



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:43 PM GMT

PDB ID : 1Y1V
Title : Refined RNA Polymerase II-TFIIS complex
Authors : Kettenberger, H.; Armache, K.-J.; Cramer, P.
Deposited on : 2004-11-19
Resolution : 3.80 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

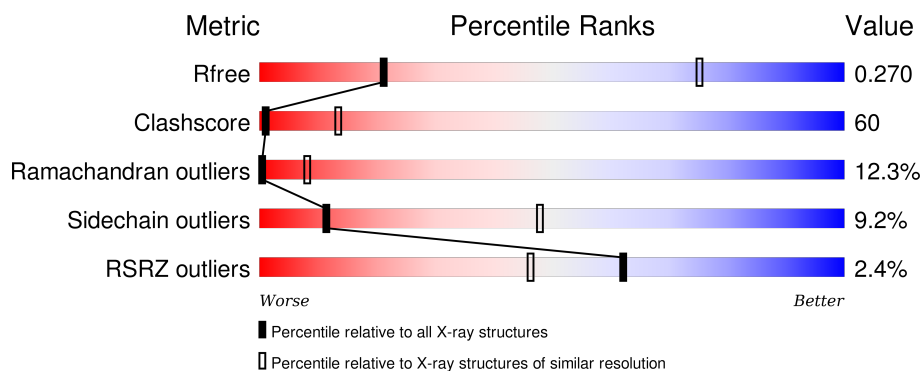
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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.



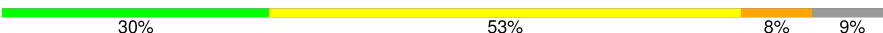
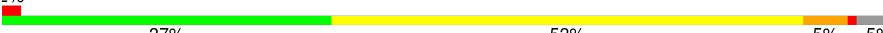
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1733	<div> <div>21%</div> <div>47%</div> <div>13%</div> <div>•</div> <div>18%</div> </div>
2	B	1224	<div>2%</div> <div>24%</div> <div>52%</div> <div>13%</div> <div>•</div> <div>9%</div>
3	C	318	<div>22%</div> <div>48%</div> <div>12%</div> <div>•</div> <div>16%</div>
4	D	221	<div>33%</div> <div>40%</div> <div>6%</div> <div>20%</div>
5	E	215	<div>%</div> <div>34%</div> <div>55%</div> <div>11%</div>

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Mol	Chain	Length	Quality of chain
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	S	179	

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	MG	S	1	-	-	-	X

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 31803 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 II largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1426	Total	C	N	O	S	0	0	0
			11214	7069	1959	2124	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1112	Total	C	N	O	S	58	0	0
			8837	5594	1548	1640	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerase II 32 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	177	Total	C	N	O	S	0	0	0
			1356	840	241	273	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II 19 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-directed RNA polymerases I/II/III subunit 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			364	224	72	64	4			

- Molecule 13 is a protein called Transcription elongation factor S-II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	S	174	Total	C	N	O	S	0	0	104
			666	454	99	108	5			

- Molecule 14 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	S	1	Total	Mg	0	0
			1	1		

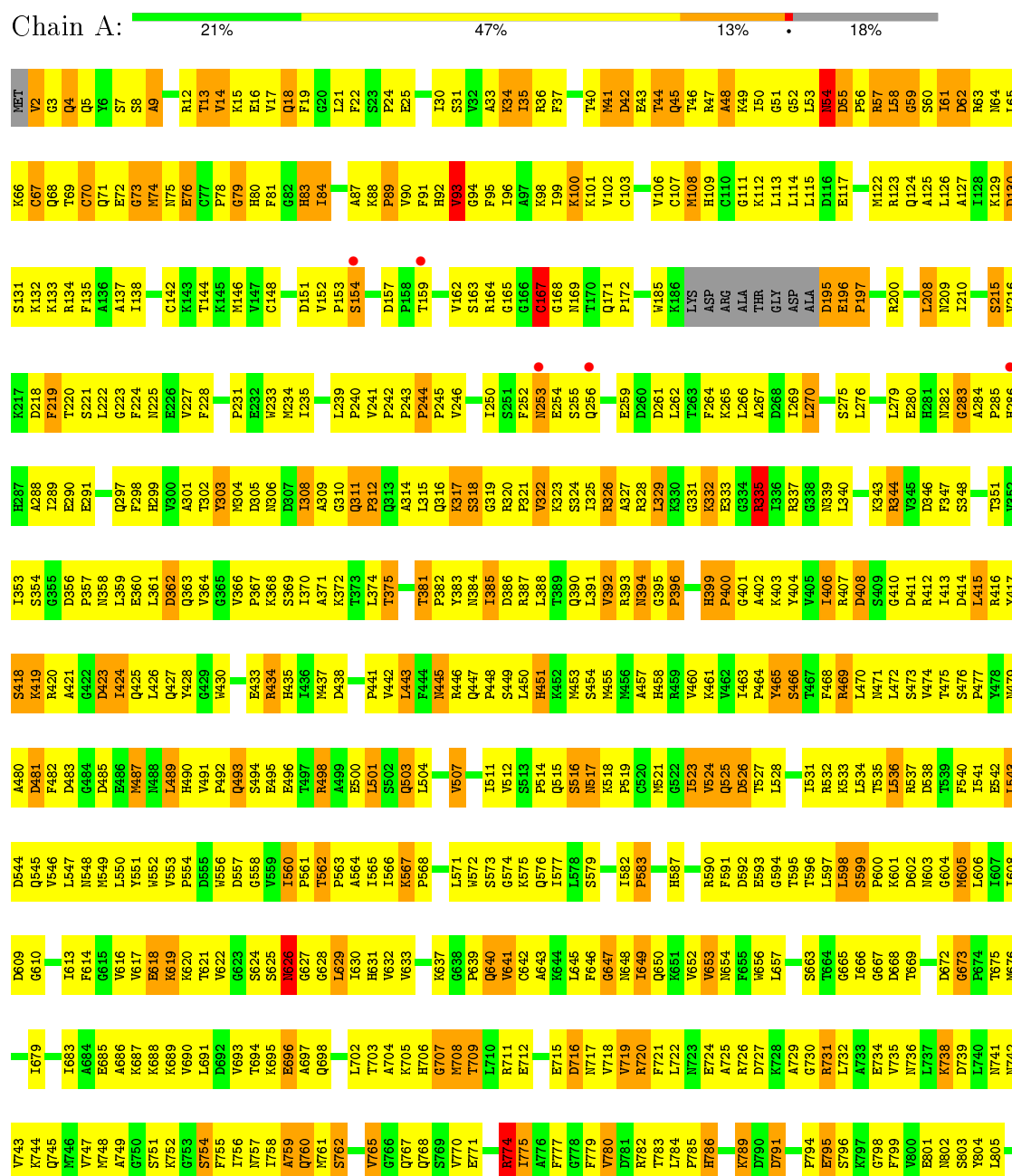
- Molecule 15 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	J	1	Total	Zn	0	0
			1	1		
15	B	1	Total	Zn	0	0
			1	1		
15	I	2	Total	Zn	0	0
			2	2		
15	C	1	Total	Zn	0	0
			1	1		
15	A	2	Total	Zn	0	0
			2	2		
15	L	1	Total	Zn	0	0
			1	1		
15	S	1	Total	Zn	0	0
			1	1		

3 Residue-property plots

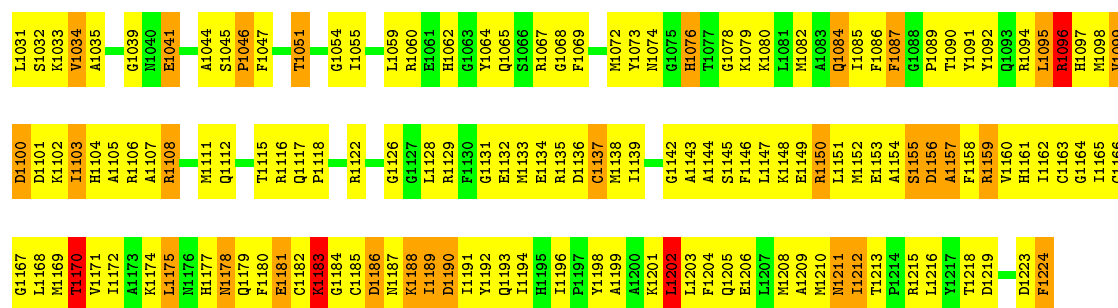
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 II largest subunit

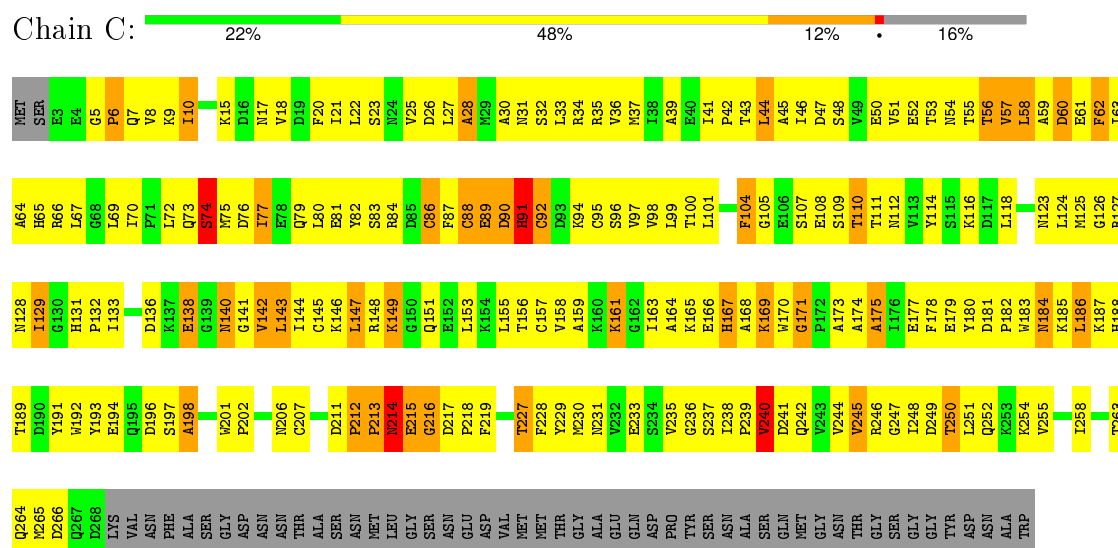




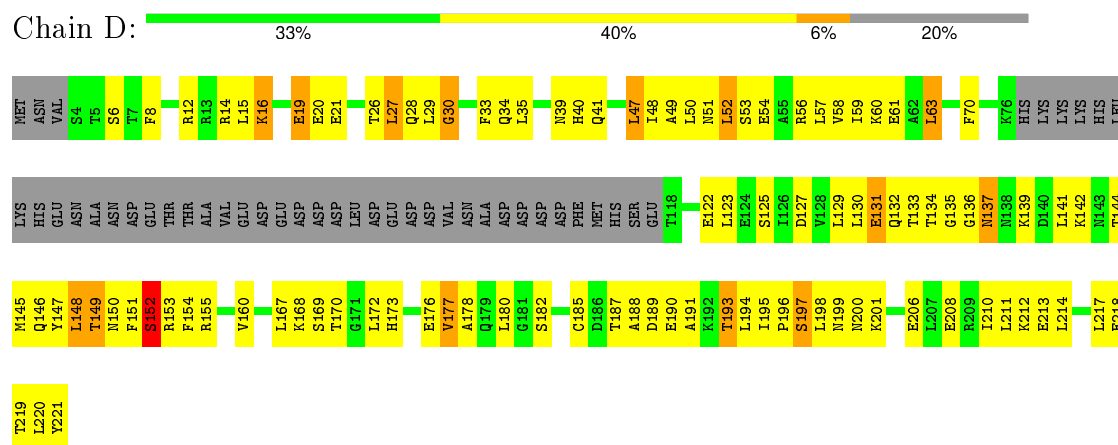




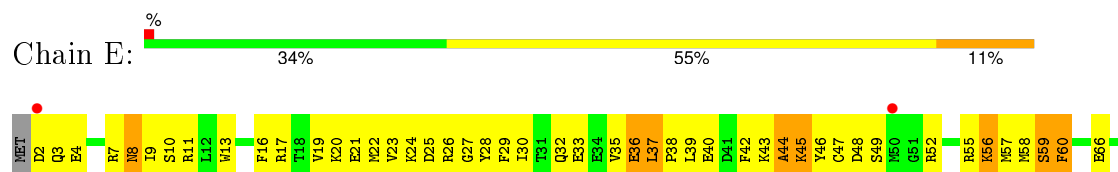
• Molecule 3: DNA-directed RNA polymerase II 45 kDa polypeptide

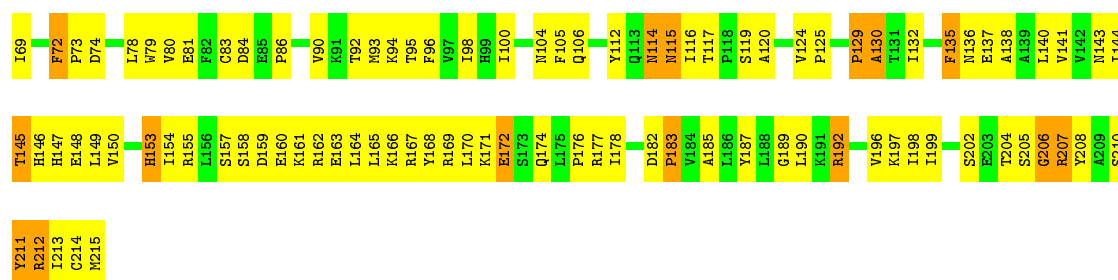


• Molecule 4: DNA-directed RNA polymerase II 32 kDa polypeptide



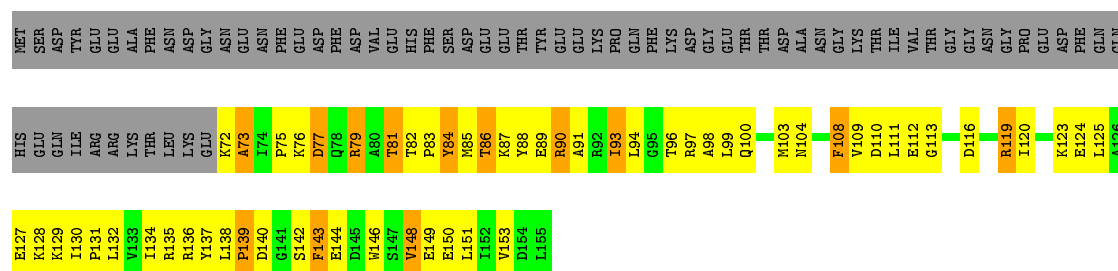
• Molecule 5: DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide





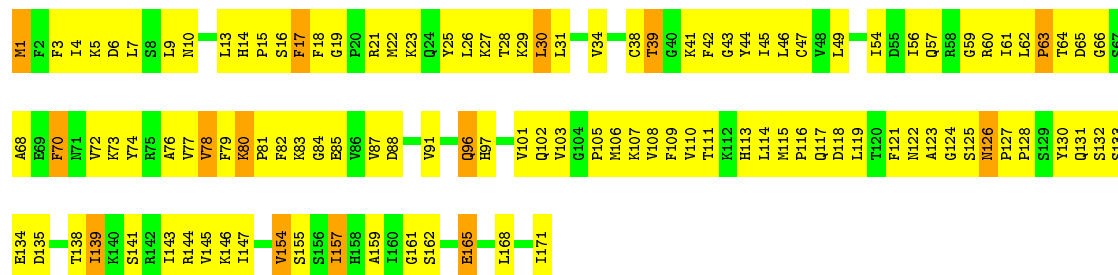
- Molecule 6: DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide

Chain F: 15% 30% 8% 46%



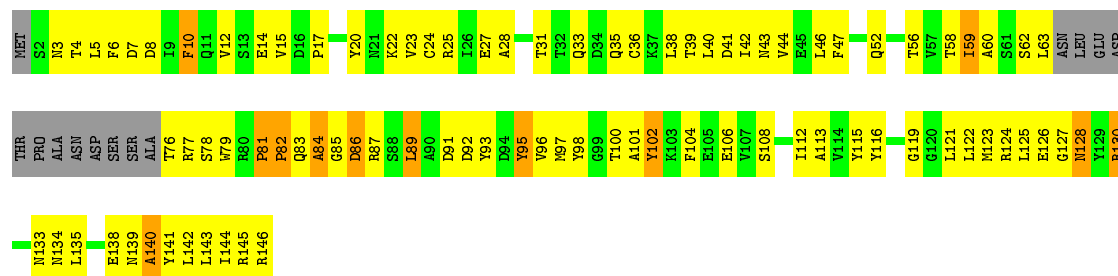
- Molecule 7: DNA-directed RNA polymerase II 19 kDa polypeptide

Chain G: 33% 59% 8%



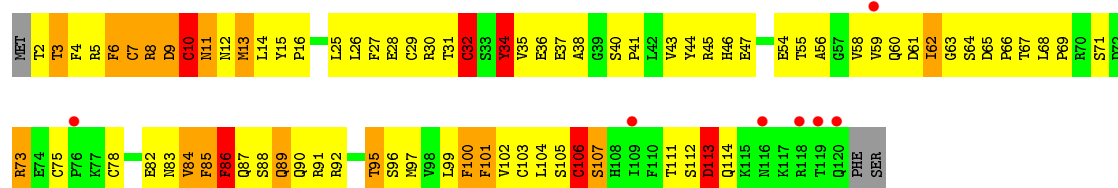
- Molecule 8: DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide

Chain H: 30% 53% 8% 9%

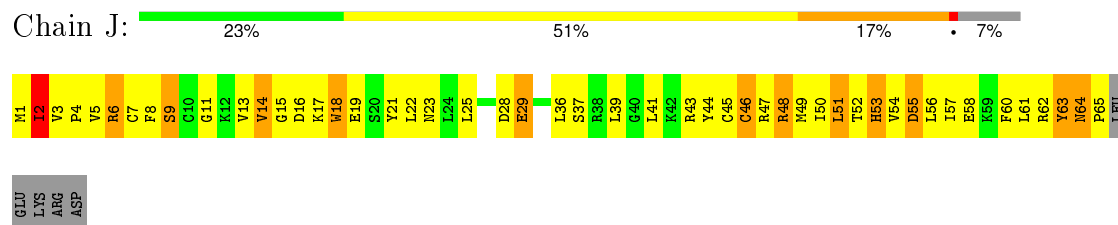


- Molecule 9: DNA-directed RNA polymerase II subunit 9

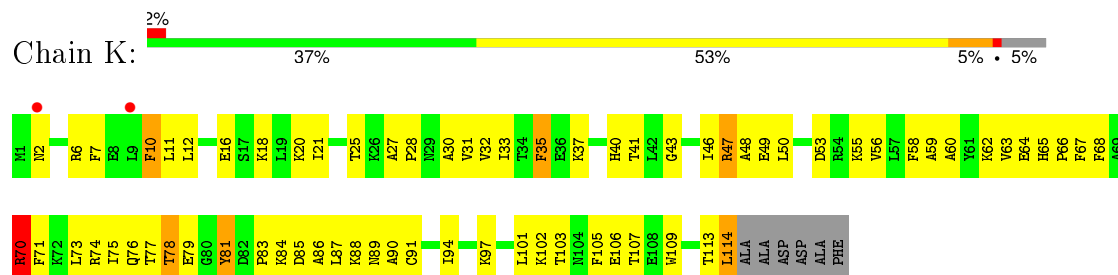
Chain I: 6% 31% 48% 13% 5%



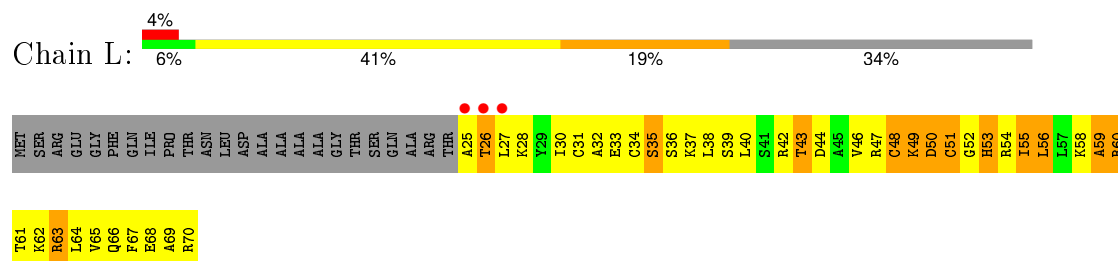
- Molecule 10: DNA-directed RNA polymerases I/II/III subunit 10



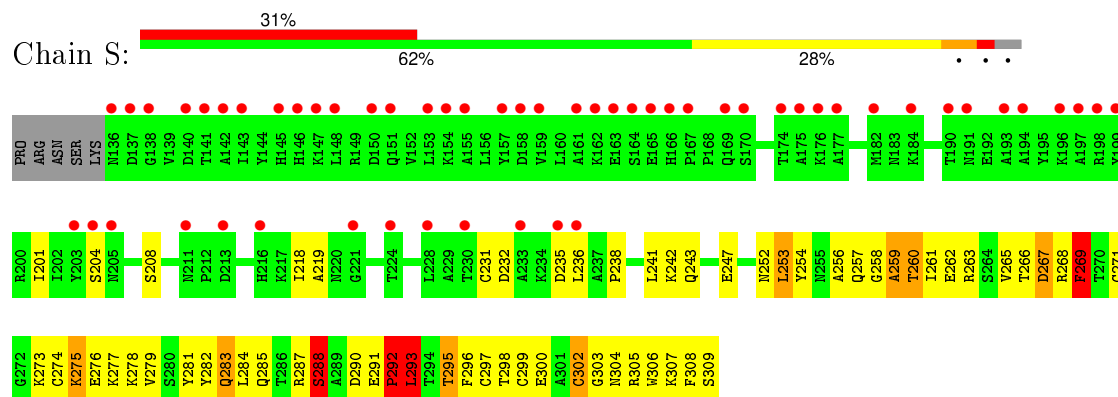
- Molecule 11: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 12: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



- Molecule 13: Transcription elongation factor S-II



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	218.90Å 395.30Å 281.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.80 49.41 – 3.74	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.80) 86.6 (49.41-3.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.75 (at 3.77Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.282 , 0.294 0.263 , 0.270	Depositor DCC
R_{free} test set	2373 reflections (2.10%)	DCC
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.208 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.216 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.12$	Xtriage
Outliers	0 of 115462 reflections	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	31803	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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	0.50	2/11417 (0.0%)	0.78	4/15442 (0.0%)
2	B	0.51	4/9009 (0.0%)	0.76	8/12146 (0.1%)
3	C	0.48	0/2133	0.77	1/2891 (0.0%)
4	D	0.41	0/1365	0.64	0/1837
5	E	0.43	0/1788	0.66	0/2406
6	F	0.52	0/691	0.77	0/933
7	G	0.49	0/1368	0.72	0/1844
8	H	0.38	0/1086	0.65	1/1470 (0.1%)
9	I	0.46	0/989	0.77	1/1331 (0.1%)
10	J	0.48	0/541	0.75	0/727
11	K	0.45	0/937	0.67	0/1265
12	L	0.54	0/366	0.79	0/485
13	S	1.31	4/571 (0.7%)	1.64	7/765 (0.9%)
All	All	0.51	10/32261 (0.0%)	0.77	22/43542 (0.1%)

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	B	0	3
13	S	0	2
All	All	0	5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	269	PHE	C-N	-16.91	0.95	1.34
2	B	467	GLY	C-O	-11.91	1.04	1.23
13	S	260	THR	CA-CB	10.48	1.80	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	468	GLU	CB-CG	8.39	1.68	1.52
13	S	268	ARG	CG-CD	6.05	1.67	1.51
13	S	267	ASP	C-O	6.03	1.34	1.23
2	B	510	LYS	CB-CG	5.59	1.67	1.52
1	A	195	ASP	N-CA	5.47	1.57	1.46
2	B	468	GLU	CG-CD	5.18	1.59	1.51
1	A	196	GLU	CB-CG	5.13	1.61	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	S	269	PHE	O-C-N	-19.02	92.27	122.70
13	S	269	PHE	C-N-CA	16.73	163.51	121.70
13	S	269	PHE	CA-C-N	16.08	152.57	117.20
1	A	195	ASP	N-CA-C	9.35	136.25	111.00
2	B	510	LYS	CB-CA-C	-7.63	95.14	110.40
2	B	510	LYS	C-N-CD	-7.44	104.24	120.60
3	C	92	CYS	CA-CB-SG	-6.79	101.77	114.00
13	S	253	LEU	CA-CB-CG	-6.79	99.67	115.30
1	A	1310	GLY	N-CA-C	-6.49	96.88	113.10
9	I	10	CYS	CA-CB-SG	6.20	125.16	114.00
2	B	468	GLU	N-CA-C	5.96	127.09	111.00
13	S	292	PRO	N-CA-C	5.96	127.59	112.10
2	B	467	GLY	CA-C-N	5.86	130.10	117.20
2	B	511	PRO	CA-N-CD	-5.81	103.37	111.50
2	B	508	LEU	C-N-CA	-5.71	107.43	121.70
1	A	344	ARG	N-CA-C	-5.58	95.93	111.00
2	B	510	LYS	C-N-CA	5.55	145.30	122.00
8	H	89	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	865	GLN	N-CA-C	-5.39	96.45	111.00
2	B	296	GLU	N-CA-C	-5.26	96.79	111.00
13	S	302	CYS	CA-CB-SG	5.18	123.32	114.00
13	S	303	GLY	N-CA-C	5.10	125.85	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	510	LYS	Mainchain
2	B	785	TYR	Sidechain
2	B	833	TYR	Sidechain
13	S	269	PHE	Sidechain,Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11214	0	11281	1514	0
2	B	8837	0	8871	1206	0
3	C	2095	0	2052	259	0
4	D	1356	0	1319	101	0
5	E	1752	0	1776	200	0
6	F	679	0	701	82	0
7	G	1340	0	1357	159	0
8	H	1068	0	1040	115	0
9	I	971	0	929	110	0
10	J	532	0	542	103	0
11	K	919	0	929	96	0
12	L	364	0	387	68	0
13	S	666	0	553	103	0
14	S	1	0	0	0	0
15	A	2	0	0	0	0
15	B	1	0	0	0	0
15	C	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	L	1	0	0	0	0
15	S	1	0	0	0	0
All	All	31803	0	31737	3771	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 60.

All (3771) 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)
13:S:260:THR:CA	13:S:260:THR:CB	1.80	1.53
13:S:269:PHE:CZ	13:S:297:CYS:SG	2.04	1.50
13:S:269:PHE:CE2	13:S:297:CYS:SG	2.14	1.39
1:A:1230:GLU:OE2	13:S:201:ILE:CA	1.75	1.32
1:A:1283:VAL:CG1	13:S:256:ALA:O	1.78	1.31
1:A:1172:LEU:CD1	13:S:204:SER:CA	2.12	1.27

