



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:44 PM EDT

PDB ID : 3HKZ / pdb_00003hgz
Title : The X-ray crystal structure of RNA polymerase from Archaea
Authors : Murakami, K.S.
Deposited on : 2009-05-26
Resolution : 3.40 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

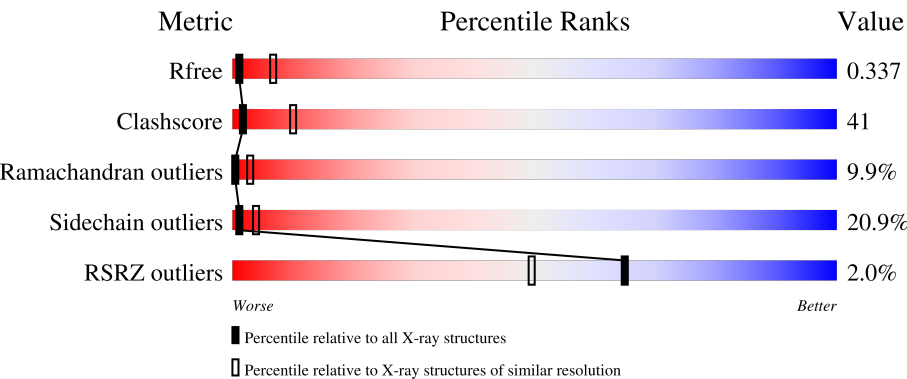
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	880	31%45%18%5%
1	I	880	29%47%17%5%
2	C	395	28%43%17%5%6% 2%
2	M	395	25%42%23%6% 2%
3	B	1124	29%47%18% 3%

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Mol	Chain	Length	Quality of chain
3	J	1124	
4	D	265	
4	O	265	
5	E	180	
5	Q	180	
6	F	113	
6	R	113	
7	G	132	
7	S	132	
8	H	84	
8	T	84	
9	K	95	
9	U	95	
10	L	92	
10	V	92	
11	N	66	
11	W	66	
12	P	48	
12	X	48	
13	Y	104	
13	Z	104	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	ZN	B	2001	-	-	X	-
14	ZN	J	2001	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	F3S	O	1001	-	-	X	-

2 Entry composition [i](#)

There are 16 unique types of molecules in this entry. The entry contains 53072 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 DNA-directed RNA polymerase subunit A'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	0	0
			6673	4248	1178	1221	26			
1	I	836	Total	C	N	O	S	0	0	0
			6673	4248	1178	1221	26			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit A''.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	370	Total	C	N	O	S	0	0	0
			2868	1818	490	551	9			
2	M	370	Total	C	N	O	S	0	0	0
			2868	1818	490	551	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	expression tag	UNP P58192
C	2	GLU	-	expression tag	UNP P58192
C	3	GLY	-	expression tag	UNP P58192
M	1	MET	-	expression tag	UNP P58192
M	2	GLU	-	expression tag	UNP P58192
M	3	GLY	-	expression tag	UNP P58192

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	1090	Total	C	N	O	S	0	0	0
			8645	5483	1529	1602	31			
3	J	1090	Total	C	N	O	S	0	0	0
			8645	5483	1529	1602	31			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	264	Total	C	N	O	S	0	0	0
			2114	1355	342	403	14			
4	O	264	Total	C	N	O	S	0	0	0
			2114	1355	342	403	14			

- Molecule 5 is a protein called DNA-directed RNA polymerase, subunit E' (RpoE1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	176	Total	C	N	O	S	0	0	0
			1402	903	236	259	4			
5	Q	176	Total	C	N	O	S	0	0	0
			1402	903	236	259	4			

- Molecule 6 is a protein called DNA-directed RNA polymerase, subunit F (RpoF).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	89	Total	C	N	O	S	0	0	0
			694	433	115	142	4			
6	R	89	Total	C	N	O	S	0	0	0
			694	433	115	142	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase, subunit G (RpoG).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	113	Total	C	N	O	S	0	0	0
			884	556	149	174	5			
7	S	113	Total	C	N	O	S	0	0	0
			884	556	149	174	5			

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	74	Total	C	N	O		0	0	0
			611	397	109	105				
8	T	74	Total	C	N	O		0	0	0
			611	397	109	105				

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	U	82	Total	C	N	O	S	0	0	0
			658	420	121	116	1			

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	92	Total	C	N	O	S	0	0	0
			723	459	121	141	2			
10	V	92	Total	C	N	O	S	0	0	0
			723	459	121	141	2			

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	N	64	Total	C	N	O	S	0	0	0
			514	326	94	88	6			
11	W	64	Total	C	N	O	S	0	0	0
			514	326	94	88	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	P	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			
12	X	43	Total	C	N	O	S	0	0	0
			346	230	58	53	5			

- Molecule 13 is a protein called DNA-directed RNA polymerase subunit 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	Y	45	Total	C	N	O	S	0	0	0
			391	245	68	77	1			
13	Z	45	Total	C	N	O	S	0	0	0
			391	245	68	77	1			

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	1	Total	Zn	0	0
			1	1		

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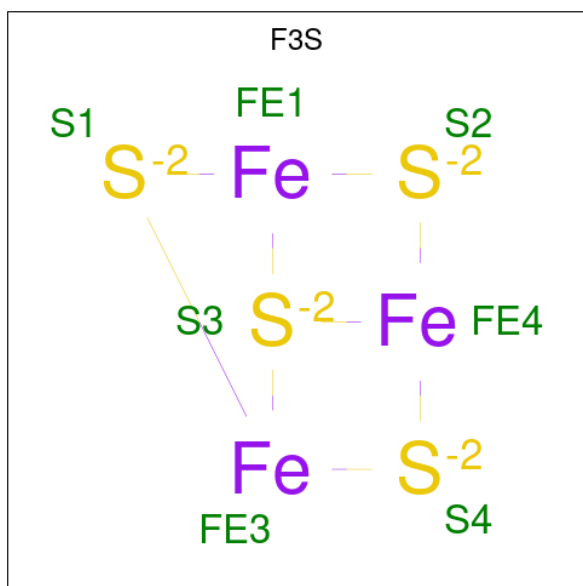
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	N	1	Total	Zn	0	0
			1	1		
14	P	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	J	1	Total	Zn	0	0
			1	1		
14	W	1	Total	Zn	0	0
			1	1		
14	X	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	I	1	Total	Mg	0	0
			1	1		

- Molecule 16 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	Fe	S	0	0
			7	3	4		

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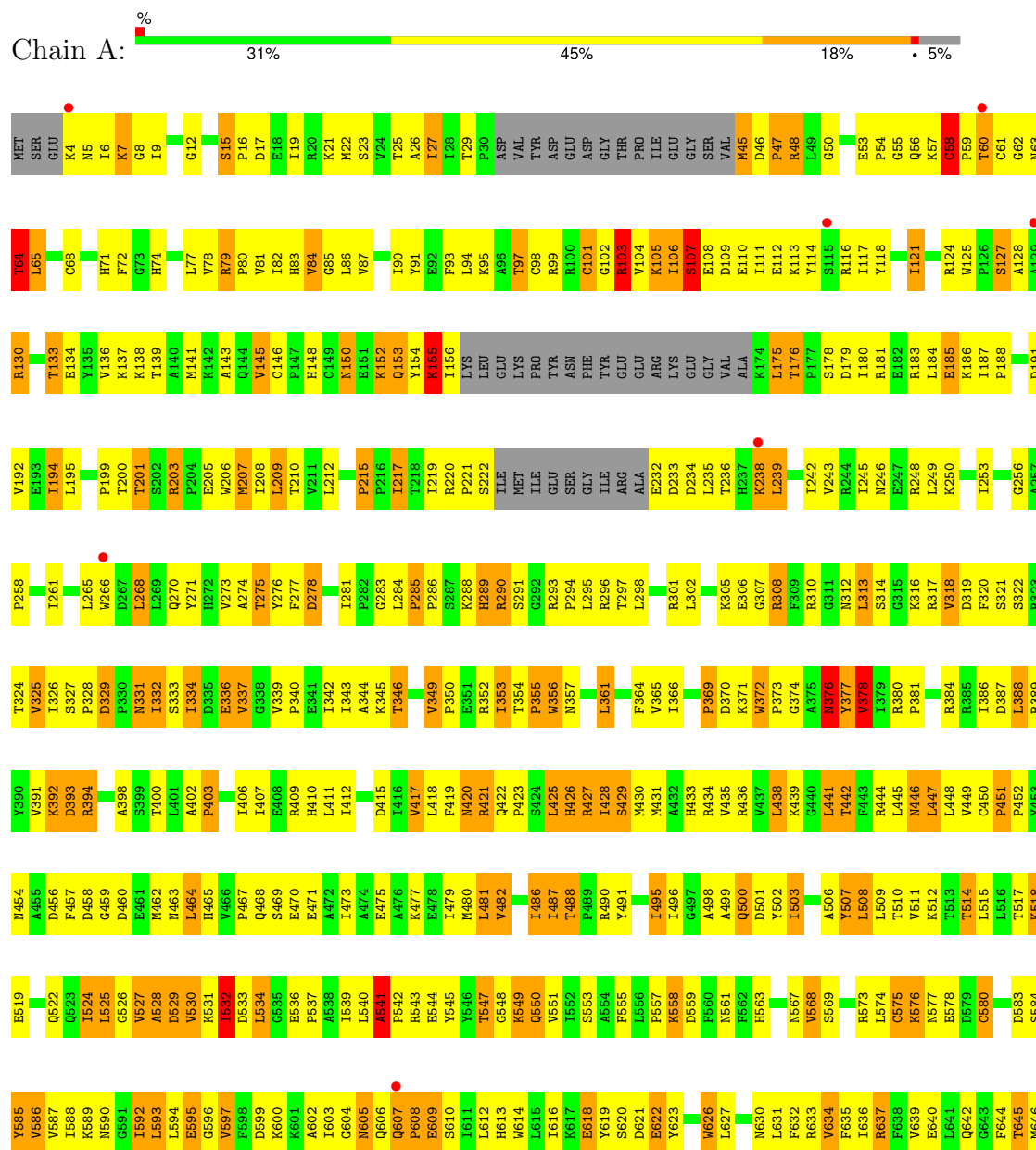
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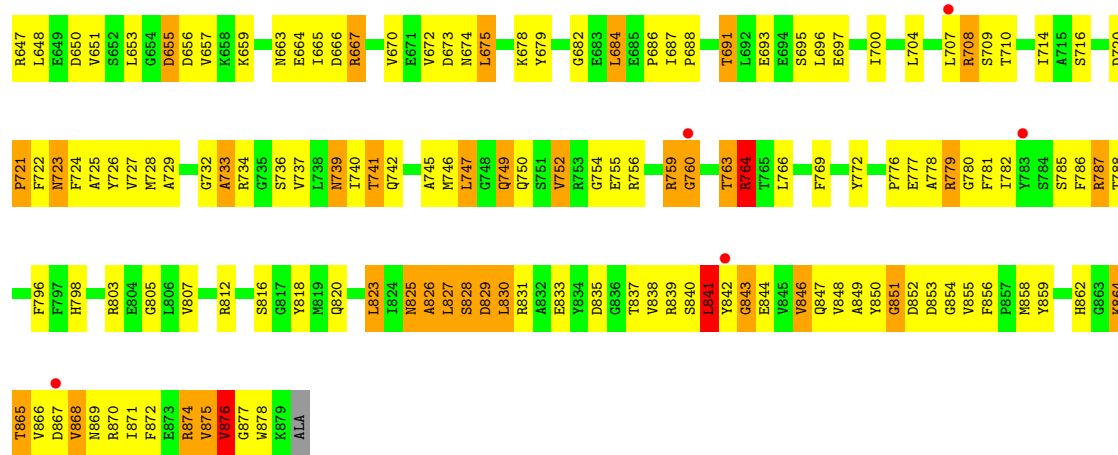
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
16	O	1	7	3	4	0	0

3 Residue-property plots

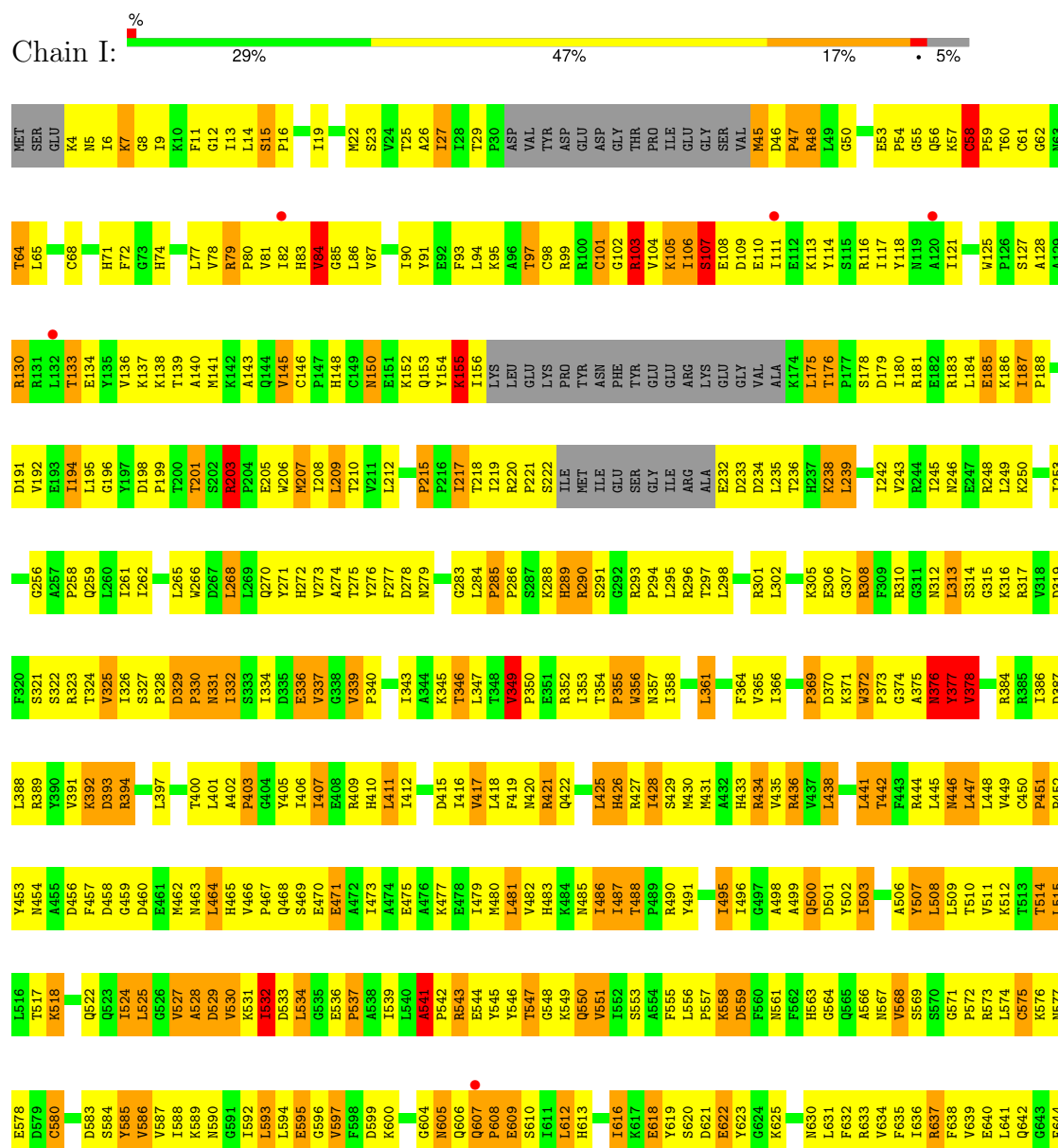
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

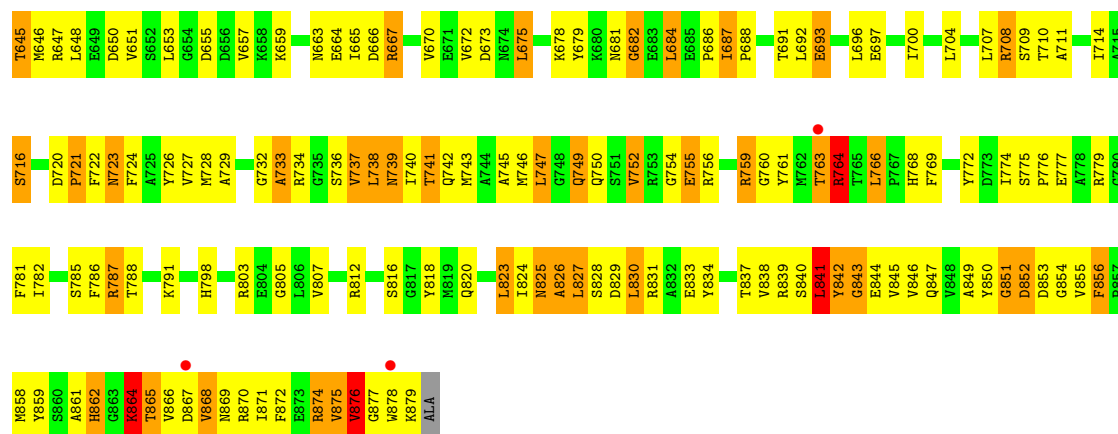
- Molecule 1: DNA-directed RNA polymerase subunit A'



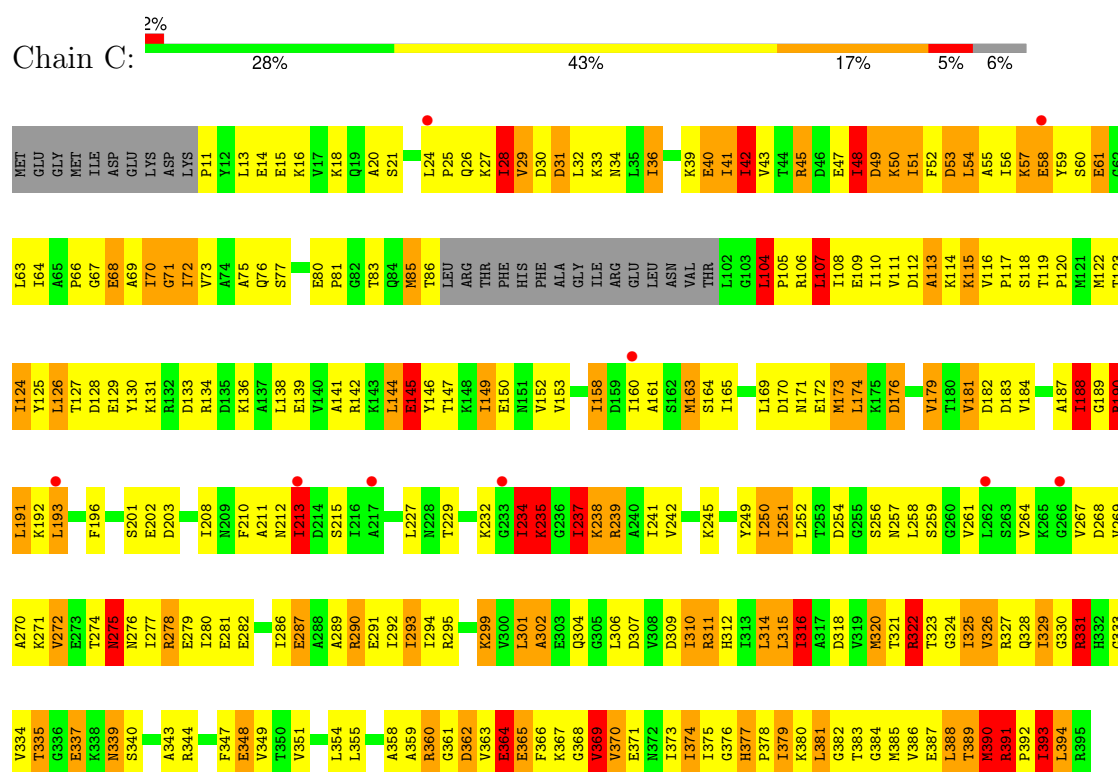


• Molecule 1: DNA-directed RNA polymerase subunit A'

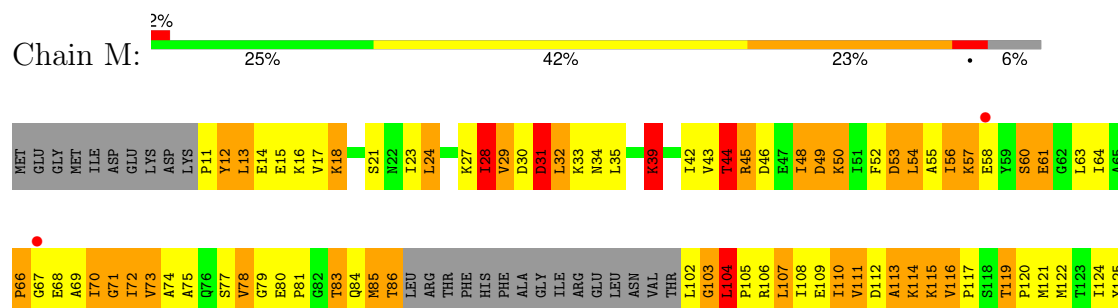


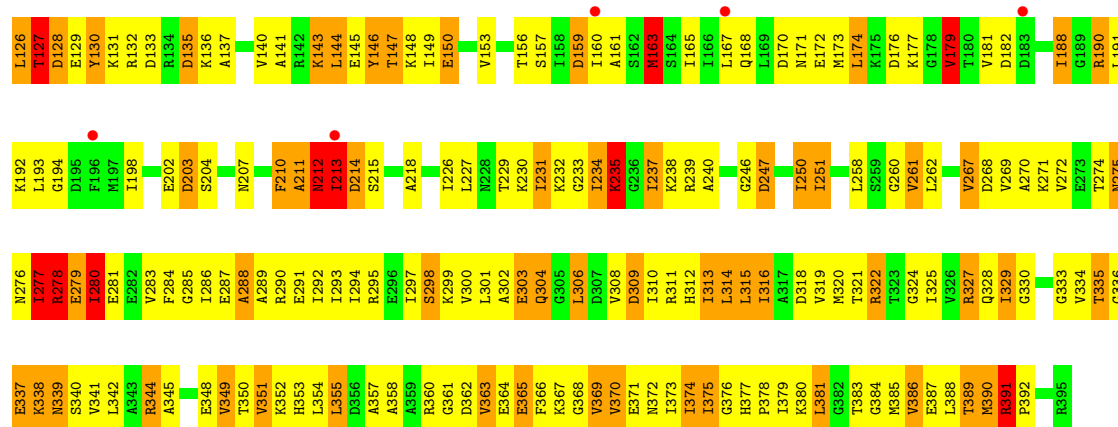


• Molecule 2: DNA-directed RNA polymerase subunit A''

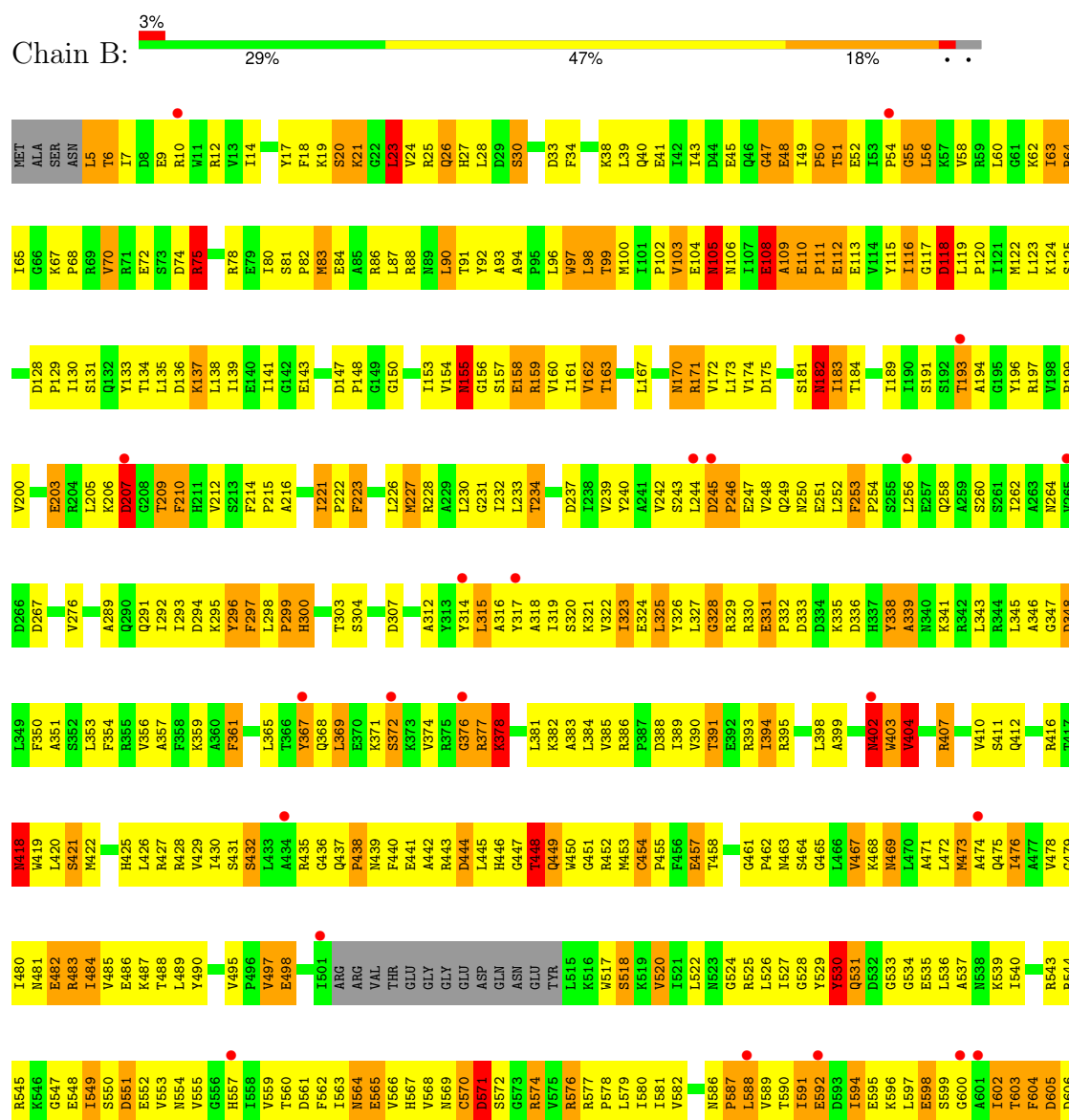


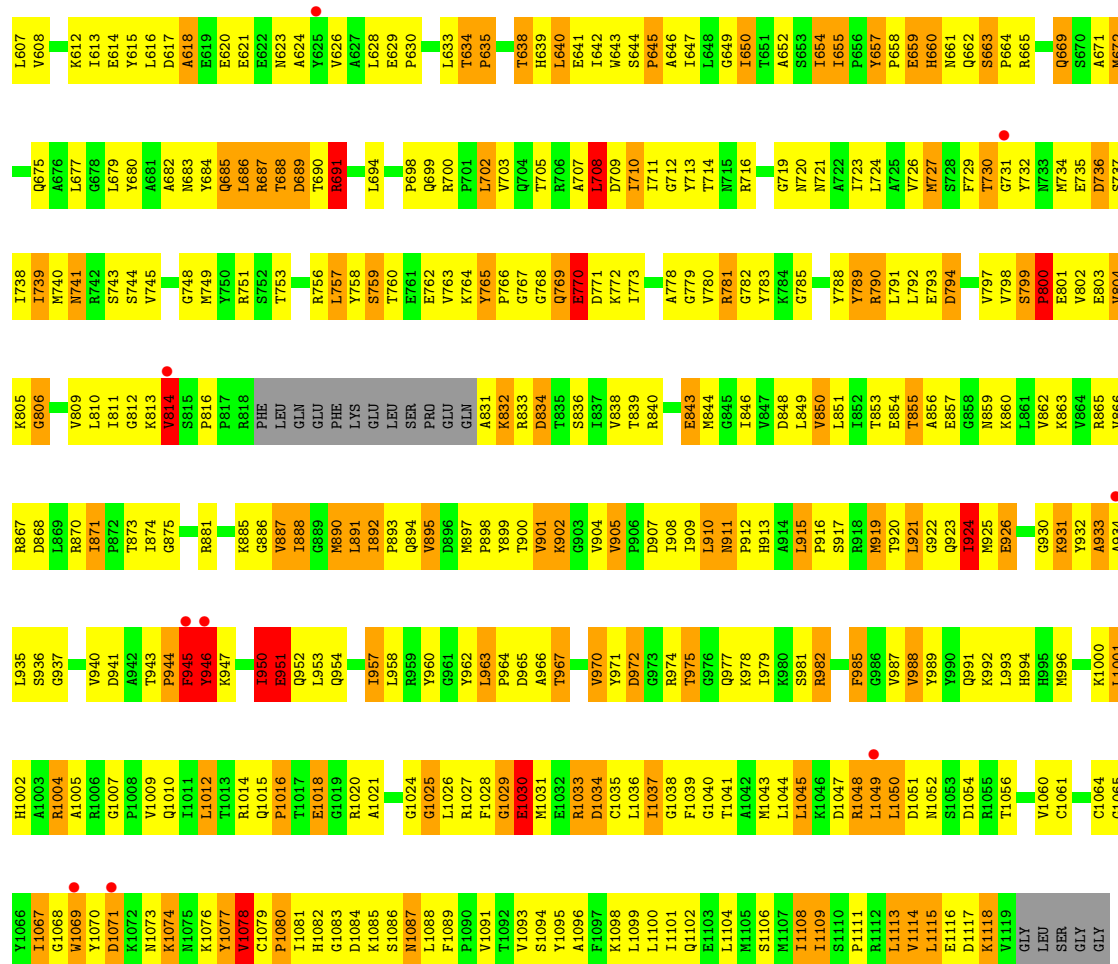
• Molecule 2: DNA-directed RNA polymerase subunit A''



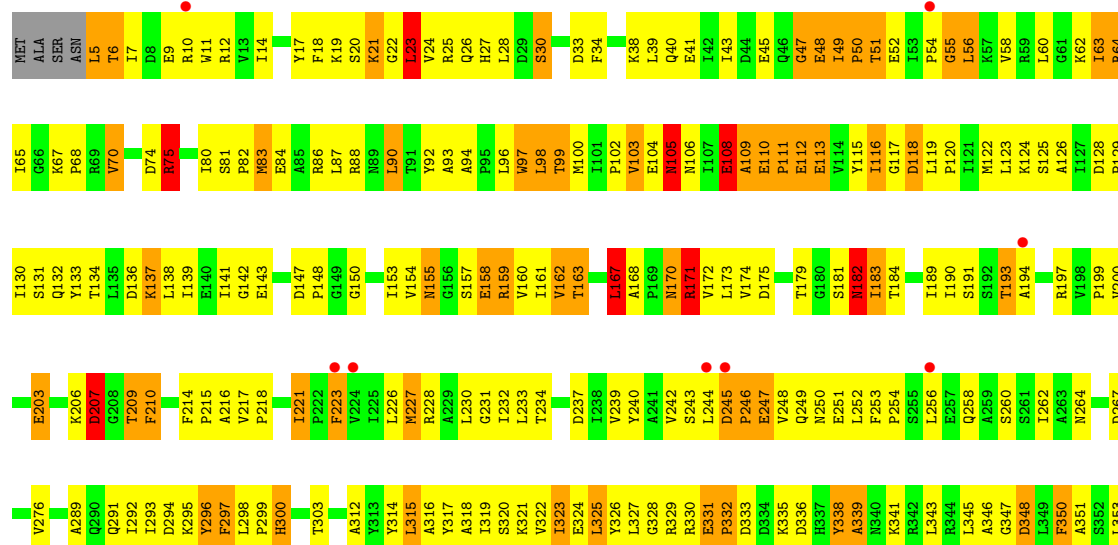


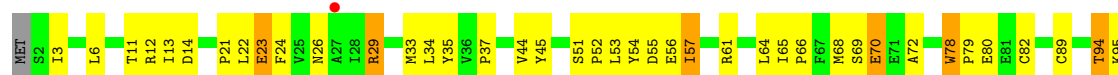
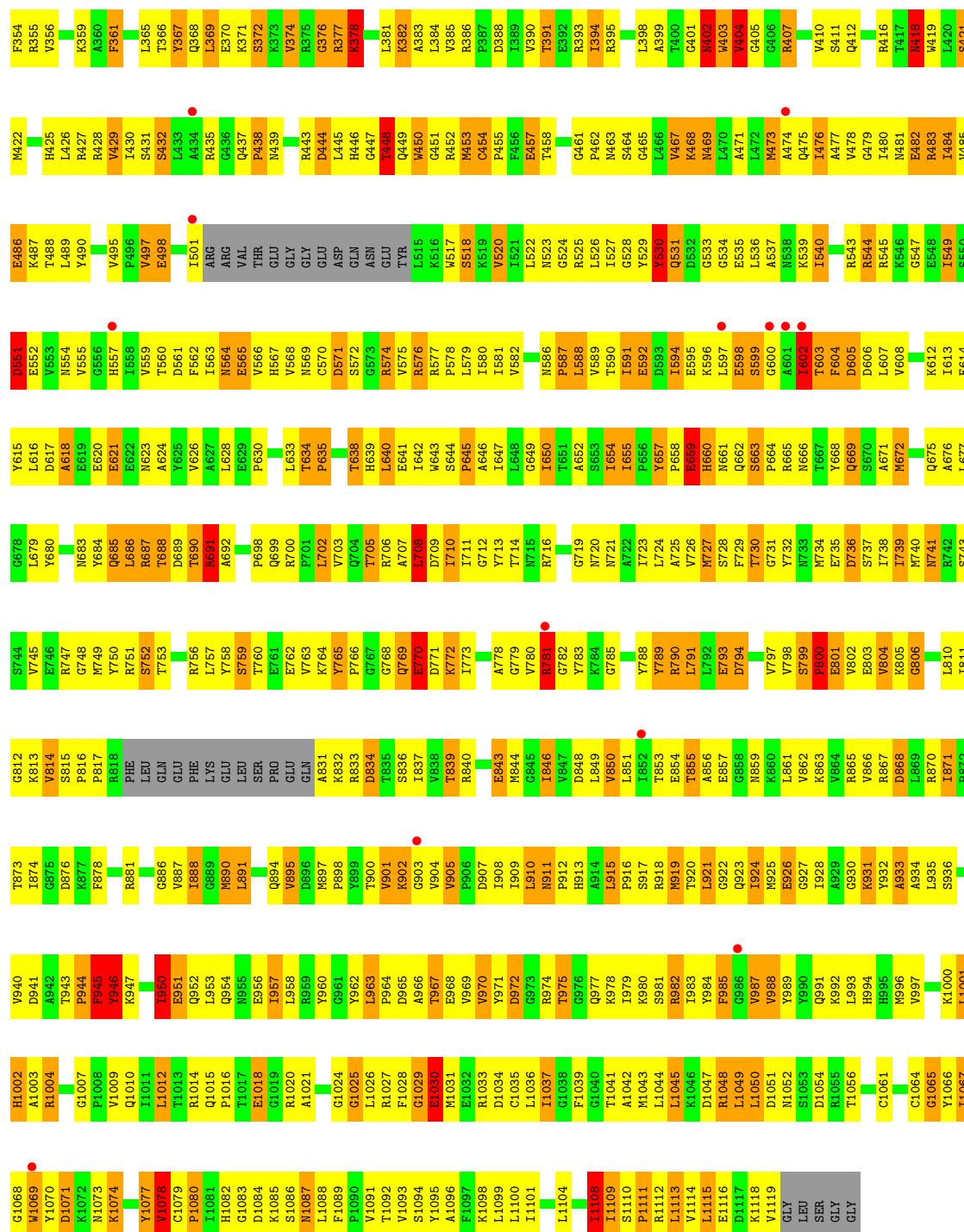
● Molecule 3: DNA-directed RNA polymerase subunit B

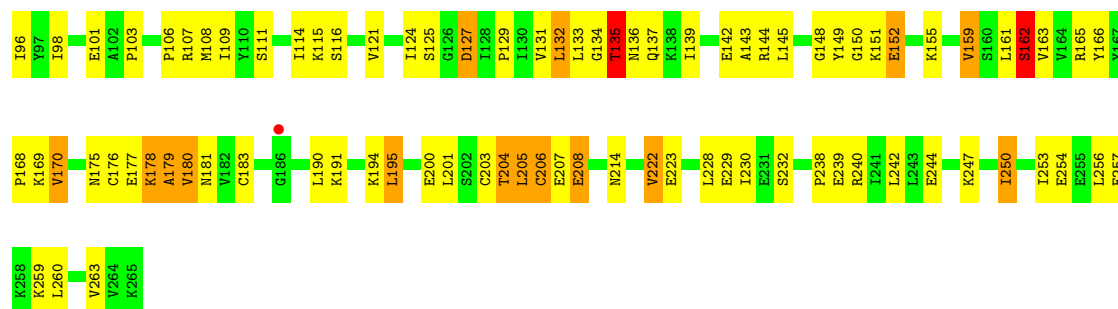




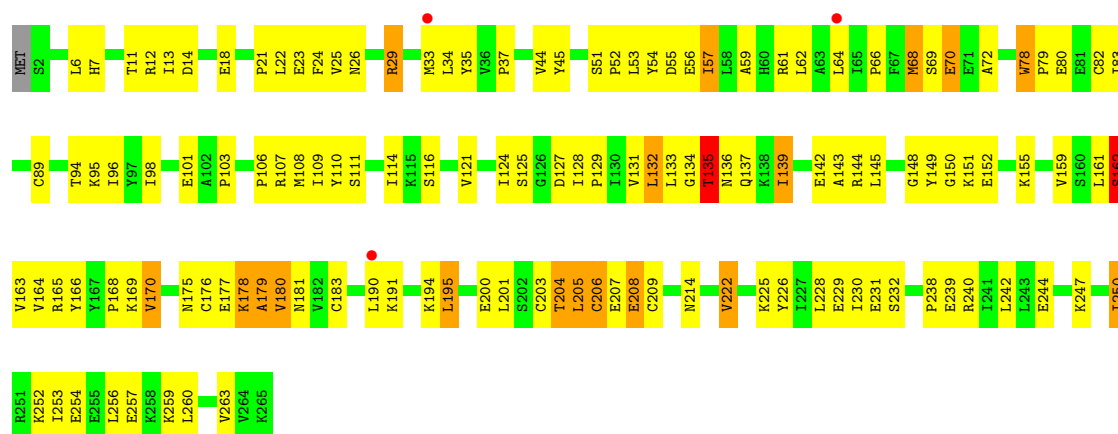
- Molecule 3: DNA-directed RNA polymerase subunit B



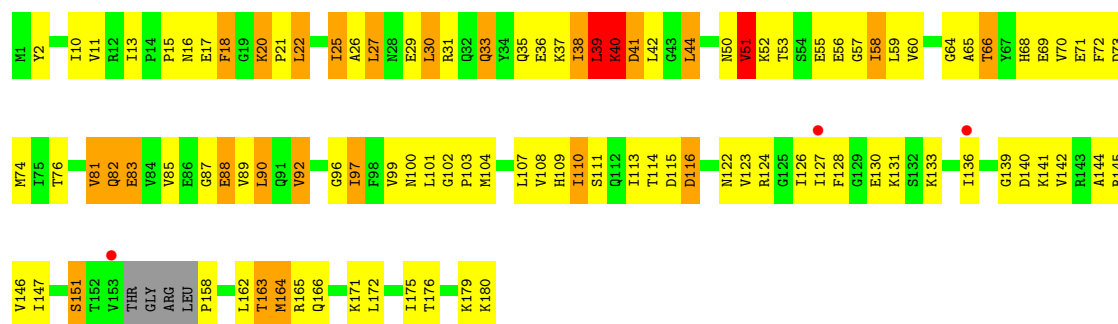




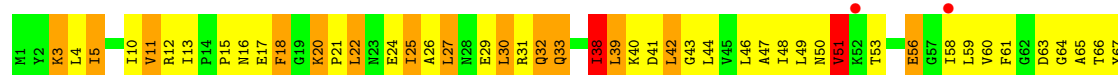
• Molecule 4: DNA-directed RNA polymerase subunit D

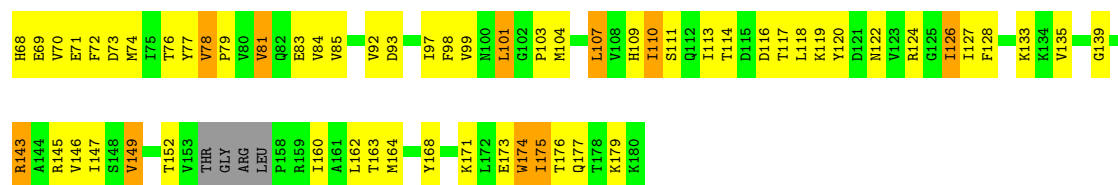


• Molecule 5: DNA-directed RNA polymerase, subunit E' (RpoE1)

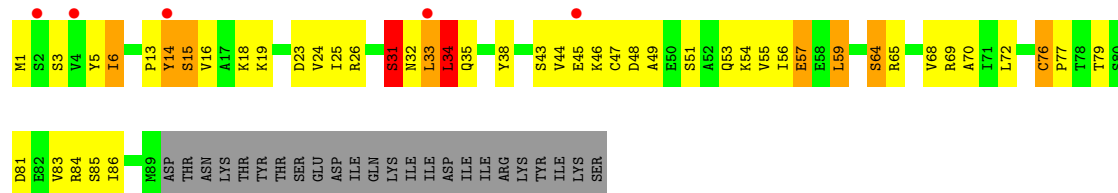


• Molecule 5: DNA-directed RNA polymerase, subunit E' (RpoE1)

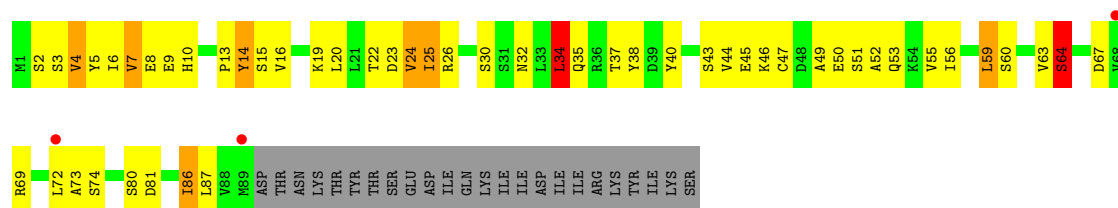




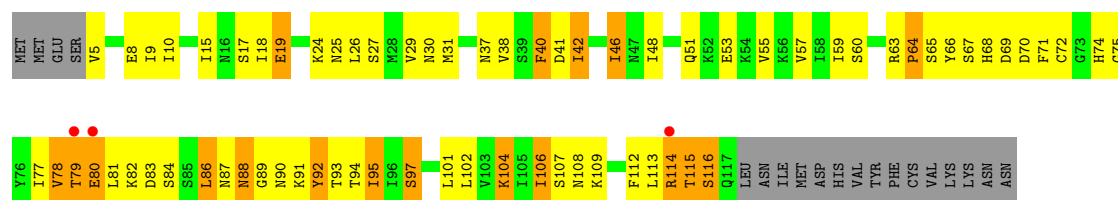
• Molecule 6: DNA-directed RNA polymerase, subunit F (RpoF)



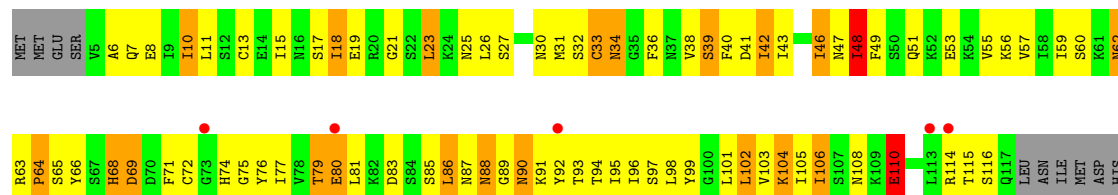
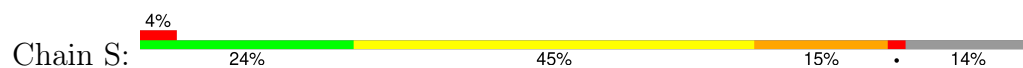
• Molecule 6: DNA-directed RNA polymerase, subunit F (RpoF)



• Molecule 7: DNA-directed RNA polymerase, subunit G (RpoG)



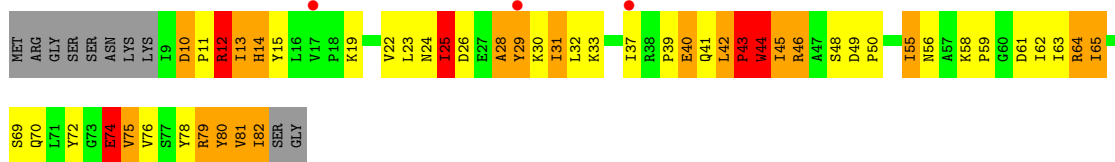
• Molecule 7: DNA-directed RNA polymerase, subunit G (RpoG)



VAL
TYR
PHE
CYS
VAL
LVS
LVS
ASN

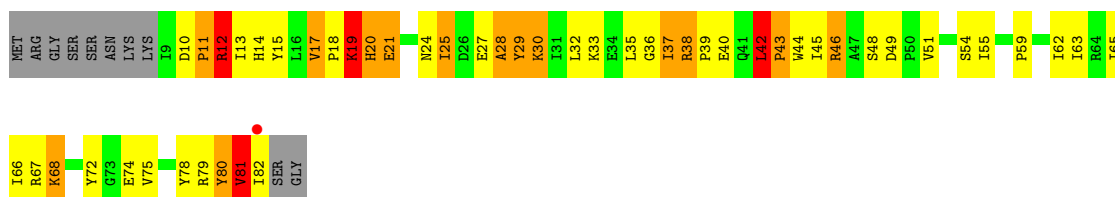
• Molecule 8: DNA-directed RNA polymerase subunit H

Chain H: 4% 29% 32% 21% 6% 12%



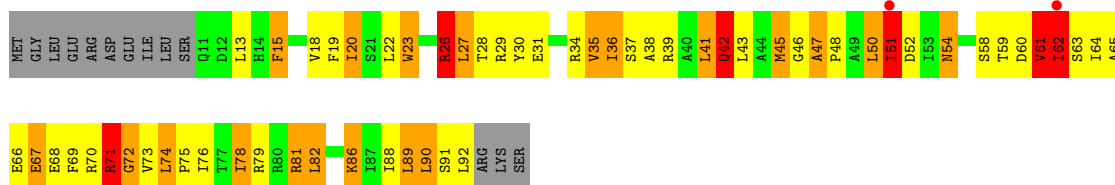
• Molecule 8: DNA-directed RNA polymerase subunit H

Chain T: % 29% 38% 17% 5% 12%



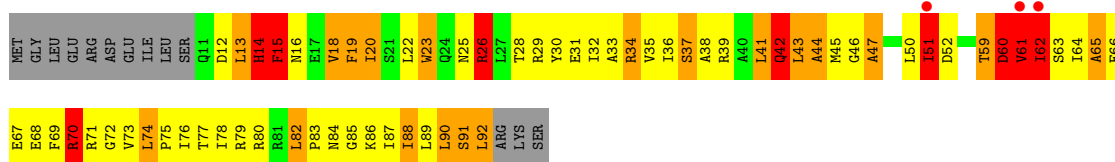
• Molecule 9: DNA-directed RNA polymerase subunit K

Chain K: 2% 24% 35% 21% 6% 14%



• Molecule 9: DNA-directed RNA polymerase subunit K

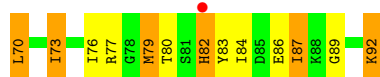
Chain U: 3% 16% 41% 20% 9% 14%



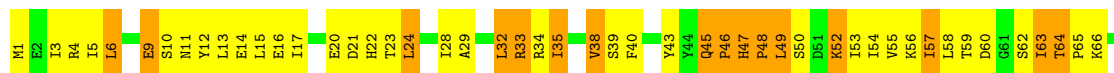
• Molecule 10: DNA-directed RNA polymerase subunit L

Chain L: % 39% 36% 25%

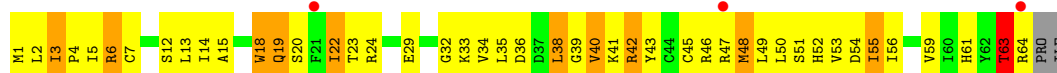




• Molecule 10: DNA-directed RNA polymerase subunit L



• Molecule 11: DNA-directed RNA polymerase subunit N



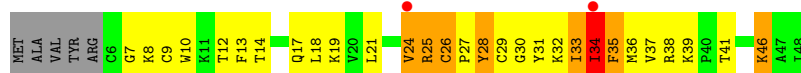
• Molecule 11: DNA-directed RNA polymerase subunit N



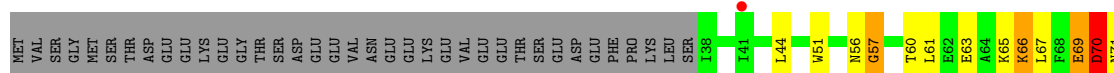
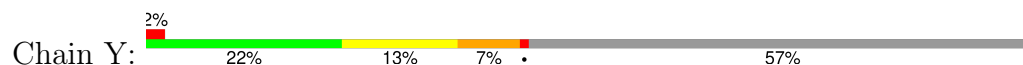
• Molecule 12: DNA-directed RNA polymerase subunit P

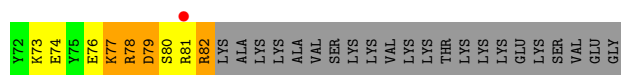


• Molecule 12: DNA-directed RNA polymerase subunit P

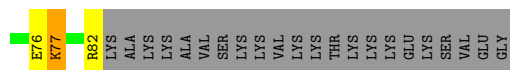
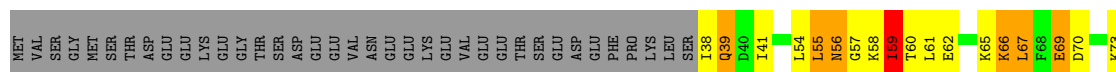
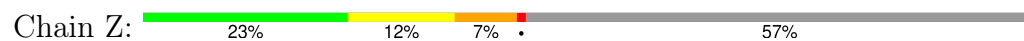


• Molecule 13: DNA-directed RNA polymerase subunit 13





- Molecule 13: DNA-directed RNA polymerase subunit 13



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.82Å 201.24Å 196.05Å 90.00° 100.92° 90.00°	Depositor
Resolution (Å)	40.00 – 3.40 40.00 – 3.40	Depositor EDS
% Data completeness (in resolution range)	80.3 (40.00-3.40) 80.3 (40.00-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.265 , 0.341 0.264 , 0.337	Depositor DCC
R_{free} test set	5323 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	53072	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, F3S, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	0/6815	1.10	40/9219 (0.4%)
1	I	0.81	1/6815 (0.0%)	1.12	45/9219 (0.5%)
2	C	0.92	2/2892 (0.1%)	1.25	22/3891 (0.6%)
2	M	0.91	1/2892 (0.0%)	1.17	15/3891 (0.4%)
3	B	0.79	0/8810	1.12	49/11921 (0.4%)
3	J	0.79	2/8810 (0.0%)	1.14	48/11921 (0.4%)
4	D	0.64	0/2152	0.95	3/2911 (0.1%)
4	O	0.66	0/2152	0.94	2/2911 (0.1%)
5	E	0.75	0/1423	1.07	7/1919 (0.4%)
5	Q	0.71	0/1423	1.01	5/1919 (0.3%)
6	F	0.71	0/701	0.99	2/949 (0.2%)
6	R	0.73	0/701	1.10	4/949 (0.4%)
7	G	0.85	0/895	1.08	2/1203 (0.2%)
7	S	0.92	0/895	1.08	4/1203 (0.3%)
8	H	0.69	0/625	1.09	4/848 (0.5%)
8	T	0.75	0/625	1.17	3/848 (0.4%)
9	K	0.80	2/667 (0.3%)	1.17	3/903 (0.3%)
9	U	0.97	2/667 (0.3%)	1.31	5/903 (0.6%)
10	L	0.68	0/733	1.05	1/986 (0.1%)
10	V	0.79	0/733	1.13	5/986 (0.5%)
11	N	0.70	0/523	1.05	2/705 (0.3%)
11	W	0.67	0/523	1.04	1/705 (0.1%)
12	P	0.80	0/354	1.13	4/475 (0.8%)
12	X	0.80	0/354	1.12	3/475 (0.6%)
13	Y	0.91	0/395	1.01	0/527
13	Z	0.82	0/395	1.14	0/527
All	All	0.79	10/53970 (0.0%)	1.11	279/72914 (0.4%)

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
2	M	0	1
3	B	0	1
3	J	0	1
7	G	0	1
9	K	0	1
9	U	0	1
All	All	0	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	28	ILE	CA-CB	7.01	1.64	1.54
9	U	62	ILE	CA-CB	6.19	1.62	1.54
9	U	51	ILE	CA-CB	6.10	1.62	1.54
9	K	51	ILE	CA-CB	5.53	1.61	1.54
3	J	1092	THR	CA-CB	5.30	1.59	1.53
2	M	66	PRO	CA-C	5.20	1.59	1.52
3	J	602	ILE	CA-CB	5.05	1.61	1.54
2	C	213	ILE	CA-CB	5.03	1.61	1.54
9	K	62	ILE	CA-CB	5.01	1.61	1.54
1	I	876	VAL	CA-CB	5.00	1.61	1.54

