Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:17 AM GMT

PDB ID	:	3HOZ
Title	:	Complete RNA polymerase II elongation complex IV with a T-U mismatch and a frayed RNA 3'-guanine
Authors	:	Sydow, J.F.; Brueckner, F.; Cheung, A.C.M.; Damsma, G.E.; Dengl, S.; Lehmann, E.; Vassylyev, D.; Cramer, P.
Deposited on	:	2009-06-03
Resolution	:	3.65 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

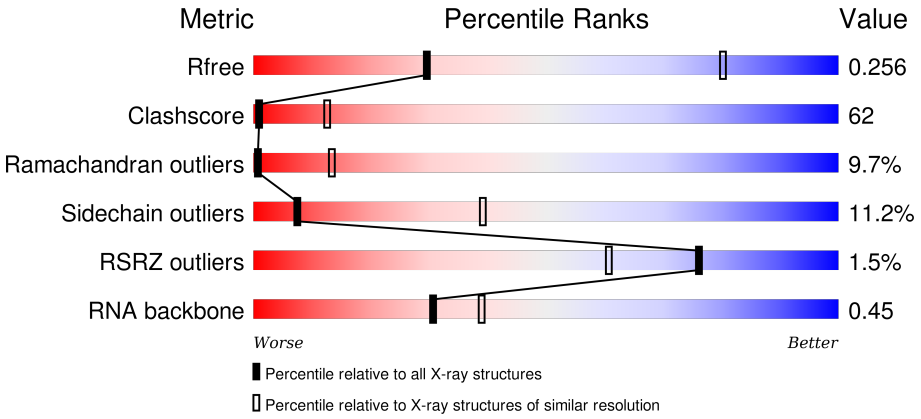
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.65 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	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (3.82-3.50)
RNA backbone	2183	1066 (4.52-2.80)

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 <=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	% 23% 47% 10% • 18%
2	B	1224	% 23% 52% 14% • 9%
3	C	347	18% 47% 11% • 23%
4	D	221	23% 45% 12% • 19%

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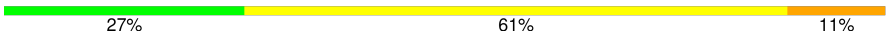
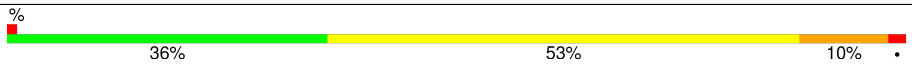
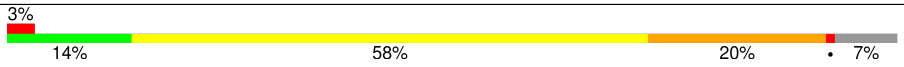
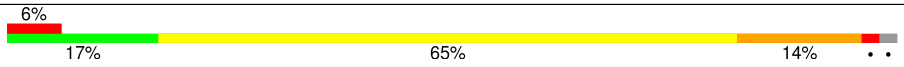
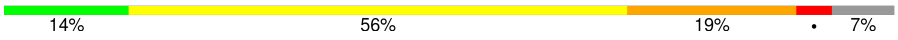
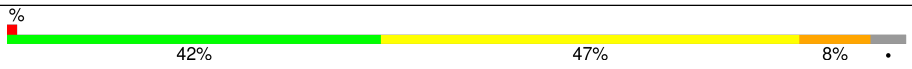
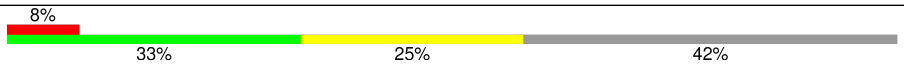
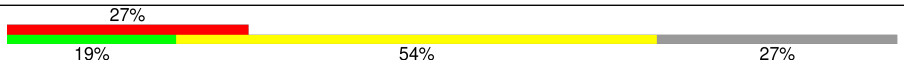
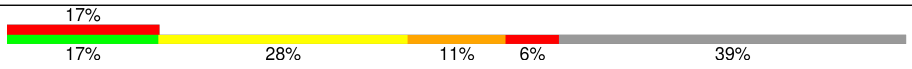
Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	N	12	
14	T	26	
15	P	18	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 31961 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 subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1418	Total	C	N	O	S	0	0	0
			11158	7030	1951	2115	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1109	Total	C	N	O	S	0	0	0
			8821	5584	1546	1636	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

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

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	EXPRESSION TAG	UNP P16370
C	-27	GLY	-	EXPRESSION TAG	UNP P16370
C	-26	SER	-	EXPRESSION TAG	UNP P16370
C	-25	HIS	-	EXPRESSION TAG	UNP P16370
C	-24	HIS	-	EXPRESSION TAG	UNP P16370
C	-23	HIS	-	EXPRESSION TAG	UNP P16370
C	-22	HIS	-	EXPRESSION TAG	UNP P16370
C	-21	HIS	-	EXPRESSION TAG	UNP P16370
C	-20	HIS	-	EXPRESSION TAG	UNP P16370
C	-19	SER	-	EXPRESSION TAG	UNP P16370
C	-18	ASN	-	EXPRESSION TAG	UNP P16370
C	-17	SER	-	EXPRESSION TAG	UNP P16370
C	-16	GLY	-	EXPRESSION TAG	UNP P16370
C	-15	LEU	-	EXPRESSION TAG	UNP P16370

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	ASN	-	EXPRESSION TAG	UNP P16370
C	-13	ASP	-	EXPRESSION TAG	UNP P16370
C	-12	ILE	-	EXPRESSION TAG	UNP P16370
C	-11	PHE	-	EXPRESSION TAG	UNP P16370
C	-10	GLU	-	EXPRESSION TAG	UNP P16370
C	-9	ALA	-	EXPRESSION TAG	UNP P16370
C	-8	GLN	-	EXPRESSION TAG	UNP P16370
C	-7	LYS	-	EXPRESSION TAG	UNP P16370
C	-6	ILE	-	EXPRESSION TAG	UNP P16370
C	-5	GLU	-	EXPRESSION TAG	UNP P16370
C	-4	TRP	-	EXPRESSION TAG	UNP P16370
C	-3	HIS	-	EXPRESSION TAG	UNP P16370
C	-2	GLU	-	EXPRESSION TAG	UNP P16370
C	-1	ASP	-	EXPRESSION TAG	UNP P16370
C	0	THR	-	EXPRESSION TAG	UNP P16370
C	1	GLY	-	EXPRESSION TAG	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	179	Total	C	N	O	S	0	0	0
			1443	892	258	291	2			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

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 subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	87	Total	C	N	O	S	0	0	0
			705	451	119	132	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

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 subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	136	Total	C	N	O	S	0	0	0
			1092	688	184	215	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

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, and III subunit RPABC5.