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:ASN:HD21	13:S:238:PRO:CA	1.48	1.25
13:S:235:ASP:CA	13:S:242:LYS:HE2	1.72	1.18
1:A:1283:VAL:HG13	13:S:256:ALA:O	1.41	1.15
7:G:138:THR:HG22	7:G:139:ILE:H	1.11	1.15
1:A:1017:LEU:HB2	5:E:206:GLY:H	1.11	1.14
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.31	1.12
4:D:40:HIS:HB3	7:G:73:LYS:HZ3	1.09	1.12
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.49	1.11
1:A:225:ASN:ND2	1:A:228:PHE:H	1.47	1.11
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.14	1.09
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.88	1.09
1:A:590:ARG:NH2	1:A:620:LYS:HB3	1.66	1.09
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.02	1.09
1:A:913:LEU:HD12	1:A:914:GLU:H	1.15	1.09
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.33	1.08
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.11	1.08
1:A:855:THR:HG21	1:A:857:ARG:HE	1.10	1.08
7:G:14:HIS:HD2	7:G:16:SER:HB2	1.15	1.08
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.15	1.07
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.28	1.07
6:F:82:THR:HG22	6:F:84:TYR:H	1.15	1.07
1:A:1172:LEU:HD13	13:S:204:SER:CA	1.81	1.06
4:D:40:HIS:HB3	7:G:73:LYS:NZ	1.69	1.06
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.86	1.05
2:B:112:LEU:HD12	2:B:113:TYR:H	1.19	1.05
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.20	1.05
1:A:47:ARG:HH12	1:A:254:GLU:HB3	1.21	1.05
13:S:235:ASP:CA	13:S:242:LYS:CE	2.34	1.05
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.19	1.04
3:C:133:ILE:HD11	3:C:237:SER:HA	1.39	1.04
2:B:839:MET:CG	2:B:1010:LEU:HD11	1.88	1.04
7:G:111:THR:HG22	7:G:113:HIS:H	1.19	1.04
1:A:834:THR:HG21	1:A:1077:THR:HG23	1.39	1.04
1:A:1135:ARG:NH1	13:S:256:ALA:HB2	1.72	1.03
1:A:901:LEU:H	1:A:926:GLN:NE2	1.54	1.03
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.39	1.02
13:S:291:GLU:N	13:S:292:PRO:HD2	1.72	1.02
2:B:508:LEU:CB	2:B:510:LYS:H	1.70	1.02
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.58	1.02
1:A:1172:LEU:HD11	13:S:204:SER:CA	1.85	1.02
2:B:1159:ARG:HD3	2:B:1193:GLN:HG3	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1199:ARG:HH22	13:S:241:LEU:HD13	1.21	1.01
2:B:589:VAL:HG12	2:B:590:HIS:H	1.24	1.00
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.43	1.00
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.43	1.00
1:A:164:ARG:HG3	1:A:165:GLY:H	1.26	1.00
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.44	1.00
1:A:53:LEU:HD23	1:A:54:ASN:N	1.76	1.00
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.44	0.99
1:A:1283:VAL:HG12	13:S:256:ALA:O	1.57	0.99
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.26	0.99
11:K:65:HIS:CD2	11:K:67:PHE:H	1.81	0.99
1:A:63:ARG:HA	1:A:74:MET:SD	2.01	0.99
2:B:510:LYS:HD2	2:B:510:LYS:O	1.60	0.99
1:A:853:ASP:OD1	1:A:855:THR:HB	1.62	0.99
1:A:1199:ARG:NH2	13:S:241:LEU:HD13	1.78	0.98
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.45	0.98
1:A:490:HIS:HB3	2:B:1150:ARG:NH1	1.79	0.98
3:C:56:THR:HG21	3:C:145:CYS:SG	2.03	0.98
2:B:65:GLU:HG3	2:B:66:ASP:H	1.27	0.98
2:B:295:GLY:H	2:B:298:LEU:HD23	1.27	0.98
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.45	0.97
2:B:839:MET:HG3	2:B:1010:LEU:HD11	1.01	0.97
1:A:225:ASN:HD22	1:A:228:PHE:H	1.03	0.97
2:B:863:GLU:OE2	2:B:873:THR:HA	1.64	0.97
1:A:913:LEU:HD12	1:A:914:GLU:N	1.81	0.96
1:A:1081:LEU:HD12	1:A:1082:ASN:OD1	1.66	0.96
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	1.78	0.96
2:B:882:THR:HG22	2:B:884:ARG:H	1.29	0.95
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.00	0.95
1:A:1172:LEU:CD2	13:S:204:SER:CA	2.44	0.95
2:B:211:VAL:O	2:B:480:SER:HA	1.65	0.95
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.31	0.95
2:B:987:LYS:HZ2	13:S:290:ASP:HB3	1.32	0.95
3:C:73:GLN:HE21	3:C:75:MET:H	1.03	0.95
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.66	0.95
2:B:583:ASN:HD21	2:B:628:THR:HB	1.29	0.95
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.45	0.94
1:A:1232:ASN:ND2	13:S:238:PRO:CA	2.29	0.94
2:B:1002:THR:HG21	2:B:1006:ILE:HD12	1.49	0.93
1:A:337:ARG:CZ	1:A:839:ARG:HH12	1.81	0.93
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:85:PHE:HD2	9:I:85:PHE:H	0.93	0.93
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.04	0.93
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.67	0.93
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.48	0.93
1:A:70:CYS:O	1:A:72:GLU:HG2	1.68	0.93
6:F:76:LYS:O	6:F:79:ARG:HD3	1.70	0.92
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.48	0.92
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.48	0.92
13:S:279:VAL:HG22	13:S:299:CYS:HA	1.50	0.92
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.84	0.92
5:E:153:HIS:O	5:E:154:ILE:HG13	1.69	0.92
2:B:1183:LYS:HE3	2:B:1183:LYS:N	1.85	0.92
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.27	0.92
7:G:14:HIS:CD2	7:G:16:SER:HB2	2.04	0.92
1:A:1341:ILE:HG23	1:A:1342:GLU:H	1.32	0.92
3:C:167:HIS:HD2	3:C:169:LYS:H	1.17	0.91
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.05	0.91
3:C:63:ILE:HA	3:C:66:ARG:HG3	1.50	0.91
2:B:168:GLY:H	2:B:450:ALA:HB1	1.34	0.91
2:B:549:THR:HG22	2:B:550:ASP:H	1.35	0.91
1:A:1362:TYR:HD1	1:A:1363:VAL:H	1.18	0.91
1:A:1329:THR:HG22	1:A:1331:SER:H	1.36	0.91
1:A:864:ILE:O	1:A:865:GLN:HG3	1.72	0.90
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.51	0.90
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.36	0.90
1:A:490:HIS:HB3	2:B:1150:ARG:HH11	1.36	0.90
11:K:65:HIS:HD2	11:K:67:PHE:H	1.10	0.90
9:I:111:THR:HG22	9:I:112:SER:H	1.37	0.90
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.52	0.89
1:A:1329:THR:N	1:A:1335:ILE:HD11	1.87	0.89
1:A:560:ILE:HG13	8:H:78:SER:HB2	1.51	0.89
1:A:666:ILE:HD12	1:A:667:GLY:H	1.35	0.89
1:A:1118:VAL:O	1:A:1305:VAL:HG13	1.71	0.89
2:B:35:SER:HA	2:B:811:TYR:HE2	1.36	0.89
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	1.88	0.89
4:D:56:ARG:HB2	4:D:148:LEU:HD22	1.52	0.89
11:K:56:VAL:HA	11:K:77:THR:HG22	1.55	0.89
1:A:708:MET:HE2	1:A:1089:VAL:HG13	1.55	0.88
2:B:1095:LEU:HD12	2:B:1095:LEU:N	1.88	0.88
10:J:6:ARG:HG2	10:J:13:VAL:HA	1.55	0.88
1:A:524:VAL:HG12	1:A:525:GLN:H	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.88
5:E:22:MET:HE3	5:E:26:ARG:NE	1.89	0.88
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.55	0.88
2:B:835:GLN:HA	2:B:1013:ASN:HD22	1.35	0.88
2:B:365:THR:HG23	2:B:367:LEU:HG	1.55	0.88
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.55	0.88
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.38	0.88
1:A:55:ASP:C	1:A:57:ARG:H	1.73	0.88
7:G:23:LYS:HG3	7:G:56:ILE:HD11	1.55	0.88
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.55	0.88
1:A:567:LYS:HB3	8:H:96:VAL:H	1.39	0.88
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.39	0.88
5:E:117:THR:HG22	5:E:119:SER:H	1.39	0.88
7:G:13:LEU:HD21	7:G:17:PHE:HB2	1.56	0.88
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.53	0.88
7:G:1:MET:HG3	7:G:85:GLU:CD	1.93	0.88
1:A:466:SER:O	2:B:1103:ILE:HD11	1.74	0.87
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.55	0.87
1:A:901:LEU:H	1:A:926:GLN:HE21	1.22	0.87
5:E:22:MET:HE3	5:E:26:ARG:HE	1.37	0.87
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.57	0.87
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.90	0.87
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.09	0.87
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.57	0.87
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.57	0.87
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.40	0.87
1:A:443:LEU:HG	2:B:1146:PHE:HE2	1.38	0.87
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.57	0.87
1:A:855:THR:HG21	1:A:857:ARG:NE	1.89	0.86
2:B:113:TYR:HB3	2:B:114:PRO:HD2	1.55	0.86
7:G:1:MET:HG3	7:G:85:GLU:OE2	1.75	0.86
1:A:587:HIS:CD2	1:A:969:GLN:HG2	2.11	0.86
3:C:213:PRO:O	3:C:214:ASN:HB2	1.74	0.86
2:B:466:TRP:O	2:B:468:GLU:N	2.08	0.86
2:B:467:GLY:O	2:B:468:GLU:HB2	1.73	0.86
9:I:29:CYS:SG	9:I:32:CYS:N	2.48	0.86
2:B:39:ARG:NH2	2:B:665:GLU:HG2	1.89	0.86
1:A:1341:ILE:HG23	1:A:1342:GLU:N	1.89	0.85
13:S:265:VAL:CG1	13:S:278:LYS:HA	2.06	0.85
2:B:880:THR:HB	2:B:934:LYS:HD2	1.56	0.85
10:J:43:ARG:HG3	10:J:45:CYS:SG	2.16	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:PHE:HE2	2:B:542:MET:HA	1.40	0.85
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.12	0.85
2:B:493:SER:HA	2:B:751:VAL:HG21	1.57	0.85
1:A:665:GLY:HA2	2:B:1026:LEU:HD21	1.58	0.85
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.44	0.85
1:A:446:ARG:HD2	1:A:480:ALA:HB2	1.58	0.85
2:B:839:MET:HG3	2:B:1010:LEU:CD1	1.98	0.85
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	1.76	0.85
2:B:955:THR:HG23	12:L:54:ARG:O	1.77	0.85
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.92	0.85
7:G:138:THR:HG22	7:G:139:ILE:N	1.91	0.85
1:A:963:ILE:HD13	1:A:1049:ILE:HG13	1.58	0.85
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.05	0.84
9:I:85:PHE:N	9:I:85:PHE:CD2	2.45	0.84
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.39	0.84
5:E:153:HIS:HB3	5:E:196:VAL:HG11	1.58	0.84
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.41	0.84
2:B:781:PHE:O	2:B:782:LEU:HG	1.78	0.84
2:B:843:GLN:HB2	2:B:993:THR:HB	1.58	0.84
2:B:766:ARG:NH2	2:B:1020:ARG:HG2	1.92	0.84
2:B:1065:GLN:HE21	2:B:1067:ARG:H	0.86	0.84
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.60	0.84
2:B:1107:ALA:O	2:B:1108:ARG:HG2	1.77	0.84
1:A:537:ARG:HD2	8:H:20:TYR:HE1	1.40	0.84
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.11	0.84
3:C:244:VAL:O	3:C:248:ILE:HG13	1.76	0.84
5:E:153:HIS:HB3	5:E:196:VAL:CG1	2.08	0.84
1:A:472:LEU:HD11	2:B:835:GLN:NE2	1.93	0.84
1:A:540:PHE:HB3	1:A:571:LEU:HD23	1.59	0.84
1:A:503:GLN:HE21	6:F:90:ARG:HH21	1.25	0.83
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.59	0.83
8:H:100:THR:HG23	8:H:138:GLU:HA	1.58	0.83
1:A:1291:VAL:HG13	1:A:1292:PRO:HD2	1.59	0.83
1:A:1116:LEU:HD23	1:A:1311:VAL:HG22	1.60	0.83
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.61	0.83
10:J:9:SER:OG	10:J:45:CYS:HB2	1.79	0.83
1:A:743:VAL:O	1:A:747:VAL:HG23	1.79	0.83
2:B:510:LYS:O	2:B:510:LYS:CD	2.25	0.82
13:S:291:GLU:H	13:S:292:PRO:HD2	1.42	0.82
2:B:510:LYS:HG2	2:B:512:ARG:H	1.43	0.82
13:S:288:SER:O	13:S:292:PRO:HD3	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ASP:OD1	10:J:17:LYS:HD2	1.80	0.82
2:B:1020:ARG:HG2	2:B:1020:ARG:HH11	1.44	0.82
9:I:111:THR:HG22	9:I:113:ASP:H	1.43	0.82
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.09	0.82
2:B:502:ILE:HG22	2:B:502:ILE:O	1.79	0.82
1:A:14:VAL:HG23	1:A:1432:GLN:NE2	1.95	0.82
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.25	0.82
2:B:295:GLY:N	2:B:298:LEU:HD23	1.94	0.81
1:A:649:ILE:O	1:A:653:VAL:HG23	1.80	0.81
6:F:86:THR:OG1	6:F:89:GLU:HG3	1.80	0.81
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.63	0.81
7:G:111:THR:HG22	7:G:113:HIS:N	1.95	0.81
1:A:1237:ILE:HG22	1:A:1238:ILE:N	1.96	0.81
2:B:816:GLU:O	2:B:817:LEU:HD23	1.80	0.81
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.44	0.81
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.10	0.81
1:A:628:GLY:O	1:A:632:VAL:HG23	1.81	0.81
9:I:56:ALA:HB2	9:I:89:GLN:CG	2.10	0.81
1:A:669:THR:O	1:A:762:SER:HB3	1.81	0.81
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.63	0.81
13:S:235:ASP:CA	13:S:242:LYS:CG	2.58	0.81
2:B:1169:MET:CE	2:B:1201:LYS:HA	2.11	0.81
1:A:78:PRO:HA	2:B:1201:LYS:NZ	1.96	0.81
1:A:1372:VAL:O	1:A:1376:THR:HG22	1.81	0.81
1:A:1317:MET:O	1:A:1322:ILE:HD11	1.80	0.81
1:A:795:GLU:CD	1:A:795:GLU:H	1.83	0.81
7:G:1:MET:HE3	7:G:80:LYS:C	2.00	0.81
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.63	0.81
9:I:6:PHE:HB3	9:I:12:ASN:O	1.80	0.81
1:A:666:ILE:HD12	1:A:667:GLY:N	1.95	0.80
2:B:510:LYS:HD2	2:B:510:LYS:C	1.98	0.80
2:B:862:GLN:HG2	2:B:963:PHE:HD1	1.45	0.80
1:A:471:ASN:O	1:A:474:VAL:HG12	1.81	0.80
1:A:399:HIS:O	1:A:401:GLY:N	2.14	0.80
9:I:58:VAL:HG12	9:I:60:GLN:H	1.47	0.80
2:B:1204:PHE:O	2:B:1208:MET:HG3	1.82	0.80
1:A:1017:LEU:HB2	5:E:206:GLY:N	1.93	0.80
6:F:82:THR:HG22	6:F:84:TYR:N	1.97	0.80
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.44	0.80
11:K:65:HIS:HD2	11:K:67:PHE:N	1.79	0.80
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:HE	1:A:339:ASN:ND2	1.79	0.79
2:B:589:VAL:HG12	2:B:590:HIS:N	1.95	0.79
2:B:508:LEU:C	2:B:510:LYS:N	2.30	0.79
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.62	0.79
1:A:56:PRO:O	1:A:57:ARG:HG3	1.82	0.79
9:I:58:VAL:HG22	9:I:62:ILE:HD12	1.63	0.79
3:C:73:GLN:NE2	3:C:75:MET:H	1.79	0.79
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.62	0.79
1:A:825:ILE:HG21	2:B:510:LYS:HE3	1.64	0.79
9:I:55:THR:HG23	9:I:100:PHE:HD2	1.48	0.79
2:B:509:ALA:O	2:B:510:LYS:HD2	1.81	0.79
2:B:508:LEU:C	2:B:510:LYS:H	1.81	0.79
2:B:359:GLU:O	2:B:362:PRO:HD3	1.82	0.79
9:I:85:PHE:HD2	9:I:85:PHE:N	1.78	0.79
3:C:133:ILE:CD1	3:C:237:SER:HA	2.12	0.79
13:S:265:VAL:HG13	13:S:278:LYS:HA	1.65	0.79
13:S:269:PHE:HZ	13:S:297:CYS:SG	1.97	0.79
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.82	0.79
1:A:299:HIS:HA	1:A:302:THR:HG22	1.65	0.79
1:A:494:SER:O	1:A:498:ARG:HG2	1.82	0.79
3:C:98:VAL:C	3:C:99:LEU:HD23	2.04	0.79
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.65	0.79
2:B:806:THR:HG22	2:B:808:ALA:H	1.48	0.79
7:G:9:LEU:HD12	7:G:10:ASN:H	1.48	0.79
2:B:613:VAL:HG13	2:B:627:PHE:O	1.84	0.78
1:A:1444:MET:HG2	7:G:60:ARG:HA	1.65	0.78
1:A:1135:ARG:NH1	13:S:256:ALA:CB	2.46	0.78
1:A:608:ILE:HB	1:A:613:ILE:HD11	1.65	0.78
2:B:593:PRO:HG2	2:B:617:ARG:NH2	1.99	0.78
1:A:537:ARG:HD2	8:H:20:TYR:CE1	2.18	0.78
3:C:167:HIS:CD2	3:C:169:LYS:H	2.02	0.78
3:C:212:PRO:HB3	3:C:213:PRO:HD2	1.64	0.78
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.48	0.78
5:E:124:VAL:HG13	5:E:132:ILE:HD12	1.64	0.78
5:E:154:ILE:H	5:E:196:VAL:HG13	1.49	0.78
13:S:271:CYS:SG	13:S:304:ASN:ND2	2.57	0.78
1:A:587:HIS:HD2	1:A:969:GLN:HG2	1.48	0.78
2:B:112:LEU:HD12	2:B:113:TYR:N	1.96	0.78
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.64	0.78
2:B:987:LYS:NZ	13:S:290:ASP:HB3	1.98	0.78
4:D:40:HIS:CB	7:G:73:LYS:HZ3	1.94	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HG22	2:B:884:ARG:N	1.99	0.78
2:B:510:LYS:HG2	2:B:512:ARG:HG3	1.64	0.78
1:A:1283:VAL:HG13	13:S:256:ALA:C	2.04	0.78
4:D:48:ILE:HG21	7:G:4:ILE:HD12	1.66	0.77
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.18	0.77
1:A:765:VAL:HG23	1:A:802:ASN:O	1.84	0.77
1:A:1127:ASP:HB3	1:A:1130:GLN:CB	2.14	0.77
1:A:1017:LEU:HB3	5:E:205:SER:HA	1.64	0.77
1:A:866:PHE:O	1:A:867:ILE:HD12	1.85	0.77
1:A:1090:ALA:HA	1:A:1093:LYS:HE3	1.66	0.77
1:A:164:ARG:HG3	1:A:165:GLY:N	1.98	0.77
2:B:508:LEU:HB3	2:B:510:LYS:H	1.48	0.77
2:B:1206:GLU:O	2:B:1209:ALA:HB3	1.83	0.77
1:A:515:GLN:O	1:A:516:SER:HB3	1.85	0.77
10:J:45:CYS:O	10:J:48:ARG:HG3	1.85	0.77
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.66	0.77
3:C:47:ASP:HA	12:L:69:ALA:CB	2.15	0.77
2:B:1106:ARG:HG3	2:B:1107:ALA:N	1.96	0.77
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.64	0.77
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.67	0.77
4:D:35:LEU:H	4:D:35:LEU:HD12	1.48	0.77
1:A:908:LEU:HD12	1:A:983:ILE:HD11	1.67	0.77
3:C:73:GLN:HE21	3:C:75:MET:N	1.82	0.76
9:I:62:ILE:HG22	9:I:62:ILE:O	1.84	0.76
7:G:121:PHE:HB2	7:G:130:TYR:CE2	2.20	0.76
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.67	0.76
1:A:590:ARG:HD3	1:A:604:GLY:HA2	1.67	0.76
1:A:830:LYS:HB2	1:A:1081:LEU:HD23	1.67	0.76
2:B:583:ASN:ND2	2:B:628:THR:HB	2.00	0.76
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.20	0.76
1:A:767:GLN:OE1	1:A:799:PHE:HB2	1.83	0.76
8:H:4:THR:HA	8:H:60:ALA:HB2	1.66	0.76
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.00	0.76
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.84	0.76
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.68	0.76
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.68	0.76
4:D:185:CYS:HA	4:D:190:GLU:OE1	1.85	0.76
2:B:1165:ILE:HG22	2:B:1166:CYS:N	1.99	0.76
1:A:963:ILE:HD11	1:A:1048:ASN:HB2	1.68	0.76
9:I:34:TYR:CD2	9:I:35:VAL:N	2.54	0.76
1:A:489:LEU:HD12	1:A:490:HIS:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:GLY:O	2:B:468:GLU:CB	2.29	0.76
1:A:1132:LYS:HE2	13:S:253:LEU:HD21	1.68	0.76
13:S:235:ASP:CA	13:S:242:LYS:HG2	2.16	0.76
2:B:1084:GLN:HE21	2:B:1084:GLN:N	1.84	0.76
1:A:106:VAL:HG13	1:A:112:LYS:O	1.86	0.76
1:A:107:CYS:H	1:A:114:LEU:HD21	1.51	0.76
5:E:7:ARG:HG3	5:E:8:ASN:N	2.00	0.76
11:K:113:THR:O	11:K:114:LEU:HB2	1.84	0.76
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.84	0.76
1:A:567:LYS:HB3	8:H:96:VAL:N	2.01	0.75
2:B:745:PRO:O	2:B:748:ILE:HG12	1.86	0.75
1:A:225:ASN:HD22	1:A:228:PHE:N	1.80	0.75
2:B:98:THR:O	2:B:126:SER:HB2	1.86	0.75
1:A:820:GLY:O	1:A:822:GLU:N	2.20	0.75
2:B:918:ILE:HD12	2:B:935:ARG:CD	2.15	0.75
1:A:1027:ALA:HB3	1:A:1030:ARG:HB2	1.68	0.75
1:A:826:ASP:O	1:A:830:LYS:HB3	1.85	0.75
2:B:1224:PHE:HE2	5:E:171:LYS:HG3	1.52	0.75
8:H:59:ILE:HG22	8:H:60:ALA:N	2.01	0.75
1:A:95:PHE:CD1	1:A:234:MET:HG2	2.20	0.75
2:B:515:HIS:CD2	2:B:517:THR:H	2.02	0.75
1:A:754:SER:H	1:A:757:ASN:HD22	1.35	0.75
1:A:1204:ASP:HA	13:S:252:ASN:HB3	1.65	0.75
2:B:705:MET:HA	2:B:705:MET:CE	2.17	0.75
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.67	0.75
2:B:39:ARG:HH21	2:B:665:GLU:HG2	1.46	0.75
3:C:90:ASP:O	3:C:91:HIS:CD2	2.39	0.75
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.68	0.75
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.17	0.75
2:B:510:LYS:HG2	2:B:512:ARG:CG	2.17	0.75
1:A:95:PHE:O	1:A:99:ILE:HG13	1.87	0.75
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.67	0.75
10:J:7:CYS:SG	10:J:49:MET:HE3	2.26	0.75
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.87	0.75
2:B:899:ILE:HD11	2:B:911:ILE:HA	1.68	0.75
1:A:1079:MET:HE2	1:A:1101:LEU:HD23	1.67	0.74
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.51	0.74
4:D:145:MET:O	4:D:149:THR:HB	1.87	0.74
9:I:101:PHE:N	9:I:101:PHE:CD1	2.55	0.74
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.69	0.74
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.21	0.74
1:A:899:VAL:CB	1:A:929:LEU:HD11	2.16	0.74
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.35	0.74
1:A:1406:VAL:HG12	1:A:1410:PHE:CE1	2.21	0.74
1:A:1135:ARG:HH12	13:S:256:ALA:HB2	1.49	0.74
3:C:50:GLU:HG2	12:L:64:LEU:HD13	1.69	0.74
2:B:563:MET:HE1	2:B:580:VAL:HB	1.69	0.74
1:A:31:SER:HA	1:A:81:PHE:O	1.87	0.74
2:B:977:GLY:HA3	2:B:1099:VAL:HB	1.70	0.74
1:A:1172:LEU:HD22	13:S:204:SER:CA	2.16	0.74
1:A:853:ASP:OD1	1:A:855:THR:N	2.21	0.74
7:G:122:ASN:ND2	7:G:125:SER:HB3	2.02	0.74
2:B:508:LEU:CB	2:B:510:LYS:N	2.50	0.74
2:B:508:LEU:HB2	2:B:510:LYS:H	1.52	0.74
1:A:68:GLN:HE22	1:A:80:HIS:CD2	2.06	0.74
1:A:1239:ARG:HH22	1:A:1241:ARG:NH2	1.85	0.74
9:I:111:THR:HG22	9:I:112:SER:N	2.03	0.74
1:A:741:ASN:HD22	1:A:744:LYS:H	1.35	0.74
1:A:897:TYR:HD1	1:A:897:TYR:N	1.85	0.74
1:A:337:ARG:CZ	1:A:839:ARG:NH1	2.50	0.74
2:B:515:HIS:HD2	2:B:517:THR:H	1.35	0.74
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.52	0.74
4:D:170:THR:CG2	4:D:172:LEU:HG	2.16	0.74
2:B:769:TYR:CE2	2:B:987:LYS:NZ	2.55	0.74
1:A:1170:ILE:HG23	1:A:1174:PHE:CE1	2.22	0.74
2:B:1142:GLY:HA3	6:F:88:TYR:HE2	1.52	0.74
1:A:858:ASN:HD22	1:A:858:ASN:C	1.90	0.74
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.68	0.73
2:B:1180:PHE:HB3	2:B:1191:ILE:HD12	1.69	0.73
7:G:145:VAL:HG12	7:G:146:LYS:N	2.03	0.73
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.69	0.73
2:B:827:ILE:HD12	2:B:1086:PHE:HD2	1.53	0.73
3:C:104:PHE:HD2	3:C:105:GLY:N	1.86	0.73
1:A:364:VAL:HG12	1:A:458:HIS:HB3	1.71	0.73
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.53	0.73
7:G:91:VAL:HG23	7:G:141:SER:O	1.88	0.73
9:I:101:PHE:H	9:I:101:PHE:HD1	1.34	0.73
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.18	0.73
8:H:36:CYS:HA	8:H:126:GLU:O	1.88	0.73
1:A:256:GLN:HE21	2:B:918:ILE:HD11	1.54	0.73
1:A:71:GLN:C	1:A:73:GLY:H	1.91	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.22	0.73
1:A:903:ASN:HD22	1:A:904:THR:N	1.87	0.73
1:A:265:LYS:HE2	1:A:322:VAL:CG1	2.19	0.73
4:D:144:THR:O	4:D:148:LEU:HB2	1.89	0.73
3:C:6:PRO:HB3	3:C:25:VAL:HG12	1.69	0.73
1:A:901:LEU:HG	1:A:926:GLN:HE21	1.53	0.73
1:A:541:ILE:HD13	1:A:549:MET:HE1	1.69	0.73
2:B:1002:THR:CG2	2:B:1006:ILE:HD12	2.19	0.72
7:G:115:MET:HB2	7:G:116:PRO:HD2	1.70	0.72
1:A:1428:VAL:HG13	2:B:1151:LEU:HD21	1.71	0.72
1:A:1420:ASP:HB3	1:A:1422:ARG:HG3	1.71	0.72
1:A:1341:ILE:CG2	1:A:1342:GLU:H	2.03	0.72
2:B:801:LYS:O	10:J:52:THR:HG23	1.89	0.72
1:A:648:ASN:O	1:A:652:VAL:HG23	1.88	0.72
1:A:979:SER:OG	1:A:980:ASP:N	2.22	0.72
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	0.72
1:A:40:THR:HG21	1:A:259:GLU:OE2	1.89	0.72
2:B:873:THR:O	2:B:914:LYS:HA	1.88	0.72
7:G:80:LYS:HG2	7:G:80:LYS:O	1.87	0.72
9:I:59:VAL:O	9:I:60:GLN:HB2	1.88	0.72
1:A:288:ALA:HA	1:A:291:GLU:OE2	1.89	0.72
1:A:1057:VAL:HG12	1:A:1058:VAL:H	1.54	0.72
5:E:213:ILE:HG12	5:E:214:CYS:H	1.54	0.72
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.19	0.72
6:F:111:LEU:HD12	6:F:111:LEU:H	1.54	0.72
1:A:1402:PHE:CE1	1:A:1403:GLU:HG3	2.24	0.72
3:C:45:ALA:CA	3:C:72:LEU:HD12	2.16	0.72
1:A:310:GLY:O	1:A:312:PRO:HD2	1.89	0.72
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.70	0.72
1:A:1385:THR:O	1:A:1388:GLY:N	2.21	0.72
1:A:370:ILE:HG23	2:B:1105:ALA:HB2	1.72	0.72
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.52	0.72
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.71	0.72
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.25	0.72
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.25	0.72
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.25	0.72
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.72	0.72
2:B:953:LEU:O	2:B:953:LEU:HD23	1.89	0.72
1:A:1086:PHE:HE2	13:S:261:ILE:HD11	1.54	0.72
7:G:43:GLY:HA3	7:G:80:LYS:HB3	1.70	0.71
2:B:1031:LEU:HA	2:B:1055:ILE:HD13	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:44:VAL:HG12	8:H:44:VAL:O	1.89	0.71
2:B:114:PRO:HG2	2:B:115:GLN:H	1.54	0.71
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.30	0.71
6:F:86:THR:HG23	6:F:89:GLU:CD	2.10	0.71
1:A:215:SER:HB3	1:A:218:ASP:OD2	1.89	0.71
2:B:957:ASN:O	2:B:959:ASP:N	2.22	0.71
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.70	0.71
1:A:666:ILE:HD11	2:B:1067:ARG:O	1.90	0.71
9:I:71:SER:OG	9:I:83:ASN:HB2	1.90	0.71
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.70	0.71
3:C:32:SER:O	3:C:36:VAL:HG23	1.89	0.71
1:A:1325:THR:O	5:E:148:GLU:HB2	1.90	0.71
1:A:375:THR:OG1	1:A:433:GLU:HB3	1.91	0.71
2:B:123:THR:O	2:B:125:SER:N	2.22	0.71
1:A:1172:LEU:HD21	13:S:204:SER:CA	2.21	0.71
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.71	0.71
2:B:1166:CYS:O	2:B:1168:LEU:N	2.22	0.71
9:I:56:ALA:HB2	9:I:89:GLN:HG3	1.72	0.71
2:B:363:HIS:O	2:B:364:ILE:HB	1.91	0.71
4:D:54:GLU:O	4:D:58:VAL:HG23	1.89	0.71
1:A:13:THR:O	2:B:1218:THR:HG22	1.90	0.71
1:A:225:ASN:ND2	1:A:228:PHE:N	2.32	0.71
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.72	0.71
1:A:1436:ILE:HD13	2:B:1139:ILE:HG23	1.73	0.71
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.00	0.71
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.05	0.71
3:C:73:GLN:NE2	3:C:74:SER:H	1.89	0.71
1:A:59:GLY:HA2	1:A:67:CYS:SG	2.30	0.71
2:B:604:ARG:NH2	2:B:613:VAL:O	2.23	0.71
1:A:90:VAL:HG12	1:A:91:PHE:N	2.03	0.71
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.21	0.71
2:B:53:GLN:HG2	2:B:547:VAL:HG22	1.72	0.71
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.06	0.70
1:A:1334:ASP:C	1:A:1336:MET:H	1.94	0.70
2:B:261:ARG:O	2:B:267:ARG:HD3	1.90	0.70
2:B:563:MET:CE	2:B:580:VAL:HB	2.21	0.70
2:B:510:LYS:HB2	2:B:511:PRO:CD	2.21	0.70
1:A:315:LEU:HD23	1:A:321:PRO:HA	1.73	0.70
1:A:351:THR:HB	2:B:1103:ILE:HD12	1.72	0.70
1:A:384:ASN:OD1	1:A:388:LEU:HD12	1.92	0.70
1:A:1147:THR:HG22	1:A:1149:ALA:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TYR:CD1	1:A:897:TYR:N	2.56	0.70
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.07	0.70
1:A:95:PHE:HD1	1:A:234:MET:HG2	1.57	0.70
1:A:370:ILE:HG22	1:A:374:LEU:CD1	2.21	0.70
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.73	0.70
8:H:102:TYR:N	8:H:102:TYR:CD2	2.58	0.70
1:A:1435:PRO:O	1:A:1436:ILE:HG13	1.91	0.70
1:A:888:GLY:O	1:A:940:ARG:NH2	2.25	0.70
2:B:496:ARG:HH11	2:B:496:ARG:HB3	1.56	0.70
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.54	0.70
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.72	0.70
1:A:339:ASN:HB3	2:B:1117:GLN:NE2	2.05	0.70
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.26	0.70
1:A:414:ASP:OD1	1:A:416:ARG:HG3	1.91	0.70
2:B:794:ASN:C	2:B:795:ILE:HD12	2.11	0.70
2:B:857:ARG:HG2	2:B:858:SER:H	1.55	0.70
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.27	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.91	0.70
1:A:608:ILE:HG23	1:A:969:GLN:OE1	1.91	0.70
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.06	0.70
1:A:698:GLN:HA	9:I:97:MET:O	1.90	0.70
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.74	0.70
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.73	0.70
1:A:852:TYR:CD1	6:F:136:ARG:HB3	2.27	0.70
1:A:1280:GLU:O	1:A:1281:ARG:O	2.10	0.70
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.04	0.70
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.56	0.70
3:C:191:TYR:HD2	3:C:201:TRP:CD1	2.09	0.70
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.74	0.70
2:B:831:SER:OG	2:B:840:ILE:HD11	1.92	0.69
2:B:510:LYS:HB2	2:B:511:PRO:HD2	1.74	0.69
1:A:78:PRO:HA	2:B:1201:LYS:HZ2	1.57	0.69
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.73	0.69
2:B:637:LEU:O	2:B:690:VAL:HG13	1.90	0.69
3:C:105:GLY:HA3	3:C:149:LYS:O	1.92	0.69
13:S:291:GLU:N	13:S:292:PRO:CD	2.53	0.69
5:E:2:ASP:O	5:E:3:GLN:HG2	1.92	0.69
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.73	0.69
2:B:546:SER:OG	2:B:631:GLY:N	2.22	0.69
1:A:855:THR:CG2	1:A:857:ARG:HE	1.99	0.69
3:C:147:LEU:HD12	3:C:151:GLN:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.22	0.69
2:B:510:LYS:CD	2:B:510:LYS:C	2.61	0.69
1:A:347:PHE:H	2:B:1107:ALA:HA	1.57	0.69
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.73	0.69
1:A:289:ILE:C	1:A:291:GLU:H	1.95	0.69
2:B:1023:VAL:O	2:B:1027:ILE:HG13	1.93	0.69
1:A:1334:ASP:O	1:A:1336:MET:N	2.25	0.69
1:A:69:THR:O	1:A:71:GLN:N	2.25	0.69
2:B:862:GLN:HG2	2:B:963:PHE:CD1	2.28	0.69
1:A:265:LYS:HD2	1:A:265:LYS:N	2.06	0.69
1:A:367:PRO:HB3	1:A:465:TYR:O	1.91	0.69
1:A:1283:VAL:HG12	1:A:1284:MET:H	1.58	0.69
9:I:56:ALA:HB2	9:I:89:GLN:HG2	1.72	0.69
1:A:92:HIS:O	1:A:94:GLY:N	2.25	0.69
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.27	0.69
11:K:12:LEU:H	11:K:12:LEU:HD12	1.58	0.69
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.74	0.69
2:B:510:LYS:CB	2:B:511:PRO:HD2	2.21	0.69
2:B:606:LYS:HD2	2:B:608:ASP:OD2	1.92	0.69
2:B:294:ASP:OD2	2:B:294:ASP:N	2.24	0.69
1:A:606:LEU:HG	1:A:613:ILE:HD12	1.74	0.69
1:A:1443:VAL:O	1:A:1444:MET:HG3	1.91	0.69
6:F:111:LEU:C	6:F:113:GLY:H	1.96	0.69
1:A:889:SER:HB3	1:A:1297:GLU:HG2	1.75	0.69
1:A:1261:LYS:HA	1:A:1264:GLU:HB3	1.73	0.69
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.28	0.69
12:L:38:LEU:O	12:L:39:SER:HB3	1.91	0.69
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.08	0.69
2:B:871:THR:HG22	2:B:872:GLU:O	1.93	0.69
7:G:123:ALA:C	7:G:125:SER:H	1.96	0.69
1:A:367:PRO:HG2	1:A:370:ILE:HG13	1.74	0.69
1:A:84:ILE:HD11	1:A:270:LEU:HD13	1.74	0.69
1:A:1135:ARG:HH11	13:S:256:ALA:HB2	1.57	0.69
2:B:112:LEU:CD1	2:B:113:TYR:H	2.03	0.69
2:B:552:MET:HA	2:B:555:ILE:HB	1.75	0.69
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.74	0.69
3:C:242:GLN:HA	3:C:245:VAL:HG23	1.73	0.69
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.23	0.69
2:B:281:PRO:HG2	2:B:284:ILE:HG13	1.74	0.69
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.23	0.69
1:A:535:THR:HG21	1:A:616:VAL:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.26	0.69
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.23	0.68
2:B:948:ILE:HG22	2:B:949:VAL:O	1.93	0.68
7:G:96:GLN:HA	7:G:121:PHE:CE2	2.28	0.68
1:A:1079:MET:CE	1:A:1101:LEU:HD23	2.23	0.68
7:G:106:MET:HG3	7:G:157:ILE:O	1.93	0.68
8:H:81:PRO:HB2	8:H:82:PRO:HD2	1.74	0.68
2:B:1165:ILE:HG22	2:B:1166:CYS:H	1.59	0.68
3:C:6:PRO:HB3	3:C:25:VAL:CG1	2.24	0.68
1:A:390:GLN:HE21	1:A:394:ASN:ND2	1.91	0.68
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.57	0.68
1:A:858:ASN:ND2	1:A:860:LEU:H	1.92	0.68
2:B:986:GLN:OE1	2:B:986:GLN:HA	1.92	0.68
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.27	0.68
2:B:821:GLN:HE22	2:B:851:PHE:H	1.42	0.68
1:A:1237:ILE:HG22	1:A:1238:ILE:H	1.55	0.68
1:A:332:LYS:HG3	1:A:333:GLU:HG2	1.75	0.68
1:A:337:ARG:NH2	1:A:839:ARG:HH12	1.90	0.68
2:B:1146:PHE:CD1	2:B:1146:PHE:O	2.47	0.68
1:A:134:ARG:HG2	1:A:134:ARG:O	1.94	0.68
2:B:773:MET:C	2:B:775:LYS:H	1.95	0.68
4:D:130:LEU:C	4:D:132:GLN:H	1.97	0.68
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.58	0.68
1:A:709:THR:HG22	1:A:712:GLU:H	1.59	0.68
6:F:97:ARG:NH2	6:F:108:PHE:HE1	1.92	0.68
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.74	0.68
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.24	0.68
1:A:901:LEU:N	1:A:926:GLN:NE2	2.36	0.68
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.56	0.68
10:J:7:CYS:SG	10:J:46:CYS:HA	2.34	0.68
1:A:1081:LEU:HD21	1:A:1098:VAL:HG21	1.74	0.68
1:A:837:ILE:HA	1:A:840:ARG:HD3	1.76	0.68
1:A:1089:VAL:O	1:A:1089:VAL:HG12	1.95	0.67
1:A:1364:ASN:OD1	1:A:1366:ARG:HD2	1.94	0.67
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.92	0.67
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.23	0.67
5:E:143:ASN:HD22	5:E:146:HIS:CE1	2.12	0.67
7:G:127:PRO:HG2	7:G:138:THR:HG21	1.74	0.67
2:B:378:LEU:HD12	2:B:378:LEU:O	1.94	0.67
2:B:1169:MET:HE1	2:B:1201:LYS:CA	2.24	0.67
1:A:1410:PHE:HA	2:B:1212:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:PRO:HG2	1:A:624:SER:O	1.94	0.67
1:A:1192:LEU:HG	1:A:1193:LEU:N	2.09	0.67
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.09	0.67
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.24	0.67
1:A:1376:THR:OG1	1:A:1377:THR:N	2.23	0.67
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.09	0.67
2:B:205:ILE:N	2:B:205:ILE:HD12	2.10	0.67
1:A:49:LYS:NZ	1:A:60:SER:HA	2.09	0.67
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.29	0.67
1:A:115:LEU:HB2	1:A:122:MET:HE1	1.75	0.67
2:B:880:THR:O	2:B:881:ASN:HB2	1.94	0.67
2:B:1010:LEU:HD12	2:B:1011:ILE:H	1.60	0.67
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.21	0.67
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.07	0.67
1:A:135:PHE:C	1:A:137:ALA:H	1.97	0.67
5:E:210:SER:C	5:E:211:TYR:CD1	2.68	0.67
3:C:73:GLN:HB3	3:C:131:HIS:H	1.60	0.67
1:A:53:LEU:HD23	1:A:54:ASN:H	1.54	0.67
1:A:55:ASP:CG	1:A:55:ASP:O	2.31	0.67
2:B:854:LEU:HB3	2:B:856:PHE:HE1	1.60	0.67
7:G:13:LEU:HD23	7:G:14:HIS:N	2.10	0.67
1:A:567:LYS:HD3	8:H:95:TYR:CG	2.30	0.67
1:A:709:THR:HB	1:A:712:GLU:HB2	1.76	0.67
7:G:91:VAL:HB	7:G:139:ILE:O	1.95	0.67
1:A:1447:GLU:OE2	7:G:23:LYS:HB2	1.94	0.67
1:A:1083:THR:HG21	1:A:1085:HIS:CE1	2.30	0.67
1:A:1118:VAL:HG12	1:A:1327:ILE:HG13	1.77	0.67
1:A:41:MET:O	1:A:50:ILE:HG13	1.94	0.67
1:A:337:ARG:HD3	2:B:1132:GLU:OE1	1.95	0.67
3:C:86:CYS:O	3:C:88:CYS:N	2.27	0.67
12:L:58:LYS:O	12:L:59:ALA:O	2.13	0.67
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.76	0.67
2:B:1159:ARG:HB3	2:B:1159:ARG:NH1	2.09	0.67
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.22	0.67
2:B:1198:TYR:CE1	2:B:1201:LYS:HD2	2.30	0.67
9:I:34:TYR:HE2	9:I:36:GLU:HB3	1.60	0.67
2:B:97:VAL:HG12	2:B:178:ASN:ND2	2.09	0.67
1:A:982:THR:O	1:A:985:ASP:HB2	1.94	0.67
1:A:829:VAL:HG13	2:B:507:LYS:HG2	1.76	0.67
2:B:654:ARG:H	2:B:657:HIS:HD2	1.41	0.67
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1104:ILE:O	1:A:1107:VAL:N	2.23	0.66
1:A:1161:THR:OG1	1:A:1170:ILE:HD11	1.95	0.66
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.76	0.66
13:S:265:VAL:HG11	13:S:278:LYS:HA	1.76	0.66
2:B:622:LYS:HE3	9:I:59:VAL:HG22	1.76	0.66
13:S:302:CYS:SG	13:S:304:ASN:ND2	2.68	0.66
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.77	0.66
7:G:73:LYS:HE2	7:G:74:TYR:O	1.95	0.66
1:A:75:ASN:O	1:A:76:GLU:HB3	1.95	0.66
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.75	0.66
1:A:1329:THR:H	1:A:1335:ILE:CD1	1.95	0.66
1:A:265:LYS:HD2	1:A:265:LYS:H	1.60	0.66
2:B:898:LEU:HB2	12:L:58:LYS:NZ	2.10	0.66
2:B:172:ILE:HD13	2:B:178:ASN:HB2	1.76	0.66
2:B:546:SER:OG	2:B:630:ALA:HA	1.95	0.66
1:A:1331:SER:OG	1:A:1333:ILE:HG22	1.94	0.66
1:A:254:GLU:HB2	2:B:935:ARG:HH22	1.60	0.66
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.10	0.66
1:A:997:LEU:HD13	1:A:1018:PHE:HE2	1.60	0.66
2:B:900:ALA:O	2:B:903:VAL:HG23	1.95	0.66
1:A:90:VAL:HG13	1:A:297:GLN:OE1	1.96	0.66
3:C:43:THR:HG22	3:C:44:LEU:N	2.10	0.66
1:A:825:ILE:C	1:A:827:THR:H	1.96	0.66
2:B:1065:GLN:HB2	3:C:201:TRP:CZ3	2.31	0.66
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.25	0.66
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.77	0.66
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.11	0.66
1:A:1283:VAL:O	1:A:1306:LEU:HA	1.96	0.66
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.25	0.66
2:B:1065:GLN:HB3	2:B:1069:PHE:O	1.95	0.66
2:B:1102:LYS:O	2:B:1103:ILE:C	2.34	0.66
9:I:58:VAL:HG13	9:I:62:ILE:CG1	2.25	0.66
2:B:705:MET:H	2:B:710:LEU:CD1	2.09	0.66
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.11	0.66
13:S:218:ILE:CA	13:S:219:ALA:CA	2.73	0.66
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.25	0.66
2:B:991:GLY:O	2:B:992:ILE:HB	1.94	0.66
1:A:63:ARG:HG2	1:A:74:MET:SD	2.36	0.66
1:A:1437:GLY:HA3	6:F:88:TYR:CD2	2.30	0.66
2:B:910:VAL:HG12	2:B:911:ILE:N	2.11	0.66
12:L:28:LYS:HB2	12:L:39:SER:HB2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:HG2	2:B:983:ARG:O	1.96	0.66
3:C:263:THR:C	3:C:265:MET:H	1.99	0.66
1:A:903:ASN:HD22	1:A:903:ASN:C	1.99	0.66
2:B:705:MET:H	2:B:710:LEU:HD12	1.61	0.66
13:S:235:ASP:CA	13:S:242:LYS:HE3	2.26	0.66
2:B:882:THR:CG2	2:B:884:ARG:HB2	2.25	0.66
2:B:589:VAL:CG1	2:B:590:HIS:H	2.06	0.66
2:B:1159:ARG:NE	2:B:1193:GLN:HE21	1.94	0.66
1:A:567:LYS:HB2	1:A:568:PRO:CD	2.25	0.66
8:H:41:ASP:O	8:H:42:ILE:HG13	1.96	0.66
2:B:616:ILE:HD12	2:B:616:ILE:N	2.11	0.66
2:B:899:ILE:CG2	2:B:903:VAL:HG21	2.25	0.66
5:E:182:ASP:O	5:E:185:ALA:N	2.28	0.66
1:A:275:SER:O	1:A:279:LEU:HG	1.96	0.66
1:A:34:LYS:HB2	1:A:36:ARG:HH21	1.60	0.66
1:A:886:ILE:HG22	1:A:887:GLY:N	2.11	0.65
1:A:264:PHE:O	1:A:267:ALA:HB3	1.96	0.65
5:E:157:SER:OG	5:E:160:GLU:HG3	1.95	0.65
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.61	0.65
1:A:591:PHE:HA	1:A:595:THR:HG21	1.77	0.65
2:B:579:ARG:HD2	2:B:586:TRP:CZ2	2.30	0.65
2:B:65:GLU:HG3	2:B:66:ASP:N	2.07	0.65
11:K:67:PHE:C	11:K:68:PHE:HD2	1.98	0.65
3:C:63:ILE:CA	3:C:66:ARG:HG3	2.26	0.65
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.26	0.65
2:B:322:PHE:HZ	9:I:30:ARG:HB3	1.61	0.65
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.79	0.65
3:C:241:ASP:O	3:C:245:VAL:HG23	1.96	0.65
2:B:23:ALA:HB1	2:B:24:PRO:CD	2.23	0.65
1:A:1291:VAL:HG13	1:A:1292:PRO:CD	2.25	0.65
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.78	0.65
5:E:78:LEU:HD23	5:E:79:TRP:N	2.11	0.65
2:B:411:PRO:O	2:B:414:ALA:HB3	1.95	0.65
4:D:137:ASN:HD22	4:D:137:ASN:C	2.00	0.65
3:C:174:ALA:O	3:C:175:ALA:HB2	1.95	0.65
1:A:107:CYS:N	1:A:114:LEU:HD21	2.11	0.65
3:C:50:GLU:HG2	12:L:64:LEU:CD1	2.25	0.65
2:B:856:PHE:N	2:B:856:PHE:CD1	2.64	0.65
2:B:294:ASP:O	2:B:296:GLU:N	2.30	0.65
2:B:687:GLU:O	2:B:689:LEU:HG	1.96	0.65
2:B:773:MET:C	2:B:775:LYS:N	2.48	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:N	1:A:56:PRO:HD3	2.11	0.65
1:A:1080:THR:HG21	13:S:284:LEU:HD13	1.77	0.65
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.29	0.65
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.36	0.65
2:B:594:ALA:HA	2:B:617:ARG:HH12	1.60	0.65
4:D:211:LEU:HD23	4:D:214:LEU:HD12	1.79	0.65
2:B:794:ASN:O	2:B:795:ILE:HD12	1.96	0.65
3:C:5:GLY:O	3:C:7:GLN:HG3	1.96	0.65
2:B:365:THR:HG23	2:B:367:LEU:H	1.61	0.65
1:A:538:ASP:OD2	8:H:22:LYS:HB2	1.96	0.65
12:L:60:ARG:HG2	12:L:61:THR:H	1.60	0.65
2:B:322:PHE:CZ	9:I:30:ARG:HB3	2.32	0.65
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.32	0.65
7:G:14:HIS:HD2	7:G:16:SER:CB	2.03	0.65
9:I:101:PHE:N	9:I:101:PHE:HD1	1.91	0.65
1:A:550:LEU:HD22	1:A:556:TRP:CE2	2.31	0.65
2:B:820:GLY:N	2:B:1091:TYR:OH	2.29	0.65
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.77	0.65
1:A:593:GLU:O	1:A:595:THR:N	2.30	0.64
1:A:47:ARG:NH2	1:A:255:SER:H	1.95	0.64
2:B:825:VAL:HG22	2:B:1010:LEU:HB3	1.79	0.64
2:B:1223:ASP:O	2:B:1224:PHE:HB2	1.96	0.64
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.10	0.64
2:B:54:PHE:CE2	2:B:59:LEU:HD13	2.32	0.64
7:G:143:ILE:HG22	7:G:144:ARG:N	2.11	0.64
1:A:855:THR:HG23	1:A:857:ARG:HG3	1.78	0.64
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.78	0.64
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.32	0.64
1:A:243:PRO:O	1:A:246:VAL:HG23	1.98	0.64
2:B:1184:GLY:C	2:B:1186:ASP:H	1.96	0.64
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.88	0.64
2:B:39:ARG:HH21	2:B:665:GLU:CG	2.10	0.64
2:B:835:GLN:HA	2:B:1013:ASN:ND2	2.10	0.64
2:B:37:PHE:HD2	2:B:542:MET:SD	2.21	0.64
4:D:47:LEU:HD13	4:D:48:ILE:H	1.63	0.64
13:S:269:PHE:HE2	13:S:297:CYS:SG	2.14	0.64
7:G:138:THR:CG2	7:G:139:ILE:H	1.95	0.64
2:B:827:ILE:HD12	2:B:1086:PHE:CD2	2.32	0.64
2:B:227:LYS:HB2	2:B:395:GLN:OE1	1.97	0.64
2:B:975:GLN:NE2	2:B:1100:ASP:OD2	2.30	0.64
1:A:550:LEU:HD22	1:A:556:TRP:NE1	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:LEU:O	1:A:1412:ALA:HB3	1.98	0.64
1:A:370:ILE:HG22	1:A:374:LEU:HD11	1.80	0.64
2:B:952:VAL:HG12	2:B:953:LEU:N	2.11	0.64
1:A:1199:ARG:HH22	13:S:241:LEU:CD1	2.02	0.64
1:A:1029:ARG:HH11	1:A:1029:ARG:CG	2.09	0.64
1:A:1423:GLY:O	1:A:1426:GLU:N	2.31	0.64
1:A:535:THR:HG21	1:A:617:VAL:H	1.63	0.64
2:B:54:PHE:HE1	2:B:414:ALA:HA	1.62	0.64
2:B:1060:ARG:HH11	2:B:1060:ARG:HG2	1.61	0.64
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.80	0.64
1:A:67:CYS:O	1:A:70:CYS:HB3	1.96	0.64
2:B:955:THR:HG22	2:B:956:THR:N	2.12	0.64
1:A:1148:ILE:O	1:A:1148:ILE:HG22	1.98	0.64
8:H:102:TYR:N	8:H:102:TYR:HD2	1.96	0.64
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.33	0.64
7:G:111:THR:CG2	7:G:113:HIS:H	2.04	0.64
1:A:567:LYS:HG3	1:A:568:PRO:HD2	1.80	0.64
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.97	0.64
2:B:315:LYS:N	2:B:316:PRO:HD2	2.11	0.64
1:A:1035:TYR:O	1:A:1037:LEU:N	2.25	0.64
3:C:179:GLU:HG2	3:C:180:TYR:N	2.12	0.64
1:A:1072:ILE:O	1:A:1075:PRO:HG2	1.98	0.64
2:B:1156:ASP:O	2:B:1157:ALA:O	2.15	0.64
2:B:1224:PHE:CE2	5:E:171:LYS:HG3	2.32	0.64
13:S:279:VAL:HG13	13:S:298:THR:O	1.98	0.64
4:D:35:LEU:N	4:D:35:LEU:HD12	2.12	0.64
2:B:261:ARG:HB3	2:B:261:ARG:NH1	2.11	0.64
13:S:282:TYR:CE2	13:S:296:PHE:HB2	2.33	0.64
1:A:768:GLN:CG	1:A:816:HIS:HA	2.22	0.64
1:A:1428:VAL:HG13	2:B:1151:LEU:CD2	2.28	0.64
3:C:235:VAL:HG13	10:J:13:VAL:HG23	1.79	0.64
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.13	0.64
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.79	0.64
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.33	0.64
1:A:1120:LEU:O	1:A:1323:ASP:HB2	1.98	0.64
1:A:853:ASP:OD1	1:A:855:THR:CB	2.40	0.64
2:B:508:LEU:HB2	2:B:510:LYS:N	2.10	0.64
5:E:177:ARG:C	5:E:212:ARG:HD3	2.18	0.64
1:A:642:CYS:O	1:A:645:LEU:N	2.27	0.64
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.78	0.64
1:A:996:ASN:C	1:A:998:LEU:HD12	2.18	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.64
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.31	0.64
2:B:859:TYR:HD1	2:B:859:TYR:H	1.44	0.64
1:A:1283:VAL:CG1	13:S:256:ALA:C	2.62	0.63
1:A:845:LEU:HD12	1:A:1069:ALA:HB2	1.80	0.63
3:C:143:LEU:HD12	3:C:145:CYS:H	1.64	0.63
1:A:17:VAL:HG23	1:A:1421:CYS:SG	2.38	0.63
9:I:113:ASP:O	9:I:114:GLN:HG3	1.98	0.63
11:K:12:LEU:HD21	11:K:18:LYS:HG2	1.80	0.63
2:B:737:THR:HG21	9:I:66:PRO:HA	1.79	0.63
2:B:390:LEU:O	2:B:392:ARG:HG3	1.97	0.63
1:A:845:LEU:HB3	1:A:848:ILE:HD12	1.80	0.63
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.28	0.63
12:L:28:LYS:HB2	12:L:39:SER:CB	2.28	0.63
2:B:117:ALA:HA	2:B:122:LEU:HD12	1.78	0.63
7:G:14:HIS:ND1	7:G:15:PRO:HD2	2.12	0.63
1:A:1080:THR:O	1:A:1081:LEU:HD22	1.97	0.63
2:B:294:ASP:C	2:B:296:GLU:H	2.01	0.63
5:E:197:LYS:HG2	5:E:197:LYS:O	1.97	0.63
2:B:37:PHE:CE2	2:B:542:MET:HA	2.27	0.63
8:H:81:PRO:CB	8:H:82:PRO:CD	2.77	0.63
3:C:35:ARG:NH1	11:K:41:THR:N	2.47	0.63
1:A:706:HIS:CE1	13:S:257:GLN:OE1	2.51	0.63
2:B:204:ILE:C	2:B:205:ILE:HD12	2.19	0.63
8:H:93:TYR:HB3	8:H:144:ILE:O	1.98	0.63
3:C:35:ARG:NH1	11:K:41:THR:H	1.96	0.63
2:B:1051:THR:HB	2:B:1054:GLY:H	1.64	0.63
1:A:637:LYS:HB3	1:A:641:VAL:HG21	1.81	0.63
7:G:6:ASP:O	7:G:7:LEU:HD23	1.98	0.63
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.34	0.63
1:A:704:ALA:O	1:A:705:LYS:HB2	1.97	0.63
2:B:508:LEU:HB2	2:B:510:LYS:CA	2.28	0.63
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.34	0.63
1:A:922:ASP:OD1	1:A:924:LYS:N	2.32	0.63
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.14	0.63
2:B:604:ARG:NH2	2:B:614:SER:HA	2.14	0.63
1:A:367:PRO:HA	1:A:463:ILE:O	1.99	0.63
13:S:279:VAL:HG13	13:S:298:THR:C	2.19	0.63
1:A:534:LEU:O	1:A:574:GLY:HA3	1.98	0.63
2:B:1149:GLU:O	2:B:1151:LEU:N	2.32	0.63
2:B:604:ARG:HH22	2:B:614:SER:HA	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1230:GLU:O	1:A:1232:ASN:N	2.32	0.62
1:A:61:ILE:O	1:A:63:ARG:N	2.32	0.62
2:B:292:ILE:HD11	2:B:327:ARG:H	1.64	0.62
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.81	0.62
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.98	0.62
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.80	0.62
2:B:254:LEU:HD23	2:B:381:MET:HE1	1.81	0.62
7:G:126:ASN:HD22	7:G:127:PRO:HA	1.63	0.62
2:B:1020:ARG:CG	2:B:1020:ARG:HH11	2.09	0.62
2:B:1099:VAL:HG22	2:B:1103:ILE:HD13	1.80	0.62
2:B:284:ILE:HD13	2:B:333:PHE:HD2	1.64	0.62
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.29	0.62
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.80	0.62
1:A:283:GLY:O	1:A:285:PRO:HD3	1.99	0.62
3:C:147:LEU:HB2	3:C:151:GLN:CB	2.29	0.62
7:G:49:LEU:HD21	7:G:77:VAL:HG23	1.80	0.62
5:E:192:ARG:HG3	5:E:192:ARG:HH11	1.64	0.62
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.12	0.62
2:B:526:GLU:OE2	2:B:752:ALA:HB2	1.98	0.62
7:G:34:VAL:HG12	7:G:45:ILE:HG21	1.80	0.62
5:E:86:PRO:O	5:E:114:ASN:HB2	1.99	0.62
9:I:87:GLN:O	9:I:89:GLN:OE1	2.18	0.62
8:H:40:LEU:CD1	8:H:123:MET:HB2	2.27	0.62
1:A:265:LYS:HE2	1:A:322:VAL:HG13	1.81	0.62
13:S:274:CYS:O	13:S:276:GLU:N	2.32	0.62
1:A:1402:PHE:O	1:A:1404:GLU:N	2.32	0.62
2:B:129:PHE:HA	2:B:165:VAL:O	1.99	0.62
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.80	0.62
1:A:1172:LEU:CG	13:S:204:SER:CA	2.77	0.62
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.68	0.62
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.80	0.62
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.33	0.62
1:A:1342:GLU:CD	5:E:198:ILE:HG21	2.18	0.62
2:B:952:VAL:HG12	2:B:953:LEU:H	1.64	0.62
1:A:1279:ILE:HD11	1:A:1316:VAL:CG2	2.29	0.62
1:A:708:MET:O	1:A:709:THR:O	2.17	0.62