All (279) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	862	HIS	N-CA-C	-10.34	102.83	114.62
9	U	60	ASP	N-CA-C	9.62	124.69	110.17
3	J	209	THR	N-CA-C	-9.35	102.97	114.75
3	B	398	LEU	N-CA-C	-9.25	103.09	114.75
1	I	605	ASN	N-CA-C	-8.96	102.48	113.15
3	J	398	LEU	N-CA-C	-8.85	103.32	114.56
2	C	377	HIS	CA-C-N	8.81	128.83	119.76
2	C	377	HIS	C-N-CA	8.81	128.83	119.76
2	M	237	ILE	N-CA-C	8.75	118.70	110.74
1	A	862	HIS	N-CA-C	-8.62	104.79	114.62
3	J	905	VAL	CA-C-N	-8.59	111.89	120.31
3	J	905	VAL	C-N-CA	-8.59	111.89	120.31
3	B	209	THR	N-CA-C	-8.53	104.00	114.75
3	J	350	PHE	N-CA-C	-8.38	103.18	113.41
1	A	846	VAL	N-CA-C	-8.24	104.48	111.56
3	B	548	GLU	N-CA-C	-8.12	105.36	114.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	536	GLU	CA-C-N	8.10	129.96	119.84
1	I	536	GLU	C-N-CA	8.10	129.96	119.84
7	G	79	THR	N-CA-C	8.09	121.45	109.24
12	X	7	GLY	N-CA-C	8.00	122.45	112.14
1	A	605	ASN	N-CA-C	-7.81	103.86	113.15
5	E	20	LYS	CA-C-N	7.80	129.60	119.84
5	E	20	LYS	C-N-CA	7.80	129.60	119.84
3	J	799	SER	CA-C-N	7.69	129.46	119.84
3	J	799	SER	C-N-CA	7.69	129.46	119.84
2	C	54	LEU	N-CA-C	-7.58	104.26	113.97
5	Q	3	LYS	N-CA-C	7.58	120.75	108.32
3	B	571	ASP	N-CA-C	7.54	126.86	110.80
3	J	571	ASP	N-CA-C	7.50	126.77	110.80
3	J	116	ILE	N-CA-C	7.32	117.40	111.62
3	B	799	SER	CA-C-N	7.30	128.96	119.84
3	B	799	SER	C-N-CA	7.30	128.96	119.84
3	J	45	GLU	N-CA-C	-7.26	104.45	113.38
10	V	33	ARG	N-CA-C	-7.25	104.42	113.55
1	I	854	GLY	N-CA-C	-7.18	104.66	115.00
1	I	349	VAL	CA-C-N	7.18	128.81	119.84
1	I	349	VAL	C-N-CA	7.18	128.81	119.84
12	P	7	GLY	N-CA-C	7.17	121.39	112.14
5	E	60	VAL	N-CA-C	7.14	117.78	108.35
1	A	580	CYS	CA-C-N	7.14	128.76	119.84
1	A	580	CYS	C-N-CA	7.14	128.76	119.84
3	B	1069	TRP	N-CA-C	7.13	117.43	108.45
3	J	1007	GLY	CA-C-N	7.09	127.13	119.90
3	J	1007	GLY	C-N-CA	7.09	127.13	119.90
8	T	42	LEU	CA-C-N	7.07	128.68	119.84
8	T	42	LEU	C-N-CA	7.07	128.68	119.84
2	M	49	ASP	N-CA-C	-7.01	103.99	112.54
3	J	207	ASP	N-CA-C	6.95	120.39	108.02
1	I	215	PRO	CA-C-N	6.85	128.40	119.84
1	I	215	PRO	C-N-CA	6.85	128.40	119.84
7	S	55	VAL	N-CA-C	6.83	117.37	108.35
3	J	834	ASP	N-CA-C	6.79	118.47	111.14
2	M	103	GLY	N-CA-C	6.77	123.63	112.66
7	S	79	THR	N-CA-C	6.74	119.97	109.52
2	C	49	ASP	N-CA-C	-6.74	104.08	112.90
3	B	1004	ARG	N-CA-C	6.74	119.81	108.02
1	I	575	CYS	N-CA-C	6.71	121.30	112.72
1	I	580	CYS	CA-C-N	6.70	128.22	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	580	CYS	C-N-CA	6.70	128.22	119.84
3	J	1078	VAL	N-CA-C	6.68	117.91	108.36
1	I	336	GLU	N-CA-C	6.66	118.90	110.24
1	I	201	THR	N-CA-C	-6.66	107.03	114.62
3	J	1069	TRP	N-CA-C	6.65	116.83	108.45
3	B	765	TYR	CA-C-N	6.64	127.09	120.52
3	B	765	TYR	C-N-CA	6.64	127.09	120.52
3	J	772	LYS	N-CA-C	6.63	118.59	109.18
9	U	73	VAL	N-CA-C	6.63	117.51	111.81
2	C	379	ILE	N-CA-C	6.55	118.52	109.80
3	B	45	GLU	N-CA-C	-6.55	105.32	113.38
2	C	322	ARG	N-CA-C	-6.53	102.10	110.53
3	B	905	VAL	CA-C-N	-6.53	113.92	120.31
3	B	905	VAL	C-N-CA	-6.53	113.92	120.31
3	B	315	LEU	N-CA-C	-6.49	104.13	111.14
1	A	215	PRO	CA-C-N	6.49	127.95	119.84
1	A	215	PRO	C-N-CA	6.49	127.95	119.84
2	M	234	ILE	N-CA-C	6.47	118.10	109.37
9	U	65	ALA	N-CA-C	-6.46	105.70	113.97
1	A	848	VAL	N-CA-C	-6.45	104.04	110.30
9	K	64	ILE	N-CA-C	-6.43	104.33	113.07
1	I	451	PRO	CA-C-N	-6.43	112.28	118.97
1	I	451	PRO	C-N-CA	-6.43	112.28	118.97
2	M	39	LYS	N-CA-C	-6.41	105.10	113.12
12	X	25	ARG	N-CA-C	6.40	114.03	108.78
1	A	622	GLU	N-CA-C	-6.38	105.51	113.55
6	R	34	LEU	N-CA-C	-6.37	106.05	113.88
3	B	339	ALA	N-CA-C	-6.36	104.23	114.09
3	J	565	GLU	N-CA-C	6.36	120.24	110.20
1	A	536	GLU	CA-C-N	6.35	127.78	119.84
1	A	536	GLU	C-N-CA	6.35	127.78	119.84
9	U	85	GLY	N-CA-C	-6.35	106.48	115.30
2	C	42	ILE	N-CA-C	6.34	117.91	111.00
3	J	765	TYR	CA-C-N	6.33	126.79	120.52
3	J	765	TYR	C-N-CA	6.33	126.79	120.52
2	C	316	ILE	CB-CA-C	-6.32	103.79	111.88
1	A	575	CYS	N-CA-C	6.30	120.78	112.72
3	J	339	ALA	N-CA-C	-6.29	104.85	114.16
2	C	68	GLU	N-CA-C	6.25	116.53	108.34
1	I	329	ASP	CA-C-N	6.25	127.66	119.84
1	I	329	ASP	C-N-CA	6.25	127.66	119.84
1	A	854	GLY	N-CA-C	-6.24	106.01	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1078	VAL	N-CA-C	6.24	117.28	108.36
10	V	13	LEU	N-CA-C	6.22	118.56	107.80
3	B	1025	GLY	N-CA-C	6.21	119.16	112.33
3	J	963	LEU	CA-C-N	6.20	127.59	119.84
3	J	963	LEU	C-N-CA	6.20	127.59	119.84
3	B	26	GLN	N-CA-C	-6.19	104.53	111.28
2	M	336	GLY	N-CA-C	-6.19	101.92	111.64
6	R	5	TYR	N-CA-C	6.18	118.48	108.34
3	B	207	ASP	N-CA-C	6.16	118.99	108.02
3	B	1037	ILE	N-CA-C	-6.16	106.22	113.42
1	I	187	ILE	CA-C-N	6.13	126.04	119.85
1	I	187	ILE	C-N-CA	6.13	126.04	119.85
1	A	250	LYS	N-CA-C	-6.12	105.85	113.38
3	B	834	ASP	N-CA-C	6.11	117.73	111.14
3	J	454	CYS	CA-C-N	6.10	125.80	119.64
3	J	454	CYS	C-N-CA	6.10	125.80	119.64
2	C	107	LEU	N-CA-C	-6.08	104.57	111.14
2	C	391	ARG	CA-C-N	-6.04	113.72	119.76
2	C	391	ARG	C-N-CA	-6.04	113.72	119.76
3	B	1007	GLY	CA-C-N	6.03	126.04	119.89
3	B	1007	GLY	C-N-CA	6.03	126.04	119.89
3	J	1025	GLY	N-CA-C	6.02	118.95	112.33
3	J	866	VAL	N-CA-C	6.01	117.30	106.61
1	A	318	VAL	N-CA-C	5.95	117.33	108.46
3	B	963	LEU	CA-C-N	5.95	126.10	119.32
3	B	963	LEU	C-N-CA	5.95	126.10	119.32
4	D	78	TRP	CA-C-N	5.95	127.28	119.84
4	D	78	TRP	C-N-CA	5.95	127.28	119.84
9	U	26	ARG	N-CA-C	5.94	123.45	110.80
1	I	451	PRO	N-CA-C	5.94	117.94	110.70
2	C	234	ILE	N-CA-C	5.90	116.37	108.11
3	J	1037	ILE	N-CA-C	-5.88	106.54	113.42
2	M	126	LEU	N-CA-C	5.86	119.50	110.42
3	B	1082	HIS	N-CA-C	5.84	119.11	109.94
1	I	843	GLY	N-CA-C	-5.84	106.44	116.01
8	T	63	ILE	N-CA-C	5.84	116.34	108.17
1	A	336	GLU	N-CA-C	5.83	117.82	110.24
12	X	35	PHE	N-CA-C	5.83	118.27	109.23
3	B	946	TYR	N-CA-C	5.81	123.18	110.80
3	J	1082	HIS	N-CA-C	5.81	119.06	109.94
3	B	116	ILE	N-CA-C	5.80	116.20	111.62
3	J	315	LEU	N-CA-C	-5.80	104.88	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	54	ASN	N-CA-C	5.79	117.81	107.80
1	I	541	ALA	CA-C-N	-5.78	113.59	119.83
1	I	541	ALA	C-N-CA	-5.78	113.59	119.83
1	A	830	LEU	N-CA-C	5.77	118.06	108.20
3	B	436	GLY	N-CA-C	-5.76	99.52	113.18
4	D	159	VAL	N-CA-C	5.76	117.05	108.46
1	A	451	PRO	N-CA-C	5.76	117.73	110.70
1	A	187	ILE	CA-C-N	5.71	125.61	119.85
1	A	187	ILE	C-N-CA	5.71	125.61	119.85
2	M	45	ARG	N-CA-C	5.69	120.94	113.20
3	J	843	GLU	N-CA-C	5.69	118.03	110.53
1	A	329	ASP	CA-C-N	5.68	126.94	119.84
1	A	329	ASP	C-N-CA	5.68	126.94	119.84
8	H	25	ILE	N-CA-C	5.67	121.13	109.34
3	B	454	CYS	CA-C-N	5.63	125.32	119.64
3	B	454	CYS	C-N-CA	5.63	125.32	119.64
6	R	46	LYS	N-CA-C	5.61	118.94	111.75
1	I	551	VAL	N-CA-C	5.59	117.00	110.62
3	B	1077	TYR	N-CA-C	5.59	118.90	111.30
5	Q	47	ALA	N-CA-C	5.58	116.72	107.73
1	A	655	ASP	CB-CA-C	-5.58	110.12	116.54
7	S	51	GLN	N-CA-C	5.58	118.08	111.33
1	I	655	ASP	CB-CA-C	-5.57	110.13	116.54
10	V	45	GLN	CA-C-N	5.57	126.80	119.84
10	V	45	GLN	C-N-CA	5.57	126.80	119.84
2	M	288	ALA	N-CA-C	-5.55	104.45	111.11
3	J	19	LYS	N-CA-C	-5.55	105.38	111.82
3	J	868	ASP	N-CA-C	5.54	117.14	107.49
3	J	1004	ARG	N-CA-C	5.52	117.68	108.02
1	A	541	ALA	CA-C-N	-5.52	114.11	119.90
1	A	541	ALA	C-N-CA	-5.52	114.11	119.90
2	M	163	MET	N-CA-C	5.52	118.13	111.40
3	J	551	ASP	N-CA-C	-5.52	107.12	112.97
8	H	14	HIS	N-CA-C	5.52	117.72	108.23
7	S	110	GLU	N-CA-C	5.51	118.26	110.50
1	A	281	ILE	CA-C-N	5.49	124.68	118.97
1	A	281	ILE	C-N-CA	5.49	124.68	118.97
5	E	58	ILE	N-CA-C	5.49	115.60	108.35
3	B	892	ILE	CA-C-N	5.49	125.46	120.03
3	B	892	ILE	C-N-CA	5.49	125.46	120.03
8	H	55	ILE	N-CA-C	5.48	115.74	107.80
10	L	15	LEU	N-CA-C	5.47	119.31	107.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	250	LYS	N-CA-C	-5.46	106.66	113.38
3	J	599	SER	N-CA-C	5.46	118.45	109.72
2	M	32	LEU	N-CA-C	-5.46	105.72	112.38
2	C	126	LEU	N-CA-C	5.44	117.55	110.53
3	B	407	ARG	N-CA-C	5.43	117.70	110.53
1	A	46	ASP	N-CA-C	5.43	120.39	108.66
3	J	108	GLU	N-CA-C	5.43	115.73	108.23
12	P	35	PHE	N-CA-C	5.43	118.29	109.06
3	B	1038	GLY	N-CA-C	-5.42	106.21	112.50
3	B	1002	HIS	N-CA-C	5.42	119.88	107.48
3	B	19	LYS	N-CA-C	-5.41	105.54	111.82
1	I	864	LYS	N-CA-C	5.41	122.32	110.80
3	B	866	VAL	N-CA-C	5.40	116.23	106.61
10	V	35	ILE	N-CA-C	5.40	116.14	107.98
5	Q	20	LYS	CA-C-N	5.40	126.59	119.84
5	Q	20	LYS	C-N-CA	5.40	126.59	119.84
3	B	924	ILE	N-CA-C	-5.40	105.11	110.62
6	R	22	THR	N-CA-C	-5.39	105.51	111.71
1	I	285	PRO	N-CA-C	5.39	117.28	110.70
11	N	18	TRP	N-CA-C	5.39	117.57	111.11
1	I	46	ASP	N-CA-C	5.37	120.35	108.27
2	C	104	LEU	CA-C-N	-5.35	113.52	119.19
2	C	104	LEU	C-N-CA	-5.35	113.52	119.19
1	I	830	LEU	N-CA-C	5.35	117.34	108.20
3	J	374	VAL	N-CA-C	-5.34	105.75	113.07
5	E	11	VAL	N-CA-C	5.34	115.47	107.51
2	M	198	ILE	N-CA-C	5.33	115.53	107.80
2	M	215	SER	N-CA-C	5.33	116.14	107.23
4	O	78	TRP	CA-C-N	5.33	126.50	119.84
4	O	78	TRP	C-N-CA	5.33	126.50	119.84
3	B	1033	ARG	N-CA-C	-5.32	105.39	111.14
3	J	171	ARG	N-CA-C	5.32	122.13	110.80
2	C	293	ILE	N-CA-C	-5.31	104.71	110.23
12	P	30	GLY	N-CA-C	-5.31	108.83	114.67
1	I	103	ARG	N-CA-C	5.30	122.09	110.80
3	B	118	ASP	N-CA-C	-5.30	99.65	108.34
1	A	285	PRO	N-CA-C	5.29	117.16	110.70
3	B	108	GLU	N-CA-C	5.28	115.52	108.23
6	F	76	CYS	CA-C-N	5.27	126.42	119.84
6	F	76	CYS	C-N-CA	5.27	126.42	119.84
3	B	565	GLU	N-CA-C	5.25	118.50	110.20
1	A	103	ARG	N-CA-C	5.25	121.99	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1077	TYR	N-CA-C	5.24	118.43	111.30
3	J	946	TYR	N-CA-C	5.24	121.97	110.80
5	E	166	GLN	CA-C-N	5.24	126.39	119.84
5	E	166	GLN	C-N-CA	5.24	126.39	119.84
3	J	832	LYS	N-CA-C	5.24	116.73	107.61
11	N	63	THR	N-CA-C	5.22	121.93	110.80
1	I	84	VAL	N-CA-C	5.22	115.94	110.62
2	M	60	SER	N-CA-C	5.22	117.38	111.02
1	I	58	CYS	CA-C-N	-5.21	116.39	121.65
1	I	58	CYS	C-N-CA	-5.21	116.39	121.65
1	I	339	VAL	N-CA-C	5.21	113.56	107.89
2	C	369	VAL	N-CA-C	5.20	115.41	110.53
3	J	118	ASP	N-CA-C	-5.19	99.83	108.34
1	I	203	ARG	CA-C-N	5.17	124.78	119.56
1	I	203	ARG	C-N-CA	5.17	124.78	119.56
3	J	981	SER	N-CA-C	5.17	118.70	111.56
3	B	832	LYS	N-CA-C	5.17	116.61	107.61
9	K	59	THR	N-CA-C	-5.17	101.43	109.24
1	A	58	CYS	CA-C-N	-5.17	116.43	121.65
1	A	58	CYS	C-N-CA	-5.17	116.43	121.65
1	A	400	THR	N-CA-C	-5.17	105.83	111.82
1	I	687	ILE	CA-C-N	5.17	126.30	119.84
1	I	687	ILE	C-N-CA	5.17	126.30	119.84
2	M	368	GLY	N-CA-C	5.16	119.16	112.25
1	I	856	PHE	CA-C-N	5.14	124.94	119.28
1	I	856	PHE	C-N-CA	5.14	124.94	119.28
1	A	153	GLN	N-CA-C	5.14	115.16	108.07
1	I	107	SER	N-CA-C	-5.13	107.07	113.38
5	Q	119	LYS	N-CA-C	5.12	118.10	109.95
2	C	237	ILE	N-CA-C	5.12	115.40	110.74
3	B	843	GLU	N-CA-C	5.12	117.29	110.53
1	A	843	GLY	N-CA-C	-5.12	107.62	116.01
3	J	1029	GLY	N-CA-C	5.12	118.61	111.14
1	I	622	GLU	N-CA-C	-5.10	107.12	113.55
1	A	201	THR	N-CA-C	-5.10	108.80	114.62
1	A	107	SER	N-CA-C	-5.10	107.11	113.38
1	I	140	ALA	N-CA-C	5.10	116.72	108.41
1	A	856	PHE	CA-C-N	5.10	124.76	119.56
1	A	856	PHE	C-N-CA	5.10	124.76	119.56
3	J	1002	HIS	N-CA-C	5.09	119.13	107.48
2	C	212	ASN	N-CA-C	5.09	117.37	110.35
12	P	25	ARG	N-CA-C	5.07	112.94	108.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	576	LYS	N-CA-C	5.07	121.59	110.80
3	B	981	SER	N-CA-C	5.07	118.55	111.56
3	B	1060	VAL	N-CA-C	5.07	115.56	108.17
3	J	450	TRP	N-CA-C	-5.07	102.36	109.96
2	C	56	ILE	N-CA-C	-5.06	105.45	110.62
11	W	63	THR	N-CA-C	5.06	121.58	110.80
3	B	1029	GLY	N-CA-C	5.05	118.51	111.14
8	H	70	GLN	N-CA-C	-5.04	107.08	113.18
7	G	74	HIS	N-CA-C	5.03	117.60	109.40
2	C	81	PRO	N-CA-C	-5.02	109.46	114.68
3	J	621	GLU	N-CA-C	-5.02	106.26	112.38

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	945	PHE	Peptide
7	G	40	PHE	Peptide
3	J	945	PHE	Peptide
9	K	26	ARG	Peptide
2	M	27	LYS	Peptide
9	U	59	THR	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6673	0	6763	631	0
1	I	6673	0	6763	647	0
2	C	2868	0	3035	284	0
2	M	2868	0	3035	344	0
3	B	8645	0	8780	868	0
3	J	8645	0	8780	915	0
4	D	2114	0	2146	125	0
4	O	2114	0	2146	131	0
5	E	1402	0	1467	84	0
5	Q	1402	0	1467	99	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	694	0	705	41	0
6	R	694	0	705	30	0
7	G	884	0	888	90	0
7	S	884	0	888	88	0
8	H	611	0	641	50	0
8	T	611	0	641	54	0
9	K	658	0	692	86	0
9	U	658	0	692	93	0
10	L	723	0	749	56	0
10	V	723	0	749	57	0
11	N	514	0	528	70	0
11	W	514	0	528	74	0
12	P	346	0	375	31	0
12	X	346	0	375	31	0
13	Y	391	0	389	28	0
13	Z	391	0	389	13	0
14	A	2	0	0	0	0
14	B	1	0	0	2	0
14	I	2	0	0	0	0
14	J	1	0	0	2	0
14	N	1	0	0	0	0
14	P	1	0	0	0	0
14	W	1	0	0	0	0
14	X	1	0	0	0	0
15	A	1	0	0	0	0
15	I	1	0	0	0	0
16	D	7	0	0	1	0
16	O	7	0	0	6	0
All	All	53072	0	54316	4372	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 41.