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 subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	0
			924	593	157	172	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called 5'-D(*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	7	Total	C	N	O	P	0	0	0
			137	68	22	41	6			

- Molecule 14 is a DNA chain called 5'-D(*AP*GP*CP*TP*C*AP*AP*GP*TP*AP*GP*TP *TP*CP*TP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
14	T	19	Total	Br	C	N	O	P	0	0	0
			387	1	185	69	114	18			

- Molecule 15 is a RNA chain called 5'-R(*UP*GP*CP*AP*UP*UP*U*CP*AP*AP*CP*CP

*AP*GP*GP*CP*UP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	11	Total	C	N	O	P	0	0	0
			232	105	44	73	10			

- Molecule 16 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

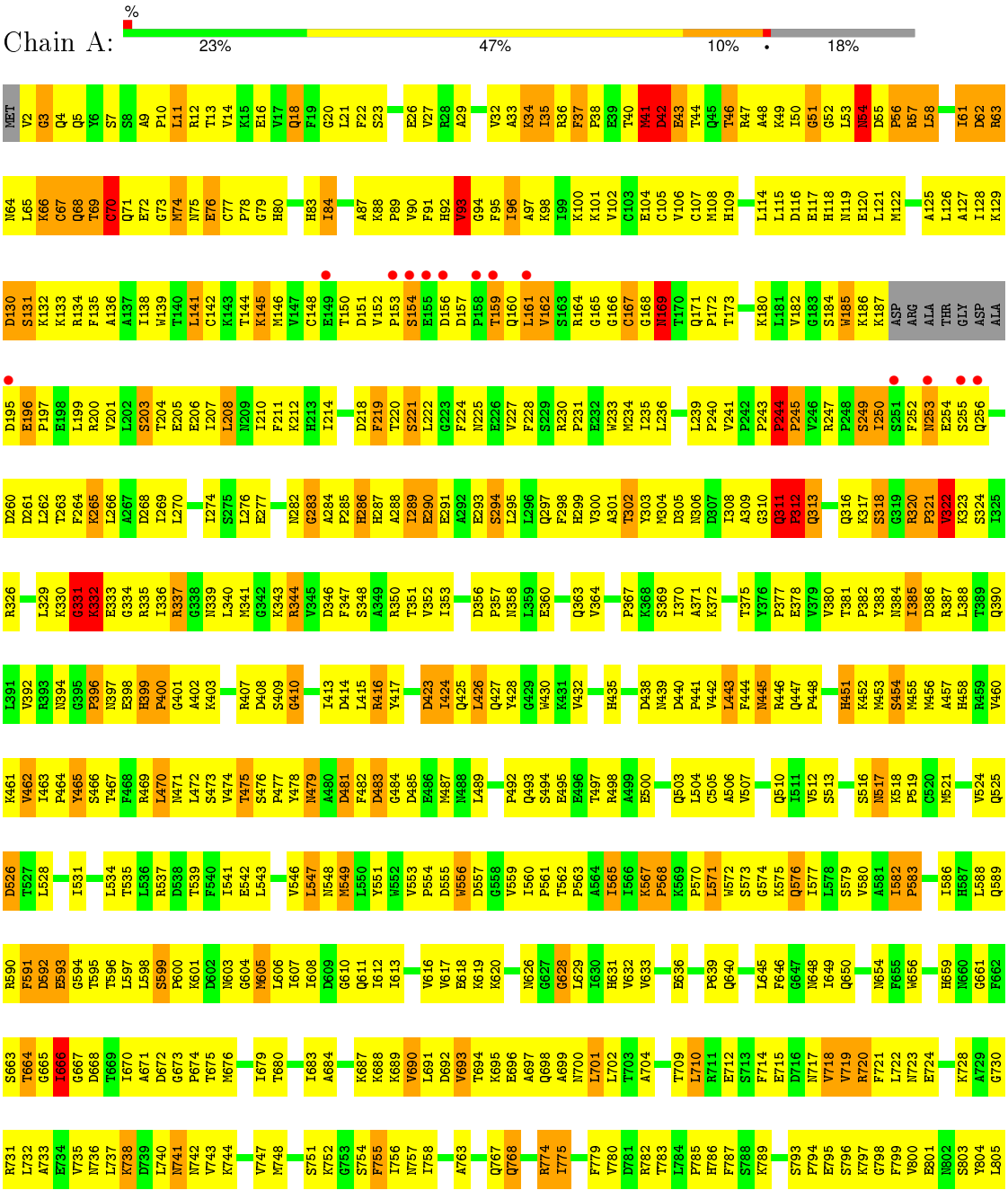
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	P	1	Total	Mg	0	0
			1	1		