2:B:780:VAL:HG12	2:B:782:LEU:O	1.99	0.62
6:F:103:MET:HE2	7:G:65:ASP:HB2	1.81	0.62
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.30	0.62
2:B:705:MET:HA	2:B:705:MET:HE2	1.81	0.62
1:A:590:ARG:HG3	1:A:590:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:MET:SD	1:A:621:THR:HG21	2.40	0.62
1:A:44:THR:O	1:A:45:GLN:HB2	1.99	0.62
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.81	0.62
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.35	0.62
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.34	0.62
1:A:998:LEU:HD12	1:A:998:LEU:H	1.65	0.62
2:B:859:TYR:CD1	2:B:859:TYR:N	2.67	0.62
1:A:21:LEU:HG	1:A:1413:GLY:O	2.00	0.62
1:A:1213:GLY:HA2	1:A:1216:ILE:HD12	1.81	0.62
1:A:1017:LEU:CB	5:E:205:SER:HA	2.29	0.62
1:A:818:MET:HG2	2:B:514:LEU:HG	1.81	0.62
2:B:763:GLN:NE2	13:S:293:LEU:HG	2.15	0.62
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.34	0.62
1:A:515:GLN:OE1	1:A:1071:SER:HA	1.99	0.62
2:B:762:ASN:HD21	2:B:1024:ALA:HB3	1.64	0.62
11:K:91:CYS:O	11:K:94:ILE:HB	1.99	0.62
6:F:97:ARG:HH22	6:F:108:PHE:HE1	1.45	0.62
1:A:886:ILE:HG13	1:A:943:LEU:CD1	2.30	0.62
2:B:1033:LYS:HD2	2:B:1087:PHE:O	2.00	0.62
2:B:37:PHE:CD1	2:B:41:LYS:HG3	2.35	0.62
1:A:90:VAL:CG1	1:A:91:PHE:N	2.63	0.62
7:G:114:LEU:HD23	7:G:161:GLY:O	2.00	0.62
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.35	0.62
1:A:897:TYR:HD2	1:A:936:LEU:HD13	1.65	0.62
7:G:80:LYS:HE2	7:G:82:PHE:CZ	2.34	0.62
1:A:289:ILE:O	1:A:291:GLU:N	2.33	0.62
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.35	0.62
2:B:601:ARG:O	2:B:605:ARG:HG3	2.00	0.62
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.35	0.62
1:A:590:ARG:HH21	1:A:620:LYS:CB	2.08	0.61
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	2.00	0.61
1:A:1019:CYS:O	1:A:1022:LEU:HB3	1.99	0.61
2:B:750:GLY:O	2:B:751:VAL:C	2.39	0.61
12:L:31:CYS:HB3	12:L:34:CYS:C	2.21	0.61
1:A:858:ASN:C	1:A:858:ASN:ND2	2.53	0.61
1:A:455:MET:HE3	2:B:1134:GLU:HG3	1.82	0.61
1:A:1001:ARG:O	1:A:1002:GLY:O	2.18	0.61
1:A:705:LYS:HA	13:S:254:TYR:OH	2.00	0.61
1:A:256:GLN:NE2	2:B:918:ILE:HD11	2.14	0.61
7:G:80:LYS:HE2	7:G:82:PHE:HZ	1.64	0.61
1:A:756:ILE:HG21	13:S:283:GLN:NE2	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.41	0.61
2:B:510:LYS:CG	2:B:512:ARG:H	2.11	0.61
1:A:866:PHE:C	1:A:867:ILE:HD12	2.21	0.61
2:B:1106:ARG:HG3	2:B:1107:ALA:H	1.65	0.61
1:A:691:LEU:O	1:A:694:THR:HB	1.99	0.61
2:B:773:MET:O	2:B:776:GLN:N	2.28	0.61
6:F:79:ARG:HG3	6:F:144:GLU:OE1	2.00	0.61
2:B:292:ILE:CD1	2:B:326:ASP:HA	2.30	0.61
2:B:541:LEU:HD12	2:B:747:MET:HE1	1.83	0.61
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.63	0.61
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.35	0.61
5:E:157:SER:C	5:E:159:ASP:H	2.04	0.61
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.81	0.61
1:A:1206:ASP:O	1:A:1207:LEU:HG	2.00	0.61
1:A:442:VAL:O	1:A:457:ALA:HA	2.00	0.61
3:C:58:LEU:CD2	3:C:58:LEU:H	2.14	0.61
4:D:40:HIS:CE1	4:D:41:GLN:HG3	2.35	0.61
3:C:248:ILE:HD13	11:K:101:LEU:HD22	1.82	0.61
1:A:50:ILE:C	1:A:52:GLY:H	2.03	0.61
1:A:489:LEU:HD12	1:A:489:LEU:C	2.21	0.61
1:A:412:ARG:NH2	2:B:1108:ARG:NH1	2.48	0.61
1:A:244:PRO:HG2	1:A:245:PRO:HD3	1.81	0.61
1:A:1081:LEU:HD11	1:A:1098:VAL:HB	1.81	0.61
1:A:91:PHE:HD2	1:A:96:ILE:HG12	1.66	0.61
1:A:852:TYR:CE2	1:A:1060:PRO:HB2	2.36	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.64	0.61
9:I:8:ARG:O	9:I:10:CYS:N	2.33	0.61
10:J:57:ILE:HG23	10:J:58:GLU:N	2.16	0.61
1:A:857:ARG:HD3	1:A:861:GLY:O	2.00	0.61
2:B:562:GLY:HA3	2:B:590:HIS:HE1	1.65	0.61
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.66	0.61
1:A:335:ARG:HE	1:A:339:ASN:HD22	1.45	0.61
2:B:899:ILE:CD1	2:B:911:ILE:HA	2.30	0.61
1:A:133:LYS:C	1:A:135:PHE:H	2.02	0.61
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.31	0.61
1:A:629:LEU:O	1:A:633:VAL:HG23	2.01	0.61
7:G:108:VAL:HG22	7:G:159:ALA:HB3	1.81	0.61
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.36	0.61
2:B:508:LEU:HB2	2:B:510:LYS:HB3	1.83	0.61
1:A:1081:LEU:CD1	1:A:1098:VAL:HB	2.30	0.61
2:B:35:SER:HA	2:B:811:TYR:CE2	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:O	1:A:531:ILE:HG22	2.01	0.61
1:A:804:TYR:OH	2:B:763:GLN:HA	2.01	0.61
8:H:23:VAL:HG13	8:H:42:ILE:O	2.00	0.61
3:C:212:PRO:CB	3:C:213:PRO:HD2	2.31	0.61
1:A:694:THR:O	1:A:698:GLN:HG3	1.99	0.61
9:I:106:CYS:O	9:I:107:SER:HB2	1.99	0.61
1:A:869:GLY:O	5:E:204:THR:HG21	2.01	0.61
2:B:496:ARG:NH1	2:B:539:LEU:HB2	2.16	0.61
4:D:134:THR:HG22	4:D:135:GLY:N	2.16	0.61
1:A:902:LEU:O	1:A:903:ASN:HB2	2.01	0.60
5:E:198:ILE:CD1	5:E:212:ARG:HH11	2.14	0.60
2:B:533:CYS:O	2:B:535:LEU:N	2.34	0.60
1:A:446:ARG:CD	1:A:480:ALA:HB2	2.31	0.60
9:I:55:THR:HG23	9:I:100:PHE:CD2	2.33	0.60
4:D:51:ASN:O	4:D:54:GLU:HB3	2.01	0.60
2:B:487:THR:HG22	2:B:488:TYR:N	2.15	0.60
10:J:57:ILE:HG23	10:J:58:GLU:H	1.66	0.60
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.83	0.60
1:A:1161:THR:C	1:A:1163:ILE:H	2.04	0.60
8:H:56:THR:O	8:H:144:ILE:HA	2.01	0.60
7:G:146:LYS:HB2	7:G:168:LEU:HD11	1.82	0.60
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.31	0.60
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.83	0.60
13:S:291:GLU:H	13:S:292:PRO:CD	2.14	0.60
2:B:510:LYS:HG2	2:B:512:ARG:CB	2.30	0.60
3:C:142:VAL:H	10:J:16:ASP:HB3	1.66	0.60
1:A:606:LEU:HB2	1:A:614:PHE:CE2	2.37	0.60
1:A:563:PRO:HG3	1:A:572:TRP:CE2	2.37	0.60
2:B:545:ILE:HG22	2:B:546:SER:O	2.01	0.60
5:E:60:PHE:CE2	5:E:80:VAL:HB	2.36	0.60
5:E:55:ARG:C	5:E:57:MET:H	2.03	0.60
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.00	0.60
1:A:786:HIS:CD2	1:A:786:HIS:N	2.69	0.60
1:A:254:GLU:CB	2:B:935:ARG:HH22	2.14	0.60
1:A:49:LYS:HE2	1:A:61:ILE:CD1	2.29	0.60
1:A:1164:PRO:HG2	1:A:1165:GLU:H	1.66	0.60
13:S:298:THR:HG23	13:S:305:ARG:HG2	1.82	0.60
8:H:113:ALA:HB2	8:H:126:GLU:HG3	1.84	0.60
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.31	0.60
1:A:225:ASN:ND2	1:A:227:VAL:H	1.98	0.60
7:G:23:LYS:HG3	7:G:56:ILE:CD1	2.28	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:LEU:HA	2:B:192:LEU:HD12	1.82	0.60
1:A:47:ARG:HH22	1:A:254:GLU:HA	1.65	0.60
1:A:761:MET:HA	1:A:804:TYR:HB2	1.83	0.60
2:B:830:TYR:HE2	2:B:1000:PRO:HD3	1.66	0.60
4:D:35:LEU:H	4:D:35:LEU:CD1	2.14	0.60
2:B:705:MET:N	2:B:710:LEU:HD12	2.16	0.60
1:A:134:ARG:O	1:A:138:ILE:HG13	2.01	0.60
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.84	0.60
6:F:72:LYS:O	6:F:73:ALA:HB3	2.02	0.60
1:A:1116:LEU:HB3	1:A:1311:VAL:HG22	1.83	0.60
13:S:287:ARG:HD3	13:S:291:GLU:OE1	2.01	0.60
2:B:1159:ARG:HE	2:B:1193:GLN:HE21	1.50	0.60
4:D:33:PHE:CE2	7:G:80:LYS:NZ	2.70	0.60
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.30	0.60
3:C:107:SER:C	3:C:109:SER:H	2.04	0.60
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.31	0.60
2:B:880:THR:HG21	2:B:934:LYS:HE3	1.82	0.60
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.30	0.60
12:L:31:CYS:HB3	12:L:35:SER:HA	1.84	0.60
1:A:820:GLY:C	1:A:822:GLU:H	2.05	0.60
1:A:144:THR:O	1:A:146:MET:HG3	2.01	0.60
1:A:1134:ILE:O	1:A:1138:ILE:HG13	2.02	0.60
1:A:863:VAL:HG12	1:A:864:ILE:N	2.17	0.60
1:A:1164:PRO:HG2	1:A:1165:GLU:HG3	1.82	0.60
1:A:332:LYS:H	1:A:337:ARG:HB3	1.67	0.60
2:B:578:THR:HG23	2:B:622:LYS:HA	1.84	0.60
4:D:210:ILE:O	4:D:214:LEU:HG	2.01	0.60
1:A:852:TYR:CE1	6:F:136:ARG:HG2	2.36	0.60
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.84	0.60
2:B:216:GLU:HA	2:B:406:LEU:HD23	1.84	0.60
1:A:863:VAL:O	1:A:864:ILE:HG12	2.02	0.60
3:C:169:LYS:NZ	12:L:69:ALA:HB3	2.16	0.60
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.37	0.60
1:A:567:LYS:HD3	8:H:95:TYR:CD2	2.37	0.60
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.31	0.60
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.37	0.60
1:A:1261:LYS:O	1:A:1264:GLU:HB3	2.01	0.60
4:D:19:GLU:O	4:D:21:GLU:N	2.35	0.60
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.00	0.59
2:B:797:TYR:C	2:B:798:TYR:HD2	2.04	0.59
1:A:1423:GLY:O	1:A:1424:VAL:C	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:VAL:CG1	1:A:1373:ASP:N	2.65	0.59
8:H:91:ASP:C	8:H:93:TYR:H	2.04	0.59
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.83	0.59
1:A:1334:ASP:C	1:A:1336:MET:N	2.55	0.59
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.84	0.59
2:B:429:PHE:HA	2:B:432:MET:HE2	1.84	0.59
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.33	0.59
1:A:1104:ILE:O	1:A:1106:ASN:N	2.35	0.59
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.26	0.59
2:B:898:LEU:HB2	12:L:58:LYS:HZ3	1.67	0.59
2:B:129:PHE:HE2	2:B:166:PHE:HD1	1.49	0.59
1:A:821:ARG:O	1:A:825:ILE:HG13	2.01	0.59
2:B:510:LYS:CB	2:B:511:PRO:CD	2.79	0.59
1:A:469:ARG:HG2	1:A:469:ARG:HH11	1.67	0.59
2:B:1183:LYS:CE	2:B:1183:LYS:N	2.62	0.59
8:H:56:THR:HB	8:H:145:ARG:HG2	1.84	0.59
8:H:59:ILE:HG22	8:H:60:ALA:H	1.64	0.59
1:A:1237:ILE:CG2	1:A:1238:ILE:H	2.15	0.59
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.31	0.59
5:E:46:TYR:CE2	5:E:58:MET:HA	2.37	0.59
4:D:176:GLU:OE2	4:D:198:LEU:HD23	2.02	0.59
1:A:40:THR:HG23	1:A:54:ASN:HD21	1.67	0.59
1:A:343:LYS:HE2	2:B:1156:ASP:OD2	2.02	0.59
10:J:41:LEU:CD1	10:J:50:ILE:HG13	2.32	0.59
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.32	0.59
9:I:111:THR:CG2	9:I:112:SER:H	2.13	0.59
2:B:807:ARG:HH11	2:B:807:ARG:HB3	1.66	0.59
1:A:475:THR:HG23	1:A:476:SER:N	2.17	0.59
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.30	0.59
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.83	0.59
2:B:310:MET:O	2:B:313:MET:HB2	2.02	0.59
7:G:6:ASP:HB3	7:G:73:LYS:HZ1	1.66	0.59
1:A:855:THR:CG2	1:A:857:ARG:HG3	2.32	0.59
2:B:1166:CYS:HB2	2:B:1168:LEU:HD12	1.84	0.59
2:B:973:ILE:HG23	2:B:974:PRO:HD2	1.84	0.59
1:A:556:TRP:C	1:A:558:GLY:H	2.05	0.59
9:I:58:VAL:HA	9:I:62:ILE:CD1	2.32	0.59
7:G:145:VAL:CG1	7:G:146:LYS:N	2.64	0.59
3:C:104:PHE:CD2	3:C:105:GLY:N	2.70	0.59
7:G:1:MET:SD	7:G:1:MET:O	2.61	0.59
2:B:46:GLN:HG3	2:B:47:GLN:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:58:LEU:N	3:C:58:LEU:CD2	2.65	0.59
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.84	0.59
1:A:834:THR:HG23	1:A:1077:THR:HA	1.85	0.59
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.84	0.59
2:B:899:ILE:HG22	2:B:900:ALA:N	2.17	0.59
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.85	0.59
1:A:391:LEU:O	1:A:394:ASN:N	2.35	0.59
1:A:868:TYR:CE1	1:A:1064:VAL:CG1	2.77	0.59
2:B:1095:LEU:CD1	2:B:1095:LEU:H	1.87	0.59
1:A:72:GLU:O	1:A:73:GLY:O	2.20	0.59
3:C:174:ALA:O	3:C:175:ALA:CB	2.51	0.59
4:D:170:THR:HG22	4:D:172:LEU:HG	1.82	0.59
2:B:546:SER:HG	2:B:630:ALA:HA	1.68	0.59
2:B:854:LEU:HB3	2:B:856:PHE:CE1	2.37	0.59
2:B:240:ILE:O	2:B:240:ILE:HG23	2.02	0.59
1:A:808:LEU:HD21	1:A:816:HIS:HD2	1.68	0.59
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.83	0.59
2:B:1160:VAL:CG1	2:B:1161:HIS:N	2.66	0.59
2:B:954:VAL:O	12:L:55:ILE:O	2.20	0.59
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.37	0.59
3:C:35:ARG:HH11	11:K:41:THR:N	2.01	0.59
1:A:1397:LEU:HA	1:A:1400:CYS:CB	2.32	0.59
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.02	0.59
2:B:113:TYR:HB3	2:B:114:PRO:CD	2.29	0.59
2:B:798:TYR:CE1	10:J:4:PRO:HB3	2.38	0.59
2:B:841:MET:O	2:B:993:THR:HG22	2.02	0.59
9:I:101:PHE:O	9:I:102:VAL:HG23	2.03	0.59
8:H:40:LEU:HD12	8:H:122:LEU:O	2.03	0.59
1:A:782:ARG:NH2	2:B:699:GLU:O	2.34	0.59
1:A:1151:GLU:HB3	1:A:1153:TYR:HE1	1.68	0.59
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.37	0.59
1:A:25:GLU:CD	1:A:25:GLU:H	2.06	0.59
1:A:1116:LEU:HB3	1:A:1311:VAL:CG2	2.33	0.58
2:B:879:ARG:O	2:B:880:THR:HB	2.03	0.58
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.26	0.58
13:S:295:THR:O	13:S:295:THR:HG22	2.02	0.58
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.03	0.58
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.85	0.58
1:A:687:LYS:O	1:A:690:VAL:HB	2.03	0.58
2:B:549:THR:HG22	2:B:550:ASP:N	2.12	0.58
1:A:667:GLY:HA3	3:C:192:TRP:CH2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:ARG:HG3	1:A:1034:GLU:OE2	2.03	0.58
1:A:528:LEU:HD23	1:A:751:SER:HA	1.85	0.58
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.43	0.58
5:E:114:ASN:O	5:E:115:ASN:HB3	2.03	0.58
1:A:1095:THR:OG1	1:A:1112:LYS:HB2	2.03	0.58
2:B:189:LEU:O	2:B:192:LEU:N	2.31	0.58
2:B:511:PRO:C	2:B:513:GLN:N	2.51	0.58
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.17	0.58
2:B:1065:GLN:HG3	2:B:1068:GLY:H	1.69	0.58
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.18	0.58
1:A:1422:ARG:HH22	2:B:1224:PHE:C	2.06	0.58
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.33	0.58
1:A:265:LYS:O	1:A:266:LEU:C	2.41	0.58
1:A:361:LEU:HG	1:A:507:VAL:HG11	1.85	0.58
6:F:111:LEU:N	6:F:111:LEU:HD12	2.18	0.58
11:K:31:VAL:HG12	11:K:32:VAL:N	2.18	0.58
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.03	0.58
1:A:360:GLU:HB2	1:A:363:GLN:HG3	1.84	0.58
10:J:19:GLU:O	10:J:23:ASN:HB2	2.03	0.58
2:B:763:GLN:HE22	13:S:293:LEU:HG	1.67	0.58
3:C:59:ALA:O	3:C:62:PHE:HB3	2.03	0.58
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.58
2:B:807:ARG:NH1	2:B:807:ARG:HB3	2.19	0.58
8:H:42:ILE:HG23	8:H:95:TYR:HE1	1.67	0.58
1:A:321:PRO:O	1:A:322:VAL:HG23	2.03	0.58
4:D:48:ILE:HG21	7:G:4:ILE:HB	1.85	0.58
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.34	0.58
1:A:535:THR:CG2	1:A:616:VAL:HA	2.33	0.58
1:A:847:ASP:HB2	1:A:859:SER:H	1.68	0.58
1:A:1127:ASP:O	1:A:1130:GLN:HB3	2.03	0.58
1:A:848:ILE:HB	1:A:1065:GLY:HA3	1.85	0.58
2:B:918:ILE:CD1	2:B:935:ARG:HD2	2.27	0.58
2:B:570:VAL:HG23	2:B:573:GLN:HB3	1.85	0.58
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	2.03	0.58
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.04	0.58
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.19	0.58
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.68	0.58
2:B:235:SER:HB3	2:B:258:LEU:HG	1.86	0.58
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.03	0.58
5:E:144:ILE:O	5:E:146:HIS:N	2.37	0.58
3:C:17:ASN:OD1	3:C:233:GLU:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:LYS:HE2	2:B:404:LYS:HA	1.85	0.58
2:B:782:LEU:HD12	2:B:788:ARG:HH11	1.67	0.58
2:B:785:TYR:HE2	10:J:60:PHE:CE1	2.22	0.58
2:B:519:TRP:C	2:B:519:TRP:CD1	2.77	0.58
1:A:666:ILE:CD1	1:A:667:GLY:N	2.66	0.58
2:B:380:TYR:OH	2:B:623:GLU:OE2	2.21	0.58
2:B:824:ILE:CG1	10:J:48:ARG:HH12	2.11	0.58
4:D:33:PHE:CE1	7:G:80:LYS:HE3	2.39	0.58
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.24	0.58
7:G:9:LEU:HD12	7:G:10:ASN:N	2.16	0.58
2:B:483:LEU:HD12	2:B:484:ASN:H	1.67	0.58
13:S:300:GLU:HG3	13:S:300:GLU:O	2.04	0.58
7:G:119:LEU:HD13	7:G:132:SER:HB2	1.86	0.58
9:I:2:THR:O	9:I:3:THR:C	2.41	0.58
1:A:827:THR:O	1:A:831:THR:HB	2.04	0.58
1:A:69:THR:C	1:A:71:GLN:N	2.57	0.58
1:A:567:LYS:CB	1:A:568:PRO:CD	2.81	0.58
5:E:13:TRP:O	5:E:16:PHE:HB3	2.03	0.58
7:G:117:GLN:O	7:G:119:LEU:N	2.37	0.58
3:C:124:LEU:O	3:C:127:ARG:HG2	2.04	0.58
1:A:1446:ASP:HB3	1:A:1449:SER:OG	2.04	0.58
1:A:446:ARG:HB2	1:A:487:MET:SD	2.43	0.58
1:A:903:ASN:ND2	1:A:905:ASP:H	2.02	0.58
1:A:55:ASP:C	1:A:57:ARG:N	2.46	0.58
2:B:1186:ASP:OD1	2:B:1186:ASP:O	2.22	0.58
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.86	0.58
1:A:744:LYS:HE2	1:A:748:MET:HE2	1.86	0.58
9:I:58:VAL:HG13	9:I:62:ILE:HG13	1.84	0.58
2:B:762:ASN:HD21	2:B:1024:ALA:CB	2.17	0.58
2:B:855:PHE:CD1	2:B:855:PHE:C	2.75	0.58
2:B:1147:LEU:HD23	2:B:1147:LEU:C	2.24	0.58
2:B:461:LEU:HD12	2:B:461:LEU:H	1.68	0.58
1:A:1316:VAL:O	1:A:1322:ILE:HD13	2.04	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.34	0.58
10:J:8:PHE:HD1	10:J:49:MET:HE1	1.69	0.58
2:B:1132:GLU:O	2:B:1135:ARG:HB3	2.04	0.58
2:B:325:GLN:HG2	9:I:31:THR:CG2	2.34	0.58
1:A:598:LEU:HD22	8:H:25:ARG:NH1	2.18	0.58
6:F:85:MET:HE1	6:F:148:VAL:HG12	1.85	0.58
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.39	0.58
2:B:708:GLU:O	2:B:710:LEU:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:162:ARG:HG2	5:E:162:ARG:HH11	1.68	0.58
3:C:82:TYR:CE1	3:C:161:LYS:HD3	2.39	0.57
2:B:992:ILE:HD13	2:B:994:TYR:CE1	2.38	0.57
2:B:603:LEU:HB3	2:B:609:ILE:HD11	1.84	0.57
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.86	0.57
8:H:84:ALA:C	8:H:86:ASP:H	2.06	0.57
2:B:903:VAL:HG12	2:B:904:ARG:N	2.17	0.57
1:A:115:LEU:HD12	1:A:142:CYS:SG	2.44	0.57
5:E:157:SER:O	5:E:159:ASP:N	2.37	0.57
2:B:57:TYR:CD1	2:B:57:TYR:N	2.72	0.57
7:G:117:GLN:C	7:G:119:LEU:H	2.07	0.57
9:I:88:SER:C	9:I:90:GLN:H	2.07	0.57
1:A:672:ASP:HB2	1:A:736:ASN:OD1	2.04	0.57
2:B:394:ASP:OD1	9:I:91:ARG:HB3	2.05	0.57
1:A:895:LYS:HG2	1:A:895:LYS:O	2.03	0.57
10:J:1:MET:H2	10:J:56:LEU:N	2.00	0.57
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.86	0.57
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.14	0.57
1:A:1421:CYS:HA	1:A:1426:GLU:HB3	1.87	0.57
9:I:59:VAL:HG12	9:I:59:VAL:O	2.04	0.57
2:B:773:MET:O	2:B:775:LYS:N	2.37	0.57
1:A:168:GLY:O	1:A:169:ASN:C	2.43	0.57
13:S:236:LEU:CA	13:S:242:LYS:HE3	2.34	0.57
1:A:818:MET:HA	2:B:514:LEU:HB3	1.87	0.57
3:C:167:HIS:CE1	12:L:70:ARG:HA	2.39	0.57
1:A:808:LEU:N	1:A:808:LEU:HD12	2.20	0.57
10:J:14:VAL:HG13	10:J:50:ILE:HD11	1.85	0.57
1:A:443:LEU:HG	2:B:1146:PHE:CE2	2.28	0.57
1:A:963:ILE:CD1	1:A:1049:ILE:HG13	2.30	0.57
8:H:100:THR:HG22	8:H:101:ALA:N	2.19	0.57
1:A:642:CYS:O	1:A:645:LEU:HB3	2.04	0.57
11:K:47:ARG:HD3	11:K:59:ALA:O	2.04	0.57
3:C:69:LEU:H	3:C:69:LEU:HD12	1.69	0.57
1:A:42:ASP:C	1:A:44:THR:H	2.07	0.57
1:A:57:ARG:O	1:A:58:LEU:O	2.21	0.57
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.05	0.57
2:B:1145:SER:C	2:B:1147:LEU:N	2.55	0.57
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.77	0.57
2:B:192:LEU:O	2:B:193:LYS:HB2	2.04	0.57
1:A:1164:PRO:O	1:A:1166:ASP:N	2.36	0.57
5:E:153:HIS:O	5:E:154:ILE:CG1	2.49	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:80:LYS:CE	7:G:82:PHE:HZ	2.17	0.57
2:B:640:VAL:O	2:B:641:GLU:C	2.41	0.57
1:A:90:VAL:HG13	1:A:297:GLN:CD	2.25	0.57
1:A:984:LYS:O	1:A:988:LEU:HB2	2.03	0.57
3:C:114:TYR:HB3	3:C:140:ASN:O	2.04	0.57
2:B:694:ASP:O	2:B:698:GLU:HB2	2.05	0.57
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.52	0.57
5:E:204:THR:CG2	5:E:205:SER:N	2.67	0.57
10:J:8:PHE:CD1	10:J:49:MET:SD	2.98	0.57
6:F:77:ASP:C	6:F:79:ARG:H	2.08	0.57
2:B:860:MET:HB2	2:B:965:LYS:HG2	1.87	0.57
3:C:196:ASP:OD1	3:C:198:ALA:HB3	2.05	0.57
7:G:109:PHE:CD1	7:G:110:VAL:N	2.71	0.57
1:A:469:ARG:NH2	2:B:991:GLY:O	2.37	0.57
2:B:296:GLU:O	2:B:299:GLU:HB2	2.04	0.57
1:A:1362:TYR:HD1	1:A:1363:VAL:N	1.85	0.57
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.87	0.57
1:A:1063:MET:CG	1:A:1436:ILE:HG23	2.35	0.57
1:A:560:ILE:HD12	8:H:79:TRP:O	2.05	0.57
9:I:6:PHE:HA	9:I:14:LEU:HG	1.85	0.57
9:I:58:VAL:HA	9:I:62:ILE:HD11	1.87	0.57
1:A:92:HIS:O	1:A:95:PHE:N	2.37	0.57
5:E:84:ASP:O	5:E:86:PRO:HD3	2.05	0.57
1:A:1359:ASP:HB3	13:S:307:LYS:HE2	1.87	0.57
2:B:557:PHE:C	2:B:557:PHE:CD2	2.77	0.57
1:A:403:LYS:O	1:A:404:TYR:CG	2.58	0.57
1:A:1335:ILE:O	1:A:1335:ILE:HG22	2.05	0.57
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.85	0.57
2:B:1085:ILE:HG22	2:B:1086:PHE:N	2.19	0.57
2:B:620:ARG:NH2	9:I:89:GLN:NE2	2.52	0.57
2:B:217:ARG:HE	2:B:405:ARG:CB	2.15	0.57
8:H:83:GLN:C	8:H:85:GLY:H	2.08	0.57
2:B:522:VAL:HG12	2:B:523:CYS:N	2.19	0.57
2:B:558:LEU:O	2:B:560:GLU:N	2.37	0.57
1:A:491:VAL:HG12	1:A:492:PRO:O	2.04	0.57
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.05	0.57
1:A:798:GLY:HA2	1:A:815:PHE:CD1	2.39	0.57
2:B:1156:ASP:HB3	2:B:1198:TYR:H	1.70	0.57
6:F:75:PRO:O	6:F:77:ASP:O	2.23	0.57
2:B:325:GLN:HG2	9:I:31:THR:HG23	1.86	0.57
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ILE:C	1:A:291:GLU:N	2.58	0.57
1:A:492:PRO:O	1:A:493:GLN:NE2	2.38	0.57
1:A:730:GLY:C	1:A:732:LEU:H	2.09	0.57
3:C:181:ASP:OD1	3:C:186:LEU:HD13	2.05	0.57
12:L:43:THR:O	12:L:43:THR:HG22	2.04	0.57
1:A:1090:ALA:CA	1:A:1093:LYS:HE3	2.34	0.56
4:D:40:HIS:CB	7:G:73:LYS:NZ	2.58	0.56
1:A:18:GLN:HG3	1:A:228:PHE:CE1	2.40	0.56
1:A:666:ILE:H	2:B:1026:LEU:HD22	1.70	0.56
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.32	0.56
1:A:1080:THR:HG22	1:A:1081:LEU:N	2.20	0.56
3:C:89:GLU:O	3:C:90:ASP:HB3	2.05	0.56
1:A:495:GLU:O	1:A:498:ARG:HG3	2.04	0.56
1:A:1203:ASN:O	1:A:1204:ASP:C	2.44	0.56
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.86	0.56
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.40	0.56
2:B:1172:ILE:O	2:B:1172:ILE:HG22	2.05	0.56
3:C:82:TYR:O	3:C:84:ARG:N	2.38	0.56
3:C:167:HIS:HD2	3:C:169:LYS:N	1.97	0.56
2:B:603:LEU:HB3	2:B:609:ILE:CD1	2.35	0.56
7:G:1:MET:CE	7:G:80:LYS:H	2.18	0.56
1:A:730:GLY:O	1:A:732:LEU:N	2.38	0.56
1:A:899:VAL:CG2	1:A:908:LEU:HD21	2.35	0.56
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.41	0.56
1:A:775:ILE:HG13	1:A:798:GLY:HA3	1.86	0.56
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.05	0.56
11:K:65:HIS:CD2	11:K:67:PHE:N	2.60	0.56
1:A:1081:LEU:HD21	1:A:1098:VAL:CG2	2.35	0.56
1:A:1051:ALA:O	1:A:1053:PHE:N	2.39	0.56
1:A:306:ASN:ND2	1:A:322:VAL:HB	2.21	0.56
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.88	0.56
12:L:62:LYS:H	12:L:62:LYS:HD2	1.70	0.56
4:D:51:ASN:ND2	4:D:54:GLU:OE2	2.38	0.56
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.86	0.56
1:A:34:LYS:CB	1:A:36:ARG:HH21	2.18	0.56
1:A:996:ASN:O	1:A:998:LEU:HD12	2.04	0.56
2:B:278:GLN:HG2	2:B:279:ASP:H	1.68	0.56
1:A:685:GLU:HG3	1:A:686:ALA:N	2.20	0.56
5:E:35:VAL:C	5:E:37:LEU:H	2.08	0.56
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.19	0.56
3:C:143:LEU:C	3:C:143:LEU:HD12	2.25	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:111:THR:HG22	9:I:113:ASP:N	2.19	0.56
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.35	0.56
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.86	0.56
2:B:247:GLY:H	2:B:418:LYS:HZ3	1.54	0.56
2:B:528:PRO:HG2	2:B:533:CYS:HA	1.88	0.56
1:A:1453:TYR:CZ	6:F:129:LYS:HA	2.40	0.56
1:A:532:ARG:HH22	1:A:745:GLN:HG2	1.69	0.56
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.34	0.56
1:A:130:ASP:O	1:A:132:LYS:N	2.39	0.56
2:B:784:ASN:O	2:B:788:ARG:HG3	2.06	0.56
10:J:57:ILE:O	10:J:60:PHE:N	2.39	0.56
2:B:766:ARG:NH2	2:B:1020:ARG:CG	2.67	0.56
2:B:511:PRO:C	2:B:513:GLN:H	2.08	0.56
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.36	0.56
1:A:1438:THR:HB	2:B:1144:ALA:CB	2.36	0.56
2:B:286:PHE:HE2	2:B:375:ALA:HB1	1.70	0.56
13:S:241:LEU:O	13:S:242:LYS:C	2.43	0.56
1:A:928:LEU:O	1:A:930:ASP:N	2.39	0.56
10:J:13:VAL:HG12	10:J:14:VAL:N	2.21	0.56
2:B:1135:ARG:O	2:B:1139:ILE:HG13	2.06	0.56
5:E:178:ILE:HG22	5:E:213:ILE:O	2.06	0.56
2:B:47:GLN:O	2:B:173:MET:HE1	2.06	0.56
2:B:857:ARG:HH21	2:B:942:ARG:NH1	2.04	0.56
5:E:19:VAL:O	5:E:23:VAL:HG23	2.06	0.56
9:I:64:SER:O	9:I:66:PRO:HD3	2.05	0.56
3:C:123:ASN:ND2	3:C:125:MET:SD	2.79	0.56
2:B:1177:HIS:C	2:B:1179:GLN:H	2.08	0.56
3:C:18:VAL:HG12	3:C:20:PHE:HD2	1.70	0.56
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.86	0.56
3:C:163:ILE:O	3:C:166:GLU:N	2.36	0.56
2:B:1020:ARG:CG	2:B:1020:ARG:NH1	2.68	0.56
1:A:98:LYS:O	1:A:102:VAL:HG23	2.05	0.56
2:B:642:ASP:O	2:B:644:GLU:N	2.30	0.56
5:E:56:LYS:HE3	5:E:84:ASP:HB2	1.87	0.56
1:A:547:LEU:HD22	11:K:58:PHE:CD1	2.40	0.56
2:B:498:THR:O	2:B:536:VAL:HG13	2.05	0.56
1:A:4:GLN:O	1:A:5:GLN:HB2	2.05	0.56
1:A:663:SER:OG	2:B:1085:ILE:HG23	2.06	0.56
2:B:377:PHE:O	2:B:380:TYR:N	2.39	0.56
1:A:936:LEU:N	1:A:936:LEU:HD23	2.21	0.56
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLN:O	1:A:73:GLY:N	2.39	0.56
7:G:1:MET:O	7:G:1:MET:HE1	2.05	0.56
2:B:37:PHE:CD2	2:B:542:MET:SD	2.99	0.56
1:A:339:ASN:CB	2:B:1117:GLN:HE22	2.19	0.56
1:A:874:ASP:CA	1:A:1058:VAL:HG23	2.36	0.56
2:B:254:LEU:HD23	2:B:381:MET:CE	2.36	0.56
9:I:90:GLN:NE2	9:I:92:ARG:HD2	2.21	0.56
1:A:1140:HIS:HB2	1:A:1276:VAL:O	2.06	0.56
3:C:82:TYR:CD1	3:C:161:LYS:HD3	2.41	0.56
3:C:242:GLN:O	3:C:246:ARG:N	2.37	0.56
2:B:766:ARG:HH21	2:B:1020:ARG:HG2	1.71	0.56
2:B:798:TYR:HE1	10:J:4:PRO:HB3	1.71	0.56
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.20	0.56
2:B:327:ARG:O	2:B:331:LEU:HD13	2.06	0.56
5:E:176:PRO:O	5:E:212:ARG:HA	2.06	0.56
1:A:567:LYS:CB	8:H:95:TYR:HA	2.36	0.56
2:B:521:LEU:HB3	2:B:633:VAL:CG1	2.36	0.56
1:A:986:ILE:HD11	1:A:1032:LEU:HD11	1.87	0.56
1:A:42:ASP:HB3	1:A:45:GLN:H	1.70	0.56
1:A:72:GLU:HB3	1:A:76:GLU:HG3	1.88	0.56
1:A:78:PRO:HB3	2:B:1201:LYS:HE3	1.88	0.56
1:A:503:GLN:C	1:A:504:LEU:HD12	2.25	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:CG1	2.32	0.56
1:A:306:ASN:HB2	1:A:324:SER:HB3	1.87	0.56
2:B:744:HIS:CG	2:B:745:PRO:HD2	2.41	0.56
7:G:114:LEU:HG	7:G:162:SER:CB	2.36	0.56
11:K:21:ILE:HG23	11:K:31:VAL:HG11	1.88	0.56
2:B:945:GLU:O	2:B:946:ASN:HB3	2.06	0.56
1:A:1044:TRP:O	1:A:1047:SER:N	2.38	0.56
1:A:861:GLY:HA3	5:E:174:GLN:NE2	2.21	0.55
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.41	0.55
2:B:1065:GLN:HG2	2:B:1069:PHE:HB2	1.88	0.55
11:K:67:PHE:C	11:K:68:PHE:CD2	2.78	0.55
2:B:635:ARG:NH2	2:B:742:GLU:OE2	2.29	0.55
12:L:30:ILE:O	12:L:56:LEU:HA	2.06	0.55
2:B:60:GLN:O	2:B:63:ILE:HG22	2.06	0.55
1:A:1127:ASP:HB3	1:A:1130:GLN:HB2	1.89	0.55
3:C:133:ILE:CD1	3:C:237:SER:CA	2.82	0.55
7:G:1:MET:CE	7:G:1:MET:O	2.54	0.55
11:K:58:PHE:HE2	11:K:74:ARG:HE	1.53	0.55
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:CG	1:A:855:THR:HB	2.25	0.55
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.42	0.55
1:A:808:LEU:CD1	1:A:808:LEU:H	2.19	0.55
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.41	0.55
8:H:5:LEU:HB2	8:H:60:ALA:H	1.71	0.55
2:B:582:VAL:HA	2:B:626:ILE:O	2.06	0.55
3:C:31:ASN:O	3:C:32:SER:C	2.45	0.55
1:A:414:ASP:OD1	1:A:416:ARG:CG	2.54	0.55
1:A:679:ILE:O	1:A:683:ILE:HG13	2.06	0.55
9:I:105:SER:O	9:I:106:CYS:HB3	2.06	0.55
2:B:847:ASP:C	2:B:849:GLY:H	2.09	0.55
1:A:708:MET:HE2	1:A:1089:VAL:CG1	2.33	0.55
2:B:118:ARG:HH11	2:B:204:ILE:HD11	1.72	0.55
1:A:823:GLY:C	1:A:825:ILE:H	2.08	0.55
1:A:71:GLN:C	1:A:73:GLY:N	2.60	0.55
1:A:1373:ASP:O	1:A:1376:THR:HG23	2.06	0.55
1:A:1341:ILE:HD12	1:A:1379:GLY:O	2.05	0.55
1:A:265:LYS:HE2	1:A:322:VAL:HG11	1.89	0.55
12:L:30:ILE:HG22	12:L:31:CYS:N	2.20	0.55
2:B:1189:ILE:HG22	2:B:1190:ASP:N	2.22	0.55
12:L:49:LYS:O	12:L:50:ASP:HB2	2.05	0.55
4:D:27:LEU:HD11	4:D:197:SER:HB2	1.89	0.55
5:E:47:CYS:HA	5:E:52:ARG:O	2.06	0.55
1:A:590:ARG:HG3	1:A:590:ARG:HH11	1.72	0.55
2:B:242:SER:OG	2:B:252:SER:O	2.23	0.55
1:A:1420:ASP:O	1:A:1421:CYS:HB2	2.07	0.55
2:B:635:ARG:HB2	2:B:636:PRO:CD	2.36	0.55
2:B:502:ILE:CG2	2:B:502:ILE:O	2.52	0.55
2:B:54:PHE:HA	2:B:58:THR:HB	1.88	0.55
1:A:1265:ASN:C	1:A:1267:MET:N	2.60	0.55
1:A:1313:LEU:O	1:A:1315:GLU:N	2.39	0.55
1:A:18:GLN:HG3	1:A:228:PHE:HE1	1.72	0.55
6:F:100:GLN:O	6:F:103:MET:HB2	2.07	0.55
6:F:84:TYR:N	6:F:84:TYR:CD1	2.73	0.55
1:A:896:ARG:O	1:A:1029:ARG:HB3	2.07	0.55
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.70	0.55
1:A:78:PRO:O	1:A:79:GLY:O	2.25	0.55
3:C:90:ASP:O	3:C:91:HIS:CG	2.60	0.55
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.89	0.55
5:E:211:TYR:CD1	5:E:211:TYR:N	2.74	0.55
3:C:9:LYS:O	3:C:10:ILE:C	2.44	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:13:LEU:HD23	7:G:14:HIS:H	1.70	0.55
3:C:46:ILE:HG13	3:C:72:LEU:HD11	1.88	0.55
3:C:166:GLU:O	3:C:167:HIS:HB2	2.07	0.55
3:C:70:ILE:HD13	3:C:144:ILE:HD11	1.88	0.55
1:A:997:LEU:HD13	1:A:1018:PHE:CE2	2.42	0.55
1:A:965:GLN:O	1:A:968:GLN:HB2	2.06	0.55
3:C:90:ASP:O	3:C:90:ASP:CG	2.43	0.55
1:A:668:ASP:CB	1:A:743:VAL:HG23	2.36	0.55
5:E:124:VAL:HG13	5:E:132:ILE:CD1	2.36	0.55
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.72	0.55
5:E:213:ILE:HG12	5:E:214:CYS:N	2.21	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.87	0.55
1:A:730:GLY:C	1:A:732:LEU:N	2.59	0.55
2:B:563:MET:HE2	2:B:587:HIS:C	2.28	0.55
2:B:378:LEU:O	2:B:382:ILE:HG13	2.07	0.55
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.89	0.55
2:B:873:THR:HG22	2:B:874:PHE:N	2.22	0.55
2:B:363:HIS:CD2	2:B:364:ILE:HG13	2.42	0.55
12:L:31:CYS:HB3	12:L:35:SER:N	2.21	0.55
1:A:390:GLN:HE21	1:A:394:ASN:HD21	1.53	0.55
3:C:58:LEU:HD23	3:C:58:LEU:H	1.71	0.55
9:I:84:VAL:O	9:I:84:VAL:HG22	2.07	0.55
1:A:848:ILE:HB	1:A:1065:GLY:CA	2.37	0.55
1:A:901:LEU:N	1:A:926:GLN:HE21	1.98	0.55
2:B:1020:ARG:NH1	2:B:1020:ARG:HG2	2.20	0.55
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.88	0.55
2:B:597:MET:SD	2:B:624:LEU:HD11	2.47	0.55
12:L:47:ARG:HH11	12:L:47:ARG:HG3	1.72	0.55
2:B:363:HIS:CD2	2:B:585:VAL:HG22	2.42	0.55
2:B:533:CYS:C	2:B:535:LEU:H	2.09	0.55
2:B:488:TYR:CE2	2:B:813:LYS:HB2	2.42	0.55
1:A:1265:ASN:C	1:A:1267:MET:H	2.09	0.55
9:I:25:LEU:HB3	9:I:38:ALA:HB2	1.89	0.55
8:H:7:ASP:O	8:H:8:ASP:HB2	2.06	0.55
2:B:781:PHE:O	2:B:782:LEU:CG	2.54	0.55
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.55	0.55
1:A:356:ASP:HB3	1:A:359:LEU:HG	1.88	0.55
2:B:800:GLN:CB	10:J:52:THR:HG21	2.33	0.55
2:B:805:THR:HA	2:B:809:MET:HE1	1.89	0.55
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.88	0.55
8:H:127:GLY:HA3	8:H:130:ARG:NH2	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1334:ASP:O	1:A:1337:GLU:N	2.40	0.55
1:A:715:GLU:O	1:A:717:ASN:N	2.39	0.55
2:B:25:ILE:HG23	2:B:29:ASP:HB3	1.89	0.55
2:B:265:SER:O	2:B:266:ALA:HB3	2.07	0.55
3:C:27:LEU:HD12	3:C:228:PHE:HE2	1.70	0.55
1:A:1017:LEU:HD23	5:E:204:THR:C	2.27	0.54
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.25	0.54
1:A:919:ILE:O	1:A:921:GLY:N	2.40	0.54
1:A:1102:LYS:HG2	1:A:1106:ASN:ND2	2.22	0.54
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.07	0.54
2:B:542:MET:HG2	2:B:747:MET:HB3	1.89	0.54
1:A:820:GLY:C	1:A:822:GLU:N	2.60	0.54
2:B:711:GLU:H	2:B:712:PRO:HD2	1.72	0.54
1:A:15:LYS:HG3	2:B:1218:THR:O	2.06	0.54
1:A:982:THR:HG22	1:A:984:LYS:H	1.73	0.54
13:S:243:GLN:O	13:S:247:GLU:HG3	2.07	0.54
1:A:1329:THR:HG22	1:A:1331:SER:N	2.15	0.54
2:B:382:ILE:O	2:B:385:LEU:HB3	2.08	0.54
3:C:67:LEU:HD23	3:C:70:ILE:HD11	1.89	0.54
5:E:124:VAL:CA	5:E:132:ILE:HD12	2.37	0.54
1:A:381:THR:HG23	1:A:382:PRO:CD	2.37	0.54
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.42	0.54
7:G:88:ASP:HA	7:G:144:ARG:HA	1.88	0.54
2:B:1017:ILE:HG22	2:B:1018:PRO:N	2.21	0.54
5:E:48:ASP:CG	5:E:49:SER:H	2.11	0.54
1:A:298:PHE:CZ	1:A:314:ALA:HB2	2.42	0.54
1:A:353:ILE:HG21	1:A:487:MET:CG	2.20	0.54
1:A:775:ILE:CG1	1:A:798:GLY:HA3	2.38	0.54
2:B:356:LEU:HA	2:B:360:PHE:HB2	1.90	0.54
1:A:49:LYS:HZ1	1:A:61:ILE:N	2.05	0.54
8:H:126:GLU:C	8:H:130:ARG:HH22	2.11	0.54
11:K:46:ILE:O	11:K:50:LEU:HB2	2.07	0.54
1:A:1397:LEU:O	1:A:1400:CYS:HB3	2.06	0.54
8:H:139:ASN:O	8:H:140:ALA:HB2	2.08	0.54
3:C:183:TRP:O	3:C:185:LYS:HG3	2.06	0.54
1:A:604:GLY:O	1:A:605:MET:HB2	2.07	0.54
1:A:855:THR:HG23	1:A:856:THR:N	2.23	0.54
7:G:18:PHE:HZ	7:G:68:ALA:HB2	1.71	0.54
3:C:250:THR:O	3:C:254:LYS:HG3	2.07	0.54
1:A:905:ASP:C	1:A:906:HIS:HD1	2.10	0.54
13:S:293:LEU:N	13:S:293:LEU:HD23	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:MET:O	1:A:42:ASP:C	2.45	0.54
2:B:1165:ILE:CG2	2:B:1166:CYS:N	2.70	0.54
3:C:143:LEU:HD12	3:C:145:CYS:N	2.22	0.54
1:A:1396:ALA:O	1:A:1398:MET:N	2.41	0.54
1:A:867:ILE:CG2	1:A:872:GLY:N	2.71	0.54
5:E:90:VAL:O	5:E:90:VAL:HG22	2.07	0.54
9:I:34:TYR:HD2	9:I:35:VAL:N	2.05	0.54
1:A:996:ASN:HA	1:A:998:LEU:CD1	2.38	0.54
1:A:597:LEU:HD12	1:A:597:LEU:N	2.21	0.54
1:A:470:LEU:CD2	1:A:487:MET:CE	2.86	0.54
1:A:1079:MET:HE2	1:A:1101:LEU:CD2	2.37	0.54
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.43	0.54
2:B:861:ASP:OD1	2:B:862:GLN:N	2.41	0.54
10:J:23:ASN:C	10:J:25:LEU:H	2.09	0.54
2:B:210:LYS:HA	2:B:481:GLN:O	2.07	0.54
5:E:39:LEU:O	5:E:42:PHE:HB3	2.08	0.54
2:B:1219:ASP:O	2:B:1219:ASP:OD1	2.25	0.54
1:A:1125:ALA:C	1:A:1127:ASP:H	2.10	0.54
1:A:1017:LEU:O	1:A:1017:LEU:HD12	2.07	0.54
3:C:39:ALA:CA	3:C:164:ALA:HB3	2.37	0.54
2:B:1099:VAL:O	2:B:1102:LYS:N	2.36	0.54
1:A:69:THR:C	1:A:71:GLN:H	2.10	0.54
3:C:174:ALA:HB2	3:C:235:VAL:HG22	1.90	0.54
2:B:865:LYS:NZ	2:B:869:SER:HA	2.23	0.54
1:A:877:HIS:CD2	1:A:1056:SER:HA	2.41	0.54
11:K:83:PRO:O	11:K:86:ALA:N	2.41	0.54
1:A:476:SER:OG	1:A:477:PRO:HD3	2.08	0.54
8:H:58:THR:HG22	8:H:59:ILE:H	1.73	0.54
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.89	0.54
7:G:81:PRO:HG3	7:G:106:MET:SD	2.47	0.54
2:B:1106:ARG:CG	2:B:1107:ALA:N	2.69	0.54
1:A:626:ASN:O	1:A:631:HIS:HB2	2.07	0.54
9:I:62:ILE:CG2	9:I:62:ILE:O	2.55	0.54
1:A:133:LYS:C	1:A:135:PHE:N	2.60	0.54
4:D:130:LEU:C	4:D:132:GLN:N	2.61	0.54
5:E:144:ILE:HG13	5:E:145:THR:H	1.72	0.54
5:E:60:PHE:HE2	5:E:80:VAL:HB	1.73	0.54
3:C:183:TRP:O	3:C:185:LYS:N	2.41	0.54
2:B:611:PRO:HB3	2:B:685:LEU:HD11	1.89	0.54
1:A:308:ILE:HG22	1:A:309:ALA:H	1.73	0.54
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:THR:O	1:A:705:LYS:HG2	2.07	0.54
3:C:44:LEU:HD23	3:C:72:LEU:HB2	1.90	0.54
6:F:84:TYR:HD1	6:F:84:TYR:N	2.06	0.54
2:B:1072:MET:HE2	2:B:1085:ILE:HB	1.89	0.54
1:A:886:ILE:HG13	1:A:943:LEU:HD12	1.90	0.54
1:A:68:GLN:C	1:A:70:CYS:H	2.09	0.54
8:H:95:TYR:HE2	8:H:97:MET:HG2	1.72	0.54
9:I:88:SER:O	9:I:90:GLN:N	2.41	0.54
8:H:14:GLU:HG2	8:H:15:VAL:N	2.22	0.54
1:A:1305:VAL:HG12	1:A:1306:LEU:N	2.23	0.54
1:A:1313:LEU:CD1	1:A:1327:ILE:HD13	2.38	0.54
2:B:555:ILE:HG22	2:B:556:THR:N	2.21	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.55	0.54
2:B:955:THR:CG2	2:B:956:THR:N	2.71	0.54
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.43	0.54
2:B:431:TYR:CE2	2:B:447:ALA:HB2	2.42	0.54
9:I:7:CYS:SG	9:I:8:ARG:O	2.66	0.54
2:B:498:THR:HB	2:B:537:LYS:O	2.08	0.54
4:D:213:GLU:O	4:D:217:LEU:HG	2.07	0.54
2:B:203:PHE:HB3	2:B:205:ILE:HD11	1.90	0.54
2:B:879:ARG:O	2:B:934:LYS:HD2	2.08	0.54
11:K:65:HIS:CD2	11:K:66:PRO:CD	2.90	0.54
2:B:1163:CYS:SG	2:B:1165:ILE:HB	2.48	0.54
2:B:1165:ILE:CG2	2:B:1185:CYS:HB3	2.38	0.54
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.54
8:H:130:ARG:HA	8:H:133:ASN:HB2	1.90	0.54
2:B:94:LYS:HG2	2:B:95:ILE:N	2.22	0.54
2:B:658:ILE:O	2:B:661:LEU:HB2	2.07	0.54
2:B:970:THR:HG22	2:B:971:THR:N	2.22	0.54
1:A:1116:LEU:CD2	1:A:1311:VAL:HG22	2.36	0.54
1:A:35:ILE:HA	1:A:52:GLY:O	2.07	0.54
2:B:1182:CYS:O	2:B:1182:CYS:SG	2.66	0.54
1:A:1376:THR:O	1:A:1377:THR:C	2.46	0.54
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.72	0.54
2:B:94:LYS:HG2	2:B:95:ILE:H	1.73	0.54
1:A:688:LYS:C	1:A:690:VAL:H	2.12	0.54
11:K:31:VAL:CG1	11:K:32:VAL:N	2.70	0.54
2:B:230:ALA:N	2:B:231:PRO:HD2	2.23	0.54
1:A:1123:GLY:O	1:A:1125:ALA:N	2.41	0.53
2:B:197:PHE:HZ	2:B:816:GLU:HG2	1.73	0.53
2:B:205:ILE:N	2:B:205:ILE:CD1	2.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1436:ILE:O	1:A:1437:GLY:C	2.46	0.53
9:I:55:THR:CG2	9:I:100:PHE:HD2	2.17	0.53
1:A:1441:PHE:HZ	6:F:89:GLU:HA	1.67	0.53
11:K:47:ARG:HH11	11:K:48:ALA:N	2.06	0.53
2:B:487:THR:HG22	2:B:488:TYR:H	1.73	0.53
11:K:58:PHE:HB3	11:K:76:GLN:HE21	1.72	0.53
2:B:203:PHE:HB3	2:B:205:ILE:CD1	2.37	0.53
1:A:1063:MET:CE	1:A:1436:ILE:HG12	2.39	0.53
6:F:77:ASP:C	6:F:79:ARG:N	2.61	0.53
8:H:116:TYR:HB2	8:H:123:MET:HB3	1.90	0.53
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.43	0.53
5:E:55:ARG:O	5:E:57:MET:N	2.41	0.53
2:B:224:GLN:O	2:B:238:ALA:HA	2.08	0.53
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.48	0.53
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.24	0.53
1:A:1305:VAL:CG1	1:A:1306:LEU:N	2.71	0.53
2:B:817:LEU:O	2:B:818:PRO:O	2.26	0.53
2:B:827:ILE:CD1	2:B:1086:PHE:HD2	2.21	0.53
1:A:41:MET:HB3	1:A:48:ALA:O	2.08	0.53
1:A:468:PHE:CE2	1:A:489:LEU:HD23	2.43	0.53
3:C:92:CYS:H	3:C:95:CYS:HG	1.57	0.53
1:A:335:ARG:HH11	2:B:1206:GLU:CD	2.10	0.53
1:A:1261:LYS:CA	1:A:1264:GLU:HB3	2.38	0.53
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.43	0.53
3:C:27:LEU:O	3:C:28:ALA:C	2.46	0.53
1:A:423:ASP:OD1	1:A:424:ILE:N	2.42	0.53
6:F:116:ASP:O	6:F:120:ILE:HG13	2.09	0.53
1:A:1454:MET:HG3	1:A:1454:MET:O	2.08	0.53
7:G:78:VAL:HG12	7:G:79:PHE:H	1.74	0.53
8:H:84:ALA:C	8:H:86:ASP:N	2.60	0.53
3:C:97:VAL:HG12	3:C:98:VAL:N	2.23	0.53
1:A:1204:ASP:HA	13:S:252:ASN:CB	2.36	0.53
4:D:123:LEU:HD23	4:D:149:THR:HG21	1.90	0.53
1:A:381:THR:HG22	1:A:383:TYR:H	1.73	0.53
1:A:392:VAL:HG21	1:A:426:LEU:HD11	1.91	0.53
9:I:103:CYS:HB3	9:I:106:CYS:SG	2.48	0.53
1:A:129:LYS:O	1:A:130:ASP:HB2	2.08	0.53
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.09	0.53
1:A:708:MET:SD	1:A:1091:SER:OG	2.66	0.53
2:B:1010:LEU:HD12	2:B:1011:ILE:N	2.23	0.53
2:B:1032:SER:C	2:B:1034:VAL:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:CA	1:A:74:MET:SD	2.89	0.53
1:A:1079:MET:HE3	1:A:1098:VAL:HG22	1.90	0.53
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.39	0.53
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.38	0.53
3:C:88:CYS:SG	3:C:91:HIS:C	2.87	0.53
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.56	0.53
1:A:135:PHE:C	1:A:137:ALA:N	2.60	0.53
1:A:1148:ILE:O	1:A:1149:ALA:HB2	2.09	0.53
4:D:129:LEU:O	4:D:132:GLN:HB2	2.08	0.53
1:A:1299:VAL:HG12	1:A:1300:LYS:H	1.74	0.53
1:A:720:ARG:O	1:A:724:GLU:HB2	2.09	0.53
4:D:14:ARG:O	4:D:16:LYS:N	2.41	0.53
3:C:144:ILE:O	3:C:145:CYS:HB2	2.08	0.53
1:A:1396:ALA:O	1:A:1399:ARG:N	2.41	0.53
1:A:503:GLN:HE21	6:F:90:ARG:NH2	2.02	0.53
1:A:867:ILE:HG22	1:A:871:ASP:N	2.24	0.53
1:A:523:ILE:HG22	1:A:528:LEU:HB2	1.88	0.53
2:B:125:SER:HA	2:B:171:PRO:HA	1.89	0.53
3:C:112:ASN:HB3	3:C:114:TYR:CE1	2.44	0.53
2:B:214:ALA:HB3	2:B:498:THR:HA	1.90	0.53
9:I:61:ASP:C	9:I:63:GLY:H	2.12	0.53
7:G:128:PRO:O	7:G:138:THR:HG23	2.09	0.53
2:B:551:PRO:C	2:B:553:PRO:HD2	2.29	0.53
5:E:154:ILE:O	5:E:196:VAL:HA	2.09	0.53
2:B:31:TRP:O	2:B:34:ILE:N	2.42	0.53
2:B:39:ARG:HG2	2:B:39:ARG:HH11	1.73	0.53
1:A:303:TYR:CE1	1:A:325:ILE:HD11	2.43	0.53
1:A:1385:THR:O	1:A:1387:HIS:N	2.42	0.53
1:A:1086:PHE:O	1:A:1087:ALA:C	2.47	0.53
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.24	0.53
1:A:151:ASP:OD1	1:A:163:SER:HB3	2.09	0.53
3:C:33:LEU:HG	3:C:37:MET:CE	2.38	0.53
10:J:57:ILE:O	10:J:60:PHE:HB2	2.09	0.53
2:B:225:VAL:HA	2:B:237:VAL:O	2.08	0.53
3:C:51:VAL:HG22	3:C:155:LEU:CD2	2.39	0.53
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.53
1:A:587:HIS:HD2	1:A:969:GLN:CG	2.19	0.53
2:B:37:PHE:HE2	2:B:542:MET:CA	2.17	0.53
7:G:123:ALA:C	7:G:125:SER:N	2.63	0.53
1:A:511:ILE:O	1:A:519:PRO:HA	2.08	0.53
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:106:CYS:SG	9:I:107:SER:N	2.82	0.53
4:D:196:PRO:C	4:D:198:LEU:H	2.11	0.53
13:S:231:CYS:CA	13:S:232:ASP:CA	2.86	0.53
1:A:47:ARG:NH1	1:A:254:GLU:HB3	2.06	0.53
2:B:273:LEU:HD21	2:B:360:PHE:CE1	2.44	0.53
10:J:48:ARG:HE	10:J:49:MET:HE2	1.73	0.53
1:A:1097:GLY:O	1:A:1100:ARG:HB3	2.09	0.53
1:A:84:ILE:HG22	1:A:239:LEU:O	2.08	0.53
2:B:856:PHE:N	2:B:856:PHE:HD1	2.06	0.53
2:B:100:PRO:HD2	2:B:180:TYR:CE1	2.43	0.53
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.09	0.53
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.74	0.53
1:A:317:LYS:O	1:A:318:SER:CB	2.57	0.53
1:A:785:PRO:HG2	2:B:703:ILE:HD12	1.91	0.53
1:A:823:GLY:O	1:A:825:ILE:N	2.41	0.53
2:B:298:LEU:CD2	2:B:298:LEU:N	2.72	0.53
2:B:906:SER:O	2:B:941:LEU:HD23	2.09	0.53
1:A:231:PRO:HA	1:A:234:MET:HE2	1.91	0.53
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.45	0.53
5:E:161:LYS:C	5:E:163:GLU:N	2.61	0.53
3:C:35:ARG:HH11	11:K:41:THR:CA	2.22	0.53
4:D:49:ALA:HB1	4:D:178:ALA:HB2	1.91	0.53
13:S:258:GLY:O	13:S:259:ALA:C	2.46	0.53
10:J:1:MET:HE2	10:J:60:PHE:HE2	1.74	0.52
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.24	0.52
3:C:133:ILE:HD11	3:C:237:SER:CA	2.24	0.52
1:A:823:GLY:HA3	13:S:285:GLN:HB2	1.90	0.52
2:B:806:THR:HG22	2:B:808:ALA:N	2.22	0.52
1:A:106:VAL:HA	1:A:114:LEU:HD21	1.90	0.52
5:E:7:ARG:O	5:E:9:ILE:N	2.42	0.52
7:G:25:TYR:O	7:G:28:THR:HB	2.09	0.52
1:A:825:ILE:C	1:A:827:THR:N	2.61	0.52
1:A:49:LYS:HZ2	1:A:60:SER:HA	1.72	0.52
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.68	0.52
1:A:1011:GLN:O	1:A:1015:VAL:HG23	2.09	0.52
1:A:964:ILE:O	1:A:968:GLN:HG2	2.09	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:HG3	1.90	0.52
1:A:262:LEU:HD22	1:A:303:TYR:HE1	1.73	0.52
5:E:124:VAL:HB	5:E:125:PRO:HD3	1.92	0.52
6:F:111:LEU:C	6:F:113:GLY:N	2.62	0.52
2:B:789:MET:HE2	2:B:965:LYS:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.49	0.52
1:A:1397:LEU:HA	1:A:1400:CYS:HB3	1.90	0.52
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.91	0.52
2:B:323:VAL:HG12	2:B:323:VAL:O	2.09	0.52
1:A:1114:PRO:O	1:A:1311:VAL:CG2	2.58	0.52
5:E:147:HIS:CD2	5:E:149:LEU:H	2.27	0.52
7:G:17:PHE:N	7:G:17:PHE:CD2	2.76	0.52
1:A:808:LEU:H	1:A:808:LEU:HD12	1.74	0.52
2:B:257:LYS:O	2:B:385:LEU:HD21	2.08	0.52
3:C:61:GLU:HA	3:C:64:ALA:HB3	1.91	0.52
1:A:751:SER:O	1:A:752:LYS:HG2	2.09	0.52
2:B:901:PRO:O	2:B:903:VAL:N	2.41	0.52
5:E:7:ARG:HG3	5:E:8:ASN:H	1.73	0.52
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.10	0.52
2:B:644:GLU:C	2:B:646:LEU:H	2.13	0.52
3:C:263:THR:C	3:C:265:MET:N	2.63	0.52
5:E:78:LEU:HD23	5:E:78:LEU:C	2.30	0.52
11:K:31:VAL:O	11:K:74:ARG:HA	2.10	0.52
2:B:558:LEU:C	2:B:560:GLU:H	2.12	0.52
3:C:9:LYS:O	3:C:10:ILE:O	2.26	0.52
2:B:347:LYS:HG3	2:B:348:ARG:H	1.74	0.52
1:A:583:PRO:O	1:A:610:GLY:HA3	2.10	0.52
1:A:853:ASP:O	1:A:854:ASN:HB2	2.09	0.52
1:A:864:ILE:O	1:A:865:GLN:CG	2.50	0.52
7:G:18:PHE:CZ	7:G:68:ALA:HB2	2.44	0.52
2:B:205:ILE:O	2:B:206:ASN:C	2.47	0.52
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.28	0.52
3:C:239:PRO:O	3:C:240:VAL:C	2.46	0.52
1:A:808:LEU:HD21	1:A:816:HIS:CD2	2.44	0.52
1:A:53:LEU:HD23	1:A:54:ASN:HB3	1.91	0.52
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.43	0.52
1:A:14:VAL:HG23	1:A:1432:GLN:HE22	1.75	0.52
1:A:477:PRO:CG	1:A:521:MET:HG2	2.39	0.52
1:A:326:ARG:HG2	1:A:327:ALA:N	2.24	0.52
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.91	0.52
4:D:185:CYS:HB3	4:D:211:LEU:CD1	2.39	0.52
7:G:146:LYS:NZ	7:G:165:GLU:OE2	2.38	0.52
3:C:31:ASN:O	3:C:34:ARG:N	2.43	0.52
2:B:57:TYR:N	2:B:57:TYR:HD1	2.06	0.52
7:G:109:PHE:CG	7:G:110:VAL:N	2.78	0.52
9:I:68:LEU:HB3	9:I:84:VAL:HG23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1310:GLY:O	1:A:1311:VAL:HG23	2.08	0.52
2:B:782:LEU:CD1	2:B:788:ARG:HH11	2.23	0.52
1:A:877:HIS:O	1:A:878:ILE:HG12	2.09	0.52
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.75	0.52
2:B:212:LEU:HD21	2:B:466:TRP:HH2	1.74	0.52
4:D:198:LEU:O	4:D:200:ASN:N	2.42	0.52
2:B:210:LYS:HD2	2:B:481:GLN:O	2.09	0.52
1:A:514:PRO:O	1:A:875:ALA:HB1	2.08	0.52
2:B:360:PHE:O	2:B:361:LEU:C	2.47	0.52
2:B:225:VAL:HG22	2:B:396:ASP:OD2	2.10	0.52
1:A:1394:THR:O	1:A:1399:ARG:NE	2.38	0.52
1:A:866:PHE:CD2	5:E:168:TYR:CE1	2.98	0.52
9:I:100:PHE:CD1	9:I:100:PHE:N	2.78	0.52
3:C:215:GLU:O	3:C:217:ASP:N	2.43	0.52
1:A:412:ARG:NH2	2:B:1108:ARG:HH12	2.07	0.52
1:A:744:LYS:HG2	1:A:748:MET:HE3	1.91	0.52
1:A:1406:VAL:CG1	1:A:1410:PHE:CE1	2.90	0.52
3:C:99:LEU:HD23	3:C:99:LEU:N	2.23	0.52
1:A:695:LYS:C	1:A:697:ALA:H	2.11	0.52
1:A:688:LYS:C	1:A:690:VAL:N	2.61	0.52
2:B:522:VAL:CG1	2:B:523:CYS:N	2.71	0.52
1:A:316:GLN:O	1:A:317:LYS:C	2.47	0.52
8:H:59:ILE:O	8:H:60:ALA:HB3	2.10	0.52
2:B:401:PHE:HD2	2:B:521:LEU:HD12	1.75	0.52
7:G:143:ILE:CG2	7:G:144:ARG:N	2.73	0.52
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.44	0.52
1:A:1073:GLY:HA2	1:A:1076:ALA:HB3	1.91	0.52
1:A:1088:GLY:O	1:A:1089:VAL:HG23	2.09	0.52
3:C:236:GLY:C	3:C:238:ILE:H	2.13	0.52
5:E:168:TYR:CB	5:E:170:LEU:HG	2.40	0.52
2:B:857:ARG:NH2	2:B:942:ARG:NH1	2.57	0.52
1:A:1213:GLY:O	1:A:1216:ILE:N	2.42	0.52
3:C:58:LEU:N	3:C:58:LEU:HD22	2.25	0.52
2:B:457:LEU:O	2:B:461:LEU:HD12	2.10	0.52
2:B:49:ASP:HA	2:B:52:ASN:HD22	1.75	0.52
10:J:55:ASP:OD2	10:J:58:GLU:HG2	2.10	0.52
1:A:785:PRO:CG	2:B:703:ILE:HD12	2.40	0.52