All (4372) 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)
8:H:29:TYR:OH	13:Y:67:LEU:HD22	1.31	1.25
4:D:183:CYS:SG	16:D:1001:F3S:S2	2.42	1.17
6:R:72:LEU:HD21	6:R:86:ILE:HD12	1.30	1.14
5:Q:147:ILE:HD11	5:Q:163:THR:HB	1.21	1.14
3:B:581:ILE:HD11	3:B:614:GLU:HB2	1.16	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:250:ILE:HD11	10:L:84:ILE:HD11	1.31	1.13
3:B:353:LEU:HA	3:B:404:VAL:HG11	1.21	1.13
3:J:353:LEU:HA	3:J:404:VAL:HG11	1.18	1.12
2:M:389:THR:HG23	9:U:77:THR:HB	1.30	1.11
3:J:759:SER:HB2	3:J:862:VAL:O	1.51	1.11
1:A:760:GLY:HA3	3:B:447:GLY:HA3	1.24	1.10
3:B:88:ARG:HD3	3:B:853:THR:HG21	1.10	1.10
3:J:922:GLY:HA2	3:J:925:MET:HB2	1.26	1.09
5:Q:53:THR:HB	5:Q:71:GLU:H	1.09	1.09
3:J:581:ILE:HD11	3:J:614:GLU:CB	1.83	1.09
9:K:90:LEU:HD23	9:K:90:LEU:H	1.09	1.09
1:I:647:ARG:HH11	3:J:965:ASP:HB2	0.96	1.09
2:C:340:SER:HB3	2:C:371:GLU:HG2	1.14	1.08
3:J:88:ARG:HD3	3:J:853:THR:HG21	1.09	1.08
2:M:146:TYR:HD2	2:M:233:GLY:O	1.35	1.08
1:I:308:ARG:HH21	3:J:1099:LEU:HD13	1.16	1.08
1:A:647:ARG:HH11	3:B:965:ASP:HB2	0.99	1.08
5:E:36:GLU:HG2	6:F:34:LEU:HD11	1.37	1.07
9:K:45:MET:HE2	9:K:45:MET:HA	1.27	1.07
5:E:39:LEU:HD11	6:F:1:MET:HA	1.35	1.06
3:J:26:GLN:O	3:J:345:LEU:HD23	1.55	1.06
1:A:418:LEU:HD21	3:B:1044:LEU:HD21	1.35	1.06
2:C:55:ALA:HA	2:C:58:GLU:HG3	1.38	1.06
3:B:26:GLN:O	3:B:345:LEU:HD23	1.56	1.06
1:I:68:CYS:SG	1:I:71:HIS:NE2	2.28	1.05
1:A:532:ILE:HD11	10:L:56:LYS:HD3	1.39	1.05
3:J:581:ILE:HD11	3:J:614:GLU:HB2	1.05	1.04
1:A:541:ALA:HB1	1:A:542:PRO:HD3	1.36	1.04
3:B:579:LEU:HD12	3:B:616:LEU:HD12	1.38	1.04
1:I:760:GLY:HA3	3:J:447:GLY:HA3	1.09	1.04
3:B:1033:ARG:NH1	3:B:1034:ASP:OD2	1.92	1.03
3:J:672:MET:HG2	3:J:993:LEU:HD21	1.37	1.03
2:M:28:ILE:HG21	9:U:14:HIS:CE1	1.93	1.02
2:C:55:ALA:HA	2:C:58:GLU:CG	1.89	1.02
1:A:877:GLY:C	3:J:377:ARG:HH12	1.65	1.02
1:A:308:ARG:HH21	3:B:1099:LEU:HD13	1.14	1.02
1:A:742:GLN:CB	3:B:919:MET:HE1	1.90	1.02
1:I:742:GLN:CB	3:J:919:MET:HE1	1.90	1.02
4:O:175:ASN:HA	4:O:195:LEU:HD11	1.39	1.02
3:B:922:GLY:HA2	3:B:925:MET:HB2	1.39	1.01
2:M:340:SER:CB	2:M:371:GLU:HG2	1.90	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:61:VAL:HG12	9:U:62:ILE:H	1.25	1.01
3:B:38:LYS:HG3	3:B:39:LEU:H	1.18	1.00
2:C:146:TYR:HB2	2:C:238:LYS:HD3	1.43	1.00
8:H:40:GLU:OE1	13:Y:66:LYS:HE2	1.61	1.00
3:J:38:LYS:HG3	3:J:39:LEU:H	1.23	1.00
3:J:702:LEU:HD22	3:J:933:ALA:HB1	1.39	1.00
3:J:1113:LEU:H	3:J:1113:LEU:HD12	1.24	1.00
3:J:569:ASN:HB3	3:J:574:ARG:HH22	1.22	1.00
5:Q:53:THR:O	5:Q:70:VAL:HG13	1.62	1.00
3:J:650:ILE:HD13	3:J:650:ILE:H	1.25	0.99
3:B:445:LEU:HD21	3:B:455:PRO:HA	1.45	0.99
7:S:63:ARG:HG3	7:S:114:ARG:HH22	1.25	0.99
1:I:647:ARG:NH1	3:J:965:ASP:HB2	1.76	0.98
3:J:458:THR:HG21	3:J:465:GLY:H	1.28	0.98
1:A:376:ASN:O	1:A:377:TYR:HB2	1.62	0.98
2:C:391:ARG:HG2	2:C:391:ARG:HH11	1.26	0.98
12:P:26:CYS:HB2	12:P:27:PRO:HD2	1.43	0.98
12:X:26:CYS:SG	12:X:29:CYS:HB2	2.02	0.98
1:A:558:LYS:HG3	3:J:104:GLU:HB2	1.42	0.98
2:C:109:GLU:O	2:C:113:ALA:HA	1.63	0.98
2:M:274:THR:HG22	2:M:275:ASN:H	1.27	0.97
12:P:46:LYS:H	12:P:46:LYS:HD2	1.29	0.97
1:A:647:ARG:NH1	3:B:965:ASP:HB2	1.78	0.97
1:I:331:ASN:O	1:I:332:ILE:HB	1.62	0.97
2:M:340:SER:HB3	2:M:371:GLU:CG	1.94	0.97
2:C:340:SER:HB3	2:C:371:GLU:CG	1.94	0.97
1:I:376:ASN:O	1:I:377:TYR:HB2	1.65	0.97
2:M:55:ALA:HA	2:M:58:GLU:HB2	1.47	0.97
2:C:329:ILE:HA	2:C:334:VAL:HG12	1.46	0.97
9:K:45:MET:HA	9:K:45:MET:CE	1.95	0.97
2:M:340:SER:HB3	2:M:371:GLU:HG2	0.98	0.97
2:C:276:ASN:HD22	2:C:279:GLU:HB2	1.29	0.97
4:D:175:ASN:HA	4:D:195:LEU:HD11	1.43	0.96
6:R:72:LEU:CD2	6:R:86:ILE:HD12	1.94	0.96
1:A:541:ALA:HB1	1:A:542:PRO:CD	1.94	0.96
2:C:126:LEU:HB2	2:C:131:LYS:HG3	1.46	0.96
1:I:541:ALA:HB1	1:I:542:PRO:HD3	1.44	0.96
3:B:581:ILE:HD11	3:B:614:GLU:CB	1.94	0.96
3:B:702:LEU:HD22	3:B:933:ALA:HB1	1.45	0.96
8:H:43:PRO:O	8:H:44:TRP:HB2	1.63	0.96
3:B:702:LEU:H	3:B:721:ASN:HD21	0.98	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:426:HIS:CE1	1:I:428:ILE:HG22	2.00	0.96
3:J:579:LEU:HD12	3:J:616:LEU:HD12	1.45	0.96
3:B:88:ARG:CD	3:B:853:THR:HG21	1.96	0.95
3:J:88:ARG:CD	3:J:853:THR:HG21	1.95	0.95
3:J:339:ALA:HB2	3:J:618:ALA:HB3	1.45	0.95
5:Q:27:LEU:HB2	5:Q:51:VAL:HG11	1.48	0.95
1:A:742:GLN:HB3	3:B:919:MET:HE1	1.48	0.95
1:I:109:ASP:O	1:I:113:LYS:HG3	1.64	0.95
9:U:69:PHE:HA	9:U:74:LEU:HD11	1.47	0.95
3:J:450:TRP:HZ2	3:J:641:GLU:OE1	1.50	0.94
3:J:104:GLU:O	3:J:105:ASN:HB2	1.63	0.94
3:B:82:PRO:HG2	3:B:143:GLU:OE1	1.67	0.94
3:B:1113:LEU:H	3:B:1113:LEU:HD12	1.28	0.94
3:J:748:GLY:HA2	3:J:751:ARG:HD2	1.47	0.94
12:P:26:CYS:SG	12:P:29:CYS:HB2	2.07	0.94
3:J:1033:ARG:NH1	3:J:1034:ASP:OD2	2.00	0.94
3:B:855:THR:HB	3:B:857:GLU:HG2	1.47	0.94
4:O:98:ILE:HD11	4:O:114:ILE:HG13	1.50	0.94
1:A:830:LEU:HD23	1:A:840:SER:HB3	1.47	0.94
3:B:650:ILE:HD13	3:B:650:ILE:H	1.32	0.94
1:I:742:GLN:HB3	3:J:919:MET:HE1	1.47	0.94
3:J:445:LEU:HD21	3:J:455:PRO:HA	1.49	0.94
3:J:749:MET:HE1	3:J:907:ASP:HB3	1.48	0.94
2:C:237:ILE:HG13	2:C:238:LYS:N	1.82	0.93
2:C:40:GLU:O	2:C:45:ARG:HG2	1.68	0.93
1:A:124:ARG:HH21	13:Y:81:ARG:HH12	1.17	0.93
9:K:82:LEU:HD23	9:K:82:LEU:H	1.32	0.93
2:M:70:ILE:CD1	2:M:70:ILE:H	1.82	0.93
2:M:126:LEU:HB2	2:M:131:LYS:HG3	1.50	0.93
3:J:88:ARG:HD3	3:J:853:THR:CG2	1.98	0.93
3:J:764:LYS:HE2	3:J:813:LYS:HE2	1.51	0.93
1:A:317:ARG:HA	3:B:1027:ARG:HA	1.51	0.93
3:J:702:LEU:H	3:J:721:ASN:HD21	0.94	0.93
2:C:391:ARG:HH11	2:C:391:ARG:CG	1.82	0.92
2:M:179:VAL:HG11	2:M:232:LYS:HZ2	1.34	0.92
3:J:855:THR:HB	3:J:857:GLU:HG2	1.51	0.92
3:J:881:ARG:HH11	3:J:989:TYR:HB3	1.34	0.92
12:X:46:LYS:H	12:X:46:LYS:HD2	1.32	0.92
1:A:595:GLU:HB2	7:G:91:LYS:HE2	1.52	0.92
1:I:760:GLY:HA3	3:J:447:GLY:CA	1.97	0.92
3:J:854:GLU:HA	3:J:859:ASN:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:88:ARG:HD3	3:B:853:THR:CG2	1.97	0.91
7:S:7:GLN:HG2	7:S:8:GLU:H	1.33	0.91
9:K:50:LEU:HD23	9:K:74:LEU:HA	1.52	0.91
1:I:541:ALA:HB1	1:I:542:PRO:CD	1.98	0.91
1:I:317:ARG:HA	3:J:1027:ARG:HA	1.51	0.91
3:B:672:MET:HG2	3:B:993:LEU:HD21	1.52	0.91
7:G:86:LEU:HD11	7:G:89:GLY:O	1.70	0.91
9:K:34:ARG:O	9:K:37:SER:HB2	1.71	0.91
1:A:365:VAL:HG23	1:A:388:LEU:HD11	1.51	0.91
3:B:749:MET:HE1	3:B:907:ASP:HB3	1.52	0.91
1:A:308:ARG:NH2	3:B:1099:LEU:HD13	1.86	0.90
1:A:541:ALA:HB2	7:G:72:CYS:H	1.36	0.90
1:A:853:ASP:HB2	2:C:311:ARG:HH12	1.36	0.90
2:C:340:SER:CB	2:C:371:GLU:HG2	2.01	0.90
3:B:104:GLU:O	3:B:105:ASN:HB2	1.71	0.90
3:B:640:LEU:HD22	3:B:641:GLU:H	1.35	0.90
3:B:687:ARG:HH11	3:B:687:ARG:HG3	1.34	0.90
1:I:594:LEU:HA	7:S:86:LEU:HD22	1.53	0.90
1:I:830:LEU:HD23	1:I:840:SER:HB3	1.50	0.90
2:M:28:ILE:HG21	9:U:14:HIS:HE1	1.36	0.90
3:B:854:GLU:HA	3:B:859:ASN:O	1.72	0.90
1:A:590:ASN:ND2	3:J:377:ARG:HB2	1.87	0.89
3:J:890:MET:HE2	3:J:891:LEU:H	1.37	0.89
4:D:96:ILE:HG22	4:D:116:SER:HA	1.54	0.89
2:M:392:PRO:HB2	5:Q:22:LEU:HD11	1.51	0.89
3:J:418:ASN:HD21	3:J:421:SER:H	1.20	0.89
1:A:872:PHE:HA	1:A:876:VAL:HB	1.55	0.89
3:J:98:LEU:HD11	3:J:100:MET:HG3	1.54	0.89
4:O:96:ILE:HG22	4:O:116:SER:HA	1.54	0.89
1:I:647:ARG:HH11	3:J:965:ASP:CB	1.85	0.88
2:C:390:MET:O	2:C:391:ARG:HB3	1.72	0.88
3:B:569:ASN:HB3	3:B:574:ARG:HH22	1.39	0.88
3:B:638:THR:HB	3:B:639:HIS:CD2	2.08	0.88
4:D:98:ILE:HD11	4:D:114:ILE:HG13	1.55	0.88
12:X:26:CYS:HB2	12:X:27:PRO:HD2	1.54	0.88
1:A:109:ASP:O	1:A:113:LYS:HG3	1.74	0.88
3:B:339:ALA:HB2	3:B:618:ALA:HB3	1.54	0.88
3:B:640:LEU:CD2	3:B:641:GLU:H	1.86	0.88
3:B:418:ASN:ND2	3:B:421:SER:H	1.71	0.88
3:B:702:LEU:H	3:B:721:ASN:ND2	1.72	0.87
4:D:111:SER:HA	4:D:114:ILE:HD13	1.54	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:82:PRO:HG2	3:J:143:GLU:OE1	1.74	0.87
3:J:418:ASN:ND2	3:J:421:SER:H	1.72	0.87
1:A:541:ALA:CB	1:A:542:PRO:CD	2.52	0.87
3:B:242:VAL:HA	3:B:316:ALA:HB1	1.55	0.87
3:J:638:THR:HB	3:J:639:HIS:CD2	2.10	0.87
4:O:209:CYS:HG	16:O:1001:F3S:FE1	0.57	0.87
1:A:512:LYS:HE2	7:G:91:LYS:HE3	1.56	0.87
3:B:759:SER:HB2	3:B:862:VAL:O	1.74	0.87
3:B:910:LEU:HD22	3:B:911:ASN:N	1.89	0.87
3:J:560:THR:HG22	3:J:562:PHE:H	1.38	0.87
3:J:1064:CYS:SG	14:J:2001:ZN:ZN	1.62	0.87
3:J:242:VAL:HA	3:J:316:ALA:HB1	1.57	0.87
2:C:241:ILE:O	2:C:251:ILE:HG13	1.73	0.87
1:I:823:LEU:HD13	2:M:75:ALA:HB1	1.56	0.87
5:Q:53:THR:HB	5:Q:71:GLU:N	1.88	0.87
1:A:369:PRO:HB3	1:A:376:ASN:HB3	1.56	0.87
1:I:632:PHE:HA	1:I:635:PHE:CD1	2.10	0.87
3:J:314:TYR:HE2	3:J:526:LEU:H	1.23	0.87
3:B:579:LEU:HD12	3:B:616:LEU:CD1	2.04	0.86
1:A:589:LYS:O	1:A:592:ILE:HG12	1.73	0.86
3:B:560:THR:HG22	3:B:562:PHE:H	1.40	0.86
3:B:595:GLU:HA	3:B:599:SER:HB3	1.56	0.86
4:D:250:ILE:HD11	10:L:84:ILE:CD1	2.03	0.86
9:K:90:LEU:HD23	9:K:90:LEU:N	1.90	0.86
3:B:314:TYR:HE2	3:B:526:LEU:H	1.21	0.86
3:B:47:GLY:HA2	3:B:58:VAL:O	1.76	0.86
1:I:308:ARG:NH2	3:J:1099:LEU:HD13	1.91	0.86
2:M:289:ALA:O	2:M:292:ILE:HG22	1.74	0.86
3:J:650:ILE:H	3:J:650:ILE:CD1	1.89	0.86
3:B:98:LEU:HD11	3:B:100:MET:HG3	1.56	0.86
3:J:851:LEU:HA	12:X:35:PHE:HB3	1.58	0.86
3:J:902:LYS:HB3	11:W:42:ARG:HD3	1.55	0.86
1:I:875:VAL:O	1:I:877:GLY:N	2.08	0.85
3:J:662:GLN:HG2	3:J:664:PRO:HD2	1.58	0.85
1:A:841:LEU:O	1:A:843:GLY:N	2.10	0.85
3:B:183:ILE:O	3:B:183:ILE:HD13	1.76	0.85
3:B:418:ASN:HD21	3:B:421:SER:H	1.16	0.85
1:I:365:VAL:HG23	1:I:388:LEU:HD11	1.58	0.85
3:J:47:GLY:HA2	3:J:58:VAL:O	1.76	0.85
8:T:42:LEU:HB2	8:T:43:PRO:HD2	1.55	0.85
4:O:111:SER:HA	4:O:114:ILE:HD13	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:589:LYS:O	1:I:592:ILE:HG12	1.77	0.85
3:J:640:LEU:HD22	3:J:641:GLU:H	1.42	0.85
3:J:529:TYR:O	3:J:530:TYR:HB3	1.76	0.85
3:J:687:ARG:HH11	3:J:687:ARG:HG3	1.40	0.85
3:J:702:LEU:H	3:J:721:ASN:ND2	1.73	0.85
3:B:451:GLY:HA3	3:B:577:ARG:HH11	1.42	0.85
3:B:748:GLY:HA2	3:B:751:ARG:HD2	1.58	0.85
2:C:340:SER:HA	2:C:364:GLU:HG2	1.59	0.85
3:B:662:GLN:HG2	3:B:664:PRO:HD2	1.57	0.85
1:I:672:VAL:HG13	1:I:700:ILE:HD12	1.58	0.85
2:M:391:ARG:HH22	9:U:39:ARG:HH11	1.20	0.84
3:J:958:LEU:HD12	3:J:964:PRO:HG3	1.59	0.84
1:A:426:HIS:CE1	1:A:428:ILE:HG22	2.11	0.84
3:B:427:ARG:HH11	3:B:650:ILE:HD12	1.42	0.84
3:B:497:VAL:HG23	3:B:528:GLY:HA2	1.60	0.84
1:A:331:ASN:O	1:A:332:ILE:HB	1.76	0.84
3:B:557:HIS:N	3:B:623:ASN:HD21	1.75	0.84
3:J:595:GLU:HA	3:J:599:SER:HB3	1.59	0.84
1:A:875:VAL:O	1:A:877:GLY:N	2.10	0.84
7:G:72:CYS:SG	7:G:114:ARG:HD3	2.17	0.84
3:J:702:LEU:N	3:J:721:ASN:HD21	1.74	0.84
5:E:50:ASN:HB2	5:E:73:ASP:OD2	1.76	0.84
2:C:388:LEU:HD11	9:K:34:ARG:HG3	1.59	0.84
1:I:426:HIS:CD2	1:I:490:ARG:HH12	1.96	0.84
1:I:667:ARG:O	1:I:670:VAL:HG22	1.77	0.84
3:B:764:LYS:HE2	3:B:813:LYS:HE2	1.60	0.84
1:I:547:THR:O	1:I:550:GLN:HB3	1.78	0.84
2:M:72:ILE:HD12	2:M:72:ILE:N	1.91	0.84
13:Z:57:GLY:HA2	13:Z:61:LEU:HG	1.59	0.84
3:J:702:LEU:CD2	3:J:933:ALA:HB1	2.07	0.83
1:I:412:ILE:O	1:I:415:ASP:HB2	1.78	0.83
1:I:418:LEU:HD21	3:J:1044:LEU:HD21	1.60	0.83
1:A:672:VAL:HG13	1:A:700:ILE:HD12	1.57	0.83
1:I:369:PRO:HB3	1:I:376:ASN:HB3	1.60	0.83
1:A:647:ARG:HH11	3:B:965:ASP:CB	1.89	0.83
4:O:13:ILE:HD11	4:O:238:PRO:HB2	1.61	0.83
3:B:253:PHE:H	3:B:254:PRO:HD2	1.42	0.83
3:B:958:LEU:HD12	3:B:964:PRO:HG3	1.59	0.83
2:M:146:TYR:CD2	2:M:233:GLY:O	2.26	0.83
3:J:90:LEU:HD11	3:J:856:ALA:H	1.43	0.83
1:I:220:ARG:NH1	1:I:236:THR:HG23	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:451:GLY:HA3	3:J:577:ARG:HH11	1.41	0.83
3:B:557:HIS:H	3:B:623:ASN:HD21	1.27	0.83
4:O:209:CYS:SG	16:O:1001:F3S:FE1	1.69	0.83
3:J:544:ARG:HH11	3:J:544:ARG:HG3	1.42	0.83
1:A:324:THR:HG22	1:A:325:VAL:H	1.43	0.83
1:I:541:ALA:CB	1:I:542:PRO:CD	2.57	0.83
3:B:870:ARG:NH1	3:B:996:MET:HB2	1.93	0.82
1:I:872:PHE:HA	1:I:876:VAL:HB	1.61	0.82
2:C:179:VAL:HG21	2:C:232:LYS:HZ2	1.42	0.82
5:E:53:THR:HG23	5:E:55:GLU:HG3	1.60	0.82
4:O:13:ILE:CD1	4:O:238:PRO:HB2	2.10	0.82
3:B:458:THR:HG21	3:B:465:GLY:H	1.44	0.82
3:B:851:LEU:HA	12:P:35:PHE:HB3	1.59	0.82
3:B:881:ARG:HH11	3:B:989:TYR:HB3	1.45	0.82
3:B:138:LEU:HA	3:B:141:ILE:HD12	1.59	0.82
3:B:450:TRP:HZ2	3:B:641:GLU:OE1	1.60	0.82
3:B:702:LEU:N	3:B:721:ASN:HD21	1.77	0.82
1:A:733:ALA:HB1	3:B:913:HIS:CE1	2.15	0.82
2:M:390:MET:HG3	5:Q:56:GLU:HG2	1.60	0.82
3:J:738:ILE:HD11	3:J:908:ILE:HG23	1.62	0.82
3:B:529:TYR:O	3:B:530:TYR:HB3	1.79	0.81
5:E:15:PRO:HG2	9:K:45:MET:HB3	1.60	0.81
9:K:71:ARG:O	9:K:73:VAL:HG13	1.80	0.81
3:B:203:GLU:OE1	3:B:203:GLU:HA	1.76	0.81
1:I:90:ILE:HD11	1:I:207:MET:HB2	1.61	0.81
1:A:412:ILE:O	1:A:415:ASP:HB2	1.80	0.81
9:K:28:THR:OG1	9:K:31:GLU:HG3	1.79	0.81
3:J:800:PRO:O	3:J:802:VAL:N	2.14	0.81
3:J:1043:MET:HE3	5:Q:61:PHE:CD2	2.15	0.81
1:A:220:ARG:NH1	1:A:236:THR:HG23	1.94	0.81
1:A:491:TYR:HB2	1:A:607:GLN:OE1	1.81	0.81
1:A:760:GLY:HA3	3:B:447:GLY:CA	2.10	0.81
5:E:36:GLU:HG2	6:F:34:LEU:CD1	2.10	0.81
5:Q:97:ILE:HD12	5:Q:113:ILE:HD11	1.62	0.81
2:C:55:ALA:HA	2:C:58:GLU:CB	2.09	0.81
2:M:170:ASP:O	2:M:174:LEU:HD11	1.81	0.81
3:J:579:LEU:HD12	3:J:616:LEU:CD1	2.10	0.81
3:J:569:ASN:HB3	3:J:574:ARG:NH2	1.95	0.81
3:J:935:LEU:HD12	3:J:957:ILE:HG22	1.63	0.81
2:M:329:ILE:HA	2:M:334:VAL:HG12	1.60	0.81
5:Q:15:PRO:HG2	9:U:45:MET:HB3	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:39:LEU:HD13	5:E:42:LEU:H	1.46	0.81
3:J:138:LEU:HA	3:J:141:ILE:HD12	1.62	0.81
2:M:48:ILE:HG12	2:M:50:LYS:HE3	1.63	0.81
6:F:35:GLN:HA	6:F:38:TYR:CD1	2.16	0.80
3:J:771:ASP:HB2	3:J:816:PRO:HD3	1.63	0.80
4:D:13:ILE:HD11	4:D:238:PRO:HB2	1.64	0.80
1:I:79:ARG:HB2	1:I:266:TRP:CE3	2.17	0.80
3:J:253:PHE:H	3:J:254:PRO:HD2	1.47	0.80
3:J:458:THR:CG2	3:J:465:GLY:H	1.95	0.80
1:I:336:GLU:HA	1:I:434:ARG:O	1.82	0.80
2:M:114:LYS:O	2:M:116:VAL:N	2.13	0.80
3:B:687:ARG:HH11	3:B:687:ARG:CG	1.94	0.80
3:J:910:LEU:HD22	3:J:911:ASN:N	1.97	0.80
1:I:853:ASP:OD2	1:I:864:LYS:HB3	1.82	0.80
3:J:813:LYS:H	3:J:836:SER:HB3	1.45	0.80
1:A:647:ARG:HH21	3:B:982:ARG:HH12	1.26	0.80
2:C:55:ALA:HA	2:C:58:GLU:HB2	1.64	0.80
3:B:90:LEU:HD11	3:B:856:ALA:H	1.47	0.80
4:D:29:ARG:HG3	4:D:162:SER:HB3	1.63	0.80
4:O:259:LYS:O	4:O:263:VAL:HG23	1.82	0.80
5:E:89:VAL:HG11	5:E:92:VAL:HG22	1.64	0.79
1:A:547:THR:O	1:A:550:GLN:HB3	1.83	0.79
1:A:549:LYS:HE2	7:G:89:GLY:HA2	1.64	0.79
1:A:733:ALA:HB1	3:B:913:HIS:HE1	1.47	0.79
1:A:742:GLN:HB2	3:B:919:MET:HE1	1.62	0.79
8:H:29:TYR:HA	8:H:32:LEU:HD12	1.61	0.79
1:I:331:ASN:O	1:I:332:ILE:CB	2.30	0.79
3:J:450:TRP:CZ2	3:J:641:GLU:OE1	2.36	0.79
1:A:426:HIS:CD2	1:A:490:ARG:HH12	1.99	0.79
5:E:87:GLY:O	5:E:88:GLU:HB2	1.81	0.79
6:R:35:GLN:HA	6:R:38:TYR:CD1	2.17	0.79
1:I:742:GLN:HB2	3:J:919:MET:HE1	1.65	0.79
3:B:539:LYS:O	3:B:543:ARG:HG3	1.83	0.79
3:J:773:ILE:HG12	3:J:813:LYS:HG2	1.64	0.79
2:M:61:GLU:O	2:M:64:ILE:HD12	1.83	0.79
2:M:110:ILE:HD11	2:M:277:ILE:HD11	1.64	0.79
3:J:665:ARG:HG3	3:J:920:THR:CG2	2.13	0.79
3:J:183:ILE:HG12	3:J:206:LYS:HB3	1.65	0.79
3:J:203:GLU:OE1	3:J:203:GLU:HA	1.82	0.79
1:A:79:ARG:HB2	1:A:266:TRP:CE3	2.17	0.79
4:D:109:ILE:HD11	4:D:133:LEU:HD12	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:491:TYR:HB2	1:I:607:GLN:OE1	1.83	0.79
9:U:91:SER:O	9:U:92:LEU:HB2	1.82	0.79
1:I:134:GLU:HA	1:I:137:LYS:HD2	1.64	0.78
1:I:353:ILE:HG13	1:I:361:LEU:HD23	1.65	0.78
1:A:61:CYS:SG	3:B:1070:TYR:HB3	2.23	0.78
1:A:206:TRP:O	1:A:208:ILE:N	2.16	0.78
1:A:525:LEU:HD11	1:A:530:VAL:HG11	1.65	0.78
3:B:702:LEU:CD2	3:B:933:ALA:HB1	2.12	0.78
1:I:541:ALA:HB2	7:S:72:CYS:H	1.46	0.78
7:G:72:CYS:SG	7:G:114:ARG:HB3	2.22	0.78
1:A:58:CYS:HB2	1:A:59:PRO:HD3	1.64	0.78
3:B:850:VAL:O	12:P:35:PHE:HB2	1.84	0.78
2:M:103:GLY:C	2:M:105:PRO:HD2	2.09	0.78
3:J:497:VAL:HG23	3:J:528:GLY:HA2	1.63	0.78
1:I:313:LEU:HB3	2:M:374:ILE:HG13	1.65	0.78
8:T:39:PRO:HB2	8:T:80:TYR:HE2	1.48	0.78
1:A:353:ILE:HG13	1:A:361:LEU:HD23	1.64	0.78
1:I:853:ASP:HB2	2:M:311:ARG:HH12	1.49	0.78
1:A:853:ASP:OD2	1:A:864:LYS:HB3	1.83	0.78
2:C:70:ILE:HA	2:C:73:VAL:HG22	1.64	0.78
1:A:541:ALA:CB	7:G:72:CYS:H	1.96	0.78
1:I:721:PRO:HA	1:I:726:TYR:HD1	1.49	0.78
4:D:13:ILE:CD1	4:D:238:PRO:HB2	2.13	0.78
1:I:324:THR:HG22	1:I:325:VAL:H	1.47	0.78
3:J:557:HIS:N	3:J:623:ASN:HD21	1.82	0.78
7:S:63:ARG:HG3	7:S:114:ARG:NH2	1.99	0.78
2:C:41:ILE:HB	2:C:42:ILE:HD12	1.64	0.77
2:C:173:MET:HA	2:C:176:ASP:HB2	1.65	0.77
3:B:38:LYS:HG3	3:B:39:LEU:N	1.98	0.77
7:G:55:VAL:HG23	7:G:116:SER:O	1.84	0.77
3:J:451:GLY:H	3:J:647:ILE:HG23	1.47	0.77
3:J:554:ASN:HD21	3:J:576:ARG:HH21	1.32	0.77
1:A:301:ARG:O	1:A:302:LEU:HG	1.84	0.77
1:A:507:TYR:O	1:A:508:LEU:HB2	1.83	0.77
2:C:391:ARG:NH2	9:K:42:GLN:HG2	1.98	0.77
1:I:828:SER:C	1:I:830:LEU:H	1.93	0.77
2:M:168:GLN:HA	2:M:204:SER:HA	1.67	0.77
2:M:345:ALA:HB1	2:M:350:THR:HG23	1.66	0.77
8:T:24:ASN:O	8:T:27:GLU:HG2	1.84	0.77
1:A:530:VAL:O	1:A:532:ILE:HG12	1.84	0.77
3:B:771:ASP:HB2	3:B:816:PRO:HD3	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:647:ARG:HH21	3:J:982:ARG:HH12	1.33	0.77
3:J:853:THR:HG22	3:J:854:GLU:H	1.48	0.77
9:K:90:LEU:H	9:K:90:LEU:CD2	1.89	0.77
3:J:317:TYR:CD2	3:J:526:LEU:HD13	2.20	0.77
3:B:935:LEU:HD12	3:B:957:ILE:HG22	1.66	0.77
1:I:823:LEU:HB3	2:M:329:ILE:HD13	1.66	0.77
1:A:667:ARG:O	1:A:670:VAL:HG22	1.85	0.77
2:C:63:LEU:O	2:C:63:LEU:HD23	1.84	0.77
3:B:962:TYR:OH	11:N:42:ARG:HD2	1.83	0.77
1:A:421:ARG:HB2	1:A:462:MET:HE3	1.64	0.77
3:B:699:GLN:NE2	11:N:48:MET:HE3	2.00	0.77
3:B:1064:CYS:SG	14:B:2001:ZN:ZN	1.74	0.77
8:H:25:ILE:HD11	8:H:61:ASP:OD1	1.85	0.77
1:A:447:LEU:HD13	3:B:734:MET:SD	2.25	0.77
3:B:853:THR:HG22	3:B:854:GLU:H	1.49	0.77
10:V:40:PHE:HB3	10:V:58:LEU:HB3	1.66	0.77
1:A:336:GLU:HA	1:A:434:ARG:O	1.85	0.77
2:C:391:ARG:H	2:C:392:PRO:HD3	1.49	0.77
3:B:813:LYS:H	3:B:836:SER:HB3	1.49	0.77
1:I:378:VAL:O	1:I:378:VAL:HG22	1.85	0.77
3:J:88:ARG:NH1	3:J:854:GLU:O	2.18	0.77
12:X:17:GLN:HB3	12:X:19:LYS:HG3	1.64	0.77
1:A:812:ARG:HE	2:C:86:THR:HG23	1.48	0.76
2:C:329:ILE:HA	2:C:334:VAL:CG1	2.15	0.76
3:J:758:TYR:O	3:J:759:SER:HB3	1.83	0.76
4:O:29:ARG:HG3	4:O:162:SER:HB3	1.68	0.76
1:A:697:GLU:OE1	1:A:756:ARG:HD3	1.85	0.76
1:I:841:LEU:O	1:I:843:GLY:N	2.18	0.76
3:J:473:MET:SD	3:J:474:ALA:N	2.58	0.76
1:I:308:ARG:HH21	3:J:1099:LEU:CD1	1.97	0.76
3:J:911:ASN:HD22	3:J:913:HIS:H	1.33	0.76
1:A:134:GLU:HA	1:A:137:LYS:HD2	1.67	0.76
3:B:630:PRO:O	3:B:633:LEU:HB3	1.84	0.76
1:I:58:CYS:HB2	1:I:59:PRO:HD3	1.66	0.76
3:J:640:LEU:CD2	3:J:641:GLU:H	1.98	0.76
1:I:760:GLY:CA	3:J:447:GLY:HA3	2.04	0.76
1:I:507:TYR:O	1:I:508:LEU:HB2	1.84	0.76
1:I:530:VAL:O	1:I:532:ILE:HG12	1.86	0.76
2:M:35:LEU:O	2:M:39:LYS:HE3	1.85	0.76
3:J:992:LYS:HE3	3:J:996:MET:SD	2.25	0.76
4:O:44:VAL:HA	4:O:143:ALA:HA	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:870:ARG:NH1	3:J:996:MET:HB2	2.00	0.76
1:A:595:GLU:CB	7:G:91:LYS:HE2	2.15	0.76
3:J:249:GLN:HG3	3:J:250:ASN:H	1.50	0.76
1:A:446:ASN:C	1:A:446:ASN:HD22	1.94	0.76
8:H:29:TYR:O	8:H:33:LYS:HG3	1.86	0.76
12:P:26:CYS:HB2	12:P:27:PRO:CD	2.14	0.76
3:J:569:ASN:CB	3:J:574:ARG:HH22	1.98	0.76
3:J:922:GLY:HA2	3:J:925:MET:CB	2.13	0.76
9:K:92:LEU:HD23	9:K:92:LEU:O	1.86	0.75
10:L:13:LEU:HB3	10:L:57:ILE:HD12	1.68	0.75
3:J:873:THR:HG22	3:J:874:ILE:N	2.01	0.75
3:B:588:LEU:HD13	3:B:612:LYS:HB3	1.67	0.75
3:B:591:ILE:HG12	3:B:612:LYS:HZ3	1.52	0.75
3:B:730:THR:HB	3:B:732:TYR:HD1	1.51	0.75
1:A:828:SER:C	1:A:830:LEU:H	1.94	0.75
3:B:183:ILE:HB	3:B:207:ASP:C	2.11	0.75
7:G:109:LYS:HZ3	3:J:378:LYS:HE3	1.51	0.75
2:M:60:SER:O	2:M:63:LEU:HB3	1.87	0.75
2:M:115:LYS:HD3	2:M:278:ARG:HB3	1.68	0.75
3:J:650:ILE:HD13	3:J:650:ILE:N	2.01	0.75
3:B:317:TYR:CD2	3:B:526:LEU:HD13	2.22	0.75
7:G:87:ASN:C	7:G:89:GLY:H	1.93	0.75
1:I:541:ALA:CB	7:S:72:CYS:H	1.98	0.75
10:V:59:THR:HG21	10:V:65:PRO:HD3	1.68	0.75
1:A:15:SER:HA	1:A:203:ARG:HH22	1.51	0.75
1:A:130:ARG:HB3	1:A:195:LEU:O	1.87	0.75
1:A:293:ARG:HH11	1:A:296:ARG:NH2	1.85	0.75
1:A:308:ARG:HH21	3:B:1099:LEU:CD1	1.94	0.75
3:B:650:ILE:H	3:B:650:ILE:CD1	2.00	0.75
3:B:773:ILE:HG12	3:B:813:LYS:HG2	1.69	0.75
2:C:377:HIS:ND1	2:C:378:PRO:HD2	2.02	0.75
1:I:220:ARG:HH11	1:I:236:THR:HG23	1.50	0.75
2:M:146:TYR:CE2	2:M:235:LYS:HB2	2.22	0.75
3:B:591:ILE:CG1	3:B:612:LYS:HZ3	1.98	0.75
1:I:326:ILE:HG21	1:I:462:MET:HG3	1.69	0.75
1:I:324:THR:HG22	1:I:325:VAL:N	2.02	0.75
3:J:539:LYS:O	3:J:543:ARG:HG3	1.87	0.75
3:J:874:ILE:H	3:J:874:ILE:HD12	1.52	0.75
1:A:525:LEU:HD12	10:L:56:LYS:HE3	1.69	0.74
1:I:234:ASP:OD2	1:I:296:ARG:HD3	1.85	0.74
3:J:38:LYS:HG3	3:J:39:LEU:N	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:390:MET:HE1	5:E:66:THR:HA	1.68	0.74
3:B:249:GLN:HG3	3:B:250:ASN:H	1.50	0.74
3:B:851:LEU:HD12	12:P:35:PHE:HD2	1.50	0.74
3:B:890:MET:HE2	3:B:891:LEU:H	1.52	0.74
3:J:427:ARG:HH11	3:J:650:ILE:HD12	1.53	0.74
1:A:525:LEU:CD1	1:A:530:VAL:HG11	2.17	0.74
2:C:389:THR:HG21	9:K:79:ARG:HH11	1.52	0.74
3:B:591:ILE:HG12	3:B:612:LYS:NZ	2.02	0.74
3:B:800:PRO:O	3:B:802:VAL:N	2.20	0.74
3:B:870:ARG:CZ	3:B:996:MET:SD	2.75	0.74
1:A:833:GLU:OE2	1:A:839:ARG:HB2	1.88	0.74
3:B:874:ILE:H	3:B:874:ILE:HD12	1.53	0.74
1:A:632:PHE:HA	1:A:635:PHE:CD1	2.22	0.74
3:B:763:VAL:HG22	3:B:770:GLU:HG3	1.68	0.74
2:M:30:ASP:O	2:M:31:ASP:HB3	1.87	0.74
10:V:3:ILE:CG2	10:V:15:LEU:HD21	2.17	0.74
7:G:80:GLU:HG2	7:G:81:LEU:H	1.52	0.74
3:J:972:ASP:OD2	3:J:974:ARG:HG2	1.87	0.74
1:A:490:ARG:HA	2:C:312:HIS:HE1	1.51	0.74
1:I:206:TRP:O	1:I:208:ILE:N	2.20	0.74
3:J:557:HIS:H	3:J:623:ASN:HD21	1.35	0.74
3:J:581:ILE:CD1	3:J:614:GLU:HB2	2.01	0.74
1:A:604:GLY:C	1:A:606:GLN:H	1.93	0.74
3:B:227:MET:HE3	3:B:312:ALA:HB1	1.67	0.74
3:B:1000:LYS:O	3:B:1001:LEU:HB2	1.86	0.74
1:I:470:GLU:O	1:I:473:ILE:HG12	1.88	0.74
2:C:60:SER:O	2:C:63:LEU:N	2.20	0.74
2:C:55:ALA:O	2:C:58:GLU:HB2	1.88	0.74
3:B:738:ILE:HD11	3:B:908:ILE:HG23	1.70	0.74
1:A:594:LEU:HA	7:G:86:LEU:HD22	1.69	0.73
5:Q:84:VAL:HG21	6:R:86:ILE:HG12	1.70	0.73
8:T:65:ILE:HD11	8:T:79:ARG:HG2	1.68	0.73
3:B:1054:ASP:HB3	3:B:1095:TYR:H	1.53	0.73
1:I:331:ASN:HD22	10:V:47:HIS:HB2	1.53	0.73
1:I:499:ALA:HB3	3:J:734:MET:CE	2.18	0.73
2:M:70:ILE:CD1	2:M:70:ILE:N	2.49	0.73
3:J:473:MET:SD	3:J:475:GLN:N	2.61	0.73
1:A:256:GLY:O	1:A:258:PRO:HD3	1.88	0.73
1:A:541:ALA:HB2	7:G:72:CYS:N	2.04	0.73
3:J:763:VAL:HG22	3:J:770:GLU:HG3	1.69	0.73
8:T:29:TYR:HA	8:T:32:LEU:HD12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:721:PRO:HA	1:A:726:TYR:HD1	1.51	0.73
3:B:451:GLY:H	3:B:647:ILE:HG23	1.53	0.73
1:I:567:ASN:N	1:I:599:ASP:OD2	2.22	0.73
3:J:687:ARG:HH11	3:J:687:ARG:CG	2.00	0.73
3:J:797:VAL:HB	12:X:36:MET:HE1	1.71	0.73
1:I:637:ARG:HD3	1:I:640:GLU:CD	2.13	0.73
3:J:708:LEU:HD13	3:J:713:TYR:HB3	1.69	0.73
7:G:30:ASN:O	7:G:31:MET:HG3	1.87	0.73
1:A:98:CYS:HA	1:A:146:CYS:SG	2.28	0.73
1:A:859:TYR:HB2	2:C:64:ILE:HG12	1.71	0.73
3:B:700:ARG:O	11:N:51:SER:HB2	1.88	0.73
1:I:604:GLY:C	1:I:606:GLN:H	1.93	0.73
2:M:70:ILE:H	2:M:70:ILE:HD12	1.52	0.73
3:J:461:GLY:O	3:J:464:SER:HB3	1.89	0.73
3:B:911:ASN:HD22	3:B:913:HIS:H	1.36	0.73
11:N:7:CYS:SG	11:N:48:MET:HG3	2.29	0.73
3:J:345:LEU:HD11	3:J:476:ILE:HG13	1.69	0.73
3:J:700:ARG:O	11:W:51:SER:HB2	1.89	0.73
7:G:83:ASP:O	7:G:93:THR:HA	1.89	0.73
1:I:245:ILE:HD13	1:I:268:LEU:HB3	1.71	0.73
1:A:846:VAL:HA	2:C:322:ARG:HE	1.54	0.73
3:B:353:LEU:HA	3:B:404:VAL:CG1	2.11	0.73
5:E:179:LYS:HE2	6:F:81:ASP:HB2	1.70	0.73
1:I:50:GLY:HA2	1:I:68:CYS:SG	2.29	0.73
3:B:210:PHE:HZ	3:B:323:ILE:HG22	1.54	0.72
1:I:301:ARG:O	1:I:302:LEU:HG	1.89	0.72
3:J:726:VAL:HG12	3:J:912:PRO:HG3	1.69	0.72
3:J:1067:ILE:HG13	3:J:1068:GLY:N	2.03	0.72
9:U:50:LEU:HD22	9:U:75:PRO:HD3	1.71	0.72
1:I:15:SER:HA	1:I:203:ARG:HH22	1.54	0.72
2:M:63:LEU:HD12	9:U:22:LEU:HD22	1.71	0.72
3:J:353:LEU:HA	3:J:404:VAL:CG1	2.10	0.72
1:A:721:PRO:HA	1:A:726:TYR:CD1	2.24	0.72
2:C:322:ARG:HH11	2:C:322:ARG:N	1.88	0.72
3:J:161:ILE:HG21	3:J:346:ALA:HA	1.71	0.72
3:J:1047:ASP:HA	3:J:1051:ASP:HB2	1.71	0.72
3:B:88:ARG:NH1	3:B:854:GLU:O	2.22	0.72
3:B:665:ARG:HG3	3:B:920:THR:CG2	2.19	0.72
3:B:687:ARG:HG3	3:B:687:ARG:NH1	2.04	0.72
1:I:632:PHE:HA	1:I:635:PHE:HD1	1.53	0.72
2:M:277:ILE:C	2:M:279:GLU:H	1.97	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:HD11	1:A:207:MET:HB2	1.70	0.72
1:A:220:ARG:HH11	1:A:236:THR:HG23	1.53	0.72
1:A:507:TYR:HB3	1:A:597:VAL:HG13	1.71	0.72
3:B:758:TYR:O	3:B:759:SER:HB3	1.88	0.72
2:M:70:ILE:N	2:M:70:ILE:HD13	2.03	0.72
8:T:30:LYS:O	8:T:33:LYS:HB2	1.90	0.72
1:I:155:LYS:H	1:I:155:LYS:HZ1	1.35	0.72
7:S:7:GLN:HG2	7:S:8:GLU:N	2.04	0.72
3:B:902:LYS:HB3	11:N:42:ARG:HD3	1.69	0.72
5:E:53:THR:HB	5:E:71:GLU:H	1.55	0.72
2:M:179:VAL:HG11	2:M:232:LYS:NZ	2.04	0.72
3:J:458:THR:HG21	3:J:465:GLY:N	2.04	0.72
5:Q:84:VAL:HG22	5:Q:145:ARG:HH11	1.54	0.72
3:J:805:LYS:HG3	3:J:844:MET:HB2	1.71	0.72
4:O:11:THR:O	4:O:238:PRO:HB3	1.90	0.72
2:C:237:ILE:HG22	2:C:257:ASN:HB2	1.72	0.72
2:C:343:ALA:HB2	2:C:371:GLU:HG3	1.71	0.72
1:A:558:LYS:HZ3	3:J:108:GLU:HG2	1.53	0.72
2:C:55:ALA:CA	2:C:58:GLU:HG3	2.19	0.72
5:E:26:ALA:O	5:E:30:LEU:HB2	1.89	0.72
7:G:63:ARG:HG3	7:G:114:ARG:HH22	1.55	0.72
3:B:522:LEU:O	3:B:525:ARG:HB3	1.90	0.71
2:M:179:VAL:HG23	2:M:182:ASP:H	1.55	0.71
3:J:873:THR:CG2	3:J:874:ILE:N	2.53	0.71
1:I:525:LEU:CD1	1:I:530:VAL:HG11	2.20	0.71
2:M:391:ARG:NH2	9:U:39:ARG:HH11	1.88	0.71
4:O:254:GLU:HG2	10:V:77:ARG:HH12	1.54	0.71
7:S:30:ASN:HA	7:S:39:SER:HB3	1.73	0.71
1:A:324:THR:HG22	1:A:325:VAL:N	2.02	0.71
1:A:502:TYR:CE1	1:A:636:ILE:HD11	2.24	0.71
1:A:567:ASN:N	1:A:599:ASP:OD2	2.21	0.71
2:M:391:ARG:HH22	9:U:39:ARG:HD2	1.55	0.71
1:A:590:ASN:ND2	3:J:377:ARG:CB	2.53	0.71
3:B:690:THR:HG22	3:B:691:ARG:HG3	1.71	0.71
1:I:90:ILE:HD11	1:I:207:MET:CB	2.20	0.71
1:I:220:ARG:HA	1:I:233:ASP:OD1	1.91	0.71
1:A:446:ASN:ND2	1:A:448:LEU:H	1.89	0.71
9:K:60:ASP:O	9:K:61:VAL:O	2.08	0.71
3:J:730:THR:HB	3:J:732:TYR:HD1	1.55	0.71
5:Q:64:GLY:H	9:U:41:LEU:HD22	1.55	0.71
3:B:1070:TYR:O	3:B:1071:ASP:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:666:ASP:O	1:I:670:VAL:HG13	1.91	0.71
3:J:739:ILE:CG2	3:J:909:ILE:HB	2.21	0.71
3:J:803:GLU:HB3	3:J:805:LYS:NZ	2.05	0.71
5:Q:135:VAL:H	5:Q:174:TRP:HZ2	1.36	0.71
10:V:4:ARG:HG2	10:V:4:ARG:HH11	1.56	0.71
1:A:846:VAL:O	2:C:322:ARG:NH2	2.23	0.71
1:A:853:ASP:HB2	2:C:311:ARG:NH1	2.05	0.71
2:C:327:ARG:HG3	2:C:334:VAL:HB	1.71	0.71
1:I:106:ILE:HG22	1:I:107:SER:H	1.56	0.71
2:M:54:LEU:O	2:M:58:GLU:HG3	1.90	0.71
12:X:46:LYS:HD2	12:X:46:LYS:N	2.06	0.71
1:A:468:GLN:HG3	3:B:1052:ASN:HD21	1.54	0.71
3:B:805:LYS:HG3	3:B:844:MET:HB2	1.71	0.71
1:I:595:GLU:CB	7:S:91:LYS:HE2	2.21	0.71
2:M:69:ALA:HB2	2:M:381:LEU:HD13	1.72	0.71
1:A:234:ASP:OD2	1:A:296:ARG:HD3	1.91	0.71
1:A:532:ILE:CD1	10:L:56:LYS:HD3	2.20	0.71
2:C:354:LEU:HD13	3:B:1104:LEU:HD21	1.73	0.71
3:B:554:ASN:HD21	3:B:576:ARG:HH21	1.39	0.71
12:P:17:GLN:HB3	12:P:19:LYS:HG3	1.73	0.71
1:I:697:GLU:OE1	1:I:756:ARG:HD3	1.91	0.71
1:A:331:ASN:O	1:A:332:ILE:CB	2.39	0.70
8:H:46:ARG:HH22	13:Y:78:ARG:HH11	1.39	0.70
1:I:238:LYS:HD3	1:I:276:TYR:HA	1.73	0.70
8:T:39:PRO:HB2	8:T:80:TYR:CE2	2.25	0.70
3:J:1000:LYS:O	3:J:1001:LEU:HB2	1.90	0.70
5:E:179:LYS:CE	6:F:81:ASP:HB2	2.21	0.70
13:Z:57:GLY:CA	13:Z:61:LEU:HG	2.21	0.70
3:B:458:THR:CG2	3:B:465:GLY:H	2.03	0.70
8:H:29:TYR:OH	13:Y:67:LEU:CD2	2.25	0.70
1:I:589:LYS:HG2	1:I:877:GLY:HA2	1.73	0.70
2:M:301:LEU:HA	2:M:304:GLN:HG3	1.71	0.70
3:J:724:LEU:HD12	3:J:908:ILE:HG22	1.73	0.70
9:U:90:LEU:N	9:U:90:LEU:HD23	2.07	0.70
1:A:828:SER:O	1:A:830:LEU:N	2.22	0.70
3:B:1004:ARG:HH11	3:B:1025:GLY:H	1.39	0.70
3:J:1070:TYR:O	3:J:1071:ASP:O	2.09	0.70
3:B:448:THR:C	3:B:450:TRP:H	1.99	0.70
3:B:1067:ILE:HG13	3:B:1068:GLY:N	2.07	0.70
10:L:24:LEU:O	10:L:28:ILE:HG12	1.90	0.70
12:P:46:LYS:HD2	12:P:46:LYS:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:525:LEU:HD11	1:I:530:VAL:HG11	1.71	0.70
1:I:704:LEU:HD22	1:I:781:PHE:CE1	2.26	0.70
2:M:377:HIS:ND1	2:M:378:PRO:HD2	2.07	0.70
3:J:1095:TYR:CE1	3:J:1098:LYS:HD2	2.26	0.70
7:S:72:CYS:SG	7:S:114:ARG:HB3	2.31	0.70
1:A:19:ILE:HA	1:A:22:MET:HE2	1.74	0.70
1:I:316:LYS:HE2	3:J:1054:ASP:OD2	1.91	0.70
1:I:733:ALA:HB1	3:J:913:HIS:CE1	2.27	0.70
1:I:827:LEU:HD11	2:M:315:LEU:HD13	1.73	0.70
2:M:277:ILE:O	2:M:279:GLU:N	2.24	0.70
1:A:50:GLY:HA2	1:A:68:CYS:SG	2.31	0.70
2:C:276:ASN:HD22	2:C:279:GLU:CB	2.05	0.70
9:K:23:TRP:CE3	9:K:23:TRP:HA	2.27	0.70
1:I:9:ILE:O	2:M:363:VAL:O	2.10	0.70
3:B:848:ASP:HB2	3:B:867:ARG:H	1.55	0.70
1:I:468:GLN:HG3	3:J:1052:ASN:HD21	1.56	0.70
1:I:594:LEU:CA	7:S:86:LEU:HD22	2.21	0.70
3:J:210:PHE:HZ	3:J:323:ILE:HG22	1.56	0.70
5:Q:18:PHE:CE2	9:U:42:GLN:HG2	2.27	0.70
2:C:269:VAL:HA	2:C:272:VAL:HG23	1.74	0.69
7:G:109:LYS:NZ	3:J:378:LYS:HE3	2.07	0.69
1:I:541:ALA:HB1	7:S:71:PHE:HA	1.73	0.69
11:W:22:ILE:HD13	11:W:23:THR:H	1.56	0.69
1:A:99:ARG:HD2	1:A:150:ASN:H	1.58	0.69
1:I:293:ARG:HH11	1:I:296:ARG:NH2	1.88	0.69
3:J:227:MET:HE3	3:J:312:ALA:HB1	1.74	0.69
3:J:1004:ARG:HH11	3:J:1025:GLY:H	1.38	0.69
2:C:69:ALA:HB2	2:C:381:LEU:HD22	1.73	0.69
3:B:480:ILE:HG22	3:B:481:ASN:N	2.07	0.69
5:E:83:GLU:H	5:E:145:ARG:HG3	1.55	0.69
9:K:38:ALA:HB1	9:K:42:GLN:HE22	1.56	0.69
2:M:70:ILE:H	2:M:70:ILE:HD13	1.57	0.69
2:M:192:LYS:C	2:M:194:GLY:H	2.00	0.69
1:A:541:ALA:HB1	7:G:71:PHE:HA	1.75	0.69
2:M:86:THR:HA	2:M:104:LEU:HD12	1.74	0.69
3:J:70:VAL:HG11	3:J:90:LEU:HD23	1.75	0.69
3:J:591:ILE:CG1	3:J:612:LYS:HZ3	2.06	0.69
3:J:812:GLY:HA2	3:J:836:SER:HB3	1.74	0.69
3:J:881:ARG:NH1	3:J:989:TYR:HB3	2.06	0.69
1:A:313:LEU:HG	2:C:374:ILE:HG23	1.73	0.69
1:A:470:GLU:O	1:A:473:ILE:HG12	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:800:PRO:HD3	3:B:850:VAL:HG23	1.74	0.69
3:B:974:ARG:HB2	10:L:22:HIS:CD2	2.27	0.69
4:D:111:SER:HA	4:D:114:ILE:CD1	2.22	0.69
1:I:4:LYS:HD2	3:J:1089:PHE:HB3	1.74	0.69
3:J:181:SER:HB3	3:J:183:ILE:HD12	1.72	0.69
3:J:930:GLY:HA2	11:W:47:ARG:HH22	1.58	0.69
1:A:364:PHE:CE1	1:A:409:ARG:HD2	2.28	0.69
1:A:510:THR:O	1:A:549:LYS:HG3	1.93	0.69
2:C:54:LEU:O	2:C:58:GLU:N	2.25	0.69
6:F:81:ASP:O	6:F:84:ARG:HG2	1.92	0.69
1:I:293:ARG:HH11	1:I:296:ARG:HH22	1.39	0.69
1:I:502:TYR:CE1	1:I:636:ILE:HD11	2.27	0.69
1:I:594:LEU:HA	7:S:86:LEU:CD2	2.22	0.69
2:M:390:MET:HB2	5:Q:56:GLU:CG	2.23	0.69
3:J:10:ARG:HB2	3:J:642:ILE:O	1.91	0.69
3:J:1015:GLN:NE2	3:J:1096:ALA:HB2	2.08	0.69
3:J:1067:ILE:HG13	3:J:1068:GLY:H	1.57	0.69
2:C:237:ILE:HG13	2:C:238:LYS:H	1.57	0.69
3:B:602:ILE:CG2	3:B:603:THR:H	2.05	0.69
1:I:541:ALA:HB2	7:S:72:CYS:N	2.08	0.69
3:J:933:ALA:HB3	11:W:47:ARG:HH12	1.58	0.69
7:S:43:ILE:O	7:S:46:ILE:HG22	1.93	0.69
10:V:83:TYR:O	10:V:87:ILE:HB	1.92	0.69
1:A:446:ASN:HD22	1:A:448:LEU:H	1.38	0.69
2:C:70:ILE:HD13	2:C:70:ILE:N	2.07	0.69
3:B:479:GLY:HA2	3:B:552:GLU:HB3	1.75	0.69
7:G:67:SER:O	7:G:69:ASP:N	2.26	0.69
1:I:696:LEU:O	1:I:700:ILE:HG12	1.93	0.69
3:J:448:THR:C	3:J:450:TRP:H	1.99	0.69
3:B:10:ARG:HB2	3:B:642:ILE:O	1.92	0.68
3:B:81:SER:HB3	3:B:84:GLU:HG3	1.74	0.68
1:I:852:ASP:HB3	8:T:75:VAL:HG21	1.76	0.68
2:M:315:LEU:O	2:M:319:VAL:HG23	1.93	0.68
3:J:17:TYR:OH	3:J:474:ALA:HA	1.93	0.68
3:J:851:LEU:HD12	12:X:35:PHE:HD2	1.56	0.68
6:R:47:CYS:HB2	6:R:52:ALA:HB2	1.76	0.68
11:W:7:CYS:SG	11:W:45:CYS:SG	2.91	0.68
1:A:245:ILE:HD13	1:A:268:LEU:HB3	1.75	0.68
1:A:293:ARG:HH11	1:A:296:ARG:HH22	1.39	0.68
3:B:708:LEU:HD13	3:B:713:TYR:HB3	1.75	0.68
11:N:18:TRP:HD1	11:N:49:LEU:HD22	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:PHE:HB2	2:M:361:GLY:O	1.93	0.68
1:I:110:GLU:HG2	1:I:113:LYS:HD2	1.75	0.68
2:M:366:PHE:CZ	2:M:375:ILE:HD12	2.28	0.68
2:M:386:VAL:HG13	9:U:34:ARG:HG2	1.74	0.68
3:J:246:PRO:C	3:J:248:VAL:H	2.02	0.68
1:A:491:TYR:HD1	1:A:607:GLN:NE2	1.92	0.68
2:C:190:ARG:HD3	2:C:191:LEU:H	1.58	0.68
3:B:253:PHE:N	3:B:254:PRO:HD2	2.08	0.68
3:B:445:LEU:HD11	3:B:455:PRO:CB	2.23	0.68
11:N:7:CYS:HB3	11:N:45:CYS:SG	2.33	0.68
3:B:361:PHE:HE1	3:B:385:VAL:HG13	1.57	0.68
5:E:179:LYS:NZ	6:F:79:THR:HB	2.09	0.68
2:M:111:VAL:HG12	2:M:329:ILE:HB	1.75	0.68
9:U:61:VAL:C	9:U:63:SER:H	2.00	0.68
4:D:230:ILE:HG13	4:D:242:LEU:HD21	1.75	0.68
1:I:68:CYS:SG	1:I:71:HIS:CE1	2.86	0.68
1:I:99:ARG:HD2	1:I:150:ASN:H	1.56	0.68
1:I:826:ALA:H	2:M:335:THR:CG2	2.07	0.68
3:J:555:VAL:O	3:J:620:GLU:HG3	1.93	0.68
3:J:602:ILE:CG2	3:J:603:THR:H	2.06	0.68
3:B:246:PRO:C	3:B:248:VAL:H	2.02	0.68
3:B:797:VAL:HB	12:P:36:MET:HE1	1.75	0.68
9:K:41:LEU:O	9:K:42:GLN:C	2.36	0.68
1:I:19:ILE:HA	1:I:22:MET:HE2	1.76	0.68
1:I:733:ALA:HB1	3:J:913:HIS:HE1	1.59	0.68
2:C:321:THR:C	2:C:322:ARG:HH11	2.02	0.68
3:B:763:VAL:HA	3:B:770:GLU:HG3	1.75	0.68
1:I:325:VAL:O	1:I:442:THR:HB	1.94	0.68
3:J:20:SER:O	3:J:25:ARG:NH2	2.24	0.68
1:A:331:ASN:ND2	3:B:732:TYR:OH	2.27	0.68
1:A:595:GLU:HB3	7:G:86:LEU:HD13	1.76	0.68
3:B:17:TYR:OH	3:B:474:ALA:HA	1.94	0.68
8:H:40:GLU:OE1	13:Y:66:LYS:CE	2.39	0.68
1:I:491:TYR:HD1	1:I:607:GLN:NE2	1.91	0.68
3:J:630:PRO:O	3:J:633:LEU:HB3	1.93	0.68
13:Z:58:LYS:O	13:Z:59:ILE:HB	1.94	0.68
1:I:575:CYS:HG	1:I:580:CYS:CB	2.06	0.68
1:I:721:PRO:HA	1:I:726:TYR:CD1	2.27	0.68
2:M:117:PRO:O	2:M:120:PRO:HG3	1.92	0.68
3:J:591:ILE:HG12	3:J:612:LYS:NZ	2.09	0.68
1:A:549:LYS:HG2	1:A:593:LEU:HD13	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:ARG:HB3	1:I:195:LEU:O	1.93	0.68
2:M:392:PRO:HD3	5:Q:56:GLU:HG3	1.75	0.68
3:J:926:GLU:HB3	3:J:988:VAL:HG22	1.76	0.68
9:K:82:LEU:H	9:K:82:LEU:CD2	2.07	0.67
1:I:141:MET:HG3	1:I:148:HIS:HA	1.76	0.67
1:I:828:SER:O	1:I:830:LEU:N	2.27	0.67
1:I:839:ARG:NH1	8:T:37:ILE:HG23	2.09	0.67
3:B:881:ARG:HD2	3:B:989:TYR:HD2	1.59	0.67
3:B:890:MET:HE3	3:B:890:MET:HA	1.75	0.67
1:I:256:GLY:O	1:I:258:PRO:HD3	1.94	0.67
1:I:328:PRO:HG3	1:I:457:PHE:CD1	2.30	0.67
2:M:55:ALA:CA	2:M:58:GLU:HB2	2.22	0.67
5:Q:31:ARG:C	5:Q:33:GLN:H	2.01	0.67
7:S:101:LEU:C	7:S:103:VAL:H	2.02	0.67
1:A:90:ILE:HD11	1:A:207:MET:CB	2.24	0.67
3:B:544:ARG:HH11	3:B:544:ARG:HG3	1.59	0.67
3:J:759:SER:HB3	3:J:863:LYS:HA	1.76	0.67
4:O:111:SER:HA	4:O:114:ILE:CD1	2.24	0.67
1:A:499:ALA:HB3	3:B:734:MET:CE	2.25	0.67
2:M:109:GLU:O	2:M:113:ALA:N	2.28	0.67
3:B:851:LEU:HD12	12:P:35:PHE:CD2	2.28	0.67
4:D:250:ILE:HA	4:D:253:ILE:HG22	1.77	0.67
2:M:373:ILE:HG13	3:J:1049:LEU:HD13	1.75	0.67
3:J:64:ARG:HG2	3:J:97:TRP:CD1	2.29	0.67
3:J:537:ALA:HB2	3:J:557:HIS:NE2	2.09	0.67
3:J:851:LEU:HD12	12:X:35:PHE:CD2	2.30	0.67
1:A:490:ARG:HG2	1:A:491:TYR:CD2	2.30	0.67
2:C:237:ILE:HG22	2:C:257:ASN:CB	2.25	0.67
2:M:355:LEU:HD22	3:J:1109:ILE:HD11	1.76	0.67
2:M:391:ARG:H	2:M:392:PRO:HD3	1.60	0.67
11:W:18:TRP:HD1	11:W:49:LEU:HD22	1.58	0.67
3:B:161:ILE:HG21	3:B:346:ALA:HA	1.77	0.67
11:N:22:ILE:HD13	11:N:23:THR:H	1.58	0.67
1:I:426:HIS:CE1	1:I:428:ILE:CG2	2.77	0.67
1:I:475:GLU:CD	2:M:383:THR:HG21	2.19	0.67
5:Q:27:LEU:HB2	5:Q:51:VAL:CG1	2.22	0.67
4:D:11:THR:O	4:D:238:PRO:HB3	1.94	0.67
2:M:55:ALA:HA	2:M:58:GLU:CB	2.21	0.67
2:M:231:ILE:HB	2:M:234:ILE:HG12	1.75	0.67
9:U:61:VAL:HG12	9:U:62:ILE:N	2.06	0.67
1:A:532:ILE:HD11	10:L:56:LYS:CD	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:291:GLN:HB3	3:B:295:LYS:HE2	1.77	0.67
3:B:933:ALA:HB3	11:N:47:ARG:HH12	1.58	0.67
3:J:38:LYS:HA	3:J:41:GLU:HG3	1.76	0.67
3:J:848:ASP:HB2	3:J:867:ARG:H	1.60	0.67
1:A:589:LYS:HG2	1:A:877:GLY:HA2	1.77	0.67
3:B:602:ILE:HG23	3:B:603:THR:H	1.59	0.67
3:J:850:VAL:O	12:X:35:PHE:HB2	1.95	0.67
3:J:890:MET:HE3	3:J:890:MET:HA	1.77	0.67
6:R:51:SER:O	6:R:55:VAL:HG23	1.94	0.67
1:A:877:GLY:C	3:J:377:ARG:NH1	2.47	0.66
3:B:602:ILE:CG2	3:B:603:THR:N	2.58	0.66
3:J:665:ARG:HG3	3:J:920:THR:HG21	1.76	0.66
3:J:962:TYR:OH	11:W:42:ARG:HD2	1.95	0.66
1:I:421:ARG:HB2	1:I:462:MET:HE3	1.78	0.66
1:I:826:ALA:HB2	2:M:335:THR:HG23	1.77	0.66
5:Q:64:GLY:N	9:U:41:LEU:HD22	2.09	0.66
3:B:451:GLY:CA	3:B:577:ARG:HH11	2.08	0.66
3:B:457:GLU:HG2	3:B:469:ASN:OD1	1.96	0.66
3:B:683:ASN:C	3:B:685:GLN:H	2.04	0.66
3:B:934:ALA:O	11:N:46:ARG:HD3	1.95	0.66
2:M:159:ASP:HB3	2:M:163:MET:HB2	1.77	0.66
2:M:391:ARG:HH22	9:U:39:ARG:NH1	1.93	0.66
3:J:451:GLY:CA	3:J:577:ARG:HH11	2.08	0.66
2:C:104:LEU:HB3	2:C:105:PRO:HD3	1.77	0.66
2:M:104:LEU:HB3	2:M:105:PRO:HD3	1.76	0.66
2:M:309:ASP:OD2	2:M:311:ARG:N	2.29	0.66
2:M:390:MET:CG	5:Q:56:GLU:HG2	2.25	0.66
3:J:253:PHE:N	3:J:254:PRO:HD2	2.09	0.66
1:A:326:ILE:HG21	1:A:462:MET:HG3	1.77	0.66
1:A:569:SER:HB2	1:A:584:SER:HG	1.59	0.66
1:A:569:SER:HB2	1:A:584:SER:OG	1.95	0.66
1:A:666:ASP:O	1:A:670:VAL:HG13	1.94	0.66
3:B:20:SER:O	3:B:25:ARG:NH2	2.28	0.66
3:B:806:GLY:O	3:B:839:THR:HB	1.95	0.66
2:M:261:VAL:O	2:M:261:VAL:HG12	1.96	0.66
1:I:4:LYS:HD3	3:J:1091:VAL:HB	1.78	0.66
1:I:722:PHE:HZ	7:S:23:LEU:HG	1.60	0.66
4:O:250:ILE:HA	4:O:253:ILE:HG22	1.78	0.66
7:S:86:LEU:HD12	7:S:91:LYS:CG	2.26	0.66
3:B:26:GLN:O	3:B:345:LEU:CD2	2.40	0.66
4:D:111:SER:CA	4:D:114:ILE:HD13	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:33:LEU:O	6:F:34:LEU:HD23	1.96	0.66
3:J:602:ILE:HG23	3:J:603:THR:H	1.61	0.66
3:J:702:LEU:HD12	11:W:51:SER:HB3	1.76	0.66
4:O:109:ILE:HD11	4:O:133:LEU:HD12	1.77	0.66
7:G:87:ASN:C	7:G:89:GLY:N	2.53	0.66
2:M:298:SER:O	2:M:302:ALA:HB2	1.96	0.66
3:J:1012:LEU:O	3:J:1095:TYR:HE2	1.79	0.66
1:A:549:LYS:CE	7:G:89:GLY:HA2	2.25	0.66
3:B:450:TRP:CZ2	3:B:641:GLU:OE1	2.47	0.66
1:I:534:LEU:HB2	10:V:39:SER:OG	1.96	0.66
1:I:549:LYS:CE	7:S:89:GLY:HA2	2.26	0.66
2:M:72:ILE:HD12	2:M:72:ILE:H	1.58	0.66
3:J:291:GLN:C	3:J:293:ILE:H	2.04	0.66
3:J:291:GLN:HB3	3:J:295:LYS:HE2	1.77	0.66
3:J:522:LEU:O	3:J:525:ARG:HB3	1.95	0.66
7:S:13:CYS:HA	7:S:33:CYS:HA	1.77	0.66
1:A:575:CYS:HG	1:A:580:CYS:CB	2.09	0.66
1:A:818:TYR:OH	2:C:348:GLU:OE2	2.12	0.66
4:D:190:LEU:CD2	4:D:195:LEU:HA	2.25	0.66
4:D:259:LYS:O	4:D:263:VAL:HG23	1.96	0.66
4:O:190:LEU:CD2	4:O:195:LEU:HA	2.26	0.66
5:Q:43:GLY:HA3	5:Q:78:VAL:HG23	1.78	0.66
1:A:106:ILE:HG22	1:A:107:SER:H	1.59	0.65
1:A:239:LEU:HD22	1:A:276:TYR:CE1	2.31	0.65
1:A:475:GLU:CD	2:C:383:THR:HG21	2.20	0.65
3:B:1015:GLN:NE2	3:B:1096:ALA:HB2	2.11	0.65
3:B:1095:TYR:CE1	3:B:1098:LYS:HD2	2.30	0.65
5:E:113:ILE:O	5:E:164:MET:HB2	1.96	0.65
8:H:29:TYR:HH	13:Y:67:LEU:HD22	1.54	0.65
9:K:71:ARG:O	9:K:72:GLY:C	2.37	0.65
1:I:345:LYS:HA	1:I:410:HIS:CD2	2.30	0.65
1:I:353:ILE:HD11	1:I:407:ILE:HG23	1.78	0.65
2:M:168:GLN:HG2	2:M:204:SER:HB3	1.78	0.65
3:J:690:THR:HG22	3:J:691:ARG:HG3	1.77	0.65
3:J:902:LYS:HB3	11:W:42:ARG:CD	2.25	0.65
1:A:647:ARG:NH2	3:B:982:ARG:HH12	1.94	0.65
3:B:569:ASN:HB3	3:B:574:ARG:NH2	2.09	0.65
4:D:44:VAL:HA	4:D:143:ALA:HA	1.77	0.65
2:M:237:ILE:HG13	2:M:238:LYS:N	2.10	0.65
2:M:354:LEU:HD22	3:J:1104:LEU:HD21	1.77	0.65
1:A:637:ARG:HD3	1:A:640:GLU:CD	2.20	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:696:LEU:O	1:A:700:ILE:HG12	1.95	0.65
1:A:837:THR:HG22	1:A:838:VAL:H	1.62	0.65
3:B:345:LEU:HD11	3:B:476:ILE:HG13	1.77	0.65
12:P:24:VAL:HG13	12:P:24:VAL:O	1.96	0.65
1:I:27:ILE:HG23	1:I:45:MET:HA	1.78	0.65
1:I:308:ARG:HG3	1:I:312:ASN:HD22	1.61	0.65
1:I:329:ASP:CG	1:I:332:ILE:HD12	2.21	0.65
1:I:515:LEU:HD13	7:S:43:ILE:HD12	1.78	0.65
3:J:781:ARG:HD3	3:J:782:GLY:H	1.61	0.65
1:A:104:VAL:HG12	1:A:104:VAL:O	1.96	0.65
1:A:141:MET:HG3	1:A:148:HIS:HA	1.78	0.65
1:A:590:ASN:HD21	3:J:377:ARG:HD2	1.61	0.65
5:E:127:ILE:HB	5:E:136:ILE:HB	1.78	0.65
1:I:841:LEU:HD11	2:M:339:ASN:HB3	1.78	0.65
3:J:587:PRO:O	3:J:588:LEU:HD23	1.96	0.65
10:L:67:ASP:HA	10:L:70:LEU:HB2	1.77	0.65
2:M:390:MET:CB	5:Q:56:GLU:HG2	2.26	0.65
3:J:298:LEU:C	3:J:300:HIS:H	2.05	0.65
5:Q:26:ALA:O	5:Q:30:LEU:HB2	1.97	0.65
3:B:739:ILE:CG2	3:B:909:ILE:HB	2.27	0.65
2:M:288:ALA:HB2	8:T:17:VAL:HB	1.77	0.65
3:J:162:VAL:HG11	3:J:412:GLN:NE2	2.10	0.65
7:S:60:SER:OG	7:S:64:PRO:HD3	1.95	0.65
1:A:827:LEU:HD11	2:C:315:LEU:HD12	1.79	0.65
1:I:635:PHE:O	1:I:639:VAL:HG23	1.97	0.65
3:J:588:LEU:HD13	3:J:612:LYS:HB3	1.79	0.65
1:A:749:GLN:H	1:A:781:PHE:HA	1.61	0.65
3:B:1047:ASP:HA	3:B:1051:ASP:HB2	1.79	0.65
3:J:147:ASP:OD2	3:J:148:PRO:HD2	1.97	0.65
3:B:245:ASP:N	3:B:246:PRO:HD3	2.12	0.65
3:B:724:LEU:HD12	3:B:908:ILE:HG22	1.78	0.65
3:J:367:TYR:CD2	3:J:367:TYR:C	2.75	0.65
3:J:602:ILE:CG2	3:J:603:THR:N	2.60	0.65
9:U:91:SER:O	9:U:92:LEU:CB	2.44	0.65
1:A:512:LYS:HE2	7:G:91:LYS:CE	2.26	0.65
3:B:552:GLU:HA	3:B:576:ARG:HH22	1.62	0.65
7:G:15:ILE:HD13	7:G:53:GLU:HB3	1.78	0.65
1:I:764:ARG:CB	1:I:764:ARG:HH11	2.09	0.65
3:J:1064:CYS:HG	14:J:2001:ZN:ZN	1.08	0.65
12:X:26:CYS:HB2	12:X:27:PRO:CD	2.26	0.65
1:A:378:VAL:O	1:A:378:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:VAL:HG23	1:A:407:ILE:HG22	1.80	0.64
2:C:299:LYS:HA	2:C:302:ALA:HB3	1.78	0.64
2:C:390:MET:O	2:C:391:ARG:CB	2.45	0.64
3:B:298:LEU:C	3:B:300:HIS:H	2.04	0.64
5:E:39:LEU:O	5:E:40:LYS:HB2	1.96	0.64
7:G:41:ASP:HB2	7:G:90:ASN:HB3	1.79	0.64
1:I:354:THR:HB	1:I:355:PRO:HD2	1.78	0.64
1:I:507:TYR:HB3	1:I:597:VAL:HG13	1.79	0.64
1:I:549:LYS:HG2	1:I:593:LEU:HD13	1.79	0.64
1:I:750:GLN:HG3	1:I:782:ILE:CD1	2.27	0.64
3:J:183:ILE:HB	3:J:207:ASP:C	2.22	0.64
3:J:840:ARG:HH11	3:J:1021:ALA:HB2	1.62	0.64
9:U:61:VAL:CG1	9:U:62:ILE:H	2.05	0.64
1:A:4:LYS:HD2	3:B:1089:PHE:HB3	1.79	0.64
1:A:345:LYS:HA	1:A:410:HIS:CD2	2.32	0.64
1:A:558:LYS:NZ	3:J:108:GLU:HG2	2.12	0.64
2:C:69:ALA:CB	2:C:381:LEU:HD22	2.27	0.64
2:C:104:LEU:O	2:C:108:ILE:HG12	1.96	0.64
4:O:133:LEU:HD21	4:O:139:ILE:HG13	1.78	0.64
7:S:83:ASP:O	7:S:93:THR:HA	1.98	0.64
1:I:446:ASN:C	1:I:446:ASN:HD22	2.05	0.64
1:A:329:ASP:CG	1:A:332:ILE:HD12	2.22	0.64
3:B:577:ARG:HE	3:B:578:PRO:HD2	1.63	0.64
3:B:881:ARG:HD2	3:B:989:TYR:CD2	2.32	0.64
8:H:78:TYR:O	8:H:79:ARG:HG2	1.98	0.64
1:I:196:GLY:O	2:M:360:ARG:HG2	1.97	0.64
9:U:19:PHE:O	9:U:20:ILE:C	2.40	0.64
10:V:32:LEU:HD13	10:V:32:LEU:O	1.98	0.64
3:B:28:LEU:HG	3:B:122:MET:CE	2.28	0.64
4:D:247:LYS:HA	4:D:250:ILE:HD12	1.78	0.64
1:I:720:ASP:C	1:I:722:PHE:H	2.04	0.64
2:M:328:GLN:O	2:M:333:GLY:HA3	1.98	0.64
3:J:336:ASP:HA	3:J:341:LYS:HE3	1.79	0.64
2:C:50:LYS:HA	2:C:53:ASP:HB2	1.79	0.64
3:B:735:GLU:O	3:B:736:ASP:C	2.40	0.64
8:H:42:LEU:HB2	8:H:43:PRO:HD2	1.78	0.64
2:M:68:GLU:HB3	9:U:30:TYR:HE1	1.62	0.64
5:Q:15:PRO:HG2	9:U:45:MET:CB	2.28	0.64
3:B:416:ARG:NH1	3:B:687:ARG:NH2	2.46	0.64
3:B:900:THR:HG22	3:B:970:VAL:HG12	1.79	0.64
1:I:133:THR:HB	1:I:137:LYS:HZ2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:647:ARG:O	1:I:650:ASP:HB2	1.96	0.64
1:I:830:LEU:CD2	1:I:840:SER:HB3	2.24	0.64
2:M:150:GLU:HG3	2:M:227:LEU:HD22	1.78	0.64
2:M:309:ASP:OD2	2:M:309:ASP:C	2.41	0.64
2:M:391:ARG:HH21	9:U:42:GLN:CG	2.11	0.64
3:J:318:ALA:O	3:J:321:LYS:HB2	1.97	0.64
3:J:890:MET:CE	3:J:891:LEU:H	2.08	0.64
1:A:678:LYS:HD2	1:A:684:LEU:HG	1.79	0.64
3:B:64:ARG:O	3:B:97:TRP:HB2	1.98	0.64
3:B:569:ASN:CB	3:B:574:ARG:HH22	2.10	0.64
3:B:657:TYR:O	3:B:660:HIS:HB2	1.97	0.64
6:F:1:MET:SD	6:F:6:ILE:HG12	2.37	0.64
7:G:101:LEU:HD12	7:G:104:LYS:NZ	2.12	0.64
1:A:27:ILE:HG23	1:A:45:MET:HA	1.79	0.64
3:B:972:ASP:OD2	3:B:974:ARG:HG2	1.97	0.64
12:X:24:VAL:HG13	12:X:24:VAL:O	1.97	0.64
3:B:116:ILE:HG22	3:B:390:VAL:HG21	1.79	0.64
3:B:239:VAL:HA	3:B:253:PHE:HE2	1.63	0.64
1:I:490:ARG:HG2	1:I:491:TYR:CD2	2.33	0.64
1:I:549:LYS:HE2	7:S:89:GLY:HA2	1.80	0.64
3:J:480:ILE:HG22	3:J:481:ASN:N	2.13	0.64
8:T:42:LEU:O	8:T:44:TRP:N	2.30	0.64
2:C:60:SER:O	2:C:63:LEU:HB3	1.98	0.63
2:C:311:ARG:HD3	2:C:311:ARG:N	2.14	0.63
3:B:930:GLY:HA2	11:N:47:ARG:HH22	1.62	0.63
2:M:68:GLU:HB3	9:U:30:TYR:CE1	2.33	0.63
3:J:591:ILE:HG12	3:J:612:LYS:HZ3	1.63	0.63
6:R:23:ASP:O	6:R:26:ARG:HB2	1.97	0.63
10:V:59:THR:CG2	10:V:65:PRO:HD3	2.28	0.63
1:I:647:ARG:NH2	3:J:982:ARG:HH12	1.97	0.63
2:M:390:MET:HA	2:M:390:MET:HE2	1.79	0.63
3:J:591:ILE:H	3:J:591:ILE:HD12	1.61	0.63
1:A:133:THR:HB	1:A:137:LYS:HZ2	1.63	0.63
1:A:156:ILE:HD11	1:A:270:GLN:HG2	1.80	0.63
1:A:353:ILE:HG13	1:A:361:LEU:CD2	2.29	0.63
2:C:359:ALA:C	2:C:361:GLY:H	2.06	0.63
3:B:99:THR:O	3:B:99:THR:HG22	1.98	0.63
3:B:537:ALA:HB2	3:B:557:HIS:NE2	2.13	0.63
4:D:131:VAL:HG22	4:D:132:LEU:N	2.13	0.63
8:H:11:PRO:O	8:H:13:ILE:N	2.29	0.63
3:J:702:LEU:HB2	3:J:721:ASN:ND2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:752:VAL:C	1:A:754:GLY:H	2.06	0.63
2:C:33:LYS:O	2:C:36:ILE:HG22	1.99	0.63
3:B:840:ARG:HH11	3:B:1021:ALA:HB2	1.62	0.63
1:I:364:PHE:CE1	1:I:409:ARG:HD2	2.34	0.63
3:J:325:LEU:HD13	3:J:330:ARG:H	1.62	0.63
3:J:638:THR:HB	3:J:639:HIS:HD2	1.62	0.63
3:J:739:ILE:HG12	3:J:890:MET:O	1.98	0.63
1:A:720:ASP:C	1:A:722:PHE:H	2.06	0.63
9:K:74:LEU:HD12	9:K:74:LEU:N	2.14	0.63
1:I:750:GLN:HG3	1:I:782:ILE:HD11	1.80	0.63
2:M:106:ARG:O	2:M:109:GLU:N	2.31	0.63
3:J:361:PHE:HE1	3:J:385:VAL:HG13	1.62	0.63
1:I:191:ASP:HA	1:I:194:ILE:HD11	1.81	0.63
1:I:512:LYS:HE2	7:S:91:LYS:CE	2.29	0.63
2:M:70:ILE:O	2:M:71:GLY:C	2.41	0.63
5:Q:109:HIS:CD2	5:Q:111:SER:H	2.17	0.63
8:T:65:ILE:HD11	8:T:79:ARG:CG	2.28	0.63
3:B:922:GLY:O	3:B:926:GLU:HB2	1.99	0.63
1:I:12:GLY:HA2	2:M:358:ALA:O	1.99	0.63
1:I:503:ILE:HD11	1:I:733:ALA:N	2.12	0.63
1:I:595:GLU:HB2	7:S:91:LYS:HE2	1.80	0.63
1:I:825:ASN:O	1:I:826:ALA:C	2.41	0.63
3:J:64:ARG:HG2	3:J:97:TRP:CG	2.33	0.63
3:J:245:ASP:N	3:J:246:PRO:HD3	2.13	0.63
1:A:110:GLU:HG2	1:A:113:LYS:HD2	1.81	0.63
2:C:183:ASP:O	2:C:187:ALA:HB2	1.98	0.63
3:B:683:ASN:O	3:B:685:GLN:N	2.32	0.63
1:I:327:SER:HB2	1:I:444:ARG:HD3	1.80	0.63
3:J:239:VAL:HA	3:J:253:PHE:HE2	1.63	0.63
3:J:922:GLY:CA	3:J:925:MET:HB2	2.17	0.63
7:S:86:LEU:HD12	7:S:91:LYS:HG2	1.81	0.63
3:B:249:GLN:HG3	3:B:250:ASN:N	2.14	0.63
6:R:34:LEU:HD22	6:R:38:TYR:CE2	2.34	0.63
1:A:316:LYS:HD2	3:B:1049:LEU:O	1.99	0.62
3:B:356:VAL:HG11	3:B:404:VAL:HG12	1.81	0.62
6:F:23:ASP:O	6:F:26:ARG:HB2	1.99	0.62
2:M:150:GLU:HG3	2:M:227:LEU:CD2	2.29	0.62
3:J:296:TYR:O	3:J:297:PHE:HB2	1.99	0.62
12:X:37:VAL:HG22	12:X:38:ARG:H	1.63	0.62
3:B:1067:ILE:HG13	3:B:1068:GLY:H	1.64	0.62
12:P:37:VAL:HG22	12:P:38:ARG:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:823:LEU:HD13	2:M:75:ALA:CB	2.27	0.62
2:M:391:ARG:HH21	9:U:42:GLN:HG2	1.64	0.62
1:A:555:PHE:CD2	1:A:631:LEU:HD13	2.34	0.62
1:A:587:VAL:HB	1:A:594:LEU:O	1.99	0.62
3:B:700:ARG:N	11:N:51:SER:O	2.31	0.62
3:B:1085:LYS:O	3:B:1086:SER:OG	2.17	0.62
7:G:101:LEU:HD12	7:G:104:LYS:HZ3	1.64	0.62
3:J:738:ILE:CD1	3:J:908:ILE:HG23	2.29	0.62
3:B:469:ASN:HD22	3:B:469:ASN:N	1.98	0.62
3:B:890:MET:CE	3:B:891:LEU:H	2.13	0.62
8:H:25:ILE:HA	8:H:28:ALA:HB3	1.81	0.62
1:I:833:GLU:HG3	1:I:839:ARG:HG3	1.81	0.62
2:M:338:LYS:HE2	2:M:338:LYS:HA	1.80	0.62
2:M:389:THR:CG2	9:U:77:THR:HB	2.17	0.62
7:S:104:LYS:NZ	7:S:104:LYS:HB3	2.14	0.62
3:B:1033:ARG:HD2	3:B:1037:ILE:HD11	1.80	0.62
3:B:1045:LEU:O	3:B:1049:LEU:HB3	1.99	0.62
1:I:483:HIS:CD2	1:I:625:LYS:HG3	2.35	0.62
3:J:81:SER:HB3	3:J:84:GLU:HG3	1.82	0.62
3:J:794:ASP:OD1	3:J:794:ASP:N	2.32	0.62
5:Q:143:ARG:CZ	5:Q:168:TYR:O	2.48	0.62
6:R:50:GLU:HA	6:R:53:GLN:HB2	1.79	0.62
1:A:865:THR:HG21	1:A:870:ARG:NH1	2.14	0.62
3:B:60:LEU:HD22	3:B:98:LEU:HD21	1.80	0.62
3:B:1012:LEU:O	3:B:1095:TYR:HE2	1.82	0.62
3:J:707:ALA:C	3:J:709:ASP:H	2.07	0.62
3:J:931:LYS:HE2	3:J:985:PHE:O	1.98	0.62
3:J:1033:ARG:HD2	3:J:1037:ILE:HD11	1.80	0.62
5:Q:83:GLU:O	5:Q:145:ARG:HA	1.99	0.62
8:T:12:ARG:HH12	8:T:55:ILE:HB	1.65	0.62
2:C:139:GLU:HA	2:C:142:ARG:HB2	1.80	0.62
3:B:356:VAL:HG22	3:B:393:ARG:HH12	1.65	0.62
3:B:473:MET:SD	3:B:475:GLN:N	2.72	0.62
3:B:650:ILE:HD13	3:B:650:ILE:N	2.11	0.62
7:G:66:TYR:HD1	7:G:114:ARG:NH1	1.98	0.62
1:I:834:TYR:CE1	9:U:80:ARG:HD3	2.34	0.62
3:J:662:GLN:O	3:J:663:SER:C	2.43	0.62
3:J:963:LEU:HD22	4:O:208:GLU:HG3	1.82	0.62
4:O:175:ASN:HA	4:O:195:LEU:CD1	2.22	0.62
11:W:22:ILE:HD13	11:W:23:THR:N	2.14	0.62
1:A:336:GLU:OE1	1:A:436:ARG:NH1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLN:O	1:A:608:PRO:C	2.43	0.62
2:C:31:ASP:O	2:C:34:ASN:N	2.33	0.62
2:C:124:ILE:HG23	2:C:272:VAL:HG22	1.82	0.62
2:C:125:TYR:HD1	2:C:271:LYS:HB3	1.64	0.62
1:I:93:PHE:HB3	1:I:184:LEU:HD21	1.80	0.62
2:M:61:GLU:C	2:M:63:LEU:H	2.06	0.62
3:J:881:ARG:HH11	3:J:989:TYR:CB	2.12	0.62
2:C:276:ASN:ND2	2:C:279:GLU:HB2	2.09	0.62
4:D:137:GLN:HE21	11:N:63:THR:HG22	1.65	0.62
1:I:376:ASN:O	1:I:377:TYR:CB	2.46	0.62
1:I:864:LYS:HG3	2:M:32:LEU:HD11	1.81	0.62
3:J:707:ALA:O	3:J:711:ILE:HG13	1.99	0.62
1:A:418:LEU:HD21	3:B:1044:LEU:CD2	2.20	0.62
3:B:296:TYR:O	3:B:297:PHE:HB2	1.99	0.62
1:I:11:PHE:HA	3:J:1110:SER:O	2.00	0.62
1:I:98:CYS:HA	1:I:146:CYS:SG	2.40	0.62
1:I:104:VAL:HG12	1:I:104:VAL:O	2.00	0.62
2:M:53:ASP:C	2:M:55:ALA:H	2.07	0.62
4:O:247:LYS:HA	4:O:250:ILE:HD12	1.81	0.62