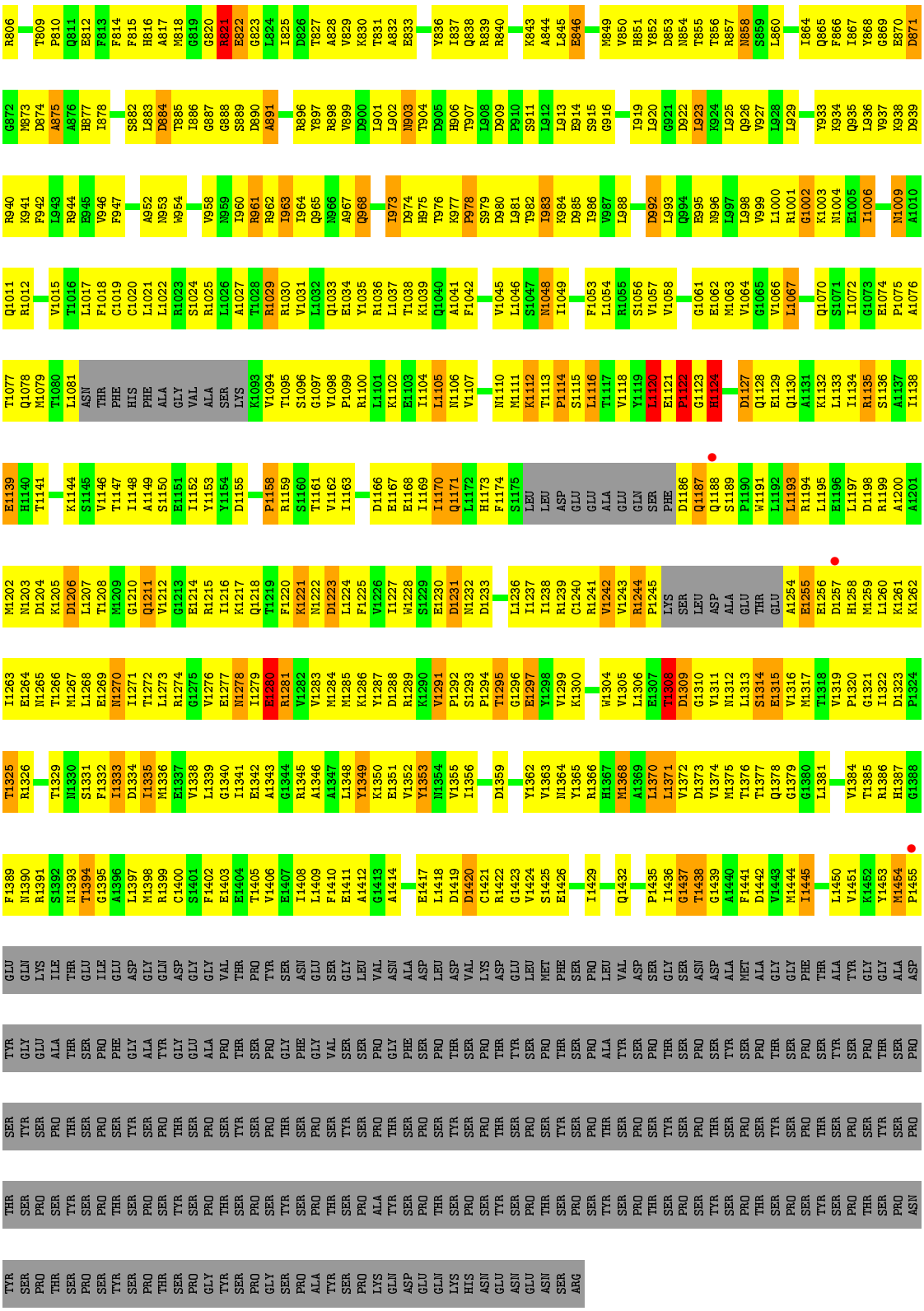
3 Residue-property plots (i)

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 subunit RPB1

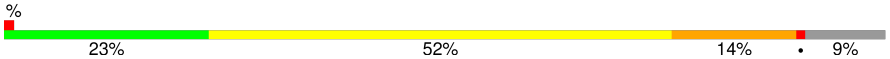
Chain A:

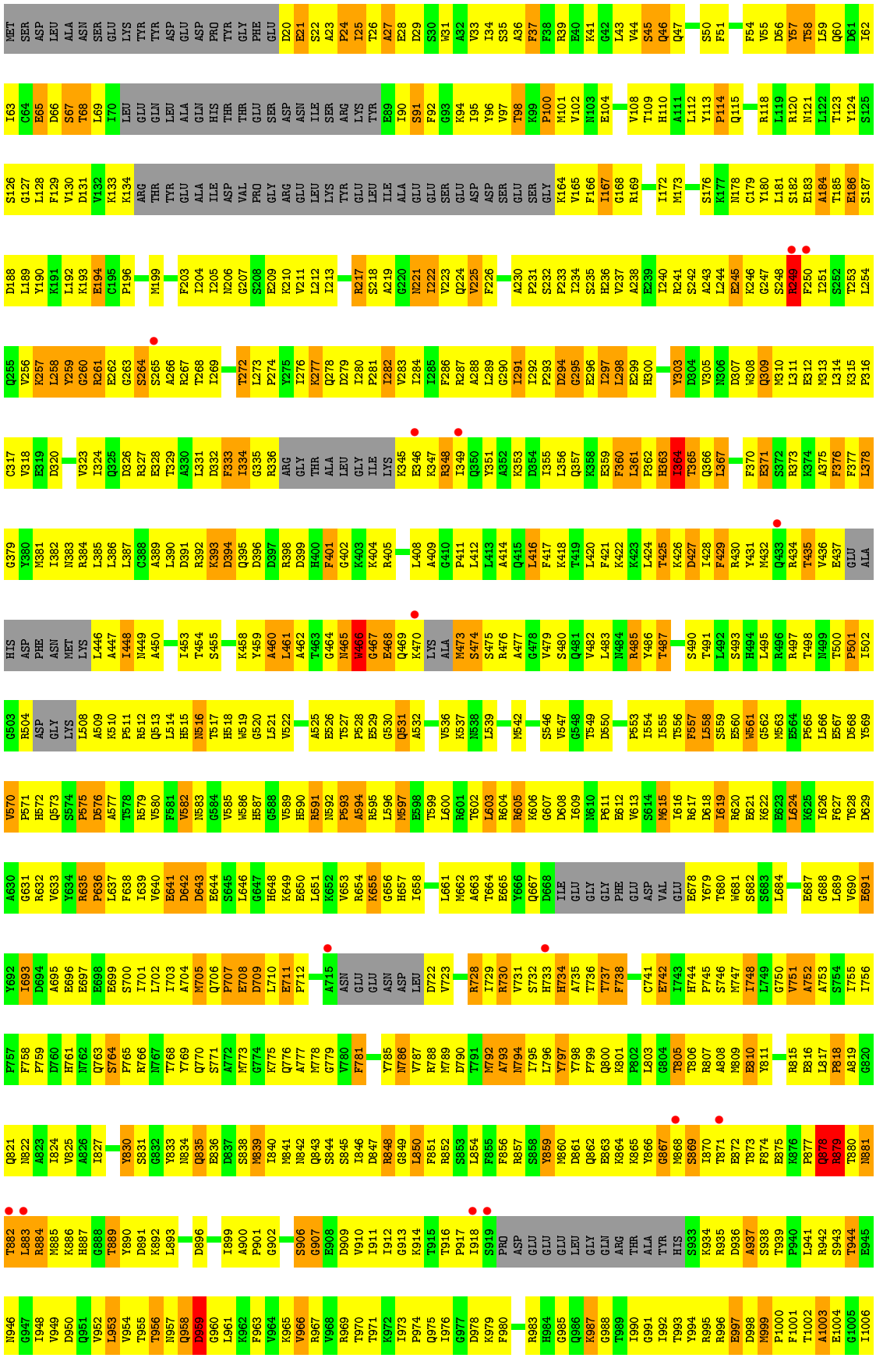


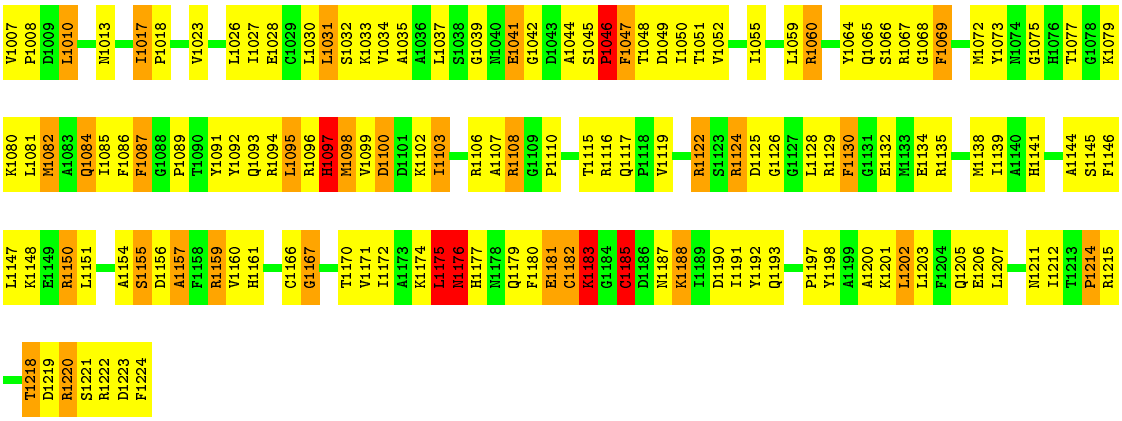


• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

Chain B:

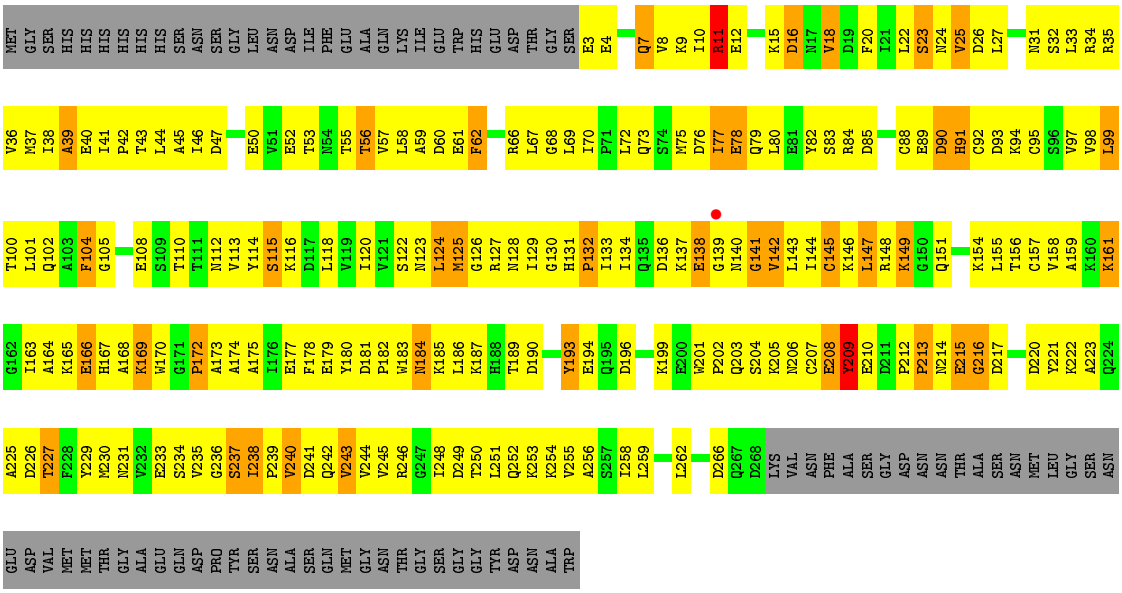






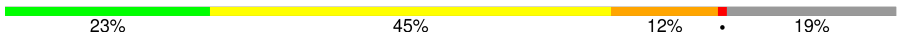
• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