2:B:865:LYS:HE2	2:B:871:THR:OG1	2.10	0.52
1:A:553:VAL:HG22	1:A:652:VAL:HG22	1.92	0.52
1:A:1444:MET:O	6:F:132:LEU:HA	2.10	0.52
2:B:1045:SER:O	2:B:1046:PRO:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:ASN:OD1	3:C:34:ARG:HD3	2.10	0.52
12:L:28:LYS:HB2	12:L:39:SER:HA	1.91	0.52
2:B:223:VAL:CG1	2:B:381:MET:HG2	2.40	0.52
5:E:55:ARG:C	5:E:57:MET:N	2.63	0.52
2:B:870:ILE:CG2	2:B:917:PRO:HG2	2.40	0.52
1:A:18:GLN:HB3	2:B:1215:ARG:HG3	1.92	0.52
2:B:508:LEU:O	2:B:510:LYS:N	2.42	0.52
1:A:55:ASP:N	1:A:56:PRO:CD	2.73	0.52
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.91	0.52
1:A:1377:THR:O	1:A:1379:GLY:N	2.42	0.52
8:H:89:LEU:C	8:H:91:ASP:H	2.12	0.52
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.92	0.52
1:A:1443:VAL:C	1:A:1444:MET:HG3	2.30	0.52
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.45	0.52
2:B:57:TYR:O	2:B:59:LEU:N	2.42	0.52
2:B:1147:LEU:O	2:B:1148:LYS:C	2.45	0.52
13:S:235:ASP:CA	13:S:242:LYS:HG3	2.38	0.51
1:A:841:LEU:O	1:A:845:LEU:HG	2.10	0.51
1:A:351:THR:HG21	2:B:1103:ILE:HG13	1.91	0.51
1:A:35:ILE:O	1:A:35:ILE:HG22	2.11	0.51
1:A:321:PRO:O	1:A:322:VAL:CB	2.57	0.51
5:E:161:LYS:C	5:E:163:GLU:H	2.14	0.51
5:E:92:THR:O	5:E:95:THR:HB	2.10	0.51
1:A:856:THR:HB	1:A:865:GLN:HB2	1.93	0.51
2:B:508:LEU:HB2	2:B:510:LYS:CB	2.40	0.51
2:B:1032:SER:C	2:B:1034:VAL:N	2.64	0.51
2:B:1034:VAL:HG23	2:B:1059:LEU:CD1	2.40	0.51
9:I:54:GLU:O	9:I:100:PHE:CE2	2.63	0.51
2:B:758:PHE:CE2	2:B:1044:ALA:CA	2.92	0.51
3:C:104:PHE:HD2	3:C:105:GLY:H	1.56	0.51
12:L:38:LEU:HG	12:L:39:SER:N	2.26	0.51
2:B:54:PHE:CE1	2:B:414:ALA:HA	2.42	0.51
1:A:675:THR:O	1:A:679:ILE:HG13	2.11	0.51
4:D:134:THR:HG22	4:D:136:GLY:H	1.75	0.51
12:L:36:SER:O	12:L:37:LYS:C	2.48	0.51
1:A:725:ALA:O	1:A:729:ALA:N	2.42	0.51
2:B:1082:MET:O	3:C:189:THR:HG23	2.10	0.51
1:A:1325:THR:CG2	1:A:1326:ARG:HG3	2.40	0.51
2:B:879:ARG:O	2:B:880:THR:CB	2.58	0.51
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.70	0.51
11:K:65:HIS:CD2	11:K:66:PRO:HD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:67:PHE:O	11:K:68:PHE:HD2	1.93	0.51
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.51
9:I:100:PHE:N	9:I:100:PHE:HD1	2.08	0.51
1:A:648:ASN:O	1:A:649:ILE:C	2.47	0.51
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.94	0.51
3:C:31:ASN:O	3:C:34:ARG:HB3	2.10	0.51
1:A:1148:ILE:O	1:A:1148:ILE:CG2	2.59	0.51
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.92	0.51
12:L:25:ALA:O	12:L:26:THR:HB	2.10	0.51
1:A:348:SER:HB2	2:B:1128:LEU:HB2	1.90	0.51
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.92	0.51
2:B:298:LEU:N	2:B:298:LEU:HD22	2.24	0.51
2:B:38:PHE:CD1	2:B:811:TYR:CD2	2.98	0.51
3:C:80:LEU:CD1	3:C:95:CYS:HA	2.40	0.51
2:B:46:GLN:CG	2:B:47:GLN:H	2.22	0.51
1:A:898:ARG:HB2	1:A:933:TYR:HE1	1.75	0.51
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.25	0.51
1:A:602:ASP:OD2	1:A:616:VAL:HG23	2.11	0.51
1:A:1005:GLU:O	1:A:1006:ILE:C	2.49	0.51
9:I:95:THR:HG22	9:I:96:SER:N	2.25	0.51
8:H:62:SER:O	8:H:63:LEU:C	2.48	0.51
11:K:87:LEU:O	11:K:87:LEU:HD12	2.09	0.51
1:A:1134:ILE:O	1:A:1135:ARG:C	2.49	0.51
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.45	0.51
1:A:56:PRO:O	1:A:57:ARG:CG	2.57	0.51
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.75	0.51
3:C:51:VAL:HG22	3:C:155:LEU:HD21	1.93	0.51
2:B:843:GLN:O	2:B:846:ILE:HB	2.11	0.51
8:H:143:LEU:N	8:H:143:LEU:HD12	2.25	0.51
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.39	0.51
7:G:123:ALA:O	7:G:125:SER:N	2.43	0.51
2:B:525:ALA:O	2:B:768:THR:HG23	2.11	0.51
11:K:35:PHE:CD1	11:K:35:PHE:N	2.79	0.51
10:J:60:PHE:O	10:J:63:TYR:HD1	1.94	0.51
1:A:901:LEU:HD22	1:A:919:ILE:HG21	1.91	0.51
1:A:1369:ALA:O	1:A:1372:VAL:HG12	2.11	0.51
3:C:213:PRO:O	3:C:214:ASN:CB	2.55	0.51
1:A:516:SER:O	1:A:517:ASN:C	2.47	0.51
2:B:708:GLU:HG3	2:B:709:ASP:H	1.76	0.51
2:B:44:VAL:O	2:B:45:SER:C	2.49	0.51
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:ARG:HH12	2:B:539:LEU:HB2	1.74	0.51
5:E:144:ILE:HG13	5:E:145:THR:N	2.26	0.51
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.46	0.51
2:B:446:LEU:HD23	2:B:446:LEU:N	2.26	0.51
2:B:424:LEU:HD22	2:B:453:ILE:HD11	1.92	0.51
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.92	0.51
1:A:986:ILE:CD1	1:A:1032:LEU:HD11	2.40	0.51
1:A:1090:ALA:O	1:A:1091:SER:OG	2.28	0.51
1:A:1323:ASP:C	1:A:1325:THR:H	2.14	0.51
1:A:470:LEU:CD2	1:A:487:MET:HE3	2.41	0.51
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.92	0.51
2:B:1065:GLN:NE2	2:B:1067:ARG:HG2	2.25	0.51
1:A:877:HIS:CG	1:A:1056:SER:HA	2.46	0.51
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.40	0.51
1:A:311:GLN:O	1:A:312:PRO:C	2.49	0.51
5:E:79:TRP:HE1	5:E:81:GLU:HB2	1.76	0.51
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.91	0.51
1:A:770:VAL:O	1:A:771:GLU:HB2	2.11	0.51
9:I:43:VAL:HG12	9:I:43:VAL:O	2.09	0.51
7:G:6:ASP:HB3	7:G:73:LYS:NZ	2.25	0.51
1:A:899:VAL:HG22	1:A:908:LEU:HD21	1.93	0.51
2:B:575:PRO:C	2:B:577:ALA:H	2.13	0.51
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.25	0.51
10:J:5:VAL:O	10:J:6:ARG:O	2.28	0.51
1:A:1372:VAL:HG12	1:A:1373:ASP:N	2.25	0.51
1:A:472:LEU:CD1	2:B:835:GLN:NE2	2.69	0.51
8:H:40:LEU:HG	8:H:41:ASP:O	2.11	0.51
3:C:60:ASP:OD2	12:L:60:ARG:NH2	2.44	0.51
2:B:857:ARG:HG2	2:B:858:SER:N	2.24	0.51
1:A:34:LYS:HG2	1:A:36:ARG:NH2	2.26	0.51
1:A:1191:TRP:HD1	1:A:1256:GLU:HB2	1.76	0.51
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.84	0.51
1:A:705:LYS:C	1:A:707:GLY:N	2.62	0.51
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.75	0.51
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.59	0.51
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.89	0.51
1:A:525:GLN:HB3	2:B:1015:HIS:HD2	1.74	0.51
1:A:556:TRP:O	1:A:558:GLY:N	2.44	0.51
2:B:1202:LEU:O	2:B:1203:LEU:C	2.49	0.51
1:A:92:HIS:O	1:A:93:VAL:C	2.48	0.51
12:L:49:LYS:O	12:L:50:ASP:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:TYR:CD2	1:A:1060:PRO:HB2	2.45	0.51
2:B:209:GLU:CD	2:B:485:ARG:HE	2.14	0.51
1:A:391:LEU:O	1:A:392:VAL:C	2.49	0.51
7:G:114:LEU:HG	7:G:162:SER:HB3	1.93	0.51
2:B:429:PHE:HA	2:B:432:MET:CE	2.40	0.51
2:B:69:LEU:HD22	2:B:429:PHE:HE1	1.74	0.51
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.40	0.51
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.46	0.51
2:B:334:ILE:O	2:B:334:ILE:HG22	2.09	0.51
1:A:1230:GLU:C	1:A:1232:ASN:H	2.14	0.51
2:B:1102:LYS:O	2:B:1103:ILE:O	2.29	0.51
2:B:798:TYR:CD1	10:J:4:PRO:HG3	2.45	0.51
10:J:46:CYS:O	10:J:49:MET:N	2.44	0.51
10:J:7:CYS:CA	10:J:49:MET:HE3	2.40	0.51
1:A:1168:GLU:OE1	13:S:208:SER:CA	2.59	0.51
1:A:1364:ASN:O	1:A:1365:TYR:C	2.49	0.51
8:H:25:ARG:HA	8:H:41:ASP:HA	1.93	0.51
1:A:1290:LYS:O	1:A:1291:VAL:HG23	2.11	0.51
1:A:474:VAL:HG22	1:A:474:VAL:O	2.10	0.51
1:A:335:ARG:NE	1:A:339:ASN:HD22	2.09	0.51
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.93	0.51
1:A:384:ASN:O	1:A:385:ILE:C	2.49	0.51
3:C:35:ARG:HD3	11:K:41:THR:HA	1.93	0.51
2:B:936:ASP:OD1	2:B:938:SER:N	2.42	0.51
1:A:1277:GLU:O	1:A:1278:ASN:HB2	2.11	0.51
1:A:496:GLU:OE1	7:G:64:THR:HA	2.11	0.51
2:B:197:PHE:CZ	2:B:816:GLU:HG2	2.46	0.50
1:A:774:ARG:O	1:A:775:ILE:C	2.49	0.50
2:B:763:GLN:C	2:B:765:PRO:HD2	2.32	0.50
1:A:42:ASP:C	1:A:44:THR:N	2.64	0.50
1:A:1167:GLU:O	1:A:1169:ILE:N	2.44	0.50
2:B:212:LEU:HD21	2:B:466:TRP:CH2	2.47	0.50
9:I:58:VAL:HG12	9:I:60:GLN:N	2.20	0.50
4:D:47:LEU:HD13	4:D:48:ILE:N	2.25	0.50
12:L:30:ILE:HG22	12:L:31:CYS:O	2.10	0.50
5:E:10:SER:O	5:E:13:TRP:HB3	2.10	0.50
4:D:52:LEU:C	4:D:54:GLU:H	2.14	0.50
7:G:49:LEU:N	7:G:49:LEU:HD23	2.25	0.50
1:A:992:ASP:O	1:A:995:GLU:HB2	2.11	0.50
3:C:168:ALA:O	3:C:170:TRP:N	2.44	0.50
1:A:167:CYS:SG	1:A:167:CYS:O	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:242:SER:HB2	2:B:362:PRO:HG2	1.93	0.50
1:A:115:LEU:HB2	1:A:122:MET:CE	2.40	0.50
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.26	0.50
4:D:51:ASN:O	4:D:52:LEU:C	2.48	0.50
2:B:546:SER:HA	2:B:612:GLU:OE2	2.11	0.50
1:A:996:ASN:HA	1:A:998:LEU:HD12	1.92	0.50
1:A:1208:THR:O	1:A:1209:MET:C	2.48	0.50
2:B:488:TYR:HE2	2:B:813:LYS:HB2	1.75	0.50
2:B:510:LYS:O	2:B:513:GLN:HB2	2.11	0.50
2:B:377:PHE:O	2:B:378:LEU:C	2.50	0.50
11:K:68:PHE:N	11:K:68:PHE:CD2	2.77	0.50
10:J:52:THR:O	10:J:53:HIS:O	2.30	0.50
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.92	0.50
7:G:70:PHE:N	7:G:70:PHE:CD1	2.79	0.50
1:A:1199:ARG:HG3	1:A:1236:LEU:HD11	1.93	0.50
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.84	0.50
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.12	0.50
2:B:269:ILE:HG22	2:B:282:ILE:HG23	1.94	0.50
2:B:996:ARG:HH22	3:C:175:ALA:HA	1.75	0.50
1:A:1424:VAL:CG2	1:A:1436:ILE:HD11	2.32	0.50
3:C:88:CYS:O	3:C:88:CYS:SG	2.70	0.50
9:I:58:VAL:HG13	9:I:62:ILE:HD12	1.93	0.50
1:A:335:ARG:HA	1:A:339:ASN:ND2	2.26	0.50
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.75	0.50
1:A:519:PRO:HG3	1:A:625:SER:O	2.12	0.50
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.25	0.50
2:B:1145:SER:C	2:B:1147:LEU:H	2.14	0.50
5:E:42:PHE:O	5:E:43:LYS:C	2.50	0.50
3:C:33:LEU:HG	3:C:37:MET:HE2	1.92	0.50
1:A:1038:THR:O	1:A:1039:LYS:C	2.49	0.50
2:B:303:TYR:N	2:B:303:TYR:CD2	2.80	0.50
1:A:406:ILE:HG22	1:A:411:ASP:O	2.11	0.50
3:C:53:THR:O	3:C:153:LEU:HA	2.10	0.50
10:J:1:MET:HE2	10:J:60:PHE:CE2	2.46	0.50
1:A:590:ARG:O	1:A:591:PHE:HB2	2.12	0.50
1:A:864:ILE:HG22	1:A:864:ILE:O	2.10	0.50
3:C:43:THR:CG2	3:C:44:LEU:N	2.74	0.50
2:B:839:MET:N	2:B:989:THR:O	2.44	0.50
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.93	0.50
2:B:1029:CYS:SG	2:B:1086:PHE:CE2	3.05	0.50
3:C:235:VAL:HG13	10:J:13:VAL:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:809:MET:O	2:B:812:LEU:N	2.37	0.50
1:A:472:LEU:CD1	2:B:835:GLN:CD	2.79	0.50
2:B:681:TRP:C	2:B:683:SER:H	2.14	0.50
2:B:48:LEU:O	2:B:51:PHE:N	2.44	0.50
2:B:1074:ASN:O	2:B:1078:GLY:N	2.44	0.50
1:A:1308:THR:HG23	1:A:1309:ASP:N	2.26	0.50
7:G:91:VAL:HA	7:G:101:VAL:HA	1.94	0.50
10:J:1:MET:HA	10:J:57:ILE:H	1.76	0.50
1:A:50:ILE:O	1:A:52:GLY:N	2.39	0.50
2:B:1149:GLU:O	2:B:1150:ARG:C	2.47	0.50
1:A:1341:ILE:O	1:A:1344:GLY:N	2.45	0.50
1:A:1344:GLY:O	1:A:1345:ARG:C	2.50	0.50
2:B:758:PHE:HE2	2:B:1044:ALA:HA	1.73	0.50
1:A:547:LEU:HD22	11:K:58:PHE:CE1	2.46	0.50
10:J:21:TYR:O	10:J:23:ASN:N	2.44	0.50
1:A:148:CYS:O	1:A:168:GLY:HA2	2.12	0.50
4:D:26:THR:O	4:D:28:GLN:HG3	2.11	0.50
1:A:1114:PRO:O	1:A:1311:VAL:HG21	2.11	0.50
1:A:1398:MET:HB2	1:A:1426:GLU:OE2	2.11	0.50
2:B:851:PHE:CD2	2:B:1094:ARG:HB2	2.46	0.50
1:A:744:LYS:HG2	1:A:748:MET:CE	2.41	0.50
1:A:265:LYS:NZ	1:A:322:VAL:HG22	2.27	0.50
5:E:3:GLN:HG3	5:E:4:GLU:N	2.27	0.50
1:A:719:VAL:O	1:A:721:PHE:N	2.45	0.50
10:J:21:TYR:C	10:J:23:ASN:H	2.15	0.50
11:K:84:LYS:O	11:K:87:LEU:HB3	2.12	0.50
1:A:709:THR:CG2	1:A:712:GLU:H	2.23	0.50
2:B:196:PRO:HG2	2:B:197:PHE:H	1.77	0.50
2:B:376:PHE:HB3	2:B:586:TRP:CZ3	2.46	0.50
1:A:1053:PHE:O	1:A:1056:SER:N	2.44	0.50
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.46	0.50
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.35	0.50
1:A:556:TRP:C	1:A:558:GLY:N	2.65	0.50
1:A:1410:PHE:C	1:A:1412:ALA:H	2.15	0.50
5:E:7:ARG:C	5:E:9:ILE:N	2.65	0.50
2:B:1022:THR:HG23	2:B:1022:THR:O	2.12	0.50
2:B:1060:ARG:NH1	2:B:1060:ARG:HG2	2.27	0.50
1:A:22:PHE:CE1	2:B:1213:THR:HG22	2.47	0.50
6:F:127:GLU:O	6:F:129:LYS:HG3	2.12	0.50
1:A:208:LEU:HG	1:A:235:ILE:HG21	1.93	0.50
4:D:53:SER:HB3	4:D:152:SER:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:ALA:O	1:A:1127:ASP:N	2.45	0.50
6:F:103:MET:O	6:F:104:ASN:HB2	2.11	0.50
2:B:877:PRO:C	2:B:878:GLN:HG3	2.31	0.50
2:B:843:GLN:O	2:B:846:ILE:N	2.44	0.50
2:B:806:THR:O	2:B:807:ARG:C	2.50	0.50
2:B:578:THR:HA	2:B:622:LYS:HB3	1.94	0.50
12:L:60:ARG:HG2	12:L:61:THR:N	2.27	0.50
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.92	0.50
1:A:12:ARG:CZ	2:B:1192:TYR:HE2	2.25	0.50
12:L:28:LYS:HB2	12:L:39:SER:CA	2.42	0.50
1:A:1213:GLY:HA2	1:A:1216:ILE:CD1	2.42	0.50
2:B:210:LYS:HE2	2:B:462:ALA:O	2.11	0.50
1:A:726:ARG:O	1:A:727:ASP:C	2.50	0.50
2:B:218:SER:O	2:B:219:ALA:O	2.29	0.50
2:B:91:SER:OG	2:B:133:LYS:HB2	2.11	0.50
1:A:853:ASP:C	1:A:853:ASP:OD1	2.51	0.49
1:A:863:VAL:HG12	1:A:865:GLN:H	1.76	0.49
3:C:84:ARG:NH2	11:K:11:LEU:HD21	2.27	0.49
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.38	0.49
2:B:999:MET:HA	2:B:999:MET:CE	2.42	0.49
3:C:63:ILE:O	3:C:64:ALA:C	2.50	0.49
2:B:1131:GLY:O	2:B:1132:GLU:C	2.50	0.49
8:H:93:TYR:N	8:H:93:TYR:CD1	2.80	0.49
1:A:347:PHE:N	2:B:1107:ALA:HA	2.26	0.49
1:A:541:ILE:HD12	1:A:577:ILE:HD11	1.94	0.49
7:G:96:GLN:HG3	7:G:97:HIS:HD2	1.76	0.49
1:A:416:ARG:O	1:A:417:TYR:HD2	1.94	0.49
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.94	0.49
4:D:134:THR:CG2	4:D:135:GLY:N	2.75	0.49
2:B:984:HIS:CD2	2:B:1025:HIS:HB2	2.47	0.49
1:A:809:THR:OG1	1:A:812:GLU:HG3	2.12	0.49
6:F:93:ILE:O	6:F:94:LEU:C	2.49	0.49
13:S:269:PHE:HE2	13:S:306:TRP:CZ2	2.30	0.49
1:A:254:GLU:HB2	2:B:935:ARG:NH2	2.25	0.49
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.94	0.49
1:A:1019:CYS:O	1:A:1022:LEU:N	2.45	0.49
1:A:1161:THR:O	1:A:1163:ILE:N	2.45	0.49
1:A:14:VAL:CG2	1:A:1430:LEU:HD13	2.42	0.49
1:A:1364:ASN:HD22	1:A:1365:TYR:N	2.10	0.49
2:B:850:LEU:HD12	2:B:851:PHE:H	1.77	0.49
9:I:113:ASP:O	9:I:114:GLN:CG	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:144:THR:OG1	7:G:105:PRO:HD3	2.12	0.49
8:H:58:THR:HB	8:H:143:LEU:HD13	1.94	0.49
3:C:86:CYS:SG	3:C:95:CYS:HB3	2.52	0.49
2:B:314:LEU:O	2:B:317:CYS:HB3	2.12	0.49
4:D:48:ILE:HG21	7:G:4:ILE:CD1	2.41	0.49
2:B:526:GLU:HG2	2:B:538:ASN:HD22	1.77	0.49
6:F:72:LYS:HB2	6:F:142:SER:HB3	1.94	0.49
2:B:25:ILE:HG23	2:B:29:ASP:CB	2.42	0.49
7:G:25:TYR:HE2	7:G:29:LYS:HD2	1.77	0.49
1:A:989:GLY:O	1:A:992:ASP:N	2.44	0.49
2:B:215:GLN:OE1	2:B:215:GLN:HA	2.12	0.49
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.93	0.49
2:B:459:TYR:CD2	2:B:459:TYR:C	2.85	0.49
1:A:755:PHE:HA	1:A:758:ILE:HG13	1.94	0.49
2:B:882:THR:HB	2:B:934:LYS:O	2.11	0.49
1:A:903:ASN:ND2	1:A:903:ASN:C	2.65	0.49
1:A:838:GLN:O	1:A:842:VAL:HG23	2.13	0.49
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.10	0.49
1:A:90:VAL:CG1	1:A:91:PHE:H	2.23	0.49
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.76	0.49
1:A:898:ARG:HB2	1:A:933:TYR:CE1	2.47	0.49
5:E:164:LEU:CD2	5:E:211:TYR:CD2	2.95	0.49
5:E:23:VAL:O	5:E:28:TYR:HB2	2.12	0.49
3:C:69:LEU:HD12	3:C:69:LEU:N	2.27	0.49
3:C:186:LEU:N	3:C:186:LEU:CD1	2.75	0.49
1:A:1041:ALA:O	1:A:1044:TRP:HB3	2.12	0.49
1:A:1360:GLY:HA3	13:S:306:TRP:HA	1.94	0.49
1:A:1127:ASP:O	1:A:1128:GLN:C	2.50	0.49
2:B:563:MET:HA	2:B:589:VAL:O	2.13	0.49
2:B:1165:ILE:HG22	2:B:1185:CYS:HB3	1.94	0.49
1:A:997:LEU:HB3	1:A:1053:PHE:CE2	2.47	0.49
2:B:583:ASN:HD21	2:B:628:THR:CB	2.13	0.49
9:I:4:PHE:CE1	9:I:13:MET:HE1	2.47	0.49
5:E:124:VAL:CG1	5:E:132:ILE:HD12	2.37	0.49
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.27	0.49
2:B:247:GLY:C	2:B:249:ARG:H	2.16	0.49
1:A:717:ASN:O	1:A:721:PHE:CD1	2.66	0.49
1:A:24:PRO:HG2	1:A:25:GLU:OE2	2.11	0.49
1:A:1285:MET:HG3	1:A:1307:GLU:OE2	2.12	0.49
1:A:564:ALA:HB2	1:A:576:GLN:OE1	2.12	0.49
1:A:470:LEU:HD11	1:A:482:PHE:CZ	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:ARG:HA	1:A:824:LEU:HD12	1.95	0.49
1:A:472:LEU:HD13	2:B:835:GLN:CD	2.33	0.49
1:A:1444:MET:HG2	7:G:60:ARG:CA	2.40	0.49
4:D:147:TYR:CZ	7:G:103:VAL:HG13	2.47	0.49
1:A:979:SER:HG	1:A:980:ASP:H	1.58	0.49
2:B:497:ARG:NH2	2:B:775:LYS:NZ	2.60	0.49
2:B:642:ASP:HA	2:B:649:LYS:HA	1.95	0.49
2:B:526:GLU:CD	2:B:752:ALA:HB2	2.32	0.49
2:B:1177:HIS:O	2:B:1179:GLN:N	2.44	0.49
5:E:72:PHE:CD1	5:E:72:PHE:N	2.80	0.49
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.77	0.49
1:A:869:GLY:O	1:A:870:GLU:HB2	2.11	0.49
3:C:73:GLN:HE21	3:C:74:SER:H	1.60	0.49
1:A:601:LYS:HB2	1:A:603:ASN:ND2	2.27	0.49
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.78	0.49
7:G:30:LEU:O	7:G:34:VAL:HG23	2.12	0.49
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.47	0.49
9:I:27:PHE:O	9:I:28:GLU:HB3	2.11	0.49
1:A:37:PHE:N	1:A:37:PHE:CD1	2.81	0.49
1:A:1090:ALA:O	1:A:1091:SER:CB	2.60	0.49
2:B:1002:THR:O	2:B:1005:GLY:N	2.32	0.49
4:D:56:ARG:NH2	4:D:155:ARG:HA	2.28	0.49
8:H:143:LEU:C	8:H:144:ILE:HG13	2.33	0.49
2:B:693:ILE:HD11	2:B:740:HIS:NE2	2.27	0.49
2:B:1106:ARG:HD3	2:B:1126:GLY:O	2.12	0.49
9:I:13:MET:HG3	9:I:14:LEU:N	2.27	0.49
1:A:321:PRO:O	1:A:322:VAL:HB	2.13	0.49
2:B:899:ILE:HG22	2:B:900:ALA:H	1.75	0.49
2:B:757:PRO:O	2:B:758:PHE:HB2	2.13	0.49
1:A:387:ARG:O	1:A:390:GLN:HB3	2.13	0.49
2:B:54:PHE:O	2:B:59:LEU:HB2	2.12	0.49
4:D:53:SER:O	4:D:57:LEU:HG	2.12	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.78	0.49
8:H:27:GLU:HA	8:H:38:LEU:O	2.12	0.49
4:D:127:ASP:O	4:D:131:GLU:HG3	2.13	0.49
1:A:88:LYS:HE3	1:A:280:GLU:OE2	2.12	0.49
1:A:1230:GLU:CD	13:S:201:ILE:CA	2.73	0.49
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.94	0.49
2:B:1059:LEU:HD23	2:B:1065:GLN:O	2.12	0.49
2:B:361:LEU:N	2:B:362:PRO:CD	2.75	0.49
1:A:877:HIS:C	1:A:878:ILE:HG13	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:681:TRP:C	2:B:683:SER:N	2.66	0.49
1:A:433:GLU:OE2	2:B:1108:ARG:NH1	2.45	0.49
1:A:626:ASN:O	1:A:628:GLY:N	2.42	0.49
2:B:910:VAL:CG1	2:B:911:ILE:N	2.76	0.49
12:L:31:CYS:HB3	12:L:35:SER:CA	2.42	0.49
4:D:170:THR:HG21	4:D:172:LEU:HG	1.94	0.49
2:B:97:VAL:CG1	2:B:178:ASN:ND2	2.74	0.49
1:A:1086:PHE:HE2	13:S:261:ILE:CD1	2.24	0.49
1:A:711:ARG:HA	9:I:97:MET:HE1	1.95	0.49
2:B:247:GLY:H	2:B:418:LYS:NZ	2.10	0.49
1:A:3:GLY:O	1:A:4:GLN:O	2.31	0.49
4:D:173:HIS:O	4:D:177:VAL:HG23	2.13	0.49
1:A:907:THR:CG2	1:A:908:LEU:N	2.75	0.49
2:B:510:LYS:HG2	2:B:512:ARG:N	2.19	0.49
2:B:1034:VAL:HG23	2:B:1059:LEU:HD12	1.95	0.49
2:B:992:ILE:CG2	2:B:994:TYR:HE1	2.26	0.49
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.94	0.49
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.95	0.49
10:J:37:SER:OG	10:J:47:ARG:NH2	2.46	0.49
2:B:446:LEU:O	2:B:447:ALA:CB	2.61	0.49
11:K:32:VAL:HG22	11:K:74:ARG:HG3	1.95	0.49
5:E:32:GLN:HG3	5:E:36:GLU:OE2	2.12	0.49
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.95	0.49
2:B:234:ILE:HD12	2:B:234:ILE:N	2.27	0.49
1:A:1198:ASP:O	1:A:1202:MET:HG2	2.13	0.49
8:H:33:GLN:C	8:H:35:GLN:H	2.16	0.49
5:E:136:ASN:OD1	5:E:137:GLU:N	2.46	0.49
1:A:481:ASP:O	1:A:485:ASP:HB2	2.13	0.49
3:C:47:ASP:O	3:C:48:SER:HB2	2.13	0.49
1:A:356:ASP:C	1:A:358:ASN:H	2.16	0.49
8:H:142:LEU:C	8:H:143:LEU:HD12	2.33	0.49
1:A:501:LEU:HD11	2:B:1146:PHE:CD2	2.48	0.49
3:C:80:LEU:HD22	3:C:129:ILE:HD13	1.94	0.49
2:B:594:ALA:CA	2:B:617:ARG:HH12	2.25	0.49
5:E:25:ASP:C	5:E:27:GLY:N	2.63	0.49
7:G:101:VAL:CG1	7:G:102:GLN:N	2.76	0.48
1:A:618:GLU:CD	1:A:618:GLU:C	2.71	0.48
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.33	0.48
1:A:525:GLN:HB3	2:B:1015:HIS:CD2	2.48	0.48
2:B:760:ASP:O	2:B:761:HIS:CD2	2.66	0.48
6:F:72:LYS:O	6:F:73:ALA:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1329:THR:O	1:A:1330:ASN:C	2.50	0.48
7:G:15:PRO:O	7:G:18:PHE:HB2	2.12	0.48
2:B:102:VAL:CG2	2:B:112:LEU:HD22	2.43	0.48
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.95	0.48
2:B:845:SER:HB3	10:J:8:PHE:O	2.13	0.48
2:B:811:TYR:N	2:B:811:TYR:CD1	2.80	0.48
12:L:30:ILE:CG2	12:L:31:CYS:N	2.75	0.48
3:C:111:THR:O	3:C:147:LEU:HD23	2.12	0.48
5:E:17:ARG:O	5:E:20:LYS:HB2	2.13	0.48
1:A:852:TYR:CE1	6:F:136:ARG:HB3	2.48	0.48
2:B:498:THR:HG22	2:B:537:LYS:H	1.78	0.48
3:C:168:ALA:C	3:C:170:TRP:H	2.17	0.48
3:C:136:ASP:OD1	3:C:138:GLU:N	2.45	0.48
1:A:1308:THR:O	1:A:1309:ASP:HB2	2.12	0.48
5:E:204:THR:HG23	5:E:205:SER:N	2.29	0.48
10:J:61:LEU:C	10:J:63:TYR:H	2.16	0.48
1:A:503:GLN:O	1:A:504:LEU:HD12	2.13	0.48
2:B:38:PHE:HD1	2:B:811:TYR:CD2	2.31	0.48
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.13	0.48
2:B:1208:MET:HA	2:B:1212:ILE:O	2.13	0.48
2:B:899:ILE:HG23	2:B:903:VAL:HG21	1.95	0.48
10:J:36:LEU:HB2	10:J:47:ARG:NH1	2.28	0.48
1:A:543:LEU:O	1:A:544:ASP:C	2.52	0.48
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.14	0.48
1:A:348:SER:HB2	2:B:1128:LEU:HD12	1.93	0.48
4:D:60:LYS:O	4:D:61:GLU:C	2.51	0.48
8:H:10:PHE:N	8:H:10:PHE:CD1	2.81	0.48
13:S:254:TYR:C	13:S:256:ALA:H	2.17	0.48
1:A:929:LEU:HD23	1:A:983:ILE:HG21	1.95	0.48
6:F:99:LEU:O	6:F:103:MET:HG2	2.14	0.48
1:A:780:VAL:O	1:A:780:VAL:HG12	2.14	0.48
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.79	0.48
3:C:164:ALA:O	3:C:167:HIS:N	2.43	0.48
2:B:976:ILE:O	2:B:990:ILE:HB	2.12	0.48
10:J:3:VAL:HG12	10:J:4:PRO:N	2.28	0.48
1:A:877:HIS:O	1:A:878:ILE:CG1	2.61	0.48
2:B:616:ILE:N	2:B:625:LYS:O	2.37	0.48
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.41	0.48
13:S:274:CYS:O	13:S:276:GLU:HG3	2.13	0.48
2:B:760:ASP:OD1	2:B:1046:PRO:HA	2.12	0.48
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.96	0.48
7:G:6:ASP:C	7:G:7:LEU:HD23	2.33	0.48
1:A:1072:ILE:C	1:A:1075:PRO:HD2	2.33	0.48
2:B:112:LEU:CD1	2:B:113:TYR:N	2.71	0.48
2:B:508:LEU:CA	2:B:510:LYS:H	2.24	0.48
3:C:173:ALA:O	3:C:174:ALA:HB3	2.13	0.48
2:B:293:PRO:C	2:B:294:ASP:O	2.47	0.48
1:A:1372:VAL:HG12	1:A:1373:ASP:H	1.78	0.48
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.44	0.48
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.48
4:D:190:GLU:O	4:D:194:LEU:HG	2.14	0.48
7:G:145:VAL:CG1	7:G:146:LYS:H	2.27	0.48
5:E:16:PHE:CE2	5:E:20:LYS:HE2	2.48	0.48
5:E:163:GLU:O	5:E:164:LEU:C	2.51	0.48
1:A:22:PHE:CD1	2:B:1213:THR:HG22	2.49	0.48
2:B:658:ILE:HG22	2:B:659:ALA:N	2.28	0.48
3:C:8:VAL:HG12	3:C:9:LYS:N	2.28	0.48
4:D:208:GLU:O	4:D:212:LYS:HG3	2.13	0.48
1:A:1272:THR:C	1:A:1273:LEU:HD12	2.34	0.48
1:A:228:PHE:CD2	1:A:228:PHE:N	2.81	0.48
1:A:863:VAL:HG12	1:A:864:ILE:H	1.77	0.48
1:A:817:ALA:O	1:A:818:MET:C	2.52	0.48
1:A:814:PHE:CD1	2:B:519:TRP:HE3	2.32	0.48
1:A:1029:ARG:HG3	1:A:1029:ARG:NH1	2.17	0.48
1:A:896:ARG:CD	1:A:897:TYR:HE1	2.12	0.48
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.41	0.48
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.96	0.48
11:K:65:HIS:CD2	11:K:66:PRO:N	2.81	0.48
1:A:1051:ALA:O	1:A:1054:LEU:N	2.47	0.48
2:B:583:ASN:OD1	2:B:628:THR:N	2.47	0.48
1:A:122:MET:O	1:A:123:ARG:C	2.51	0.48
8:H:83:GLN:O	8:H:85:GLY:N	2.44	0.48
1:A:873:MET:HG2	1:A:957:PRO:HG3	1.96	0.48
3:C:263:THR:O	3:C:265:MET:N	2.47	0.48
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.95	0.48
13:S:254:TYR:O	13:S:256:ALA:N	2.47	0.48
13:S:236:LEU:CA	13:S:242:LYS:NZ	2.77	0.48
2:B:764:SER:N	2:B:765:PRO:HD2	2.29	0.48
1:A:821:ARG:CB	1:A:821:ARG:HH11	2.25	0.48
1:A:42:ASP:OD1	1:A:45:GLN:HA	2.13	0.48
2:B:797:TYR:HB3	2:B:798:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.96	0.48
11:K:81:TYR:OH	11:K:86:ALA:HA	2.13	0.48
8:H:89:LEU:O	8:H:91:ASP:N	2.39	0.48
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.65	0.48
8:H:82:PRO:O	8:H:83:GLN:HB2	2.13	0.48
1:A:1057:VAL:CG1	1:A:1058:VAL:N	2.76	0.48
6:F:111:LEU:O	6:F:113:GLY:N	2.47	0.48
1:A:939:ASP:O	1:A:940:ARG:C	2.50	0.48
2:B:525:ALA:O	2:B:527:THR:HG22	2.13	0.48
3:C:168:ALA:C	3:C:170:TRP:N	2.67	0.48
2:B:371:GLU:H	2:B:371:GLU:CD	2.17	0.48
2:B:825:VAL:CG1	2:B:826:ALA:N	2.77	0.48
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.95	0.48
1:A:821:ARG:O	1:A:821:ARG:HG3	2.12	0.48
2:B:509:ALA:O	2:B:510:LYS:O	2.32	0.48
2:B:1149:GLU:C	2:B:1151:LEU:N	2.67	0.48
1:A:375:THR:HA	1:A:434:ARG:O	2.14	0.48
2:B:619:ILE:C	2:B:621:GLU:H	2.17	0.48
1:A:1059:HIS:O	1:A:1061:GLY:N	2.46	0.48
3:C:22:LEU:HD13	3:C:230:MET:CE	2.44	0.48
5:E:46:TYR:CD2	5:E:58:MET:HG2	2.48	0.48
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.29	0.48
4:D:196:PRO:C	4:D:198:LEU:N	2.67	0.48
2:B:458:LYS:O	2:B:459:TYR:C	2.50	0.48
1:A:437:MET:O	1:A:438:ASP:C	2.50	0.48
1:A:329:LEU:HD23	1:A:329:LEU:N	2.28	0.48
1:A:1313:LEU:O	1:A:1314:SER:C	2.52	0.48
1:A:590:ARG:HD3	1:A:604:GLY:CA	2.41	0.48
1:A:823:GLY:C	1:A:825:ILE:N	2.66	0.48
2:B:273:LEU:HD21	2:B:360:PHE:CD1	2.48	0.48
1:A:68:GLN:NE2	1:A:80:HIS:CD2	2.79	0.48
3:C:67:LEU:HD11	3:C:155:LEU:CD1	2.44	0.48
2:B:295:GLY:H	2:B:298:LEU:CD2	2.13	0.48
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.38	0.48
2:B:294:ASP:C	2:B:296:GLU:N	2.68	0.48
1:A:14:VAL:HG21	1:A:1430:LEU:HD13	1.96	0.48
2:B:681:TRP:O	2:B:683:SER:N	2.46	0.48
2:B:617:ARG:NE	2:B:619:ILE:HG12	2.29	0.48
12:L:39:SER:O	12:L:40:LEU:HG	2.14	0.48
11:K:21:ILE:HG23	11:K:31:VAL:CG1	2.44	0.48
1:A:1265:ASN:O	1:A:1267:MET:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:109:VAL:HG12	6:F:110:ASP:N	2.29	0.48
8:H:106:GLU:HG2	8:H:112:ILE:HG12	1.96	0.48
13:S:253:LEU:O	13:S:256:ALA:HB3	2.14	0.48
1:A:779:PHE:O	1:A:780:VAL:C	2.52	0.48
3:C:143:LEU:HD21	3:C:146:LYS:CE	2.43	0.48
10:J:7:CYS:HA	10:J:49:MET:HE3	1.95	0.48
2:B:1002:THR:HG22	2:B:1006:ILE:O	2.14	0.48
1:A:315:LEU:HD22	1:A:319:GLY:O	2.13	0.48
2:B:910:VAL:HG12	2:B:911:ILE:H	1.79	0.48
4:D:185:CYS:HB3	4:D:211:LEU:HD13	1.95	0.48
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.96	0.48
7:G:88:ASP:HB3	7:G:144:ARG:HB2	1.95	0.48
1:A:1293:SER:OG	1:A:1295:THR:CG2	2.62	0.48
2:B:465:ASN:HD22	2:B:465:ASN:N	2.12	0.48
10:J:57:ILE:CA	10:J:60:PHE:CD2	2.90	0.47
3:C:42:PRO:HA	3:C:163:ILE:CG2	2.44	0.47
1:A:356:ASP:HB2	1:A:469:ARG:HG2	1.96	0.47
2:B:806:THR:HG22	2:B:808:ALA:HB3	1.94	0.47
2:B:540:SER:HA	2:B:749:LEU:O	2.14	0.47
6:F:132:LEU:O	6:F:148:VAL:HG22	2.14	0.47
1:A:261:ASP:O	1:A:264:PHE:HB2	2.13	0.47
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.14	0.47
1:A:418:SER:O	1:A:421:ALA:N	2.46	0.47
5:E:44:ALA:O	5:E:45:LYS:HB2	2.13	0.47
1:A:393:ARG:O	1:A:395:GLY:N	2.47	0.47
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.96	0.47
1:A:1283:VAL:CG1	1:A:1284:MET:H	2.24	0.47
1:A:1116:LEU:HA	1:A:1329:THR:HA	1.96	0.47
1:A:928:LEU:O	1:A:931:GLU:N	2.47	0.47
3:C:242:GLN:CA	3:C:245:VAL:HG23	2.43	0.47
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.27	0.47
2:B:1159:ARG:CD	2:B:1193:GLN:HE21	2.26	0.47
2:B:1150:ARG:HE	2:B:1150:ARG:HA	1.79	0.47
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.96	0.47
2:B:689:LEU:O	2:B:690:VAL:HG23	2.14	0.47
2:B:942:ARG:O	2:B:944:THR:N	2.48	0.47
5:E:157:SER:C	5:E:159:ASP:N	2.68	0.47
2:B:486:TYR:CG	2:B:1096:ARG:NH2	2.82	0.47
2:B:810:GLU:HG3	2:B:815:ARG:HH22	1.79	0.47
9:I:2:THR:HG22	9:I:2:THR:O	2.14	0.47
3:C:79:GLN:O	3:C:127:ARG:NH1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:LEU:O	2:B:461:LEU:CD1	2.61	0.47
3:C:27:LEU:O	3:C:30:ALA:N	2.47	0.47
2:B:1017:ILE:HG22	2:B:1018:PRO:CD	2.44	0.47
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.95	0.47
2:B:510:LYS:HD3	2:B:510:LYS:O	2.13	0.47
3:C:191:TYR:CD2	3:C:201:TRP:CD1	2.97	0.47
2:B:992:ILE:HG21	2:B:994:TYR:HE1	1.79	0.47
1:A:1104:ILE:O	1:A:1105:LEU:C	2.53	0.47
1:A:993:LEU:HD11	1:A:997:LEU:HD21	1.96	0.47
2:B:168:GLY:N	2:B:450:ALA:HB1	2.14	0.47
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.36	0.47
7:G:1:MET:HE1	7:G:80:LYS:H	1.79	0.47
1:A:81:PHE:CE2	1:A:242:PRO:HA	2.48	0.47
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.50	0.47
1:A:419:LYS:HG3	1:A:420:ARG:N	2.28	0.47
1:A:1090:ALA:CB	1:A:1093:LYS:HE3	2.43	0.47
1:A:852:TYR:CD2	1:A:1060:PRO:CB	2.97	0.47
1:A:1006:ILE:HD11	5:E:163:GLU:CG	2.44	0.47
2:B:413:LEU:O	2:B:414:ALA:C	2.52	0.47
1:A:1263:ILE:O	1:A:1267:MET:HG3	2.15	0.47
1:A:789:LYS:HE3	9:I:67:THR:HB	1.97	0.47
1:A:944:ARG:NE	1:A:1298:TYR:HE1	2.12	0.47
8:H:128:ASN:CG	8:H:128:ASN:O	2.52	0.47
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.94	0.47
1:A:1335:ILE:O	1:A:1335:ILE:CG2	2.63	0.47
11:K:65:HIS:CD2	11:K:65:HIS:C	2.87	0.47
2:B:1033:LYS:HB2	2:B:1089:PRO:HD2	1.97	0.47
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.47
12:L:58:LYS:HG2	12:L:58:LYS:O	2.15	0.47
4:D:51:ASN:O	4:D:52:LEU:O	2.33	0.47
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.35	0.47
12:L:27:LEU:HD13	12:L:37:LYS:HE2	1.96	0.47
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.96	0.47
1:A:1157:ASP:C	1:A:1159:ARG:H	2.18	0.47
1:A:125:ALA:O	1:A:127:ALA:N	2.48	0.47
1:A:814:PHE:C	1:A:814:PHE:CD2	2.88	0.47
2:B:798:TYR:CD2	2:B:798:TYR:N	2.83	0.47
1:A:1051:ALA:C	1:A:1053:PHE:N	2.67	0.47
1:A:399:HIS:CB	1:A:400:PRO:CD	2.87	0.47
1:A:606:LEU:CB	1:A:614:PHE:CE2	2.97	0.47
1:A:962:ARG:O	1:A:964:ILE:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:314:LEU:O	2:B:315:LYS:C	2.53	0.47
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.44	0.47
2:B:1210:MET:O	2:B:1212:ILE:N	2.47	0.47
2:B:363:HIS:NE2	2:B:364:ILE:HG13	2.29	0.47
2:B:619:ILE:O	2:B:621:GLU:N	2.47	0.47
2:B:903:VAL:CG1	2:B:904:ARG:N	2.76	0.47
1:A:1057:VAL:CG1	1:A:1058:VAL:H	2.26	0.47
1:A:711:ARG:HA	9:I:97:MET:CE	2.44	0.47
1:A:1280:GLU:O	1:A:1281:ARG:C	2.52	0.47
1:A:535:THR:HG23	1:A:575:LYS:HG2	1.96	0.47
2:B:752:ALA:HB1	2:B:771:SER:HB3	1.96	0.47
1:A:1216:ILE:O	1:A:1219:THR:HB	2.14	0.47
3:C:227:THR:C	3:C:228:PHE:CD1	2.87	0.47
1:A:447:GLN:HB3	1:A:448:PRO:HA	1.97	0.47
1:A:1129:GLU:C	1:A:1131:ALA:N	2.67	0.47
1:A:1330:ASN:C	1:A:1330:ASN:OD1	2.52	0.47
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	1.96	0.47
1:A:794:PRO:C	1:A:796:SER:H	2.18	0.47
1:A:814:PHE:O	1:A:817:ALA:HB3	2.15	0.47
1:A:253:ASN:OD1	2:B:884:ARG:HD2	2.14	0.47
2:B:221:ASN:OD1	2:B:242:SER:HA	2.14	0.47
1:A:53:LEU:HD23	1:A:54:ASN:CB	2.45	0.47
1:A:897:TYR:HD2	1:A:936:LEU:CD1	2.28	0.47
2:B:298:LEU:CD2	2:B:298:LEU:H	2.27	0.47
1:A:1102:LYS:C	1:A:1106:ASN:HD22	2.18	0.47
1:A:1081:LEU:HD21	1:A:1098:VAL:CB	2.44	0.47
5:E:167:ARG:O	5:E:168:TYR:HD2	1.97	0.47
1:A:650:GLN:O	1:A:654:ASN:HB2	2.14	0.47
9:I:5:ARG:O	9:I:14:LEU:HD12	2.13	0.47
1:A:302:THR:HA	1:A:305:ASP:O	2.14	0.47
11:K:113:THR:O	11:K:114:LEU:CB	2.58	0.47
2:B:1191:ILE:C	2:B:1192:TYR:CD1	2.88	0.47
1:A:1388:GLY:O	1:A:1391:ARG:HG2	2.15	0.47
8:H:102:TYR:HD2	8:H:102:TYR:H	1.51	0.47
2:B:544:CYS:O	2:B:545:ILE:HG13	2.15	0.47
1:A:1227:ILE:O	1:A:1228:TRP:HB3	2.14	0.47
2:B:847:ASP:OD2	11:K:6:ARG:NH2	2.48	0.47
7:G:62:LEU:HB3	7:G:63:PRO:HD2	1.95	0.47
8:H:39:THR:HB	8:H:124:ARG:HB3	1.97	0.47
2:B:371:GLU:OE1	2:B:371:GLU:N	2.48	0.47
3:C:206:ASN:OD1	3:C:229:TYR:CD2	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:HIS:O	2:B:1137:CYS:SG	2.73	0.47
4:D:220:LEU:O	4:D:221:TYR:HD1	1.97	0.47
6:F:124:GLU:HB3	6:F:130:ILE:HG12	1.95	0.47
6:F:124:GLU:O	6:F:130:ILE:HG13	2.14	0.47
1:A:795:GLU:CD	1:A:795:GLU:N	2.59	0.47
1:A:254:GLU:H	2:B:935:ARG:HH12	1.63	0.47
2:B:831:SER:HB2	2:B:833:TYR:HD1	1.79	0.47
2:B:1155:SER:OG	2:B:1156:ASP:N	2.47	0.47
10:J:8:PHE:CE1	10:J:49:MET:SD	3.08	0.47
5:E:177:ARG:O	5:E:212:ARG:HD3	2.15	0.47
2:B:899:ILE:HG22	2:B:903:VAL:HG21	1.95	0.47
1:A:95:PHE:HD1	1:A:234:MET:CG	2.25	0.47
1:A:937:VAL:C	1:A:939:ASP:N	2.68	0.47
11:K:12:LEU:HD23	11:K:16:GLU:O	2.14	0.47
5:E:143:ASN:OD1	5:E:187:TYR:CE1	2.68	0.47
3:C:109:SER:O	3:C:110:THR:O	2.32	0.47
5:E:93:MET:C	5:E:95:THR:N	2.68	0.47
2:B:51:PHE:O	2:B:52:ASN:C	2.53	0.47
9:I:65:ASP:OD1	9:I:67:THR:OG1	2.21	0.47
6:F:128:LYS:HD3	6:F:149:GLU:O	2.15	0.47
1:A:1282:VAL:O	1:A:1283:VAL:HG22	2.14	0.47
2:B:781:PHE:CD1	2:B:781:PHE:C	2.88	0.47
1:A:254:GLU:O	2:B:935:ARG:NH1	2.45	0.47
2:B:839:MET:HE2	2:B:1010:LEU:HD21	1.95	0.47
1:A:759:ALA:O	1:A:761:MET:N	2.47	0.47
6:F:90:ARG:CG	6:F:91:ALA:N	2.78	0.47
6:F:77:ASP:O	6:F:79:ARG:N	2.47	0.47
2:B:850:LEU:HD12	2:B:851:PHE:N	2.30	0.47
5:E:124:VAL:CG1	5:E:132:ILE:HB	2.43	0.47
4:D:51:ASN:C	4:D:52:LEU:O	2.52	0.47
1:A:543:LEU:HD11	1:A:547:LEU:HD11	1.96	0.47
6:F:94:LEU:HD23	6:F:94:LEU:HA	1.64	0.47
1:A:7:SER:O	1:A:8:SER:C	2.54	0.47
6:F:103:MET:CE	7:G:65:ASP:HB2	2.44	0.47
2:B:834:ASN:HA	2:B:838:SER:O	2.15	0.47
2:B:1103:ILE:O	2:B:1122:ARG:NH1	2.48	0.47
10:J:14:VAL:O	10:J:16:ASP:N	2.48	0.47
10:J:18:TRP:HA	10:J:18:TRP:CE3	2.49	0.47
1:A:1398:MET:O	1:A:1401:SER:OG	2.22	0.47
1:A:335:ARG:NE	1:A:339:ASN:ND2	2.57	0.47
1:A:222:LEU:O	1:A:224:PHE:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:VAL:CG1	2:B:178:ASN:HD21	2.28	0.47
1:A:1402:PHE:CD1	1:A:1403:GLU:HG3	2.50	0.47
4:D:130:LEU:O	4:D:132:GLN:N	2.48	0.47
2:B:95:ILE:HG13	2:B:130:VAL:CG2	2.44	0.47
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.26	0.47
3:C:107:SER:C	3:C:109:SER:N	2.69	0.47
10:J:23:ASN:C	10:J:25:LEU:N	2.68	0.47
3:C:112:ASN:CB	3:C:114:TYR:CE1	2.98	0.47
4:D:189:ASP:O	4:D:193:THR:HB	2.14	0.47
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.50	0.47
11:K:78:THR:O	11:K:79:GLU:C	2.53	0.47
1:A:946:VAL:HG12	1:A:947:PHE:N	2.29	0.47
1:A:1162:VAL:HG12	1:A:1162:VAL:O	2.15	0.47
13:S:269:PHE:CZ	13:S:308:PHE:CE1	3.03	0.46
1:A:1283:VAL:CG1	1:A:1284:MET:N	2.78	0.46
1:A:928:LEU:O	1:A:929:LEU:C	2.53	0.46
1:A:936:LEU:H	1:A:936:LEU:HD23	1.78	0.46
1:A:830:LYS:HB2	1:A:1081:LEU:CD2	2.43	0.46
1:A:500:GLU:O	1:A:504:LEU:HB2	2.15	0.46
1:A:1342:GLU:CG	5:E:198:ILE:HG21	2.45	0.46
2:B:43:LEU:HD11	2:B:811:TYR:O	2.15	0.46
5:E:90:VAL:HG23	5:E:120:ALA:HA	1.97	0.46
1:A:626:ASN:O	1:A:631:HIS:CB	2.63	0.46
2:B:1204:PHE:CE1	2:B:1216:LEU:HD11	2.50	0.46
6:F:135:ARG:HD3	6:F:143:PHE:CD2	2.51	0.46
6:F:85:MET:HE1	6:F:148:VAL:CG1	2.45	0.46
5:E:7:ARG:CG	5:E:8:ASN:N	2.76	0.46
2:B:202:TYR:CE1	2:B:209:GLU:HG2	2.50	0.46
2:B:654:ARG:H	2:B:657:HIS:CD2	2.28	0.46
1:A:24:PRO:HG2	1:A:25:GLU:CD	2.35	0.46
1:A:809:THR:HG23	1:A:812:GLU:OE1	2.15	0.46
1:A:548:ASN:HA	11:K:60:ALA:HB1	1.97	0.46
2:B:285:ILE:O	2:B:288:ALA:HB3	2.15	0.46
1:A:1327:ILE:HG22	5:E:147:HIS:CE1	2.51	0.46
13:S:236:LEU:CA	13:S:242:LYS:CE	2.93	0.46
2:B:785:TYR:HA	2:B:788:ARG:HG3	1.97	0.46
1:A:863:VAL:O	1:A:864:ILE:CG1	2.63	0.46
1:A:808:LEU:N	1:A:808:LEU:CD1	2.78	0.46
2:B:1034:VAL:CG1	2:B:1035:ALA:N	2.78	0.46
1:A:894:GLU:C	1:A:896:ARG:H	2.18	0.46
1:A:80:HIS:O	1:A:243:PRO:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:99:LEU:C	9:I:100:PHE:HD1	2.18	0.46
9:I:83:ASN:HA	9:I:102:VAL:O	2.16	0.46
11:K:83:PRO:O	11:K:86:ALA:HB3	2.15	0.46
8:H:89:LEU:C	8:H:91:ASP:N	2.68	0.46
1:A:549:MET:O	1:A:550:LEU:C	2.53	0.46
1:A:647:GLY:O	1:A:650:GLN:HB2	2.14	0.46
1:A:370:ILE:HG23	2:B:1105:ALA:CB	2.41	0.46
1:A:535:THR:O	1:A:536:LEU:O	2.34	0.46
2:B:58:THR:O	2:B:62:ILE:HG13	2.14	0.46
1:A:881:GLN:NE2	1:A:958:VAL:O	2.42	0.46
1:A:696:GLU:HG2	1:A:696:GLU:O	2.15	0.46
13:S:269:PHE:CE2	13:S:297:CYS:CB	2.96	0.46
1:A:1311:VAL:HG11	1:A:1329:THR:HG21	1.96	0.46
2:B:834:ASN:O	2:B:838:SER:O	2.34	0.46
1:A:43:GLU:O	1:A:44:THR:HB	2.15	0.46
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.50	0.46
1:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.77	0.46
7:G:81:PRO:HA	7:G:85:GLU:OE1	2.15	0.46
3:C:95:CYS:O	3:C:96:SER:HB3	2.15	0.46
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.81	0.46
5:E:7:ARG:C	5:E:9:ILE:H	2.19	0.46
12:L:48:CYS:O	12:L:50:ASP:N	2.47	0.46
5:E:144:ILE:C	5:E:146:HIS:H	2.19	0.46
1:A:1220:PHE:CE2	1:A:1263:ILE:HG23	2.50	0.46
1:A:317:LYS:O	1:A:318:SER:HB3	2.14	0.46
1:A:344:ARG:HA	2:B:1129:ARG:HA	1.98	0.46
2:B:753:ALA:O	2:B:756:ILE:N	2.46	0.46
2:B:27:ALA:O	2:B:30:SER:OG	2.29	0.46
2:B:788:ARG:HE	2:B:788:ARG:HB3	1.52	0.46
1:A:618:GLU:O	1:A:621:THR:N	2.46	0.46
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.96	0.46
2:B:378:LEU:HD12	2:B:378:LEU:C	2.35	0.46
2:B:871:THR:HG22	2:B:872:GLU:N	2.31	0.46
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.46	0.46
2:B:281:PRO:O	2:B:283:VAL:N	2.48	0.46
2:B:293:PRO:O	2:B:294:ASP:O	2.33	0.46
7:G:1:MET:HE3	7:G:80:LYS:O	2.14	0.46
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.45	0.46
2:B:789:MET:CE	2:B:965:LYS:HB3	2.46	0.46
1:A:414:ASP:O	1:A:416:ARG:N	2.48	0.46
2:B:313:MET:HE2	2:B:390:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:29:LEU:N	4:D:29:LEU:HD23	2.30	0.46
2:B:1079:LYS:HE3	3:C:188:HIS:CE1	2.51	0.46
1:A:100:LYS:O	1:A:101:LYS:C	2.54	0.46
1:A:103:CYS:SG	1:A:108:MET:CE	3.04	0.46
11:K:63:VAL:O	11:K:63:VAL:HG23	2.15	0.46
10:J:61:LEU:O	10:J:63:TYR:N	2.48	0.46
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.18	0.46
1:A:1169:ILE:O	1:A:1170:ILE:C	2.54	0.46
6:F:87:LYS:HG3	6:F:88:TYR:CD1	2.51	0.46
9:I:99:LEU:HB2	9:I:101:PHE:CE1	2.50	0.46
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.80	0.46
5:E:197:LYS:O	5:E:199:ILE:HG13	2.16	0.46
1:A:567:LYS:HE3	8:H:46:LEU:HD12	1.97	0.46
1:A:563:PRO:HB2	1:A:565:ILE:O	2.16	0.46
1:A:645:LEU:O	1:A:646:PHE:C	2.54	0.46
1:A:647:GLY:O	1:A:648:ASN:C	2.54	0.46
12:L:30:ILE:O	12:L:56:LEU:HD23	2.15	0.46
2:B:760:ASP:O	2:B:761:HIS:CG	2.69	0.46
5:E:16:PHE:O	5:E:17:ARG:C	2.54	0.46
2:B:770:GLN:CD	2:B:983:ARG:HA	2.36	0.46
3:C:228:PHE:N	3:C:228:PHE:CD1	2.83	0.46
5:E:24:LYS:HG3	5:E:25:ASP:N	2.30	0.46
4:D:154:PHE:HB2	4:D:160:VAL:HG22	1.97	0.46
8:H:76:THR:HG22	8:H:76:THR:O	2.14	0.46
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.96	0.46
3:C:251:LEU:O	3:C:254:LYS:N	2.49	0.46
2:B:510:LYS:HD3	2:B:513:GLN:H	1.80	0.46
1:A:896:ARG:CD	1:A:897:TYR:CE1	2.93	0.46
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.45	0.46
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.45	0.46
2:B:863:GLU:O	2:B:961:LEU:HD22	2.15	0.46
2:B:281:PRO:HG2	2:B:284:ILE:CG1	2.44	0.46
1:A:867:ILE:CG2	1:A:872:GLY:H	2.29	0.46
5:E:22:MET:HE3	5:E:26:ARG:CZ	2.42	0.46
12:L:54:ARG:HG3	12:L:54:ARG:NH1	2.29	0.46
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.97	0.46
2:B:1023:VAL:HG12	2:B:1027:ILE:HG13	1.97	0.46
1:A:460:VAL:CG1	1:A:461:LYS:N	2.79	0.46
1:A:715:GLU:O	1:A:718:VAL:N	2.48	0.46
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.46
1:A:738:LYS:HZ1	3:C:194:GLU:C	2.18	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:31:THR:O	8:H:31:THR:HG22	2.15	0.46
1:A:907:THR:HG22	1:A:908:LEU:N	2.30	0.46
1:A:351:THR:HB	2:B:1103:ILE:CD1	2.43	0.46
2:B:994:TYR:HB2	2:B:999:MET:CE	2.46	0.46
1:A:399:HIS:O	1:A:400:PRO:C	2.54	0.46
8:H:143:LEU:O	8:H:144:ILE:HG13	2.16	0.46
1:A:550:LEU:HD11	1:A:561:PRO:HD2	1.98	0.46
9:I:11:ASN:O	9:I:12:ASN:ND2	2.48	0.46
6:F:132:LEU:HD22	7:G:61:ILE:HD11	1.97	0.46
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.51	0.46
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.80	0.46
9:I:69:PRO:O	9:I:84:VAL:HA	2.14	0.46
4:D:53:SER:HB3	4:D:153:ARG:H	1.81	0.46
7:G:27:LYS:O	7:G:31:LEU:HG	2.16	0.46
2:B:20:ASP:C	2:B:22:SER:H	2.19	0.46
1:A:1116:LEU:HB2	1:A:1329:THR:OG1	2.16	0.46
1:A:707:GLY:O	1:A:708:MET:O	2.34	0.46
2:B:189:LEU:O	2:B:192:LEU:HB2	2.15	0.46
2:B:882:THR:O	2:B:883:LEU:CB	2.63	0.46
2:B:992:ILE:HD13	2:B:994:TYR:HE1	1.81	0.46
1:A:76:GLU:O	1:A:76:GLU:CG	2.63	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.56	0.46
5:E:90:VAL:HB	5:E:119:SER:HB2	1.98	0.46
4:D:33:PHE:CZ	7:G:80:LYS:NZ	2.84	0.46
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.72	0.46
2:B:683:SER:O	2:B:687:GLU:HB2	2.16	0.46
1:A:285:PRO:CG	1:A:288:ALA:HB3	2.40	0.46
3:C:147:LEU:HD23	3:C:147:LEU:N	2.31	0.46
1:A:1083:THR:O	1:A:1084:PHE:O	2.34	0.46
3:C:114:TYR:CD1	3:C:114:TYR:N	2.83	0.46
2:B:558:LEU:C	2:B:560:GLU:N	2.70	0.46
1:A:100:LYS:O	1:A:103:CYS:N	2.49	0.46
1:A:983:ILE:HG22	1:A:983:ILE:O	2.15	0.46
7:G:18:PHE:HA	7:G:22:MET:CE	2.45	0.46
7:G:56:ILE:O	7:G:57:GLN:HB2	2.15	0.46
3:C:15:LYS:O	3:C:240:VAL:HG22	2.16	0.46
3:C:163:ILE:O	3:C:164:ALA:C	2.54	0.46
2:B:510:LYS:HD3	2:B:513:GLN:N	2.31	0.46
2:B:274:PRO:O	2:B:275:TYR:HB2	2.16	0.46
2:B:385:LEU:O	2:B:385:LEU:HD12	2.15	0.46
1:A:63:ARG:HA	1:A:74:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	2.19	0.46
2:B:613:VAL:HG22	2:B:628:THR:HA	1.98	0.46
5:E:153:HIS:C	5:E:154:ILE:HG13	2.34	0.46
1:A:646:PHE:O	1:A:647:GLY:C	2.55	0.46
9:I:34:TYR:C	9:I:34:TYR:CD2	2.90	0.46
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.79	0.46
1:A:385:ILE:HG22	1:A:386:ASP:N	2.29	0.46
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.46	0.46
8:H:98:TYR:HE1	8:H:139:ASN:HA	1.80	0.46
1:A:1129:GLU:HG3	1:A:1132:LYS:HE3	1.97	0.46
1:A:1119:TYR:CD2	1:A:1305:VAL:HG21	2.51	0.46
11:K:10:PHE:CD2	11:K:10:PHE:N	2.84	0.46
1:A:921:GLY:O	1:A:922:ASP:C	2.55	0.46
1:A:243:PRO:CB	1:A:244:PRO:HD2	2.46	0.46
1:A:566:ILE:O	1:A:567:LYS:O	2.34	0.46
7:G:80:LYS:HA	7:G:81:PRO:HD2	1.74	0.46
3:C:80:LEU:O	3:C:80:LEU:HG	2.16	0.46
1:A:642:CYS:O	1:A:643:ALA:C	2.54	0.46
2:B:546:SER:HA	2:B:612:GLU:CD	2.35	0.46
1:A:1227:ILE:CG2	1:A:1228:TRP:N	2.78	0.46
1:A:695:LYS:C	1:A:697:ALA:N	2.69	0.46
1:A:809:THR:HB	1:A:810:PRO:HD2	1.97	0.46
9:I:15:TYR:O	9:I:28:GLU:HG2	2.16	0.46
1:A:1067:LEU:O	1:A:1068:ALA:C	2.54	0.46
1:A:1330:ASN:OD1	1:A:1331:SER:N	2.49	0.45
1:A:18:GLN:CB	2:B:1215:ARG:HB2	2.45	0.45
2:B:1020:ARG:HH12	13:S:291:GLU:HA	1.81	0.45
1:A:1081:LEU:CD1	1:A:1099:PRO:HD3	2.46	0.45
1:A:1170:ILE:HG23	1:A:1174:PHE:HE1	1.77	0.45
1:A:1437:GLY:CA	6:F:88:TYR:CD2	2.97	0.45
2:B:1182:CYS:O	2:B:1183:LYS:C	2.53	0.45
1:A:871:ASP:CG	1:A:1366:ARG:HH22	2.19	0.45
3:C:94:LYS:HB2	3:C:94:LYS:HE3	1.67	0.45
4:D:48:ILE:CG2	7:G:4:ILE:HB	2.46	0.45
1:A:1191:TRP:HB3	1:A:1260:LEU:HD23	1.97	0.45
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.99	0.45
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.36	0.45
1:A:811:GLN:O	1:A:812:GLU:C	2.55	0.45
1:A:512:VAL:HG11	1:A:876:ALA:O	2.16	0.45
11:K:70:ARG:HG3	11:K:70:ARG:O	2.16	0.45
2:B:1111:MET:O	2:B:1112:GLN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:202:SER:HB3	5:E:205:SER:O	2.15	0.45
1:A:353:ILE:HG13	1:A:482:PHE:CD2	2.51	0.45
3:C:43:THR:HG22	3:C:44:LEU:H	1.81	0.45
3:C:46:ILE:HD13	3:C:157:CYS:CB	2.46	0.45
2:B:880:THR:HB	2:B:934:LYS:CD	2.36	0.45
2:B:838:SER:HA	2:B:989:THR:O	2.17	0.45
1:A:915:SER:O	1:A:919:ILE:HG13	2.16	0.45
2:B:386:LEU:O	2:B:388:CYS:N	2.50	0.45
8:H:91:ASP:C	8:H:93:TYR:N	2.70	0.45
1:A:321:PRO:O	1:A:322:VAL:CG2	2.63	0.45
2:B:906:SER:O	2:B:907:GLY:O	2.34	0.45
2:B:172:ILE:CG2	2:B:173:MET:N	2.79	0.45
2:B:313:MET:CE	2:B:390:LEU:HD21	2.46	0.45
5:E:25:ASP:C	5:E:27:GLY:H	2.17	0.45
1:A:33:ALA:O	1:A:83:HIS:HD2	1.99	0.45
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.29	0.45
2:B:551:PRO:HG2	2:B:552:MET:H	1.81	0.45
1:A:44:THR:HG22	1:A:44:THR:O	2.16	0.45
2:B:806:THR:HG22	2:B:808:ALA:CB	2.46	0.45
1:A:556:TRP:CE2	1:A:558:GLY:HA2	2.51	0.45
1:A:515:GLN:O	1:A:516:SER:CB	2.58	0.45
12:L:59:ALA:O	12:L:60:ARG:O	2.34	0.45
2:B:520:GLY:H	2:B:748:ILE:HG22	1.81	0.45
3:C:22:LEU:CD2	3:C:25:VAL:HG21	2.47	0.45
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.50	0.45
1:A:1213:GLY:O	1:A:1214:GLU:C	2.54	0.45
11:K:88:LYS:O	11:K:91:CYS:N	2.49	0.45
10:J:21:TYR:C	10:J:23:ASN:N	2.70	0.45
1:A:791:ASP:C	1:A:791:ASP:OD1	2.55	0.45
1:A:1329:THR:O	1:A:1331:SER:N	2.49	0.45
2:B:1026:LEU:HD23	2:B:1086:PHE:CE2	2.52	0.45
2:B:1169:MET:CE	2:B:1201:LYS:CA	2.89	0.45
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.16	0.45
2:B:284:ILE:HG12	2:B:324:ILE:HD12	1.98	0.45
2:B:1115:THR:HG22	2:B:1117:GLN:CG	2.46	0.45
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.99	0.45
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.97	0.45
2:B:1164:GLY:HA3	2:B:1190:ASP:OD2	2.16	0.45
2:B:170:LEU:HG	2:B:170:LEU:O	2.14	0.45
2:B:202:TYR:N	2:B:202:TYR:CD2	2.84	0.45
1:A:1210:GLY:O	1:A:1214:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:33:ILE:HB	11:K:35:PHE:HE1	1.81	0.45
1:A:1359:ASP:HB2	1:A:1361:SER:OG	2.16	0.45
1:A:1451:VAL:C	1:A:1453:TYR:H	2.19	0.45
1:A:362:ASP:N	1:A:362:ASP:OD2	2.48	0.45
1:A:1115:SER:OG	1:A:1116:LEU:N	2.49	0.45
7:G:126:ASN:HA	7:G:127:PRO:C	2.36	0.45
2:B:816:GLU:O	2:B:817:LEU:CD2	2.59	0.45
2:B:293:PRO:HG2	2:B:296:GLU:OE1	2.16	0.45
1:A:560:ILE:CG1	8:H:78:SER:HB2	2.36	0.45
2:B:615:MET:HA	2:B:625:LYS:O	2.16	0.45
6:F:143:PHE:C	6:F:143:PHE:CD1	2.90	0.45
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.98	0.45