1:A:289:HIS:HB2	1:A:295:LEU:HD21	1.81	0.61
1:A:866:VAL:HG12	1:A:869:ASN:H	1.65	0.61
3:B:367:TYR:CD2	3:B:367:TYR:C	2.77	0.61
3:B:702:LEU:HD12	11:N:51:SER:HB3	1.79	0.61
8:H:29:TYR:HA	8:H:32:LEU:CD1	2.30	0.61
9:K:82:LEU:HD23	9:K:82:LEU:N	2.10	0.61
1:I:502:TYR:HE1	1:I:636:ILE:HD11	1.65	0.61
3:J:806:GLY:O	3:J:839:THR:HB	2.00	0.61
3:J:881:ARG:HD2	3:J:989:TYR:HD2	1.64	0.61
7:S:15:ILE:HD13	7:S:53:GLU:HB3	1.80	0.61
1:A:710:THR:O	1:A:714:ILE:HG12	2.00	0.61
2:C:125:TYR:CD1	2:C:271:LYS:HB3	2.36	0.61
2:C:390:MET:HG3	5:E:57:GLY:N	2.16	0.61
3:B:21:LYS:HE2	3:B:475:GLN:OE1	2.00	0.61
3:B:291:GLN:C	3:B:293:ILE:H	2.08	0.61
3:B:587:PRO:O	3:B:588:LEU:HD23	2.00	0.61
2:M:49:ASP:O	2:M:52:PHE:N	2.32	0.61
3:J:289:ALA:O	3:J:293:ILE:HG12	2.00	0.61
3:J:679:LEU:HD23	3:J:716:ARG:HG2	1.81	0.61
4:O:131:VAL:HA	11:W:2:LEU:HD11	1.81	0.61
5:Q:110:ILE:HD13	5:Q:113:ILE:HG21	1.82	0.61
1:A:506:ALA:HA	1:A:635:PHE:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:812:ARG:NE	2:C:86:THR:HG23	2.14	0.61
1:A:833:GLU:HG3	1:A:839:ARG:HG3	1.82	0.61
1:I:239:LEU:HD22	1:I:276:TYR:CE1	2.35	0.61
2:M:13:LEU:HD23	2:M:16:LYS:HZ2	1.64	0.61
3:J:484:ILE:H	3:J:484:ILE:HD12	1.65	0.61
3:J:763:VAL:HA	3:J:770:GLU:HG3	1.83	0.61
10:V:3:ILE:HG23	10:V:15:LEU:HD21	1.82	0.61
1:A:825:ASN:O	1:A:826:ALA:C	2.44	0.61
3:B:356:VAL:CG1	3:B:404:VAL:HG12	2.31	0.61
7:G:63:ARG:HA	7:G:114:ARG:NH2	2.16	0.61
1:I:426:HIS:HD2	1:I:490:ARG:HH12	1.45	0.61
1:A:238:LYS:HD3	1:A:276:TYR:HA	1.81	0.61
1:A:827:LEU:HD11	2:C:315:LEU:CD1	2.30	0.61
2:C:107:LEU:O	2:C:110:ILE:HG22	2.00	0.61
2:C:391:ARG:CG	2:C:391:ARG:NH1	2.50	0.61
3:B:448:THR:O	3:B:450:TRP:N	2.33	0.61
9:K:50:LEU:HD23	9:K:75:PRO:HD3	1.83	0.61
1:I:371:LYS:NZ	1:I:373:PRO:HD3	2.16	0.61
1:I:501:ASP:OD2	3:J:913:HIS:CD2	2.54	0.61
2:M:127:THR:OG1	2:M:130:TYR:O	2.19	0.61
2:M:309:ASP:OD2	2:M:310:ILE:N	2.34	0.61
1:A:85:GLY:HA3	2:C:355:LEU:CD1	2.31	0.61
2:C:270:ALA:HA	8:H:14:HIS:ND1	2.15	0.61
3:B:557:HIS:H	3:B:623:ASN:ND2	1.97	0.61
3:B:662:GLN:O	3:B:663:SER:C	2.44	0.61
3:B:739:ILE:HG23	3:B:909:ILE:HB	1.81	0.61
1:I:604:GLY:C	1:I:606:GLN:N	2.58	0.61
2:M:269:VAL:HA	2:M:272:VAL:HG23	1.81	0.61
2:M:274:THR:HG22	2:M:275:ASN:N	2.09	0.61
3:J:28:LEU:HG	3:J:122:MET:CE	2.30	0.61
3:J:934:ALA:O	11:W:46:ARG:HD3	1.99	0.61
3:J:965:ASP:O	3:J:967:THR:N	2.33	0.61
7:S:87:ASN:C	7:S:89:GLY:H	2.09	0.61
2:C:311:ARG:HD3	2:C:311:ARG:H	1.66	0.61
4:D:106:PRO:HA	4:D:134:GLY:HA2	1.81	0.61
6:F:19:LYS:HG3	6:F:49:ALA:HB2	1.83	0.61
1:I:632:PHE:HA	1:I:635:PHE:CE1	2.35	0.61
3:J:450:TRP:HZ3	3:J:621:GLU:OE2	1.84	0.61
4:O:23:GLU:OE1	10:V:34:ARG:NH2	2.34	0.61
10:V:74:GLU:HA	10:V:77:ARG:HE	1.65	0.61
1:A:105:LYS:NZ	1:A:108:GLU:HB2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:LYS:O	2:C:20:ALA:HB3	2.01	0.61
6:F:14:TYR:N	6:F:14:TYR:HD1	1.98	0.61
1:I:720:ASP:O	1:I:722:PHE:N	2.33	0.61
3:B:6:THR:HG22	3:B:7:ILE:H	1.66	0.61
3:B:28:LEU:HG	3:B:122:MET:HE1	1.83	0.61
6:F:14:TYR:N	6:F:14:TYR:CD1	2.69	0.61
8:H:49:ASP:OD2	8:H:50:PRO:HD2	2.01	0.61
10:L:7:LYS:HE3	10:L:12:TYR:HE2	1.65	0.61
3:J:686:LEU:HD12	3:J:686:LEU:H	1.64	0.61
4:O:111:SER:CA	4:O:114:ILE:HD13	2.27	0.61
11:W:7:CYS:SG	11:W:48:MET:HG3	2.41	0.61
1:A:176:THR:O	1:A:180:ILE:HG13	2.00	0.61
1:A:191:ASP:HA	1:A:194:ILE:HD11	1.81	0.61
2:C:70:ILE:N	2:C:70:ILE:CD1	2.64	0.61
1:I:595:GLU:HB3	7:S:91:LYS:HE2	1.82	0.61
1:I:856:PHE:CE2	2:M:73:VAL:HG21	2.35	0.61
1:I:866:VAL:HG12	1:I:869:ASN:H	1.65	0.61
3:J:495:VAL:O	3:J:528:GLY:HA3	2.01	0.61
8:T:12:ARG:NH1	8:T:55:ILE:HB	2.15	0.61
1:A:121:ILE:HG21	13:Y:66:LYS:HE3	1.81	0.60
3:B:458:THR:HG21	3:B:465:GLY:N	2.15	0.60
11:N:7:CYS:SG	11:N:45:CYS:SG	2.99	0.60
1:I:856:PHE:HE2	2:M:73:VAL:HG21	1.65	0.60
2:M:104:LEU:HB3	2:M:105:PRO:CD	2.30	0.60
2:M:237:ILE:HG13	2:M:238:LYS:H	1.66	0.60
3:J:163:THR:HG23	3:J:428:ARG:O	2.01	0.60
3:J:249:GLN:HG3	3:J:250:ASN:N	2.15	0.60
3:J:683:ASN:C	3:J:685:GLN:H	2.09	0.60
3:J:881:ARG:HD2	3:J:989:TYR:CD2	2.36	0.60
5:Q:13:ILE:HG23	5:Q:25:ILE:HG21	1.83	0.60
1:A:506:ALA:HA	1:A:635:PHE:CD2	2.36	0.60
1:A:853:ASP:CB	2:C:311:ARG:HH12	2.12	0.60
1:I:155:LYS:H	1:I:155:LYS:NZ	1.99	0.60
1:I:734:ARG:HG3	3:J:917:SER:HB3	1.82	0.60
3:J:81:SER:O	3:J:84:GLU:HB2	2.01	0.60
3:J:381:LEU:C	3:J:383:ALA:H	2.09	0.60
1:A:328:PRO:HG3	1:A:457:PHE:CD1	2.36	0.60
1:A:531:LYS:O	1:A:532:ILE:HB	2.00	0.60
1:A:640:GLU:OE1	3:B:974:ARG:NH1	2.34	0.60
3:B:759:SER:HB3	3:B:863:LYS:HA	1.81	0.60
3:B:873:THR:HG22	3:B:874:ILE:N	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:45:MET:HE2	9:K:45:MET:CA	2.17	0.60
1:I:58:CYS:CB	1:I:59:PRO:HD3	2.31	0.60
1:A:798:HIS:HE2	3:B:663:SER:H	1.50	0.60
3:B:160:VAL:O	3:B:411:SER:HA	2.02	0.60
3:B:803:GLU:HB3	3:B:805:LYS:NZ	2.16	0.60
8:H:23:LEU:HB2	8:H:62:ILE:O	2.01	0.60
2:M:303:GLU:O	2:M:304:GLN:HG2	2.01	0.60
3:J:60:LEU:HD22	3:J:98:LEU:HD21	1.82	0.60
3:J:87:LEU:HD23	3:J:688:THR:CG2	2.31	0.60
3:J:958:LEU:HD21	4:O:181:ASN:O	2.01	0.60
5:Q:110:ILE:O	5:Q:113:ILE:HG22	2.00	0.60
9:U:87:ILE:HG22	9:U:87:ILE:O	2.01	0.60
3:B:707:ALA:O	3:B:711:ILE:HG13	2.01	0.60
3:B:781:ARG:HD3	3:B:782:GLY:H	1.67	0.60
3:B:1100:LEU:O	3:B:1101:ILE:C	2.44	0.60
9:K:41:LEU:O	9:K:43:LEU:N	2.34	0.60
3:J:356:VAL:HG22	3:J:393:ARG:HH12	1.65	0.60
3:J:1004:ARG:NH1	3:J:1024:GLY:HA2	2.16	0.60
2:C:392:PRO:HG3	5:E:66:THR:HG21	1.82	0.60
3:B:197:ARG:HB2	3:B:199:PRO:HD3	1.84	0.60
3:B:741:ASN:OD1	3:B:743:SER:N	2.34	0.60
5:E:144:ALA:HB2	5:E:164:MET:HE3	1.83	0.60
1:I:531:LYS:O	1:I:532:ILE:HB	2.00	0.60
1:I:798:HIS:HE2	3:J:663:SER:H	1.48	0.60
3:J:902:LYS:HB2	11:W:42:ARG:NH1	2.15	0.60
7:S:80:GLU:CG	7:S:81:LEU:H	2.14	0.60
1:A:81:VAL:HG12	1:A:270:GLN:HG3	1.84	0.60
1:A:859:TYR:CB	2:C:64:ILE:HG12	2.32	0.60
3:B:163:THR:HG23	3:B:428:ARG:O	2.02	0.60
2:M:286:ILE:HD12	8:T:45:ILE:HG13	1.84	0.60
1:A:71:HIS:ND1	3:B:1070:TYR:HE2	1.98	0.60
1:A:155:LYS:H	1:A:155:LYS:NZ	1.99	0.60
1:A:491:TYR:CB	1:A:607:GLN:OE1	2.50	0.60
3:B:40:GLN:HE22	3:B:62:LYS:HA	1.66	0.60
7:G:80:GLU:O	7:G:81:LEU:HD12	2.00	0.60
1:I:847:GLN:HG2	2:M:318:ASP:OD1	2.02	0.60
1:A:376:ASN:O	1:A:377:TYR:CB	2.43	0.60
1:A:632:PHE:HA	1:A:635:PHE:HD1	1.63	0.60
1:A:868:VAL:HG22	2:C:39:LYS:NZ	2.17	0.60
3:B:38:LYS:HA	3:B:41:GLU:HG3	1.84	0.60
3:B:555:VAL:O	3:B:620:GLU:HG3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:660:HIS:CE1	3:B:925:MET:HE1	2.36	0.60
3:B:686:LEU:HD12	3:B:686:LEU:H	1.67	0.60
5:E:66:THR:CG2	5:E:68:HIS:NE2	2.64	0.60
2:M:53:ASP:C	2:M:55:ALA:N	2.59	0.60
3:J:197:ARG:HB2	3:J:199:PRO:HD3	1.83	0.60
3:J:971:TYR:CZ	4:O:165:ARG:HA	2.37	0.60
3:J:1071:ASP:C	3:J:1073:ASN:H	2.09	0.60
9:U:41:LEU:O	9:U:45:MET:HG2	2.01	0.60
9:K:90:LEU:N	9:K:90:LEU:CD2	2.57	0.60
10:L:1:MET:HA	10:L:18:GLU:O	2.01	0.60
1:I:447:LEU:HD13	3:J:734:MET:SD	2.42	0.60
1:I:510:THR:O	1:I:549:LYS:HG3	2.02	0.60
1:I:752:VAL:C	1:I:754:GLY:H	2.10	0.60
2:M:133:ASP:HB2	2:M:136:LYS:HG2	1.84	0.60
3:J:83:MET:HG3	3:J:142:GLY:O	2.01	0.60
1:A:93:PHE:HB3	1:A:184:LEU:HD21	1.84	0.59
1:A:220:ARG:HA	1:A:233:ASP:OD1	2.02	0.59
1:I:317:ARG:NH1	3:J:1018:GLU:HG3	2.17	0.59
1:I:839:ARG:HH12	8:T:37:ILE:HG23	1.65	0.59
2:M:390:MET:CB	5:Q:56:GLU:CG	2.80	0.59
9:U:44:ALA:O	9:U:45:MET:HE2	2.01	0.59
1:A:133:THR:HB	1:A:137:LYS:NZ	2.16	0.59
1:A:354:THR:HB	1:A:355:PRO:HD2	1.84	0.59
3:B:484:ILE:H	3:B:484:ILE:HD12	1.67	0.59
3:B:881:ARG:HH11	3:B:989:TYR:CB	2.15	0.59
7:G:87:ASN:O	7:G:89:GLY:N	2.35	0.59
1:I:355:PRO:O	1:I:356:TRP:CD1	2.55	0.59
1:I:849:ALA:HB2	9:U:15:PHE:CD1	2.37	0.59
2:M:318:ASP:O	2:M:322:ARG:CD	2.50	0.59
3:J:75:ARG:H	3:J:75:ARG:HE	1.47	0.59
3:J:230:LEU:HD13	3:J:312:ALA:HA	1.82	0.59
10:V:72:ALA:HA	10:V:75:ASN:HB2	1.82	0.59
1:A:284:LEU:N	1:A:285:PRO:HD2	2.17	0.59
1:A:450:CYS:HB2	1:A:451:PRO:HD3	1.84	0.59
1:I:84:VAL:HG11	1:I:274:ALA:HB1	1.83	0.59
1:I:290:ARG:HD2	1:I:291:SER:N	2.16	0.59
1:I:678:LYS:HD2	1:I:684:LEU:HG	1.84	0.59
2:M:330:GLY:O	2:M:335:THR:OG1	2.20	0.59
3:J:183:ILE:O	3:J:183:ILE:HD13	2.03	0.59
3:J:479:GLY:HA2	3:J:552:GLU:HB3	1.84	0.59
3:J:902:LYS:HE2	11:W:41:LYS:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:799:SER:O	3:B:800:PRO:O	2.19	0.59
2:M:144:LEU:HA	2:M:146:TYR:CE2	2.37	0.59
3:J:448:THR:O	3:J:450:TRP:N	2.35	0.59
3:J:577:ARG:HE	3:J:578:PRO:HD2	1.66	0.59
3:J:1004:ARG:HH12	3:J:1016:PRO:HB3	1.67	0.59
3:J:1113:LEU:H	3:J:1113:LEU:CD1	2.03	0.59
4:O:183:CYS:SG	16:O:1001:F3S:S1	3.00	0.59
1:A:58:CYS:CB	1:A:59:PRO:HD3	2.29	0.59
1:A:558:LYS:HG3	3:J:104:GLU:CB	2.26	0.59
2:C:390:MET:HB2	5:E:56:GLU:HG2	1.85	0.59
3:B:75:ARG:H	3:B:75:ARG:HE	1.50	0.59
3:B:473:MET:SD	3:B:474:ALA:N	2.76	0.59
1:I:491:TYR:CB	1:I:607:GLN:OE1	2.49	0.59
1:I:608:PRO:C	1:I:609:GLU:HG2	2.27	0.59
2:M:11:PRO:C	2:M:13:LEU:H	2.10	0.59
2:M:78:VAL:O	2:M:81:PRO:HD2	2.01	0.59
2:M:277:ILE:C	2:M:279:GLU:N	2.57	0.59
3:J:315:LEU:O	3:J:319:ILE:HG12	2.02	0.59
5:Q:53:THR:OG1	5:Q:71:GLU:HB2	2.03	0.59
5:Q:110:ILE:HG23	5:Q:118:LEU:HB3	1.84	0.59
1:A:316:LYS:HE2	3:B:1054:ASP:OD2	2.03	0.59
1:A:502:TYR:HE1	1:A:636:ILE:HD11	1.66	0.59
3:B:68:PRO:HD3	3:B:129:PRO:HG2	1.85	0.59
3:B:729:PHE:C	3:B:731:GLY:H	2.11	0.59
4:D:69:SER:HA	4:D:72:ALA:HB3	1.84	0.59
9:K:54:ASN:HD21	9:K:58:SER:HB2	1.67	0.59
9:K:74:LEU:HD12	9:K:74:LEU:H	1.65	0.59
1:I:518:LYS:HE2	1:I:544:GLU:HB2	1.83	0.59
2:M:389:THR:HG21	9:U:79:ARG:HH11	1.67	0.59
3:J:98:LEU:C	3:J:98:LEU:HD13	2.27	0.59
3:J:660:HIS:CE1	3:J:925:MET:HE1	2.36	0.59
3:J:700:ARG:N	11:W:51:SER:O	2.36	0.59
6:R:30:SER:OG	6:R:34:LEU:HB3	2.02	0.59
1:A:249:LEU:HB3	1:A:266:TRP:CH2	2.38	0.59
1:A:720:ASP:O	1:A:722:PHE:N	2.33	0.59
4:D:131:VAL:HA	11:N:2:LEU:HD11	1.84	0.59
9:K:50:LEU:CD2	9:K:75:PRO:HD3	2.33	0.59
1:I:659:LYS:O	1:I:663:ASN:HB2	2.02	0.59
1:I:847:GLN:OE1	1:I:850:TYR:HA	2.02	0.59
5:E:141:LYS:HB2	5:E:172:LEU:HG	1.85	0.59
1:I:522:GLN:HG2	10:V:40:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:812:ARG:HE	2:M:86:THR:HG23	1.68	0.59
11:W:18:TRP:CD1	11:W:49:LEU:HD22	2.38	0.59
1:A:97:THR:HG22	1:A:99:ARG:H	1.67	0.59
1:A:321:SER:O	1:A:322:SER:HB2	2.03	0.59
1:A:530:VAL:O	1:A:530:VAL:HG13	2.02	0.59
1:A:644:PHE:HA	1:A:724:PHE:CE2	2.37	0.59
1:A:750:GLN:HG3	1:A:782:ILE:CD1	2.32	0.59
3:B:123:LEU:O	3:B:125:SER:N	2.36	0.59
7:G:40:PHE:HA	7:G:92:TYR:HD1	1.68	0.59
1:I:826:ALA:H	2:M:335:THR:HG22	1.66	0.59
3:J:900:THR:HG22	3:J:970:VAL:HG12	1.84	0.59
2:C:55:ALA:CA	2:C:58:GLU:HB2	2.31	0.59
3:B:707:ALA:C	3:B:709:ASP:H	2.10	0.59
3:B:730:THR:HB	3:B:732:TYR:CD1	2.36	0.59
4:D:51:SER:HB2	4:D:52:PRO:HD2	1.85	0.59
13:Y:67:LEU:O	13:Y:71:ASN:ND2	2.36	0.59
1:I:508:LEU:O	1:I:514:THR:HG23	2.03	0.59
2:M:188:ILE:HG23	2:M:190:ARG:H	1.68	0.59
3:J:325:LEU:HD11	3:J:331:GLU:H	1.67	0.59
4:O:259:LYS:O	4:O:263:VAL:CG2	2.51	0.59
8:T:59:PRO:HA	8:T:81:VAL:HB	1.84	0.59
3:B:171:ARG:HH22	3:B:569:ASN:HD21	1.49	0.58
8:H:31:ILE:HD11	9:K:13:LEU:HG	1.84	0.58
1:I:816:SER:OG	2:M:83:THR:HG22	2.02	0.58
2:M:202:GLU:O	2:M:203:ASP:HB2	2.03	0.58
3:J:416:ARG:NH1	3:J:687:ARG:NH2	2.51	0.58
5:Q:64:GLY:H	9:U:41:LEU:CD2	2.16	0.58
10:V:6:LEU:HB2	10:V:14:GLU:O	2.03	0.58
1:A:704:LEU:HD22	1:A:781:PHE:CE1	2.38	0.58
2:C:268:ASP:OD1	2:C:270:ALA:HB3	2.03	0.58
2:C:321:THR:O	2:C:321:THR:HG22	2.02	0.58
3:B:183:ILE:HG12	3:B:206:LYS:HB3	1.84	0.58
3:B:1069:TRP:CD1	3:B:1088:LEU:HD22	2.38	0.58
3:B:1071:ASP:C	3:B:1073:ASN:H	2.11	0.58
1:I:530:VAL:O	1:I:530:VAL:HG13	2.02	0.58
3:J:12:ARG:HH11	3:J:596:LYS:HG2	1.68	0.58
3:J:99:THR:O	3:J:99:THR:HG22	2.02	0.58
3:J:193:THR:HG21	3:J:197:ARG:H	1.68	0.58
3:J:325:LEU:HD22	3:J:330:ARG:HG3	1.85	0.58
4:O:180:VAL:HG21	4:O:190:LEU:HG	1.85	0.58
1:A:491:TYR:HD1	1:A:607:GLN:HE22	1.49	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:PRO:C	1:A:609:GLU:HG2	2.27	0.58
2:C:373:ILE:HG12	3:B:1049:LEU:HD13	1.85	0.58
3:B:419:TRP:CZ3	3:B:712:GLY:HA3	2.38	0.58
3:B:569:ASN:HB3	3:B:574:ARG:HH12	1.68	0.58
6:F:13:PRO:HG2	6:F:16:VAL:HG23	1.85	0.58
1:I:512:LYS:HE2	7:S:91:LYS:HE3	1.85	0.58
1:I:549:LYS:NZ	7:S:89:GLY:HA2	2.17	0.58
1:I:575:CYS:HG	1:I:580:CYS:HG	0.80	0.58
1:I:749:GLN:H	1:I:781:PHE:HA	1.69	0.58
2:M:112:ASP:HA	2:M:328:GLN:HB3	1.86	0.58
3:J:325:LEU:CD1	3:J:331:GLU:H	2.16	0.58
4:O:131:VAL:HG22	4:O:132:LEU:N	2.18	0.58
1:A:48:ARG:HB2	1:A:59:PRO:HB3	1.84	0.58
2:C:15:GLU:HG3	2:C:18:LYS:HD2	1.85	0.58
3:B:381:LEU:C	3:B:383:ALA:H	2.11	0.58
1:I:345:LYS:NZ	1:I:370:ASP:O	2.35	0.58
1:I:569:SER:HB2	1:I:584:SER:OG	2.02	0.58
3:J:87:LEU:HD23	3:J:688:THR:HG21	1.86	0.58
4:O:69:SER:HA	4:O:72:ALA:HB3	1.85	0.58
9:U:90:LEU:HD23	9:U:90:LEU:H	1.68	0.58
1:A:301:ARG:HH12	1:A:312:ASN:HD21	1.52	0.58
1:A:830:LEU:CD2	1:A:840:SER:HB3	2.26	0.58
3:B:183:ILE:CG1	3:B:206:LYS:HB3	2.33	0.58
3:B:518:SER:HB3	3:B:564:ASN:ND2	2.19	0.58
1:I:106:ILE:HG22	1:I:107:SER:N	2.17	0.58
3:J:160:VAL:O	3:J:411:SER:HA	2.03	0.58
4:O:239:GLU:HA	4:O:242:LEU:HD12	1.85	0.58
5:Q:147:ILE:CD1	5:Q:163:THR:HB	2.15	0.58
1:A:155:LYS:H	1:A:155:LYS:HZ1	1.52	0.58
1:A:392:LYS:O	1:A:394:ARG:HB2	2.04	0.58
1:A:509:LEU:O	1:A:548:GLY:HA3	2.03	0.58
2:C:115:LYS:O	2:C:115:LYS:HG3	2.03	0.58
3:B:739:ILE:HG12	3:B:890:MET:O	2.03	0.58
5:E:97:ILE:HD13	5:E:136:ILE:HG21	1.85	0.58
1:I:83:HIS:HB3	1:I:86:LEU:HB2	1.86	0.58
1:I:859:TYR:HB2	2:M:64:ILE:CG2	2.33	0.58
2:M:104:LEU:O	2:M:108:ILE:HG12	2.03	0.58
3:J:367:TYR:C	3:J:367:TYR:HD2	2.10	0.58
3:J:557:HIS:H	3:J:623:ASN:ND2	2.01	0.58
3:J:992:LYS:CE	3:J:996:MET:SD	2.91	0.58
7:S:15:ILE:HG13	7:S:31:MET:HE2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:873:THR:CG2	3:B:874:ILE:N	2.65	0.58
8:H:46:ARG:NH2	13:Y:78:ARG:HH11	2.00	0.58
1:I:353:ILE:HG13	1:I:361:LEU:CD2	2.32	0.58
1:I:803:ARG:HG2	3:J:444:ASP:HA	1.86	0.58
2:M:310:ILE:HG22	2:M:314:LEU:CD2	2.32	0.58
3:J:762:GLU:O	3:J:764:LYS:HG3	2.03	0.58
3:J:764:LYS:HZ1	3:J:814:VAL:H	1.49	0.58
6:R:3:SER:OG	6:R:4:VAL:N	2.36	0.58
3:B:445:LEU:HD11	3:B:455:PRO:HB3	1.86	0.58
3:B:794:ASP:OD1	3:B:794:ASP:N	2.31	0.58
1:I:301:ARG:HH12	1:I:312:ASN:HD21	1.52	0.58
1:I:785:SER:H	1:I:788:THR:HB	1.68	0.58
2:M:295:ARG:HA	2:M:298:SER:HB2	1.86	0.58
4:O:98:ILE:CD1	4:O:114:ILE:HG13	2.30	0.58
5:Q:3:LYS:HB2	6:R:10:HIS:O	2.04	0.58
3:B:489:LEU:HD11	3:B:568:VAL:HG21	1.84	0.58
5:E:108:VAL:HG22	5:E:162:LEU:HB2	1.85	0.58
1:I:387:ASP:OD2	1:I:388:LEU:N	2.34	0.58
2:M:373:ILE:O	3:J:1049:LEU:HD11	2.04	0.58
2:M:392:PRO:HG3	5:Q:68:HIS:HE1	1.69	0.58
3:J:28:LEU:HA	3:J:122:MET:HE1	1.85	0.58
3:J:1119:VAL:HG22	5:Q:10:ILE:HD13	1.85	0.58
1:A:589:LYS:O	1:A:592:ILE:CG1	2.49	0.58
1:A:647:ARG:HB2	1:A:650:ASP:CG	2.29	0.58
2:C:389:THR:HG21	9:K:79:ARG:NH1	2.18	0.58
3:B:895:VAL:HG11	4:D:34:LEU:HD21	1.86	0.58
1:I:97:THR:HG22	1:I:99:ARG:H	1.69	0.58
1:I:524:ILE:CG2	1:I:634:VAL:HG13	2.34	0.58
1:I:607:GLN:O	1:I:608:PRO:C	2.47	0.58
3:J:376:GLY:O	3:J:377:ARG:HB3	2.02	0.58
3:J:1045:LEU:O	3:J:1049:LEU:HB3	2.04	0.58
9:U:82:LEU:HD12	9:U:86:LYS:HB3	1.85	0.58
11:W:7:CYS:HB3	11:W:45:CYS:SG	2.44	0.58
3:B:28:LEU:HA	3:B:122:MET:HE1	1.86	0.57
3:B:87:LEU:HD23	3:B:688:THR:CG2	2.34	0.57
3:B:738:ILE:HG23	3:B:888:ILE:HA	1.86	0.57
1:I:289:HIS:HB2	1:I:295:LEU:HD21	1.86	0.57
2:M:103:GLY:HA2	2:M:106:ARG:CB	2.34	0.57
3:J:40:GLN:HE22	3:J:62:LYS:HA	1.69	0.57
3:J:457:GLU:HG2	3:J:469:ASN:OD1	2.04	0.57
3:J:489:LEU:HD11	3:J:568:VAL:HG21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:881:ARG:NH1	3:J:989:TYR:CB	2.67	0.57
3:J:978:LYS:HZ3	4:O:205:LEU:HD13	1.68	0.57
3:J:1031:MET:O	3:J:1034:ASP:HB2	2.04	0.57
4:O:230:ILE:HG13	4:O:242:LEU:HD21	1.85	0.57
8:T:19:LYS:H	8:T:19:LYS:HD2	1.69	0.57
1:A:355:PRO:O	1:A:356:TRP:CD1	2.57	0.57
2:C:49:ASP:O	2:C:52:PHE:N	2.36	0.57
2:C:391:ARG:HB3	9:K:75:PRO:O	2.03	0.57
1:I:4:LYS:HD2	3:J:1089:PHE:CB	2.35	0.57
3:J:83:MET:HE2	3:J:683:ASN:HD22	1.68	0.57
1:A:319:ASP:HB2	3:B:1052:ASN:HB3	1.86	0.57
2:C:234:ILE:O	2:C:235:LYS:HG3	2.04	0.57
2:C:270:ALA:HA	8:H:14:HIS:CG	2.39	0.57
1:I:249:LEU:HB3	1:I:266:TRP:CH2	2.39	0.57
1:I:477:LYS:O	1:I:481:LEU:HB2	2.03	0.57
1:I:587:VAL:HB	1:I:594:LEU:O	2.05	0.57
1:I:865:THR:HG21	1:I:870:ARG:NH1	2.19	0.57
2:M:21:SER:O	2:M:33:LYS:HE3	2.04	0.57
3:J:324:GLU:O	3:J:325:LEU:HB2	2.04	0.57
3:J:801:GLU:HG3	12:X:38:ARG:NH2	2.19	0.57
3:J:922:GLY:O	3:J:926:GLU:HB2	2.02	0.57
1:A:503:ILE:HD11	1:A:733:ALA:N	2.19	0.57
1:A:594:LEU:CA	7:G:86:LEU:HD22	2.33	0.57
1:A:785:SER:H	1:A:788:THR:HB	1.70	0.57
3:B:14:ILE:HG13	3:B:18:PHE:CE2	2.40	0.57
3:B:119:LEU:HD12	3:B:120:PRO:HD2	1.86	0.57
3:B:348:ASP:OD2	3:B:348:ASP:N	2.38	0.57
3:B:812:GLY:HA2	3:B:836:SER:HB3	1.85	0.57
3:B:853:THR:HG23	12:P:32:LYS:O	2.04	0.57
9:K:91:SER:O	9:K:92:LEU:CB	2.51	0.57
2:M:212:ASN:C	2:M:214:ASP:H	2.12	0.57
2:M:289:ALA:O	2:M:290:ARG:C	2.48	0.57
12:X:17:GLN:C	12:X:19:LYS:H	2.12	0.57
1:A:327:SER:HB2	1:A:444:ARG:HD3	1.85	0.57
1:A:477:LYS:O	1:A:481:LEU:HB2	2.05	0.57
1:A:488:THR:HB	1:A:495:ILE:HB	1.86	0.57
1:A:555:PHE:HD2	1:A:631:LEU:HD13	1.69	0.57
3:B:64:ARG:HG2	3:B:97:TRP:CD1	2.39	0.57
3:B:172:VAL:HG22	3:B:189:ILE:HD11	1.85	0.57
3:B:289:ALA:O	3:B:293:ILE:HG12	2.05	0.57
3:B:367:TYR:C	3:B:367:TYR:HD2	2.13	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:658:PRO:O	3:B:660:HIS:N	2.35	0.57
1:I:637:ARG:NH1	3:J:974:ARG:HH22	2.02	0.57
2:M:392:PRO:CD	5:Q:56:GLU:HG3	2.34	0.57
3:J:119:LEU:HD12	3:J:120:PRO:HD2	1.85	0.57
3:J:210:PHE:CZ	3:J:323:ILE:HG22	2.39	0.57
1:A:851:GLY:C	1:A:853:ASP:H	2.11	0.57
2:C:340:SER:HA	2:C:364:GLU:CG	2.34	0.57
3:B:43:ILE:O	3:B:43:ILE:HG22	2.04	0.57
3:B:159:ARG:HD3	3:B:399:ALA:HA	1.86	0.57
3:B:402:ASN:HB2	3:B:410:VAL:CG2	2.34	0.57
3:B:495:VAL:O	3:B:528:GLY:HA3	2.04	0.57
8:H:63:ILE:CG2	8:H:64:ARG:N	2.67	0.57
3:J:6:THR:HG22	3:J:7:ILE:H	1.69	0.57
3:J:451:GLY:CA	3:J:577:ARG:NH1	2.68	0.57
3:J:943:THR:HG22	3:J:944:PRO:HD2	1.87	0.57
5:Q:18:PHE:HE2	9:U:42:GLN:HG2	1.70	0.57
1:A:490:ARG:HG3	2:C:77:SER:HB3	1.86	0.57
2:C:70:ILE:HA	2:C:73:VAL:CG2	2.33	0.57
2:C:85:MET:HE1	2:C:107:LEU:HD12	1.86	0.57
3:B:68:PRO:HA	3:B:93:ALA:O	2.05	0.57
1:I:249:LEU:HD22	1:I:266:TRP:CE2	2.40	0.57
1:I:781:PHE:C	1:I:781:PHE:CD2	2.83	0.57
1:I:833:GLU:OE2	1:I:839:ARG:HB2	2.05	0.57
3:J:702:LEU:HD22	3:J:933:ALA:CB	2.27	0.57
11:W:6:ARG:HG2	11:W:11:GLY:O	2.05	0.57
1:A:426:HIS:CE1	1:A:428:ILE:CG2	2.85	0.57
3:B:315:LEU:O	3:B:319:ILE:HG12	2.04	0.57
3:B:376:GLY:O	3:B:377:ARG:HB3	2.05	0.57
3:B:727:MET:CE	3:B:898:PRO:HG3	2.35	0.57
13:Y:71:ASN:HA	13:Y:74:GLU:CD	2.29	0.57
1:I:426:HIS:O	1:I:429:SER:HB2	2.04	0.57
2:M:107:LEU:O	2:M:111:VAL:HG23	2.04	0.57
3:J:26:GLN:O	3:J:345:LEU:CD2	2.42	0.57
1:A:98:CYS:O	1:A:99:ARG:HB2	2.05	0.57
1:A:575:CYS:HG	1:A:580:CYS:HB3	1.70	0.57
1:A:734:ARG:HG3	3:B:917:SER:HB3	1.85	0.57
1:A:803:ARG:HG2	3:B:444:ASP:HA	1.86	0.57
1:A:878:TRP:N	3:J:377:ARG:HH12	2.00	0.57
2:C:373:ILE:HD13	3:B:1033:ARG:HD3	1.87	0.57
3:B:64:ARG:HG2	3:B:97:TRP:CG	2.39	0.57
3:B:116:ILE:HD12	3:B:361:PHE:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:88:GLU:H	5:E:99:VAL:HG13	1.68	0.57
6:F:15:SER:HA	6:F:18:LYS:NZ	2.19	0.57
7:G:80:GLU:HG2	7:G:81:LEU:N	2.20	0.57
1:I:6:ILE:HD11	3:J:1091:VAL:HG11	1.86	0.57
1:I:352:ARG:HA	1:I:406:ILE:HA	1.86	0.57
3:J:82:PRO:HG3	3:J:130:ILE:CD1	2.35	0.57
3:J:116:ILE:HG22	3:J:390:VAL:HG21	1.85	0.57
3:J:197:ARG:HH22	3:J:359:LYS:HG2	1.70	0.57
3:J:338:TYR:HB2	3:J:448:THR:HG21	1.87	0.57
3:J:683:ASN:O	3:J:685:GLN:N	2.38	0.57
3:J:727:MET:HE3	3:J:898:PRO:HG3	1.85	0.57
3:J:1054:ASP:HB3	3:J:1095:TYR:H	1.69	0.57
5:Q:30:LEU:HD21	5:Q:72:PHE:CE1	2.40	0.57
1:A:106:ILE:HG22	1:A:107:SER:N	2.20	0.57
2:C:355:LEU:CD2	3:B:1109:ILE:HD11	2.35	0.57
3:B:291:GLN:O	3:B:295:LYS:HG2	2.05	0.57
4:D:134:GLY:N	4:D:137:GLN:OE1	2.23	0.57
2:M:103:GLY:HA3	2:M:300:VAL:HG13	1.87	0.57
3:J:445:LEU:HD11	3:J:455:PRO:CB	2.34	0.57
1:A:594:LEU:HA	7:G:86:LEU:CD2	2.33	0.56
1:A:764:ARG:CB	1:A:764:ARG:HH11	2.18	0.56
2:C:70:ILE:O	2:C:71:GLY:C	2.48	0.56
2:C:110:ILE:HD11	2:C:277:ILE:HD11	1.86	0.56
2:C:139:GLU:HG2	2:C:142:ARG:HD2	1.86	0.56
3:B:699:GLN:HB2	3:B:720:ASN:HA	1.87	0.56
4:D:53:LEU:HD22	4:D:57:ILE:CG2	2.35	0.56
4:D:101:GLU:O	4:D:107:ARG:NH1	2.36	0.56
1:I:176:THR:O	1:I:180:ILE:HG13	2.04	0.56
1:I:764:ARG:HH11	1:I:764:ARG:HB2	1.69	0.56
3:J:870:ARG:CZ	3:J:996:MET:SD	2.93	0.56
5:Q:42:LEU:HD23	5:Q:42:LEU:H	1.69	0.56
7:S:17:SER:HB2	7:S:19:GLU:HG3	1.86	0.56
9:U:43:LEU:C	9:U:45:MET:H	2.13	0.56
1:A:369:PRO:HA	1:A:410:HIS:HE1	1.70	0.56
1:A:502:TYR:CE2	3:B:734:MET:HE1	2.41	0.56
3:B:193:THR:HG21	3:B:197:ARG:H	1.70	0.56
4:D:133:LEU:HD21	4:D:139:ILE:HG13	1.87	0.56
1:I:446:ASN:ND2	1:I:448:LEU:H	2.03	0.56
1:I:853:ASP:HB2	2:M:311:ARG:NH1	2.20	0.56
3:J:64:ARG:O	3:J:97:TRP:HB2	2.05	0.56
3:J:181:SER:O	3:J:182:ASN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:183:ILE:O	3:J:183:ILE:CD1	2.53	0.56
3:J:727:MET:HE3	3:J:898:PRO:CG	2.36	0.56
3:J:739:ILE:HG23	3:J:909:ILE:HB	1.86	0.56
7:S:18:ILE:O	7:S:18:ILE:HG22	2.05	0.56
1:A:728:MET:HE3	3:B:913:HIS:HA	1.86	0.56
1:A:749:GLN:N	1:A:781:PHE:HA	2.21	0.56
3:B:157:SER:O	3:B:158:GLU:HB2	2.04	0.56
3:B:419:TRP:HZ3	3:B:712:GLY:HA3	1.70	0.56
3:B:457:GLU:OE1	3:B:652:ALA:HB2	2.06	0.56
3:B:591:ILE:H	3:B:591:ILE:HD12	1.70	0.56
3:B:910:LEU:CD2	3:B:911:ASN:N	2.66	0.56
4:D:94:THR:OG1	4:D:95:LYS:N	2.39	0.56
1:I:116:ARG:HE	1:I:117:ILE:HG12	1.71	0.56
1:I:392:LYS:O	1:I:394:ARG:HB2	2.06	0.56
1:I:512:LYS:HE2	7:S:91:LYS:NZ	2.19	0.56
1:I:710:THR:O	1:I:714:ILE:HG12	2.06	0.56
1:I:870:ARG:NH2	2:M:57:LYS:O	2.38	0.56
2:M:262:LEU:HD23	2:M:269:VAL:HG11	1.86	0.56
2:M:390:MET:HB2	5:Q:56:GLU:HG2	1.87	0.56
3:J:171:ARG:HH22	3:J:569:ASN:HD21	1.53	0.56
3:J:710:ILE:HD13	3:J:710:ILE:H	1.69	0.56
4:O:51:SER:HB2	4:O:52:PRO:HD2	1.87	0.56
4:O:96:ILE:CG1	4:O:143:ALA:HB3	2.36	0.56
5:Q:124:ARG:HE	5:Q:126:ILE:HD13	1.71	0.56
1:A:220:ARG:N	1:A:221:PRO:HD3	2.20	0.56
3:B:1036:LEU:HD22	3:B:1041:THR:HG21	1.87	0.56
5:E:179:LYS:NZ	6:F:81:ASP:HB2	2.20	0.56
7:G:82:LYS:HB2	7:G:95:ILE:HG13	1.86	0.56
9:K:23:TRP:HA	9:K:23:TRP:HE3	1.69	0.56
1:I:81:VAL:HG23	1:I:209:LEU:HB2	1.87	0.56
1:I:557:PRO:HD3	1:I:623:TYR:OH	2.05	0.56
1:I:569:SER:HB2	1:I:584:SER:HG	1.69	0.56
5:Q:113:ILE:O	5:Q:164:MET:HB2	2.05	0.56
1:A:345:LYS:HG2	1:A:410:HIS:CD2	2.41	0.56
1:A:816:SER:OG	2:C:83:THR:HA	2.06	0.56
3:B:81:SER:O	3:B:84:GLU:HB2	2.06	0.56
3:B:230:LEU:HD13	3:B:312:ALA:HA	1.88	0.56
3:B:451:GLY:CA	3:B:577:ARG:NH1	2.68	0.56
3:B:855:THR:O	3:B:856:ALA:C	2.48	0.56
9:K:35:VAL:HG22	9:K:36:ILE:HD13	1.88	0.56
11:N:22:ILE:HD13	11:N:23:THR:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LYS:HE2	1:A:544:GLU:HB2	1.87	0.56
1:A:612:LEU:HD23	1:A:612:LEU:C	2.31	0.56
2:C:376:GLY:HA2	3:B:1049:LEU:HD21	1.87	0.56
3:B:544:ARG:HB2	3:B:549:ILE:HG22	1.88	0.56
7:G:79:THR:HG22	7:G:80:GLU:H	1.70	0.56
8:H:40:GLU:HG2	8:H:41:GLN:N	2.20	0.56
1:I:727:VAL:O	1:I:729:ALA:O	2.23	0.56
3:J:68:PRO:HD3	3:J:129:PRO:HG2	1.87	0.56
3:J:765:TYR:CG	3:J:766:PRO:HD2	2.41	0.56
3:J:943:THR:CG2	3:J:944:PRO:HD2	2.35	0.56
3:J:946:TYR:HD2	3:J:947:LYS:H	1.54	0.56
4:O:253:ILE:HG13	10:V:73:ILE:HD13	1.88	0.56
8:T:29:TYR:OH	13:Z:67:LEU:HD13	2.05	0.56
9:U:12:ASP:O	9:U:13:LEU:C	2.47	0.56
1:A:4:LYS:HD3	3:B:1091:VAL:HB	1.88	0.56
3:B:83:MET:O	3:B:87:LEU:HD12	2.06	0.56
3:B:719:GLY:O	3:B:989:TYR:CE1	2.59	0.56
3:B:921:LEU:C	3:B:923:GLN:H	2.13	0.56
3:B:1004:ARG:HH12	3:B:1016:PRO:HB3	1.70	0.56
11:N:3:ILE:HG22	11:N:4:PRO:HD2	1.88	0.56
1:I:575:CYS:CB	1:I:580:CYS:HG	2.18	0.56
1:I:828:SER:C	1:I:830:LEU:N	2.61	0.56
3:J:699:GLN:NE2	11:W:48:MET:HE3	2.21	0.56
3:J:735:GLU:O	3:J:736:ASP:C	2.49	0.56
3:J:741:ASN:OD1	3:J:743:SER:N	2.39	0.56
1:A:563:HIS:HB2	1:A:872:PHE:HE2	1.70	0.56
2:C:383:THR:HG22	3:B:1040:GLY:O	2.05	0.56
2:C:387:GLU:OE1	9:K:81:ARG:HD2	2.06	0.56
9:K:19:PHE:O	9:K:20:ILE:C	2.49	0.56
1:I:55:GLY:O	1:I:57:LYS:N	2.39	0.56
1:I:220:ARG:N	1:I:221:PRO:HD3	2.21	0.56
2:M:14:GLU:O	2:M:17:VAL:HG12	2.05	0.56
2:M:24:LEU:HD13	2:M:33:LYS:HA	1.88	0.56
2:M:72:ILE:N	2:M:72:ILE:CD1	2.63	0.56
2:M:80:GLU:HB3	2:M:81:PRO:HD3	1.87	0.56
3:J:402:ASN:HB2	3:J:410:VAL:CG2	2.36	0.56
3:J:644:SER:C	3:J:646:ALA:H	2.14	0.56
3:J:741:ASN:OD1	3:J:741:ASN:C	2.49	0.56
5:Q:11:VAL:HG12	5:Q:12:ARG:H	1.70	0.56
9:U:33:ALA:O	9:U:35:VAL:N	2.39	0.56
10:V:80:THR:O	10:V:84:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:SER:HA	1:A:203:ARG:NH2	2.19	0.56
1:A:91:TYR:OH	1:A:153:GLN:O	2.12	0.56
1:A:288:LYS:HG2	1:A:294:PRO:HA	1.88	0.56
2:C:30:ASP:O	2:C:31:ASP:HB3	2.05	0.56
2:C:70:ILE:CD1	2:C:70:ILE:H	2.19	0.56
2:C:238:LYS:HB2	2:C:239:ARG:CZ	2.36	0.56
2:C:386:VAL:HG11	9:K:31:GLU:HA	1.88	0.56
3:B:43:ILE:HG13	3:B:63:ILE:CD1	2.36	0.56
4:D:34:LEU:HA	4:D:150:GLY:HA3	1.88	0.56
1:I:509:LEU:O	1:I:548:GLY:HA3	2.05	0.56
2:M:159:ASP:HB3	2:M:163:MET:CB	2.35	0.56
3:J:365:LEU:O	3:J:369:LEU:HB2	2.06	0.56
3:J:687:ARG:HG3	3:J:687:ARG:NH1	2.11	0.56
1:A:155:LYS:CB	1:A:156:ILE:HA	2.35	0.56
2:C:286:ILE:O	2:C:289:ALA:HB3	2.05	0.56
3:B:12:ARG:HH11	3:B:596:LYS:HG2	1.70	0.56
4:D:129:PRO:HG2	11:N:15:ALA:HB1	1.88	0.56
13:Y:63:GLU:O	13:Y:67:LEU:HD13	2.06	0.56
1:I:155:LYS:CB	1:I:156:ILE:HA	2.35	0.56
1:I:317:ARG:HB2	3:J:1016:PRO:HB2	1.87	0.56
1:I:345:LYS:HG2	1:I:410:HIS:CD2	2.41	0.56
1:I:491:TYR:HD1	1:I:607:GLN:HE22	1.53	0.56
1:I:610:SER:O	1:I:613:HIS:HB3	2.06	0.56
1:I:831:ARG:NH2	2:M:385:MET:HG3	2.20	0.56
3:J:82:PRO:HG3	3:J:130:ILE:HD11	1.88	0.56
2:C:146:TYR:CE1	2:C:237:ILE:HG12	2.41	0.55
3:B:325:LEU:HD13	3:B:330:ARG:H	1.70	0.55
1:I:156:ILE:HD11	1:I:270:GLN:HG2	1.88	0.55
1:I:215:PRO:HB2	1:I:219:ILE:HD11	1.88	0.55
1:I:563:HIS:HB2	1:I:872:PHE:HE2	1.71	0.55
3:J:24:VAL:HG21	3:J:426:LEU:HD13	1.87	0.55
3:J:934:ALA:HB2	11:W:47:ARG:HD3	1.87	0.55
11:W:4:PRO:HG2	11:W:48:MET:HE1	1.88	0.55
1:A:249:LEU:HD13	1:A:266:TRP:CE3	2.41	0.55
3:B:197:ARG:HH22	3:B:359:LYS:HG2	1.71	0.55
3:B:210:PHE:CZ	3:B:323:ILE:HG22	2.38	0.55
3:B:318:ALA:O	3:B:321:LYS:HB2	2.06	0.55
3:B:760:THR:OG1	3:B:813:LYS:HD2	2.06	0.55
3:B:848:ASP:OD1	3:B:865:ARG:CZ	2.54	0.55
5:E:39:LEU:HD22	5:E:41:ASP:H	1.69	0.55
1:I:81:VAL:HG12	1:I:270:GLN:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:94:LEU:HD11	1:I:180:ILE:HG23	1.88	0.55
3:J:902:LYS:CB	11:W:42:ARG:NH1	2.69	0.55
3:J:922:GLY:O	3:J:926:GLU:N	2.34	0.55
1:A:610:SER:O	1:A:613:HIS:HB3	2.05	0.55
1:A:650:ASP:HB3	1:A:723:ASN:ND2	2.21	0.55
3:B:762:GLU:O	3:B:764:LYS:HG3	2.06	0.55
1:I:98:CYS:O	1:I:99:ARG:HB2	2.06	0.55
2:M:285:GLY:HA2	8:T:49:ASP:OD2	2.06	0.55
2:M:384:GLY:HA2	5:Q:61:PHE:CZ	2.41	0.55
3:J:28:LEU:HG	3:J:122:MET:HE1	1.88	0.55
3:J:552:GLU:HA	3:J:576:ARG:HH22	1.71	0.55
4:O:137:GLN:HE21	11:W:63:THR:HG22	1.71	0.55
6:R:14:TYR:N	6:R:14:TYR:CD1	2.74	0.55
1:A:604:GLY:C	1:A:606:GLN:N	2.62	0.55
3:B:390:VAL:O	3:B:394:ILE:HB	2.06	0.55
1:I:25:THR:HG22	1:I:27:ILE:H	1.71	0.55
1:I:293:ARG:HD3	1:I:296:ARG:HH22	1.71	0.55
1:I:305:LYS:HA	1:I:310:ARG:HD2	1.88	0.55
1:I:849:ALA:HB2	9:U:15:PHE:CG	2.40	0.55
2:M:28:ILE:HG13	9:U:18:VAL:HG21	1.89	0.55
3:J:730:THR:HB	3:J:732:TYR:CD1	2.38	0.55
3:J:1009:VAL:HB	3:J:1014:ARG:O	2.06	0.55
3:J:1074:LYS:HE2	3:J:1074:LYS:HA	1.88	0.55
4:O:34:LEU:HD22	4:O:151:LYS:HB2	1.87	0.55
1:A:81:VAL:HG23	1:A:209:LEU:HB2	1.86	0.55
1:A:113:LYS:HA	1:A:116:ARG:HB3	1.88	0.55
1:A:426:HIS:HD2	1:A:490:ARG:HH12	1.51	0.55
1:A:549:LYS:HB2	7:G:88:ASN:O	2.06	0.55
2:C:366:PHE:O	2:C:368:GLY:N	2.39	0.55
3:B:154:VAL:O	3:B:155:ASN:C	2.50	0.55
3:B:950:ILE:O	3:B:952:GLN:N	2.39	0.55
3:B:1031:MET:O	3:B:1034:ASP:HB2	2.07	0.55
4:D:239:GLU:HA	4:D:242:LEU:HD12	1.89	0.55
1:I:26:ALA:HA	1:I:74:HIS:CE1	2.41	0.55
3:J:106:ASN:O	3:J:108:GLU:HG3	2.07	0.55
3:J:582:VAL:HG13	3:J:586:ASN:N	2.21	0.55
3:J:745:VAL:HG21	3:J:891:LEU:HD11	1.88	0.55
3:J:910:LEU:HD22	3:J:911:ASN:H	1.70	0.55
10:V:59:THR:HG21	10:V:65:PRO:CD	2.35	0.55
1:A:58:CYS:HB2	1:A:59:PRO:CD	2.36	0.55
1:A:532:ILE:HG23	10:L:40:PHE:CG	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:318:ASP:O	2:C:322:ARG:CZ	2.54	0.55
3:B:978:LYS:HZ3	4:D:205:LEU:HD13	1.71	0.55
4:D:253:ILE:HD11	10:L:76:ILE:HD12	1.88	0.55
7:G:79:THR:HG22	7:G:80:GLU:N	2.20	0.55
1:I:337:VAL:HG21	1:I:419:PHE:CD1	2.41	0.55
1:I:704:LEU:HD13	1:I:781:PHE:HD1	1.72	0.55
2:M:390:MET:O	2:M:391:ARG:HB3	2.04	0.55
3:J:921:LEU:C	3:J:923:GLN:H	2.13	0.55
7:S:6:ALA:HB1	7:S:62:ASN:OD1	2.07	0.55
8:T:46:ARG:HD2	8:T:48:SER:HB2	1.87	0.55
1:A:25:THR:HG22	1:A:27:ILE:H	1.71	0.55
2:C:146:TYR:HD1	2:C:238:LYS:H	1.55	0.55
2:C:213:ILE:O	2:C:213:ILE:HG22	2.07	0.55
3:B:560:THR:HG22	3:B:562:PHE:N	2.17	0.55
7:G:86:LEU:HD12	7:G:91:LYS:HG3	1.88	0.55
5:Q:46:LEU:HD11	5:Q:77:TYR:HB2	1.88	0.55
5:Q:97:ILE:CD1	5:Q:113:ILE:HD11	2.34	0.55
3:B:122:MET:HE3	3:B:150:GLY:HA2	1.89	0.55
3:B:726:VAL:HG12	3:B:912:PRO:HG3	1.88	0.55
3:B:1113:LEU:H	3:B:1113:LEU:CD1	2.07	0.55
11:N:42:ARG:CG	11:N:43:TYR:H	2.19	0.55
1:I:84:VAL:CG1	1:I:274:ALA:HB1	2.36	0.55
1:I:595:GLU:HB3	7:S:86:LEU:HD13	1.89	0.55
2:M:369:VAL:HG21	3:J:1037:ILE:HG21	1.87	0.55
3:J:657:TYR:O	3:J:660:HIS:HB2	2.06	0.55
3:J:764:LYS:NZ	3:J:772:LYS:O	2.40	0.55
3:J:963:LEU:HD21	4:O:206:CYS:SG	2.47	0.55
10:V:38:VAL:HG13	10:V:58:LEU:O	2.06	0.55
11:W:3:ILE:HG22	11:W:4:PRO:HD2	1.88	0.55
13:Z:76:GLU:O	13:Z:77:LYS:HB3	2.07	0.55
1:A:595:GLU:N	7:G:86:LEU:HD22	2.22	0.55
1:A:763:THR:CG2	1:A:772:TYR:HA	2.37	0.55
2:C:257:ASN:OD1	2:C:259:SER:HB2	2.07	0.55
3:B:765:TYR:CG	3:B:766:PRO:HD2	2.42	0.55
3:B:946:TYR:HD2	3:B:947:LYS:H	1.55	0.55
11:N:7:CYS:CB	11:N:45:CYS:SG	2.95	0.55
4:O:21:PRO:HG3	10:V:79:MET:SD	2.47	0.55
4:O:106:PRO:HA	4:O:134:GLY:HA2	1.87	0.55
1:A:249:LEU:HD22	1:A:266:TRP:CE2	2.42	0.55
1:A:387:ASP:OD2	1:A:388:LEU:N	2.35	0.55
1:A:501:ASP:OD2	3:B:913:HIS:CD2	2.60	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:VAL:HG22	2:C:39:LYS:HZ1	1.72	0.55
3:B:139:ILE:HD13	11:N:61:HIS:CD2	2.42	0.55
10:L:59:THR:CG2	10:L:65:PRO:HD3	2.35	0.55
1:I:589:LYS:O	1:I:592:ILE:CG1	2.54	0.55
2:M:124:ILE:HG21	2:M:267:VAL:HG13	1.89	0.55
3:J:43:ILE:O	3:J:43:ILE:HG22	2.06	0.55
1:A:540:LEU:HB3	7:G:66:TYR:OH	2.06	0.54
3:B:147:ASP:OD2	3:B:148:PRO:HD2	2.07	0.54
3:B:346:ALA:O	3:B:350:PHE:N	2.36	0.54
5:E:27:LEU:HB2	5:E:51:VAL:HG11	1.89	0.54
11:N:35:LEU:CD2	11:N:40:VAL:HG21	2.37	0.54
1:I:203:ARG:HG3	1:I:205:GLU:HB2	1.88	0.54
1:I:555:PHE:CD2	1:I:631:LEU:HD13	2.42	0.54
2:M:311:ARG:H	2:M:311:ARG:HD3	1.72	0.54
3:J:603:THR:O	3:J:604:PHE:C	2.49	0.54
3:J:616:LEU:HD11	3:J:639:HIS:CE1	2.41	0.54
3:J:672:MET:HA	3:J:675:GLN:HB2	1.88	0.54
3:J:799:SER:O	3:J:800:PRO:O	2.25	0.54
4:O:134:GLY:N	4:O:137:GLN:OE1	2.23	0.54
3:B:70:VAL:HG11	3:B:90:LEU:HD23	1.90	0.54
3:B:727:MET:CE	3:B:898:PRO:CG	2.85	0.54
3:B:800:PRO:HB2	12:P:38:ARG:HA	1.87	0.54
3:B:1010:GLN:OE1	3:B:1010:GLN:HA	2.07	0.54
3:J:157:SER:O	3:J:158:GLU:HB2	2.07	0.54
3:J:159:ARG:HD3	3:J:399:ALA:HA	1.89	0.54
3:J:365:LEU:HG	3:J:369:LEU:HD12	1.90	0.54
4:O:254:GLU:CG	10:V:77:ARG:HH12	2.20	0.54
9:U:82:LEU:HD11	9:U:88:ILE:HD11	1.88	0.54
1:A:525:LEU:C	1:A:527:VAL:H	2.16	0.54
3:B:365:LEU:O	3:B:369:LEU:HB2	2.07	0.54
1:I:249:LEU:HD13	1:I:266:TRP:CE3	2.42	0.54
1:I:868:VAL:O	1:I:871:ILE:HG22	2.06	0.54
3:J:172:VAL:HG22	3:J:189:ILE:HD11	1.89	0.54
3:J:855:THR:O	3:J:856:ALA:C	2.48	0.54
5:Q:29:GLU:O	5:Q:33:GLN:HG3	2.07	0.54
11:W:35:LEU:CD2	11:W:40:VAL:HG21	2.37	0.54
1:A:116:ARG:HE	1:A:117:ILE:HG12	1.73	0.54
1:A:448:LEU:HD23	1:A:498:ALA:HA	1.88	0.54
3:B:588:LEU:CD1	3:B:612:LYS:HB3	2.37	0.54
6:F:55:VAL:O	6:F:59:LEU:HB2	2.08	0.54
2:M:146:TYR:HB2	2:M:238:LYS:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:291:GLU:HA	2:M:294:ILE:HD12	1.90	0.54
3:J:582:VAL:HG13	3:J:586:ASN:H	1.73	0.54
5:Q:66:THR:HG22	5:Q:68:HIS:NE2	2.21	0.54
1:A:84:VAL:CG1	1:A:274:ALA:HB1	2.37	0.54
1:A:84:VAL:HG11	1:A:274:ALA:HB1	1.88	0.54
1:A:470:GLU:HB2	9:K:41:LEU:HD12	1.89	0.54
1:A:507:TYR:O	1:A:508:LEU:CB	2.56	0.54
2:C:107:LEU:O	2:C:111:VAL:HG23	2.07	0.54
3:B:904:VAL:HG21	11:N:42:ARG:HE	1.72	0.54
3:B:910:LEU:HD22	3:B:911:ASN:H	1.68	0.54
1:I:446:ASN:HD22	1:I:447:LEU:N	2.05	0.54
2:M:52:PHE:O	2:M:56:ILE:HG12	2.08	0.54
2:M:63:LEU:HD21	9:U:23:TRP:HZ3	1.72	0.54
3:J:457:GLU:OE1	3:J:652:ALA:HB2	2.08	0.54
3:J:518:SER:HB3	3:J:564:ASN:ND2	2.22	0.54
3:J:812:GLY:HA2	3:J:836:SER:CB	2.36	0.54
1:A:102:GLY:H	1:A:103:ARG:HE	1.54	0.54
1:A:508:LEU:O	1:A:514:THR:HG23	2.08	0.54
3:B:200:VAL:O	3:B:200:VAL:HG13	2.08	0.54
3:B:463:ASN:HB3	3:B:467:VAL:CG1	2.38	0.54
3:B:690:THR:O	3:B:691:ARG:C	2.50	0.54
6:F:65:ARG:O	6:F:69:ARG:HG3	2.07	0.54
9:K:31:GLU:O	9:K:35:VAL:HG13	2.07	0.54
10:L:46:PRO:HD2	10:L:53:ILE:HA	1.90	0.54
1:I:764:ARG:NH1	1:I:769:PHE:O	2.40	0.54
1:I:781:PHE:C	1:I:781:PHE:HD2	2.14	0.54
3:J:368:GLN:O	3:J:372:SER:HB3	2.07	0.54
3:J:729:PHE:C	3:J:731:GLY:H	2.15	0.54
4:O:96:ILE:HG13	4:O:143:ALA:HB3	1.89	0.54
1:A:239:LEU:CD2	1:A:276:TYR:HE1	2.20	0.54
1:A:563:HIS:HB2	1:A:872:PHE:CE2	2.42	0.54
3:B:139:ILE:HG21	11:N:61:HIS:HD2	1.72	0.54
4:D:175:ASN:HA	4:D:195:LEU:CD1	2.26	0.54
2:M:309:ASP:OD2	2:M:311:ARG:HD3	2.08	0.54
7:S:86:LEU:HD12	7:S:91:LYS:HG3	1.90	0.54
10:V:1:MET:HB3	10:V:20:GLU:OE1	2.08	0.54
1:A:352:ARG:HA	1:A:406:ILE:HA	1.90	0.54
1:A:752:VAL:C	1:A:754:GLY:N	2.66	0.54
2:C:134:ARG:O	2:C:138:LEU:HG	2.08	0.54
2:C:322:ARG:H	2:C:322:ARG:HD2	1.73	0.54
6:F:56:ILE:HD11	6:F:70:ALA:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:560:THR:HG22	3:J:562:PHE:N	2.16	0.54
3:J:803:GLU:HB3	3:J:805:LYS:HZ1	1.72	0.54
4:O:209:CYS:SG	16:O:1001:F3S:S2	3.06	0.54
7:S:56:LYS:O	7:S:115:THR:HA	2.06	0.54
7:S:87:ASN:C	7:S:89:GLY:N	2.65	0.54
1:A:12:GLY:HA2	2:C:358:ALA:O	2.08	0.54
2:C:61:GLU:C	2:C:63:LEU:H	2.16	0.54
3:B:926:GLU:HB3	3:B:988:VAL:HG22	1.89	0.54
1:I:15:SER:HA	1:I:203:ARG:NH2	2.21	0.54
1:I:448:LEU:HD23	1:I:498:ALA:HA	1.89	0.54
3:J:800:PRO:HD3	3:J:850:VAL:HG23	1.88	0.54
3:J:803:GLU:HB3	3:J:805:LYS:HZ2	1.68	0.54
2:C:321:THR:C	2:C:322:ARG:NH1	2.66	0.54
4:D:205:LEU:O	4:D:207:GLU:N	2.40	0.54
8:H:24:ASN:O	8:H:26:ASP:N	2.41	0.54
1:I:529:ASP:CG	1:I:529:ASP:O	2.51	0.54
2:M:337:GLU:OE1	2:M:337:GLU:N	2.41	0.54
2:M:388:LEU:HD21	9:U:35:VAL:HG12	1.90	0.54
3:J:228:ARG:NH2	3:J:233:LEU:O	2.41	0.54
3:J:680:TYR:HE1	3:J:687:ARG:HH12	1.56	0.54
3:J:699:GLN:HB2	3:J:720:ASN:HA	1.90	0.54
4:O:176:CYS:H	4:O:195:LEU:HD21	1.73	0.54
6:R:56:ILE:HG23	6:R:69:ARG:HD2	1.90	0.54
3:B:582:VAL:HG13	3:B:586:ASN:N	2.23	0.53
4:D:116:SER:OG	4:D:121:VAL:O	2.20	0.53
1:I:133:THR:HB	1:I:137:LYS:NZ	2.23	0.53
2:M:290:ARG:HB2	2:M:321:THR:HG21	1.90	0.53
3:J:356:VAL:HG11	3:J:404:VAL:HG12	1.91	0.53
11:W:42:ARG:CG	11:W:43:TYR:H	2.21	0.53
1:A:95:LYS:NZ	1:A:152:LYS:HB3	2.23	0.53
1:A:374:GLY:C	1:A:410:HIS:ND1	2.66	0.53
1:A:558:LYS:CG	3:J:104:GLU:HB2	2.28	0.53
1:A:637:ARG:NH1	3:B:974:ARG:HH22	2.06	0.53
1:A:644:PHE:HA	1:A:724:PHE:HE2	1.73	0.53
1:A:827:LEU:HG	2:C:75:ALA:HB2	1.89	0.53
3:B:669:GLN:NE2	3:B:881:ARG:HA	2.23	0.53
1:I:502:TYR:CE2	3:J:734:MET:HE1	2.42	0.53
2:M:301:LEU:O	2:M:304:GLN:HB2	2.09	0.53
2:M:373:ILE:HD12	3:J:1049:LEU:HD22	1.90	0.53
3:J:356:VAL:CG1	3:J:404:VAL:HG12	2.38	0.53
3:J:932:TYR:CD2	3:J:932:TYR:O	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:180:VAL:CG2	4:O:190:LEU:HG	2.38	0.53
4:O:190:LEU:HD22	4:O:195:LEU:HA	1.89	0.53
9:U:44:ALA:C	9:U:45:MET:HE2	2.33	0.53
1:A:337:VAL:HG23	1:A:433:HIS:ND1	2.23	0.53
1:A:350:PRO:HG3	1:A:468:GLN:NE2	2.23	0.53
1:A:402:ALA:O	1:A:403:PRO:C	2.50	0.53
3:B:103:VAL:O	3:B:103:VAL:HG12	2.08	0.53
3:B:922:GLY:HA2	3:B:925:MET:CB	2.26	0.53
5:E:88:GLU:H	5:E:99:VAL:CG1	2.22	0.53
1:I:369:PRO:HG3	1:I:389:ARG:HA	1.89	0.53
3:J:346:ALA:O	3:J:350:PHE:N	2.42	0.53
3:J:895:VAL:HG21	4:O:34:LEU:HD21	1.90	0.53
1:A:595:GLU:HB2	7:G:91:LYS:CE	2.31	0.53
1:A:750:GLN:HG3	1:A:782:ILE:HD11	1.89	0.53
2:C:145:GLU:HA	2:C:239:ARG:H	1.73	0.53
3:B:321:LYS:HA	3:B:324:GLU:HB3	1.90	0.53
3:B:946:TYR:HD2	3:B:947:LYS:N	2.06	0.53
1:I:637:ARG:HH11	3:J:974:ARG:HH22	1.56	0.53
2:M:337:GLU:CD	2:M:338:LYS:H	2.16	0.53
3:J:321:LYS:HA	3:J:324:GLU:HB3	1.90	0.53
3:J:473:MET:HE1	3:J:475:GLN:O	2.07	0.53
3:J:490:TYR:HE1	3:J:527:ILE:CG2	2.21	0.53
3:J:727:MET:CE	3:J:898:PRO:HG3	2.39	0.53
7:S:85:SER:HB3	7:S:92:TYR:HB2	1.90	0.53
11:W:44:CYS:SG	11:W:45:CYS:N	2.81	0.53
1:A:764:ARG:NH1	1:A:769:PHE:O	2.42	0.53
2:C:299:LYS:CA	2:C:302:ALA:HB3	2.38	0.53
3:B:87:LEU:HD23	3:B:688:THR:HG21	1.91	0.53
3:B:94:ALA:O	3:B:119:LEU:N	2.39	0.53
3:B:1069:TRP:HE1	3:B:1088:LEU:HB3	1.73	0.53
3:B:1077:TYR:O	3:B:1077:TYR:HD1	1.91	0.53
4:D:22:LEU:C	4:D:24:PHE:H	2.16	0.53
7:G:40:PHE:CE2	7:G:113:LEU:HD21	2.44	0.53
1:I:91:TYR:OH	1:I:153:GLN:O	2.18	0.53
3:J:27:HIS:HD2	3:J:346:ALA:HB2	1.74	0.53
3:J:446:HIS:O	3:J:447:GLY:C	2.50	0.53
3:J:663:SER:HB3	3:J:664:PRO:HD3	1.89	0.53
3:J:946:TYR:HD2	3:J:947:LYS:N	2.06	0.53
3:J:1069:TRP:CD1	3:J:1088:LEU:HD22	2.43	0.53
5:Q:109:HIS:HD2	5:Q:111:SER:H	1.56	0.53
6:R:14:TYR:N	6:R:14:TYR:HD1	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:SER:HB2	2:C:360:ARG:NH1	2.23	0.53
3:B:578:PRO:HB3	3:B:615:TYR:CE1	2.44	0.53
3:B:943:THR:CG2	3:B:944:PRO:HD2	2.38	0.53
9:K:70:ARG:C	9:K:72:GLY:H	2.16	0.53
1:I:584:SER:OG	1:I:585:TYR:N	2.40	0.53
3:J:760:THR:OG1	3:J:813:LYS:HD2	2.08	0.53
1:A:58:CYS:CB	1:A:59:PRO:CD	2.86	0.53
1:A:94:LEU:HD11	1:A:180:ILE:HG23	1.90	0.53
2:C:144:LEU:O	2:C:145:GLU:C	2.51	0.53
3:B:368:GLN:O	3:B:372:SER:HB3	2.08	0.53
3:B:937:GLY:HA2	11:N:50:LEU:HD11	1.90	0.53
6:F:48:ASP:H	6:F:51:SER:HG	1.56	0.53
6:F:54:LYS:HA	6:F:57:GLU:HB2	1.91	0.53
1:I:61:CYS:SG	3:J:1070:TYR:HB3	2.48	0.53
3:J:390:VAL:O	3:J:394:ILE:HB	2.08	0.53
8:T:45:ILE:HG22	8:T:81:VAL:N	2.24	0.53
1:A:26:ALA:HA	1:A:74:HIS:CE1	2.44	0.53
2:C:76:GLN:O	2:C:80:GLU:N	2.37	0.53
2:C:190:ARG:CD	2:C:191:LEU:H	2.21	0.53
2:C:328:GLN:O	2:C:333:GLY:HA3	2.09	0.53
3:B:474:ALA:HB2	3:B:578:PRO:HG3	1.91	0.53
5:E:17:GLU:OE2	5:E:20:LYS:NZ	2.24	0.53
1:I:874:ARG:HE	2:M:53:ASP:CB	2.21	0.53
2:M:119:THR:N	2:M:120:PRO:HD3	2.24	0.53
2:M:173:MET:HE3	2:M:177:LYS:NZ	2.24	0.53
2:M:212:ASN:HD22	2:M:213:ILE:N	2.07	0.53
2:M:329:ILE:HA	2:M:334:VAL:CG1	2.35	0.53
3:J:54:PRO:O	3:J:56:LEU:N	2.42	0.53
3:J:971:TYR:CE2	3:J:978:LYS:HB3	2.44	0.53
7:S:21:GLY:HA3	7:S:26:LEU:HD12	1.90	0.53
9:U:82:LEU:HB2	9:U:84:ASN:HB2	1.91	0.53
1:A:113:LYS:HG2	1:A:116:ARG:CZ	2.38	0.53
1:A:215:PRO:HB2	1:A:219:ILE:HD11	1.91	0.53
2:C:55:ALA:C	2:C:58:GLU:HB2	2.33	0.53
4:D:190:LEU:HD22	4:D:195:LEU:HA	1.91	0.53
1:I:209:LEU:HD13	1:I:273:VAL:HG11	1.91	0.53
1:I:541:ALA:N	7:S:72:CYS:O	2.42	0.53
1:I:644:PHE:HA	1:I:724:PHE:CE2	2.44	0.53
1:I:827:LEU:HD13	2:M:319:VAL:HG21	1.90	0.53
2:M:122:MET:HG2	2:M:274:THR:HG23	1.90	0.53
2:M:370:VAL:O	2:M:373:ILE:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:391:ARG:H	2:M:392:PRO:CD	2.22	0.53
3:J:43:ILE:HG13	3:J:63:ILE:CD1	2.39	0.53
3:J:1069:TRP:HE1	3:J:1088:LEU:HB3	1.73	0.53
4:O:34:LEU:HA	4:O:150:GLY:HA3	1.91	0.53
13:Z:59:ILE:HA	13:Z:62:GLU:CD	2.34	0.53
1:A:290:ARG:HD2	1:A:291:SER:N	2.24	0.53
1:A:458:ASP:HA	3:B:886:GLY:HA2	1.90	0.53
1:A:647:ARG:HB2	1:A:650:ASP:OD1	2.09	0.53
3:B:448:THR:C	3:B:450:TRP:N	2.67	0.53
3:B:560:THR:HG22	3:B:561:ASP:N	2.24	0.53
3:B:954:GLN:HA	3:B:957:ILE:HD11	1.90	0.53
11:N:1:MET:HE2	11:N:56:ILE:HG13	1.90	0.53
1:I:392:LYS:O	1:I:393:ASP:C	2.52	0.53
1:I:450:CYS:N	1:I:451:PRO:CD	2.72	0.53
1:I:458:ASP:HA	3:J:886:GLY:HA2	1.91	0.53
2:M:190:ARG:CZ	2:M:191:LEU:HG	2.39	0.53
3:J:1004:ARG:NH1	3:J:1025:GLY:H	2.05	0.53
1:A:620:SER:C	1:A:622:GLU:H	2.15	0.52
3:B:762:GLU:HG2	3:B:772:LYS:HA	1.91	0.52
11:N:18:TRP:CD1	11:N:49:LEU:HD22	2.39	0.52
1:I:268:LEU:HD23	1:I:271:TYR:HD1	1.74	0.52
1:I:336:GLU:OE1	1:I:436:ARG:NH1	2.43	0.52
1:I:364:PHE:HD2	1:I:373:PRO:O	1.93	0.52
1:I:378:VAL:HG23	1:I:407:ILE:HG22	1.91	0.52
1:I:501:ASP:HB2	3:J:734:MET:SD	2.49	0.52
1:I:752:VAL:C	1:I:754:GLY:N	2.66	0.52
1:I:775:SER:OG	1:I:776:PRO:HD2	2.10	0.52
2:M:13:LEU:HD23	2:M:16:LYS:NZ	2.24	0.52
3:J:83:MET:O	3:J:87:LEU:HD12	2.09	0.52
3:J:448:THR:C	3:J:450:TRP:N	2.67	0.52
8:T:11:PRO:HD2	8:T:12:ARG:HD3	1.90	0.52
1:A:345:LYS:NZ	1:A:370:ASP:O	2.35	0.52
1:A:417:VAL:HG13	1:A:464:LEU:HD13	1.91	0.52
3:B:591:ILE:O	3:B:594:ILE:HG12	2.09	0.52
3:B:602:ILE:HG22	3:B:603:THR:N	2.24	0.52
3:B:702:LEU:HD13	11:N:47:ARG:HD2	1.91	0.52
4:D:111:SER:C	4:D:114:ILE:HD13	2.34	0.52
4:D:253:ILE:CD1	10:L:76:ILE:HD12	2.39	0.52
5:E:130:GLU:HA	5:E:133:LYS:HE2	1.90	0.52
1:I:620:SER:C	1:I:622:GLU:H	2.18	0.52
1:I:679:TYR:OH	1:I:693:GLU:HG2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:61:GLU:C	2:M:63:LEU:N	2.68	0.52
3:J:246:PRO:C	3:J:248:VAL:N	2.68	0.52
1:A:828:SER:C	1:A:830:LEU:N	2.61	0.52
3:B:48:GLU:HG2	3:B:58:VAL:HB	1.91	0.52
3:B:425:HIS:HA	3:B:428:ARG:HD3	1.91	0.52
3:B:461:GLY:O	3:B:464:SER:HB3	2.09	0.52
3:B:895:VAL:HG21	4:D:34:LEU:HD21	1.92	0.52
3:B:1069:TRP:CH2	3:B:1077:TYR:HB2	2.44	0.52
5:E:66:THR:HG23	5:E:68:HIS:CE1	2.44	0.52
3:J:533:GLY:O	3:J:535:GLU:N	2.41	0.52
3:J:834:ASP:O	3:J:836:SER:N	2.38	0.52
4:O:29:ARG:HG3	4:O:162:SER:O	2.10	0.52
4:O:134:GLY:O	4:O:135:THR:C	2.52	0.52
12:X:26:CYS:HG	12:X:29:CYS:HB2	1.73	0.52
1:A:490:ARG:HA	2:C:312:HIS:CE1	2.39	0.52
2:C:153:VAL:HG13	2:C:153:VAL:O	2.09	0.52
2:C:237:ILE:CG1	2:C:238:LYS:N	2.63	0.52
3:B:971:TYR:CE2	3:B:978:LYS:HB3	2.45	0.52
5:E:51:VAL:O	5:E:53:THR:N	2.41	0.52
5:E:179:LYS:HZ2	6:F:79:THR:HB	1.74	0.52
12:P:9:CYS:HB3	12:P:12:THR:O	2.10	0.52
1:I:349:VAL:HG21	1:I:409:ARG:NH2	2.24	0.52
1:I:750:GLN:CG	1:I:782:ILE:CD1	2.88	0.52
3:J:474:ALA:HB2	3:J:578:PRO:HG3	1.90	0.52
3:J:1083:GLY:C	3:J:1085:LYS:H	2.16	0.52
4:O:129:PRO:HG2	11:W:15:ALA:HB1	1.90	0.52
1:A:239:LEU:CD2	1:A:276:TYR:CE1	2.92	0.52
1:A:549:LYS:HB2	1:A:549:LYS:HZ3	1.74	0.52
1:A:647:ARG:O	1:A:650:ASP:HB2	2.08	0.52
2:C:124:ILE:O	2:C:251:ILE:HG22	2.10	0.52
2:C:392:PRO:HG2	5:E:22:LEU:HD21	1.91	0.52
3:B:82:PRO:CG	3:B:143:GLU:OE1	2.48	0.52
3:B:435:ARG:HB3	3:B:437:GLN:HB2	1.90	0.52
3:B:677:LEU:HD12	3:B:992:LYS:HD3	1.90	0.52
9:K:38:ALA:C	9:K:42:GLN:NE2	2.67	0.52
1:I:426:HIS:ND1	1:I:428:ILE:HG22	2.24	0.52
1:I:448:LEU:O	1:I:496:ILE:HG23	2.10	0.52
1:I:563:HIS:HB2	1:I:872:PHE:CE2	2.44	0.52
2:M:112:ASP:O	2:M:113:ALA:CB	2.58	0.52
2:M:372:ASN:O	2:M:375:ILE:HG22	2.09	0.52
3:J:21:LYS:HE2	3:J:475:GLN:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:38:ALA:HB1	9:U:42:GLN:HE22	1.75	0.52
11:W:1:MET:HE2	11:W:56:ILE:HG13	1.91	0.52
1:A:446:ASN:O	1:A:448:LEU:N	2.42	0.52
2:C:355:LEU:HD23	3:B:1109:ILE:HD11	1.91	0.52
3:B:162:VAL:HG11	3:B:412:GLN:NE2	2.25	0.52
3:B:603:THR:O	3:B:604:PHE:C	2.52	0.52
3:B:727:MET:HE3	3:B:898:PRO:CG	2.39	0.52
10:L:69:LEU:O	10:L:73:ILE:N	2.36	0.52
1:I:457:PHE:HB2	3:J:737:SER:HB2	1.91	0.52
1:I:488:THR:HG23	1:I:490:ARG:H	1.75	0.52
1:I:825:ASN:O	1:I:827:LEU:N	2.43	0.52
3:J:368:GLN:NE2	3:J:386:ARG:HE	2.08	0.52
5:Q:18:PHE:CD2	9:U:47:ALA:HB1	2.45	0.52
11:W:43:TYR:HA	11:W:46:ARG:HB2	1.91	0.52
1:A:95:LYS:HZ1	1:A:152:LYS:HB3	1.74	0.52
1:A:215:PRO:HB3	3:B:1106:SER:HB3	1.90	0.52
1:A:369:PRO:HG3	1:A:389:ARG:HA	1.91	0.52
1:A:446:ASN:C	1:A:446:ASN:ND2	2.65	0.52
2:C:261:VAL:O	2:C:261:VAL:HG12	2.10	0.52
3:B:369:LEU:HG	3:B:384:LEU:HD13	1.91	0.52
3:B:582:VAL:HG11	3:B:633:LEU:HD11	1.91	0.52
3:B:682:ALA:O	11:N:59:VAL:HG13	2.10	0.52
3:B:902:LYS:HE2	11:N:41:LYS:HB3	1.91	0.52
4:D:96:ILE:HG13	4:D:143:ALA:HB3	1.91	0.52
4:D:131:VAL:HG22	4:D:132:LEU:H	1.73	0.52
10:L:76:ILE:O	10:L:77:ARG:C	2.53	0.52
1:I:378:VAL:O	1:I:378:VAL:CG2	2.55	0.52
1:I:664:GLU:OE1	1:I:707:LEU:HD22	2.09	0.52
2:M:153:VAL:HG23	2:M:168:GLN:O	2.10	0.52
3:J:96:LEU:HB2	3:J:117:GLY:H	1.75	0.52
3:J:130:ILE:HA	3:J:133:TYR:CE1	2.45	0.52
3:J:215:PRO:O	3:J:216:ALA:HB3	2.10	0.52
3:J:369:LEU:HG	3:J:384:LEU:HD13	1.91	0.52
3:J:849:LEU:HB3	3:J:865:ARG:HB3	1.91	0.52
4:O:101:GLU:O	4:O:107:ARG:NH1	2.43	0.52
1:A:353:ILE:CG1	1:A:361:LEU:HD23	2.37	0.52
1:A:855:VAL:HG22	2:C:64:ILE:HB	1.92	0.52
3:B:850:VAL:O	12:P:35:PHE:CB	2.57	0.52
4:D:21:PRO:HG3	10:L:79:MET:SD	2.49	0.52
4:D:180:VAL:HG21	4:D:190:LEU:HG	1.92	0.52
5:E:81:VAL:O	5:E:82:GLN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:71:PHE:O	7:G:114:ARG:HA	2.10	0.52
1:I:77:LEU:HD12	1:I:210:THR:C	2.35	0.52
1:I:761:TYR:OH	3:J:621:GLU:OE1	2.20	0.52
2:M:103:GLY:HA2	2:M:106:ARG:HB3	1.90	0.52
3:J:193:THR:HG21	3:J:197:ARG:N	2.25	0.52
3:J:848:ASP:OD1	3:J:865:ARG:CZ	2.57	0.52
3:J:902:LYS:HB2	11:W:42:ARG:HH11	1.75	0.52
3:J:1061:CYS:HA	3:J:1088:LEU:HD23	1.92	0.52
7:S:101:LEU:C	7:S:103:VAL:N	2.66	0.52
1:A:155:LYS:HA	1:A:156:ILE:O	2.10	0.52
1:A:495:ILE:HG13	1:A:495:ILE:O	2.10	0.52
1:A:632:PHE:HA	1:A:635:PHE:CE1	2.45	0.52
1:A:868:VAL:HG13	2:C:39:LYS:HE2	1.92	0.52
3:B:367:TYR:HD2	3:B:367:TYR:O	1.93	0.52
3:B:950:ILE:C	3:B:952:GLN:N	2.67	0.52
4:D:96:ILE:CG1	4:D:143:ALA:HB3	2.40	0.52
9:K:69:PHE:HA	9:K:74:LEU:HD11	1.92	0.52
9:K:86:LYS:N	9:K:86:LYS:HD2	2.25	0.52
1:I:337:VAL:HG12	1:I:339:VAL:HG23	1.91	0.52
1:I:507:TYR:HB2	1:I:511:VAL:HG13	1.92	0.52
1:I:763:THR:CG2	1:I:772:TYR:HA	2.40	0.52
2:M:106:ARG:O	2:M:107:LEU:C	2.52	0.52
2:M:344:ARG:HB3	2:M:353:HIS:CD2	2.44	0.52
3:J:911:ASN:HD21	3:J:913:HIS:HD2	1.57	0.52
3:B:368:GLN:HE22	3:B:386:ARG:HH21	1.57	0.52
3:B:471:ALA:O	3:B:473:MET:HG3	2.10	0.52
3:B:789:TYR:O	3:B:791:LEU:N	2.43	0.52
3:B:943:THR:HG22	3:B:944:PRO:HD2	1.91	0.52
4:D:176:CYS:H	4:D:195:LEU:HD21	1.74	0.52
10:L:32:LEU:HD11	10:L:69:LEU:HD12	1.92	0.52
1:I:71:HIS:ND1	3:J:1070:TYR:HE2	2.07	0.52
1:I:441:LEU:HD12	3:J:873:THR:HG21	1.92	0.52
1:I:506:ALA:O	1:I:510:THR:HG23	2.10	0.52
2:M:145:GLU:O	2:M:147:THR:N	2.43	0.52
7:S:42:ILE:HD12	7:S:46:ILE:HG21	1.91	0.52
1:A:83:HIS:HB3	1:A:86:LEU:HB2	1.92	0.51
1:A:507:TYR:OH	1:A:727:VAL:HG13	2.09	0.51
1:A:557:PRO:HD3	1:A:623:TYR:OH	2.10	0.51
1:A:590:ASN:CG	3:J:377:ARG:HB2	2.34	0.51
3:B:27:HIS:HD2	3:B:346:ALA:HB2	1.75	0.51
3:B:579:LEU:O	3:B:613:ILE:HG23	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:644:SER:C	3:B:646:ALA:H	2.17	0.51
3:B:685:GLN:HE22	3:B:867:ARG:HH22	1.58	0.51
4:D:204:THR:O	4:D:206:CYS:N	2.43	0.51
7:G:29:VAL:HB	7:G:40:PHE:HD1	1.75	0.51
8:H:63:ILE:HG22	8:H:64:ARG:N	2.25	0.51
1:I:95:LYS:HB3	1:I:138:LYS:HG3	1.92	0.51
1:I:533:ASP:O	1:I:534:LEU:C	2.52	0.51
1:I:728:MET:CE	3:J:913:HIS:HA	2.40	0.51
1:I:837:THR:HG22	1:I:838:VAL:H	1.75	0.51
3:J:94:ALA:O	3:J:119:LEU:N	2.37	0.51
3:J:602:ILE:HG22	3:J:603:THR:N	2.25	0.51
3:J:800:PRO:HB2	12:X:38:ARG:HA	1.92	0.51
1:A:541:ALA:CA	7:G:72:CYS:H	2.23	0.51
2:C:390:MET:C	2:C:391:ARG:CD	2.83	0.51
4:D:250:ILE:CD1	10:L:84:ILE:CD1	2.83	0.51
7:G:86:LEU:HD12	7:G:91:LYS:CG	2.39	0.51
1:I:737:VAL:HG23	1:I:738:LEU:HD22	1.93	0.51
3:J:419:TRP:CZ3	3:J:712:GLY:HA3	2.45	0.51
3:J:624:ALA:HB1	3:J:639:HIS:CD2	2.45	0.51
4:O:134:GLY:O	4:O:135:THR:O	2.28	0.51
5:Q:31:ARG:O	5:Q:33:GLN:N	2.42	0.51
1:A:446:ASN:HD22	1:A:447:LEU:N	2.08	0.51
1:A:541:ALA:CB	7:G:71:PHE:HA	2.40	0.51
2:C:391:ARG:H	2:C:392:PRO:CD	2.22	0.51
3:B:738:ILE:CD1	3:B:908:ILE:HG23	2.39	0.51
3:B:745:VAL:HG21	3:B:891:LEU:HD11	1.91	0.51
9:K:67:GLU:CD	9:K:70:ARG:HH21	2.17	0.51
1:I:486:ILE:HG12	1:I:496:ILE:HB	1.93	0.51
1:I:594:LEU:O	1:I:595:GLU:HG2	2.10	0.51
2:M:55:ALA:C	2:M:58:GLU:HB2	2.35	0.51
2:M:388:LEU:HD21	9:U:35:VAL:CG1	2.39	0.51
3:J:116:ILE:HD12	3:J:361:PHE:CZ	2.46	0.51
5:Q:79:PRO:HG2	5:Q:149:VAL:HG21	1.92	0.51
11:W:42:ARG:HG3	11:W:43:TYR:H	1.74	0.51
1:A:558:LYS:H	1:A:558:LYS:CD	2.23	0.51
2:C:392:PRO:HB2	5:E:22:LEU:HD11	1.93	0.51
3:B:855:THR:C	3:B:857:GLU:N	2.66	0.51
5:E:64:GLY:O	9:K:42:GLN:OE1	2.28	0.51
7:G:46:ILE:O	7:G:46:ILE:CG2	2.58	0.51
1:I:105:LYS:NZ	1:I:108:GLU:HB2	2.25	0.51
2:M:55:ALA:CB	2:M:58:GLU:OE2	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:55:ALA:O	2:M:58:GLU:HB2	2.10	0.51
2:M:146:TYR:CZ	2:M:235:LYS:HB2	2.45	0.51
2:M:376:GLY:HA2	3:J:1049:LEU:HD21	1.91	0.51
3:J:92:TYR:O	3:J:92:TYR:CD2	2.63	0.51
3:J:367:TYR:HD2	3:J:367:TYR:O	1.93	0.51
3:J:569:ASN:HB3	3:J:574:ARG:HH12	1.76	0.51
3:J:963:LEU:HD22	3:J:982:ARG:NH2	2.26	0.51
1:A:238:LYS:HE2	1:A:297:THR:HG22	1.92	0.51
2:C:278:ARG:O	2:C:278:ARG:HD2	2.11	0.51
3:B:170:ASN:HB3	3:B:300:HIS:HE1	1.76	0.51
3:B:246:PRO:C	3:B:248:VAL:N	2.68	0.51
3:B:517:TRP:HD1	3:B:531:GLN:H	1.59	0.51
7:G:17:SER:HB2	7:G:19:GLU:HG2	1.92	0.51