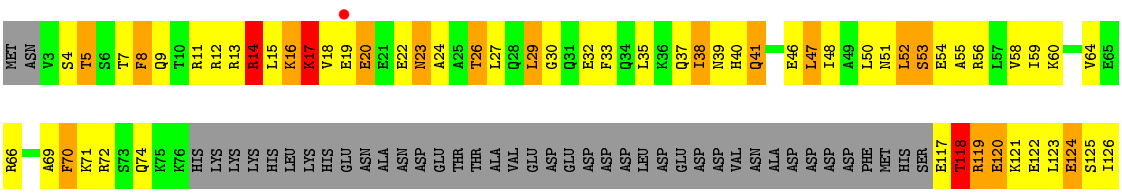
Chain C:

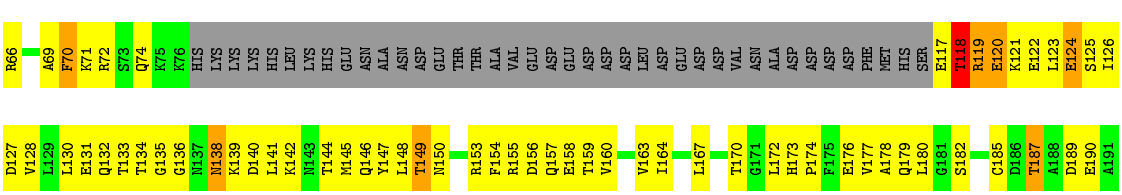


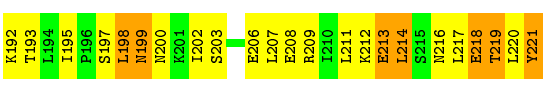
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

Chain D:



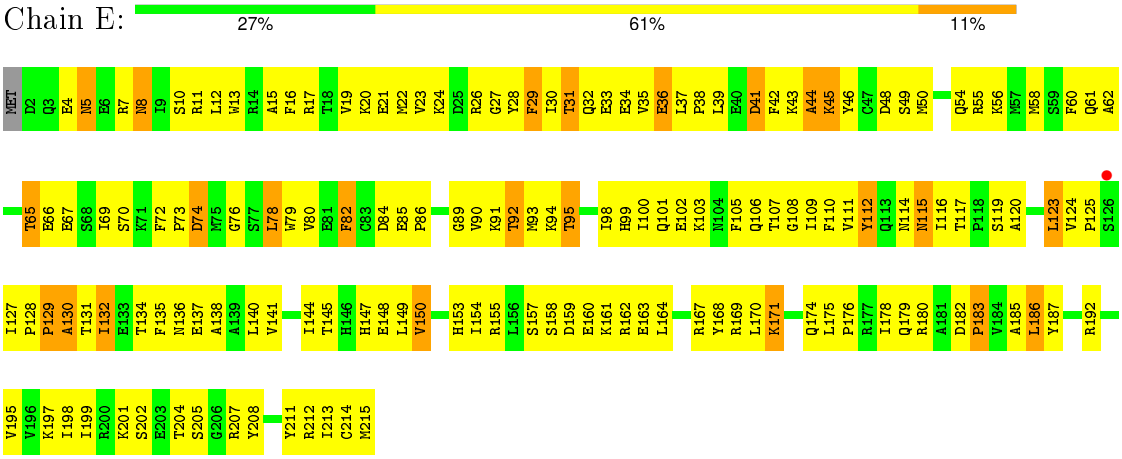






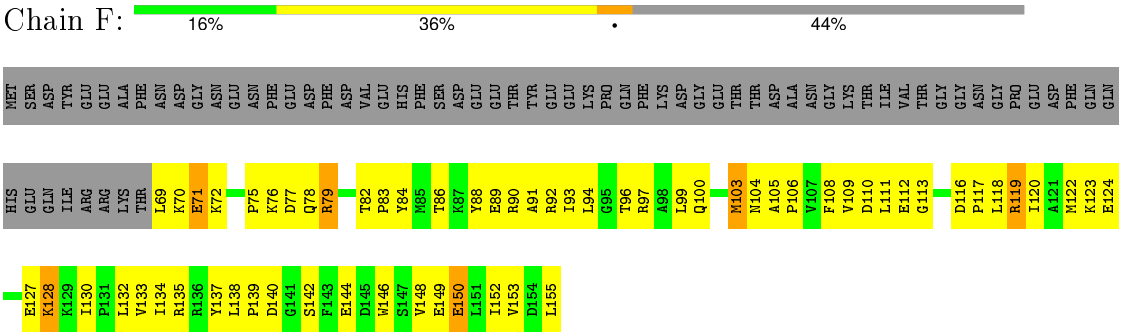
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



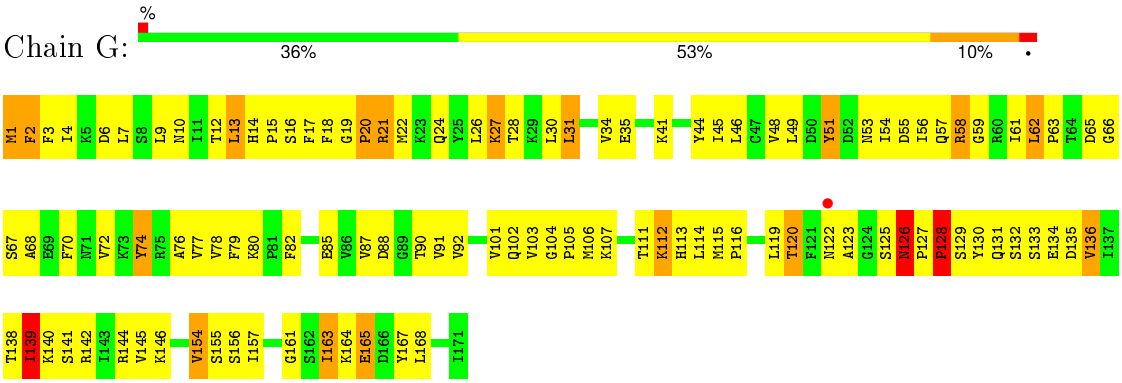
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