12:L:52:GLY:O	12:L:53:HIS:C	2.54	0.45
1:A:937:VAL:HG12	1:A:938:LYS:N	2.30	0.45
1:A:1242:VAL:O	1:A:1243:VAL:HB	2.17	0.45
12:L:28:LYS:HG3	12:L:39:SER:OG	2.15	0.45
1:A:777:PHE:CE2	1:A:782:ARG:HA	2.51	0.45
1:A:298:PHE:HZ	1:A:314:ALA:HB2	1.80	0.45
1:A:19:PHE:O	1:A:1416:ALA:HA	2.17	0.45
2:B:255:GLN:O	2:B:271:ALA:HB1	2.17	0.45
3:C:158:VAL:O	3:C:158:VAL:HG12	2.17	0.45
1:A:1122:PRO:O	1:A:1123:GLY:C	2.54	0.45
3:C:46:ILE:HD13	3:C:157:CYS:HB3	1.99	0.45
1:A:834:THR:CG2	1:A:1077:THR:HA	2.46	0.45
1:A:42:ASP:CG	1:A:45:GLN:HA	2.37	0.45
1:A:1016:THR:O	1:A:1018:PHE:N	2.49	0.45
2:B:1181:GLU:OE1	2:B:1183:LYS:HG3	2.17	0.45
2:B:217:ARG:C	2:B:217:ARG:HD2	2.37	0.45
2:B:901:PRO:O	2:B:902:GLY:C	2.53	0.45
1:A:95:PHE:CD1	1:A:234:MET:CG	2.96	0.45
5:E:135:PHE:CB	5:E:140:LEU:HD11	2.47	0.45
1:A:1173:HIS:CG	1:A:1227:ILE:HG23	2.51	0.45
1:A:1151:GLU:HB3	1:A:1153:TYR:CE1	2.50	0.45
1:A:688:LYS:O	1:A:690:VAL:N	2.50	0.45
7:G:132:SER:HB3	7:G:135:ASP:HB2	1.97	0.45
9:I:88:SER:C	9:I:90:GLN:N	2.70	0.45
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.51	0.45
4:D:122:GLU:HA	4:D:125:SER:OG	2.17	0.45
1:A:1121:GLU:O	1:A:1122:PRO:O	2.35	0.45
1:A:1115:SER:O	1:A:1329:THR:HG23	2.17	0.45
1:A:760:GLN:O	1:A:804:TYR:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:975:GLN:HG2	2:B:976:ILE:H	1.82	0.45
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.98	0.45
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.80	0.45
5:E:171:LYS:O	5:E:172:GLU:C	2.55	0.45
2:B:280:ILE:HG23	2:B:281:PRO:HD2	1.99	0.45
5:E:117:THR:O	5:E:120:ALA:N	2.45	0.45
7:G:1:MET:HE3	7:G:80:LYS:H	1.81	0.45
7:G:82:PHE:O	7:G:84:GLY:N	2.50	0.45
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.82	0.45
2:B:578:THR:HG23	2:B:622:LYS:CA	2.47	0.45
1:A:849:MET:O	1:A:851:HIS:HD2	1.99	0.45
11:K:90:ALA:O	11:K:94:ILE:HG13	2.17	0.45
4:D:176:GLU:O	4:D:180:LEU:HB2	2.17	0.45
1:A:1293:SER:OG	1:A:1295:THR:HG23	2.17	0.45
13:S:273:LYS:C	13:S:275:LYS:H	2.18	0.45
1:A:1271:ILE:CG2	1:A:1271:ILE:O	2.65	0.45
1:A:1313:LEU:HD11	1:A:1327:ILE:HD13	1.99	0.45
1:A:353:ILE:HG23	1:A:485:ASP:O	2.16	0.45
3:C:44:LEU:HG	3:C:159:ALA:HB1	1.99	0.45
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.51	0.45
1:A:783:THR:O	1:A:784:LEU:HD23	2.16	0.45
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.17	0.45
1:A:52:GLY:O	1:A:56:PRO:HG2	2.17	0.45
1:A:30:ILE:HD11	2:B:1168:LEU:HD13	1.99	0.45
1:A:1011:GLN:NE2	1:A:1015:VAL:CG2	2.65	0.45
5:E:198:ILE:CD1	5:E:212:ARG:NH1	2.78	0.45
8:H:95:TYR:HE2	8:H:97:MET:CG	2.29	0.45
5:E:117:THR:HG22	5:E:119:SER:N	2.20	0.45
3:C:214:ASN:HB3	3:C:217:ASP:OD2	2.16	0.45
2:B:958:GLN:C	2:B:960:GLY:H	2.19	0.45
3:C:88:CYS:SG	3:C:91:HIS:N	2.90	0.45
1:A:668:ASP:HA	1:A:741:ASN:OD1	2.17	0.45
11:K:35:PHE:N	11:K:35:PHE:HD1	2.15	0.45
2:B:1178:ASN:O	2:B:1179:GLN:C	2.55	0.45
1:A:1143:LEU:HD12	1:A:1146:VAL:HG23	1.99	0.45
2:B:489:SER:OG	2:B:490:SER:N	2.49	0.45
13:S:260:THR:CA	13:S:260:THR:HB	2.20	0.45
1:A:244:PRO:CG	1:A:245:PRO:HD3	2.47	0.45
2:B:1006:ILE:HG13	2:B:1006:ILE:H	1.19	0.45
2:B:851:PHE:O	2:B:974:PRO:HD3	2.17	0.45
9:I:55:THR:HG22	9:I:56:ALA:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.17	0.45
8:H:23:VAL:HG22	8:H:43:ASN:HA	1.99	0.45
8:H:100:THR:HG22	8:H:101:ALA:H	1.79	0.45
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.52	0.45
1:A:324:SER:O	1:A:325:ILE:C	2.52	0.45
2:B:710:LEU:O	2:B:711:GLU:HG2	2.17	0.45
2:B:964:VAL:HG12	2:B:965:LYS:N	2.32	0.45
2:B:855:PHE:CD1	2:B:856:PHE:N	2.85	0.45
7:G:39:THR:C	7:G:41:LYS:N	2.70	0.45
1:A:925:LEU:C	1:A:927:VAL:H	2.20	0.45
1:A:1115:SER:HA	1:A:1308:THR:HG23	1.99	0.45
1:A:706:HIS:ND1	13:S:257:GLN:HB2	2.32	0.45
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.46	0.45
2:B:563:MET:HE3	2:B:580:VAL:HB	1.99	0.45
2:B:975:GLN:HG2	2:B:976:ILE:N	2.32	0.45
2:B:990:ILE:HG22	2:B:992:ILE:H	1.81	0.45
2:B:824:ILE:CD1	10:J:48:ARG:NH1	2.80	0.45
1:A:1081:LEU:CD2	1:A:1098:VAL:HG21	2.45	0.45
2:B:1183:LYS:CE	2:B:1183:LYS:H	2.27	0.45
1:A:866:PHE:HD2	5:E:168:TYR:CE1	2.33	0.45
2:B:800:GLN:HB2	2:B:821:GLN:HA	1.99	0.45
2:B:843:GLN:O	2:B:844:SER:C	2.56	0.45
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.52	0.45
8:H:95:TYR:CE2	8:H:97:MET:CG	3.00	0.45
1:A:563:PRO:HB3	1:A:571:LEU:O	2.17	0.45
2:B:745:PRO:O	2:B:748:ILE:CG1	2.61	0.45
2:B:758:PHE:O	2:B:760:ASP:N	2.49	0.45
4:D:51:ASN:OD1	4:D:52:LEU:O	2.34	0.45
1:A:1261:LYS:C	1:A:1264:GLU:H	2.20	0.45
3:C:170:TRP:O	3:C:171:GLY:C	2.54	0.45
9:I:15:TYR:CD1	9:I:15:TYR:N	2.85	0.45
1:A:789:LYS:HD2	9:I:67:THR:OG1	2.17	0.45
1:A:125:ALA:C	1:A:127:ALA:H	2.20	0.45
2:B:598:GLU:HG2	2:B:598:GLU:O	2.17	0.45
4:D:40:HIS:CE1	4:D:41:GLN:HE21	2.34	0.44
2:B:785:TYR:CE2	10:J:60:PHE:CE1	3.04	0.44
3:C:77:ILE:HG23	3:C:161:LYS:HE3	2.00	0.44
2:B:828:ALA:HB2	2:B:1085:ILE:HG21	2.00	0.44
2:B:977:GLY:CA	2:B:1099:VAL:HB	2.44	0.44
1:A:51:GLY:HA2	1:A:56:PRO:HA	1.99	0.44
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1101:LEU:HD12	1:A:1101:LEU:O	2.17	0.44
6:F:88:TYR:N	6:F:88:TYR:CD1	2.85	0.44
4:D:141:LEU:O	4:D:144:THR:HB	2.16	0.44
2:B:615:MET:C	2:B:616:ILE:HD12	2.36	0.44
2:B:1160:VAL:CG1	2:B:1161:HIS:H	2.30	0.44
3:C:52:GLU:HA	12:L:64:LEU:HD22	1.99	0.44
1:A:465:TYR:N	11:K:2:ASN:HB3	2.32	0.44
1:A:384:ASN:O	1:A:386:ASP:N	2.50	0.44
2:B:390:LEU:O	2:B:391:ASP:C	2.54	0.44
2:B:753:ALA:HA	2:B:756:ILE:HG13	1.99	0.44
1:A:673:GLY:O	1:A:676:MET:HB2	2.16	0.44
1:A:1132:LYS:CE	13:S:253:LEU:HD21	2.43	0.44
2:B:981:ALA:CB	2:B:987:LYS:HA	2.46	0.44
1:A:814:PHE:CD1	2:B:519:TRP:CE3	3.05	0.44
3:C:73:GLN:NE2	3:C:75:MET:N	2.54	0.44
1:A:78:PRO:O	1:A:78:PRO:HG2	2.17	0.44
1:A:1170:ILE:O	1:A:1174:PHE:HD1	2.00	0.44
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.47	0.44
1:A:1226:VAL:C	1:A:1227:ILE:HG13	2.37	0.44
1:A:576:GLN:O	1:A:579:SER:HB2	2.18	0.44
1:A:108:MET:O	1:A:109:HIS:HB2	2.16	0.44
2:B:186:GLU:O	2:B:187:SER:C	2.55	0.44
1:A:470:LEU:HD11	1:A:482:PHE:CE2	2.52	0.44
7:G:14:HIS:CG	7:G:15:PRO:HD2	2.53	0.44
2:B:555:ILE:HD11	2:B:587:HIS:NE2	2.32	0.44
10:J:3:VAL:CG2	10:J:18:TRP:CG	2.99	0.44
1:A:1161:THR:HG1	1:A:1170:ILE:HD11	1.82	0.44
1:A:1436:ILE:HD13	2:B:1139:ILE:CG2	2.45	0.44
2:B:542:MET:CG	2:B:747:MET:HB3	2.48	0.44
4:D:147:TYR:CE1	7:G:103:VAL:HG13	2.53	0.44
1:A:381:THR:O	1:A:384:ASN:N	2.45	0.44
2:B:1073:TYR:CE2	2:B:1080:LYS:HG2	2.53	0.44
13:S:283:GLN:HG2	13:S:295:THR:OG1	2.17	0.44
2:B:408:LEU:HA	2:B:408:LEU:HD12	1.76	0.44
2:B:373:ARG:HG3	2:B:566:LEU:HD23	2.00	0.44
1:A:573:SER:CB	8:H:119:GLY:O	2.65	0.44
2:B:372:SER:O	2:B:376:PHE:HD1	2.00	0.44
1:A:666:ILE:N	2:B:1026:LEU:HD22	2.32	0.44
2:B:1150:ARG:NE	2:B:1150:ARG:HA	2.33	0.44
1:A:1354:ASN:O	1:A:1355:VAL:C	2.54	0.44
2:B:604:ARG:O	2:B:606:LYS:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1437:GLY:O	1:A:1438:THR:C	2.56	0.44
2:B:287:ARG:NH1	2:B:324:ILE:O	2.50	0.44
2:B:806:THR:C	2:B:808:ALA:N	2.68	0.44
3:C:91:HIS:HB2	3:C:96:SER:OG	2.18	0.44
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.53	0.44
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.46	0.44
3:C:178:PHE:O	3:C:179:GLU:HB2	2.16	0.44
1:A:1209:MET:O	1:A:1210:GLY:C	2.55	0.44
13:S:269:PHE:HZ	13:S:308:PHE:CE1	2.35	0.44
7:G:101:VAL:HG12	7:G:102:GLN:N	2.32	0.44
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.99	0.44
10:J:1:MET:N	10:J:56:LEU:N	2.65	0.44
1:A:786:HIS:CE1	2:B:519:TRP:CZ2	3.05	0.44
1:A:1434:ALA:HA	1:A:1435:PRO:HD3	1.91	0.44
2:B:821:GLN:HE22	2:B:851:PHE:N	2.09	0.44
2:B:806:THR:O	2:B:808:ALA:N	2.51	0.44
2:B:1107:ALA:O	2:B:1108:ARG:O	2.36	0.44
3:C:80:LEU:HD11	3:C:95:CYS:CA	2.47	0.44
7:G:96:GLN:HA	7:G:121:PHE:CD2	2.52	0.44
1:A:12:ARG:NE	2:B:1192:TYR:HE2	2.15	0.44
2:B:642:ASP:C	2:B:644:GLU:H	2.19	0.44
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.44	0.44
2:B:394:ASP:OD2	9:I:91:ARG:HD2	2.17	0.44
1:A:967:ALA:N	1:A:1044:TRP:HZ3	2.16	0.44
2:B:233:PRO:HG2	2:B:234:ILE:CD1	2.47	0.44
2:B:371:GLU:N	2:B:371:GLU:CD	2.70	0.44
1:A:843:LYS:HD2	1:A:843:LYS:HA	1.89	0.44
2:B:882:THR:O	2:B:883:LEU:HB2	2.17	0.44
3:C:75:MET:HE2	3:C:239:PRO:HD3	1.99	0.44
1:A:834:THR:CG2	1:A:1077:THR:HG23	2.29	0.44
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.17	0.44
2:B:360:PHE:C	2:B:360:PHE:CD2	2.91	0.44
1:A:896:ARG:NH2	1:A:1030:ARG:NH2	2.66	0.44
2:B:999:MET:HE3	2:B:999:MET:HA	2.00	0.44
1:A:76:GLU:O	1:A:76:GLU:HG3	2.18	0.44
2:B:798:TYR:HD2	2:B:798:TYR:N	2.16	0.44
2:B:874:PHE:HA	2:B:913:GLY:O	2.17	0.44
1:A:1099:PRO:O	1:A:1102:LYS:HB3	2.17	0.44
2:B:324:ILE:CG2	2:B:325:GLN:N	2.81	0.44
2:B:1182:CYS:O	2:B:1183:LYS:O	2.36	0.44
4:D:47:LEU:CD1	4:D:48:ILE:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:50:GLU:HB3	3:C:156:THR:HB	1.98	0.44
1:A:384:ASN:CG	1:A:388:LEU:HD12	2.37	0.44
2:B:67:SER:O	2:B:68:THR:C	2.56	0.44
1:A:847:ASP:N	1:A:847:ASP:OD1	2.48	0.44
3:C:21:ILE:HG22	3:C:21:ILE:O	2.17	0.44
7:G:14:HIS:CD2	7:G:16:SER:H	2.34	0.44
3:C:44:LEU:HD23	3:C:72:LEU:CB	2.48	0.44
1:A:164:ARG:CG	1:A:165:GLY:H	2.01	0.44
2:B:293:PRO:O	2:B:296:GLU:HB3	2.18	0.44
1:A:1342:GLU:HG2	5:E:198:ILE:HD13	1.99	0.44
5:E:177:ARG:HD3	5:E:215:MET:HG3	1.99	0.44
1:A:475:THR:CG2	1:A:476:SER:N	2.81	0.44
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.53	0.44
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.52	0.44
2:B:230:ALA:N	2:B:231:PRO:CD	2.81	0.44
1:A:1343:ALA:HB2	5:E:150:VAL:HG22	1.98	0.44
8:H:38:LEU:HD12	8:H:39:THR:H	1.82	0.44
1:A:1313:LEU:HD12	1:A:1327:ILE:HD13	1.99	0.44
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.18	0.44
1:A:43:GLU:O	1:A:44:THR:CB	2.66	0.44
3:C:175:ALA:HB3	10:J:43:ARG:NH2	2.33	0.44
10:J:45:CYS:SG	10:J:46:CYS:N	2.91	0.44
1:A:525:GLN:O	1:A:526:ASP:C	2.56	0.44
5:E:117:THR:C	5:E:119:SER:H	2.21	0.44
7:G:1:MET:CE	7:G:80:LYS:O	2.66	0.44
12:L:47:ARG:NH2	12:L:54:ARG:HE	2.16	0.44
1:A:718:VAL:O	1:A:721:PHE:HB2	2.18	0.44
1:A:1206:ASP:HB2	1:A:1274:ARG:HH22	1.83	0.44
1:A:1210:GLY:O	1:A:1211:GLN:C	2.56	0.44
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.83	0.44
11:K:7:PHE:O	11:K:11:LEU:HB2	2.18	0.44
3:C:247:GLY:C	3:C:249:ASP:N	2.72	0.44
1:A:55:ASP:O	1:A:57:ARG:N	2.51	0.44
1:A:1104:ILE:C	1:A:1106:ASN:N	2.71	0.44
3:C:211:ASP:HA	3:C:212:PRO:HD3	1.84	0.44
3:C:80:LEU:HD11	3:C:96:SER:N	2.33	0.44
1:A:668:ASP:CG	1:A:742:ASN:HD22	2.19	0.44
4:D:146:GLN:O	4:D:150:ASN:N	2.51	0.44
2:B:952:VAL:CG1	2:B:953:LEU:N	2.79	0.44
12:L:40:LEU:HD22	12:L:44:ASP:CB	2.47	0.44
5:E:207:ARG:NH1	5:E:207:ARG:HB3	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:80:VAL:HG12	5:E:81:GLU:N	2.33	0.44
2:B:781:PHE:HD1	2:B:782:LEU:HG	1.83	0.43
1:A:814:PHE:CE1	2:B:519:TRP:HA	2.52	0.43
2:B:1085:ILE:CG2	2:B:1086:PHE:N	2.80	0.43
2:B:1084:GLN:OE1	3:C:191:TYR:HA	2.17	0.43
1:A:49:LYS:HZ1	1:A:60:SER:CA	2.31	0.43
9:I:71:SER:O	9:I:83:ASN:ND2	2.51	0.43
3:C:98:VAL:O	3:C:99:LEU:HD23	2.18	0.43
12:L:30:ILE:CD1	12:L:59:ALA:HB2	2.42	0.43
1:A:135:PHE:CE1	1:A:222:LEU:HD22	2.53	0.43
1:A:98:LYS:O	1:A:99:ILE:C	2.56	0.43
11:K:88:LYS:O	11:K:89:ASN:C	2.56	0.43
1:A:185:TRP:O	1:A:197:PRO:HA	2.18	0.43
8:H:38:LEU:HD12	8:H:124:ARG:O	2.18	0.43
1:A:1152:ILE:HG13	9:I:44:TYR:HD2	1.83	0.43
1:A:449:SER:O	2:B:1133:MET:HB3	2.18	0.43
5:E:138:ALA:HA	5:E:141:VAL:CG2	2.47	0.43
1:A:64:ASN:O	1:A:65:LEU:C	2.56	0.43
1:A:708:MET:HE3	1:A:1090:ALA:O	2.18	0.43
1:A:1329:THR:C	1:A:1331:SER:N	2.71	0.43
3:C:62:PHE:O	3:C:65:HIS:HB3	2.17	0.43
1:A:877:HIS:C	1:A:878:ILE:CG1	2.86	0.43
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.18	0.43
2:B:39:ARG:HG2	2:B:39:ARG:NH1	2.34	0.43
1:A:1406:VAL:HG12	1:A:1410:PHE:CD1	2.52	0.43
2:B:546:SER:HG	2:B:631:GLY:H	1.56	0.43
5:E:92:THR:HG22	5:E:92:THR:O	2.18	0.43
5:E:21:GLU:O	5:E:24:LYS:HG2	2.19	0.43
7:G:47:CYS:O	7:G:76:ALA:HB1	2.19	0.43
1:A:693:VAL:O	1:A:693:VAL:HG12	2.18	0.43
1:A:396:PRO:HB3	1:A:402:ALA:O	2.18	0.43
1:A:1116:LEU:HD12	1:A:1116:LEU:C	2.38	0.43
2:B:987:LYS:O	2:B:987:LYS:HG2	2.18	0.43
1:A:814:PHE:HE1	2:B:519:TRP:HA	1.83	0.43
3:C:169:LYS:NZ	12:L:69:ALA:CB	2.81	0.43
13:S:293:LEU:N	13:S:293:LEU:CD2	2.81	0.43
2:B:395:GLN:HG2	2:B:396:ASP:H	1.83	0.43
1:A:43:GLU:HB2	1:A:46:THR:HB	2.00	0.43
1:A:1239:ARG:HB3	1:A:1239:ARG:NH1	2.33	0.43
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.39	0.43
2:B:911:ILE:HG23	2:B:966:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:901:PRO:HB2	12:L:60:ARG:HA	2.00	0.43
2:B:789:MET:CE	2:B:965:LYS:O	2.65	0.43
1:A:218:ASP:HA	1:A:221:SER:HG	1.83	0.43
2:B:482:VAL:O	2:B:483:LEU:C	2.57	0.43
12:L:38:LEU:O	12:L:39:SER:CB	2.58	0.43
11:K:30:ALA:HA	11:K:75:ILE:O	2.18	0.43
11:K:32:VAL:HA	11:K:73:LEU:O	2.18	0.43
7:G:119:LEU:HD12	7:G:131:GLN:O	2.18	0.43
1:A:720:ARG:HD2	13:S:262:GLU:HB3	1.99	0.43
2:B:465:ASN:N	2:B:465:ASN:ND2	2.65	0.43
5:E:29:PHE:O	5:E:30:ILE:HG13	2.18	0.43
1:A:971:PHE:CE2	1:A:1040:GLN:HG2	2.53	0.43
1:A:353:ILE:HD13	1:A:487:MET:HG3	2.00	0.43
3:C:144:ILE:O	3:C:145:CYS:CB	2.66	0.43
10:J:7:CYS:SG	10:J:49:MET:CE	3.01	0.43
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.99	0.43
1:A:567:LYS:HD3	8:H:95:TYR:HA	1.99	0.43
7:G:1:MET:HE3	7:G:80:LYS:N	2.33	0.43
1:A:962:ARG:O	1:A:965:GLN:N	2.51	0.43
2:B:59:LEU:CD1	2:B:417:PHE:CE2	3.01	0.43
13:S:296:PHE:CD1	13:S:296:PHE:N	2.86	0.43
10:J:25:LEU:O	10:J:29:GLU:HA	2.18	0.43
2:B:214:ALA:HA	2:B:408:LEU:HD12	2.00	0.43
2:B:215:GLN:OE1	2:B:499:ASN:HB3	2.18	0.43
8:H:38:LEU:HD13	8:H:125:LEU:HD13	2.00	0.43
11:K:106:GLU:O	11:K:107:THR:C	2.56	0.43
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.99	0.43
1:A:1121:GLU:O	1:A:1122:PRO:C	2.57	0.43
1:A:706:HIS:C	1:A:708:MET:H	2.22	0.43
1:A:845:LEU:HD22	1:A:1374:VAL:HG21	2.00	0.43
3:C:44:LEU:HG	3:C:45:ALA:N	2.34	0.43
3:C:237:SER:O	3:C:238:ILE:HG13	2.18	0.43
3:C:242:GLN:HA	3:C:245:VAL:CG2	2.45	0.43
2:B:509:ALA:C	2:B:510:LYS:HD2	2.36	0.43
2:B:258:LEU:HG	2:B:258:LEU:O	2.18	0.43
2:B:976:ILE:HG22	2:B:977:GLY:N	2.34	0.43
1:A:42:ASP:HB3	1:A:45:GLN:N	2.33	0.43
1:A:58:LEU:O	1:A:59:GLY:O	2.36	0.43
4:D:56:ARG:CB	4:D:148:LEU:HD22	2.37	0.43
7:G:1:MET:SD	7:G:79:PHE:CD1	3.12	0.43
2:B:540:SER:HB3	2:B:747:MET:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:PHE:CB	1:A:571:LEU:HD23	2.39	0.43
2:B:591:ARG:O	2:B:592:ASN:C	2.57	0.43
2:B:634:TYR:CE1	2:B:692:TYR:CD1	3.06	0.43
1:A:1001:ARG:HH11	1:A:1001:ARG:HG2	1.83	0.43
2:B:1145:SER:O	2:B:1147:LEU:N	2.51	0.43
2:B:695:ALA:O	2:B:698:GLU:HB3	2.18	0.43
2:B:847:ASP:C	2:B:849:GLY:N	2.72	0.43
1:A:88:LYS:HA	1:A:89:PRO:HD2	1.72	0.43
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	2.00	0.43
1:A:108:MET:SD	1:A:210:ILE:HD13	2.59	0.43
2:B:787:VAL:HG12	2:B:787:VAL:O	2.19	0.43
1:A:735:VAL:HG12	1:A:735:VAL:O	2.18	0.43
2:B:780:VAL:HG21	10:J:56:LEU:HD11	1.99	0.43
2:B:777:ALA:HA	2:B:1095:LEU:CA	2.45	0.43
1:A:862:ASN:HA	5:E:174:GLN:O	2.19	0.43
3:C:242:GLN:HB3	3:C:246:ARG:HG3	1.99	0.43
2:B:508:LEU:O	2:B:509:ALA:C	2.51	0.43
1:A:1080:THR:HG22	1:A:1081:LEU:H	1.81	0.43
1:A:1101:LEU:HD11	1:A:1105:LEU:HD11	2.00	0.43
2:B:287:ARG:NH2	2:B:325:GLN:HE22	2.16	0.43
5:E:198:ILE:HD11	5:E:212:ARG:HH11	1.84	0.43
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.52	0.43
12:L:63:ARG:O	12:L:63:ARG:HG3	2.19	0.43
2:B:952:VAL:CG1	2:B:953:LEU:H	2.31	0.43
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	2.00	0.43
2:B:644:GLU:C	2:B:646:LEU:N	2.71	0.43
1:A:1192:LEU:CG	1:A:1193:LEU:N	2.81	0.43
2:B:390:LEU:O	2:B:392:ARG:N	2.51	0.43
1:A:703:THR:HB	1:A:705:LYS:HE2	2.01	0.43
1:A:353:ILE:HG13	1:A:482:PHE:HD2	1.83	0.43
2:B:1099:VAL:CG1	2:B:1100:ASP:H	2.24	0.43
2:B:597:MET:O	2:B:599:THR:N	2.52	0.43
1:A:525:GLN:CD	2:B:836:GLU:HG2	2.39	0.43
8:H:145:ARG:O	8:H:146:ARG:HB2	2.18	0.43
6:F:86:THR:O	6:F:89:GLU:HB2	2.18	0.43
1:A:115:LEU:O	1:A:122:MET:HE2	2.18	0.43
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.54	0.43
2:B:758:PHE:C	2:B:760:ASP:N	2.72	0.43
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.83	0.43
1:A:416:ARG:C	1:A:417:TYR:CD2	2.92	0.43
1:A:989:GLY:C	1:A:991:LYS:N	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:62:LYS:O	11:K:62:LYS:HG3	2.19	0.43
1:A:2:VAL:HG21	2:B:1158:PHE:N	2.34	0.43
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.19	0.43
1:A:1064:VAL:O	1:A:1065:GLY:C	2.55	0.43
2:B:114:PRO:O	2:B:115:GLN:C	2.57	0.43
2:B:376:PHE:HE2	2:B:569:TYR:HD2	1.65	0.43
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.49	0.43
1:A:49:LYS:NZ	1:A:60:SER:CA	2.81	0.43
2:B:872:GLU:CD	2:B:914:LYS:HE2	2.39	0.43
2:B:624:LEU:HA	2:B:624:LEU:HD12	1.79	0.43
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.84	0.43
3:C:97:VAL:HG12	3:C:98:VAL:H	1.84	0.43
1:A:231:PRO:C	1:A:233:TRP:N	2.72	0.43
2:B:545:ILE:C	2:B:634:TYR:HE2	2.22	0.43
1:A:426:LEU:O	1:A:427:GLN:HG2	2.19	0.43
2:B:1076:HIS:CD2	11:K:40:HIS:NE2	2.86	0.43
1:A:1208:THR:O	1:A:1211:GLN:N	2.52	0.43
2:B:486:TYR:CD1	2:B:1096:ARG:NH2	2.86	0.43
1:A:722:LEU:O	1:A:725:ALA:HB3	2.19	0.43
6:F:134:ILE:N	6:F:146:TRP:O	2.50	0.43
2:B:20:ASP:O	2:B:22:SER:N	2.48	0.43
1:A:157:ASP:C	1:A:159:THR:H	2.22	0.43
1:A:1230:GLU:C	1:A:1232:ASN:N	2.71	0.43
10:J:54:VAL:HG12	10:J:56:LEU:HD23	2.00	0.43
1:A:1450:LEU:HD11	6:F:108:PHE:CZ	2.54	0.43
1:A:253:ASN:HB2	2:B:935:ARG:NH1	2.34	0.43
2:B:236:HIS:O	2:B:237:VAL:HG23	2.18	0.43
2:B:995:ARG:O	2:B:997:GLU:N	2.52	0.43
2:B:798:TYR:HE2	3:C:62:PHE:CE2	2.37	0.43
1:A:1051:ALA:O	1:A:1052:GLN:C	2.56	0.43
1:A:1373:ASP:HA	1:A:1376:THR:CG2	2.49	0.43
9:I:111:THR:CG2	9:I:112:SER:N	2.74	0.43
2:B:758:PHE:HB2	2:B:1024:ALA:HB1	2.00	0.43
1:A:858:ASN:O	1:A:860:LEU:N	2.52	0.43
2:B:485:ARG:HH11	2:B:485:ARG:HG3	1.83	0.43
2:B:526:GLU:HG2	2:B:538:ASN:HB2	2.01	0.43
1:A:582:ILE:O	1:A:583:PRO:O	2.36	0.43
1:A:496:GLU:OE1	7:G:63:PRO:O	2.37	0.43
1:A:955:PRO:HG2	1:A:955:PRO:O	2.18	0.43
1:A:841:LEU:HD13	1:A:1072:ILE:HB	2.00	0.43
1:A:1074:GLU:N	1:A:1075:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.49	0.43
1:A:919:ILE:O	1:A:920:LEU:C	2.57	0.43
3:C:59:ALA:O	3:C:62:PHE:CB	2.67	0.43
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.81	0.43
1:A:1348:LEU:HG	1:A:1372:VAL:HG23	2.01	0.43
1:A:751:SER:OG	2:B:1015:HIS:CE1	2.72	0.43
8:H:97:MET:SD	8:H:121:LEU:HD12	2.59	0.43
12:L:50:ASP:O	12:L:52:GLY:N	2.52	0.43
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.49	0.43
1:A:536:LEU:HG	1:A:536:LEU:H	1.51	0.43
2:B:63:ILE:O	2:B:67:SER:HB3	2.19	0.43
2:B:166:PHE:C	2:B:167:ILE:HG13	2.39	0.43
1:A:1021:LEU:O	1:A:1024:SER:HB3	2.19	0.43
2:B:936:ASP:CG	2:B:938:SER:H	2.23	0.43
4:D:26:THR:O	4:D:28:GLN:N	2.52	0.43
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.54	0.43
3:C:76:ASP:HB2	3:C:128:ASN:O	2.18	0.43
5:E:129:PRO:O	5:E:130:ALA:C	2.57	0.43
13:S:281:TYR:CD1	13:S:281:TYR:C	2.93	0.43
10:J:64:ASN:CB	10:J:65:PRO:CD	2.74	0.42
1:A:784:LEU:HD11	1:A:815:PHE:CE2	2.54	0.42
3:C:241:ASP:O	3:C:244:VAL:HB	2.19	0.42
2:B:1159:ARG:CD	2:B:1193:GLN:HG3	2.31	0.42
1:A:343:LYS:HE2	2:B:1156:ASP:HB2	2.01	0.42
1:A:1169:ILE:HD11	1:A:1229:SER:HB3	2.01	0.42
2:B:324:ILE:HG22	2:B:325:GLN:N	2.34	0.42
5:E:154:ILE:HG22	5:E:155:ARG:O	2.19	0.42
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.39	0.42
1:A:1444:MET:HG2	7:G:59:GLY:O	2.19	0.42
1:A:261:ASP:O	1:A:264:PHE:N	2.51	0.42
1:A:366:VAL:O	1:A:463:ILE:HG12	2.19	0.42
1:A:715:GLU:C	1:A:717:ASN:N	2.71	0.42
1:A:996:ASN:C	1:A:998:LEU:H	2.22	0.42
11:K:35:PHE:HD1	11:K:35:PHE:H	1.67	0.42
1:A:1446:ASP:HB3	1:A:1449:SER:HG	1.84	0.42
2:B:1017:ILE:HG22	2:B:1018:PRO:HD3	2.01	0.42
1:A:727:ASP:O	1:A:731:ARG:HG3	2.18	0.42
8:H:27:GLU:HG2	8:H:39:THR:HG23	2.00	0.42
1:A:1384:VAL:O	1:A:1384:VAL:HG12	2.19	0.42
1:A:1129:GLU:O	1:A:1131:ALA:N	2.52	0.42
1:A:1282:VAL:C	1:A:1283:VAL:CG2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:LYS:C	1:A:707:GLY:H	2.23	0.42
5:E:205:SER:O	5:E:206:GLY:C	2.56	0.42
6:F:100:GLN:HG2	7:G:66:GLY:HA3	2.01	0.42
2:B:1085:ILE:HD12	2:B:1085:ILE:N	2.34	0.42
3:C:63:ILE:O	3:C:67:LEU:HG	2.19	0.42
2:B:597:MET:C	2:B:599:THR:H	2.22	0.42
2:B:292:ILE:N	2:B:293:PRO:HD2	2.34	0.42
9:I:111:THR:HG21	9:I:113:ASP:HB2	2.00	0.42
1:A:600:PRO:HA	8:H:25:ARG:NH2	2.34	0.42
1:A:304:MET:O	1:A:326:ARG:HB3	2.19	0.42
5:E:182:ASP:O	5:E:185:ALA:HB3	2.19	0.42
2:B:1073:TYR:N	2:B:1073:TYR:CD1	2.87	0.42
2:B:1076:HIS:ND1	2:B:1076:HIS:N	2.66	0.42
3:C:197:SER:O	3:C:198:ALA:C	2.58	0.42
1:A:533:LYS:HE3	1:A:745:GLN:NE2	2.34	0.42
1:A:8:SER:O	1:A:9:ALA:C	2.57	0.42
2:B:176:SER:O	2:B:182:SER:HB3	2.19	0.42
13:S:254:TYR:C	13:S:256:ALA:N	2.73	0.42
1:A:483:ASP:HB2	2:B:987:LYS:CG	2.48	0.42
1:A:783:THR:HG21	1:A:815:PHE:CE2	2.53	0.42
1:A:47:ARG:CZ	1:A:255:SER:H	2.31	0.42
2:B:549:THR:CG2	2:B:550:ASP:H	2.17	0.42
1:A:526:ASP:HB3	1:A:657:LEU:HD23	2.01	0.42
1:A:472:LEU:O	1:A:475:THR:HG22	2.19	0.42
8:H:58:THR:HG22	8:H:59:ILE:N	2.35	0.42
1:A:527:THR:O	1:A:653:VAL:HG11	2.19	0.42
1:A:515:GLN:HB3	1:A:1071:SER:OG	2.20	0.42
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.99	0.42
1:A:107:CYS:HB2	1:A:171:GLN:HG2	2.01	0.42
2:B:222:ILE:O	2:B:240:ILE:HA	2.19	0.42
2:B:1003:ALA:HA	3:C:178:PHE:O	2.19	0.42
2:B:431:TYR:CD2	2:B:447:ALA:HB2	2.54	0.42
1:A:1272:THR:HG22	1:A:1273:LEU:N	2.34	0.42
5:E:147:HIS:HD2	5:E:149:LEU:H	1.67	0.42
1:A:928:LEU:C	1:A:930:ASP:N	2.70	0.42
2:B:702:LEU:C	2:B:703:ILE:HG13	2.39	0.42
2:B:295:GLY:HA2	2:B:298:LEU:HB2	2.01	0.42
10:J:52:THR:O	10:J:53:HIS:C	2.57	0.42
1:A:608:ILE:O	1:A:609:ASP:C	2.58	0.42
2:B:949:VAL:HG12	2:B:950:ASP:N	2.34	0.42
1:A:370:ILE:O	1:A:371:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:32:ALA:CB	12:L:55:ILE:HD12	2.48	0.42
2:B:546:SER:HG	2:B:630:ALA:CA	2.33	0.42
5:E:25:ASP:O	5:E:27:GLY:N	2.52	0.42
1:A:1067:LEU:O	1:A:1067:LEU:HD12	2.20	0.42
4:D:63:LEU:HD13	4:D:133:THR:OG1	2.19	0.42
6:F:103:MET:CE	7:G:66:GLY:H	2.32	0.42
3:C:236:GLY:C	3:C:238:ILE:N	2.73	0.42
3:C:245:VAL:C	3:C:247:GLY:N	2.73	0.42
2:B:235:SER:OG	2:B:236:HIS:CD2	2.72	0.42
1:A:40:THR:CG2	1:A:259:GLU:OE2	2.65	0.42
1:A:52:GLY:N	1:A:56:PRO:HG3	2.35	0.42
10:J:6:ARG:HB3	10:J:11:GLY:O	2.20	0.42
2:B:603:LEU:HD13	2:B:608:ASP:HB2	2.00	0.42
9:I:73:ARG:HH12	9:I:112:SER:HB2	1.83	0.42
2:B:615:MET:HA	2:B:626:ILE:HA	2.01	0.42
2:B:744:HIS:HD2	2:B:746:SER:CB	2.32	0.42
1:A:1213:GLY:O	1:A:1215:ARG:N	2.53	0.42
1:A:1453:TYR:CE2	6:F:129:LYS:HA	2.54	0.42
2:B:259:TYR:N	2:B:259:TYR:CD1	2.88	0.42
11:K:105:PHE:O	11:K:106:GLU:C	2.57	0.42
1:A:1007:ILE:C	1:A:1009:ASN:N	2.71	0.42
3:C:258:ILE:N	3:C:258:ILE:HD12	2.35	0.42
1:A:929:LEU:HD13	1:A:929:LEU:O	2.19	0.42
6:F:97:ARG:O	6:F:98:ALA:C	2.57	0.42
1:A:252:PHE:HB2	1:A:256:GLN:HB3	2.01	0.42
2:B:1162:ILE:HG22	2:B:1163:CYS:O	2.19	0.42
1:A:1081:LEU:HA	1:A:1081:LEU:HD13	1.84	0.42
1:A:1164:PRO:O	1:A:1167:GLU:HG3	2.19	0.42
2:B:283:VAL:O	2:B:284:ILE:C	2.57	0.42
2:B:843:GLN:HA	2:B:846:ILE:HG13	2.02	0.42
3:C:86:CYS:C	3:C:88:CYS:N	2.72	0.42
1:A:231:PRO:O	1:A:233:TRP:N	2.52	0.42
9:I:26:LEU:CD2	9:I:37:GLU:HA	2.41	0.42
1:A:873:MET:C	1:A:1058:VAL:HG23	2.40	0.42
7:G:30:LEU:HD13	7:G:72:VAL:HG11	2.01	0.42
2:B:533:CYS:C	2:B:535:LEU:N	2.72	0.42
1:A:695:LYS:O	1:A:697:ALA:N	2.53	0.42
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.18	0.42
1:A:1134:ILE:O	1:A:1137:ALA:N	2.48	0.42
5:E:147:HIS:O	5:E:148:GLU:C	2.57	0.42
1:A:1017:LEU:HD23	5:E:204:THR:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:ASP:HA	1:A:926:GLN:HE22	1.84	0.42
2:B:1065:GLN:HG3	2:B:1067:ARG:H	1.83	0.42
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.54	0.42
1:A:526:ASP:OD2	2:B:829:CYS:HB3	2.20	0.42
7:G:106:MET:HG2	7:G:107:LYS:N	2.34	0.42
2:B:582:VAL:HG23	2:B:626:ILE:CB	2.39	0.42
1:A:962:ARG:O	1:A:963:ILE:C	2.58	0.42
2:B:680:THR:HB	2:B:681:TRP:H	1.58	0.42
1:A:325:ILE:O	1:A:328:ARG:HB2	2.20	0.42
4:D:146:GLN:O	4:D:147:TYR:C	2.58	0.42
5:E:135:PHE:CD1	5:E:135:PHE:N	2.88	0.42
7:G:145:VAL:HG12	7:G:146:LYS:H	1.82	0.42
2:B:1031:LEU:HD13	2:B:1055:ILE:HD11	2.00	0.42
2:B:634:TYR:HE1	2:B:692:TYR:CD1	2.38	0.42
5:E:185:ALA:O	5:E:190:LEU:HG	2.18	0.42
5:E:162:ARG:CG	5:E:162:ARG:HH11	2.32	0.42
1:A:532:ARG:HD3	1:A:749:ALA:HB2	2.00	0.42
1:A:282:ASN:O	1:A:284:ALA:N	2.53	0.42
1:A:605:MET:HB2	1:A:605:MET:HE2	1.78	0.42
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.52	0.42
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.84	0.42
1:A:1080:THR:C	1:A:1081:LEU:HD22	2.40	0.42
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.49	0.42
1:A:566:ILE:O	1:A:567:LYS:C	2.57	0.42
3:C:91:HIS:O	3:C:91:HIS:CD2	2.73	0.42
2:B:315:LYS:HE2	9:I:4:PHE:CD2	2.55	0.42
1:A:322:VAL:CG1	1:A:323:LYS:N	2.82	0.42
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.03	0.42
1:A:933:TYR:C	1:A:935:GLN:N	2.72	0.42
5:E:144:ILE:C	5:E:146:HIS:N	2.72	0.42
11:K:40:HIS:O	11:K:41:THR:C	2.58	0.42
3:C:183:TRP:O	3:C:184:ASN:C	2.58	0.42
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	2.02	0.42
2:B:730:ARG:O	2:B:731:VAL:O	2.38	0.42
6:F:138:LEU:O	6:F:140:ASP:N	2.52	0.42
1:A:893:PHE:CD2	1:A:893:PHE:C	2.92	0.42
7:G:21:ARG:HD3	7:G:21:ARG:HA	1.92	0.42
1:A:117:GLU:H	1:A:117:GLU:CD	2.23	0.42
1:A:1116:LEU:O	1:A:1308:THR:HG22	2.19	0.42
1:A:870:GLU:HG2	5:E:208:TYR:CE2	2.55	0.42
1:A:900:ASP:HA	1:A:926:GLN:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:ALA:CB	2:B:24:PRO:CD	2.95	0.42
1:A:886:ILE:HG13	1:A:943:LEU:HD13	2.00	0.42
2:B:628:THR:O	2:B:629:ASP:O	2.38	0.42
1:A:1348:LEU:HG	1:A:1372:VAL:CG2	2.50	0.42
1:A:598:LEU:CD2	8:H:25:ARG:NH1	2.83	0.42
8:H:95:TYR:HB3	8:H:144:ILE:HB	2.00	0.42
7:G:44:TYR:HE1	7:G:157:ILE:HB	1.83	0.42
12:L:54:ARG:HH11	12:L:54:ARG:HG3	1.85	0.42
1:A:92:HIS:HB3	1:A:95:PHE:HB2	2.02	0.42
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.54	0.42
2:B:644:GLU:O	2:B:646:LEU:N	2.53	0.42
2:B:642:ASP:HB3	2:B:649:LYS:CE	2.49	0.42
2:B:1090:THR:O	2:B:1091:TYR:C	2.57	0.42
11:K:58:PHE:CB	11:K:76:GLN:HE21	2.32	0.42
3:C:181:ASP:N	3:C:182:PRO:CD	2.83	0.42
1:A:542:GLU:HG2	1:A:542:GLU:H	1.66	0.42
1:A:1131:ALA:O	1:A:1132:LYS:C	2.58	0.42
1:A:483:ASP:OD2	1:A:485:ASP:OD1	2.38	0.42
1:A:254:GLU:N	2:B:935:ARG:HH22	2.17	0.42
1:A:825:ILE:O	1:A:827:THR:N	2.52	0.42
1:A:70:CYS:O	1:A:71:GLN:C	2.58	0.42
5:E:197:LYS:O	5:E:197:LYS:CG	2.64	0.42
2:B:835:GLN:HE21	2:B:835:GLN:HB2	1.57	0.42
4:D:33:PHE:CE1	7:G:80:LYS:CE	3.02	0.42
2:B:1115:THR:CG2	2:B:1117:GLN:HB2	2.50	0.42
2:B:591:ARG:O	2:B:593:PRO:HD3	2.19	0.42
1:A:518:LYS:HE2	1:A:624:SER:O	2.20	0.42
12:L:53:HIS:O	12:L:55:ILE:HG12	2.20	0.42
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.37	0.42
1:A:1215:ARG:HA	1:A:1215:ARG:HD2	1.87	0.42
1:A:419:LYS:HG3	1:A:420:ARG:H	1.84	0.42
7:G:27:LYS:HE2	7:G:54:ILE:HB	2.02	0.42
1:A:216:VAL:O	1:A:219:PHE:HB2	2.20	0.42
1:A:552:TRP:O	1:A:554:PRO:HD3	2.20	0.42
12:L:66:GLN:C	12:L:67:PHE:CD1	2.94	0.42
1:A:716:ASP:O	1:A:716:ASP:OD1	2.37	0.42
2:B:939:THR:HA	2:B:940:PRO:HD2	1.92	0.42
1:A:1125:ALA:C	1:A:1127:ASP:N	2.72	0.41
1:A:1282:VAL:HG22	1:A:1308:THR:HA	2.01	0.41
2:B:785:TYR:HE2	10:J:60:PHE:CZ	2.38	0.41
3:C:249:ASP:O	3:C:252:GLN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:MET:O	3:C:246:ARG:NH2	2.31	0.41
2:B:1098:MET:O	2:B:1099:VAL:C	2.59	0.41
2:B:31:TRP:HA	2:B:31:TRP:CE3	2.55	0.41
2:B:616:ILE:CD1	2:B:616:ILE:N	2.81	0.41
2:B:419:THR:HG21	2:B:468:GLU:OE2	2.20	0.41
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.20	0.41
6:F:86:THR:O	6:F:89:GLU:N	2.51	0.41
1:A:324:SER:O	1:A:327:ALA:HB3	2.19	0.41
2:B:593:PRO:O	2:B:594:ALA:C	2.59	0.41
12:L:62:LYS:O	12:L:63:ARG:C	2.58	0.41
1:A:114:LEU:O	1:A:115:LEU:HG	2.20	0.41
1:A:874:ASP:HA	1:A:1058:VAL:HG23	2.01	0.41
2:B:172:ILE:HG22	2:B:173:MET:N	2.35	0.41
2:B:57:TYR:HD1	2:B:57:TYR:H	1.67	0.41
1:A:675:THR:O	1:A:675:THR:HG22	2.19	0.41
2:B:487:THR:CG2	2:B:488:TYR:N	2.82	0.41
1:A:1143:LEU:HD23	1:A:1267:MET:O	2.19	0.41
2:B:373:ARG:CG	2:B:566:LEU:HD23	2.50	0.41
1:A:726:ARG:O	1:A:729:ALA:N	2.53	0.41
2:B:492:LEU:O	2:B:495:LEU:N	2.42	0.41
1:A:1450:LEU:HD21	7:G:19:GLY:O	2.20	0.41
3:C:164:ALA:O	3:C:165:LYS:C	2.57	0.41
1:A:901:LEU:CG	1:A:926:GLN:HE21	2.28	0.41
2:B:510:LYS:HE2	2:B:513:GLN:OE1	2.21	0.41
2:B:1098:MET:O	2:B:1101:ASP:HB2	2.20	0.41
9:I:55:THR:HG22	9:I:56:ALA:H	1.84	0.41
2:B:806:THR:N	2:B:809:MET:HE3	2.35	0.41
1:A:567:LYS:CE	8:H:46:LEU:HB2	2.50	0.41
1:A:546:VAL:HG21	1:A:572:TRP:CD2	2.55	0.41
1:A:320:ARG:HH21	1:A:323:LYS:NZ	2.17	0.41
9:I:16:PRO:HA	9:I:26:LEU:O	2.21	0.41
2:B:544:CYS:O	2:B:545:ILE:CG1	2.68	0.41
3:C:18:VAL:O	3:C:20:PHE:CD2	2.73	0.41
1:A:209:ASN:O	1:A:210:ILE:C	2.58	0.41
1:A:408:ASP:C	1:A:410:GLY:H	2.23	0.41
2:B:866:TYR:O	2:B:868:MET:N	2.53	0.41
1:A:1092:LYS:HD2	1:A:1092:LYS:HA	1.82	0.41
2:B:174:LEU:HD11	2:B:204:ILE:CD1	2.49	0.41
2:B:1032:SER:O	2:B:1034:VAL:N	2.53	0.41
2:B:1102:LYS:C	2:B:1103:ILE:O	2.58	0.41
2:B:1201:LYS:HE2	2:B:1205:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:117:THR:C	5:E:119:SER:N	2.73	0.41
1:A:606:LEU:HB3	1:A:614:PHE:CD2	2.55	0.41
4:D:149:THR:O	4:D:149:THR:HG23	2.20	0.41
2:B:45:SER:O	2:B:46:GLN:C	2.58	0.41
5:E:16:PHE:CD1	5:E:58:MET:HE2	2.55	0.41
2:B:170:LEU:HA	2:B:171:PRO:HD2	1.87	0.41
11:K:12:LEU:HD11	11:K:18:LYS:HE2	2.02	0.41
4:D:195:ILE:O	4:D:198:LEU:HG	2.21	0.41
1:A:1397:LEU:HA	1:A:1400:CYS:HB2	1.99	0.41
2:B:849:GLY:O	2:B:852:ARG:HG3	2.20	0.41
3:C:8:VAL:CG1	3:C:9:LYS:N	2.83	0.41
4:D:217:LEU:O	4:D:219:THR:N	2.54	0.41
2:B:303:TYR:HD2	2:B:303:TYR:N	2.18	0.41
4:D:151:PHE:O	4:D:152:SER:O	2.38	0.41
2:B:233:PRO:HG2	2:B:234:ILE:HD12	2.02	0.41
1:A:7:SER:HB2	2:B:1175:LEU:CD2	2.49	0.41
13:S:269:PHE:CE2	13:S:306:TRP:CZ2	3.08	0.41
4:D:40:HIS:CG	4:D:41:GLN:N	2.89	0.41
7:G:7:LEU:O	7:G:73:LYS:HD2	2.20	0.41
1:A:784:LEU:C	1:A:786:HIS:H	2.23	0.41
2:B:700:SER:C	2:B:701:ILE:CG2	2.89	0.41
1:A:254:GLU:H	2:B:935:ARG:NH1	2.18	0.41
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.73	0.41
10:J:43:ARG:HG2	10:J:46:CYS:SG	2.61	0.41
9:I:101:PHE:O	9:I:102:VAL:CG2	2.67	0.41
2:B:34:ILE:O	2:B:35:SER:C	2.58	0.41
2:B:809:MET:O	2:B:811:TYR:N	2.54	0.41
1:A:550:LEU:HD22	1:A:556:TRP:CD1	2.55	0.41
3:C:80:LEU:HD12	3:C:95:CYS:HA	2.01	0.41
1:A:630:ILE:HG23	1:A:642:CYS:SG	2.60	0.41
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.50	0.41
2:B:515:HIS:CG	2:B:516:ASN:N	2.88	0.41
2:B:770:GLN:OE1	2:B:983:ARG:HA	2.20	0.41
5:E:143:ASN:ND2	5:E:146:HIS:ND1	2.68	0.41
2:B:1060:ARG:C	2:B:1062:HIS:H	2.22	0.41
3:C:255:VAL:HG21	11:K:94:ILE:HG21	2.03	0.41
11:K:85:ASP:O	11:K:89:ASN:ND2	2.54	0.41
1:A:1260:LEU:HG	1:A:1260:LEU:O	2.20	0.41
1:A:809:THR:O	1:A:810:PRO:C	2.58	0.41
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.56	0.41
2:B:121:ASN:HA	2:B:207:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.55	0.41
1:A:703:THR:O	1:A:704:ALA:C	2.59	0.41
1:A:618:GLU:O	1:A:619:LYS:C	2.59	0.41
2:B:702:LEU:HA	2:B:702:LEU:HD12	1.85	0.41
2:B:575:PRO:HG2	2:B:576:ASP:H	1.84	0.41
3:C:249:ASP:O	3:C:250:THR:C	2.58	0.41
2:B:282:ILE:HD13	2:B:382:ILE:HD13	2.01	0.41
1:A:44:THR:O	1:A:45:GLN:CB	2.65	0.41
2:B:995:ARG:O	2:B:996:ARG:C	2.59	0.41
6:F:75:PRO:C	6:F:77:ASP:N	2.74	0.41
1:A:1377:THR:O	1:A:1378:GLN:C	2.57	0.41
2:B:365:THR:CG2	2:B:367:LEU:HG	2.38	0.41
5:E:116:ILE:HG22	5:E:117:THR:N	2.35	0.41
3:C:215:GLU:O	3:C:216:GLY:C	2.59	0.41
2:B:956:THR:HG22	2:B:960:GLY:HA2	2.02	0.41
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.35	0.41
1:A:266:LEU:O	1:A:267:ALA:C	2.58	0.41
1:A:324:SER:O	1:A:327:ALA:N	2.53	0.41
2:B:952:VAL:O	2:B:953:LEU:HB3	2.20	0.41
1:A:889:SER:C	1:A:891:ALA:N	2.72	0.41
2:B:62:ILE:HG23	2:B:418:LYS:CG	2.49	0.41
5:E:33:GLU:C	5:E:35:VAL:N	2.72	0.41
6:F:150:GLU:O	6:F:151:LEU:C	2.59	0.41
1:A:1279:ILE:CD1	1:A:1316:VAL:HG21	2.48	0.41
2:B:700:SER:O	2:B:701:ILE:HG22	2.20	0.41
3:C:241:ASP:HB3	11:K:109:TRP:CH2	2.55	0.41
2:B:274:PRO:CG	2:B:359:GLU:HB3	2.51	0.41
2:B:830:TYR:HD1	2:B:830:TYR:HA	1.68	0.41
1:A:1362:TYR:CE1	1:A:1364:ASN:HA	2.56	0.41
11:K:55:LYS:O	11:K:77:THR:HG22	2.20	0.41
1:A:475:THR:O	1:A:479:ASN:N	2.53	0.41
1:A:598:LEU:O	1:A:599:SER:C	2.58	0.41
7:G:1:MET:SD	7:G:79:PHE:CE1	3.14	0.41
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.86	0.41
12:L:31:CYS:SG	12:L:34:CYS:N	2.93	0.41
8:H:83:GLN:C	8:H:85:GLY:N	2.74	0.41
1:A:361:LEU:HG	1:A:507:VAL:CG1	2.51	0.41
5:E:114:ASN:O	5:E:115:ASN:CB	2.68	0.41
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.35	0.41
1:A:445:ASN:ND2	1:A:455:MET:HE3	2.35	0.41
1:A:1397:LEU:H	1:A:1397:LEU:HG	1.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1260:LEU:CG	1:A:1260:LEU:O	2.68	0.41
1:A:151:ASP:OD1	1:A:163:SER:CB	2.68	0.41
6:F:138:LEU:O	6:F:139:PRO:C	2.59	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
1:A:368:LYS:O	1:A:369:SER:C	2.58	0.41
4:D:167:LEU:C	4:D:169:SER:H	2.24	0.41
5:E:165:LEU:O	5:E:166:LYS:C	2.58	0.41
1:A:960:ILE:O	1:A:960:ILE:HG22	2.20	0.41
1:A:1116:LEU:H	1:A:1308:THR:CG2	2.18	0.41
1:A:1120:LEU:N	1:A:1120:LEU:HD12	2.36	0.41
7:G:5:LYS:HG3	7:G:7:LEU:HD21	2.02	0.41
10:J:57:ILE:CG2	10:J:58:GLU:N	2.84	0.41
1:A:825:ILE:O	1:A:828:ALA:N	2.49	0.41
1:A:78:PRO:O	1:A:79:GLY:C	2.58	0.41
2:B:599:THR:O	2:B:603:LEU:HB2	2.20	0.41
2:B:604:ARG:C	2:B:606:LYS:H	2.24	0.41
1:A:1419:ASP:OD1	1:A:1426:GLU:OE1	2.39	0.41
1:A:839:ARG:O	1:A:842:VAL:HB	2.21	0.41
2:B:293:PRO:CG	2:B:296:GLU:OE1	2.68	0.41
1:A:1427:ASN:O	1:A:1430:LEU:N	2.43	0.41
9:I:86:PHE:HB2	9:I:87:GLN:H	1.67	0.41
1:A:443:LEU:HB2	1:A:501:LEU:HD21	2.03	0.41
1:A:541:ILE:CD1	1:A:577:ILE:HD11	2.51	0.41
4:D:50:LEU:HD11	7:G:4:ILE:CG1	2.51	0.41
1:A:231:PRO:C	1:A:233:TRP:H	2.23	0.41
5:E:211:TYR:HD1	5:E:211:TYR:N	2.19	0.41
3:C:8:VAL:HG12	3:C:10:ILE:H	1.86	0.41
4:D:59:ILE:O	4:D:60:LYS:C	2.58	0.41
3:C:229:TYR:CD1	3:C:229:TYR:N	2.89	0.41
5:E:66:GLU:HA	5:E:69:ILE:HD12	2.02	0.41
1:A:1187:GLN:HG3	1:A:1188:GLN:H	1.85	0.41
11:K:71:PHE:C	11:K:71:PHE:CD1	2.94	0.41
13:S:308:PHE:O	13:S:309:SER:CB	2.69	0.41
2:B:114:PRO:CG	2:B:115:GLN:H	2.25	0.41
2:B:360:PHE:CE2	2:B:361:LEU:HB2	2.55	0.41
2:B:386:LEU:C	2:B:388:CYS:N	2.73	0.41
2:B:824:ILE:HG22	2:B:1087:PHE:CE2	2.55	0.41
1:A:1018:PHE:O	1:A:1019:CYS:C	2.59	0.41
1:A:1167:GLU:O	1:A:1168:GLU:C	2.58	0.41
8:H:96:VAL:HA	8:H:142:LEU:O	2.21	0.41
8:H:3:ASN:HB3	8:H:4:THR:H	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:97:HIS:CD2	7:G:97:HIS:N	2.89	0.41
1:A:135:PHE:O	1:A:137:ALA:N	2.54	0.41
2:B:401:PHE:C	2:B:403:LYS:H	2.24	0.41
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.41
2:B:543:SER:C	2:B:544:CYS:SG	2.99	0.41
2:B:526:GLU:CD	2:B:752:ALA:CB	2.89	0.41
1:A:24:PRO:HG2	1:A:25:GLU:OE1	2.20	0.41
1:A:582:ILE:HA	1:A:583:PRO:HD2	1.84	0.41
1:A:7:SER:HB2	2:B:1175:LEU:HD22	2.02	0.41
9:I:45:ARG:HE	9:I:47:GLU:HG3	1.85	0.41
8:H:104:PHE:HZ	8:H:135:LEU:O	2.04	0.41
1:A:883:LEU:HA	1:A:883:LEU:HD23	1.87	0.41
1:A:1114:PRO:O	1:A:1115:SER:O	2.38	0.41
1:A:1308:THR:OG1	1:A:1309:ASP:N	2.53	0.41
1:A:18:GLN:OE1	1:A:18:GLN:C	2.59	0.41
7:G:18:PHE:HA	7:G:22:MET:HE3	2.03	0.41
2:B:102:VAL:O	2:B:109:THR:HG23	2.21	0.41
2:B:1064:TYR:O	2:B:1065:GLN:C	2.59	0.41
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.51	0.41
2:B:23:ALA:CB	2:B:24:PRO:HD2	2.31	0.41
1:A:1027:ALA:O	1:A:1030:ARG:N	2.54	0.41
1:A:49:LYS:HZ1	1:A:60:SER:C	2.23	0.41
1:A:73:GLY:O	1:A:74:MET:C	2.59	0.41
1:A:35:ILE:HD12	1:A:241:VAL:CG2	2.50	0.41
10:J:18:TRP:HA	10:J:18:TRP:HE3	1.85	0.41
3:C:61:GLU:HG2	3:C:62:PHE:N	2.36	0.41
2:B:1004:GLU:CB	2:B:1006:ILE:HD11	2.51	0.41
2:B:1142:GLY:O	2:B:1144:ALA:N	2.54	0.41
2:B:38:PHE:O	2:B:39:ARG:C	2.59	0.41
2:B:635:ARG:HH11	2:B:635:ARG:CG	2.33	0.41
1:A:562:THR:HA	1:A:563:PRO:HD3	1.84	0.41
1:A:556:TRP:CD2	1:A:558:GLY:HA2	2.55	0.41
4:D:34:GLN:O	4:D:47:LEU:HD23	2.21	0.41
4:D:47:LEU:CD1	7:G:3:PHE:HD2	2.33	0.41
12:L:60:ARG:CG	12:L:61:THR:H	2.29	0.41
1:A:218:ASP:HA	1:A:221:SER:OG	2.21	0.41
2:B:857:ARG:O	2:B:858:SER:HB3	2.21	0.41
1:A:996:ASN:CA	1:A:998:LEU:HD12	2.51	0.41
2:B:90:ILE:HD11	2:B:432:MET:SD	2.60	0.41
2:B:535:LEU:HA	2:B:535:LEU:HD23	1.87	0.41
1:A:544:ASP:CG	1:A:545:GLN:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.51	0.41
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.78	0.41
3:C:69:LEU:H	3:C:69:LEU:CD1	2.32	0.41
1:A:130:ASP:C	1:A:132:LYS:H	2.24	0.41
1:A:1451:VAL:O	1:A:1453:TYR:N	2.54	0.41
2:B:408:LEU:O	2:B:412:LEU:HG	2.21	0.41
3:C:26:ASP:O	3:C:27:LEU:C	2.58	0.41
1:A:420:ARG:O	1:A:424:ILE:HG13	2.21	0.41
7:G:62:LEU:HB3	7:G:63:PRO:CD	2.50	0.41
5:E:112:TYR:HE1	5:E:136:ASN:HD22	1.69	0.41
5:E:24:LYS:CG	5:E:25:ASP:N	2.84	0.41
1:A:393:ARG:C	1:A:395:GLY:N	2.75	0.41
1:A:103:CYS:SG	1:A:108:MET:HE3	2.61	0.41
7:G:39:THR:HB	7:G:42:PHE:H	1.86	0.41
1:A:971:PHE:N	1:A:971:PHE:CD1	2.88	0.41
2:B:1152:MET:O	2:B:1154:ALA:N	2.54	0.41
6:F:123:LYS:C	6:F:125:LEU:N	2.73	0.41
11:K:27:ALA:HB1	11:K:28:PRO:HD2	2.03	0.41
2:B:792:MET:O	2:B:793:ALA:HB2	2.20	0.41
1:A:704:ALA:O	1:A:705:LYS:CB	2.66	0.41
1:A:1072:ILE:O	1:A:1075:PRO:CG	2.66	0.41
1:A:922:ASP:OD1	1:A:922:ASP:C	2.60	0.41
11:K:65:HIS:NE2	11:K:67:PHE:CG	2.88	0.41
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.21	0.41
10:J:48:ARG:C	10:J:48:ARG:HD2	2.41	0.41
2:B:212:LEU:HD23	2:B:212:LEU:HA	1.73	0.41
1:A:90:VAL:HG12	1:A:91:PHE:O	2.20	0.41
1:A:937:VAL:O	1:A:938:LYS:C	2.58	0.41
2:B:483:LEU:HD12	2:B:484:ASN:N	2.35	0.41
5:E:59:SER:O	5:E:60:PHE:HB3	2.21	0.41
5:E:93:MET:O	5:E:94:LYS:C	2.59	0.41
1:A:1191:TRP:HA	1:A:1191:TRP:CE3	2.56	0.41
1:A:967:ALA:HA	1:A:1044:TRP:CZ3	2.56	0.41
3:C:27:LEU:HA	3:C:228:PHE:CE2	2.56	0.41
13:S:258:GLY:O	13:S:259:ALA:O	2.38	0.41
2:B:351:TYR:O	2:B:355:ILE:HG13	2.20	0.41
1:A:7:SER:CB	2:B:1175:LEU:HD22	2.51	0.41
1:A:1318:THR:HB	5:E:141:VAL:HG11	2.03	0.41
1:A:1142:THR:O	1:A:1145:SER:OG	2.27	0.41
1:A:113:LEU:HA	1:A:113:LEU:HD23	1.96	0.41
1:A:706:HIS:CD2	1:A:706:HIS:H	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:GLY:C	1:A:708:MET:HG3	2.41	0.40
1:A:848:ILE:O	1:A:1065:GLY:N	2.39	0.40
2:B:878:GLN:O	2:B:879:ARG:C	2.58	0.40
1:A:920:LEU:CD2	1:A:920:LEU:C	2.89	0.40
1:A:1161:THR:CG2	1:A:1163:ILE:HG13	2.51	0.40
1:A:1165:GLU:H	1:A:1165:GLU:HG3	1.58	0.40
1:A:599:SER:HA	1:A:600:PRO:HD2	1.86	0.40
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.47	0.40
5:E:124:VAL:HB	5:E:125:PRO:CD	2.50	0.40
2:B:1023:VAL:O	2:B:1027:ILE:N	2.50	0.40
3:C:22:LEU:HD13	3:C:230:MET:HE1	2.02	0.40
1:A:1147:THR:HG22	1:A:1148:ILE:N	2.36	0.40
1:A:935:GLN:C	1:A:937:VAL:N	2.71	0.40
2:B:222:ILE:O	2:B:240:ILE:HG13	2.21	0.40
1:A:1037:LEU:HD23	1:A:1037:LEU:N	2.36	0.40
2:B:121:ASN:HA	2:B:207:GLY:CA	2.51	0.40
2:B:329:THR:O	2:B:332:ASP:HB3	2.21	0.40
1:A:1327:ILE:HG22	5:E:147:HIS:HE1	1.85	0.40
7:G:22:MET:O	7:G:23:LYS:C	2.59	0.40
2:B:114:PRO:HG3	2:B:194:GLU:HG3	2.03	0.40
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.99	0.40
2:B:508:LEU:HB3	2:B:510:LYS:N	2.25	0.40
2:B:1198:TYR:O	2:B:1199:ALA:C	2.59	0.40
2:B:873:THR:CG2	2:B:874:PHE:N	2.84	0.40
6:F:88:TYR:HD1	6:F:88:TYR:H	1.67	0.40
5:E:153:HIS:HB3	5:E:196:VAL:HG13	1.99	0.40
1:A:1004:ASN:HD22	5:E:167:ARG:HD2	1.78	0.40
2:B:842:ASN:O	2:B:846:ILE:HG13	2.21	0.40
2:B:38:PHE:CE2	2:B:43:LEU:HD23	2.57	0.40
1:A:477:PRO:HG3	1:A:521:MET:HG2	2.03	0.40
8:H:47:PHE:CD2	8:H:95:TYR:HD1	2.39	0.40
2:B:687:GLU:O	2:B:688:GLY:C	2.59	0.40
3:C:80:LEU:CD1	3:C:95:CYS:CA	2.99	0.40
1:A:626:ASN:HB3	1:A:627:GLY:H	1.71	0.40
2:B:903:VAL:O	2:B:948:ILE:HG23	2.21	0.40
9:I:34:TYR:HE2	9:I:36:GLU:CB	2.32	0.40
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.86	0.40
5:E:144:ILE:H	5:E:144:ILE:HG12	1.68	0.40
2:B:247:GLY:N	2:B:418:LYS:HZ3	2.17	0.40
13:S:282:TYR:O	13:S:282:TYR:CG	2.73	0.40
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ASN:HB2	1:A:455:MET:HG2	2.03	0.40
7:G:132:SER:O	7:G:134:GLU:N	2.54	0.40
1:A:130:ASP:C	1:A:132:LYS:N	2.75	0.40
2:B:847:ASP:O	2:B:849:GLY:N	2.55	0.40
1:A:639:PRO:HG2	1:A:640:GLN:H	1.85	0.40
2:B:564:GLU:O	2:B:565:PRO:C	2.58	0.40
2:B:796:LEU:HA	2:B:796:LEU:HD12	1.82	0.40
1:A:942:PHE:C	1:A:942:PHE:CD2	2.94	0.40
7:G:5:LYS:CG	7:G:7:LEU:HD21	2.51	0.40
3:C:43:THR:CG2	3:C:44:LEU:H	2.34	0.40
6:F:82:THR:HA	6:F:83:PRO:HD3	1.82	0.40
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.84	0.40
11:K:101:LEU:O	11:K:102:LYS:C	2.58	0.40
2:B:1194:ILE:HD12	2:B:1196:ILE:CG2	2.52	0.40
2:B:996:ARG:HH22	3:C:175:ALA:CA	2.34	0.40
10:J:13:VAL:HG12	10:J:14:VAL:H	1.86	0.40
1:A:1019:CYS:O	1:A:1022:LEU:CB	2.68	0.40
1:A:1435:PRO:C	1:A:1436:ILE:HG13	2.40	0.40
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.51	0.40
1:A:515:GLN:HB2	1:A:1071:SER:HB3	2.02	0.40
10:J:47:ARG:HG2	10:J:47:ARG:HH11	1.85	0.40
2:B:515:HIS:HD2	2:B:517:THR:N	2.12	0.40
12:L:32:ALA:HB3	12:L:55:ILE:CG1	2.52	0.40
1:A:933:TYR:C	1:A:935:GLN:H	2.24	0.40
2:B:496:ARG:NH1	2:B:496:ARG:HB3	2.30	0.40
1:A:34:LYS:HD3	1:A:34:LYS:H	1.86	0.40
5:E:60:PHE:HE2	5:E:80:VAL:CB	2.35	0.40
1:A:532:ARG:NH2	1:A:745:GLN:HG2	2.36	0.40
4:D:29:LEU:O	4:D:30:GLY:O	2.39	0.40
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.50	0.40
7:G:154:VAL:HB	7:G:155:SER:H	1.71	0.40
2:B:213:ILE:HA	2:B:213:ILE:HD13	1.81	0.40
4:D:188:ALA:O	4:D:191:ALA:N	2.55	0.40
1:A:1129:GLU:O	1:A:1130:GLN:C	2.60	0.40
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.25	0.40
6:F:97:ARG:O	6:F:100:GLN:N	2.54	0.40
7:G:13:LEU:HD12	7:G:26:LEU:HD21	2.03	0.40
6:F:99:LEU:HD21	7:G:66:GLY:N	2.37	0.40
1:A:254:GLU:H	2:B:935:ARG:HH22	1.70	0.40
1:A:757:ASN:O	1:A:761:MET:HG3	2.20	0.40
2:B:763:GLN:OE1	13:S:292:PRO:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:HIS:HE1	2:B:389:ALA:HA	1.83	0.40
1:A:932:GLU:HG3	1:A:936:LEU:HD21	2.02	0.40
1:A:42:ASP:O	1:A:44:THR:N	2.38	0.40
2:B:1183:LYS:HA	2:B:1186:ASP:HA	2.04	0.40
2:B:1013:ASN:OD1	2:B:1014:PRO:HD2	2.21	0.40
4:D:50:LEU:HD11	7:G:4:ILE:HG13	2.03	0.40
4:D:52:LEU:O	4:D:54:GLU:N	2.46	0.40
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.52	0.40
2:B:216:GLU:HB2	2:B:406:LEU:CD2	2.51	0.40
10:J:21:TYR:HB2	10:J:39:LEU:HD13	2.02	0.40
1:A:493:GLN:HE21	1:A:493:GLN:CA	2.33	0.40
5:E:37:LEU:HA	5:E:38:PRO:HD2	1.94	0.40
2:B:661:LEU:C	2:B:663:ALA:N	2.75	0.40
1:A:803:SER:C	1:A:805:LEU:N	2.75	0.40
2:B:530:GLY:O	2:B:532:ALA:N	2.54	0.40
2:B:349:ILE:HG22	2:B:349:ILE:O	2.20	0.40
1:A:1116:LEU:HG	1:A:1116:LEU:O	2.22	0.40
1:A:1138:ILE:CG2	1:A:1316:VAL:HG13	2.52	0.40
6:F:103:MET:HE3	7:G:15:PRO:HG2	2.03	0.40
2:B:377:PHE:C	2:B:379:GLY:N	2.71	0.40
1:A:79:GLY:C	1:A:243:PRO:HG3	2.42	0.40
1:A:1347:ALA:O	1:A:1348:LEU:C	2.60	0.40
1:A:867:ILE:HG22	1:A:871:ASP:H	1.85	0.40
2:B:800:GLN:CB	10:J:52:THR:CG2	2.98	0.40
1:A:599:SER:HB2	1:A:603:ASN:H	1.87	0.40
1:A:501:LEU:HD11	2:B:1146:PHE:CE2	2.56	0.40
12:L:61:THR:HG22	12:L:63:ARG:N	2.37	0.40
2:B:516:ASN:H	2:B:516:ASN:HD22	1.70	0.40
2:B:1192:TYR:N	2:B:1192:TYR:CD1	2.89	0.40
1:A:461:LYS:O	1:A:463:ILE:HG23	2.22	0.40
2:B:240:ILE:O	2:B:240:ILE:CG2	2.68	0.40
2:B:533:CYS:SG	2:B:534:GLY:N	2.95	0.40
5:E:93:MET:O	5:E:96:PHE:N	2.55	0.40
11:K:20:LYS:HB2	11:K:20:LYS:HE3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1418/1733 (82%)	914 (64%)	316 (22%)	188 (13%)	0	6
2	B	1096/1224 (90%)	726 (66%)	223 (20%)	147 (13%)	0	6
3	C	264/318 (83%)	169 (64%)	62 (24%)	33 (12%)	0	8
4	D	173/221 (78%)	129 (75%)	27 (16%)	17 (10%)	1	14
5	E	212/215 (99%)	141 (66%)	50 (24%)	21 (10%)	1	13
6	F	82/155 (53%)	60 (73%)	15 (18%)	7 (8%)	1	17
7	G	169/171 (99%)	123 (73%)	34 (20%)	12 (7%)	1	23
8	H	129/146 (88%)	93 (72%)	26 (20%)	10 (8%)	1	20
9	I	117/122 (96%)	80 (68%)	22 (19%)	15 (13%)	0	7
10	J	63/70 (90%)	36 (57%)	14 (22%)	13 (21%)	0	2
11	K	112/120 (93%)	82 (73%)	25 (22%)	5 (4%)	3	34
12	L	44/70 (63%)	18 (41%)	14 (32%)	12 (27%)	0	0
13	S	68/179 (38%)	51 (75%)	10 (15%)	7 (10%)	1	12
All	All	3947/4744 (83%)	2622 (66%)	838 (21%)	487 (12%)	0	8