1:I:7:LYS:HE2	2:M:365:GLU:OE2	2.11	0.51
1:I:438:LEU:HD21	1:I:444:ARG:CZ	2.40	0.51
1:I:525:LEU:C	1:I:527:VAL:H	2.18	0.51
3:J:970:VAL:HG22	3:J:979:ILE:HG12	1.92	0.51
3:J:978:LYS:HG2	4:O:166:TYR:CE2	2.46	0.51
1:A:317:ARG:NH1	3:B:1018:GLU:HG3	2.26	0.51
1:A:557:PRO:HA	1:A:558:LYS:HZ2	1.75	0.51
2:C:277:ILE:C	2:C:279:GLU:H	2.19	0.51
3:B:356:VAL:HG22	3:B:393:ARG:NH1	2.25	0.51
3:B:665:ARG:HG3	3:B:920:THR:HG21	1.91	0.51
3:B:1074:LYS:HE2	3:B:1074:LYS:HA	1.93	0.51
1:I:98:CYS:HB3	1:I:101:CYS:H	1.76	0.51
1:I:217:ILE:C	1:I:219:ILE:H	2.18	0.51
2:M:149:ILE:HB	2:M:227:LEU:HA	1.92	0.51
3:J:469:ASN:HD22	3:J:469:ASN:N	2.07	0.51
3:J:1043:MET:HE2	3:J:1043:MET:HA	1.93	0.51
4:O:137:GLN:NE2	11:W:63:THR:HG22	2.26	0.51
1:A:209:LEU:HD13	1:A:273:VAL:HG11	1.92	0.51
1:A:290:ARG:NH1	1:A:291:SER:HB2	2.25	0.51
1:A:528:ALA:HB3	1:A:630:ASN:HD21	1.74	0.51
1:A:659:LYS:O	1:A:663:ASN:HB2	2.09	0.51
2:C:11:PRO:O	2:C:14:GLU:HG3	2.11	0.51
3:B:260:SER:C	3:B:262:ILE:H	2.19	0.51
3:B:330:ARG:HA	3:B:563:ILE:HD11	1.93	0.51
3:B:1004:ARG:NH1	3:B:1024:GLY:HA2	2.25	0.51
3:B:1009:VAL:HB	3:B:1014:ARG:O	2.09	0.51
3:B:1029:GLY:O	3:B:1030:GLU:C	2.53	0.51
5:E:87:GLY:O	5:E:88:GLU:CB	2.55	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:69:SER:HB2	8:H:75:VAL:HG22	1.93	0.51
1:I:290:ARG:NH1	1:I:291:SER:HB2	2.25	0.51
1:I:853:ASP:HB3	1:I:855:VAL:H	1.76	0.51
2:M:369:VAL:O	2:M:373:ILE:HB	2.11	0.51
2:M:384:GLY:HA2	5:Q:61:PHE:HZ	1.75	0.51
3:J:435:ARG:HB3	3:J:437:GLN:HB2	1.93	0.51
5:Q:15:PRO:HB2	9:U:45:MET:O	2.10	0.51
5:Q:120:TYR:CZ	5:Q:122:ASN:HA	2.46	0.51
9:U:39:ARG:HE	9:U:68:GLU:CD	2.18	0.51
1:A:371:LYS:NZ	1:A:373:PRO:HD3	2.26	0.51
1:A:539:ILE:HB	1:A:545:TYR:HB2	1.93	0.51
2:C:301:LEU:O	2:C:304:GLN:N	2.44	0.51
3:B:931:LYS:HE2	3:B:985:PHE:O	2.10	0.51
6:F:77:PRO:HG3	6:F:83:VAL:HG22	1.93	0.51
8:H:78:TYR:C	8:H:79:ARG:HG2	2.35	0.51
9:K:61:VAL:O	9:K:62:ILE:HB	2.11	0.51
9:K:91:SER:O	9:K:92:LEU:HB3	2.11	0.51
1:I:502:TYR:CD2	3:J:734:MET:HE1	2.45	0.51
1:I:532:ILE:HG23	10:V:40:PHE:CD2	2.46	0.51
1:I:741:THR:O	1:I:742:GLN:C	2.54	0.51
1:I:859:TYR:HB2	2:M:64:ILE:HG23	1.93	0.51
2:M:121:MET:H	2:M:275:ASN:ND2	2.09	0.51
2:M:286:ILE:HG13	8:T:49:ASP:OD2	2.11	0.51
3:J:904:VAL:HG22	11:W:44:CYS:HB3	1.93	0.51
6:R:13:PRO:HB3	6:R:73:ALA:HB3	1.92	0.51
9:U:41:LEU:O	9:U:42:GLN:C	2.54	0.51
2:C:49:ASP:O	2:C:51:ILE:N	2.44	0.51
2:C:72:ILE:CG2	2:C:76:GLN:OE1	2.59	0.51
3:B:683:ASN:C	3:B:685:GLN:N	2.64	0.51
3:B:699:GLN:HE21	11:N:48:MET:HE3	1.76	0.51
3:B:710:ILE:HD13	3:B:710:ILE:H	1.76	0.51
3:B:834:ASP:O	3:B:836:SER:N	2.39	0.51
6:F:64:SER:H	6:F:69:ARG:HH21	1.59	0.51
9:K:54:ASN:HD21	9:K:58:SER:CB	2.24	0.51
1:I:465:HIS:CD2	3:J:1048:ARG:HD2	2.46	0.51
1:I:749:GLN:N	1:I:781:PHE:HA	2.25	0.51
3:J:14:ILE:HG13	3:J:18:PHE:CE2	2.46	0.51
3:J:232:ILE:HG23	3:J:237:ASP:HB3	1.92	0.51
5:Q:50:ASN:HB2	5:Q:73:ASP:OD2	2.11	0.51
1:A:293:ARG:HD3	1:A:296:ARG:HH22	1.76	0.51
1:A:305:LYS:HA	1:A:310:ARG:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:THR:CG2	1:A:325:VAL:N	2.73	0.51
3:B:67:LYS:HB3	3:B:68:PRO:HD2	1.93	0.51
3:B:699:GLN:HA	11:N:51:SER:O	2.11	0.51
3:B:875:GLY:HA2	3:B:887:VAL:HG13	1.93	0.51
3:B:897:MET:HE2	3:B:897:MET:HA	1.93	0.51
3:B:932:TYR:CD2	3:B:932:TYR:O	2.64	0.51
5:E:110:ILE:O	5:E:113:ILE:HG22	2.11	0.51
1:I:290:ARG:HD2	1:I:291:SER:H	1.76	0.51
1:I:723:ASN:O	1:I:724:PHE:C	2.51	0.51
2:M:24:LEU:HD11	2:M:58:GLU:OE1	2.12	0.51
2:M:286:ILE:HG12	2:M:324:GLY:O	2.10	0.51
3:J:729:PHE:O	3:J:731:GLY:N	2.43	0.51
3:J:950:ILE:O	3:J:952:GLN:N	2.45	0.51
3:J:975:THR:OG1	3:J:977:GLN:HG2	2.11	0.51
10:V:82:HIS:O	10:V:86:GLU:N	2.43	0.51
1:A:525:LEU:HG	10:L:40:PHE:HZ	1.75	0.50
2:C:359:ALA:C	2:C:361:GLY:N	2.66	0.50
3:B:68:PRO:CD	3:B:129:PRO:HG2	2.40	0.50
3:B:325:LEU:HD11	3:B:331:GLU:H	1.76	0.50
3:B:582:VAL:HG13	3:B:586:ASN:H	1.76	0.50
3:B:870:ARG:HH11	3:B:996:MET:HB2	1.74	0.50
4:D:131:VAL:CG2	4:D:132:LEU:H	2.24	0.50
8:H:65:ILE:HD11	8:H:79:ARG:HG2	1.92	0.50
1:I:78:VAL:HG23	1:I:266:TRP:HZ3	1.75	0.50
1:I:851:GLY:C	1:I:853:ASP:H	2.19	0.50
3:J:291:GLN:O	3:J:295:LYS:HG2	2.10	0.50
3:J:699:GLN:HA	11:W:51:SER:O	2.11	0.50
3:J:762:GLU:HG2	3:J:772:LYS:HA	1.93	0.50
8:T:45:ILE:O	8:T:81:VAL:HA	2.12	0.50
1:A:549:LYS:CB	7:G:88:ASN:O	2.60	0.50
2:C:52:PHE:HA	2:C:55:ALA:HB3	1.93	0.50
2:C:150:GLU:HB2	2:C:227:LEU:HB3	1.93	0.50
3:B:579:LEU:CD1	3:B:616:LEU:HD12	2.26	0.50
3:B:849:LEU:HB3	3:B:865:ARG:HB3	1.94	0.50
4:D:250:ILE:CD1	10:L:84:ILE:HD11	2.21	0.50
7:G:37:ASN:O	7:G:94:THR:HA	2.10	0.50
7:G:40:PHE:CZ	7:G:115:THR:HG21	2.46	0.50
1:I:506:ALA:HA	1:I:635:PHE:CE2	2.46	0.50
3:J:560:THR:CG2	3:J:561:ASP:N	2.74	0.50
4:O:12:ARG:HA	4:O:230:ILE:O	2.11	0.50
8:T:42:LEU:CB	8:T:43:PRO:HD2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ARG:HB2	3:B:1016:PRO:HB2	1.93	0.50
1:A:353:ILE:HD11	1:A:407:ILE:HG23	1.92	0.50
1:A:450:CYS:N	1:A:451:PRO:CD	2.74	0.50
3:B:325:LEU:HD22	3:B:330:ARG:HG3	1.93	0.50
3:B:729:PHE:O	3:B:731:GLY:N	2.44	0.50
3:B:763:VAL:HA	3:B:770:GLU:CG	2.41	0.50
4:D:134:GLY:O	4:D:135:THR:C	2.54	0.50
6:F:15:SER:HA	6:F:18:LYS:HZ1	1.76	0.50
10:L:40:PHE:HB3	10:L:58:LEU:HB3	1.93	0.50
1:I:238:LYS:HE2	1:I:297:THR:HG22	1.94	0.50
1:I:239:LEU:CD2	1:I:276:TYR:CE1	2.94	0.50
1:I:324:THR:CG2	1:I:325:VAL:H	2.22	0.50
1:I:524:ILE:O	1:I:525:LEU:HD22	2.11	0.50
1:I:644:PHE:HA	1:I:724:PHE:HE2	1.77	0.50
1:I:859:TYR:HB3	2:M:64:ILE:HG12	1.93	0.50
2:M:297:ILE:O	2:M:298:SER:C	2.55	0.50
3:J:54:PRO:O	3:J:55:GLY:C	2.54	0.50
3:J:103:VAL:O	3:J:103:VAL:HG12	2.10	0.50
3:J:517:TRP:HD1	3:J:531:GLN:H	1.59	0.50
7:S:57:VAL:HG13	7:S:115:THR:HG22	1.92	0.50
9:U:34:ARG:C	9:U:37:SER:HB2	2.36	0.50
1:A:337:VAL:HG21	1:A:419:PHE:CD1	2.46	0.50
3:B:361:PHE:CE1	3:B:385:VAL:HG13	2.44	0.50
1:I:288:LYS:HG2	1:I:294:PRO:HA	1.92	0.50
3:J:448:THR:HG22	3:J:452:ARG:HD2	1.93	0.50
9:U:41:LEU:O	9:U:43:LEU:N	2.44	0.50
13:Z:76:GLU:O	13:Z:77:LYS:CB	2.58	0.50
1:A:486:ILE:O	1:A:486:ILE:HD13	2.11	0.50
1:A:653:LEU:HD11	1:A:745:ALA:HB2	1.94	0.50
1:A:723:ASN:O	1:A:724:PHE:C	2.54	0.50
2:C:11:PRO:HB2	2:C:14:GLU:OE1	2.10	0.50
3:B:533:GLY:O	3:B:535:GLU:N	2.45	0.50
3:B:900:THR:OG1	3:B:904:VAL:HB	2.12	0.50
4:D:131:VAL:CG2	4:D:132:LEU:N	2.74	0.50
5:E:179:LYS:HZ3	6:F:79:THR:HB	1.77	0.50
8:H:58:LYS:HB2	8:H:61:ASP:HB2	1.93	0.50
1:I:446:ASN:HD22	1:I:448:LEU:H	1.59	0.50
2:M:339:ASN:OD1	2:M:339:ASN:N	2.42	0.50
3:J:330:ARG:NH2	3:J:565:GLU:OE1	2.44	0.50
3:J:377:ARG:O	3:J:378:LYS:HB2	2.12	0.50
3:J:453:MET:HG2	3:J:468:LYS:HD2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:228:LEU:O	4:O:229:GLU:HG3	2.11	0.50
7:S:80:GLU:HG3	7:S:81:LEU:H	1.76	0.50
3:B:26:GLN:C	3:B:345:LEU:HD23	2.34	0.50
3:B:226:LEU:O	3:B:230:LEU:HD12	2.12	0.50
3:B:813:LYS:O	3:B:814:VAL:HG23	2.12	0.50
3:B:934:ALA:HB2	11:N:47:ARG:HD3	1.92	0.50
7:G:66:TYR:HB2	7:G:70:ASP:OD1	2.12	0.50
1:I:284:LEU:N	1:I:285:PRO:HD2	2.27	0.50
1:I:465:HIS:NE2	3:J:1028:PHE:HD1	2.10	0.50
1:I:507:TYR:O	1:I:508:LEU:CB	2.57	0.50
1:I:653:LEU:HD11	1:I:745:ALA:HB2	1.94	0.50
2:M:238:LYS:HB2	2:M:239:ARG:NH1	2.27	0.50
2:M:349:VAL:CG2	2:M:352:LYS:HB2	2.42	0.50
3:J:34:PHE:HE1	3:J:351:ALA:HA	1.75	0.50
3:J:497:VAL:HG12	3:J:498:GLU:N	2.25	0.50
3:J:557:HIS:CE1	3:J:566:VAL:HG13	2.47	0.50
3:J:560:THR:HG22	3:J:561:ASP:N	2.25	0.50
3:J:1069:TRP:CH2	3:J:1077:TYR:HB2	2.46	0.50
10:V:15:LEU:HB3	10:V:55:VAL:CG2	2.41	0.50
1:A:468:GLN:HB2	3:B:1047:ASP:OD2	2.12	0.50
1:A:502:TYR:CD2	3:B:734:MET:HE1	2.46	0.50
1:A:739:ASN:O	3:B:919:MET:HE3	2.12	0.50
2:C:122:MET:SD	2:C:256:SER:HA	2.52	0.50
3:B:1067:ILE:CG2	3:B:1080:PRO:HG2	2.41	0.50
5:E:29:GLU:O	5:E:33:GLN:HG3	2.11	0.50
7:G:40:PHE:HZ	7:G:115:THR:HG21	1.77	0.50
10:L:45:GLN:O	10:L:46:PRO:O	2.30	0.50
1:I:369:PRO:HA	1:I:410:HIS:HE1	1.77	0.50
1:I:547:THR:HG21	7:S:89:GLY:HA3	1.93	0.50
1:I:640:GLU:OE1	3:J:974:ARG:NH1	2.45	0.50
3:J:239:VAL:HA	3:J:253:PHE:CE2	2.46	0.50
3:J:473:MET:HA	3:J:577:ARG:NH2	2.27	0.50
3:J:738:ILE:HG23	3:J:888:ILE:HA	1.92	0.50
3:J:747:ARG:NH1	11:W:8:PHE:O	2.44	0.50
5:Q:168:TYR:O	5:Q:175:ILE:HD13	2.11	0.50
6:R:24:VAL:C	6:R:26:ARG:H	2.20	0.50
8:T:17:VAL:HG21	8:T:51:VAL:HG21	1.92	0.50
1:A:372:TRP:O	1:A:374:GLY:N	2.45	0.50
1:A:392:LYS:O	1:A:393:ASP:C	2.54	0.50
1:A:446:ASN:O	1:A:447:LEU:C	2.55	0.50
2:C:133:ASP:HB2	2:C:136:LYS:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:GLU:HG2	2:C:239:ARG:HA	1.94	0.50
3:B:125:SER:O	3:B:131:SER:HB2	2.12	0.50
3:B:171:ARG:HB3	3:B:524:GLY:HA3	1.94	0.50
3:B:298:LEU:C	3:B:300:HIS:N	2.70	0.50
3:B:497:VAL:HG12	3:B:498:GLU:N	2.26	0.50
3:B:560:THR:CG2	3:B:561:ASP:N	2.74	0.50
3:B:579:LEU:CD1	3:B:616:LEU:CD1	2.85	0.50
3:B:762:GLU:HG3	3:B:773:ILE:HG13	1.93	0.50
4:D:180:VAL:CG2	4:D:190:LEU:HG	2.42	0.50
8:H:45:ILE:N	8:H:79:ARG:HB3	2.27	0.50
1:I:532:ILE:HG22	10:V:58:LEU:HD22	1.93	0.50
1:I:532:ILE:HG13	10:V:12:TYR:OH	2.12	0.50
1:I:826:ALA:HB1	2:M:334:VAL:HG13	1.94	0.50
4:O:37:PRO:HA	4:O:148:GLY:O	2.12	0.50
5:Q:31:ARG:C	5:Q:33:GLN:N	2.68	0.50
1:A:4:LYS:HD2	3:B:1089:PHE:CB	2.42	0.50
1:A:188:PRO:O	1:A:192:VAL:HG23	2.12	0.50
2:C:393:ILE:HG22	2:C:394:LEU:H	1.76	0.50
3:B:214:PHE:CD1	3:B:215:PRO:HD2	2.47	0.50
3:B:221:ILE:HD13	3:B:221:ILE:N	2.26	0.50
3:B:345:LEU:HD12	3:B:345:LEU:N	2.27	0.50
3:B:432:SER:HB3	3:B:435:ARG:HH21	1.77	0.50
3:B:624:ALA:HB1	3:B:639:HIS:CD2	2.47	0.50
5:E:51:VAL:C	5:E:53:THR:H	2.19	0.50
8:H:25:ILE:HA	8:H:28:ALA:CB	2.42	0.50
9:K:26:ARG:HB3	9:K:27:LEU:HD12	1.94	0.50
1:I:58:CYS:CB	1:I:59:PRO:CD	2.89	0.50
1:I:220:ARG:HH11	1:I:236:THR:CG2	2.22	0.50
1:I:259:GLN:HA	1:I:262:ILE:HG22	1.94	0.50
2:M:135:ASP:C	2:M:137:ALA:H	2.20	0.50
2:M:168:GLN:HG2	2:M:204:SER:CB	2.42	0.50
2:M:276:ASN:O	2:M:279:GLU:HB3	2.12	0.50
3:J:348:ASP:OD2	3:J:348:ASP:N	2.45	0.50
3:J:740:MET:O	3:J:891:LEU:HA	2.11	0.50
3:J:769:GLN:O	3:J:770:GLU:HB3	2.11	0.50
4:O:191:LYS:HB2	4:O:194:LYS:HD2	1.94	0.50
5:Q:113:ILE:HG23	5:Q:114:THR:N	2.27	0.50
3:B:654:ILE:HG13	3:B:708:LEU:HD21	1.93	0.49
3:B:740:MET:O	3:B:891:LEU:HA	2.12	0.49
3:B:769:GLN:O	3:B:770:GLU:HB3	2.10	0.49
5:E:109:HIS:CD2	5:E:111:SER:H	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:N:4:PRO:HG2	11:N:48:MET:HE1	1.92	0.49
1:I:409:ARG:NH2	1:I:415:ASP:OD2	2.45	0.49
1:I:716:SER:CB	1:I:726:TYR:OH	2.60	0.49
2:M:386:VAL:HB	9:U:31:GLU:HG2	1.94	0.49
3:J:128:ASP:OD1	3:J:130:ILE:HB	2.12	0.49
3:J:544:ARG:HG3	3:J:544:ARG:NH1	2.17	0.49
4:O:35:TYR:O	4:O:149:TYR:HD2	1.95	0.49
4:O:125:SER:O	4:O:127:ASP:N	2.45	0.49
9:U:31:GLU:CD	9:U:78:ILE:HG21	2.37	0.49
1:A:86:LEU:HD22	1:A:207:MET:HE3	1.94	0.49
1:A:425:LEU:O	1:A:426:HIS:HB2	2.11	0.49
1:A:831:ARG:NH2	2:C:385:MET:HG3	2.27	0.49
2:C:126:LEU:HG	2:C:249:TYR:O	2.12	0.49
7:G:79:THR:CG2	7:G:80:GLU:H	2.25	0.49
1:I:417:VAL:HG13	1:I:464:LEU:HD13	1.94	0.49
2:M:238:LYS:HB2	2:M:239:ARG:CZ	2.42	0.49
3:J:314:TYR:HE2	3:J:526:LEU:N	2.02	0.49
3:J:475:GLN:HG2	3:J:476:ILE:H	1.77	0.49
1:A:206:TRP:C	1:A:208:ILE:H	2.20	0.49
1:A:283:GLY:C	1:A:285:PRO:HD2	2.37	0.49
1:A:325:VAL:O	1:A:442:THR:HB	2.11	0.49
2:C:122:MET:HG2	2:C:274:THR:HG23	1.95	0.49
3:B:655:ILE:HG12	3:B:669:GLN:HG2	1.94	0.49
1:I:353:ILE:CG1	1:I:361:LEU:HD23	2.39	0.49
2:M:357:ALA:O	2:M:362:ASP:HB2	2.13	0.49
3:J:759:SER:CB	3:J:862:VAL:O	2.42	0.49
3:J:904:VAL:HG21	11:W:42:ARG:HG2	1.94	0.49
4:O:257:GLU:O	4:O:260:LEU:HB3	2.12	0.49
10:V:21:ASP:OD1	10:V:22:HIS:N	2.45	0.49
1:A:6:ILE:HD11	3:B:1091:VAL:HG11	1.93	0.49
1:A:23:SER:HA	1:A:72:PHE:O	2.11	0.49
1:A:501:ASP:OD2	3:B:913:HIS:HD2	1.95	0.49
1:A:728:MET:CE	3:B:913:HIS:HA	2.41	0.49
2:C:179:VAL:HG23	2:C:182:ASP:H	1.77	0.49
3:B:338:TYR:CZ	3:B:341:LYS:NZ	2.81	0.49
3:B:430:ILE:HG22	3:B:431:SER:O	2.12	0.49
3:B:753:THR:HG23	3:B:868:ASP:H	1.77	0.49
3:B:764:LYS:NZ	3:B:772:LYS:O	2.45	0.49
1:I:48:ARG:HB2	1:I:59:PRO:HB3	1.93	0.49
1:I:331:ASN:ND2	3:J:732:TYR:OH	2.45	0.49
1:I:499:ALA:HB3	3:J:734:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:349:VAL:HG21	2:M:352:LYS:HB2	1.93	0.49
3:J:477:ALA:HB3	3:J:574:ARG:CG	2.42	0.49
7:S:31:MET:N	7:S:38:VAL:O	2.45	0.49
10:V:14:GLU:OE1	10:V:56:LYS:HG2	2.12	0.49
10:V:69:LEU:O	10:V:72:ALA:N	2.45	0.49
1:A:188:PRO:HD2	1:A:191:ASP:HB2	1.95	0.49
1:A:324:THR:CG2	1:A:325:VAL:H	2.21	0.49
1:A:337:VAL:HG12	1:A:339:VAL:HG23	1.95	0.49
1:A:449:VAL:O	1:A:449:VAL:HG12	2.12	0.49
2:C:327:ARG:HH21	2:C:337:GLU:HG3	1.77	0.49
3:B:551:ASP:OD2	3:B:551:ASP:N	2.44	0.49
3:B:588:LEU:HD22	3:B:612:LYS:HG2	1.95	0.49
3:B:965:ASP:O	3:B:967:THR:N	2.46	0.49
5:E:42:LEU:HD22	5:E:74:MET:HE1	1.94	0.49
11:N:38:LEU:HD23	11:N:39:GLY:N	2.27	0.49
1:I:239:LEU:CD2	1:I:276:TYR:HE1	2.24	0.49
1:I:319:ASP:HB2	3:J:1052:ASN:HB3	1.93	0.49
1:I:487:ILE:O	1:I:858:MET:HG3	2.13	0.49
1:I:506:ALA:HA	1:I:635:PHE:CD2	2.48	0.49
1:I:528:ALA:HB3	1:I:630:ASN:HD21	1.78	0.49
1:I:647:ARG:HB2	1:I:650:ASP:CG	2.37	0.49
2:M:39:LYS:O	2:M:43:VAL:HG23	2.12	0.49
2:M:75:ALA:O	2:M:79:GLY:N	2.29	0.49
2:M:322:ARG:C	2:M:324:GLY:H	2.21	0.49
2:M:376:GLY:HA3	3:J:1050:LEU:HD13	1.94	0.49
2:M:390:MET:HB3	2:M:392:PRO:HD3	1.95	0.49
3:J:325:LEU:HD12	3:J:328:GLY:HA2	1.95	0.49
3:J:677:LEU:HD21	3:J:994:HIS:HB3	1.94	0.49
3:J:790:ARG:HH22	12:X:39:LYS:HE3	1.77	0.49
3:J:790:ARG:NH2	12:X:39:LYS:HE3	2.27	0.49
3:J:927:GLY:HA2	3:J:987:VAL:O	2.12	0.49
3:J:969:VAL:HG21	4:O:205:LEU:HB3	1.95	0.49
4:O:169:LYS:HG2	4:O:222:VAL:HG22	1.94	0.49
11:W:7:CYS:CB	11:W:45:CYS:SG	3.01	0.49
1:A:86:LEU:HB3	1:A:207:MET:HE2	1.93	0.49
1:A:488:THR:HG23	1:A:490:ARG:H	1.77	0.49
1:A:826:ALA:HB1	2:C:334:VAL:HG13	1.94	0.49
2:C:120:PRO:HA	2:C:275:ASN:ND2	2.27	0.49
2:C:322:ARG:N	2:C:322:ARG:HD2	2.27	0.49
3:B:123:LEU:C	3:B:125:SER:H	2.20	0.49
3:B:520:VAL:HG12	3:B:527:ILE:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:881:ARG:NH1	3:B:989:TYR:CB	2.75	0.49
4:D:228:LEU:O	4:D:229:GLU:HG3	2.13	0.49
5:E:83:GLU:N	5:E:145:ARG:HG3	2.25	0.49
7:G:86:LEU:CD1	7:G:91:LYS:HG3	2.42	0.49
9:K:27:LEU:HD21	9:K:78:ILE:HD13	1.95	0.49
1:I:353:ILE:HA	1:I:357:ASN:HD21	1.77	0.49
1:I:372:TRP:O	1:I:374:GLY:N	2.45	0.49
3:J:789:TYR:O	3:J:791:LEU:N	2.45	0.49
3:J:797:VAL:CB	12:X:36:MET:HE1	2.40	0.49
3:J:855:THR:C	3:J:857:GLU:N	2.70	0.49
10:V:46:PRO:O	10:V:47:HIS:HB3	2.10	0.49
1:A:203:ARG:HG3	1:A:205:GLU:HB2	1.94	0.49
1:A:234:ASP:C	1:A:236:THR:H	2.19	0.49
1:A:575:CYS:CB	1:A:580:CYS:SG	3.01	0.49
1:A:607:GLN:HB2	1:A:608:PRO:CD	2.43	0.49
1:A:853:ASP:HB3	1:A:855:VAL:H	1.76	0.49
3:B:480:ILE:CG2	3:B:481:ASN:N	2.75	0.49
5:E:92:VAL:HG13	5:E:97:ILE:HG23	1.94	0.49
6:F:18:LYS:HZ3	6:F:45:GLU:HG2	1.77	0.49
8:H:12:ARG:HH22	8:H:55:ILE:HD12	1.77	0.49
8:H:72:TYR:C	8:H:74:GLU:H	2.21	0.49
2:M:72:ILE:H	2:M:72:ILE:CD1	2.24	0.49
2:M:314:LEU:O	2:M:315:LEU:C	2.53	0.49
3:J:533:GLY:C	3:J:535:GLU:H	2.19	0.49
3:J:574:ARG:O	3:J:574:ARG:HG3	2.12	0.49
4:O:176:CYS:H	4:O:195:LEU:CD2	2.26	0.49
1:A:308:ARG:HG3	1:A:312:ASN:HD22	1.78	0.49
2:C:237:ILE:CG1	2:C:238:LYS:H	2.25	0.49
3:B:727:MET:HE3	3:B:898:PRO:HG3	1.93	0.49
2:M:28:ILE:HG21	9:U:14:HIS:ND1	2.26	0.49
3:J:26:GLN:C	3:J:345:LEU:HD23	2.34	0.49
3:J:260:SER:C	3:J:262:ILE:H	2.20	0.49
3:J:578:PRO:HB3	3:J:615:TYR:CE1	2.47	0.49
3:J:910:LEU:CD2	3:J:911:ASN:N	2.73	0.49
3:J:950:ILE:C	3:J:952:GLN:N	2.70	0.49
8:T:42:LEU:HB2	8:T:43:PRO:CD	2.38	0.49
9:U:63:SER:HA	9:U:66:GLU:HG3	1.95	0.49
1:A:55:GLY:O	1:A:57:LYS:N	2.46	0.49
3:B:193:THR:HG21	3:B:197:ARG:N	2.28	0.49
4:D:169:LYS:HG2	4:D:222:VAL:HG22	1.94	0.49
5:E:82:GLN:H	5:E:146:VAL:HB	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:471:GLU:OE1	9:U:41:LEU:HD13	2.13	0.49
1:I:525:LEU:HA	1:I:527:VAL:HG23	1.94	0.49
1:I:527:VAL:HB	1:I:530:VAL:HB	1.95	0.49
1:I:728:MET:HE3	3:J:913:HIS:HA	1.94	0.49
3:J:853:THR:HG23	12:X:32:LYS:O	2.12	0.49
3:J:972:ASP:O	3:J:975:THR:HG23	2.13	0.49
3:J:975:THR:O	4:O:26:ASN:ND2	2.46	0.49
1:A:4:LYS:NZ	3:B:1115:LEU:HB3	2.27	0.49
1:A:486:ILE:HG12	1:A:496:ILE:HB	1.93	0.49
1:A:486:ILE:HG12	1:A:496:ILE:HD12	1.94	0.49
1:A:584:SER:OG	1:A:585:TYR:N	2.43	0.49
1:A:704:LEU:HD13	1:A:781:PHE:HD1	1.77	0.49
1:A:847:GLN:OE1	1:A:850:TYR:HA	2.12	0.49
1:A:868:VAL:O	1:A:871:ILE:HG22	2.12	0.49
7:G:8:GLU:O	7:G:9:ILE:HG13	2.12	0.49
7:G:30:ASN:C	7:G:31:MET:HG3	2.38	0.49
1:I:446:ASN:O	1:I:448:LEU:N	2.46	0.49
1:I:501:ASP:OD2	3:J:913:HIS:HD2	1.94	0.49
1:I:549:LYS:HB2	7:S:88:ASN:O	2.13	0.49
1:I:847:GLN:HE22	2:M:314:LEU:HB3	1.78	0.49
2:M:342:LEU:CD2	2:M:374:ILE:HG21	2.43	0.49
3:J:227:MET:CE	3:J:232:ILE:HG13	2.43	0.49
3:J:419:TRP:HZ3	3:J:712:GLY:HA3	1.77	0.49
3:J:644:SER:N	3:J:645:PRO:CD	2.76	0.49
3:J:965:ASP:C	3:J:967:THR:H	2.21	0.49
6:R:72:LEU:HD23	6:R:86:ILE:HD12	1.90	0.49
8:T:40:GLU:OE1	13:Z:66:LYS:NZ	2.46	0.49
1:A:16:PRO:HD3	1:A:206:TRP:CD1	2.48	0.48
1:A:353:ILE:HA	1:A:357:ASN:HD21	1.77	0.48
1:A:831:ARG:HH21	2:C:385:MET:HB2	1.77	0.48
2:C:312:HIS:O	2:C:316:ILE:HG12	2.13	0.48
2:C:390:MET:HG3	5:E:57:GLY:H	1.78	0.48
3:B:244:LEU:C	3:B:246:PRO:HD3	2.38	0.48
3:B:764:LYS:HZ3	3:B:814:VAL:H	1.59	0.48
3:B:958:LEU:HD21	4:D:181:ASN:O	2.13	0.48
3:B:971:TYR:CZ	4:D:165:ARG:HA	2.48	0.48
3:B:1061:CYS:HA	3:B:1088:LEU:HD23	1.95	0.48
4:D:108:MET:HE3	11:N:19:GLN:NE2	2.27	0.48
7:G:60:SER:O	7:G:112:PHE:HD1	1.96	0.48
1:I:8:GLY:HA2	2:M:365:GLU:HA	1.94	0.48
1:I:402:ALA:O	1:I:403:PRO:C	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:352:LYS:O	2:M:353:HIS:C	2.56	0.48
2:M:392:PRO:HG3	5:Q:68:HIS:CE1	2.47	0.48
3:J:325:LEU:O	3:J:326:TYR:C	2.56	0.48
7:S:69:ASP:OD2	7:S:69:ASP:N	2.45	0.48
1:A:78:VAL:HG23	1:A:266:TRP:HZ3	1.77	0.48
1:A:422:GLN:NE2	1:A:463:ASN:HD21	2.10	0.48
1:A:831:ARG:HH21	2:C:385:MET:CG	2.26	0.48
3:B:1004:ARG:NH1	3:B:1025:GLY:H	2.07	0.48
4:D:111:SER:O	4:D:114:ILE:HD13	2.13	0.48
1:I:145:VAL:O	1:I:145:VAL:HG22	2.12	0.48
1:I:337:VAL:HG23	1:I:433:HIS:ND1	2.28	0.48
1:I:528:ALA:C	1:I:530:VAL:H	2.21	0.48
1:I:543:ARG:HH11	1:I:545:TYR:HE1	1.61	0.48
1:I:739:ASN:O	3:J:919:MET:HE3	2.13	0.48
2:M:35:LEU:O	2:M:39:LYS:CG	2.61	0.48
2:M:313:ILE:HA	2:M:316:ILE:HG13	1.94	0.48
3:J:617:ASP:O	3:J:618:ALA:HB2	2.13	0.48
3:J:669:GLN:NE2	3:J:881:ARG:HA	2.28	0.48
7:S:64:PRO:C	7:S:114:ARG:HH11	2.21	0.48
1:A:124:ARG:HH21	13:Y:81:ARG:NH1	1.98	0.48
1:A:837:THR:HG22	1:A:838:VAL:N	2.28	0.48
2:C:146:TYR:HE1	2:C:237:ILE:HG12	1.76	0.48
2:C:390:MET:HB2	5:E:56:GLU:CG	2.43	0.48
3:B:482:GLU:O	3:B:483:ARG:C	2.56	0.48
3:B:840:ARG:NH1	3:B:1021:ALA:HB2	2.28	0.48
3:B:1069:TRP:HE1	3:B:1088:LEU:CB	2.25	0.48
10:L:80:THR:O	10:L:83:TYR:HB3	2.13	0.48
1:I:353:ILE:CD1	1:I:407:ILE:HG23	2.42	0.48
2:M:55:ALA:HA	2:M:58:GLU:CG	2.43	0.48
1:A:268:LEU:HD23	1:A:271:TYR:HD1	1.78	0.48
1:A:357:ASN:HD22	1:A:361:LEU:HD22	1.78	0.48
1:A:781:PHE:C	1:A:781:PHE:CD2	2.91	0.48
2:C:112:ASP:O	2:C:113:ALA:CB	2.60	0.48
3:B:34:PHE:HE1	3:B:351:ALA:HA	1.78	0.48
3:B:249:GLN:CG	3:B:250:ASN:H	2.23	0.48
3:B:446:HIS:O	3:B:447:GLY:C	2.56	0.48
3:B:475:GLN:HG2	3:B:476:ILE:H	1.78	0.48
3:B:741:ASN:OD1	3:B:741:ASN:C	2.56	0.48
6:F:69:ARG:HA	6:F:72:LEU:HD12	1.94	0.48
10:L:47:HIS:O	10:L:48:PRO:C	2.56	0.48
1:I:575:CYS:CB	1:I:580:CYS:SG	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:637:ARG:HH11	3:J:974:ARG:NH2	2.11	0.48
2:M:28:ILE:CG1	9:U:18:VAL:HG21	2.43	0.48
3:J:17:TYR:HH	3:J:474:ALA:HA	1.77	0.48
3:J:50:PRO:C	3:J:52:GLU:H	2.21	0.48
3:J:67:LYS:HB3	3:J:68:PRO:HD2	1.94	0.48
3:J:75:ARG:HE	3:J:75:ARG:N	2.11	0.48
3:J:191:SER:HB3	3:J:300:HIS:NE2	2.29	0.48
3:J:368:GLN:HE22	3:J:386:ARG:HH21	1.61	0.48
3:J:579:LEU:O	3:J:613:ILE:HG23	2.13	0.48
3:J:654:ILE:CG2	3:J:881:ARG:HG2	2.43	0.48
4:O:66:PRO:HG2	11:W:13:LEU:HD11	1.95	0.48
4:O:116:SER:OG	4:O:121:VAL:O	2.21	0.48
1:A:95:LYS:HB3	1:A:138:LYS:HG3	1.95	0.48
1:A:672:VAL:O	1:A:673:ASP:C	2.56	0.48
1:A:723:ASN:ND2	1:A:723:ASN:C	2.72	0.48
2:C:27:LYS:O	2:C:29:VAL:HG23	2.13	0.48
3:B:450:TRP:HZ3	3:B:621:GLU:OE2	1.97	0.48
3:B:680:TYR:HE1	3:B:687:ARG:HH12	1.60	0.48
4:D:257:GLU:O	4:D:260:LEU:HB3	2.13	0.48
9:K:28:THR:OG1	9:K:31:GLU:CG	2.58	0.48
11:N:33:LYS:HA	11:N:36:ASP:HB2	1.96	0.48
1:I:645:THR:OG1	1:I:646:MET:N	2.46	0.48
1:I:824:ILE:O	1:I:828:SER:HB3	2.13	0.48
3:J:551:ASP:OD2	3:J:551:ASP:N	2.47	0.48
3:J:555:VAL:HA	3:J:567:HIS:O	2.12	0.48
3:J:683:ASN:C	3:J:685:GLN:N	2.68	0.48
3:J:702:LEU:HD13	11:W:47:ARG:HD2	1.96	0.48
4:O:205:LEU:O	4:O:207:GLU:N	2.46	0.48
5:Q:38:ILE:O	5:Q:39:LEU:CB	2.61	0.48
7:S:59:ILE:O	7:S:59:ILE:HG22	2.13	0.48
8:T:18:PRO:HB2	8:T:67:ARG:HA	1.95	0.48
11:W:20:SER:O	11:W:24:ARG:HG3	2.14	0.48
1:A:57:LYS:HB3	1:A:62:GLY:HA2	1.94	0.48
1:A:512:LYS:N	1:A:583:ASP:OD2	2.46	0.48
3:B:106:ASN:O	3:B:108:GLU:HG3	2.12	0.48
3:B:644:SER:N	3:B:645:PRO:CD	2.76	0.48
3:B:657:TYR:HE2	3:B:946:TYR:CZ	2.30	0.48
3:B:1083:GLY:C	3:B:1085:LYS:H	2.22	0.48
4:D:240:ARG:O	4:D:244:GLU:HG2	2.13	0.48
5:E:163:THR:HG23	5:E:165:ARG:H	1.77	0.48
7:G:66:TYR:HD1	7:G:114:ARG:HH11	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:K:61:VAL:HG12	9:K:62:ILE:H	1.77	0.48
1:I:102:GLY:H	1:I:103:ARG:HE	1.60	0.48
1:I:116:ARG:O	1:I:130:ARG:NH2	2.46	0.48
1:I:428:ILE:HD11	1:I:485:ASN:HB3	1.95	0.48
2:M:270:ALA:HA	8:T:14:HIS:ND1	2.28	0.48
3:J:591:ILE:O	3:J:594:ILE:HG12	2.13	0.48
6:R:20:LEU:O	6:R:23:ASP:HB2	2.13	0.48
8:T:44:TRP:O	8:T:79:ARG:HD3	2.13	0.48
10:V:48:PRO:C	10:V:50:SER:H	2.21	0.48
1:A:61:CYS:SG	3:B:1070:TYR:CB	3.00	0.48
3:B:181:SER:O	3:B:182:ASN:HB2	2.13	0.48
3:B:473:MET:HA	3:B:577:ARG:NH2	2.29	0.48
4:D:178:LYS:O	4:D:180:VAL:N	2.46	0.48
6:F:46:LYS:HD3	6:F:76:CYS:HB2	1.96	0.48
2:M:246:GLY:O	2:M:247:ASP:C	2.57	0.48
3:J:102:PRO:HD2	3:J:109:ALA:HB3	1.95	0.48
3:J:1100:LEU:O	3:J:1101:ILE:C	2.56	0.48
4:O:131:VAL:HG22	4:O:132:LEU:H	1.79	0.48
1:A:533:ASP:O	1:A:534:LEU:C	2.56	0.48
1:A:826:ALA:HB2	2:C:335:THR:HG23	1.95	0.48
3:B:123:LEU:C	3:B:125:SER:N	2.71	0.48
3:B:191:SER:HB3	3:B:300:HIS:NE2	2.28	0.48
3:B:240:TYR:HD2	3:B:244:LEU:HD23	1.79	0.48
3:B:325:LEU:CD1	3:B:331:GLU:H	2.25	0.48
3:B:336:ASP:HA	3:B:341:LYS:HE3	1.94	0.48
3:B:540:ILE:HG21	3:B:555:VAL:HG21	1.94	0.48
12:P:17:GLN:C	12:P:19:LYS:H	2.19	0.48
1:I:57:LYS:HB3	1:I:62:GLY:HA2	1.95	0.48
3:J:139:ILE:HG21	11:W:61:HIS:HD2	1.79	0.48
3:J:291:GLN:C	3:J:293:ILE:N	2.71	0.48
3:J:330:ARG:HA	3:J:563:ILE:HD11	1.95	0.48
3:J:654:ILE:HG22	3:J:881:ARG:HG2	1.95	0.48
8:T:68:LYS:HA	8:T:74:GLU:HA	1.96	0.48
8:T:78:TYR:OH	9:U:12:ASP:HB3	2.14	0.48
1:A:99:ARG:HG2	1:A:183:ARG:NH1	2.29	0.48
1:A:116:ARG:O	1:A:130:ARG:NH2	2.47	0.48
2:C:322:ARG:HA	8:H:43:PRO:O	2.13	0.48
3:B:294:ASP:O	3:B:303:THR:HG23	2.13	0.48
3:B:550:SER:HB3	3:B:553:VAL:HG23	1.95	0.48
5:E:140:ASP:HB3	5:E:171:LYS:HG3	1.95	0.48
1:I:87:VAL:HG21	1:I:156:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:ARG:CZ	1:I:206:TRP:HB2	2.43	0.48
1:I:500:GLN:HB2	3:J:913:HIS:ND1	2.28	0.48
1:I:647:ARG:HB2	1:I:650:ASP:OD1	2.13	0.48
2:M:286:ILE:O	2:M:289:ALA:HB3	2.13	0.48
3:J:108:GLU:OE2	3:J:108:GLU:C	2.56	0.48
3:J:425:HIS:HA	3:J:428:ARG:HD3	1.96	0.48
3:J:848:ASP:CG	3:J:867:ARG:HH11	2.20	0.48
5:Q:39:LEU:HD23	5:Q:41:ASP:H	1.79	0.48
8:T:45:ILE:HB	8:T:79:ARG:HB3	1.96	0.48
1:A:831:ARG:HH21	2:C:385:MET:CB	2.27	0.48
2:C:179:VAL:CG2	2:C:232:LYS:HZ2	2.20	0.48
2:C:330:GLY:O	2:C:331:ARG:C	2.57	0.48
2:C:354:LEU:HD13	3:B:1104:LEU:CD2	2.43	0.48
3:B:361:PHE:C	3:B:361:PHE:CD2	2.92	0.48
3:B:480:ILE:HG22	3:B:481:ASN:H	1.77	0.48
3:B:1036:LEU:HD22	3:B:1041:THR:CG2	2.43	0.48
7:G:80:GLU:CG	7:G:81:LEU:N	2.77	0.48
1:I:93:PHE:HB3	1:I:184:LEU:CD2	2.44	0.48
1:I:354:THR:HB	1:I:355:PRO:CD	2.44	0.48
1:I:539:ILE:HB	1:I:545:TYR:HB2	1.94	0.48
2:M:103:GLY:CA	2:M:106:ARG:HB3	2.44	0.48
3:J:298:LEU:C	3:J:300:HIS:N	2.71	0.48
3:J:813:LYS:O	3:J:814:VAL:HG23	2.13	0.48
3:J:900:THR:OG1	3:J:904:VAL:HB	2.14	0.48
3:J:1029:GLY:O	3:J:1031:MET:N	2.47	0.48
4:D:55:ASP:HB3	12:P:45:VAL:HG21	1.96	0.47
8:H:80:TYR:CD1	8:H:81:VAL:O	2.67	0.47
10:L:35:ILE:O	10:L:36:SER:C	2.57	0.47
1:I:332:ILE:HA	1:I:436:ARG:HH12	1.78	0.47
1:I:353:ILE:HD11	1:I:407:ILE:CG2	2.45	0.47
3:J:86:ARG:HG3	3:J:153:ILE:HD13	1.96	0.47
3:J:520:VAL:HG12	3:J:527:ILE:HB	1.94	0.47
3:J:904:VAL:CG2	11:W:42:ARG:HG2	2.44	0.47
9:U:28:THR:OG1	9:U:31:GLU:HG3	2.15	0.47
1:A:194:ILE:H	1:A:194:ILE:HG13	1.34	0.47
1:A:199:PRO:O	1:A:200:THR:OG1	2.23	0.47
1:A:420:ASN:HB2	1:A:430:MET:HG2	1.96	0.47
1:A:524:ILE:O	1:A:525:LEU:HD22	2.14	0.47
3:B:634:THR:N	3:B:635:PRO:HD3	2.29	0.47
3:B:848:ASP:CG	3:B:867:ARG:HH11	2.22	0.47
5:E:96:GLY:HA2	5:E:110:ILE:HG12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:45:GLN:HE22	10:L:48:PRO:HD3	1.78	0.47
1:I:23:SER:HA	1:I:72:PHE:O	2.14	0.47
1:I:830:LEU:HD22	1:I:846:VAL:HG21	1.96	0.47
2:M:289:ALA:O	2:M:292:ILE:CG2	2.56	0.47
3:J:325:LEU:HA	3:J:329:ARG:H	1.79	0.47
3:J:443:ARG:NH2	3:J:462:PRO:O	2.47	0.47
3:J:727:MET:CE	3:J:898:PRO:CG	2.92	0.47
3:J:897:MET:HE2	3:J:897:MET:HA	1.95	0.47
3:J:904:VAL:HG21	11:W:42:ARG:HE	1.78	0.47
5:Q:12:ARG:HG3	5:Q:67:TYR:CZ	2.49	0.47
5:Q:38:ILE:O	5:Q:39:LEU:HB2	2.14	0.47
7:S:68:HIS:ND1	7:S:68:HIS:N	2.46	0.47
10:V:12:TYR:CD1	10:V:57:ILE:O	2.68	0.47
10:V:73:ILE:HG22	10:V:74:GLU:N	2.29	0.47
1:A:457:PHE:HB2	3:B:737:SER:HB2	1.96	0.47
1:A:490:ARG:HD3	2:C:77:SER:HA	1.97	0.47
1:A:529:ASP:CG	1:A:529:ASP:O	2.57	0.47
1:A:691:THR:O	1:A:695:SER:OG	2.30	0.47
2:C:15:GLU:O	2:C:18:LYS:N	2.47	0.47
2:C:376:GLY:HA3	3:B:1050:LEU:HD13	1.95	0.47
3:B:345:LEU:O	3:B:346:ALA:C	2.57	0.47
3:B:600:GLY:C	3:B:602:ILE:H	2.22	0.47
3:B:617:ASP:O	3:B:618:ALA:HB2	2.14	0.47
3:B:1113:LEU:HD12	3:B:1113:LEU:N	2.11	0.47
3:B:1117:ASP:O	3:B:1118:LYS:HB3	2.14	0.47
7:G:31:MET:HB2	7:G:38:VAL:O	2.14	0.47
9:K:50:LEU:O	9:K:51:ILE:C	2.56	0.47
11:N:42:ARG:HG3	11:N:43:TYR:H	1.80	0.47
1:I:104:VAL:HG12	1:I:137:LYS:HA	1.97	0.47
1:I:467:PRO:HA	3:J:1048:ARG:NH2	2.29	0.47
1:I:524:ILE:O	1:I:525:LEU:CD2	2.62	0.47
2:M:48:ILE:HG22	2:M:49:ASP:H	1.78	0.47
2:M:237:ILE:C	2:M:238:LYS:HG2	2.40	0.47
3:J:48:GLU:HG3	3:J:365:LEU:HD23	1.95	0.47
3:J:294:ASP:O	3:J:303:THR:HG23	2.14	0.47
3:J:813:LYS:N	3:J:836:SER:HB3	2.20	0.47
3:J:954:GLN:HA	3:J:957:ILE:HD11	1.95	0.47
4:O:131:VAL:CG2	4:O:132:LEU:N	2.78	0.47
4:O:240:ARG:O	4:O:244:GLU:HG2	2.14	0.47
1:A:99:ARG:HG2	1:A:183:ARG:HH12	1.79	0.47
1:A:105:LYS:HZ3	1:A:108:GLU:HB2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ALA:C	1:A:530:VAL:H	2.22	0.47
1:A:559:ASP:OD2	3:J:109:ALA:HA	2.15	0.47
1:A:750:GLN:CG	1:A:782:ILE:CD1	2.92	0.47
1:A:833:GLU:CG	1:A:839:ARG:HG3	2.44	0.47
2:C:31:ASP:C	2:C:33:LYS:N	2.71	0.47
3:B:9:GLU:O	3:B:10:ARG:C	2.58	0.47
3:B:855:THR:CB	3:B:857:GLU:HG2	2.31	0.47
5:E:72:PHE:HE1	5:E:74:MET:SD	2.37	0.47
10:L:3:ILE:HG13	10:L:17:ILE:HD13	1.96	0.47
11:N:3:ILE:HG22	11:N:4:PRO:CD	2.43	0.47
1:I:14:LEU:HB3	3:J:1108:ILE:HG23	1.96	0.47
1:I:541:ALA:CA	7:S:72:CYS:H	2.26	0.47
2:M:35:LEU:O	2:M:39:LYS:HG2	2.15	0.47
3:J:200:VAL:O	3:J:200:VAL:HG13	2.13	0.47
1:A:98:CYS:HB3	1:A:101:CYS:H	1.79	0.47
1:A:425:LEU:HD22	2:C:83:THR:HG21	1.96	0.47
2:C:123:THR:HG22	2:C:252:LEU:HD23	1.96	0.47
3:B:191:SER:HB3	3:B:300:HIS:CD2	2.49	0.47
3:B:232:ILE:HG23	3:B:237:ASP:HB3	1.94	0.47
3:B:377:ARG:O	3:B:378:LYS:HB2	2.13	0.47
3:B:902:LYS:HB3	11:N:42:ARG:CD	2.42	0.47
1:I:113:LYS:HA	1:I:116:ARG:HB3	1.95	0.47
1:I:490:ARG:NH1	2:M:80:GLU:HG3	2.29	0.47
1:I:723:ASN:ND2	1:I:723:ASN:C	2.72	0.47
2:M:15:GLU:HA	2:M:18:LYS:HE3	1.95	0.47
3:J:123:LEU:C	3:J:125:SER:N	2.72	0.47
3:J:289:ALA:O	3:J:293:ILE:CG1	2.62	0.47
3:J:320:SER:O	3:J:320:SER:OG	2.32	0.47
3:J:356:VAL:HG22	3:J:393:ARG:NH1	2.29	0.47
3:J:804:VAL:HG11	3:J:810:LEU:HD21	1.97	0.47
3:J:1054:ASP:HB2	3:J:1094:SER:HA	1.97	0.47
6:R:16:VAL:HG22	6:R:53:GLN:HE21	1.79	0.47
10:V:35:ILE:HD13	10:V:75:ASN:OD1	2.14	0.47
1:A:664:GLU:OE1	1:A:707:LEU:HD22	2.14	0.47
3:B:92:TYR:O	3:B:92:TYR:CD2	2.68	0.47
3:B:324:GLU:O	3:B:325:LEU:HB2	2.14	0.47
3:B:679:LEU:HD23	3:B:716:ARG:HG2	1.97	0.47
3:B:813:LYS:N	3:B:836:SER:HB3	2.25	0.47
3:B:881:ARG:NH1	3:B:989:TYR:HB3	2.22	0.47
3:B:958:LEU:C	3:B:958:LEU:HD23	2.39	0.47
4:D:176:CYS:H	4:D:195:LEU:CD2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:28:ILE:CG2	9:U:14:HIS:HE1	2.18	0.47
2:M:355:LEU:N	2:M:355:LEU:HD23	2.29	0.47
3:J:48:GLU:HG2	3:J:58:VAL:HB	1.95	0.47
3:J:1069:TRP:HE1	3:J:1088:LEU:CB	2.28	0.47
11:W:33:LYS:HA	11:W:36:ASP:HB2	1.96	0.47
1:A:99:ARG:HE	1:A:183:ARG:NH2	2.12	0.47
1:A:319:ASP:O	1:A:320:PHE:HB2	2.15	0.47
2:C:11:PRO:HB2	2:C:14:GLU:CD	2.40	0.47
2:C:271:LYS:O	2:C:272:VAL:C	2.57	0.47
2:C:393:ILE:H	2:C:393:ILE:HG13	1.56	0.47
3:B:54:PRO:O	3:B:56:LEU:N	2.48	0.47
3:B:557:HIS:N	3:B:623:ASN:ND2	2.53	0.47
3:B:594:ILE:HB	3:B:599:SER:HB2	1.97	0.47
3:B:663:SER:HB3	3:B:664:PRO:HD3	1.96	0.47
3:B:702:LEU:HD22	3:B:933:ALA:CB	2.32	0.47
3:B:898:PRO:HA	3:B:971:TYR:O	2.14	0.47
3:B:930:GLY:HA3	3:B:987:VAL:HB	1.97	0.47
3:B:972:ASP:HB3	3:B:975:THR:HG23	1.97	0.47
9:K:82:LEU:HD23	9:K:86:LYS:O	2.15	0.47
13:Y:65:LYS:C	13:Y:67:LEU:H	2.23	0.47
13:Y:65:LYS:C	13:Y:67:LEU:N	2.73	0.47
1:I:217:ILE:C	1:I:219:ILE:N	2.73	0.47
1:I:321:SER:O	1:I:322:SER:HB2	2.14	0.47
1:I:433:HIS:HE2	1:I:453:TYR:HH	1.57	0.47
1:I:438:LEU:HD12	10:V:47:HIS:NE2	2.30	0.47
1:I:500:GLN:HG2	3:J:734:MET:HE3	1.97	0.47
1:I:763:THR:HG23	1:I:779:ARG:HH12	1.80	0.47
3:J:64:ARG:H	3:J:97:TRP:HB2	1.80	0.47
3:J:291:GLN:HB3	3:J:295:LYS:CE	2.44	0.47
3:J:368:GLN:HE22	3:J:386:ARG:HE	1.62	0.47
3:J:463:ASN:HB3	3:J:467:VAL:CG1	2.44	0.47
3:J:971:TYR:CE2	4:O:165:ARG:HA	2.49	0.47
3:J:1087:ASN:C	3:J:1088:LEU:HG	2.39	0.47
4:O:108:MET:HE3	11:W:19:GLN:NE2	2.29	0.47
5:Q:128:PHE:HE2	5:Q:133:LYS:HD3	1.80	0.47
8:T:25:ILE:HA	8:T:28:ALA:HB3	1.97	0.47
8:T:42:LEU:HD13	8:T:79:ARG:O	2.14	0.47
11:W:35:LEU:HD22	11:W:40:VAL:HG21	1.97	0.47
12:X:12:THR:O	12:X:14:THR:N	2.37	0.47
1:A:349:VAL:HG21	1:A:415:ASP:OD2	2.15	0.47
1:A:727:VAL:O	1:A:729:ALA:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:130:ILE:HA	3:B:133:TYR:CE1	2.50	0.47
9:K:41:LEU:C	9:K:43:LEU:N	2.73	0.47
1:I:238:LYS:HZ3	1:I:276:TYR:HA	1.80	0.47
1:I:841:LEU:HB3	1:I:842:TYR:H	1.54	0.47
1:I:845:VAL:O	8:T:43:PRO:HD3	2.15	0.47
3:J:412:GLN:HG3	3:J:425:HIS:NE2	2.30	0.47
3:J:657:TYR:O	3:J:658:PRO:C	2.57	0.47
3:J:972:ASP:OD2	3:J:974:ARG:CG	2.59	0.47
4:O:94:THR:O	4:O:95:LYS:HG3	2.15	0.47
4:O:256:LEU:HD13	10:V:3:ILE:HD12	1.97	0.47
5:Q:179:LYS:HD3	6:R:81:ASP:HB2	1.97	0.47
10:V:46:PRO:HD2	10:V:52:LYS:O	2.15	0.47
1:A:763:THR:HG21	1:A:772:TYR:HA	1.97	0.47
3:B:96:LEU:O	3:B:115:TYR:HA	2.15	0.47
3:B:239:VAL:HA	3:B:253:PHE:CE2	2.48	0.47
3:B:946:TYR:CD2	3:B:947:LYS:N	2.82	0.47
9:K:42:GLN:O	9:K:45:MET:HB2	2.15	0.47
9:K:82:LEU:CD2	9:K:82:LEU:N	2.72	0.47
10:L:49:LEU:O	10:L:50:SER:HB3	2.15	0.47
1:I:568:VAL:HG21	1:I:597:VAL:HG11	1.96	0.47
1:I:612:LEU:HD23	1:I:612:LEU:C	2.39	0.47
3:J:401:GLY:O	3:J:402:ASN:O	2.32	0.47
3:J:902:LYS:CB	11:W:42:ARG:HH11	2.27	0.47
3:J:926:GLU:HB3	3:J:988:VAL:CG2	2.43	0.47
5:Q:110:ILE:CG2	5:Q:118:LEU:HB3	2.45	0.47
7:S:41:ASP:HB2	7:S:91:LYS:H	1.80	0.47
12:X:28:TYR:O	12:X:29:CYS:C	2.57	0.47
1:A:8:GLY:HA2	2:C:365:GLU:HA	1.96	0.47
1:A:524:ILE:O	1:A:525:LEU:CD2	2.63	0.47
1:A:870:ARG:NH2	2:C:57:LYS:O	2.48	0.47
2:C:189:GLY:O	2:C:190:ARG:HB2	2.15	0.47
3:B:98:LEU:HD11	3:B:100:MET:CG	2.38	0.47
3:B:298:LEU:O	3:B:300:HIS:N	2.48	0.47
3:B:391:THR:O	3:B:394:ILE:HG22	2.15	0.47
3:B:437:GLN:OE1	3:B:438:PRO:HD2	2.15	0.47
3:B:574:ARG:O	3:B:574:ARG:HG3	2.14	0.47
3:B:677:LEU:HD21	3:B:994:HIS:HB3	1.97	0.47
3:B:781:ARG:HB2	3:B:831:ALA:N	2.30	0.47
4:D:37:PRO:HA	4:D:148:GLY:O	2.14	0.47
5:E:13:ILE:HG23	5:E:25:ILE:HG21	1.97	0.47
5:E:18:PHE:CD2	9:K:47:ALA:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:15:ILE:HG22	7:G:51:GLN:O	2.15	0.47
1:I:85:GLY:HA3	2:M:355:LEU:HD12	1.96	0.47
1:I:234:ASP:C	1:I:236:THR:H	2.22	0.47
1:I:595:GLU:HB2	7:S:91:LYS:CE	2.45	0.47
1:I:833:GLU:CG	1:I:839:ARG:HG3	2.45	0.47
3:J:633:LEU:C	3:J:635:PRO:CD	2.88	0.47
3:J:930:GLY:O	11:W:47:ARG:NH1	2.48	0.47
3:J:1012:LEU:O	3:J:1095:TYR:CE2	2.64	0.47
3:J:1085:LYS:O	3:J:1086:SER:OG	2.30	0.47
11:W:10:CYS:HB3	11:W:44:CYS:SG	2.55	0.47
1:A:16:PRO:HD3	1:A:206:TRP:HD1	1.80	0.46
1:A:594:LEU:O	1:A:595:GLU:HG2	2.15	0.46
3:B:797:VAL:CB	12:P:36:MET:HE1	2.45	0.46
3:B:921:LEU:O	3:B:923:GLN:N	2.46	0.46
3:B:963:LEU:HD22	3:B:982:ARG:NH2	2.30	0.46
4:D:45:TYR:HB2	4:D:142:GLU:O	2.15	0.46
11:N:38:LEU:HD23	11:N:39:GLY:H	1.80	0.46
1:I:87:VAL:O	1:I:91:TYR:HB2	2.15	0.46
1:I:874:ARG:HE	2:M:53:ASP:HB3	1.79	0.46
3:J:418:ASN:ND2	3:J:418:ASN:C	2.73	0.46
3:J:840:ARG:NH1	3:J:1021:ALA:HB2	2.29	0.46
3:J:946:TYR:CD2	3:J:947:LYS:N	2.83	0.46
4:O:53:LEU:HD22	4:O:57:ILE:CG2	2.44	0.46
9:U:63:SER:C	9:U:65:ALA:H	2.22	0.46
10:V:60:ASP:C	10:V:62:SER:H	2.22	0.46
12:X:25:ARG:HD2	12:X:30:GLY:HA2	1.96	0.46
1:A:457:PHE:C	1:A:459:GLY:H	2.21	0.46
2:C:152:VAL:O	2:C:152:VAL:HG22	2.14	0.46
2:C:163:MET:N	2:C:164:SER:HA	2.28	0.46
2:C:337:GLU:OE1	2:C:337:GLU:N	2.47	0.46
3:B:88:ARG:HG2	12:P:33:ILE:HD11	1.97	0.46
4:D:134:GLY:O	4:D:135:THR:O	2.33	0.46
4:D:144:ARG:C	4:D:145:LEU:HD12	2.41	0.46
5:E:113:ILE:HG23	5:E:114:THR:N	2.30	0.46
1:I:428:ILE:HG23	1:I:452:PRO:HB2	1.96	0.46
1:I:537:PRO:O	7:S:74:HIS:NE2	2.47	0.46
2:M:140:VAL:O	2:M:143:LYS:HB2	2.16	0.46
2:M:287:GLU:OE2	8:T:79:ARG:CZ	2.63	0.46
2:M:318:ASP:O	2:M:322:ARG:HD2	2.15	0.46
3:J:249:GLN:CG	3:J:250:ASN:H	2.24	0.46
3:J:582:VAL:HG11	3:J:633:LEU:HD11	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:669:GLN:C	3:J:671:ALA:H	2.23	0.46
3:J:881:ARG:CD	3:J:989:TYR:HD2	2.27	0.46
3:J:1067:ILE:CG2	3:J:1080:PRO:HG2	2.45	0.46
1:A:759:ARG:NH2	1:A:763:THR:OG1	2.48	0.46
3:B:227:MET:CE	3:B:232:ILE:HG13	2.46	0.46
3:B:698:PRO:HG2	11:N:55:ILE:HD12	1.96	0.46
3:B:953:LEU:O	3:B:957:ILE:HG12	2.14	0.46
4:D:53:LEU:HD22	4:D:57:ILE:HG21	1.97	0.46
4:D:137:GLN:NE2	11:N:63:THR:HG22	2.30	0.46
4:D:170:VAL:HG23	4:D:200:GLU:HG3	1.96	0.46
4:D:254:GLU:HG2	10:L:77:ARG:NH1	2.31	0.46
2:M:295:ARG:O	2:M:299:LYS:HB2	2.16	0.46
3:J:170:ASN:O	3:J:171:ARG:O	2.34	0.46
3:J:191:SER:HB3	3:J:300:HIS:CD2	2.51	0.46
3:J:873:THR:CG2	3:J:874:ILE:H	2.26	0.46
3:J:1010:GLN:HA	3:J:1010:GLN:OE1	2.15	0.46
4:O:64:LEU:O	11:W:6:ARG:HD2	2.15	0.46
4:O:206:CYS:O	4:O:207:GLU:HB2	2.15	0.46
9:U:70:ARG:CZ	9:U:70:ARG:HB3	2.46	0.46
1:A:9:ILE:O	2:C:363:VAL:O	2.33	0.46
1:A:425:LEU:HD12	1:A:425:LEU:H	1.80	0.46
1:A:672:VAL:HG11	1:A:776:PRO:HD3	1.98	0.46
1:A:781:PHE:C	1:A:781:PHE:HD2	2.23	0.46
2:C:68:GLU:HB3	9:K:30:TYR:CZ	2.50	0.46
2:C:321:THR:O	2:C:321:THR:CG2	2.63	0.46
2:C:390:MET:O	2:C:391:ARG:HD2	2.15	0.46
3:B:473:MET:HE1	3:B:475:GLN:O	2.16	0.46
4:D:29:ARG:HG3	4:D:162:SER:O	2.16	0.46
2:M:268:ASP:OD1	2:M:270:ALA:HB3	2.15	0.46
2:M:341:VAL:HG11	2:M:357:ALA:HB1	1.97	0.46
3:J:116:ILE:HG23	3:J:361:PHE:CZ	2.50	0.46
3:J:170:ASN:HB3	3:J:300:HIS:HE1	1.80	0.46
3:J:248:VAL:HG21	3:J:329:ARG:HH22	1.80	0.46
3:J:569:ASN:HB3	3:J:574:ARG:CZ	2.45	0.46
3:J:764:LYS:HZ2	3:J:772:LYS:C	2.23	0.46
4:O:208:GLU:N	16:O:1001:F3S:S2	2.88	0.46
1:A:599:ASP:H	1:A:602:ALA:HB3	1.80	0.46
1:A:830:LEU:HD23	1:A:840:SER:CB	2.34	0.46
2:C:72:ILE:HG23	2:C:76:GLN:OE1	2.15	0.46
3:B:54:PRO:O	3:B:55:GLY:C	2.58	0.46
3:B:256:LEU:C	3:B:258:GLN:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:633:LEU:C	3:B:635:PRO:CD	2.89	0.46
3:B:721:ASN:HB3	11:N:47:ARG:HE	1.80	0.46
3:B:870:ARG:NE	3:B:996:MET:SD	2.88	0.46
3:B:910:LEU:CD2	3:B:911:ASN:H	2.25	0.46
3:B:937:GLY:HA3	11:N:32:GLY:CA	2.46	0.46
3:B:1077:TYR:O	3:B:1077:TYR:CD1	2.69	0.46
13:Y:57:GLY:HA2	13:Y:61:LEU:HD21	1.97	0.46
1:I:58:CYS:HB2	1:I:59:PRO:CD	2.39	0.46
1:I:433:HIS:NE2	1:I:453:TYR:OH	2.43	0.46
1:I:486:ILE:HG12	1:I:496:ILE:HD12	1.97	0.46
1:I:631:LEU:O	1:I:634:VAL:HB	2.15	0.46
2:M:231:ILE:HD12	2:M:231:ILE:H	1.81	0.46
3:J:162:VAL:HG11	3:J:412:GLN:HE21	1.80	0.46
3:J:343:LEU:HD22	3:J:575:VAL:HG22	1.98	0.46
3:J:603:THR:C	3:J:605:ASP:N	2.73	0.46
3:J:723:ILE:HG12	3:J:907:ASP:OD2	2.16	0.46
3:J:848:ASP:HB2	3:J:867:ARG:HB2	1.98	0.46
5:Q:79:PRO:HG3	5:Q:160:ILE:HG12	1.98	0.46
1:A:764:ARG:HH11	1:A:764:ARG:HB2	1.80	0.46
2:C:391:ARG:HB2	9:K:75:PRO:HB2	1.96	0.46
3:B:330:ARG:NH2	3:B:565:GLU:OE1	2.48	0.46
3:B:402:ASN:HB2	3:B:410:VAL:HB	1.97	0.46
3:B:640:LEU:CD2	3:B:641:GLU:N	2.67	0.46
3:B:992:LYS:HE3	3:B:996:MET:SD	2.55	0.46
4:D:254:GLU:HG2	10:L:77:ARG:HH12	1.80	0.46
5:E:39:LEU:HD12	5:E:42:LEU:HG	1.96	0.46
9:K:86:LYS:HD2	9:K:86:LYS:H	1.81	0.46
10:L:61:GLY:O	10:L:62:SER:C	2.58	0.46
1:I:13:ILE:HG13	1:I:207:MET:HG2	1.97	0.46
1:I:187:ILE:HA	1:I:188:PRO:HD3	1.70	0.46
1:I:316:LYS:HD2	3:J:1049:LEU:O	2.15	0.46
2:M:48:ILE:HG22	2:M:49:ASP:N	2.31	0.46
2:M:86:THR:HA	2:M:104:LEU:CD1	2.42	0.46
3:J:11:TRP:O	3:J:14:ILE:HG22	2.16	0.46
3:J:24:VAL:HG21	3:J:426:LEU:CD1	2.46	0.46
3:J:154:VAL:O	3:J:155:ASN:C	2.59	0.46
3:J:158:GLU:OE2	3:J:416:ARG:NH1	2.45	0.46
3:J:214:PHE:CD1	3:J:215:PRO:HD2	2.51	0.46
3:J:663:SER:CB	3:J:664:PRO:HD3	2.46	0.46
3:J:781:ARG:CD	3:J:782:GLY:H	2.26	0.46
3:J:971:TYR:CZ	3:J:978:LYS:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:252:LYS:HD2	10:V:24:LEU:HD23	1.97	0.46
6:R:59:LEU:HD22	6:R:69:ARG:HD3	1.97	0.46
8:T:45:ILE:HG22	8:T:81:VAL:H	1.79	0.46
9:U:61:VAL:C	9:U:62:ILE:HG12	2.41	0.46
2:C:51:ILE:H	2:C:51:ILE:HG13	1.34	0.46
2:C:269:VAL:O	8:H:14:HIS:HB3	2.15	0.46
3:B:133:TYR:HD2	3:B:137:LYS:HB3	1.80	0.46
3:B:291:GLN:C	3:B:293:ILE:N	2.74	0.46
3:B:848:ASP:HB2	3:B:867:ARG:HB2	1.97	0.46
4:D:178:LYS:O	4:D:179:ALA:C	2.59	0.46
5:E:142:VAL:HA	5:E:171:LYS:HA	1.98	0.46
6:F:18:LYS:NZ	6:F:45:GLU:HG2	2.29	0.46
13:Y:51:TRP:CD1	13:Y:51:TRP:H	2.33	0.46
1:I:374:GLY:C	1:I:410:HIS:ND1	2.74	0.46
3:J:586:ASN:HA	3:J:587:PRO:HD3	1.82	0.46
3:J:587:PRO:C	3:J:588:LEU:HG	2.40	0.46
3:J:691:ARG:NH1	3:J:756:ARG:NH2	2.64	0.46
3:J:707:ALA:C	3:J:709:ASP:N	2.73	0.46
3:J:855:THR:CB	3:J:857:GLU:HG2	2.34	0.46
8:T:46:ARG:HD3	8:T:48:SER:H	1.80	0.46
9:U:39:ARG:HG3	9:U:39:ARG:O	2.16	0.46
1:A:141:MET:HE3	1:A:148:HIS:HB3	1.97	0.46
1:A:145:VAL:O	1:A:145:VAL:HG22	2.16	0.46
2:C:28:ILE:HG23	2:C:30:ASP:CG	2.41	0.46
3:B:289:ALA:O	3:B:293:ILE:CG1	2.64	0.46
3:B:655:ILE:HG23	3:B:881:ARG:O	2.16	0.46
5:E:115:ASP:O	5:E:116:ASP:HB2	2.16	0.46
11:N:20:SER:O	11:N:24:ARG:HG3	2.16	0.46
1:I:371:LYS:HZ3	1:I:373:PRO:HD3	1.80	0.46
1:I:495:ILE:O	1:I:495:ILE:HG13	2.16	0.46
2:M:12:TYR:C	2:M:13:LEU:HG	2.41	0.46
3:J:751:ARG:HG2	3:J:871:ILE:HG23	1.97	0.46
3:J:762:GLU:HG3	3:J:773:ILE:HG13	1.96	0.46
4:O:80:GLU:HA	4:O:83:ILE:HD12	1.97	0.46
5:Q:43:GLY:CA	5:Q:78:VAL:HG23	2.46	0.46
10:V:9:GLU:O	10:V:11:ASN:N	2.49	0.46
2:C:281:GLU:OE1	2:C:326:VAL:HG12	2.15	0.46
3:B:248:VAL:HG21	3:B:329:ARG:HH22	1.80	0.46
3:B:440:PHE:C	3:B:442:ALA:H	2.23	0.46
5:E:124:ARG:HG3	5:E:126:ILE:CG1	2.46	0.46
7:G:9:ILE:HD13	7:G:104:LYS:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:SER:HA	7:G:92:TYR:O	2.16	0.46
10:L:47:HIS:O	10:L:49:LEU:N	2.49	0.46
13:Y:71:ASN:O	13:Y:74:GLU:HB2	2.15	0.46
1:I:445:LEU:HD21	1:I:450:CYS:HA	1.97	0.46
2:M:173:MET:HE3	2:M:177:LYS:HZ1	1.80	0.46
3:J:325:LEU:HD21	3:J:332:PRO:HD3	1.97	0.46
3:J:402:ASN:HB2	3:J:410:VAL:HB	1.98	0.46
4:O:111:SER:C	4:O:114:ILE:HD13	2.41	0.46
4:O:131:VAL:CG2	4:O:132:LEU:H	2.29	0.46
7:S:103:VAL:O	7:S:103:VAL:HG13	2.16	0.46
8:T:80:TYR:O	8:T:81:VAL:HG23	2.16	0.46
9:U:82:LEU:HB3	9:U:83:PRO:HD2	1.97	0.46
1:A:329:ASP:CB	1:A:332:ILE:HD12	2.45	0.46
1:A:487:ILE:O	1:A:858:MET:HG3	2.15	0.46
1:A:532:ILE:HG23	10:L:40:PHE:CD2	2.51	0.46
3:B:48:GLU:HG3	3:B:365:LEU:HD23	1.97	0.46
3:B:170:ASN:O	3:B:171:ARG:O	2.34	0.46
3:B:174:VAL:HG12	3:B:175:ASP:N	2.31	0.46
3:B:533:GLY:C	3:B:535:GLU:H	2.23	0.46
3:B:638:THR:HB	3:B:639:HIS:HD2	1.68	0.46
3:B:895:VAL:HG11	4:D:34:LEU:CD2	2.46	0.46
4:D:133:LEU:HD22	4:D:137:GLN:HB3	1.98	0.46
12:P:26:CYS:CB	12:P:27:PRO:HD2	2.30	0.46
12:P:33:ILE:O	12:P:34:ILE:C	2.59	0.46
1:I:209:LEU:HD11	1:I:277:PHE:HE2	1.80	0.46
1:I:475:GLU:OE2	3:J:1043:MET:HB2	2.16	0.46
3:J:81:SER:OG	3:J:141:ILE:CG2	2.64	0.46
3:J:658:PRO:O	3:J:660:HIS:N	2.44	0.46
3:J:661:ASN:ND2	3:J:921:LEU:O	2.48	0.46
3:J:738:ILE:HD12	3:J:739:ILE:H	1.81	0.46
3:J:1029:GLY:O	3:J:1030:GLU:C	2.59	0.46
9:U:43:LEU:C	9:U:45:MET:N	2.73	0.46
9:U:50:LEU:H	9:U:50:LEU:HD12	1.79	0.46
12:X:9:CYS:HB3	12:X:12:THR:O	2.16	0.46
1:A:45:MET:O	1:A:47:PRO:HD3	2.15	0.45
1:A:199:PRO:C	1:A:201:THR:H	2.24	0.45
1:A:553:SER:OG	1:A:592:ILE:HA	2.15	0.45
3:B:23:LEU:HB3	3:B:24:VAL:H	1.52	0.45
3:B:96:LEU:HB2	3:B:117:GLY:H	1.80	0.45
3:B:200:VAL:O	3:B:200:VAL:CG1	2.64	0.45
3:B:419:TRP:HZ3	3:B:712:GLY:C	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:422:MET:HE2	3:B:422:MET:HB3	1.77	0.45
3:B:557:HIS:CE1	3:B:566:VAL:HG13	2.52	0.45
3:B:657:TYR:O	3:B:658:PRO:C	2.56	0.45
3:B:881:ARG:CD	3:B:989:TYR:HD2	2.27	0.45
3:B:1054:ASP:HB2	3:B:1094:SER:HA	1.98	0.45
4:D:191:LYS:HB2	4:D:194:LYS:HD2	1.97	0.45
6:F:14:TYR:O	6:F:18:LYS:HE3	2.16	0.45
7:G:80:GLU:C	7:G:81:LEU:HD12	2.41	0.45
7:G:94:THR:HG21	7:G:101:LEU:HD11	1.98	0.45
9:K:82:LEU:HD21	9:K:88:ILE:HG12	1.98	0.45
10:L:82:HIS:O	10:L:86:GLU:N	2.48	0.45
11:N:6:ARG:HA	11:N:12:SER:O	2.15	0.45
1:I:105:LYS:HZ3	1:I:108:GLU:HB2	1.79	0.45
1:I:181:ARG:HG3	1:I:208:ILE:HB	1.98	0.45
1:I:434:ARG:HE	1:I:434:ARG:HB3	1.40	0.45
1:I:722:PHE:CZ	7:S:23:LEU:HG	2.45	0.45
2:M:31:ASP:C	2:M:33:LYS:N	2.72	0.45
2:M:322:ARG:HD2	2:M:322:ARG:N	2.32	0.45
3:J:123:LEU:C	3:J:125:SER:H	2.24	0.45
3:J:338:TYR:CZ	3:J:341:LYS:NZ	2.84	0.45
3:J:422:MET:HE2	3:J:422:MET:HB3	1.83	0.45
3:J:430:ILE:HG22	3:J:431:SER:O	2.16	0.45
3:J:437:GLN:OE1	3:J:438:PRO:HD2	2.17	0.45
3:J:1004:ARG:NH1	3:J:1016:PRO:HB3	2.30	0.45
1:A:217:ILE:C	1:A:219:ILE:H	2.24	0.45
1:A:342:ILE:O	1:A:345:LYS:N	2.49	0.45
2:C:339:ASN:OD1	2:C:339:ASN:N	2.32	0.45
3:B:472:LEU:HD12	3:B:646:ALA:HA	1.99	0.45
3:B:570:CYS:HB3	3:B:571:ASP:H	1.59	0.45
3:B:587:PRO:C	3:B:588:LEU:HG	2.40	0.45
3:B:633:LEU:HD13	3:B:640:LEU:HG	1.99	0.45
8:H:69:SER:HB2	8:H:75:VAL:CG2	2.46	0.45
9:K:50:LEU:CD2	9:K:74:LEU:HA	2.36	0.45
13:Y:57:GLY:HA2	13:Y:61:LEU:CD2	2.46	0.45
1:I:518:LYS:H	1:I:518:LYS:HG2	1.61	0.45
1:I:618:GLU:O	1:I:619:TYR:CG	2.69	0.45
1:I:708:ARG:O	1:I:711:ALA:HB3	2.17	0.45
2:M:70:ILE:HA	2:M:73:VAL:HG22	1.97	0.45
2:M:290:ARG:HG3	2:M:321:THR:HG21	1.98	0.45
3:J:110:GLU:HA	3:J:111:PRO:HA	1.51	0.45
3:J:246:PRO:O	3:J:248:VAL:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:419:TRP:HZ3	3:J:712:GLY:C	2.24	0.45
3:J:672:MET:CG	3:J:993:LEU:HD21	2.27	0.45
3:J:925:MET:HE3	3:J:950:ILE:HG12	1.99	0.45
3:J:983:ILE:HG22	3:J:984:TYR:O	2.17	0.45
3:J:1036:LEU:HD22	3:J:1041:THR:HG21	1.98	0.45
9:U:61:VAL:O	9:U:63:SER:N	2.42	0.45
11:W:35:LEU:HD22	11:W:46:ARG:HG3	1.99	0.45
2:C:49:ASP:CG	3:J:382:LYS:HE2	2.41	0.45
3:B:691:ARG:NH1	3:B:756:ARG:NH2	2.65	0.45
3:B:950:ILE:C	3:B:952:GLN:H	2.24	0.45
7:G:75:GLY:HA3	7:G:86:LEU:O	2.16	0.45
10:L:7:LYS:HE3	10:L:12:TYR:CE2	2.48	0.45
3:J:123:LEU:O	3:J:125:SER:N	2.49	0.45
3:J:125:SER:O	3:J:126:ALA:C	2.59	0.45
3:J:182:ASN:HD22	3:J:182:ASN:N	2.14	0.45
3:J:264:ASN:H	3:J:267:ASP:HB2	1.81	0.45
3:J:346:ALA:O	3:J:350:PHE:HB2	2.16	0.45
3:J:921:LEU:O	3:J:923:GLN:N	2.48	0.45
5:Q:27:LEU:HD21	5:Q:31:ARG:NH2	2.31	0.45
7:S:66:TYR:N	7:S:66:TYR:CD1	2.83	0.45
1:A:71:HIS:ND1	3:B:1070:TYR:CE2	2.82	0.45
1:A:805:GLY:C	1:A:807:VAL:H	2.24	0.45
5:E:44:LEU:C	5:E:44:LEU:HD12	2.41	0.45
9:K:30:TYR:N	9:K:30:TYR:CD1	2.85	0.45
12:P:37:VAL:HG22	12:P:38:ARG:N	2.31	0.45
1:I:346:THR:HG21	3:J:1003:ALA:HB1	1.97	0.45
1:I:371:LYS:HZ2	1:I:373:PRO:HD3	1.81	0.45
1:I:839:ARG:NH1	8:T:37:ILE:CG2	2.78	0.45
3:J:96:LEU:HD21	3:J:119:LEU:HB2	1.98	0.45
3:J:256:LEU:C	3:J:258:GLN:H	2.24	0.45
3:J:343:LEU:HB2	3:J:476:ILE:HG21	1.99	0.45
3:J:544:ARG:HB2	3:J:549:ILE:HG22	1.99	0.45
3:J:633:LEU:HD13	3:J:640:LEU:HG	1.98	0.45
3:J:644:SER:C	3:J:646:ALA:N	2.74	0.45
3:J:685:GLN:HE22	3:J:867:ARG:HH22	1.64	0.45
3:J:894:GLN:HE21	4:O:33:MET:HE2	1.80	0.45
7:S:86:LEU:HG	7:S:87:ASN:N	2.31	0.45
1:A:93:PHE:HB3	1:A:184:LEU:CD2	2.46	0.45
1:A:525:LEU:HA	1:A:527:VAL:HG23	1.97	0.45
2:C:359:ALA:O	2:C:361:GLY:N	2.49	0.45
3:B:215:PRO:O	3:B:216:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:314:TYR:HE2	3:B:526:LEU:N	2.02	0.45
3:B:544:ARG:NH2	3:B:620:GLU:OE2	2.50	0.45
3:B:661:ASN:ND2	3:B:921:LEU:O	2.48	0.45
3:B:702:LEU:HB2	3:B:721:ASN:ND2	2.32	0.45
4:D:53:LEU:HD11	11:N:2:LEU:HD12	1.98	0.45
1:I:155:LYS:HA	1:I:156:ILE:O	2.17	0.45
1:I:486:ILE:HA	1:I:496:ILE:HD12	1.99	0.45
1:I:759:ARG:HE	1:I:759:ARG:HB3	1.57	0.45
3:J:133:TYR:HD2	3:J:137:LYS:HB3	1.81	0.45
3:J:361:PHE:C	3:J:361:PHE:CD2	2.95	0.45
3:J:691:ARG:NH1	3:J:756:ARG:HH21	2.15	0.45
13:Z:61:LEU:O	13:Z:65:LYS:HB2	2.16	0.45
1:A:527:VAL:HB	1:A:530:VAL:HB	1.98	0.45
1:A:634:VAL:O	1:A:635:PHE:C	2.60	0.45
3:B:98:LEU:CD1	3:B:100:MET:HG3	2.37	0.45
3:B:554:ASN:ND2	3:B:576:ARG:HH21	2.11	0.45
3:B:569:ASN:HB3	3:B:574:ARG:NH1	2.29	0.45
3:B:669:GLN:C	3:B:671:ALA:H	2.25	0.45
3:B:803:GLU:HB3	3:B:805:LYS:HZ2	1.80	0.45
3:B:930:GLY:CA	11:N:47:ARG:HH22	2.29	0.45
4:D:34:LEU:HD22	4:D:151:LYS:HB2	1.99	0.45
8:H:13:ILE:HG23	8:H:14:HIS:CE1	2.51	0.45
13:Y:69:GLU:O	13:Y:70:ASP:C	2.60	0.45
1:I:16:PRO:HD3	1:I:206:TRP:CD1	2.52	0.45
1:I:279:ASN:ND2	1:I:295:LEU:O	2.49	0.45
1:I:512:LYS:N	1:I:583:ASP:OD2	2.50	0.45
1:I:672:VAL:O	1:I:673:ASP:C	2.60	0.45
3:J:381:LEU:C	3:J:383:ALA:N	2.75	0.45
3:J:768:GLY:O	3:J:769:GLN:HB2	2.15	0.45
4:O:11:THR:HG22	4:O:232:SER:HB3	1.98	0.45
5:Q:15:PRO:HG3	5:Q:64:GLY:O	2.15	0.45
5:Q:63:ASP:C	5:Q:65:ALA:H	2.24	0.45
5:Q:101:LEU:HD21	5:Q:162:LEU:HD11	1.99	0.45
10:V:84:ILE:O	10:V:87:ILE:HG22	2.17	0.45
1:A:5:ASN:O	3:B:1116:GLU:N	2.50	0.45
1:A:354:THR:HB	1:A:355:PRO:CD	2.46	0.45
1:A:732:GLY:O	1:A:733:ALA:C	2.60	0.45
1:A:866:VAL:O	1:A:867:ASP:C	2.60	0.45
3:B:555:VAL:HA	3:B:567:HIS:O	2.17	0.45
3:B:1012:LEU:O	3:B:1095:TYR:CE2	2.68	0.45
3:B:1069:TRP:NE1	3:B:1088:LEU:HD13	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:151:LYS:O	4:D:152:GLU:C	2.60	0.45
4:D:178:LYS:C	4:D:180:VAL:N	2.75	0.45
11:N:35:LEU:HD23	11:N:40:VAL:HG21	1.98	0.45
13:Y:71:ASN:HA	13:Y:74:GLU:OE1	2.16	0.45
1:I:827:LEU:HD12	2:M:71:GLY:HA2	1.99	0.45
2:M:28:ILE:H	2:M:28:ILE:HG12	1.60	0.45
2:M:146:TYR:HB2	2:M:238:LYS:HZ3	1.82	0.45
2:M:210:PHE:HB3	2:M:211:ALA:H	1.54	0.45
3:J:240:TYR:HD2	3:J:244:LEU:HD23	1.82	0.45
3:J:900:THR:HG21	3:J:968:GLU:OE2	2.16	0.45
6:R:72:LEU:C	6:R:74:SER:H	2.25	0.45
10:V:4:ARG:HH11	10:V:4:ARG:CG	2.27	0.45
11:W:18:TRP:CZ2	11:W:22:ILE:HG13	2.52	0.45
1:A:130:ARG:HB3	1:A:195:LEU:C	2.42	0.45
1:A:634:VAL:HG12	1:A:635:PHE:N	2.32	0.45
1:A:741:THR:O	1:A:742:GLN:C	2.59	0.45
2:C:171:ASN:HA	2:C:174:LEU:HB3	1.98	0.45
3:B:97:TRP:O	3:B:98:LEU:HB3	2.17	0.45
10:L:49:LEU:H	10:L:49:LEU:HD22	1.82	0.45
10:L:87:ILE:HD13	10:L:87:ILE:HA	1.79	0.45
11:N:35:LEU:HD22	11:N:40:VAL:HG21	1.98	0.45
1:I:206:TRP:C	1:I:208:ILE:H	2.25	0.45
1:I:430:MET:O	1:I:431:MET:HG3	2.16	0.45
1:I:447:LEU:HD11	3:J:731:GLY:O	2.16	0.45
1:I:556:LEU:HA	1:I:557:PRO:HD3	1.90	0.45
2:M:55:ALA:HB2	2:M:58:GLU:OE2	2.17	0.45
2:M:226:ILE:HB	2:M:227:LEU:HD12	1.97	0.45
3:J:34:PHE:HA	3:J:38:LYS:HB3	1.98	0.45
3:J:454:CYS:HB2	3:J:649:GLY:N	2.32	0.45
3:J:555:VAL:HG22	3:J:568:VAL:HA	1.99	0.45
3:J:758:TYR:O	3:J:759:SER:CB	2.60	0.45
3:J:778:ALA:HA	3:J:783:TYR:CE1	2.51	0.45
3:J:930:GLY:CA	11:W:47:ARG:HH22	2.27	0.45
1:A:456:ASP:OD1	1:A:460:ASP:OD2	2.35	0.45
2:C:26:GLN:C	2:C:28:ILE:N	2.74	0.45
3:B:5:LEU:O	3:B:5:LEU:HD22	2.17	0.45
3:B:148:PRO:HG3	3:B:422:MET:CE	2.47	0.45
3:B:657:TYR:HB3	3:B:660:HIS:CD2	2.52	0.45
4:D:22:LEU:C	4:D:24:PHE:N	2.74	0.45
4:D:78:TRP:O	4:D:80:GLU:N	2.50	0.45
4:D:125:SER:OG	4:D:127:ASP:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:66:THR:CG2	5:E:68:HIS:CE1	2.99	0.45
10:L:92:LYS:HA	10:L:92:LYS:HE3	1.98	0.45
1:I:327:SER:HB2	1:I:444:ARG:CD	2.47	0.45
1:I:483:HIS:HD2	1:I:625:LYS:HG3	1.79	0.45
3:J:21:LYS:HA	3:J:25:ARG:CZ	2.47	0.45
3:J:221:ILE:HD13	3:J:221:ILE:N	2.31	0.45
3:J:226:LEU:O	3:J:230:LEU:HD12	2.17	0.45
3:J:298:LEU:O	3:J:300:HIS:N	2.50	0.45
3:J:429:VAL:HG11	3:J:453:MET:HE1	1.99	0.45
3:J:781:ARG:HB2	3:J:831:ALA:N	2.32	0.45
3:J:956:GLU:O	3:J:960:TYR:HD1	2.00	0.45
4:O:170:VAL:HG23	4:O:200:GLU:HG3	1.99	0.45
9:U:84:ASN:HB3	9:U:86:LYS:HB2	1.99	0.45