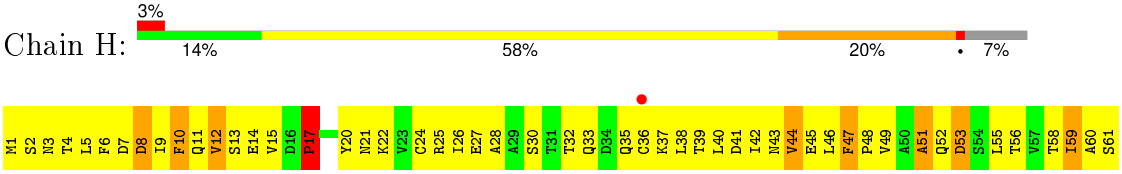
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

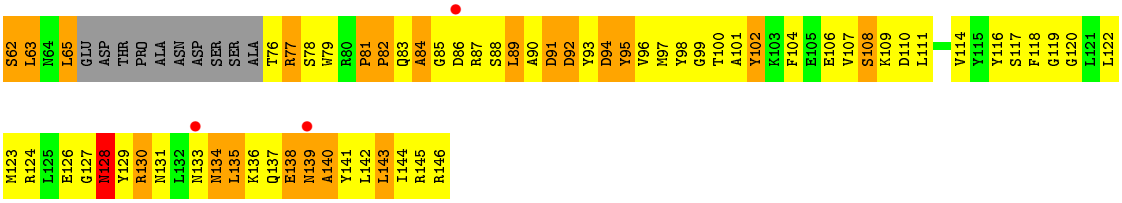
Chain G:



• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3

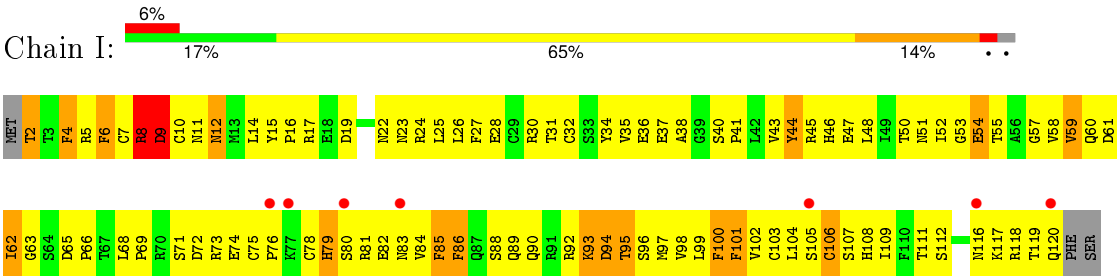
Chain H:





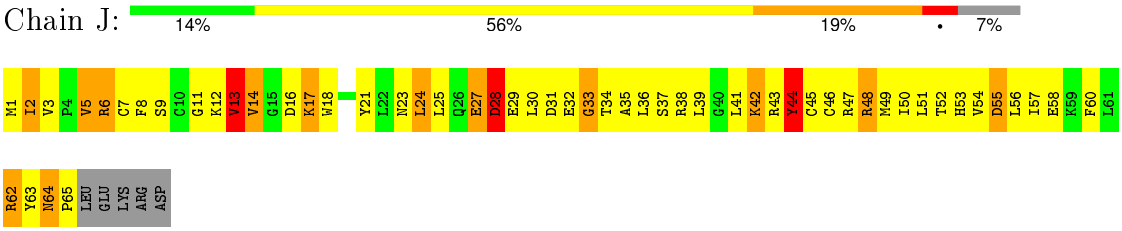
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

Chain I:



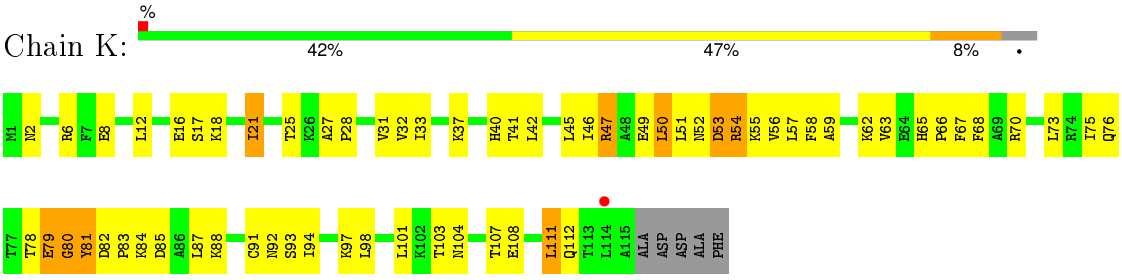
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



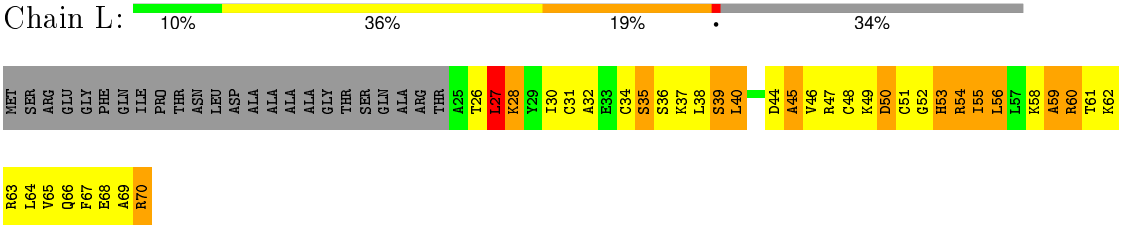
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11

Chain K:



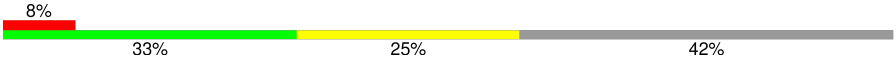
• Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4

Chain L:

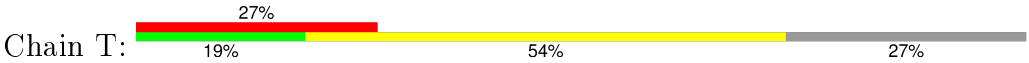


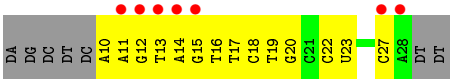
• Molecule 13: 5'-D(*AP*CP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3'

Chain N:



• Molecule 14: 5'-D(*AP*GP*CP*TP*C*AP*AP*GP*TP*AP*GP*TP*TP*CP*TP*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3'





• Molecule 15: 5'-R(*UP*GP*CP*AP*UP*UP*U*CP*AP*AP*CP*CP*AP*GP*GP*CP*UP*G)-3'

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	221.43Å 393.75Å 281.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.65 49.84 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-3.65) 100.0 (49.84-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 3.67Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.253 0.213 , 0.256	Depositor DCC
R_{free} test set	2674 reflections (2.01%)	DCC
Wilson B-factor (Å^2)	88.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 112.9	EDS
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.025 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 135971 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	31961	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, ZN, BRU

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	0.51	0/11358	0.79	4/15360 (0.0%)
2	B	0.49	0/8991	0.74	4/12121 (0.0%)
3	C	0.50	0/2133	0.74	1/2891 (0.0%)
4	D	0.48	0/1453	0.77	1/1947 (0.1%)
5	E	0.48	0/1788	0.71	2/2406 (0.1%)
6	F	0.57	0/717	0.83	1/967 (0.1%)
7	G	0.54	0/1368	0.81	1/1844 (0.1%)
8	H	0.45	0/1110	0.74	0/1502
9	I	0.44	0/989	0.72	0/1331
10	J	0.51	0/541	0.85	1/727 (0.1%)
11	K	0.49	0/942	0.68	0/1272
12	L	0.56	0/365	0.82	0/485
13	N	0.60	0/152	0.90	0/232
14	T	0.58	0/410	0.82	0/629
15	P	0.57	0/259	0.82	1/402 (0.2%)
All	All	0.50	0/32576	0.76	16/44116 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	J	0	1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	26	THR	N-CA-C	-6.48	93.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	39	ALA	N-CA-C	6.32	128.07	111.00
1	A	331	GLY	N-CA-C	5.96	128.00	113.10
7	G	65	ASP	N-CA-C	-5.92	95.02	111.00
1	A	3	GLY	N-CA-C	-5.78	98.65	113.10
1	A	56	PRO	N-CA-C	-5.52	97.74	112.10
5	E	171	LYS	N-CA-C	-5.47	96.22	111.00
5	E	186	LEU	CA-CB-CG	-5.35	102.99	115.30
6	F	71	GLU	N-CA-C	-5.33	96.62	111.00
2	B	624	LEU	CA-CB-CG	-5.30	103.11	115.30
15	P	2	A	C2'-C3'-O3'	5.26	122.11	113.70
2	B	1130	PHE	N-CA-C	-5.25	96.82	111.00
1	A	311	GLN	N-CA-C	5.25	125.17	111.00
2	B	1185	CYS	N-CA-C	-5.16	97.06	111.00
10	J	5	VAL	N-CA-C	-5.14	97.13	111.00
2	B	363	HIS	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	J	44	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11158	0	11228	1381	0
2	B	8821	0	8850	1234	0
3	C	2095	0	2051	306	0
4	D	1443	0	1466	213	0
5	E	1752	0	1776	214	0
6	F	705	0	731	92	0
7	G	1340	0	1357	168	0
8	H	1092	0	1069	179	0
9	I	971	0	929	137	0
10	J	532	0	542	112	0
11	K	924	0	934	105	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	363	0	388	83	0
13	N	137	0	82	4	0
14	T	387	0	214	25	0
15	P	232	0	122	14	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	P	1	0	0	0	0
All	All	31961	0	31739	3920	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 62.