All (487) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	48	ALA
1	A	55	ASP
1	A	58	LEU
1	A	62	ASP
1	A	70	CYS
1	A	73	GLY
1	A	76	GLU
1	A	93	VAL
1	A	130	ASP

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Mol	Chain	Res	Type
1	A	286	HIS
1	A	311	GLN
1	A	322	VAL
1	A	385	ILE
1	A	399	HIS
1	A	423	ASP
1	A	516	SER
1	A	525	GLN
1	A	536	LEU
1	A	567	LYS
1	A	583	PRO
1	A	626	ASN
1	A	709	THR
1	A	780	VAL
1	A	821	ARG
1	A	920	LEU
1	A	1002	GLY
1	A	1036	ARG
1	A	1115	SER
1	A	1122	PRO
1	A	1124	HIS
1	A	1165	GLU
1	A	1167	GLU
1	A	1212	VAL
1	A	1223	ASP
1	A	1231	ASP
1	A	1242	VAL
1	A	1281	ARG
1	A	1308	THR
1	A	1309	ASP
1	A	1335	ILE
1	A	1341	ILE
1	A	1366	ARG
1	A	1377	THR
1	A	1378	GLN
1	A	1386	ARG
1	A	1392	SER
1	A	1396	ALA
1	A	1397	LEU
1	A	1403	GLU
1	A	1405	THR
1	A	1424	VAL