1:A:332:ILE:HA	1:A:436:ARG:HH12	1.82	0.45
1:A:575:CYS:CB	1:A:580:CYS:HG	2.30	0.45
1:A:586:VAL:HA	1:A:596:GLY:HA3	1.99	0.45
1:A:820:GLN:O	1:A:823:LEU:HD12	2.17	0.45
2:C:170:ASP:OD1	2:C:171:ASN:N	2.46	0.45
2:C:282:GLU:O	8:H:50:PRO:HG3	2.17	0.45
3:B:50:PRO:C	3:B:52:GLU:H	2.25	0.45
3:B:291:GLN:HB3	3:B:295:LYS:CE	2.44	0.45
3:B:353:LEU:CA	3:B:404:VAL:HG11	2.16	0.45
3:B:687:ARG:NH1	3:B:689:ASP:OD1	2.49	0.45
3:B:707:ALA:C	3:B:709:ASP:N	2.75	0.45
3:B:792:LEU:HD21	3:B:809:VAL:HG12	1.98	0.45
3:B:950:ILE:O	3:B:951:GLU:C	2.60	0.45
1:I:181:ARG:O	1:I:185:GLU:HG3	2.17	0.45
1:I:371:LYS:HZ2	1:I:373:PRO:CD	2.30	0.45
1:I:457:PHE:C	1:I:459:GLY:H	2.24	0.45
1:I:508:LEU:HB3	1:I:638:PHE:HE2	1.81	0.45
1:I:564:GLY:O	1:I:586:VAL:N	2.47	0.45
1:I:607:GLN:HB2	1:I:608:PRO:CD	2.47	0.45
2:M:106:ARG:O	2:M:109:GLU:HB2	2.16	0.45
2:M:388:LEU:CD2	9:U:35:VAL:HG12	2.47	0.45
3:J:248:VAL:HA	3:J:251:GLU:CD	2.42	0.45
3:J:554:ASN:O	3:J:569:ASN:N	2.48	0.45
3:J:569:ASN:HB3	3:J:574:ARG:NH1	2.32	0.45
3:J:600:GLY:C	3:J:602:ILE:H	2.24	0.45
3:J:797:VAL:HG12	3:J:798:VAL:N	2.31	0.45
4:O:178:LYS:O	4:O:180:VAL:N	2.50	0.45
7:S:87:ASN:O	7:S:89:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:33:ILE:O	12:X:34:ILE:C	2.60	0.45
1:A:238:LYS:HZ2	1:A:276:TYR:HA	1.82	0.44
2:C:258:LEU:HD22	2:C:279:GLU:HG2	1.99	0.44
2:C:347:PHE:CE2	2:C:348:GLU:HG3	2.53	0.44
3:B:108:GLU:O	3:B:110:GLU:N	2.51	0.44
3:B:239:VAL:HG22	3:B:253:PHE:HD2	1.82	0.44
3:B:545:ARG:C	3:B:547:GLY:H	2.25	0.44
3:B:921:LEU:C	3:B:923:GLN:N	2.76	0.44
3:B:936:SER:HA	3:B:960:TYR:CE2	2.53	0.44
5:E:2:TYR:N	5:E:2:TYR:CD1	2.85	0.44
9:K:39:ARG:HD3	9:K:74:LEU:HD23	1.98	0.44
1:I:528:ALA:O	1:I:530:VAL:HG12	2.16	0.44
1:I:641:LEU:O	3:J:980:LYS:HB2	2.17	0.44
1:I:764:ARG:HB2	1:I:764:ARG:NH1	2.33	0.44
2:M:289:ALA:HA	2:M:292:ILE:HG22	1.99	0.44
3:J:814:VAL:HG22	3:J:833:ARG:O	2.17	0.44
4:O:54:TYR:O	4:O:55:ASP:C	2.60	0.44
4:O:78:TRP:N	4:O:78:TRP:CD1	2.85	0.44
8:T:28:ALA:C	8:T:30:LYS:H	2.25	0.44
1:A:475:GLU:CD	3:B:1043:MET:HB2	2.42	0.44
1:A:648:LEU:HB2	3:B:924:ILE:HG21	1.99	0.44
2:C:318:ASP:OD2	2:C:322:ARG:NH2	2.51	0.44
3:B:86:ARG:HG3	3:B:153:ILE:HD13	1.98	0.44
3:B:243:SER:O	3:B:249:GLN:OE1	2.35	0.44
3:B:295:LYS:C	3:B:296:TYR:HD1	2.25	0.44
3:B:319:ILE:C	3:B:321:LYS:H	2.25	0.44
3:B:325:LEU:HD12	3:B:328:GLY:HA2	1.98	0.44
3:B:490:TYR:HE1	3:B:527:ILE:CG2	2.30	0.44
6:F:23:ASP:HA	6:F:26:ARG:HD2	2.00	0.44
7:G:64:PRO:O	7:G:114:ARG:HD2	2.18	0.44
9:K:19:PHE:C	9:K:19:PHE:CD2	2.95	0.44
1:I:16:PRO:HD3	1:I:206:TRP:HD1	1.83	0.44
1:I:452:PRO:HG3	1:I:496:ILE:HG12	2.00	0.44
3:J:244:LEU:C	3:J:246:PRO:HD3	2.42	0.44
3:J:402:ASN:O	3:J:403:TRP:HB2	2.18	0.44
3:J:634:THR:N	3:J:635:PRO:HD3	2.33	0.44
7:S:10:ILE:H	7:S:10:ILE:HD12	1.81	0.44
11:W:18:TRP:C	11:W:20:SER:H	2.24	0.44
1:A:346:THR:O	3:B:1005:ALA:HB2	2.17	0.44
1:A:441:LEU:HD12	3:B:873:THR:HG21	2.00	0.44
1:A:500:GLN:HG3	1:A:501:ASP:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:GLN:HG2	3:B:734:MET:HE3	1.99	0.44
1:A:620:SER:C	1:A:622:GLU:N	2.74	0.44
1:A:665:ILE:HG13	1:A:666:ASP:N	2.32	0.44
3:B:554:ASN:O	3:B:569:ASN:N	2.49	0.44
4:D:34:LEU:O	4:D:150:GLY:N	2.49	0.44
7:G:75:GLY:HA3	7:G:87:ASN:HA	1.98	0.44
1:I:347:LEU:HD13	1:I:466:VAL:CG2	2.47	0.44
1:I:561:ASN:HD22	1:I:590:ASN:H	1.65	0.44
3:J:68:PRO:HA	3:J:93:ALA:O	2.16	0.44
3:J:657:TYR:HE2	3:J:946:TYR:CZ	2.35	0.44
3:J:1104:LEU:HB3	3:J:1109:ILE:HB	1.99	0.44
7:S:42:ILE:HD13	7:S:42:ILE:HA	1.85	0.44
9:U:38:ALA:O	9:U:41:LEU:N	2.50	0.44
1:A:647:ARG:HD3	3:B:965:ASP:HB3	1.99	0.44
1:A:827:LEU:CD2	2:C:75:ALA:HB2	2.47	0.44
1:A:878:TRP:NE1	3:J:377:ARG:HD3	2.31	0.44
2:C:32:LEU:O	2:C:36:ILE:HB	2.17	0.44
2:C:310:ILE:O	2:C:314:LEU:HD23	2.16	0.44
3:B:82:PRO:HG3	3:B:130:ILE:CD1	2.47	0.44
3:B:249:GLN:HB2	3:B:253:PHE:CZ	2.52	0.44
3:B:343:LEU:HB2	3:B:476:ILE:HG21	2.00	0.44
3:B:368:GLN:NE2	3:B:386:ARG:HE	2.16	0.44
3:B:419:TRP:HZ3	3:B:712:GLY:CA	2.28	0.44
3:B:595:GLU:CA	3:B:599:SER:HB3	2.39	0.44
3:B:943:THR:C	3:B:945:PHE:H	2.26	0.44
3:B:971:TYR:CZ	3:B:978:LYS:HB3	2.52	0.44
3:B:975:THR:OG1	3:B:977:GLN:HG2	2.17	0.44
4:D:35:TYR:O	4:D:149:TYR:HD2	2.01	0.44
7:G:66:TYR:C	7:G:66:TYR:CD2	2.95	0.44
8:H:62:ILE:HG22	8:H:80:TYR:HA	1.99	0.44
8:H:82:ILE:HD13	8:H:82:ILE:HA	1.87	0.44
1:I:634:VAL:O	1:I:635:PHE:C	2.61	0.44
2:M:70:ILE:HG12	2:M:315:LEU:HD11	2.00	0.44
2:M:149:ILE:O	2:M:153:VAL:HG12	2.18	0.44
3:J:487:LYS:C	3:J:489:LEU:N	2.75	0.44
3:J:655:ILE:HG23	3:J:881:ARG:O	2.17	0.44
3:J:753:THR:HG23	3:J:868:ASP:H	1.82	0.44
3:J:1069:TRP:HE3	3:J:1070:TYR:N	2.14	0.44
7:S:72:CYS:HA	7:S:114:ARG:HA	1.99	0.44
8:T:80:TYR:CD1	8:T:81:VAL:O	2.70	0.44
13:Z:69:GLU:O	13:Z:73:LYS:NZ	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:ARG:O	1:A:185:GLU:HG3	2.17	0.44
1:A:209:LEU:HD11	1:A:277:PHE:HE2	1.82	0.44
1:A:275:THR:HA	1:A:278:ASP:O	2.18	0.44
2:C:188:ILE:HB	2:C:189:GLY:H	1.65	0.44
3:B:12:ARG:HB2	3:B:592:GLU:OE2	2.17	0.44
3:B:804:VAL:HG11	3:B:810:LEU:HD21	1.99	0.44
3:B:911:ASN:HD21	3:B:913:HIS:HD2	1.65	0.44
3:B:963:LEU:HD22	4:D:208:GLU:HG3	2.00	0.44
6:F:1:MET:HE1	6:F:5:TYR:C	2.43	0.44
1:I:249:LEU:HD21	1:I:265:LEU:HB2	1.99	0.44
1:I:425:LEU:HD12	1:I:425:LEU:H	1.81	0.44
1:I:747:LEU:HD22	1:I:786:PHE:CE1	2.53	0.44
2:M:141:ALA:HB2	2:M:251:ILE:HD11	1.99	0.44
3:J:108:GLU:HB2	3:J:109:ALA:H	1.65	0.44
3:J:480:ILE:HG22	3:J:481:ASN:H	1.83	0.44
3:J:484:ILE:H	3:J:484:ILE:CD1	2.27	0.44
3:J:554:ASN:ND2	3:J:576:ARG:HH21	2.06	0.44
3:J:668:TYR:O	3:J:671:ALA:HB3	2.17	0.44
3:J:958:LEU:C	3:J:958:LEU:HD23	2.42	0.44
1:A:409:ARG:NH2	1:A:415:ASP:OD2	2.49	0.44
1:A:448:LEU:O	1:A:496:ILE:HG23	2.17	0.44
1:A:498:ALA:HB3	1:A:603:ILE:O	2.18	0.44
1:A:506:ALA:O	1:A:510:THR:HG23	2.18	0.44
1:A:526:GLY:HA2	10:L:44:TYR:CD1	2.53	0.44
1:A:559:ASP:C	1:A:559:ASP:OD1	2.61	0.44
1:A:723:ASN:ND2	1:A:725:ALA:H	2.15	0.44
1:A:874:ARG:HG3	2:C:54:LEU:HB2	1.99	0.44
3:B:24:VAL:HG21	3:B:426:LEU:HD13	2.00	0.44
3:B:75:ARG:HE	3:B:75:ARG:N	2.15	0.44
3:B:139:ILE:HD13	11:N:61:HIS:HD2	1.80	0.44
3:B:183:ILE:HG22	3:B:209:THR:N	2.33	0.44
5:E:179:LYS:HZ3	6:F:81:ASP:HB2	1.82	0.44
1:I:184:LEU:O	1:I:186:LYS:N	2.50	0.44
1:I:586:VAL:HA	1:I:596:GLY:HA3	1.99	0.44
1:I:728:MET:HE1	3:J:912:PRO:O	2.17	0.44
1:I:763:THR:HG21	1:I:772:TYR:HA	1.99	0.44
1:I:864:LYS:NZ	2:M:29:VAL:HA	2.33	0.44
1:I:870:ARG:CZ	2:M:57:LYS:O	2.66	0.44
2:M:109:GLU:OE2	2:M:117:PRO:HA	2.16	0.44
2:M:125:TYR:HD2	2:M:250:ILE:HG23	1.82	0.44
2:M:192:LYS:C	2:M:194:GLY:N	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:383:THR:HG22	3:J:1042:ALA:H	1.82	0.44
3:J:111:PRO:O	3:J:112:GLU:CB	2.64	0.44
3:J:557:HIS:N	3:J:623:ASN:ND2	2.57	0.44
3:J:658:PRO:HB2	3:J:666:ASN:ND2	2.33	0.44
11:W:38:LEU:HD23	11:W:39:GLY:N	2.32	0.44
1:A:337:VAL:HG23	1:A:433:HIS:CG	2.52	0.44
2:C:113:ALA:HB3	2:C:328:GLN:NE2	2.32	0.44
3:B:727:MET:HE1	3:B:898:PRO:CG	2.47	0.44
3:B:759:SER:CB	3:B:862:VAL:O	2.56	0.44
3:B:1001:LEU:O	3:B:1020:ARG:HD3	2.17	0.44
3:B:1071:ASP:C	3:B:1073:ASN:N	2.76	0.44
1:I:5:ASN:O	3:J:1116:GLU:N	2.51	0.44
1:I:416:ILE:HD11	1:I:477:LYS:HG3	2.00	0.44
2:M:31:ASP:C	2:M:31:ASP:OD1	2.59	0.44
2:M:210:PHE:O	2:M:211:ALA:C	2.61	0.44
3:J:910:LEU:CD2	3:J:911:ASN:H	2.30	0.44
3:J:932:TYR:CD2	3:J:953:LEU:HD22	2.52	0.44
8:T:46:ARG:CD	8:T:48:SER:HB2	2.47	0.44
9:U:61:VAL:C	9:U:63:SER:N	2.69	0.44
11:W:3:ILE:HG22	11:W:4:PRO:CD	2.48	0.44
1:A:175:LEU:HD23	1:A:176:THR:H	1.82	0.44
1:A:364:PHE:HD2	1:A:373:PRO:O	2.00	0.44
1:A:524:ILE:CG2	1:A:634:VAL:HG13	2.48	0.44
1:A:679:TYR:OH	1:A:693:GLU:HG2	2.17	0.44
1:A:829:ASP:HA	2:C:369:VAL:HG13	1.99	0.44
3:B:812:GLY:HA2	3:B:836:SER:CB	2.47	0.44
3:B:970:VAL:HG22	3:B:979:ILE:HG12	2.00	0.44
5:E:107:LEU:O	5:E:162:LEU:N	2.50	0.44
7:G:66:TYR:CD1	7:G:114:ARG:NH1	2.82	0.44
11:N:22:ILE:H	11:N:22:ILE:HD12	1.82	0.44
1:I:4:LYS:NZ	3:J:1115:LEU:HB3	2.32	0.44
1:I:456:ASP:OD1	1:I:460:ASP:OD2	2.35	0.44
1:I:875:VAL:O	1:I:876:VAL:C	2.59	0.44
2:M:115:LYS:HD3	2:M:278:ARG:HD2	2.00	0.44
3:J:27:HIS:O	3:J:28:LEU:C	2.61	0.44
3:J:68:PRO:CD	3:J:129:PRO:HG2	2.47	0.44
3:J:83:MET:HE2	3:J:683:ASN:ND2	2.31	0.44
3:J:122:MET:HE3	3:J:150:GLY:HA2	1.99	0.44
3:J:705:THR:HG22	3:J:706:ARG:H	1.83	0.44
3:J:785:GLY:HA3	3:J:788:TYR:HE2	1.82	0.44
3:J:936:SER:HA	3:J:960:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:56:GLU:HA	5:Q:68:HIS:ND1	2.33	0.44
8:T:44:TRP:HA	8:T:80:TYR:HB3	2.00	0.44
13:Z:38:ILE:O	13:Z:39:GLN:HB2	2.17	0.44
1:A:4:LYS:HG2	1:A:5:ASN:N	2.32	0.44
1:A:105:LYS:HZ2	1:A:108:GLU:HB2	1.81	0.44
1:A:500:GLN:HB2	3:B:913:HIS:CG	2.53	0.44
1:A:588:ILE:HA	1:A:592:ILE:O	2.17	0.44
1:A:637:ARG:HH11	3:B:974:ARG:HH22	1.66	0.44
1:A:747:LEU:HD23	1:A:747:LEU:N	2.33	0.44
3:B:251:GLU:C	3:B:252:LEU:HG	2.43	0.44
3:B:586:ASN:HA	3:B:587:PRO:HD3	1.80	0.44
4:D:64:LEU:O	11:N:6:ARG:HD2	2.18	0.44
4:D:168:PRO:HG3	4:D:203:CYS:O	2.18	0.44
5:E:15:PRO:CG	9:K:45:MET:HB3	2.41	0.44
7:G:26:LEU:HD13	7:G:27:SER:N	2.32	0.44
13:Y:67:LEU:HA	13:Y:70:ASP:HB2	2.00	0.44
13:Y:69:GLU:O	13:Y:73:LYS:HG2	2.18	0.44
1:I:650:ASP:HB3	1:I:723:ASN:ND2	2.32	0.44
2:M:286:ILE:CD1	8:T:45:ILE:HG13	2.48	0.44
3:J:134:THR:O	3:J:138:LEU:HD12	2.18	0.44
3:J:249:GLN:HB2	3:J:253:PHE:CZ	2.53	0.44
3:J:720:ASN:HD22	3:J:720:ASN:N	2.16	0.44
3:J:1071:ASP:C	3:J:1073:ASN:N	2.73	0.44
5:Q:27:LEU:HD21	5:Q:31:ARG:CZ	2.48	0.44
10:V:63:ILE:HG22	10:V:64:THR:H	1.83	0.44
10:V:72:ALA:O	10:V:75:ASN:HB2	2.18	0.44
1:A:333:SER:O	1:A:334:ILE:C	2.60	0.43
1:A:426:HIS:O	1:A:429:SER:HB2	2.18	0.43
3:B:253:PHE:N	3:B:254:PRO:CD	2.79	0.43
3:B:814:VAL:HG22	3:B:833:ARG:O	2.18	0.43
9:K:19:PHE:C	9:K:19:PHE:HD2	2.26	0.43
10:L:87:ILE:C	10:L:89:GLY:N	2.74	0.43
1:I:600:LYS:HB2	1:I:732:GLY:HA3	1.99	0.43
1:I:859:TYR:HB2	2:M:64:ILE:HG21	2.00	0.43
1:I:874:ARG:HA	1:I:874:ARG:HD3	1.76	0.43
2:M:391:ARG:NH2	9:U:39:ARG:HD2	2.27	0.43
3:J:9:GLU:O	3:J:10:ARG:C	2.61	0.43
3:J:432:SER:HB3	3:J:435:ARG:HH21	1.81	0.43
3:J:921:LEU:C	3:J:923:GLN:N	2.76	0.43
4:O:59:ALA:O	4:O:62:LEU:HB2	2.18	0.43
1:A:239:LEU:HD23	1:A:276:TYR:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LYS:NZ	7:G:89:GLY:HA2	2.33	0.43
3:B:92:TYR:OH	3:B:128:ASP:OD2	2.35	0.43
3:B:154:VAL:O	3:B:156:GLY:N	2.52	0.43
4:D:44:VAL:HG13	4:D:143:ALA:HB2	2.00	0.43
7:G:57:VAL:HG12	7:G:57:VAL:O	2.18	0.43
11:N:35:LEU:HD22	11:N:46:ARG:HG3	2.00	0.43
1:I:665:ILE:HG13	1:I:666:ASP:N	2.33	0.43
1:I:866:VAL:O	1:I:867:ASP:C	2.61	0.43
3:J:139:ILE:HD13	11:W:61:HIS:CD2	2.53	0.43
3:J:361:PHE:CE1	3:J:385:VAL:HG13	2.50	0.43
3:J:721:ASN:HB3	11:W:47:ARG:HE	1.82	0.43
3:J:895:VAL:HG11	4:O:34:LEU:HD21	2.00	0.43
4:O:45:TYR:HB2	4:O:142:GLU:O	2.18	0.43
5:Q:98:PHE:CE1	5:Q:107:LEU:HD13	2.53	0.43
5:Q:171:LYS:HE2	5:Q:173:GLU:HB2	1.99	0.43
10:V:45:GLN:HG3	10:V:45:GLN:O	2.19	0.43
1:A:626:TRP:O	1:A:627:LEU:C	2.62	0.43
1:A:828:SER:OG	1:A:829:ASP:N	2.51	0.43
2:C:286:ILE:HD12	8:H:45:ILE:HG13	1.99	0.43
2:C:287:GLU:OE2	8:H:79:ARG:CZ	2.66	0.43
3:B:6:THR:HB	3:B:9:GLU:CB	2.48	0.43
3:B:134:THR:O	3:B:138:LEU:HD12	2.18	0.43
3:B:898:PRO:HB2	3:B:970:VAL:HG21	2.00	0.43
3:B:899:TYR:CE1	3:B:971:TYR:HB2	2.53	0.43
5:E:27:LEU:HD21	5:E:31:ARG:NH1	2.33	0.43
9:K:71:ARG:HH11	9:K:71:ARG:HB2	1.83	0.43
10:L:15:LEU:HB3	10:L:55:VAL:HG23	2.01	0.43
1:I:194:ILE:H	1:I:194:ILE:HG13	1.42	0.43
1:I:272:HIS:HA	1:I:275:THR:HB	2.00	0.43
1:I:397:LEU:HA	1:I:400:THR:OG1	2.18	0.43
1:I:475:GLU:OE1	3:J:1043:MET:N	2.48	0.43
1:I:588:ILE:HA	1:I:592:ILE:O	2.18	0.43
1:I:755:GLU:CD	1:I:756:ARG:H	2.26	0.43
2:M:391:ARG:NH2	9:U:39:ARG:NH1	2.58	0.43
3:J:183:ILE:HG22	3:J:209:THR:N	2.33	0.43
3:J:950:ILE:C	3:J:952:GLN:H	2.26	0.43
3:J:971:TYR:CD2	4:O:164:VAL:O	2.72	0.43
5:Q:11:VAL:HG12	5:Q:12:ARG:N	2.31	0.43
6:R:15:SER:O	6:R:19:LYS:HG2	2.18	0.43
11:W:6:ARG:HA	11:W:12:SER:O	2.18	0.43
11:W:35:LEU:HD23	11:W:40:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:X:17:GLN:C	12:X:19:LYS:N	2.76	0.43
1:A:438:LEU:HD21	1:A:444:ARG:CZ	2.47	0.43
1:A:541:ALA:HB3	1:A:542:PRO:CD	2.44	0.43
2:C:111:VAL:HG12	2:C:329:ILE:HB	1.99	0.43
3:B:43:ILE:HG13	3:B:63:ILE:HD12	2.00	0.43
3:B:55:GLY:O	3:B:105:ASN:N	2.51	0.43
3:B:356:VAL:O	3:B:357:ALA:C	2.61	0.43
3:B:580:ILE:HG13	3:B:642:ILE:HD13	2.00	0.43
3:B:589:VAL:O	3:B:590:THR:C	2.61	0.43
3:B:629:GLU:HB3	3:B:630:PRO:HD2	2.00	0.43
3:B:672:MET:HA	3:B:675:GLN:HB2	2.00	0.43
3:B:925:MET:HE3	3:B:950:ILE:HG12	2.00	0.43
9:K:70:ARG:C	9:K:72:GLY:N	2.76	0.43
11:N:43:TYR:HA	11:N:46:ARG:HB2	1.99	0.43
1:I:90:ILE:CD1	1:I:207:MET:HB2	2.41	0.43
1:I:323:ARG:H	3:J:1002:HIS:HB2	1.82	0.43
3:J:136:ASP:HA	3:J:139:ILE:HD12	2.01	0.43
3:J:247:GLU:C	3:J:249:GLN:N	2.76	0.43
3:J:594:ILE:HB	3:J:599:SER:HB2	2.00	0.43
3:J:803:GLU:HG2	3:J:846:ILE:HG13	1.99	0.43
1:A:64:THR:HB	1:A:65:LEU:H	1.48	0.43
1:A:112:GLU:O	1:A:116:ARG:HB2	2.18	0.43
1:A:646:MET:HE1	3:B:916:PRO:HD3	2.01	0.43
1:A:849:ALA:HB2	9:K:15:PHE:CD1	2.54	0.43
3:B:183:ILE:HG12	3:B:207:ASP:N	2.33	0.43
3:B:296:TYR:N	3:B:296:TYR:CD1	2.87	0.43
3:B:445:LEU:HD11	3:B:455:PRO:HB2	2.00	0.43
3:B:597:LEU:O	3:B:598:GLU:HB2	2.19	0.43
3:B:757:LEU:HD21	3:B:863:LYS:HB3	2.01	0.43
5:E:36:GLU:CG	6:F:34:LEU:HD11	2.27	0.43
5:E:175:ILE:O	5:E:175:ILE:HG22	2.18	0.43
6:F:84:ARG:HG3	6:F:85:SER:N	2.32	0.43
9:K:34:ARG:C	9:K:37:SER:HB2	2.38	0.43
9:K:61:VAL:HG12	9:K:62:ILE:N	2.33	0.43
2:M:274:THR:CG2	2:M:275:ASN:H	2.07	0.43
2:M:390:MET:HE3	5:Q:59:LEU:N	2.34	0.43
3:J:148:PRO:HG3	3:J:422:MET:CE	2.47	0.43
3:J:296:TYR:N	3:J:296:TYR:CD1	2.87	0.43
3:J:405:GLY:C	3:J:407:ARG:H	2.27	0.43
3:J:890:MET:HG3	3:J:891:LEU:N	2.32	0.43
5:Q:171:LYS:HB3	5:Q:174:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:R:64:SER:H	6:R:69:ARG:HH21	1.66	0.43
10:V:78:GLY:O	10:V:81:SER:HB2	2.18	0.43
1:A:217:ILE:C	1:A:219:ILE:N	2.77	0.43
1:A:353:ILE:CD1	1:A:407:ILE:HG23	2.47	0.43
2:C:24:LEU:HD13	2:C:33:LYS:HA	2.01	0.43
3:B:191:SER:CB	3:B:300:HIS:CD2	3.01	0.43
3:B:873:THR:HG23	3:B:874:ILE:HD12	2.00	0.43
3:B:875:GLY:HA2	3:B:887:VAL:CG1	2.48	0.43
6:F:64:SER:N	6:F:69:ARG:HH21	2.16	0.43
11:N:53:VAL:HG23	11:N:55:ILE:HG23	2.01	0.43
1:I:188:PRO:O	1:I:192:VAL:HG23	2.19	0.43
1:I:347:LEU:HB2	1:I:411:LEU:HD22	2.01	0.43
1:I:646:MET:HE1	3:J:916:PRO:HD3	2.00	0.43
1:I:823:LEU:O	1:I:824:ILE:C	2.61	0.43
2:M:145:GLU:HG3	2:M:240:ALA:HB3	2.00	0.43
3:J:675:GLN:HG2	3:J:994:HIS:NE2	2.33	0.43
1:A:249:LEU:HD21	1:A:265:LEU:HB2	2.01	0.43
1:A:517:THR:HG22	1:A:519:GLU:H	1.84	0.43
1:A:635:PHE:O	1:A:639:VAL:HG23	2.19	0.43
1:A:835:ASP:HA	9:K:20:ILE:CD1	2.49	0.43
2:C:146:TYR:HD1	2:C:238:LYS:N	2.17	0.43
3:B:81:SER:OG	3:B:141:ILE:CG2	2.67	0.43
3:B:381:LEU:C	3:B:383:ALA:N	2.76	0.43
3:B:654:ILE:HG22	3:B:881:ARG:HG2	2.01	0.43
3:B:685:GLN:NE2	3:B:867:ARG:HH22	2.17	0.43
3:B:687:ARG:HH11	3:B:687:ARG:CB	2.31	0.43
3:B:1004:ARG:NH1	3:B:1016:PRO:HB3	2.34	0.43
4:D:6:LEU:HB3	4:D:14:ASP:HB2	2.00	0.43
5:E:20:LYS:HA	5:E:21:PRO:HD2	1.68	0.43
9:K:46:GLY:O	9:K:47:ALA:C	2.62	0.43
1:I:571:GLY:HA3	1:I:572:PRO:HD2	1.91	0.43
1:I:853:ASP:CB	2:M:311:ARG:HH12	2.26	0.43
3:J:5:LEU:O	3:J:5:LEU:HD22	2.18	0.43
3:J:217:VAL:HA	3:J:218:PRO:HD3	1.90	0.43
3:J:295:LYS:C	3:J:296:TYR:HD1	2.27	0.43
3:J:698:PRO:HB2	11:W:53:VAL:CG2	2.47	0.43
3:J:763:VAL:HA	3:J:770:GLU:CG	2.48	0.43
3:J:1077:TYR:O	3:J:1077:TYR:HD1	2.02	0.43
5:Q:146:VAL:HG12	5:Q:147:ILE:N	2.34	0.43
1:A:631:LEU:O	1:A:634:VAL:HB	2.19	0.43
2:C:238:LYS:O	2:C:239:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:325:LEU:O	3:B:326:TYR:C	2.61	0.43
3:B:600:GLY:C	3:B:602:ILE:N	2.77	0.43
3:B:644:SER:C	3:B:646:ALA:N	2.76	0.43
3:B:935:LEU:O	11:N:46:ARG:NH1	2.51	0.43
3:B:1074:LYS:HB3	3:B:1076:LYS:HE2	2.01	0.43
4:D:94:THR:CG2	4:D:145:LEU:HB2	2.49	0.43
6:F:18:LYS:HD3	6:F:45:GLU:CD	2.43	0.43
8:H:41:GLN:O	8:H:42:LEU:HB3	2.19	0.43
9:K:68:GLU:HG3	9:K:74:LEU:HG	2.00	0.43
9:K:89:LEU:H	9:K:89:LEU:HG	1.77	0.43
11:N:52:HIS:CE1	11:N:54:ASP:H	2.36	0.43
12:P:28:TYR:O	12:P:29:CYS:C	2.61	0.43
1:I:365:VAL:HG11	1:I:401:LEU:HD11	2.01	0.43
1:I:812:ARG:NE	2:M:86:THR:HG23	2.31	0.43
3:J:253:PHE:N	3:J:254:PRO:CD	2.80	0.43
3:J:402:ASN:O	3:J:403:TRP:CB	2.66	0.43
3:J:665:ARG:HH21	3:J:918:ARG:NE	2.15	0.43
3:J:764:LYS:NZ	3:J:814:VAL:H	2.14	0.43
3:J:1069:TRP:HB2	3:J:1078:VAL:O	2.18	0.43
3:J:1083:GLY:O	3:J:1084:ASP:HB2	2.18	0.43
4:O:133:LEU:HD22	4:O:137:GLN:HB3	2.01	0.43
7:S:90:ASN:OD1	7:S:90:ASN:N	2.41	0.43
8:T:20:HIS:O	8:T:21:GLU:HG3	2.19	0.43
1:A:98:CYS:CA	1:A:146:CYS:SG	3.05	0.43
1:A:349:VAL:HG21	1:A:409:ARG:NH2	2.33	0.43
1:A:415:ASP:H	1:A:435:VAL:HG12	1.84	0.43
1:A:426:HIS:ND1	1:A:428:ILE:HG22	2.30	0.43
1:A:785:SER:C	1:A:787:ARG:N	2.73	0.43
3:B:88:ARG:CD	3:B:853:THR:CG2	2.77	0.43
3:B:134:THR:O	3:B:135:LEU:C	2.61	0.43
3:B:549:ILE:HD13	3:B:549:ILE:HA	1.75	0.43
4:D:61:ARG:HG2	4:D:61:ARG:HH11	1.82	0.43
5:E:15:PRO:O	5:E:16:ASN:C	2.62	0.43
7:G:109:LYS:NZ	3:J:378:LYS:CE	2.78	0.43
13:Y:77:LYS:NZ	13:Y:77:LYS:HB3	2.34	0.43
13:Y:82:ARG:HA	13:Y:82:ARG:HE	1.83	0.43
1:I:259:GLN:HA	1:I:262:ILE:CG2	2.49	0.43
1:I:541:ALA:CB	7:S:71:PHE:HA	2.46	0.43
1:I:681:ASN:O	1:I:682:GLY:C	2.61	0.43
2:M:21:SER:O	2:M:33:LYS:CE	2.67	0.43
2:M:148:LYS:HE3	2:M:231:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:14:ILE:O	3:J:17:TYR:HB3	2.18	0.43
3:J:181:SER:O	3:J:182:ASN:CB	2.67	0.43
3:J:246:PRO:HD2	3:J:247:GLU:H	1.84	0.43
3:J:480:ILE:CG2	3:J:481:ASN:N	2.80	0.43
3:J:522:LEU:HD13	3:J:523:ASN:HB2	2.01	0.43
3:J:589:VAL:O	3:J:590:THR:C	2.61	0.43
3:J:871:ILE:H	3:J:871:ILE:HG13	1.62	0.43
8:T:38:ARG:HB3	8:T:40:GLU:HG2	2.00	0.43
1:A:77:LEU:HD12	1:A:210:THR:C	2.43	0.43
1:A:353:ILE:O	1:A:403:PRO:HA	2.19	0.43
1:A:502:TYR:CD1	1:A:632:PHE:HB3	2.53	0.43
1:A:796:PHE:CZ	3:B:445:LEU:HD13	2.54	0.43
2:C:11:PRO:O	2:C:14:GLU:CG	2.67	0.43
2:C:181:VAL:O	2:C:184:VAL:HG12	2.19	0.43
3:B:248:VAL:HA	3:B:251:GLU:CD	2.44	0.43
3:B:402:ASN:O	3:B:403:TRP:CB	2.67	0.43
3:B:735:GLU:HA	3:B:735:GLU:OE2	2.18	0.43
3:B:1054:ASP:HB3	3:B:1095:TYR:N	2.26	0.43
6:F:13:PRO:HG2	6:F:16:VAL:CG2	2.48	0.43
1:I:71:HIS:ND1	3:J:1070:TYR:CE2	2.86	0.43
1:I:375:ALA:O	1:I:377:TYR:N	2.52	0.43
1:I:507:TYR:HA	1:I:510:THR:H	1.84	0.43
1:I:672:VAL:O	1:I:675:LEU:N	2.51	0.43
2:M:373:ILE:CD1	3:J:1049:LEU:HD22	2.49	0.43
3:J:55:GLY:O	3:J:105:ASN:N	2.51	0.43
3:J:388:ASP:HB3	3:J:391:THR:HB	2.01	0.43
3:J:416:ARG:NH1	3:J:687:ARG:HH21	2.17	0.43
3:J:445:LEU:HD11	3:J:455:PRO:HB3	2.01	0.43
3:J:461:GLY:HA3	3:J:462:PRO:HD3	1.91	0.43
4:O:144:ARG:C	4:O:145:LEU:HD12	2.44	0.43
5:Q:38:ILE:HB	5:Q:39:LEU:H	1.43	0.43
7:S:33:CYS:HB2	7:S:36:PHE:O	2.19	0.43
13:Z:59:ILE:HA	13:Z:62:GLU:OE2	2.19	0.43
1:A:87:VAL:O	1:A:91:TYR:HB2	2.18	0.42
1:A:340:PRO:HB2	1:A:343:ILE:HG12	2.00	0.42
1:A:525:LEU:C	1:A:527:VAL:N	2.77	0.42
1:A:875:VAL:HB	1:A:876:VAL:H	1.71	0.42
2:C:60:SER:O	2:C:63:LEU:CB	2.64	0.42
2:C:361:GLY:O	2:C:362:ASP:O	2.37	0.42
3:B:663:SER:CB	3:B:664:PRO:HD3	2.48	0.42
3:B:690:THR:CG2	3:B:691:ARG:HG3	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:83:GLU:O	5:E:145:ARG:HA	2.19	0.42
7:G:86:LEU:HG	7:G:87:ASN:N	2.34	0.42
12:P:12:THR:O	12:P:14:THR:N	2.39	0.42
1:I:517:THR:HG22	1:I:518:LYS:N	2.34	0.42
2:M:15:GLU:O	2:M:16:LYS:C	2.62	0.42
2:M:85:MET:HE1	2:M:107:LEU:HD12	2.00	0.42
2:M:117:PRO:HD3	2:M:276:ASN:ND2	2.34	0.42
2:M:292:ILE:HG23	2:M:293:ILE:H	1.83	0.42
3:J:50:PRO:C	3:J:52:GLU:N	2.77	0.42
3:J:96:LEU:O	3:J:115:TYR:HA	2.19	0.42
3:J:171:ARG:HB3	3:J:524:GLY:HA3	2.00	0.42
3:J:174:VAL:HG12	3:J:175:ASP:N	2.34	0.42
3:J:251:GLU:C	3:J:252:LEU:HG	2.43	0.42
3:J:545:ARG:C	3:J:547:GLY:H	2.27	0.42
3:J:690:THR:O	3:J:691:ARG:C	2.62	0.42
3:J:790:ARG:C	3:J:790:ARG:HE	2.27	0.42
3:J:970:VAL:O	3:J:979:ILE:HG13	2.19	0.42
4:O:178:LYS:HE2	4:O:178:LYS:HB2	1.89	0.42
11:W:52:HIS:NE2	11:W:54:ASP:HB2	2.34	0.42
12:X:37:VAL:HG22	12:X:38:ARG:N	2.32	0.42
1:A:84:VAL:O	1:A:87:VAL:HG12	2.19	0.42
1:A:234:ASP:C	1:A:236:THR:N	2.77	0.42
1:A:763:THR:HG23	1:A:779:ARG:HH12	1.85	0.42
3:B:110:GLU:HA	3:B:111:PRO:HA	1.57	0.42
3:B:246:PRO:O	3:B:248:VAL:N	2.47	0.42
3:B:544:ARG:HB2	3:B:549:ILE:CG2	2.48	0.42
3:B:797:VAL:HG12	3:B:798:VAL:N	2.33	0.42
4:D:64:LEU:HD22	11:N:6:ARG:HD3	2.01	0.42
10:L:59:THR:HG22	10:L:65:PRO:HD3	1.99	0.42
1:I:349:VAL:HG21	1:I:415:ASP:OD2	2.18	0.42
1:I:357:ASN:HD22	1:I:361:LEU:HD22	1.83	0.42
1:I:555:PHE:HD2	1:I:631:LEU:HD13	1.81	0.42
1:I:558:LYS:HA	1:I:590:ASN:O	2.19	0.42
1:I:826:ALA:H	2:M:335:THR:HG23	1.83	0.42
1:I:879:LYS:NZ	2:M:44:THR:HB	2.34	0.42
2:M:174:LEU:HB2	2:M:179:VAL:HG13	2.00	0.42
3:J:191:SER:CB	3:J:300:HIS:CD2	3.01	0.42
3:J:617:ASP:O	3:J:618:ALA:CB	2.66	0.42
9:U:46:GLY:O	9:U:47:ALA:O	2.38	0.42
12:X:33:ILE:HD13	12:X:33:ILE:HA	1.90	0.42
1:A:63:ASN:ND2	3:B:1071:ASP:CG	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:ARG:O	1:A:788:THR:C	2.62	0.42
2:C:391:ARG:HH22	9:K:42:GLN:HG2	1.82	0.42
3:B:94:ALA:O	3:B:118:ASP:HA	2.19	0.42
3:B:446:HIS:HD2	3:B:448:THR:OG1	2.02	0.42
4:D:256:LEU:O	4:D:257:GLU:C	2.63	0.42
7:G:42:ILE:HD13	7:G:46:ILE:HG21	2.00	0.42
1:I:620:SER:C	1:I:622:GLU:N	2.76	0.42
2:M:146:TYR:O	2:M:238:LYS:HD2	2.19	0.42
3:J:418:ASN:HD21	3:J:421:SER:N	2.00	0.42
3:J:533:GLY:C	3:J:535:GLU:N	2.78	0.42
3:J:597:LEU:O	3:J:598:GLU:HB2	2.19	0.42
3:J:657:TYR:HB3	3:J:660:HIS:CD2	2.55	0.42
3:J:759:SER:CB	3:J:863:LYS:HA	2.47	0.42
4:O:68:MET:CE	4:O:68:MET:HA	2.49	0.42
4:O:110:TYR:HA	4:O:128:ILE:O	2.19	0.42
4:O:128:ILE:CG1	11:W:16:ASP:HB3	2.49	0.42
1:A:17:ASP:O	1:A:21:LYS:HG3	2.19	0.42
1:A:637:ARG:HH11	3:B:974:ARG:HH12	1.68	0.42
1:A:722:PHE:CD2	7:G:24:LYS:HG3	2.55	0.42
3:B:435:ARG:CB	3:B:439:ASN:HD21	2.32	0.42
3:B:781:ARG:HD3	3:B:832:LYS:O	2.20	0.42
3:B:962:TYR:HH	11:N:42:ARG:HD2	1.81	0.42
4:D:115:LYS:O	4:D:116:SER:HB3	2.18	0.42
5:E:31:ARG:O	5:E:35:GLN:HB2	2.19	0.42
7:G:57:VAL:O	7:G:59:ILE:HG13	2.19	0.42
7:G:83:ASP:HB3	7:G:94:THR:HB	2.02	0.42
10:L:70:LEU:HA	10:L:73:ILE:HB	2.01	0.42
10:L:82:HIS:O	10:L:83:TYR:C	2.62	0.42
1:I:155:LYS:HB3	1:I:156:ILE:HA	2.02	0.42
1:I:175:LEU:HD23	1:I:176:THR:H	1.84	0.42
1:I:199:PRO:C	1:I:201:THR:H	2.28	0.42
1:I:490:ARG:HG3	2:M:77:SER:HB3	2.01	0.42
1:I:507:TYR:OH	1:I:727:VAL:HG13	2.19	0.42
1:I:648:LEU:HB2	3:J:924:ILE:HG21	2.01	0.42
1:I:716:SER:HB3	1:I:726:TYR:OH	2.19	0.42
3:J:579:LEU:CD1	3:J:616:LEU:CD1	2.91	0.42
3:J:930:GLY:HA3	3:J:987:VAL:HB	2.01	0.42
4:O:25:VAL:HG21	4:O:226:TYR:HD1	1.84	0.42
4:O:78:TRP:O	4:O:80:GLU:N	2.53	0.42
7:S:33:CYS:HB3	7:S:34:ASN:H	1.62	0.42
7:S:64:PRO:C	7:S:114:ARG:NH1	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:V:45:GLN:HA	10:V:46:PRO:HD2	1.73	0.42
1:A:7:LYS:HE2	2:C:365:GLU:CD	2.44	0.42
1:A:57:LYS:HD2	1:A:60:THR:HA	2.01	0.42
1:A:452:PRO:HG3	1:A:496:ILE:HG12	2.01	0.42
2:C:70:ILE:HD13	2:C:71:GLY:H	1.83	0.42
3:B:173:LEU:HA	3:B:333:ASP:OD2	2.19	0.42
3:B:181:SER:HB3	3:B:183:ILE:CD1	2.50	0.42
3:B:196:TYR:CE1	3:B:303:THR:HB	2.54	0.42
3:B:616:LEU:HD11	3:B:639:HIS:CE1	2.54	0.42
3:B:624:ALA:HB1	3:B:639:HIS:HD2	1.84	0.42
3:B:738:ILE:HD12	3:B:739:ILE:H	1.84	0.42
3:B:741:ASN:OD1	3:B:744:SER:N	2.44	0.42
4:D:12:ARG:HA	4:D:230:ILE:O	2.19	0.42
4:D:259:LYS:O	4:D:263:VAL:CG2	2.64	0.42
1:I:141:MET:HE3	1:I:148:HIS:HB3	2.00	0.42
1:I:313:LEU:HD12	1:I:313:LEU:HA	1.90	0.42
1:I:340:PRO:HB2	1:I:343:ILE:HG12	2.00	0.42
2:M:318:ASP:O	2:M:322:ARG:NE	2.53	0.42
3:J:132:GLN:OE1	3:J:132:GLN:HA	2.19	0.42
3:J:264:ASN:HB2	3:J:267:ASP:H	1.84	0.42
3:J:345:LEU:O	3:J:346:ALA:C	2.62	0.42
3:J:501:ILE:HD12	3:J:501:ILE:N	2.35	0.42
3:J:624:ALA:HB1	3:J:639:HIS:HD2	1.84	0.42
1:A:648:LEU:O	1:A:651:VAL:HG12	2.19	0.42
1:A:851:GLY:C	1:A:853:ASP:N	2.77	0.42
2:C:126:LEU:CD1	2:C:249:TYR:HB2	2.50	0.42
2:C:146:TYR:CE2	2:C:235:LYS:HB2	2.54	0.42
2:C:179:VAL:HG23	2:C:182:ASP:HB2	2.01	0.42
3:B:6:THR:HB	3:B:9:GLU:H	1.85	0.42
3:B:644:SER:O	3:B:647:ILE:HG13	2.20	0.42
3:B:1015:GLN:HE21	3:B:1096:ALA:HB2	1.80	0.42
8:H:30:LYS:HA	8:H:33:LYS:HE2	2.01	0.42
11:N:22:ILE:N	11:N:22:ILE:CD1	2.83	0.42
2:M:63:LEU:HD12	9:U:22:LEU:CD2	2.43	0.42
2:M:322:ARG:HG3	8:T:43:PRO:HA	2.01	0.42
3:J:174:VAL:HG11	3:J:325:LEU:HD23	2.02	0.42
3:J:243:SER:O	3:J:249:GLN:OE1	2.37	0.42
3:J:435:ARG:CB	3:J:439:ASN:HD21	2.32	0.42
3:J:588:LEU:HD22	3:J:612:LYS:HG2	2.01	0.42
3:J:1009:VAL:HB	3:J:1014:ARG:C	2.45	0.42
4:O:111:SER:OG	4:O:125:SER:O	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:159:VAL:HG23	4:O:231:GLU:C	2.44	0.42
5:Q:128:PHE:CE2	5:Q:133:LYS:HD3	2.55	0.42
9:U:18:VAL:HG12	9:U:22:LEU:HD12	2.01	0.42
1:A:618:GLU:O	1:A:619:TYR:CG	2.72	0.42
1:A:727:VAL:O	1:A:728:MET:C	2.62	0.42
2:C:21:SER:O	2:C:25:PRO:HD3	2.19	0.42
3:B:338:TYR:HB2	3:B:448:THR:HG21	2.02	0.42
3:B:365:LEU:HG	3:B:369:LEU:HD12	2.02	0.42
3:B:768:GLY:O	3:B:769:GLN:HB2	2.19	0.42
3:B:778:ALA:HA	3:B:783:TYR:CE1	2.55	0.42
7:G:79:THR:CG2	7:G:80:GLU:N	2.82	0.42
1:I:220:ARG:NH1	1:I:236:THR:CG2	2.74	0.42
1:I:871:ILE:HG13	2:M:54:LEU:HD11	2.01	0.42
2:M:392:PRO:HG2	5:Q:22:LEU:HD21	2.01	0.42
3:J:22:GLY:O	3:J:23:LEU:C	2.62	0.42
3:J:92:TYR:OH	3:J:128:ASP:OD2	2.36	0.42
3:J:382:LYS:O	3:J:382:LYS:HG2	2.19	0.42
3:J:793:GLU:HB3	3:J:794:ASP:H	1.72	0.42
7:S:42:ILE:HD11	7:S:71:PHE:CZ	2.55	0.42
10:V:3:ILE:HD13	10:V:17:ILE:HG23	2.01	0.42
1:A:104:VAL:HG12	1:A:137:LYS:HA	2.02	0.42
1:A:320:PHE:CE2	3:B:1005:ALA:HB1	2.55	0.42
1:A:380:ARG:HB3	1:A:381:PRO:HD2	2.01	0.42
1:A:394:ARG:O	1:A:398:ALA:HB2	2.20	0.42
1:A:427:ARG:NH1	2:C:73:VAL:HG11	2.34	0.42
1:A:827:LEU:CG	2:C:75:ALA:HB2	2.49	0.42
2:C:106:ARG:HH21	2:C:117:PRO:HB3	1.85	0.42
2:C:149:ILE:O	2:C:153:VAL:HG12	2.19	0.42
2:C:389:THR:O	2:C:390:MET:O	2.37	0.42
3:B:136:ASP:HA	3:B:139:ILE:HD12	2.01	0.42
3:B:386:ARG:HB3	3:B:389:ILE:HD11	2.02	0.42
3:B:1069:TRP:HE3	3:B:1070:TYR:N	2.18	0.42
4:D:21:PRO:O	4:D:24:PHE:HB3	2.20	0.42
4:D:107:ARG:N	4:D:133:LEU:O	2.51	0.42
4:D:206:CYS:O	4:D:207:GLU:HB2	2.20	0.42
7:G:18:ILE:HG22	7:G:18:ILE:O	2.18	0.42
1:I:488:THR:HB	1:I:495:ILE:HB	2.02	0.42
1:I:559:ASP:C	1:I:559:ASP:OD1	2.61	0.42
3:J:537:ALA:HB2	3:J:557:HIS:CD2	2.55	0.42
4:O:128:ILE:HG12	11:W:16:ASP:HB3	2.01	0.42
1:A:85:GLY:HA3	2:C:355:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLY:O	1:A:551:VAL:HG12	2.20	0.42
1:A:835:ASP:HA	9:K:20:ILE:HD13	2.02	0.42
2:C:190:ARG:HD3	2:C:191:LEU:N	2.31	0.42
2:C:202:GLU:O	2:C:203:ASP:HB2	2.20	0.42
3:B:24:VAL:HG11	3:B:426:LEU:HD13	2.01	0.42
3:B:111:PRO:O	3:B:112:GLU:CB	2.68	0.42
3:B:205:LEU:HD23	3:B:212:VAL:HG22	2.01	0.42
3:B:298:LEU:N	3:B:299:PRO:HD3	2.35	0.42
3:B:388:ASP:HB3	3:B:391:THR:HB	2.01	0.42
3:B:418:ASN:HD21	3:B:420:LEU:HB3	1.84	0.42
3:B:458:THR:CG2	3:B:464:SER:HA	2.49	0.42
3:B:1029:GLY:O	3:B:1031:MET:N	2.52	0.42
8:H:10:ASP:OD1	8:H:10:ASP:C	2.62	0.42
11:N:22:ILE:H	11:N:22:ILE:CD1	2.33	0.42
11:N:24:ARG:HD2	11:N:34:VAL:HG13	2.02	0.42
1:I:861:ALA:CB	1:I:866:VAL:HG23	2.49	0.42
2:M:239:ARG:HE	2:M:239:ARG:HB2	1.71	0.42
2:M:258:LEU:HB2	2:M:279:GLU:HG2	2.01	0.42
2:M:283:VAL:C	2:M:284:PHE:HD1	2.28	0.42
3:J:173:LEU:HA	3:J:333:ASP:OD2	2.19	0.42
3:J:435:ARG:HB3	3:J:439:ASN:HD21	1.84	0.42
3:J:485:VAL:C	3:J:487:LYS:H	2.28	0.42
3:J:752:SER:OG	3:J:753:THR:N	2.53	0.42
3:J:928:ILE:HD13	3:J:954:GLN:HE21	1.84	0.42
4:O:178:LYS:O	4:O:179:ALA:C	2.63	0.42
7:S:42:ILE:HD11	7:S:71:PHE:CE1	2.55	0.42
1:A:655:ASP:HB3	1:A:656:ASP:H	1.61	0.42
1:A:672:VAL:O	1:A:675:LEU:N	2.52	0.42
1:A:823:LEU:HD13	2:C:75:ALA:O	2.18	0.42
2:C:109:GLU:O	2:C:113:ALA:CA	2.51	0.42
3:B:264:ASN:H	3:B:267:ASP:HB2	1.85	0.42
3:B:354:PHE:CD1	3:B:354:PHE:C	2.98	0.42
3:B:469:ASN:N	3:B:469:ASN:ND2	2.67	0.42
3:B:658:PRO:C	3:B:660:HIS:N	2.76	0.42
3:B:1064:CYS:SG	3:B:1081:ILE:HD12	2.60	0.42
3:B:1099:LEU:O	3:B:1102:GLN:HB2	2.20	0.42
7:G:57:VAL:HG13	7:G:115:THR:HG22	2.02	0.42
10:L:3:ILE:H	10:L:3:ILE:HD12	1.85	0.42
10:L:29:ALA:HA	10:L:32:LEU:HB2	2.02	0.42
1:I:188:PRO:HD2	1:I:191:ASP:HB2	2.00	0.42
1:I:212:LEU:CD2	1:I:242:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:550:GLN:NE2	7:S:88:ASN:ND2	2.68	0.42
1:I:553:SER:OG	1:I:592:ILE:HA	2.20	0.42
3:J:87:LEU:HD22	3:J:851:LEU:HD13	2.02	0.42
3:J:130:ILE:O	3:J:131:SER:C	2.62	0.42
3:J:354:PHE:O	3:J:355:ARG:C	2.63	0.42
3:J:482:GLU:O	3:J:483:ARG:C	2.63	0.42
3:J:540:ILE:HG21	3:J:555:VAL:HG21	2.01	0.42
3:J:580:ILE:HA	3:J:613:ILE:HD13	2.01	0.42
3:J:1004:ARG:HD3	3:J:1004:ARG:C	2.45	0.42
4:O:53:LEU:HD11	11:W:2:LEU:HD12	2.01	0.42
7:S:75:GLY:HA3	7:S:87:ASN:HA	2.02	0.42
1:A:181:ARG:HG3	1:A:208:ILE:HB	2.00	0.41
1:A:355:PRO:O	1:A:357:ASN:OD1	2.37	0.41
1:A:425:LEU:CD2	2:C:83:THR:HG21	2.50	0.41
1:A:439:LYS:H	1:A:439:LYS:HG3	1.57	0.41
3:B:116:ILE:HD12	3:B:361:PHE:HZ	1.83	0.41
3:B:388:ASP:OD1	3:B:391:THR:OG1	2.25	0.41
3:B:430:ILE:HG22	3:B:431:SER:N	2.35	0.41
3:B:454:CYS:HB2	3:B:649:GLY:N	2.35	0.41
3:B:785:GLY:HA3	3:B:788:TYR:HE2	1.84	0.41
3:B:874:ILE:H	3:B:874:ILE:CD1	2.17	0.41
3:B:975:THR:O	4:D:26:ASN:ND2	2.53	0.41
8:H:64:ARG:HG3	8:H:78:TYR:HE2	1.84	0.41
9:K:74:LEU:HD22	9:K:76:ILE:HD12	2.01	0.41
1:I:349:VAL:HA	1:I:350:PRO:HD2	1.80	0.41
1:I:364:PHE:CD2	1:I:373:PRO:O	2.73	0.41
1:I:449:VAL:O	1:I:449:VAL:HG12	2.20	0.41
1:I:548:GLY:HA2	1:I:551:VAL:HG12	2.02	0.41
1:I:644:PHE:HB3	3:J:728:SER:OG	2.20	0.41
1:I:648:LEU:C	1:I:650:ASP:N	2.78	0.41
3:J:6:THR:HB	3:J:9:GLU:CB	2.50	0.41
3:J:750:TYR:O	3:J:992:LYS:NZ	2.52	0.41
3:J:764:LYS:NZ	3:J:814:VAL:O	2.35	0.41
3:J:898:PRO:HB2	3:J:970:VAL:HG21	2.02	0.41
4:O:204:THR:O	4:O:206:CYS:N	2.53	0.41
1:A:327:SER:HB2	1:A:444:ARG:CD	2.47	0.41
1:A:422:GLN:HA	1:A:423:PRO:C	2.44	0.41
1:A:445:LEU:HD21	1:A:450:CYS:HA	2.02	0.41
1:A:609:GLU:HB3	1:A:614:TRP:CZ2	2.55	0.41
3:B:723:ILE:HG12	3:B:907:ASP:OD2	2.19	0.41
3:B:790:ARG:HE	3:B:790:ARG:C	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:45:TYR:CD1	12:P:44:ILE:HG12	2.54	0.41
4:D:94:THR:O	4:D:95:LYS:HG3	2.20	0.41
4:D:125:SER:O	4:D:127:ASP:N	2.52	0.41
10:L:59:THR:HG21	10:L:65:PRO:HD3	2.02	0.41
1:I:45:MET:O	1:I:47:PRO:HD3	2.20	0.41
1:I:485:ASN:HD21	3:J:1039:PHE:HE2	1.67	0.41
1:I:486:ILE:HD12	1:I:616:ILE:HD13	2.02	0.41
1:I:708:ARG:HG3	1:I:709:SER:N	2.35	0.41
1:I:839:ARG:NH2	9:U:83:PRO:HG3	2.35	0.41
2:M:234:ILE:H	2:M:234:ILE:HG13	1.65	0.41
3:J:366:THR:O	3:J:370:GLU:HG3	2.19	0.41
3:J:738:ILE:HD12	3:J:739:ILE:N	2.34	0.41
3:J:764:LYS:HD3	3:J:815:SER:HB3	2.02	0.41
3:J:811:ILE:HB	3:J:837:ILE:HB	2.02	0.41
3:J:1065:GLY:O	3:J:1112:ARG:HA	2.20	0.41
6:R:7:VAL:HG12	6:R:8:GLU:N	2.33	0.41
7:S:48:ILE:C	7:S:49:PHE:CG	2.98	0.41
13:Z:55:LEU:HB3	13:Z:56:ASN:H	1.63	0.41
1:A:153:GLN:HG2	1:A:154:TYR:H	1.85	0.41
2:C:57:LYS:HA	2:C:57:LYS:HE3	2.02	0.41
2:C:320:MET:HA	2:C:327:ARG:HG2	2.02	0.41
2:C:337:GLU:N	2:C:337:GLU:CD	2.79	0.41
3:B:157:SER:O	3:B:158:GLU:CB	2.67	0.41
3:B:485:VAL:C	3:B:487:LYS:H	2.28	0.41
3:B:764:LYS:HZ1	3:B:772:LYS:C	2.28	0.41
10:L:51:ASP:C	10:L:52:LYS:HG3	2.45	0.41
12:P:26:CYS:CB	12:P:27:PRO:CD	2.87	0.41
1:I:153:GLN:HG2	1:I:154:TYR:H	1.85	0.41
1:I:283:GLY:C	1:I:285:PRO:HD2	2.45	0.41
1:I:352:ARG:HD3	1:I:406:ILE:HG12	2.02	0.41
1:I:500:GLN:HG3	1:I:501:ASP:H	1.85	0.41
1:I:742:GLN:HG2	1:I:747:LEU:HA	2.02	0.41
1:I:763:THR:C	1:I:764:ARG:HG2	2.44	0.41
1:I:874:ARG:HE	2:M:53:ASP:HB2	1.85	0.41
2:M:80:GLU:CB	2:M:81:PRO:HD3	2.50	0.41
2:M:389:THR:HG21	9:U:79:ARG:NH1	2.34	0.41
3:J:28:LEU:CA	3:J:122:MET:HE1	2.50	0.41
3:J:88:ARG:HG2	12:X:33:ILE:HD11	2.02	0.41
3:J:138:LEU:HA	3:J:141:ILE:CD1	2.43	0.41
3:J:549:ILE:HD13	3:J:549:ILE:HA	1.80	0.41
4:O:256:LEU:CD1	10:V:3:ILE:HD12	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:20:LYS:HA	5:Q:21:PRO:HD2	1.80	0.41
7:S:104:LYS:O	7:S:106:ILE:N	2.54	0.41
9:U:60:ASP:O	9:U:61:VAL:O	2.38	0.41
10:V:45:GLN:HB3	10:V:53:ILE:HG22	2.01	0.41
1:A:212:LEU:CD2	1:A:242:ILE:HD13	2.50	0.41
1:A:290:ARG:HD2	1:A:291:SER:H	1.84	0.41
1:A:778:ALA:O	1:A:780:GLY:N	2.53	0.41
2:C:309:ASP:OD2	2:C:311:ARG:HD3	2.21	0.41
3:B:402:ASN:O	3:B:403:TRP:HB2	2.21	0.41
3:B:729:PHE:C	3:B:731:GLY:N	2.78	0.41
3:B:972:ASP:O	3:B:975:THR:HG23	2.20	0.41
1:I:329:ASP:CB	1:I:332:ILE:HD12	2.49	0.41
1:I:541:ALA:CB	1:I:542:PRO:HD2	2.46	0.41
1:I:600:LYS:HE3	1:I:732:GLY:HA2	2.00	0.41
1:I:742:GLN:HB2	3:J:919:MET:CE	2.44	0.41
1:I:879:LYS:HD3	1:I:879:LYS:HA	1.90	0.41
3:J:64:ARG:CG	3:J:97:TRP:CD1	3.01	0.41
3:J:97:TRP:O	3:J:98:LEU:HB3	2.20	0.41
3:J:133:TYR:CD2	3:J:141:ILE:HD11	2.56	0.41
3:J:319:ILE:C	3:J:321:LYS:H	2.28	0.41
3:J:654:ILE:HG13	3:J:708:LEU:HD21	2.03	0.41
3:J:659:GLU:O	3:J:660:HIS:CD2	2.72	0.41
3:J:719:GLY:O	3:J:989:TYR:CE1	2.74	0.41
3:J:800:PRO:HG2	12:X:37:VAL:HA	2.02	0.41
3:J:1015:GLN:HE21	3:J:1096:ALA:HB2	1.81	0.41
7:S:36:PHE:CD2	7:S:96:ILE:HD11	2.54	0.41
1:A:87:VAL:HG21	1:A:156:ILE:O	2.20	0.41
1:A:125:TRP:CZ3	8:H:82:ILE:HG21	2.56	0.41
1:A:155:LYS:HB3	1:A:156:ILE:HA	2.01	0.41
1:A:220:ARG:HH11	1:A:236:THR:CG2	2.27	0.41
1:A:342:ILE:C	1:A:344:ALA:N	2.76	0.41
1:A:465:HIS:NE2	3:B:1028:PHE:HD1	2.19	0.41
1:A:645:THR:OG1	1:A:646:MET:N	2.54	0.41
2:C:40:GLU:H	2:C:40:GLU:HG2	1.62	0.41
3:B:589:VAL:O	3:B:592:GLU:N	2.54	0.41
3:B:617:ASP:O	3:B:618:ALA:CB	2.67	0.41
3:B:654:ILE:CG2	3:B:881:ARG:HG2	2.51	0.41
3:B:751:ARG:HG2	3:B:871:ILE:HG23	2.01	0.41
3:B:894:GLN:HE21	4:D:33:MET:HE2	1.86	0.41
3:B:963:LEU:HD21	4:D:206:CYS:SG	2.60	0.41
4:D:65:ILE:HA	4:D:66:PRO:HD3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:102:GLY:HA3	5:E:103:PRO:HD3	1.95	0.41
10:L:59:THR:HG21	10:L:63:ILE:O	2.19	0.41
1:I:239:LEU:HD23	1:I:276:TYR:HE1	1.85	0.41
1:I:422:GLN:NE2	1:I:463:ASN:HD21	2.19	0.41
1:I:768:HIS:NE2	3:J:450:TRP:CZ2	2.79	0.41
1:I:870:ARG:HH21	2:M:61:GLU:H	1.69	0.41
2:M:261:VAL:O	2:M:261:VAL:CG1	2.67	0.41
3:J:669:GLN:C	3:J:671:ALA:N	2.78	0.41
4:O:6:LEU:HB3	4:O:14:ASP:HB2	2.02	0.41
6:R:40:TYR:CD2	6:R:40:TYR:C	2.97	0.41
6:R:55:VAL:HG12	6:R:59:LEU:HD12	2.02	0.41
7:S:34:ASN:OD1	7:S:34:ASN:N	2.53	0.41
8:T:35:LEU:O	8:T:36:GLY:C	2.62	0.41
10:V:47:HIS:O	10:V:49:LEU:N	2.53	0.41
1:A:568:VAL:HG21	1:A:597:VAL:HG11	2.01	0.41
1:A:708:ARG:HG3	1:A:709:SER:N	2.34	0.41
1:A:831:ARG:NH2	2:C:385:MET:CG	2.83	0.41
3:B:130:ILE:O	3:B:131:SER:C	2.62	0.41
3:B:487:LYS:C	3:B:489:LEU:N	2.78	0.41
3:B:987:VAL:HG11	11:N:47:ARG:NE	2.36	0.41
4:D:11:THR:HG22	4:D:232:SER:HB3	2.03	0.41
4:D:69:SER:O	4:D:70:GLU:C	2.63	0.41
4:D:178:LYS:HE2	4:D:178:LYS:HB2	1.92	0.41
4:D:223:GLU:H	4:D:223:GLU:HG3	1.69	0.41
9:K:39:ARG:HB3	9:K:65:ALA:HB1	2.03	0.41
13:Y:79:ASP:HB3	13:Y:80:SER:H	1.72	0.41
1:I:198:ASP:HA	1:I:199:PRO:HD2	1.99	0.41
1:I:418:LEU:HD23	1:I:430:MET:HE1	2.01	0.41
1:I:820:GLN:O	1:I:823:LEU:HD12	2.19	0.41
2:M:258:LEU:HB2	2:M:279:GLU:CG	2.49	0.41
2:M:312:HIS:O	2:M:316:ILE:HG12	2.20	0.41
3:J:52:GLU:HB2	3:J:56:LEU:HB3	2.02	0.41
3:J:130:ILE:HA	3:J:133:TYR:CD1	2.54	0.41
3:J:918:ARG:O	3:J:920:THR:HG23	2.21	0.41
4:O:178:LYS:H	4:O:178:LYS:NZ	2.18	0.41
7:S:26:LEU:HD22	7:S:42:ILE:O	2.21	0.41
7:S:76:TYR:CZ	7:S:110:GLU:HG3	2.56	0.41
7:S:104:LYS:HB3	7:S:104:LYS:HZ2	1.84	0.41
9:U:70:ARG:O	9:U:72:GLY:N	2.53	0.41
11:W:18:TRP:O	11:W:20:SER:N	2.50	0.41
1:A:77:LEU:HD23	1:A:246:ASN:HD21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HD12	1:A:313:LEU:HA	1.93	0.41
1:A:326:ILE:HG21	1:A:462:MET:CG	2.48	0.41
1:A:728:MET:HE1	3:B:912:PRO:O	2.21	0.41
1:A:747:LEU:HD22	1:A:786:PHE:CE1	2.56	0.41
2:C:158:ILE:HD11	2:C:165:ILE:HG23	2.02	0.41
3:B:448:THR:HG22	3:B:452:ARG:HD2	2.03	0.41
3:B:764:LYS:NZ	3:B:814:VAL:H	2.19	0.41
3:B:790:ARG:HH22	12:P:39:LYS:HE3	1.85	0.41
3:B:867:ARG:NH2	4:D:54:TYR:CE2	2.89	0.41
3:B:890:MET:HE2	3:B:891:LEU:N	2.29	0.41
3:B:1033:ARG:HH11	3:B:1033:ARG:HG3	1.85	0.41
3:B:1069:TRP:HB2	3:B:1078:VAL:O	2.20	0.41
3:B:1085:LYS:HG2	3:B:1086:SER:N	2.36	0.41
4:D:34:LEU:O	4:D:150:GLY:HA3	2.21	0.41
4:D:35:TYR:HE2	10:L:23:THR:HG21	1.86	0.41
8:H:69:SER:HB3	8:H:72:TYR:H	1.85	0.41
9:K:47:ALA:HA	9:K:48:PRO:HD2	1.95	0.41
1:I:77:LEU:HD23	1:I:246:ASN:HD21	1.85	0.41
1:I:402:ALA:O	1:I:405:TYR:HD1	2.03	0.41
1:I:425:LEU:O	1:I:426:HIS:HB2	2.20	0.41
1:I:563:HIS:ND1	1:I:876:VAL:HG13	2.36	0.41
1:I:876:VAL:C	1:I:878:TRP:N	2.79	0.41
2:M:125:TYR:HD1	2:M:271:LYS:HB2	1.85	0.41
2:M:212:ASN:C	2:M:214:ASP:N	2.78	0.41
2:M:279:GLU:O	2:M:280:ILE:C	2.64	0.41
2:M:320:MET:O	2:M:327:ARG:HG2	2.21	0.41
3:J:81:SER:OG	3:J:141:ILE:HG23	2.20	0.41
3:J:92:TYR:O	3:J:92:TYR:HD2	2.02	0.41
3:J:158:GLU:CD	3:J:416:ARG:NH1	2.79	0.41
3:J:167:LEU:HB2	3:J:168:ALA:H	1.74	0.41
3:J:490:TYR:CE1	3:J:527:ILE:CG2	3.03	0.41
3:J:962:TYR:HH	11:W:42:ARG:HD2	1.86	0.41
3:J:1109:ILE:O	3:J:1111:PRO:HD3	2.21	0.41
4:O:69:SER:O	4:O:70:GLU:C	2.64	0.41
5:Q:66:THR:CG2	5:Q:68:HIS:NE2	2.84	0.41
5:Q:103:PRO:HD3	6:R:37:THR:HG23	2.03	0.41
1:A:125:TRP:HD1	1:A:128:ALA:HB3	1.85	0.41
1:A:430:MET:O	1:A:431:MET:HG3	2.21	0.41
1:A:431:MET:CE	1:A:482:VAL:HG13	2.50	0.41
1:A:507:TYR:HB2	1:A:511:VAL:HG13	2.01	0.41
1:A:541:ALA:CB	1:A:542:PRO:HD2	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:ASN:HA	1:A:588:ILE:O	2.20	0.41
1:A:763:THR:HG22	1:A:772:TYR:HA	2.01	0.41
2:C:276:ASN:O	2:C:279:GLU:HB3	2.20	0.41
2:C:323:THR:O	2:C:325:ILE:N	2.54	0.41
2:C:382:GLY:C	2:C:384:GLY:H	2.26	0.41
3:B:264:ASN:HB2	3:B:267:ASP:H	1.85	0.41
3:B:661:ASN:HD22	3:B:920:THR:HA	1.86	0.41
3:B:838:VAL:CG1	3:B:839:THR:N	2.83	0.41
3:B:892:ILE:HA	3:B:893:PRO:HD3	1.96	0.41
4:D:159:VAL:HG23	4:D:232:SER:HA	2.03	0.41
5:E:171:LYS:HG2	5:E:172:LEU:H	1.85	0.41
9:K:63:SER:HA	9:K:66:GLU:HG3	2.03	0.41
13:Y:69:GLU:HB3	13:Y:73:LYS:NZ	2.36	0.41
3:J:49:ILE:H	3:J:49:ILE:HG13	1.65	0.41
3:J:223:PHE:CD2	3:J:256:LEU:HD22	2.56	0.41
3:J:816:PRO:HA	3:J:817:PRO:HD3	1.85	0.41
3:J:997:VAL:O	3:J:1000:LYS:O	2.39	0.41
4:O:21:PRO:HB3	10:V:34:ARG:HH21	1.84	0.41
4:O:35:TYR:HE2	10:V:23:THR:HG21	1.85	0.41
5:Q:5:ILE:O	5:Q:74:MET:N	2.53	0.41
11:W:22:ILE:HD12	11:W:22:ILE:H	1.86	0.41
1:A:4:LYS:HZ2	3:B:1115:LEU:HB3	1.85	0.41
1:A:371:LYS:HZ2	1:A:373:PRO:HD3	1.84	0.41
1:A:378:VAL:O	1:A:378:VAL:CG2	2.67	0.41
1:A:575:CYS:O	1:A:577:ASN:N	2.54	0.41
1:A:670:VAL:O	1:A:674:ASN:ND2	2.54	0.41
2:C:61:GLU:C	2:C:63:LEU:N	2.78	0.41
2:C:125:TYR:HD1	2:C:271:LYS:CB	2.30	0.41
2:C:126:LEU:HD11	2:C:249:TYR:HB2	2.03	0.41
2:C:245:LYS:HB2	2:C:250:ILE:HD11	2.03	0.41
2:C:293:ILE:O	2:C:294:ILE:C	2.64	0.41
3:B:14:ILE:O	3:B:17:TYR:HB3	2.21	0.41
3:B:34:PHE:CE1	3:B:351:ALA:HA	2.56	0.41
3:B:78:ARG:HH22	12:P:30:GLY:HA3	1.85	0.41
3:B:82:PRO:HG3	3:B:130:ILE:HD11	2.02	0.41
3:B:91:THR:O	3:B:92:TYR:C	2.63	0.41
3:B:102:PRO:HD2	3:B:109:ALA:HB3	2.01	0.41
3:B:222:PRO:O	3:B:223:PHE:C	2.63	0.41
3:B:228:ARG:NH2	3:B:233:LEU:O	2.50	0.41
3:B:580:ILE:HB	3:B:640:LEU:HB3	2.03	0.41
3:B:793:GLU:HB3	3:B:794:ASP:H	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1114:VAL:C	3:B:1115:LEU:HD23	2.46	0.41
5:E:51:VAL:C	5:E:53:THR:N	2.79	0.41
7:G:102:LEU:HA	7:G:106:ILE:HG21	2.03	0.41
7:G:107:SER:O	7:G:109:LYS:N	2.37	0.41
11:N:14:ILE:HD13	11:N:14:ILE:HA	1.93	0.41
1:I:4:LYS:HG2	1:I:5:ASN:N	2.36	0.41
1:I:86:LEU:HD13	1:I:207:MET:HG2	2.02	0.41
1:I:234:ASP:C	1:I:236:THR:N	2.79	0.41
1:I:329:ASP:HA	1:I:330:PRO:HD3	1.74	0.41
1:I:537:PRO:HA	1:I:546:TYR:CD2	2.55	0.41
1:I:859:TYR:CB	2:M:64:ILE:HG12	2.50	0.41
2:M:130:TYR:HD2	2:M:130:TYR:HA	1.77	0.41
2:M:146:TYR:O	2:M:238:LYS:CD	2.69	0.41
2:M:174:LEU:CB	2:M:179:VAL:HG13	2.50	0.41
3:J:99:THR:HG23	3:J:111:PRO:HB3	2.03	0.41
3:J:321:LYS:CA	3:J:324:GLU:HB3	2.51	0.41
3:J:402:ASN:HB3	3:J:403:TRP:H	1.46	0.41
3:J:419:TRP:HZ3	3:J:712:GLY:CA	2.34	0.41
3:J:471:ALA:O	3:J:473:MET:HG3	2.21	0.41
3:J:580:ILE:HG13	3:J:642:ILE:HD13	2.03	0.41
3:J:589:VAL:O	3:J:592:GLU:N	2.54	0.41
4:O:61:ARG:HH11	4:O:61:ARG:HG2	1.86	0.41
4:O:168:PRO:HG3	4:O:203:CYS:O	2.21	0.41
5:Q:110:ILE:O	5:Q:118:LEU:HD22	2.21	0.41
5:Q:163:THR:O	5:Q:164:MET:HG3	2.21	0.41
7:S:83:ASP:N	7:S:94:THR:O	2.49	0.41
9:U:32:ILE:O	9:U:36:ILE:HG12	2.20	0.41
1:A:114:TYR:O	1:A:118:TYR:HB2	2.20	0.41
1:A:184:LEU:O	1:A:186:LYS:N	2.54	0.41
1:A:371:LYS:HD3	1:A:372:TRP:N	2.36	0.41
1:A:467:PRO:HA	3:B:1048:ARG:NH2	2.36	0.41
1:A:764:ARG:NH2	3:B:624:ALA:O	2.54	0.41
2:C:49:ASP:O	2:C:50:LYS:C	2.64	0.41
3:B:304:SER:OG	3:B:307:ASP:OD2	2.39	0.41
3:B:978:LYS:HG2	4:D:166:TYR:CE2	2.56	0.41
4:D:78:TRP:N	4:D:78:TRP:CD1	2.86	0.41
8:H:39:PRO:HB2	8:H:80:TYR:CE2	2.56	0.41
12:P:24:VAL:O	12:P:24:VAL:CG1	2.67	0.41
1:I:561:ASN:ND2	1:I:590:ASN:H	2.18	0.41
1:I:716:SER:HB2	1:I:726:TYR:OH	2.22	0.41
1:I:805:GLY:C	1:I:807:VAL:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:126:LEU:O	2:M:127:THR:C	2.63	0.41
2:M:258:LEU:HD12	2:M:258:LEU:HA	1.90	0.41
3:J:88:ARG:CD	3:J:853:THR:CG2	2.78	0.41
3:J:600:GLY:C	3:J:602:ILE:N	2.78	0.41
3:J:867:ARG:NH2	4:O:54:TYR:CE2	2.89	0.41
3:J:1113:LEU:HD12	3:J:1113:LEU:N	2.08	0.41
4:O:44:VAL:HG13	4:O:143:ALA:HB2	2.03	0.41
4:O:256:LEU:O	4:O:257:GLU:C	2.63	0.41
5:Q:3:LYS:HB2	5:Q:3:LYS:HE3	1.60	0.41
9:U:18:VAL:HG12	9:U:22:LEU:CD1	2.50	0.41
9:U:42:GLN:HE21	9:U:42:GLN:HB2	1.78	0.41
10:V:4:ARG:HG2	10:V:4:ARG:NH1	2.29	0.41
1:A:8:GLY:O	3:B:1114:VAL:HG22	2.21	0.40
1:A:53:GLU:O	1:A:55:GLY:N	2.54	0.40
1:A:447:LEU:HD11	3:B:731:GLY:O	2.20	0.40
3:B:81:SER:OG	3:B:141:ILE:HG23	2.21	0.40
3:B:138:LEU:HA	3:B:141:ILE:CD1	2.41	0.40
3:B:221:ILE:HA	3:B:222:PRO:HD3	1.95	0.40
3:B:443:ARG:NH2	3:B:462:PRO:O	2.54	0.40
3:B:446:HIS:H	3:B:449:GLN:NE2	2.19	0.40
3:B:489:LEU:HD23	3:B:489:LEU:HA	1.87	0.40
3:B:691:ARG:NH1	3:B:756:ARG:HH21	2.18	0.40
3:B:932:TYR:CD2	3:B:953:LEU:HD22	2.56	0.40
4:D:23:GLU:O	10:L:27:LEU:HD13	2.21	0.40
1:I:99:ARG:HG2	1:I:183:ARG:NH1	2.35	0.40
1:I:114:TYR:O	1:I:118:TYR:HB2	2.20	0.40
1:I:125:TRP:HD1	1:I:128:ALA:HB3	1.86	0.40
1:I:446:ASN:O	1:I:447:LEU:C	2.64	0.40
1:I:499:ALA:H	1:I:502:TYR:HD2	1.69	0.40
1:I:608:PRO:HA	1:I:862:HIS:CE1	2.56	0.40
1:I:651:VAL:HG21	1:I:743:MET:HB3	2.02	0.40
1:I:787:ARG:O	1:I:788:THR:C	2.64	0.40
2:M:103:GLY:HA2	2:M:106:ARG:HB2	2.02	0.40
2:M:344:ARG:HB3	2:M:353:HIS:NE2	2.36	0.40
3:J:157:SER:O	3:J:158:GLU:CB	2.68	0.40
3:J:658:PRO:HB2	3:J:666:ASN:HD21	1.86	0.40
4:O:22:LEU:C	4:O:24:PHE:H	2.29	0.40
4:O:131:VAL:HA	11:W:2:LEU:CD1	2.49	0.40
4:O:178:LYS:C	4:O:180:VAL:N	2.79	0.40
4:O:183:CYS:HB2	16:O:1001:F3S:S1	2.61	0.40
9:U:23:TRP:CE3	9:U:23:TRP:HA	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:3:ILE:HD11	11:W:18:TRP:CE3	2.56	0.40
1:A:58:CYS:SG	1:A:59:PRO:CD	3.10	0.40
1:A:203:ARG:CZ	1:A:206:TRP:HB2	2.50	0.40
1:A:522:GLN:HG2	10:L:40:PHE:CE1	2.56	0.40
2:C:141:ALA:O	2:C:145:GLU:HB2	2.21	0.40
3:B:174:VAL:HG11	3:B:325:LEU:HD23	2.03	0.40
3:B:420:LEU:O	3:B:421:SER:C	2.62	0.40
3:B:936:SER:O	11:N:32:GLY:HA3	2.21	0.40
3:B:1083:GLY:O	3:B:1084:ASP:HB2	2.21	0.40
5:E:90:LEU:HD12	5:E:100:ASN:HB2	2.01	0.40
6:F:31:SER:HB2	6:F:32:ASN:H	1.70	0.40
9:K:63:SER:O	9:K:66:GLU:HB2	2.21	0.40
1:I:471:GLU:OE1	9:U:41:LEU:CD1	2.70	0.40
1:I:500:GLN:HB2	3:J:913:HIS:CG	2.56	0.40
1:I:575:CYS:O	1:I:577:ASN:N	2.52	0.40
2:M:167:LEU:HD12	2:M:207:ASN:HD21	1.87	0.40
2:M:298:SER:O	2:M:301:LEU:HD12	2.22	0.40
3:J:655:ILE:HG12	3:J:669:GLN:HG2	2.03	0.40
3:J:680:TYR:CE2	3:J:692:ALA:HB1	2.56	0.40
3:J:707:ALA:O	3:J:709:ASP:N	2.54	0.40
3:J:876:ASP:HB2	3:J:878:PHE:HE1	1.86	0.40
3:J:1001:LEU:O	3:J:1020:ARG:HD3	2.21	0.40
4:O:176:CYS:N	4:O:195:LEU:HD21	2.37	0.40
5:Q:110:ILE:HD12	5:Q:118:LEU:HA	2.04	0.40
7:S:36:PHE:CG	7:S:96:ILE:HD11	2.56	0.40
8:T:17:VAL:HA	8:T:18:PRO:HD3	1.83	0.40
11:W:21:PHE:O	11:W:25:VAL:HG23	2.21	0.40
1:A:81:VAL:O	1:A:209:LEU:N	2.54	0.40
1:A:480:MET:HG2	3:B:1039:PHE:CE1	2.56	0.40
1:A:500:GLN:O	1:A:501:ASP:C	2.64	0.40
2:C:108:ILE:O	2:C:109:GLU:C	2.65	0.40
2:C:391:ARG:NH1	2:C:391:ARG:HG3	2.33	0.40
3:B:245:ASP:N	3:B:246:PRO:CD	2.83	0.40
3:B:249:GLN:O	3:B:253:PHE:CD1	2.74	0.40
3:B:353:LEU:HD12	3:B:404:VAL:HG13	2.03	0.40
3:B:669:GLN:C	3:B:671:ALA:N	2.80	0.40
3:B:902:LYS:HB2	11:N:42:ARG:NH1	2.37	0.40
5:E:38:ILE:O	5:E:39:LEU:HB2	2.20	0.40
5:E:151:SER:HB3	5:E:158:PRO:N	2.36	0.40
1:I:105:LYS:HB3	1:I:109:ASP:OD1	2.21	0.40
1:I:326:ILE:HG21	1:I:462:MET:CG	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:704:LEU:HD22	1:I:781:PHE:CD1	2.55	0.40
1:I:818:TYR:OH	2:M:348:GLU:OE2	2.25	0.40
2:M:53:ASP:O	2:M:55:ALA:N	2.54	0.40
2:M:148:LYS:HG2	2:M:230:LYS:O	2.21	0.40
3:J:1015:GLN:HG2	3:J:1054:ASP:OD1	2.21	0.40
5:Q:39:LEU:HD13	5:Q:42:LEU:HD21	2.02	0.40
5:Q:64:GLY:O	9:U:42:GLN:HG3	2.21	0.40
6:R:63:VAL:HG12	6:R:63:VAL:O	2.21	0.40
1:A:288:LYS:HG2	1:A:294:PRO:CA	2.52	0.40
1:A:318:VAL:HG23	1:A:321:SER:HB2	2.03	0.40
3:B:234:THR:O	3:B:237:ASP:HB2	2.22	0.40
3:B:320:SER:O	3:B:320:SER:OG	2.33	0.40
3:B:457:GLU:HG2	3:B:469:ASN:CG	2.45	0.40
3:B:603:THR:C	3:B:605:ASP:N	2.77	0.40
3:B:781:ARG:CD	3:B:782:GLY:H	2.33	0.40
3:B:803:GLU:HB3	3:B:805:LYS:HZ1	1.82	0.40
3:B:811:ILE:O	3:B:836:SER:HB2	2.21	0.40
3:B:1087:ASN:C	3:B:1088:LEU:HG	2.46	0.40
1:I:217:ILE:O	1:I:219:ILE:N	2.54	0.40
1:I:312:ASN:HA	1:I:315:GLY:O	2.21	0.40
1:I:446:ASN:C	1:I:448:LEU:N	2.80	0.40
1:I:475:GLU:CD	3:J:1043:MET:HB2	2.46	0.40
1:I:566:ALA:HB1	1:I:599:ASP:OD2	2.21	0.40
1:I:645:THR:HG22	1:I:724:PHE:CZ	2.55	0.40
3:J:554:ASN:HD22	3:J:574:ARG:HH11	1.69	0.40
3:J:811:ILE:O	3:J:836:SER:HB2	2.21	0.40
3:J:963:LEU:HA	3:J:964:PRO:HD3	1.96	0.40
3:J:1066:TYR:CE1	3:J:1112:ARG:HD3	2.55	0.40
4:O:18:GLU:HB2	4:O:225:LYS:HE3	2.02	0.40
4:O:94:THR:CG2	4:O:145:LEU:HB2	2.52	0.40
8:T:80:TYR:C	8:T:81:VAL:HG23	2.47	0.40
1:A:600:LYS:HB2	1:A:732:GLY:HA3	2.03	0.40
1:A:733:ALA:CB	3:B:913:HIS:HE1	2.26	0.40
2:C:48:ILE:H	2:C:50:LYS:HG3	1.87	0.40
2:C:237:ILE:C	2:C:238:LYS:HG2	2.47	0.40
2:C:290:ARG:HG3	2:C:321:THR:HG21	2.04	0.40
2:C:370:VAL:O	2:C:374:ILE:HD12	2.22	0.40
3:B:329:ARG:HD2	3:B:562:PHE:HB3	2.04	0.40
3:B:430:ILE:HD13	3:B:467:VAL:HB	2.02	0.40
3:B:463:ASN:HB3	3:B:467:VAL:HG12	2.02	0.40
3:B:485:VAL:C	3:B:487:LYS:N	2.79	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:904:VAL:HG21	11:N:42:ARG:HG2	2.03	0.40
3:B:965:ASP:C	3:B:967:THR:H	2.30	0.40
3:B:1064:CYS:HG	14:B:2001:ZN:ZN	1.29	0.40
5:E:147:ILE:HD11	5:E:163:THR:HG22	2.03	0.40
13:Y:57:GLY:CA	13:Y:61:LEU:HD21	2.51	0.40
1:I:53:GLU:O	1:I:55:GLY:N	2.55	0.40
1:I:253:ILE:HG12	1:I:266:TRP:HZ2	1.87	0.40
1:I:353:ILE:HG21	1:I:358:ILE:HD12	2.04	0.40
1:I:415:ASP:H	1:I:435:VAL:HG12	1.85	0.40
1:I:480:MET:HE2	1:I:480:MET:HB3	1.79	0.40
1:I:539:ILE:HG21	7:S:46:ILE:HD11	2.04	0.40
1:I:766:LEU:HD22	1:I:766:LEU:HA	2.01	0.40
1:I:785:SER:C	1:I:787:ARG:N	2.78	0.40
3:J:116:ILE:HD12	3:J:361:PHE:HZ	1.86	0.40
3:J:223:PHE:CE1	3:J:319:ILE:HG13	2.57	0.40
3:J:676:ALA:O	3:J:677:LEU:HD23	2.21	0.40
3:J:725:ALA:O	3:J:909:ILE:HG23	2.21	0.40
3:J:853:THR:O	3:J:861:LEU:N	2.55	0.40
3:J:895:VAL:HG11	4:O:34:LEU:CG	2.52	0.40
5:Q:92:VAL:HG12	5:Q:93:ASP:H	1.85	0.40
10:V:29:ALA:O	10:V:33:ARG:HG3	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	828/880 (94%)	597 (72%)	154 (19%)	77 (9%)	0	3
1	I	828/880 (94%)	594 (72%)	157 (19%)	77 (9%)	0	3
2	C	366/395 (93%)	225 (62%)	92 (25%)	49 (13%)	0	1
2	M	366/395 (93%)	232 (63%)	84 (23%)	50 (14%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	1084/1124 (96%)	752 (69%)	215 (20%)	117 (11%)	0	2
3	J	1084/1124 (96%)	752 (69%)	217 (20%)	115 (11%)	0	2
4	D	262/265 (99%)	199 (76%)	50 (19%)	13 (5%)	1	10
4	O	262/265 (99%)	198 (76%)	53 (20%)	11 (4%)	2	14
5	E	172/180 (96%)	125 (73%)	35 (20%)	12 (7%)	1	6
5	Q	172/180 (96%)	128 (74%)	34 (20%)	10 (6%)	1	8
6	F	87/113 (77%)	57 (66%)	25 (29%)	5 (6%)	1	9
6	R	87/113 (77%)	59 (68%)	19 (22%)	9 (10%)	0	2
7	G	111/132 (84%)	82 (74%)	22 (20%)	7 (6%)	1	7
7	S	111/132 (84%)	84 (76%)	16 (14%)	11 (10%)	0	3
8	H	72/84 (86%)	46 (64%)	12 (17%)	14 (19%)	0	0
8	T	72/84 (86%)	39 (54%)	20 (28%)	13 (18%)	0	0
9	K	80/95 (84%)	50 (62%)	21 (26%)	9 (11%)	0	2
9	U	80/95 (84%)	43 (54%)	18 (22%)	19 (24%)	0	0
10	L	90/92 (98%)	66 (73%)	16 (18%)	8 (9%)	0	3
10	V	90/92 (98%)	58 (64%)	28 (31%)	4 (4%)	2	13
11	N	62/66 (94%)	41 (66%)	17 (27%)	4 (6%)	1	6
11	W	62/66 (94%)	43 (69%)	15 (24%)	4 (6%)	1	6
12	P	41/48 (85%)	29 (71%)	8 (20%)	4 (10%)	0	3
12	X	41/48 (85%)	28 (68%)	8 (20%)	5 (12%)	0	1
13	Y	43/104 (41%)	26 (60%)	13 (30%)	4 (9%)	0	3
13	Z	43/104 (41%)	30 (70%)	11 (26%)	2 (5%)	2	12
All	All	6596/7156 (92%)	4583 (70%)	1360 (21%)	653 (10%)	0	3

