)	414 (6%)	5 (0%)	58	88

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	169	PRO
3	B	168	ASP
7	F	168	TYR
6	E	114	GLU
6	E	115	VAL

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	G	174/178 (98%)	173 (99%)	1 (1%)	89	94
2	A	293/300 (98%)	292 (100%)	1 (0%)	94	96
3	B	289/298 (97%)	286 (99%)	3 (1%)	80	90
4	C	297/333 (89%)	292 (98%)	5 (2%)	66	84
5	D	301/321 (94%)	298 (99%)	3 (1%)	80	90
6	E	300/333 (90%)	297 (99%)	3 (1%)	80	90
7	F	308/326 (94%)	304 (99%)	4 (1%)	73	87
8	U	639/720 (89%)	636 (100%)	3 (0%)	91	95
9	V	164/164 (100%)	164 (100%)	0	100	100
10	W	416/416 (100%)	413 (99%)	3 (1%)	87	93
11	X	331/331 (100%)	331 (100%)	0	100	100
12	Y	334/334 (100%)	333 (100%)	1 (0%)	94	96
13	Z	257/257 (100%)	256 (100%)	1 (0%)	93	95
14	a	334/334 (100%)	334 (100%)	0	100	100
15	b	167/167 (100%)	166 (99%)	1 (1%)	89	94
16	c	252/252 (100%)	251 (100%)	1 (0%)	93	95
17	d	121/121 (100%)	120 (99%)	1 (1%)	85	92
18	e	63/63 (100%)	63 (100%)	0	100	100
19	f	579/714 (81%)	563 (97%)	16 (3%)	49	74
All	All	5619/5962 (94%)	5572 (99%)	47 (1%)	86	92

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	117	ASN
2	A	108	ASP
3	B	168	ASP
3	B	260	LEU
3	B	355	LEU
4	C	248	MET
4	C	287	LYS
4	C	293	MET
4	C	311	ILE
4	C	376	VAL
5	D	230	VAL
5	D	353	ASN
5	D	370	ILE
6	E	216	ARG
6	E	262	ASN
6	E	322	LYS
7	F	85	THR
7	F	168	TYR
7	F	180	ARG
7	F	323	ASN
8	U	397	THR
8	U	427	LEU
8	U	616	ARG
10	W	33	LYS
10	W	116	THR
10	W	211	THR
12	Y	343	LEU
13	Z	90	ARG
15	b	25	ARG
16	c	282	ARG
17	d	190	LEU
19	f	39	LYS
19	f	89	MET
19	f	184	LEU
19	f	188	VAL
19	f	275	MET
19	f	314	TYR
19	f	391	LEU
19	f	460	ASP
19	f	473	ASN
19	f	493	ASN
19	f	565	ASN

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Mol	Chain	Res	Type
19	f	569	LYS
19	f	639	LYS
19	f	696	LEU
19	f	745	LEU
19	f	788	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	100	ASN
1	G	117	ASN
2	A	165	GLN
2	A	314	ASN
3	B	131	HIS
3	B	193	GLN
3	B	241	ASN
3	B	315	GLN
4	C	22	GLN
5	D	65	GLN
5	D	133	HIS
5	D	175	GLN
5	D	286	GLN
5	D	301	GLN
5	D	353	ASN
6	E	45	ASN
6	E	124	HIS
6	E	262	ASN
7	F	323	ASN
7	F	428	GLN
8	U	247	GLN
8	U	259	GLN
8	U	340	GLN
8	U	415	HIS
8	U	453	HIS
8	U	500	ASN
8	U	754	HIS
8	U	801	GLN
9	V	329	HIS
10	W	86	ASN
10	W	218	ASN
10	W	236	HIS
11	X	349	HIS

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Mol	Chain	Res	Type
11	X	406	ASN
12	Y	178	ASN
12	Y	363	ASN
13	Z	189	GLN
13	Z	194	GLN
13	Z	282	ASN
14	a	35	HIS
14	a	152	HIS
14	a	264	ASN
14	a	288	HIS
15	b	29	GLN
15	b	34	ASN
15	b	76	HIS
15	b	99	HIS
15	b	149	ASN
16	c	183	HIS
16	c	241	ASN
16	c	254	ASN
17	d	141	GLN
19	f	180	GLN
19	f	301	HIS
19	f	327	ASN
19	f	405	HIS
19	f	475	ASN
19	f	493	ASN
19	f	566	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
11	X	1
10	W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	W	205:ILE	C	206:SER	N	3.19
1	X	311:ALA	C	312:GLU	N	3.16