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Mol	Chain	Res	Type
2	B	43	LEU
2	B	45	SER
2	B	58	THR
2	B	67	SER
2	B	108	VAL
2	B	124	TYR
2	B	186	GLU
2	B	219	ALA
2	B	261	ARG
2	B	367	LEU
2	B	391	ASP
2	B	466	TRP
2	B	467	GLY
2	B	468	GLU
2	B	474	SER
2	B	510	LYS
2	B	530	GLY
2	B	531	GLN
2	B	571	PRO
2	B	591	ARG
2	B	620	ARG
2	B	629	ASP
2	B	636	PRO
2	B	643	ASP
2	B	648	HIS
2	B	709	ASP
2	B	727	LYS
2	B	731	VAL
2	B	751	VAL
2	B	752	ALA
2	B	818	PRO
2	B	901	PRO
2	B	943	SER
2	B	958	GLN
2	B	992	ILE
2	B	1046	PRO
2	B	1108	ARG
2	B	1157	ALA
2	B	1167	GLY
2	B	1171	VAL
2	B	1175	LEU
2	B	1181	GLU

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Mol	Chain	Res	Type
2	B	1188	LYS
2	B	1211	ASN
3	C	10	ILE
3	C	60	ASP
3	C	81	GLU
3	C	83	SER
3	C	87	PHE
3	C	110	THR
3	C	149	LYS
3	C	167	HIS
3	C	175	ALA
3	C	184	ASN
3	C	213	PRO
3	C	214	ASN
3	C	215	GLU
3	C	216	GLY
4	D	12	ARG
4	D	15	LEU
4	D	20	GLU
4	D	152	SER
5	E	130	ALA
5	E	158	SER
6	F	81	THR
7	G	118	ASP
8	H	81	PRO
8	H	84	ALA
8	H	140	ALA
9	I	9	ASP
9	I	11	ASN
9	I	84	VAL
10	J	6	ARG
10	J	15	GLY
10	J	53	HIS
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
13	S	275	LYS
13	S	292	PRO
1	A	42	ASP
1	A	44	THR