All (653) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	PRO
1	A	56	GLN
1	A	58	CYS
1	A	64	THR
1	A	145	VAL
1	A	207	MET
1	A	332	ILE

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Mol	Chain	Res	Type
1	A	376	ASN
1	A	377	TYR
1	A	426	HIS
1	A	508	LEU
1	A	528	ALA
1	A	532	ILE
1	A	541	ALA
1	A	585	TYR
1	A	608	PRO
1	A	746	MET
1	A	829	ASP
1	A	842	TYR
1	A	865	THR
1	A	876	VAL
2	C	28	ILE
2	C	31	ASP
2	C	48	ILE
2	C	50	LYS
2	C	66	PRO
2	C	104	LEU
2	C	113	ALA
2	C	127	THR
2	C	188	ILE
2	C	191	LEU
2	C	193	LEU
2	C	211	ALA
2	C	275	ASN
2	C	306	LEU
2	C	324	GLY
2	C	362	ASP
2	C	364	GLU
2	C	365	GLU
2	C	390	MET
2	C	391	ARG
3	B	23	LEU
3	B	97	TRP
3	B	124	LYS
3	B	171	ARG
3	B	297	PHE
3	B	300	HIS
3	B	325	LEU
3	B	347	GLY

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Mol	Chain	Res	Type
3	B	372	SER
3	B	378	LYS
3	B	382	LYS
3	B	402	ASN
3	B	403	TRP
3	B	448	THR
3	B	473	MET
3	B	483	ARG
3	B	571	ASP
3	B	602	ILE
3	B	659	GLU
3	B	663	SER
3	B	730	THR
3	B	790	ARG
3	B	800	PRO
3	B	801	GLU
3	B	945	PHE
3	B	966	ALA
3	B	1030	GLU
3	B	1056	THR
3	B	1071	ASP
3	B	1114	VAL
3	B	1118	LYS
4	D	135	THR
4	D	152	GLU
4	D	205	LEU
5	E	39	LEU
5	E	88	GLU
5	E	116	ASP
6	F	3	SER
7	G	68	HIS
7	G	88	ASN
7	G	108	ASN
8	H	12	ARG
8	H	25	ILE
8	H	28	ALA
8	H	43	PRO
9	K	42	GLN
9	K	51	ILE
9	K	61	VAL
9	K	62	ILE
9	K	72	GLY