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Mol	Chain	Res	Type
1	A	45	GLN
1	A	54	ASN
1	A	57	ARG
1	A	61	ILE
1	A	74	MET
1	A	79	GLY
1	A	111	GLY
1	A	126	LEU
1	A	131	SER
1	A	154	SER
1	A	219	PHE
1	A	223	GLY
1	A	244	PRO
1	A	290	GLU
1	A	317	LYS
1	A	318	SER
1	A	331	GLY
1	A	332	LYS
1	A	335	ARG
1	A	400	PRO
1	A	415	LEU
1	A	418	SER
1	A	419	LYS
1	A	424	ILE
1	A	473	SER
1	A	557	ASP
1	A	594	GLY
1	A	598	LEU
1	A	619	LYS
1	A	708	MET
1	A	716	ASP
1	A	720	ARG
1	A	738	LYS
1	A	760	GLN
1	A	765	VAL
1	A	775	ILE
1	A	824	LEU
1	A	846	GLU
1	A	847	ASP
1	A	859	SER
1	A	864	ILE
1	A	875	ALA

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Mol	Chain	Res	Type
1	A	929	LEU
1	A	968	GLN
1	A	979	SER
1	A	1006	ILE
1	A	1016	THR
1	A	1052	GLN
1	A	1084	PHE
1	A	1089	VAL
1	A	1104	ILE
1	A	1105	LEU
1	A	1126	ALA
1	A	1128	GLN
1	A	1164	PRO
1	A	1168	GLU
1	A	1169	ILE
1	A	1170	ILE
1	A	1224	LEU
1	A	1314	SER
1	A	1365	TYR
1	A	1376	THR
2	B	21	GLU
2	B	46	GLN
2	B	65	GLU
2	B	68	THR
2	B	114	PRO
2	B	229	ALA
2	B	258	LEU
2	B	260	GLY
2	B	266	ALA
2	B	294	ASP
2	B	322	PHE
2	B	504	ARG
2	B	509	ALA
2	B	526	GLU
2	B	534	GLY
2	B	559	SER
2	B	605	ARG
2	B	613	VAL
2	B	641	GLU
2	B	810	GLU
2	B	867	GLY
2	B	869	SER

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Mol	Chain	Res	Type
2	B	880	THR
2	B	881	ASN
2	B	891	ASP
2	B	902	GLY
2	B	903	VAL
2	B	907	GLY
2	B	1018	PRO
2	B	1041	GLU
2	B	1096	ARG
2	B	1099	VAL
2	B	1150	ARG
2	B	1156	ASP
2	B	1170	THR
2	B	1183	LYS
2	B	1186	ASP
2	B	1190	ASP
3	C	74	SER
3	C	141	GLY
3	C	161	LYS
4	D	6	SER
4	D	8	PHE
4	D	16	LYS
4	D	19	GLU
4	D	30	GLY
4	D	199	ASN
4	D	218	GLU
5	E	36	GLU
5	E	45	LYS
5	E	59	SER
5	E	106	GLN
5	E	145	THR
5	E	189	GLY
5	E	206	GLY
6	F	131	PRO
7	G	83	LYS
7	G	154	VAL
8	H	59	ILE
8	H	77	ARG
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
9	I	3	THR

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Mol	Chain	Res	Type
9	I	34	TYR
9	I	62	ILE
9	I	89	GLN
9	I	106	CYS
9	I	107	SER
10	J	2	ILE
10	J	62	ARG
11	K	37	LYS
11	K	103	THR
12	L	43	THR
12	L	51	CYS
12	L	56	LEU
13	S	259	ALA
1	A	59	GLY
1	A	66	LYS
1	A	89	PRO
1	A	124	GLN
1	A	167	CYS
1	A	283	GLY
1	A	394	ASN
1	A	396	PRO
1	A	517	ASN
1	A	543	LEU
1	A	592	ASP
1	A	640	GLN
1	A	647	GLY
1	A	707	GLY
1	A	731	ARG
1	A	774	ARG
1	A	903	ASN
1	A	1017	LEU
1	A	1060	PRO
1	A	1062	GLU
1	A	1131	ALA
1	A	1221	LYS
1	A	1229	SER
1	A	1452	LYS
2	B	115	GLN
2	B	131	ASP
2	B	176	SER
2	B	206	ASN
2	B	295	GLY

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Mol	Chain	Res	Type
2	B	308	TRP
2	B	334	ILE
2	B	365	THR
2	B	369	GLY
2	B	469	GLN
2	B	480	SER
2	B	551	PRO
2	B	598	GLU
2	B	645	SER
2	B	682	SER
2	B	688	GLY
2	B	711	GLU
2	B	712	PRO
2	B	738	PHE
2	B	761	HIS
2	B	792	MET
2	B	822	ASN
2	B	996	ARG
2	B	1017	ILE
2	B	1153	GLU
2	B	1155	SER
2	B	1189	ILE
3	C	6	PRO
3	C	28	ALA
3	C	91	HIS
3	C	169	LYS
3	C	202	PRO
3	C	212	PRO
3	C	218	PRO
3	C	264	GLN
4	D	52	LEU
5	E	8	ASN
5	E	44	ALA
5	E	56	LYS
5	E	74	ASP
5	E	192	ARG
7	G	17	PHE
7	G	139	ILE
7	G	147	ILE
9	I	7	CYS
9	I	113	ASP
10	J	22	LEU

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Mol	Chain	Res	Type
12	L	35	SER
12	L	49	LYS
13	S	295	THR
1	A	35	ILE
1	A	67	CYS
1	A	100	LYS
1	A	196	GLU
1	A	253	ASN
1	A	312	PRO
1	A	465	TYR
1	A	526	ASP
1	A	605	MET
1	A	986	ILE
1	A	1040	GLN
1	A	1139	GLU
1	A	1206	ASP
1	A	1266	THR
1	A	1280	GLU
1	A	1302	PRO
2	B	387	LEU
2	B	409	ALA
2	B	430	ARG
2	B	754	SER
2	B	848	ARG
2	B	884	ARG
2	B	946	ASN
2	B	1029	CYS
2	B	1143	ALA
2	B	1178	ASN
2	B	1202	LEU
3	C	90	ASP
3	C	198	ALA
3	C	227	THR
3	C	240	VAL
4	D	131	GLU
4	D	168	LYS
5	E	73	PRO
5	E	115	ASN
6	F	73	ALA
6	F	112	GLU
7	G	133	SER
8	H	92	ASP

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Mol	Chain	Res	Type
9	I	32	CYS
9	I	73	ARG
9	I	86	PHE
9	I	95	THR
10	J	9	SER
10	J	29	GLU
10	J	51	LEU
10	J	63	TYR
11	K	64	GLU
12	L	42	ARG
13	S	288	SER
1	A	84	ILE
1	A	197	PRO
1	A	696	GLU
1	A	759	ALA
1	A	789	LYS
1	A	795	GLU
1	A	808	LEU
1	A	817	ALA
1	A	958	VAL
1	A	1160	SER
1	A	1188	GLN
1	A	1435	PRO
2	B	22	SER
2	B	56	ASP
2	B	368	GLU
2	B	483	LEU
2	B	490	SER
2	B	565	PRO
2	B	878	GLN
2	B	879	ARG
2	B	883	LEU
2	B	1019	SER
2	B	1100	ASP
3	C	148	ARG
4	D	27	LEU
4	D	142	LYS
5	E	40	GLU
5	E	172	GLU
5	E	183	PRO
6	F	108	PHE
7	G	30	LEU

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Mol	Chain	Res	Type
7	G	124	GLY
7	G	165	GLU
8	H	52	GLN
11	K	70	ARG
13	S	277	LYS
13	S	293	LEU
1	A	599	SER
1	A	641	VAL
1	A	719	VAL
1	A	1162	VAL
1	A	1338	VAL
2	B	171	PRO
2	B	282	ILE
2	B	450	ALA
2	B	543	SER
2	B	694	ASP
2	B	758	PHE
2	B	906	SER
2	B	1103	ILE
2	B	1118	PRO
3	C	126	GLY
3	C	171	GLY
4	D	201	LYS
6	F	139	PRO
10	J	18	TRP
12	L	26	THR
12	L	46	VAL
1	A	507	VAL
1	A	1057	VAL
2	B	635	ARG
3	C	142	VAL
6	F	93	ILE
1	A	9	ALA
1	A	653	VAL
1	A	886	ILE
1	A	963	ILE
1	A	1158	PRO
2	B	985	GLY
5	E	37	LEU
7	G	63	PRO
1	A	392	VAL
1	A	673	GLY

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Mol	Chain	Res	Type
1	A	1379	GLY
2	B	410	GLY
2	B	502	ILE
2	B	552	MET
2	B	974	PRO
1	A	250	ILE
1	A	649	ILE
1	A	1031	VAL
10	J	14	VAL
11	K	43	GLY
1	A	357	PRO
1	A	1061	GLY
2	B	575	PRO
7	G	157	ILE
5	E	129	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	1246/1520 (82%)	1133 (91%)	113 (9%)	12	48
2	B	964/1061 (91%)	880 (91%)	84 (9%)	13	50
3	C	234/274 (85%)	205 (88%)	29 (12%)	6	33
4	D	140/200 (70%)	126 (90%)	14 (10%)	9	43
5	E	196/197 (100%)	184 (94%)	12 (6%)	23	65
6	F	74/137 (54%)	63 (85%)	11 (15%)	4	26
7	G	152/152 (100%)	143 (94%)	9 (6%)	24	66
8	H	117/128 (91%)	110 (94%)	7 (6%)	24	65
9	I	113/116 (97%)	97 (86%)	16 (14%)	4	29
10	J	60/65 (92%)	55 (92%)	5 (8%)	14	52
11	K	99/102 (97%)	91 (92%)	8 (8%)	15	54
12	L	40/57 (70%)	33 (82%)	7 (18%)	2	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	S	62/156 (40%)	55 (89%)	7 (11%)	7	38
All	All	3497/4165 (84%)	3175 (91%)	322 (9%)	11	48

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	13	THR
1	A	14	VAL
1	A	18	GLN
1	A	34	LYS
1	A	41	MET
1	A	54	ASN
1	A	62	ASP
1	A	83	HIS
1	A	93	VAL
1	A	108	MET
1	A	167	CYS
1	A	195	ASP
1	A	200	ARG
1	A	208	LEU
1	A	215	SER
1	A	220	THR
1	A	270	LEU
1	A	303	TYR
1	A	308	ILE
1	A	326	ARG
1	A	329	LEU
1	A	335	ARG
1	A	354	SER
1	A	362	ASP
1	A	375	THR
1	A	381	THR
1	A	406	ILE
1	A	408	ASP
1	A	425	GLN
1	A	434	ARG
1	A	443	LEU
1	A	445	ASN
1	A	450	LEU
1	A	451	HIS
1	A	453	MET

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Mol	Chain	Res	Type
1	A	454	SER
1	A	466	SER
1	A	469	ARG
1	A	481	ASP
1	A	487	MET
1	A	489	LEU
1	A	493	GLN
1	A	498	ARG
1	A	501	LEU
1	A	503	GLN
1	A	523	ILE
1	A	524	VAL
1	A	560	ILE
1	A	562	THR
1	A	596	THR
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	734	GLU
1	A	739	ASP
1	A	754	SER
1	A	762	SER
1	A	774	ARG
1	A	786	HIS
1	A	791	ASP
1	A	816	HIS
1	A	821	ARG
1	A	831	THR
1	A	833	GLU
1	A	845	LEU
1	A	852	TYR
1	A	854	ASN
1	A	858	ASN
1	A	879	GLU
1	A	890	ASP
1	A	897	TYR
1	A	903	ASN
1	A	906	HIS
1	A	920	LEU
1	A	929	LEU
1	A	936	LEU
1	A	949	ASP

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Mol	Chain	Res	Type
1	A	969	GLN
1	A	1029	ARG
1	A	1035	TYR
1	A	1048	ASN
1	A	1050	GLU
1	A	1058	VAL
1	A	1081	LEU
1	A	1082	ASN
1	A	1110	ASN
1	A	1111	MET
1	A	1114	PRO
1	A	1116	LEU
1	A	1122	PRO
1	A	1127	ASP
1	A	1142	THR
1	A	1155	ASP
1	A	1166	ASP
1	A	1236	LEU
1	A	1264	GLU
1	A	1271	ILE
1	A	1274	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1298	TYR
1	A	1300	LYS
1	A	1325	THR
1	A	1333	ILE
1	A	1353	TYR
1	A	1358	SER
1	A	1362	TYR
1	A	1364	ASN
1	A	1372	VAL
1	A	1376	THR
1	A	1445	ILE
1	A	1447	GLU
2	B	44	VAL
2	B	57	TYR
2	B	128	LEU
2	B	175	ARG
2	B	194	GLU
2	B	217	ARG
2	B	223	VAL

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Mol	Chain	Res	Type
2	B	261	ARG
2	B	268	THR
2	B	286	PHE
2	B	294	ASP
2	B	298	LEU
2	B	365	THR
2	B	371	GLU
2	B	378	LEU
2	B	393	LYS
2	B	401	PHE
2	B	408	LEU
2	B	419	THR
2	B	427	ASP
2	B	429	PHE
2	B	463	THR
2	B	466	TRP
2	B	476	ARG
2	B	485	ARG
2	B	496	ARG
2	B	498	THR
2	B	510	LYS
2	B	511	PRO
2	B	582	VAL
2	B	603	LEU
2	B	615	MET
2	B	629	ASP
2	B	635	ARG
2	B	636	PRO
2	B	644	GLU
2	B	658	ILE
2	B	682	SER
2	B	724	ASP
2	B	737	THR
2	B	742	GLU
2	B	743	ILE
2	B	748	ILE
2	B	751	VAL
2	B	766	ARG
2	B	815	ARG
2	B	830	TYR
2	B	835	GLN
2	B	839	MET

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Mol	Chain	Res	Type
2	B	855	PHE
2	B	856	PHE
2	B	859	TYR
2	B	878	GLN
2	B	895	ASP
2	B	901	PRO
2	B	909	ASP
2	B	939	THR
2	B	953	LEU
2	B	986	GLN
2	B	987	LYS
2	B	993	THR
2	B	997	GLU
2	B	999	MET
2	B	1002	THR
2	B	1006	ILE
2	B	1026	LEU
2	B	1034	VAL
2	B	1047	PHE
2	B	1051	THR
2	B	1076	HIS
2	B	1084	GLN
2	B	1087	PHE
2	B	1092	TYR
2	B	1095	LEU
2	B	1096	ARG
2	B	1104	HIS
2	B	1137	CYS
2	B	1138	MET
2	B	1159	ARG
2	B	1170	THR
2	B	1183	LYS
2	B	1202	LEU
2	B	1212	ILE
2	B	1224	PHE
3	C	23	SER
3	C	44	LEU
3	C	54	ASN
3	C	55	THR
3	C	56	THR
3	C	57	VAL
3	C	58	LEU

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Mol	Chain	Res	Type
3	C	62	PHE
3	C	74	SER
3	C	77	ILE
3	C	86	CYS
3	C	88	CYS
3	C	89	GLU
3	C	91	HIS
3	C	100	THR
3	C	104	PHE
3	C	108	GLU
3	C	129	ILE
3	C	138	GLU
3	C	140	ASN
3	C	143	LEU
3	C	147	LEU
3	C	186	LEU
3	C	193	TYR
3	C	214	ASN
3	C	240	VAL
3	C	245	VAL
3	C	250	THR
3	C	266	ASP
4	D	47	LEU
4	D	63	LEU
4	D	70	PHE
4	D	137	ASN
4	D	139	LYS
4	D	148	LEU
4	D	149	THR
4	D	152	SER
4	D	177	VAL
4	D	182	SER
4	D	187	THR
4	D	193	THR
4	D	197	SER
4	D	206	GLU
5	E	60	PHE
5	E	72	PHE
5	E	83	CYS
5	E	104	ASN
5	E	114	ASN
5	E	135	PHE

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Mol	Chain	Res	Type
5	E	153	HIS
5	E	169	ARG
5	E	183	PRO
5	E	207	ARG
5	E	211	TYR
5	E	212	ARG
6	F	77	ASP
6	F	79	ARG
6	F	81	THR
6	F	84	TYR
6	F	86	THR
6	F	90	ARG
6	F	96	THR
6	F	119	ARG
6	F	143	PHE
6	F	148	VAL
6	F	153	VAL
7	G	1	MET
7	G	38	CYS
7	G	39	THR
7	G	70	PHE
7	G	78	VAL
7	G	80	LYS
7	G	96	GLN
7	G	126	ASN
7	G	171	ILE
8	H	10	PHE
8	H	86	ASP
8	H	95	TYR
8	H	102	TYR
8	H	130	ARG
8	H	134	ASN
8	H	141	TYR
9	I	6	PHE
9	I	8	ARG
9	I	9	ASP
9	I	10	CYS
9	I	13	MET
9	I	32	CYS
9	I	34	TYR
9	I	46	HIS
9	I	75	CYS

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Mol	Chain	Res	Type
9	I	78	CYS
9	I	85	PHE
9	I	86	PHE
9	I	100	PHE
9	I	101	PHE
9	I	106	CYS
9	I	113	ASP
10	J	2	ILE
10	J	28	ASP
10	J	46	CYS
10	J	48	ARG
10	J	55	ASP
11	K	10	PHE
11	K	25	THR
11	K	35	PHE
11	K	47	ARG
11	K	70	ARG
11	K	78	THR
11	K	81	TYR
11	K	114	LEU
12	L	33	GLU
12	L	48	CYS
12	L	51	CYS
12	L	55	ILE
12	L	63	ARG
12	L	65	VAL
12	L	68	GLU
13	S	263	ARG
13	S	266	THR
13	S	267	ASP
13	S	283	GLN
13	S	288	SER
13	S	292	PRO
13	S	293	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	80	HIS
1	A	83	HIS
1	A	92	HIS

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Mol	Chain	Res	Type
1	A	213	HIS
1	A	225	ASN
1	A	256	GLN
1	A	299	HIS
1	A	339	ASN
1	A	394	ASN
1	A	435	HIS
1	A	445	ASN
1	A	451	HIS
1	A	493	GLN
1	A	503	GLN
1	A	587	HIS
1	A	603	ASN
1	A	611	GLN
1	A	631	HIS
1	A	654	ASN
1	A	659	HIS
1	A	741	ASN
1	A	757	ASN
1	A	786	HIS
1	A	851	HIS
1	A	858	ASN
1	A	877	HIS
1	A	903	ASN
1	A	926	GLN
1	A	1048	ASN
1	A	1085	HIS
1	A	1106	ASN
1	A	1232	ASN
1	A	1432	GLN
2	B	52	ASN
2	B	60	GLN
2	B	121	ASN
2	B	178	ASN
2	B	236	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN

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Mol	Chain	Res	Type
2	B	657	HIS
2	B	744	HIS
2	B	821	GLN
2	B	835	GLN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1065	GLN
2	B	1084	GLN
2	B	1117	GLN
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	252	GLN
4	D	28	GLN
4	D	39	ASN
4	D	40	HIS
4	D	51	ASN
4	D	137	ASN
5	E	101	GLN
5	E	104	ASN
5	E	114	ASN
5	E	143	ASN
5	E	147	HIS
7	G	14	HIS
7	G	53	ASN
7	G	97	HIS
7	G	122	ASN
7	G	126	ASN
9	I	12	ASN
9	I	83	ASN
9	I	89	GLN
9	I	90	GLN
11	K	65	HIS
11	K	76	GLN

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Mol	Chain	Res	Type
11	K	89	ASN
13	S	283	GLN
13	S	285	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	1426/1733 (82%)	-0.17	6 (0%) 93 87	1, 54, 131, 183	0
2	B	1104/1224 (90%)	-0.04	22 (1%) 68 53	4, 67, 147, 180	0
3	C	266/318 (83%)	-0.16	0 100 100	17, 61, 118, 143	0
4	D	177/221 (80%)	-0.16	0 100 100	23, 78, 141, 157	0
5	E	214/215 (99%)	-0.06	2 (0%) 85 74	10, 93, 155, 173	0
6	F	84/155 (54%)	-0.32	0 100 100	1, 40, 79, 101	0
7	G	171/171 (100%)	-0.12	0 100 100	25, 56, 96, 113	0
8	H	133/146 (91%)	0.25	0 100 100	60, 115, 156, 175	0
9	I	119/122 (97%)	0.31	7 (5%) 26 15	45, 109, 153, 196	0
10	J	65/70 (92%)	-0.21	0 100 100	30, 56, 107, 124	0
11	K	114/120 (95%)	-0.09	2 (1%) 71 56	21, 67, 121, 129	0
12	L	46/70 (65%)	0.30	3 (6%) 22 13	51, 117, 149, 169	0
13	S	174/179 (97%)	1.89	55 (31%) 1 1	50, 50, 110, 125	0
All	All	4093/4744 (86%)	-0.01	97 (2%) 62 46	1, 64, 141, 196	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	S	141	THR	18.9
13	S	162	LYS	13.8
13	S	164	SER	11.0
13	S	145	HIS	10.9
13	S	142	ALA	10.3
13	S	138	GLY	9.9
13	S	161	ALA	9.6
13	S	230	THR	8.3
13	S	137	ASP	7.6

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Mol	Chain	Res	Type	RSRZ
13	S	136	ASN	7.1
13	S	146	HIS	7.1
13	S	235	ASP	7.1
13	S	155	ALA	6.8
13	S	163	GLU	6.7
13	S	151	GLN	6.1
9	I	120	GLN	5.6
13	S	221	GLY	5.3
13	S	196	LYS	5.1
9	I	119	THR	4.9
13	S	204	SER	4.9
13	S	175	ALA	4.6
13	S	184	LYS	4.5
12	L	25	ALA	4.4
11	K	9	LEU	4.3
2	B	882	THR	4.3
1	A	1176	LEU	4.2
13	S	198	ARG	4.1
13	S	199	TYR	4.1
13	S	190	THR	4.0
13	S	140	ASP	4.0
13	S	193	ALA	4.0
13	S	165	GLU	3.9
2	B	246	LYS	3.8
13	S	167	PRO	3.7
13	S	213	ASP	3.7
9	I	116	ASN	3.7
2	B	734	HIS	3.6
2	B	715	ALA	3.6
5	E	50	MET	3.5
1	A	253	ASN	3.5
12	L	27	LEU	3.5
13	S	177	ALA	3.4
13	S	197	ALA	3.4
13	S	147	LYS	3.3
13	S	182	MET	3.2
2	B	919	SER	3.2
13	S	159	VAL	3.1
13	S	176	LYS	3.1
13	S	154	LYS	3.0
9	I	118	ARG	3.0
13	S	236	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	247	GLY	3.0
2	B	349	ILE	2.9
13	S	143	ILE	2.8
9	I	76	PRO	2.8
2	B	509	ALA	2.7
12	L	26	THR	2.7
13	S	211	ASN	2.7
1	A	286	HIS	2.7
2	B	346	GLU	2.7
13	S	150	ASP	2.7
13	S	157	TYR	2.7
2	B	106	ASP	2.7
2	B	714	GLU	2.6
13	S	174	THR	2.6
2	B	709	ASP	2.5
13	S	191	ASN	2.5
13	S	216	HIS	2.5
9	I	59	VAL	2.5
13	S	169	GLN	2.5
2	B	248	SER	2.4
2	B	724	ASP	2.4
13	S	153	LEU	2.4
13	S	194	ALA	2.3
1	A	154	SER	2.3
2	B	883	LEU	2.3
2	B	475	SER	2.3
2	B	723	VAL	2.2
2	B	725	PRO	2.2
13	S	166	HIS	2.2
5	E	2	ASP	2.2
2	B	881	ASN	2.2
2	B	733	HIS	2.1
13	S	205	ASN	2.1
1	A	256	GLN	2.1
2	B	587	HIS	2.1
13	S	228	LEU	2.1
11	K	2	ASN	2.1
13	S	170	SER	2.1
13	S	203	TYR	2.1
1	A	159	THR	2.1
9	I	109	ILE	2.1
13	S	148	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	250	PHE	2.1
13	S	158	ASP	2.1
13	S	224	THR	2.0
13	S	233	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
14	MG	S	1	1/1	0.83	0.61	11.38	91,91,91,91	0
15	ZN	B	1307	1/1	0.99	0.16	-0.76	15,15,15,15	0
15	ZN	S	310	1/1	0.98	0.14	-1.09	94,94,94,94	0
15	ZN	L	105	1/1	0.99	0.11	-1.47	68,68,68,68	0
15	ZN	A	1735	1/1	0.99	0.17	-1.56	15,15,15,15	0
15	ZN	C	319	1/1	0.99	0.15	-1.67	20,20,20,20	0
15	ZN	J	101	1/1	0.99	0.12	-1.86	16,16,16,16	0
15	ZN	I	203	1/1	0.99	0.11	-1.98	63,63,63,63	0
15	ZN	I	204	1/1	0.91	0.13	-2.09	97,97,97,97	0
15	ZN	A	1734	1/1	0.98	0.11	-3.10	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.