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Mol	Chain	Res	Type
10	L	10	SER
10	L	36	SER
10	L	46	PRO
10	L	48	PRO
11	N	29	GLU
12	P	26	CYS
12	P	34	ILE
1	I	47	PRO
1	I	56	GLN
1	I	58	CYS
1	I	64	THR
1	I	145	VAL
1	I	207	MET
1	I	332	ILE
1	I	377	TYR
1	I	426	HIS
1	I	508	LEU
1	I	528	ALA
1	I	532	ILE
1	I	541	ALA
1	I	585	TYR
1	I	595	GLU
1	I	607	GLN
1	I	608	PRO
1	I	721	PRO
1	I	733	ALA
1	I	746	MET
1	I	825	ASN
1	I	826	ALA
1	I	829	ASP
1	I	842	TYR
1	I	865	THR
1	I	876	VAL
2	M	28	ILE
2	M	31	ASP
2	M	48	ILE
2	M	54	LEU
2	M	66	PRO
2	M	104	LEU
2	M	113	ALA
2	M	115	LYS
2	M	127	THR

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Mol	Chain	Res	Type
2	M	146	TYR
2	M	213	ILE
2	M	306	LEU
2	M	365	GLU
2	M	391	ARG
3	J	23	LEU
3	J	97	TRP
3	J	112	GLU
3	J	124	LYS
3	J	171	ARG
3	J	297	PHE
3	J	300	HIS
3	J	325	LEU
3	J	372	SER
3	J	378	LYS
3	J	402	ASN
3	J	403	TRP
3	J	448	THR
3	J	473	MET
3	J	483	ARG
3	J	530	TYR
3	J	571	ASP
3	J	602	ILE
3	J	659	GLU
3	J	663	SER
3	J	730	THR
3	J	790	ARG
3	J	800	PRO
3	J	801	GLU
3	J	945	PHE
3	J	966	ALA
3	J	1030	GLU
3	J	1056	THR
3	J	1071	ASP
3	J	1111	PRO
3	J	1114	VAL
3	J	1118	LYS
4	O	135	THR
4	O	152	GLU
4	O	205	LEU
5	Q	32	GLN
5	Q	39	LEU

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Mol	Chain	Res	Type
5	Q	40	LYS
6	R	7	VAL
6	R	32	ASN
6	R	64	SER
7	S	65	SER
7	S	88	ASN
7	S	108	ASN
8	T	15	TYR
8	T	21	GLU
8	T	43	PRO
9	U	14	HIS
9	U	15	PHE
9	U	20	ILE
9	U	26	ARG
9	U	34	ARG
9	U	42	GLN
9	U	47	ALA
9	U	51	ILE
9	U	59	THR
9	U	61	VAL
11	W	29	GLU
12	X	26	CYS
12	X	34	ILE
13	Z	59	ILE
13	Z	77	LYS
1	A	27	ILE
1	A	150	ASN
1	A	155	LYS
1	A	185	GLU
1	A	307	GLY
1	A	355	PRO
1	A	378	VAL
1	A	392	LYS
1	A	393	ASP
1	A	447	LEU
1	A	529	ASP
1	A	534	LEU
1	A	576	LYS
1	A	595	GLU
1	A	607	GLN
1	A	621	ASP
1	A	682	GLY

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Mol	Chain	Res	Type
1	A	721	PRO
1	A	733	ALA
1	A	749	GLN
1	A	763	THR
1	A	764	ARG
1	A	825	ASN
1	A	826	ALA
1	A	841	LEU
2	C	115	LYS
2	C	190	ARG
2	C	210	PHE
2	C	264	VAL
2	C	299	LYS
2	C	331	ARG
2	C	360	ARG
2	C	367	LYS
3	B	30	SER
3	B	47	GLY
3	B	50	PRO
3	B	55	GLY
3	B	74	ASP
3	B	105	ASN
3	B	109	ALA
3	B	112	GLU
3	B	158	GLU
3	B	167	LEU
3	B	246	PRO
3	B	292	ILE
3	B	404	VAL
3	B	418	ASN
3	B	482	GLU
3	B	530	TYR
3	B	534	GLY
3	B	574	ARG
3	B	587	PRO
3	B	604	PHE
3	B	605	ASP
3	B	618	ALA
3	B	684	TYR
3	B	691	ARG
3	B	708	LEU
3	B	736	ASP

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Mol	Chain	Res	Type
3	B	806	GLY
3	B	933	ALA
3	B	951	GLU
3	B	1001	LEU
3	B	1065	GLY
3	B	1111	PRO
4	D	103	PRO
4	D	206	CYS
5	E	40	LYS
5	E	65	ALA
5	E	82	GLN
5	E	122	ASN
5	E	139	GLY
7	G	97	SER
8	H	56	ASN
8	H	74	GLU
8	H	80	TYR
8	H	81	VAL
9	K	47	ALA
10	L	50	SER
10	L	62	SER
11	N	63	THR
13	Y	66	LYS
1	I	27	ILE
1	I	80	PRO
1	I	150	ASN
1	I	155	LYS
1	I	185	GLU
1	I	307	GLY
1	I	372	TRP
1	I	376	ASN
1	I	378	VAL
1	I	392	LYS
1	I	393	ASP
1	I	447	LEU
1	I	454	ASN
1	I	482	VAL
1	I	529	ASP
1	I	534	LEU
1	I	576	LYS
1	I	621	ASP
1	I	682	GLY

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Mol	Chain	Res	Type
1	I	741	THR
1	I	749	GLN
1	I	764	ARG
1	I	841	LEU
2	M	44	THR
2	M	128	ASP
2	M	211	ALA
2	M	212	ASN
2	M	235	LYS
2	M	247	ASP
2	M	280	ILE
2	M	281	GLU
2	M	304	GLN
2	M	351	VAL
3	J	30	SER
3	J	50	PRO
3	J	51	THR
3	J	55	GLY
3	J	74	ASP
3	J	105	ASN
3	J	109	ALA
3	J	158	GLU
3	J	167	LEU
3	J	246	PRO
3	J	292	ILE
3	J	347	GLY
3	J	382	LYS
3	J	404	VAL
3	J	418	ASN
3	J	457	GLU
3	J	482	GLU
3	J	534	GLY
3	J	574	ARG
3	J	587	PRO
3	J	604	PHE
3	J	605	ASP
3	J	618	ALA
3	J	684	TYR
3	J	708	LEU
3	J	736	ASP
3	J	806	GLY
3	J	933	ALA

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Mol	Chain	Res	Type
3	J	951	GLU
3	J	972	ASP
3	J	1001	LEU
3	J	1065	GLY
4	O	162	SER
4	O	179	ALA
6	R	49	ALA
7	S	80	GLU
7	S	97	SER
7	S	105	ILE
8	T	28	ALA
8	T	29	TYR
9	U	25	ASN
9	U	71	ARG
10	V	28	ILE
10	V	66	LYS
11	W	63	THR
1	A	80	PRO
1	A	106	ILE
1	A	121	ILE
1	A	286	PRO
1	A	356	TRP
1	A	372	TRP
1	A	454	ASN
1	A	514	THR
1	A	688	PRO
1	A	741	THR
1	A	852	ASP
2	C	58	GLU
2	C	145	GLU
2	C	192	LYS
2	C	196	PHE
2	C	235	LYS
2	C	272	VAL
2	C	290	ARG
2	C	302	ALA
3	B	51	THR
3	B	75	ARG
3	B	110	GLU
3	B	155	ASN
3	B	170	ASN
3	B	182	ASN

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Mol	Chain	Res	Type
3	B	184	THR
3	B	247	GLU
3	B	276	VAL
3	B	449	GLN
3	B	559	VAL
3	B	660	HIS
3	B	769	GLN
3	B	901	VAL
3	B	921	LEU
3	B	1080	PRO
4	D	23	GLU
4	D	70	GLU
4	D	179	ALA
5	E	52	LYS
6	F	43	SER
7	G	48	ILE
8	H	44	TRP
9	K	26	ARG
9	K	27	LEU
9	K	71	ARG
12	P	13	PHE
13	Y	56	ASN
13	Y	70	ASP
1	I	97	THR
1	I	106	ILE
1	I	235	LEU
1	I	356	TRP
1	I	514	THR
1	I	688	PRO
1	I	763	THR
1	I	864	LYS
2	M	50	LYS
2	M	71	GLY
2	M	114	LYS
2	M	278	ARG
2	M	279	GLU
2	M	337	GLU
2	M	367	LYS
3	J	47	GLY
3	J	75	ARG
3	J	110	GLU
3	J	170	ASN

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Mol	Chain	Res	Type
3	J	182	ASN
3	J	184	THR
3	J	231	GLY
3	J	247	GLU
3	J	276	VAL
3	J	332	PRO
3	J	449	GLN
3	J	559	VAL
3	J	657	TYR
3	J	660	HIS
3	J	691	ARG
3	J	759	SER
3	J	769	GLN
3	J	888	ILE
3	J	921	LEU
3	J	1080	PRO
4	O	103	PRO
4	O	206	CYS
5	Q	16	ASN
5	Q	56	GLU
5	Q	116	ASP
7	S	47	ASN
7	S	102	LEU
8	T	19	LYS
8	T	20	HIS
8	T	54	SER
8	T	81	VAL
9	U	13	LEU
9	U	16	ASN
9	U	44	ALA
12	X	13	PHE
12	X	28	TYR
1	A	54	PRO
1	A	97	THR
1	A	103	ARG
1	A	235	LEU
1	A	524	ILE
1	A	626	TRP
1	A	645	THR
1	A	686	PRO
2	C	45	ARG
2	C	67	GLY

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Mol	Chain	Res	Type
2	C	238	LYS
3	B	111	PRO
3	B	210	PHE
3	B	223	PHE
3	B	231	GLY
3	B	331	GLU
3	B	338	TYR
3	B	376	GLY
3	B	657	TYR
3	B	759	SER
3	B	860	LYS
3	B	1048	ARG
3	B	1087	ASN
4	D	162	SER
4	D	177	GLU
5	E	131	LYS
6	F	34	LEU
6	F	57	GLU
8	H	10	ASP
8	H	15	TYR
8	H	29	TYR
8	H	79	ARG
10	L	6	LEU
11	N	19	GLN
12	P	28	TYR
1	I	103	ARG
1	I	218	THR
1	I	286	PRO
1	I	355	PRO
1	I	537	PRO
1	I	686	PRO
1	I	852	ASP
2	M	12	TYR
2	M	144	LEU
2	M	193	LEU
2	M	210	PHE
2	M	218	ALA
3	J	98	LEU
3	J	111	PRO
3	J	113	GLU
3	J	331	GLU
3	J	338	TYR

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Mol	Chain	Res	Type
3	J	486	GLU
3	J	901	VAL
4	O	7	HIS
4	O	70	GLU
5	Q	81	VAL
5	Q	139	GLY
6	R	25	ILE
6	R	43	SER
6	R	80	SER
7	S	48	ILE
7	S	99	TYR
8	T	12	ARG
9	U	19	PHE
11	W	6	ARG
11	W	19	GLN
1	A	391	VAL
1	A	403	PRO
1	A	482	VAL
1	A	537	PRO
1	A	543	ARG
1	A	779	ARG
2	C	144	LEU
2	C	161	ALA
2	C	213	ILE
2	C	239	ARG
2	C	348	GLU
3	B	98	LEU
3	B	103	VAL
3	B	194	ALA
3	B	441	GLU
3	B	635	PRO
3	B	915	LEU
3	B	1034	ASP
4	D	127	ASP
6	F	31	SER
11	N	6	ARG
1	I	54	PRO
1	I	143	ALA
1	I	524	ILE
1	I	543	ARG
1	I	645	THR
2	M	74	ALA

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Mol	Chain	Res	Type
2	M	298	SER
3	J	103	VAL
3	J	194	ALA
3	J	210	PHE
3	J	376	GLY
3	J	598	GLU
3	J	635	PRO
3	J	770	GLU
3	J	781	ARG
3	J	915	LEU
4	O	177	GLU
5	Q	38	ILE
8	T	80	TYR
1	A	143	ALA
2	C	114	LYS
2	C	128	ASP
3	B	332	PRO
3	B	377	ARG
3	B	438	PRO
3	B	598	GLU
3	B	703	VAL
3	B	770	GLU
3	B	779	GLY
3	B	972	ASP
4	D	79	PRO
4	D	94	THR
5	E	51	VAL
1	I	334	ILE
1	I	391	VAL
1	I	403	PRO
1	I	851	GLY
2	M	161	ALA
2	M	203	ASP
2	M	363	VAL
2	M	364	GLU
3	J	223	PHE
3	J	377	ARG
3	J	438	PRO
3	J	703	VAL
3	J	779	GLY
3	J	793	GLU
3	J	1048	ARG

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Mol	Chain	Res	Type
3	J	1087	ASN
6	R	60	SER
8	T	11	PRO
9	U	70	ARG
12	X	18	LEU
1	A	530	VAL
1	A	851	GLY
2	C	71	GLY
3	B	299	PRO
3	B	328	GLY
3	B	591	ILE
3	B	814	VAL
3	B	944	PRO
3	B	950	ILE
8	H	59	PRO
1	I	121	ILE
2	M	24	LEU
2	M	67	GLY
2	M	119	THR
2	M	179	VAL
2	M	181	VAL
3	J	299	PRO
3	J	903	GLY
3	J	950	ILE
3	J	1108	ILE
3	B	767	GLY
3	B	1108	ILE
10	L	28	ILE
1	I	530	VAL
2	M	277	ILE
6	R	4	VAL
7	S	64	PRO
8	T	10	ASP
1	A	334	ILE
1	A	369	PRO
2	C	393	ILE
3	B	253	PHE
7	G	64	PRO
7	G	78	VAL
13	Y	57	GLY
2	M	260	GLY
2	M	261	VAL

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Mol	Chain	Res	Type
3	J	645	PRO
3	J	944	PRO
5	Q	51	VAL
9	U	64	ILE
10	V	48	PRO
2	C	181	VAL
3	B	645	PRO
3	B	888	ILE
5	E	25	ILE
1	I	330	PRO
1	I	369	PRO
3	J	591	ILE
9	U	62	ILE
10	V	46	PRO
1	A	760	GLY
4	O	79	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	729/766 (95%)	585 (80%)	144 (20%)	1	5
1	I	729/766 (95%)	583 (80%)	146 (20%)	1	4
2	C	318/340 (94%)	226 (71%)	92 (29%)	0	1
2	M	318/340 (94%)	222 (70%)	96 (30%)	0	0
3	B	937/965 (97%)	756 (81%)	181 (19%)	1	5
3	J	937/965 (97%)	752 (80%)	185 (20%)	1	5
4	D	241/242 (100%)	216 (90%)	25 (10%)	7	24
4	O	241/242 (100%)	216 (90%)	25 (10%)	7	24
5	E	156/159 (98%)	121 (78%)	35 (22%)	1	3
5	Q	156/159 (98%)	116 (74%)	40 (26%)	0	1
6	F	82/106 (77%)	67 (82%)	15 (18%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	R	82/106 (77%)	68 (83%)	14 (17%)	2	9
7	G	105/125 (84%)	86 (82%)	19 (18%)	2	7
7	S	105/125 (84%)	77 (73%)	28 (27%)	0	1
8	H	67/75 (89%)	48 (72%)	19 (28%)	0	1
8	T	67/75 (89%)	51 (76%)	16 (24%)	1	2
9	K	72/84 (86%)	48 (67%)	24 (33%)	0	0
9	U	72/84 (86%)	47 (65%)	25 (35%)	0	0
10	L	81/81 (100%)	63 (78%)	18 (22%)	1	3
10	V	81/81 (100%)	60 (74%)	21 (26%)	0	1
11	N	58/60 (97%)	48 (83%)	10 (17%)	2	8
11	W	58/60 (97%)	48 (83%)	10 (17%)	2	8
12	P	39/43 (91%)	32 (82%)	7 (18%)	2	7
12	X	39/43 (91%)	30 (77%)	9 (23%)	1	2
13	Y	43/97 (44%)	34 (79%)	9 (21%)	1	4
13	Z	43/97 (44%)	31 (72%)	12 (28%)	0	1
All	All	5856/6286 (93%)	4631 (79%)	1225 (21%)	1	4

All (1225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	15	SER
1	A	29	THR
1	A	45	MET
1	A	48	ARG
1	A	58	CYS
1	A	60	THR
1	A	64	THR
1	A	65	LEU
1	A	79	ARG
1	A	82	ILE
1	A	84	VAL
1	A	101	CYS
1	A	103	ARG
1	A	105	LYS
1	A	107	SER
1	A	111	ILE

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Mol	Chain	Res	Type
1	A	127	SER
1	A	130	ARG
1	A	133	THR
1	A	136	VAL
1	A	139	THR
1	A	152	LYS
1	A	155	LYS
1	A	175	LEU
1	A	176	THR
1	A	178	SER
1	A	179	ASP
1	A	194	ILE
1	A	203	ARG
1	A	209	LEU
1	A	217	ILE
1	A	222	SER
1	A	232	GLU
1	A	238	LYS
1	A	239	LEU
1	A	243	VAL
1	A	248	ARG
1	A	253	ILE
1	A	261	ILE
1	A	268	LEU
1	A	275	THR
1	A	278	ASP
1	A	289	HIS
1	A	290	ARG
1	A	298	LEU
1	A	306	GLU
1	A	308	ARG
1	A	313	LEU
1	A	314	SER
1	A	325	VAL
1	A	331	ASN
1	A	337	VAL
1	A	346	THR
1	A	349	VAL
1	A	353	ILE
1	A	361	LEU
1	A	366	ILE
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	378	VAL
1	A	384	ARG
1	A	386	ILE
1	A	388	LEU
1	A	394	ARG
1	A	411	LEU
1	A	417	VAL
1	A	420	ASN
1	A	421	ARG
1	A	425	LEU
1	A	427	ARG
1	A	428	ILE
1	A	429	SER
1	A	438	LEU
1	A	441	LEU
1	A	442	THR
1	A	446	ASN
1	A	464	LEU
1	A	469	SER
1	A	471	GLU
1	A	479	ILE
1	A	481	LEU
1	A	486	ILE
1	A	487	ILE
1	A	488	THR
1	A	495	ILE
1	A	500	GLN
1	A	503	ILE
1	A	507	TYR
1	A	515	LEU
1	A	518	LYS
1	A	525	LEU
1	A	527	VAL
1	A	532	ILE
1	A	547	THR
1	A	549	LYS
1	A	550	GLN
1	A	558	LYS
1	A	568	VAL
1	A	573	ARG
1	A	574	LEU
1	A	578	GLU

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Mol	Chain	Res	Type
1	A	586	VAL
1	A	592	ILE
1	A	593	LEU
1	A	597	VAL
1	A	605	ASN
1	A	609	GLU
1	A	616	ILE
1	A	618	GLU
1	A	633	ARG
1	A	634	VAL
1	A	637	ARG
1	A	642	GLN
1	A	657	VAL
1	A	667	ARG
1	A	675	LEU
1	A	684	LEU
1	A	687	ILE
1	A	691	THR
1	A	708	ARG
1	A	716	SER
1	A	723	ASN
1	A	736	SER
1	A	737	VAL
1	A	739	ASN
1	A	740	ILE
1	A	747	LEU
1	A	752	VAL
1	A	755	GLU
1	A	759	ARG
1	A	764	ARG
1	A	766	LEU
1	A	777	GLU
1	A	787	ARG
1	A	823	LEU
1	A	827	LEU
1	A	828	SER
1	A	841	LEU
1	A	844	GLU
1	A	864	LYS
1	A	868	VAL
1	A	874	ARG
1	A	875	VAL

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Mol	Chain	Res	Type
1	A	876	VAL
2	C	13	LEU
2	C	29	VAL
2	C	36	ILE
2	C	40	GLU
2	C	41	ILE
2	C	42	ILE
2	C	43	VAL
2	C	47	GLU
2	C	48	ILE
2	C	51	ILE
2	C	53	ASP
2	C	57	LYS
2	C	59	TYR
2	C	61	GLU
2	C	70	ILE
2	C	72	ILE
2	C	85	MET
2	C	104	LEU
2	C	107	LEU
2	C	116	VAL
2	C	118	SER
2	C	119	THR
2	C	124	ILE
2	C	129	GLU
2	C	130	TYR
2	C	145	GLU
2	C	147	THR
2	C	149	ILE
2	C	158	ILE
2	C	160	ILE
2	C	163	MET
2	C	169	LEU
2	C	172	GLU
2	C	173	MET
2	C	174	LEU
2	C	176	ASP
2	C	179	VAL
2	C	188	ILE
2	C	190	ARG
2	C	193	LEU
2	C	201	SER

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Mol	Chain	Res	Type
2	C	208	ILE
2	C	215	SER
2	C	229	THR
2	C	234	ILE
2	C	235	LYS
2	C	237	ILE
2	C	242	VAL
2	C	250	ILE
2	C	251	ILE
2	C	254	ASP
2	C	267	VAL
2	C	275	ASN
2	C	278	ARG
2	C	280	ILE
2	C	287	GLU
2	C	291	GLU
2	C	292	ILE
2	C	295	ARG
2	C	301	LEU
2	C	307	ASP
2	C	310	ILE
2	C	311	ARG
2	C	314	LEU
2	C	315	LEU
2	C	316	ILE
2	C	320	MET
2	C	322	ARG
2	C	325	ILE
2	C	326	VAL
2	C	329	ILE
2	C	331	ARG
2	C	335	THR
2	C	337	GLU
2	C	339	ASN
2	C	344	ARG
2	C	349	VAL
2	C	351	VAL
2	C	364	GLU
2	C	369	VAL
2	C	370	VAL
2	C	374	ILE
2	C	375	ILE

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Mol	Chain	Res	Type
2	C	379	ILE
2	C	380	LYS
2	C	381	LEU
2	C	388	LEU
2	C	389	THR
2	C	390	MET
2	C	391	ARG
2	C	393	ILE
2	C	394	LEU
3	B	5	LEU
3	B	6	THR
3	B	20	SER
3	B	21	LYS
3	B	23	LEU
3	B	30	SER
3	B	33	ASP
3	B	48	GLU
3	B	49	ILE
3	B	51	THR
3	B	56	LEU
3	B	63	ILE
3	B	64	ARG
3	B	65	ILE
3	B	70	VAL
3	B	72	GLU
3	B	75	ARG
3	B	80	ILE
3	B	83	MET
3	B	90	LEU
3	B	99	THR
3	B	105	ASN
3	B	108	GLU
3	B	113	GLU
3	B	118	ASP
3	B	137	LYS
3	B	155	ASN
3	B	159	ARG
3	B	162	VAL
3	B	163	THR
3	B	182	ASN
3	B	183	ILE
3	B	193	THR

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Mol	Chain	Res	Type
3	B	203	GLU
3	B	207	ASP
3	B	221	ILE
3	B	227	MET
3	B	234	THR
3	B	245	ASP
3	B	296	TYR
3	B	322	VAL
3	B	323	ILE
3	B	327	LEU
3	B	335	LYS
3	B	348	ASP
3	B	361	PHE
3	B	367	TYR
3	B	369	LEU
3	B	371	LYS
3	B	374	VAL
3	B	378	LYS
3	B	391	THR
3	B	394	ILE
3	B	395	ARG
3	B	402	ASN
3	B	404	VAL
3	B	407	ARG
3	B	418	ASN
3	B	421	SER
3	B	429	VAL
3	B	432	SER
3	B	444	ASP
3	B	448	THR
3	B	453	MET
3	B	457	GLU
3	B	467	VAL
3	B	468	LYS
3	B	469	ASN
3	B	476	ILE
3	B	478	VAL
3	B	484	ILE
3	B	486	GLU
3	B	488	THR
3	B	497	VAL
3	B	498	GLU

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Mol	Chain	Res	Type
3	B	518	SER
3	B	520	VAL
3	B	530	TYR
3	B	531	GLN
3	B	536	LEU
3	B	549	ILE
3	B	551	ASP
3	B	564	ASN
3	B	570	CYS
3	B	572	SER
3	B	576	ARG
3	B	588	LEU
3	B	592	GLU
3	B	594	ILE
3	B	603	THR
3	B	606	ASP
3	B	607	LEU
3	B	608	VAL
3	B	626	VAL
3	B	628	LEU
3	B	634	THR
3	B	638	THR
3	B	640	LEU
3	B	643	TRP
3	B	650	ILE
3	B	654	ILE
3	B	655	ILE
3	B	659	GLU
3	B	669	GLN
3	B	672	MET
3	B	685	GLN
3	B	686	LEU
3	B	687	ARG
3	B	688	THR
3	B	689	ASP
3	B	691	ARG
3	B	694	LEU
3	B	702	LEU
3	B	705	THR
3	B	708	LEU
3	B	710	ILE
3	B	714	THR

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Mol	Chain	Res	Type
3	B	727	MET
3	B	739	ILE
3	B	741	ASN
3	B	757	LEU
3	B	770	GLU
3	B	780	VAL
3	B	781	ARG
3	B	789	TYR
3	B	794	ASP
3	B	800	PRO
3	B	804	VAL
3	B	814	VAL
3	B	843	GLU
3	B	846	ILE
3	B	850	VAL
3	B	855	THR
3	B	871	ILE
3	B	885	LYS
3	B	887	VAL
3	B	890	MET
3	B	891	LEU
3	B	895	VAL
3	B	901	VAL
3	B	902	LYS
3	B	905	VAL
3	B	910	LEU
3	B	911	ASN
3	B	915	LEU
3	B	919	MET
3	B	924	ILE
3	B	926	GLU
3	B	931	LYS
3	B	940	VAL
3	B	941	ASP
3	B	945	PHE
3	B	946	TYR
3	B	950	ILE
3	B	951	GLU
3	B	957	ILE
3	B	967	THR
3	B	970	VAL
3	B	975	THR

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Mol	Chain	Res	Type
3	B	982	ARG
3	B	985	PHE
3	B	988	VAL
3	B	991	GLN
3	B	1012	LEU
3	B	1016	PRO
3	B	1018	GLU
3	B	1026	LEU
3	B	1030	GLU
3	B	1035	CYS
3	B	1045	LEU
3	B	1049	LEU
3	B	1050	LEU
3	B	1067	ILE
3	B	1074	LYS
3	B	1078	VAL
3	B	1079	CYS
3	B	1093	VAL
3	B	1108	ILE
3	B	1109	ILE
3	B	1113	LEU
3	B	1115	LEU
4	D	3	ILE
4	D	29	ARG
4	D	56	GLU
4	D	57	ILE
4	D	68	MET
4	D	82	CYS
4	D	89	CYS
4	D	124	ILE
4	D	132	LEU
4	D	135	THR
4	D	136	ASN
4	D	155	LYS
4	D	161	LEU
4	D	162	SER
4	D	163	VAL
4	D	170	VAL
4	D	178	LYS
4	D	180	VAL
4	D	195	LEU
4	D	201	LEU

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Mol	Chain	Res	Type
4	D	204	THR
4	D	208	GLU
4	D	214	ASN
4	D	222	VAL
4	D	250	ILE
5	E	10	ILE
5	E	18	PHE
5	E	22	LEU
5	E	27	LEU
5	E	30	LEU
5	E	33	GLN
5	E	37	LYS
5	E	38	ILE
5	E	39	LEU
5	E	40	LYS
5	E	41	ASP
5	E	44	LEU
5	E	51	VAL
5	E	58	ILE
5	E	59	LEU
5	E	66	THR
5	E	69	GLU
5	E	70	VAL
5	E	76	THR
5	E	81	VAL
5	E	83	GLU
5	E	85	VAL
5	E	90	LEU
5	E	92	VAL
5	E	97	ILE
5	E	101	LEU
5	E	104	MET
5	E	110	ILE
5	E	123	VAL
5	E	128	PHE
5	E	151	SER
5	E	163	THR
5	E	164	MET
5	E	176	THR
5	E	180	LYS
6	F	6	ILE
6	F	14	TYR

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Mol	Chain	Res	Type
6	F	15	SER
6	F	24	VAL
6	F	25	ILE
6	F	31	SER
6	F	33	LEU
6	F	34	LEU
6	F	44	VAL
6	F	47	CYS
6	F	53	GLN
6	F	59	LEU
6	F	64	SER
6	F	68	VAL
6	F	86	ILE
7	G	5	VAL
7	G	10	ILE
7	G	19	GLU
7	G	25	ASN
7	G	42	ILE
7	G	46	ILE
7	G	65	SER
7	G	77	ILE
7	G	78	VAL
7	G	80	GLU
7	G	86	LEU
7	G	92	TYR
7	G	95	ILE
7	G	97	SER
7	G	104	LYS
7	G	106	ILE
7	G	114	ARG
7	G	115	THR
7	G	116	SER
8	H	12	ARG
8	H	13	ILE
8	H	19	LYS
8	H	22	VAL
8	H	31	ILE
8	H	37	ILE
8	H	40	GLU
8	H	42	LEU
8	H	43	PRO
8	H	44	TRP

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Mol	Chain	Res	Type
8	H	45	ILE
8	H	46	ARG
8	H	48	SER
8	H	64	ARG
8	H	65	ILE
8	H	74	GLU
8	H	75	VAL
8	H	76	VAL
8	H	82	ILE
9	K	15	PHE
9	K	18	VAL
9	K	20	ILE
9	K	22	LEU
9	K	23	TRP
9	K	29	ARG
9	K	35	VAL
9	K	36	ILE
9	K	41	LEU
9	K	42	GLN
9	K	45	MET
9	K	50	LEU
9	K	51	ILE
9	K	52	ASP
9	K	61	VAL
9	K	67	GLU
9	K	71	ARG
9	K	74	LEU
9	K	78	ILE
9	K	81	ARG
9	K	82	LEU
9	K	86	LYS
9	K	89	LEU
9	K	90	LEU
10	L	5	ILE
10	L	9	GLU
10	L	17	ILE
10	L	24	LEU
10	L	44	TYR
10	L	45	GLN
10	L	47	HIS
10	L	49	LEU
10	L	53	ILE

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Mol	Chain	Res	Type
10	L	55	VAL
10	L	57	ILE
10	L	69	LEU
10	L	70	LEU
10	L	73	ILE
10	L	79	MET
10	L	82	HIS
10	L	87	ILE
10	L	92	LYS
11	N	3	ILE
11	N	5	ILE
11	N	13	LEU
11	N	22	ILE
11	N	38	LEU
11	N	40	VAL
11	N	42	ARG
11	N	48	MET
11	N	55	ILE
11	N	64	ARG
12	P	8	LYS
12	P	10	TRP
12	P	21	LEU
12	P	24	VAL
12	P	31	TYR
12	P	34	ILE
12	P	46	LYS
13	Y	44	LEU
13	Y	60	THR
13	Y	69	GLU
13	Y	70	ASP
13	Y	76	GLU
13	Y	77	LYS
13	Y	78	ARG
13	Y	79	ASP
13	Y	82	ARG
1	I	7	LYS
1	I	15	SER
1	I	29	THR
1	I	45	MET
1	I	48	ARG
1	I	58	CYS
1	I	60	THR

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Mol	Chain	Res	Type
1	I	64	THR
1	I	65	LEU
1	I	79	ARG
1	I	82	ILE
1	I	84	VAL
1	I	101	CYS
1	I	103	ARG
1	I	105	LYS
1	I	107	SER
1	I	111	ILE
1	I	127	SER
1	I	130	ARG
1	I	133	THR
1	I	136	VAL
1	I	139	THR
1	I	152	LYS
1	I	155	LYS
1	I	175	LEU
1	I	176	THR
1	I	178	SER
1	I	179	ASP
1	I	194	ILE
1	I	203	ARG
1	I	209	LEU
1	I	217	ILE
1	I	222	SER
1	I	232	GLU
1	I	238	LYS
1	I	239	LEU
1	I	243	VAL
1	I	248	ARG
1	I	261	ILE
1	I	268	LEU
1	I	278	ASP
1	I	289	HIS
1	I	290	ARG
1	I	298	LEU
1	I	306	GLU
1	I	308	ARG
1	I	313	LEU
1	I	314	SER
1	I	325	VAL

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Mol	Chain	Res	Type
1	I	331	ASN
1	I	337	VAL
1	I	346	THR
1	I	349	VAL
1	I	361	LEU
1	I	366	ILE
1	I	376	ASN
1	I	377	TYR
1	I	378	VAL
1	I	384	ARG
1	I	386	ILE
1	I	394	ARG
1	I	407	ILE
1	I	411	LEU
1	I	417	VAL
1	I	420	ASN
1	I	421	ARG
1	I	425	LEU
1	I	427	ARG
1	I	428	ILE
1	I	434	ARG
1	I	436	ARG
1	I	438	LEU
1	I	441	LEU
1	I	442	THR
1	I	446	ASN
1	I	464	LEU
1	I	469	SER
1	I	471	GLU
1	I	479	ILE
1	I	481	LEU
1	I	486	ILE
1	I	487	ILE
1	I	488	THR
1	I	495	ILE
1	I	500	GLN
1	I	503	ILE
1	I	507	TYR
1	I	515	LEU
1	I	518	LYS
1	I	525	LEU
1	I	527	VAL

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Mol	Chain	Res	Type
1	I	532	ILE
1	I	547	THR
1	I	550	GLN
1	I	558	LYS
1	I	559	ASP
1	I	568	VAL
1	I	573	ARG
1	I	574	LEU
1	I	578	GLU
1	I	586	VAL
1	I	593	LEU
1	I	597	VAL
1	I	605	ASN
1	I	609	GLU
1	I	612	LEU
1	I	616	ILE
1	I	618	GLU
1	I	633	ARG
1	I	637	ARG
1	I	642	GLN
1	I	657	VAL
1	I	667	ARG
1	I	675	LEU
1	I	684	LEU
1	I	687	ILE
1	I	691	THR
1	I	692	LEU
1	I	693	GLU
1	I	708	ARG
1	I	716	SER
1	I	723	ASN
1	I	736	SER
1	I	737	VAL
1	I	738	LEU
1	I	739	ASN
1	I	740	ILE
1	I	747	LEU
1	I	752	VAL
1	I	755	GLU
1	I	759	ARG
1	I	764	ARG
1	I	766	LEU

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Mol	Chain	Res	Type
1	I	774	ILE
1	I	777	GLU
1	I	787	ARG
1	I	791	LYS
1	I	823	LEU
1	I	827	LEU
1	I	841	LEU
1	I	844	GLU
1	I	864	LYS
1	I	868	VAL
1	I	874	ARG
1	I	875	VAL
1	I	876	VAL
2	M	13	LEU
2	M	18	LYS
2	M	23	ILE
2	M	28	ILE
2	M	29	VAL
2	M	31	ASP
2	M	34	ASN
2	M	39	LYS
2	M	42	ILE
2	M	44	THR
2	M	45	ARG
2	M	46	ASP
2	M	53	ASP
2	M	56	ILE
2	M	57	LYS
2	M	61	GLU
2	M	70	ILE
2	M	72	ILE
2	M	73	VAL
2	M	78	VAL
2	M	83	THR
2	M	84	GLN
2	M	85	MET
2	M	86	THR
2	M	102	LEU
2	M	104	LEU
2	M	107	LEU
2	M	110	ILE
2	M	111	VAL

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Mol	Chain	Res	Type
2	M	116	VAL
2	M	127	THR
2	M	128	ASP
2	M	129	GLU
2	M	130	TYR
2	M	132	ARG
2	M	135	ASP
2	M	143	LYS
2	M	147	THR
2	M	150	GLU
2	M	156	THR
2	M	157	SER
2	M	159	ASP
2	M	160	ILE
2	M	163	MET
2	M	165	ILE
2	M	171	ASN
2	M	172	GLU
2	M	174	LEU
2	M	176	ASP
2	M	179	VAL
2	M	188	ILE
2	M	190	ARG
2	M	212	ASN
2	M	213	ILE
2	M	214	ASP
2	M	229	THR
2	M	231	ILE
2	M	235	LYS
2	M	250	ILE
2	M	251	ILE
2	M	267	VAL
2	M	275	ASN
2	M	277	ILE
2	M	278	ARG
2	M	280	ILE
2	M	303	GLU
2	M	306	LEU
2	M	308	VAL
2	M	309	ASP
2	M	313	ILE
2	M	314	LEU

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Mol	Chain	Res	Type
2	M	315	LEU
2	M	316	ILE
2	M	322	ARG
2	M	325	ILE
2	M	327	ARG
2	M	329	ILE
2	M	335	THR
2	M	338	LYS
2	M	339	ASN
2	M	344	ARG
2	M	349	VAL
2	M	351	VAL
2	M	355	LEU
2	M	369	VAL
2	M	370	VAL
2	M	374	ILE
2	M	375	ILE
2	M	379	ILE
2	M	380	LYS
2	M	381	LEU
2	M	386	VAL
2	M	387	GLU
2	M	389	THR
2	M	390	MET
2	M	391	ARG
3	J	5	LEU
3	J	6	THR
3	J	21	LYS
3	J	23	LEU
3	J	30	SER
3	J	33	ASP
3	J	48	GLU
3	J	49	ILE
3	J	51	THR
3	J	56	LEU
3	J	63	ILE
3	J	64	ARG
3	J	65	ILE
3	J	70	VAL
3	J	75	ARG
3	J	80	ILE
3	J	83	MET

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Mol	Chain	Res	Type
3	J	90	LEU
3	J	99	THR
3	J	105	ASN
3	J	108	GLU
3	J	113	GLU
3	J	118	ASP
3	J	137	LYS
3	J	155	ASN
3	J	159	ARG
3	J	162	VAL
3	J	163	THR
3	J	167	LEU
3	J	179	THR
3	J	182	ASN
3	J	183	ILE
3	J	190	ILE
3	J	193	THR
3	J	203	GLU
3	J	207	ASP
3	J	221	ILE
3	J	227	MET
3	J	234	THR
3	J	245	ASP
3	J	296	TYR
3	J	322	VAL
3	J	323	ILE
3	J	327	LEU
3	J	335	LYS
3	J	348	ASP
3	J	361	PHE
3	J	367	TYR
3	J	369	LEU
3	J	371	LYS
3	J	374	VAL
3	J	378	LYS
3	J	391	THR
3	J	394	ILE
3	J	395	ARG
3	J	402	ASN
3	J	404	VAL
3	J	407	ARG
3	J	418	ASN

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Mol	Chain	Res	Type
3	J	421	SER
3	J	429	VAL
3	J	432	SER
3	J	444	ASP
3	J	448	THR
3	J	453	MET
3	J	467	VAL
3	J	468	LYS
3	J	469	ASN
3	J	476	ILE
3	J	478	VAL
3	J	484	ILE
3	J	486	GLU
3	J	488	THR
3	J	497	VAL
3	J	498	GLU
3	J	518	SER
3	J	520	VAL
3	J	530	TYR
3	J	531	GLN
3	J	536	LEU
3	J	540	ILE
3	J	544	ARG
3	J	549	ILE
3	J	551	ASP
3	J	564	ASN
3	J	570	CYS
3	J	572	SER
3	J	576	ARG
3	J	588	LEU
3	J	592	GLU
3	J	594	ILE
3	J	603	THR
3	J	606	ASP
3	J	607	LEU
3	J	608	VAL
3	J	626	VAL
3	J	628	LEU
3	J	634	THR
3	J	638	THR
3	J	640	LEU
3	J	643	TRP

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Mol	Chain	Res	Type
3	J	650	ILE
3	J	654	ILE
3	J	655	ILE
3	J	659	GLU
3	J	669	GLN
3	J	672	MET
3	J	685	GLN
3	J	686	LEU
3	J	687	ARG
3	J	688	THR
3	J	689	ASP
3	J	690	THR
3	J	691	ARG
3	J	702	LEU
3	J	705	THR
3	J	708	LEU
3	J	710	ILE
3	J	714	THR
3	J	727	MET
3	J	739	ILE
3	J	741	ASN
3	J	752	SER
3	J	757	LEU
3	J	770	GLU
3	J	780	VAL
3	J	781	ARG
3	J	789	TYR
3	J	791	LEU
3	J	794	ASP
3	J	800	PRO
3	J	804	VAL
3	J	814	VAL
3	J	839	THR
3	J	843	GLU
3	J	846	ILE
3	J	850	VAL
3	J	855	THR
3	J	871	ILE
3	J	887	VAL
3	J	890	MET
3	J	891	LEU
3	J	895	VAL

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Mol	Chain	Res	Type
3	J	901	VAL
3	J	902	LYS
3	J	905	VAL
3	J	910	LEU
3	J	911	ASN
3	J	915	LEU
3	J	919	MET
3	J	924	ILE
3	J	926	GLU
3	J	931	LYS
3	J	940	VAL
3	J	941	ASP
3	J	945	PHE
3	J	946	TYR
3	J	950	ILE
3	J	951	GLU
3	J	957	ILE
3	J	967	THR
3	J	970	VAL
3	J	975	THR
3	J	982	ARG
3	J	985	PHE
3	J	987	VAL
3	J	988	VAL
3	J	991	GLN
3	J	1012	LEU
3	J	1018	GLU
3	J	1026	LEU
3	J	1030	GLU
3	J	1035	CYS
3	J	1045	LEU
3	J	1049	LEU
3	J	1050	LEU
3	J	1067	ILE
3	J	1074	LYS
3	J	1078	VAL
3	J	1079	CYS
3	J	1093	VAL
3	J	1108	ILE
3	J	1109	ILE
3	J	1113	LEU
3	J	1115	LEU

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Mol	Chain	Res	Type
4	O	29	ARG
4	O	56	GLU
4	O	57	ILE
4	O	68	MET
4	O	82	CYS
4	O	89	CYS
4	O	124	ILE
4	O	132	LEU
4	O	135	THR
4	O	136	ASN
4	O	139	ILE
4	O	155	LYS
4	O	161	LEU
4	O	162	SER
4	O	163	VAL
4	O	170	VAL
4	O	178	LYS
4	O	180	VAL
4	O	195	LEU
4	O	201	LEU
4	O	204	THR
4	O	208	GLU
4	O	214	ASN
4	O	222	VAL
4	O	250	ILE
5	Q	4	LEU
5	Q	5	ILE
5	Q	11	VAL
5	Q	17	GLU
5	Q	18	PHE
5	Q	22	LEU
5	Q	24	GLU
5	Q	25	ILE
5	Q	27	LEU
5	Q	30	LEU
5	Q	32	GLN
5	Q	33	GLN
5	Q	38	ILE
5	Q	42	LEU
5	Q	44	LEU
5	Q	48	ILE
5	Q	49	LEU

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Mol	Chain	Res	Type
5	Q	51	VAL
5	Q	58	ILE
5	Q	60	VAL
5	Q	69	GLU
5	Q	76	THR
5	Q	78	VAL
5	Q	81	VAL
5	Q	85	VAL
5	Q	99	VAL
5	Q	101	LEU
5	Q	104	MET
5	Q	107	LEU
5	Q	110	ILE
5	Q	117	THR
5	Q	126	ILE
5	Q	127	ILE
5	Q	143	ARG
5	Q	149	VAL
5	Q	152	THR
5	Q	174	TRP
5	Q	175	ILE
5	Q	176	THR
5	Q	177	GLN
6	R	2	SER
6	R	6	ILE
6	R	9	GLU
6	R	14	TYR
6	R	24	VAL
6	R	25	ILE
6	R	34	LEU
6	R	44	VAL
6	R	45	GLU
6	R	59	LEU
6	R	64	SER
6	R	67	ASP
6	R	86	ILE
6	R	87	LEU
7	S	10	ILE
7	S	11	LEU
7	S	18	ILE
7	S	23	LEU
7	S	25	ASN

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Mol	Chain	Res	Type
7	S	27	SER
7	S	32	SER
7	S	33	CYS
7	S	34	ASN
7	S	39	SER
7	S	40	PHE
7	S	42	ILE
7	S	46	ILE
7	S	48	ILE
7	S	62	ASN
7	S	68	HIS
7	S	69	ASP
7	S	77	ILE
7	S	79	THR
7	S	86	LEU
7	S	90	ASN
7	S	95	ILE
7	S	98	LEU
7	S	102	LEU
7	S	104	LYS
7	S	106	ILE
7	S	110	GLU
7	S	116	SER
8	T	12	ARG
8	T	13	ILE
8	T	17	VAL
8	T	19	LYS
8	T	25	ILE
8	T	30	LYS
8	T	37	ILE
8	T	38	ARG
8	T	42	LEU
8	T	46	ARG
8	T	62	ILE
8	T	66	ILE
8	T	68	LYS
8	T	72	TYR
8	T	81	VAL
8	T	82	ILE
9	U	14	HIS
9	U	15	PHE
9	U	18	VAL

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Mol	Chain	Res	Type
9	U	23	TRP
9	U	26	ARG
9	U	29	ARG
9	U	37	SER
9	U	41	LEU
9	U	42	GLN
9	U	43	LEU
9	U	51	ILE
9	U	52	ASP
9	U	60	ASP
9	U	61	VAL
9	U	62	ILE
9	U	67	GLU
9	U	70	ARG
9	U	74	LEU
9	U	76	ILE
9	U	82	LEU
9	U	88	ILE
9	U	89	LEU
9	U	90	LEU
9	U	91	SER
9	U	92	LEU
10	V	5	ILE
10	V	6	LEU
10	V	9	GLU
10	V	10	SER
10	V	16	GLU
10	V	24	LEU
10	V	32	LEU
10	V	38	VAL
10	V	43	TYR
10	V	47	HIS
10	V	49	LEU
10	V	52	LYS
10	V	54	ILE
10	V	57	ILE
10	V	63	ILE
10	V	64	THR
10	V	70	LEU
10	V	73	ILE
10	V	79	MET
10	V	87	ILE

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Mol	Chain	Res	Type
10	V	92	LYS
11	W	3	ILE
11	W	5	ILE
11	W	13	LEU
11	W	22	ILE
11	W	38	LEU
11	W	40	VAL
11	W	42	ARG
11	W	48	MET
11	W	55	ILE
11	W	64	ARG
12	X	8	LYS
12	X	10	TRP
12	X	21	LEU
12	X	24	VAL
12	X	31	TYR
12	X	33	ILE
12	X	34	ILE
12	X	41	THR
12	X	46	LYS
13	Z	39	GLN
13	Z	41	ILE
13	Z	54	LEU
13	Z	55	LEU
13	Z	56	ASN
13	Z	59	ILE
13	Z	60	THR
13	Z	66	LYS
13	Z	67	LEU
13	Z	69	GLU
13	Z	70	ASP
13	Z	82	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (168) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	63	ASN
1	A	119	ASN
1	A	148	HIS
1	A	246	ASN
1	A	259	GLN

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Mol	Chain	Res	Type
1	A	312	ASN
1	A	331	ASN
1	A	367	ASN
1	A	376	ASN
1	A	420	ASN
1	A	422	GLN
1	A	446	ASN
1	A	465	HIS
1	A	485	ASN
1	A	561	ASN
1	A	567	ASN
1	A	582	HIS
1	A	590	ASN
1	A	677	GLN
1	A	723	ASN
1	A	749	GLN
2	C	38	ASN
2	C	84	GLN
2	C	207	ASN
2	C	209	ASN
2	C	212	ASN
2	C	275	ASN
2	C	276	ASN
2	C	328	GLN
2	C	332	HIS
2	C	353	HIS
3	B	26	GLN
3	B	27	HIS
3	B	40	GLN
3	B	164	GLN
3	B	182	ASN
3	B	291	GLN
3	B	300	HIS
3	B	396	HIS
3	B	412	GLN
3	B	418	ASN
3	B	439	ASN
3	B	446	HIS
3	B	449	GLN
3	B	554	ASN
3	B	564	ASN
3	B	567	HIS

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Mol	Chain	Res	Type
3	B	569	ASN
3	B	610	GLN
3	B	623	ASN
3	B	637	HIS
3	B	639	HIS
3	B	660	HIS
3	B	666	ASN
3	B	669	GLN
3	B	685	GLN
3	B	715	ASN
3	B	720	ASN
3	B	721	ASN
3	B	911	ASN
3	B	913	HIS
3	B	1015	GLN
3	B	1052	ASN
3	B	1087	ASN
4	D	104	ASN
5	E	16	ASN
5	E	23	ASN
5	E	33	GLN
5	E	109	HIS
5	E	112	GLN
6	F	61	ASN
7	G	62	ASN
7	G	88	ASN
8	H	20	HIS
9	K	42	GLN
9	K	54	ASN
10	L	22	HIS
11	N	19	GLN
11	N	57	ASN
13	Y	71	ASN
1	I	5	ASN
1	I	56	GLN
1	I	63	ASN
1	I	148	HIS
1	I	259	GLN
1	I	312	ASN
1	I	331	ASN
1	I	357	ASN
1	I	367	ASN

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Mol	Chain	Res	Type
1	I	376	ASN
1	I	410	HIS
1	I	420	ASN
1	I	422	GLN
1	I	426	HIS
1	I	446	ASN
1	I	465	HIS
1	I	468	GLN
1	I	483	HIS
1	I	485	ASN
1	I	561	ASN
1	I	567	ASN
1	I	590	ASN
1	I	677	GLN
1	I	723	ASN
2	M	26	GLN
2	M	207	ASN
2	M	209	ASN
2	M	212	ASN
2	M	228	ASN
2	M	276	ASN
2	M	328	GLN
2	M	332	HIS
2	M	353	HIS
3	J	26	GLN
3	J	27	HIS
3	J	40	GLN
3	J	106	ASN
3	J	164	GLN
3	J	182	ASN
3	J	211	HIS
3	J	291	GLN
3	J	300	HIS
3	J	368	GLN
3	J	412	GLN
3	J	418	ASN
3	J	439	ASN
3	J	446	HIS
3	J	449	GLN
3	J	531	GLN
3	J	554	ASN
3	J	564	ASN

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Mol	Chain	Res	Type
3	J	567	HIS
3	J	569	ASN
3	J	586	ASN
3	J	610	GLN
3	J	623	ASN
3	J	637	HIS
3	J	639	HIS
3	J	660	HIS
3	J	666	ASN
3	J	669	GLN
3	J	685	GLN
3	J	715	ASN
3	J	720	ASN
3	J	721	ASN
3	J	911	ASN
3	J	913	HIS
3	J	954	GLN
3	J	1015	GLN
3	J	1052	ASN
4	O	26	ASN
4	O	104	ASN
4	O	199	ASN
5	Q	33	GLN
5	Q	82	GLN
5	Q	100	ASN
5	Q	109	HIS
5	Q	112	GLN
6	R	53	GLN
7	S	88	ASN
7	S	117	GLN
8	T	70	GLN
9	U	14	HIS
9	U	16	ASN
9	U	42	GLN
9	U	55	ASN
11	W	57	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\# Z > 2$
16	F3S	D	1001	4	0,9,9	-	-	-		
16	F3S	O	1001	4	0,9,9	-	-	-		

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
16	F3S	D	1001	4	-	-	0/3/3/3
16	F3S	O	1001	4	-	-	0/3/3/3

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.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	1001	F3S	1	0
16	O	1001	F3S	6	0

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	836/880 (95%)	0.05	12 (1%) 73 59	28, 71, 105, 133	0
1	I	836/880 (95%)	0.05	8 (0%) 79 66	28, 71, 106, 133	0
2	C	370/395 (93%)	0.17	9 (2%) 59 45	37, 78, 130, 138	0
2	M	370/395 (93%)	0.20	7 (1%) 66 51	38, 79, 130, 138	0
3	B	1090/1124 (96%)	0.10	31 (2%) 55 41	33, 66, 117, 149	0
3	J	1090/1124 (96%)	0.06	21 (1%) 66 51	33, 67, 117, 149	0
4	D	264/265 (99%)	0.18	2 (0%) 82 71	57, 86, 121, 139	0
4	O	264/265 (99%)	0.21	3 (1%) 78 65	57, 86, 121, 139	0
5	E	176/180 (97%)	0.22	3 (1%) 69 54	58, 98, 140, 143	0
5	Q	176/180 (97%)	0.19	2 (1%) 78 65	58, 98, 139, 142	0
6	F	89/113 (78%)	0.47	5 (5%) 30 23	100, 127, 132, 133	0
6	R	89/113 (78%)	0.50	3 (3%) 48 35	100, 127, 132, 133	0
7	G	113/132 (85%)	0.33	3 (2%) 56 42	65, 88, 108, 112	0
7	S	113/132 (85%)	0.34	5 (4%) 39 28	66, 88, 108, 112	0
8	H	74/84 (88%)	0.14	3 (4%) 41 29	66, 81, 99, 102	0
8	T	74/84 (88%)	0.18	1 (1%) 73 59	66, 81, 99, 102	0
9	K	82/95 (86%)	-0.13	2 (2%) 59 45	41, 57, 86, 94	0
9	U	82/95 (86%)	-0.13	3 (3%) 45 32	43, 58, 87, 93	0
10	L	92/92 (100%)	-0.24	1 (1%) 78 65	53, 73, 103, 107	0
10	V	92/92 (100%)	-0.15	0 100 100	54, 73, 103, 107	0
11	N	64/66 (96%)	0.19	3 (4%) 36 27	62, 80, 103, 124	0
11	W	64/66 (96%)	0.20	3 (4%) 36 27	62, 80, 103, 124	0
12	P	43/48 (89%)	0.64	1 (2%) 61 46	66, 89, 103, 110	0
12	X	43/48 (89%)	0.47	2 (4%) 36 27	66, 89, 103, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	Y	45/104 (43%)	0.56	2 (4%) 39 28	98, 108, 124, 125	0
13	Z	45/104 (43%)	0.47	0 100 100	98, 108, 124, 124	0
All	All	6676/7156 (93%)	0.12	135 (2%) 65 49	28, 76, 127, 149	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	X	34	ILE	4.7
3	B	1069	TRP	4.6
3	B	600	GLY	4.3
3	B	557	HIS	4.2
3	J	557	HIS	3.9
9	K	51	ILE	3.8
1	A	266	TRP	3.6
7	S	73	GLY	3.6
3	J	194	ALA	3.6
7	S	80	GLU	3.6
3	J	501	ILE	3.5
11	N	47	ARG	3.5
1	A	867	ASP	3.5
3	B	625	TYR	3.4
6	R	72	LEU	3.4
3	J	474	ALA	3.3
11	N	21	PHE	3.2
3	J	256	LEU	3.2
1	A	783	TYR	3.1
12	P	33	ILE	3.1
3	B	501	ILE	3.1
9	K	62	ILE	3.0
3	B	245	ASP	3.0
3	B	376	GLY	3.0
9	U	62	ILE	3.0
3	B	256	LEU	2.9
3	B	54	PRO	2.9
4	O	64	LEU	2.8
1	A	238	LYS	2.8
1	A	842	TYR	2.8
3	B	314	TYR	2.8
6	F	4	VAL	2.8
3	J	852	ILE	2.7
1	A	60	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	607	GLN	2.7
13	Y	41	ILE	2.7
13	Y	81	ARG	2.7
3	J	601	ALA	2.7
1	A	4	LYS	2.7
7	S	92	TYR	2.7
2	C	24	LEU	2.7
2	M	58	GLU	2.7
1	I	111	ILE	2.6
7	G	80	GLU	2.6
3	B	434	ALA	2.6
11	W	21	PHE	2.6
2	C	213	ILE	2.6
5	E	153	VAL	2.5
2	M	213	ILE	2.5
2	C	160	ILE	2.5
3	B	731	GLY	2.5
7	G	114	ARG	2.5
8	H	17	VAL	2.5
4	O	190	LEU	2.5
2	C	58	GLU	2.5
3	J	245	ASP	2.5
6	F	33	LEU	2.5
6	F	2	SER	2.4
5	E	127	ILE	2.4
5	Q	58	ILE	2.4
6	R	89	MET	2.4
5	E	136	ILE	2.4
3	J	597	LEU	2.4
3	J	224	VAL	2.4
2	M	160	ILE	2.3
2	C	266	GLY	2.3
8	H	29	TYR	2.3
3	B	945	PHE	2.3
3	B	592	GLU	2.3
12	X	24	VAL	2.3
1	A	115	SER	2.3
3	B	367	TYR	2.3
1	I	132	LEU	2.3
3	B	244	LEU	2.3
3	J	244	LEU	2.3
3	B	588	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	J	781	ARG	2.3
3	B	193	THR	2.2
3	J	602	ILE	2.2
1	A	760	GLY	2.2
3	B	474	ALA	2.2
3	J	10	ARG	2.2
3	B	265	VAL	2.2
9	U	51	ILE	2.2
3	J	223	PHE	2.2
3	B	10	ARG	2.2
3	B	601	ALA	2.2
3	B	1071	ASP	2.2
3	J	1069	TRP	2.2
1	I	763	THR	2.2
1	A	607	GLN	2.2
4	D	27	ALA	2.2
7	S	114	ARG	2.2
3	B	946	TYR	2.1
8	H	37	ILE	2.1
11	W	5	ILE	2.1
1	A	129	ALA	2.1
1	I	120	ALA	2.1
6	R	68	VAL	2.1
3	B	317	TYR	2.1
2	C	262	LEU	2.1
3	J	434	ALA	2.1
3	J	600	GLY	2.1
3	J	986	GLY	2.1
3	B	814	VAL	2.1
8	T	82	ILE	2.1
2	C	217	ALA	2.1
3	B	1049	LEU	2.1
4	O	33	MET	2.1
3	B	934	ALA	2.1
1	I	82	ILE	2.1
2	C	193	LEU	2.1
7	S	113	LEU	2.1
11	N	64	ARG	2.1
11	W	64	ARG	2.1
3	B	207	ASP	2.1
4	D	186	GLY	2.1
2	M	196	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
5	Q	52	LYS	2.0
9	U	61	VAL	2.0
3	B	372	SER	2.0
1	A	707	LEU	2.0
3	B	402	ASN	2.0
10	L	82	HIS	2.0
2	M	183	ASP	2.0
2	C	233	GLY	2.0
3	J	903	GLY	2.0
2	M	167	LEU	2.0
1	I	878	TRP	2.0
6	F	14	TYR	2.0
7	G	79	THR	2.0
1	I	867	ASP	2.0
2	M	67	GLY	2.0
3	J	54	PRO	2.0
6	F	45	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	I	1002	1/1	0.96	0.10	78,78,78,78	0
14	ZN	I	1001	1/1	0.98	0.13	57,57,57,57	0
14	ZN	A	1002	1/1	0.98	0.10	69,69,69,69	0
16	F3S	D	1001	7/7	0.98	0.04	79,81,82,84	0
16	F3S	O	1001	7/7	0.98	0.04	104,105,106,106	0
14	ZN	J	2001	1/1	0.99	0.04	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	ZN	W	1001	1/1	0.99	0.06	63,63,63,63	0
14	ZN	X	1001	1/1	0.99	0.03	54,54,54,54	0
14	ZN	A	1001	1/1	0.99	0.10	46,46,46,46	0
14	ZN	B	2001	1/1	0.99	0.06	66,66,66,66	0
15	MG	A	1003	1/1	1.00	0.06	2,2,2,2	0
15	MG	I	1003	1/1	1.00	0.08	2,2,2,2	0
14	ZN	P	1001	1/1	1.00	0.06	33,33,33,33	0
14	ZN	N	1001	1/1	1.00	0.07	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.