All (3920) 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)
2:B:508:LEU:HD13	2:B:510:LYS:HE2	1.26	1.16
1:A:53:LEU:HD23	1:A:54:ASN:N	1.61	1.16
2:B:744:HIS:HD2	2:B:745:PRO:HD2	1.07	1.14
1:A:1208:THR:HB	1:A:1211:GLN:HG3	1.24	1.13
2:B:559:SER:HA	2:B:563:MET:HB3	1.15	1.13
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.85	1.11
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.25	1.11
2:B:806:THR:HG22	2:B:808:ALA:H	1.12	1.10
1:A:53:LEU:HD23	1:A:54:ASN:H	0.96	1.09
3:C:112:ASN:HB3	3:C:114:TYR:HE1	1.10	1.09
8:H:4:THR:HA	8:H:60:ALA:HB2	1.32	1.08
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.17	1.08
2:B:744:HIS:CD2	2:B:745:PRO:HD2	1.89	1.07
3:C:112:ASN:HB3	3:C:114:TYR:CE1	1.89	1.07
1:A:1242:VAL:HG12	1:A:1243:VAL:N	1.68	1.05
2:B:261:ARG:HH11	2:B:261:ARG:HB3	1.19	1.05
2:B:345:LYS:HG2	2:B:346:GLU:H	1.17	1.05
5:E:117:THR:HG22	5:E:119:SER:H	1.21	1.05
1:A:567:LYS:HE3	1:A:568:PRO:HD2	1.38	1.05
6:F:90:ARG:HD3	6:F:155:LEU:HD13	1.38	1.05
1:A:567:LYS:HB3	8:H:96:VAL:H	1.21	1.04
1:A:1206:ASP:HB3	1:A:1274:ARG:HH22	1.19	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.40	1.03
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.39	1.02
10:J:64:ASN:HB3	10:J:65:PRO:CD	1.90	1.01
1:A:1242:VAL:HG12	1:A:1243:VAL:H	0.85	1.01
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.08	1.01
1:A:265:LYS:HE3	1:A:265:LYS:N	1.74	1.01
2:B:710:LEU:HA	2:B:733:HIS:HB3	1.41	1.00
7:G:26:LEU:HD12	7:G:56:ILE:HD11	1.37	1.00
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.43	1.00
1:A:1244:ARG:HE	1:A:1245:PRO:HD2	1.21	1.00
5:E:56:LYS:HE2	5:E:84:ASP:HB2	1.40	1.00
1:A:1242:VAL:CG1	1:A:1243:VAL:H	1.71	1.00
2:B:510:LYS:CG	2:B:511:PRO:HD3	1.92	0.99
1:A:1445:ILE:HD12	1:A:1445:ILE:H	1.28	0.99
1:A:323:LYS:H	1:A:323:LYS:HD2	1.21	0.99
2:B:510:LYS:HG3	2:B:511:PRO:HD3	1.00	0.99
1:A:12:ARG:HB3	2:B:1218:THR:HG22	1.40	0.98
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.43	0.98
1:A:244:PRO:HB2	1:A:245:PRO:HD3	1.43	0.98
1:A:381:THR:HG22	1:A:383:TYR:H	1.23	0.98
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.94	0.97
1:A:41:MET:HB3	1:A:49:LYS:HA	1.44	0.97
7:G:34:VAL:HG11	7:G:74:TYR:HE1	1.30	0.97
7:G:139:ILE:HG23	7:G:140:LYS:HG3	1.46	0.97
2:B:882:THR:HG23	2:B:884:ARG:H	1.22	0.97
1:A:783:THR:HG21	1:A:796:SER:O	1.65	0.97
2:B:770:GLN:OE1	2:B:983:ARG:HA	1.64	0.96
2:B:806:THR:N	2:B:809:MET:HE3	1.80	0.96
7:G:138:THR:HG22	7:G:139:ILE:N	1.80	0.96
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	1.65	0.96
2:B:622:LYS:HE2	9:I:59:VAL:HG22	1.47	0.96
2:B:289:LEU:HD13	2:B:375:ALA:HB2	1.46	0.95
10:J:53:HIS:HD2	10:J:54:VAL:N	1.63	0.95
2:B:243:ALA:HB2	2:B:251:ILE:HD13	1.45	0.95
2:B:1187:ASN:O	2:B:1188:LYS:HB2	1.64	0.95
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.49	0.95
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.48	0.94
4:D:220:LEU:CD2	4:D:221:TYR:H	1.80	0.94
1:A:672:ASP:HB3	1:A:736:ASN:OD1	1.68	0.94
1:A:344:ARG:HB3	1:A:344:ARG:HH11	1.30	0.94
1:A:351:THR:HG22	2:B:1103:ILE:HA	1.47	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:510:LYS:HG3	2:B:511:PRO:CD	1.96	0.93
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.48	0.93
1:A:41:MET:CB	1:A:49:LYS:HA	1.98	0.93
1:A:1187:GLN:HB2	1:A:1244:ARG:HG2	1.48	0.93
1:A:66:LYS:HZ3	1:A:68:GLN:H	1.01	0.93
1:A:1329:THR:HG22	1:A:1331:SER:H	1.30	0.93
3:C:177:GLU:HG3	3:C:231:ASN:HB3	1.51	0.93
1:A:629:LEU:O	1:A:633:VAL:HG23	1.69	0.93
1:A:98:LYS:O	1:A:102:VAL:HG23	1.69	0.93
7:G:15:PRO:HA	7:G:18:PHE:CD1	2.04	0.93
2:B:865:LYS:HB2	2:B:961:LEU:HD11	1.52	0.92
6:F:77:ASP:O	6:F:78:GLN:HB2	1.66	0.92
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.48	0.92
1:A:913:LEU:HD12	1:A:914:GLU:H	1.32	0.92
7:G:138:THR:HG22	7:G:139:ILE:H	1.31	0.92
1:A:66:LYS:NZ	1:A:68:GLN:H	1.68	0.92
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.02	0.92
2:B:737:THR:HG21	9:I:66:PRO:HA	1.52	0.92
4:D:60:LYS:HE3	4:D:126:ILE:HD11	1.52	0.92
4:D:14:ARG:HB3	4:D:14:ARG:HH11	1.34	0.92
1:A:549:MET:HE3	1:A:656:TRP:HD1	1.35	0.91
1:A:182:VAL:HG22	1:A:201:VAL:HA	1.52	0.91
1:A:1095:THR:HG21	1:A:1112:LYS:HB2	1.52	0.91
1:A:1094:VAL:HG22	1:A:1113:THR:HG21	1.51	0.91
5:E:22:MET:HE1	5:E:26:ARG:HH21	1.34	0.91
1:A:154:SER:HB3	1:A:162:VAL:HG21	1.50	0.91
1:A:1063:MET:SD	1:A:1436:ILE:HG12	2.10	0.91
2:B:800:GLN:HB3	10:J:52:THR:CG2	2.00	0.91
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.53	0.91
2:B:773:MET:SD	2:B:987:LYS:HD2	2.11	0.91
2:B:642:ASP:HB3	2:B:649:LYS:HD2	1.53	0.91
3:C:57:VAL:HG11	10:J:60:PHE:HB3	1.51	0.90
12:L:40:LEU:HD13	12:L:44:ASP:HB3	1.53	0.90
2:B:241:ARG:HA	2:B:253:THR:HG22	1.53	0.90
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.53	0.90
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.50	0.90
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.53	0.90
15:P:10:U:H5'	15:P:11:G:O3'	1.71	0.90
1:A:107:CYS:HA	1:A:171:GLN:NE2	1.85	0.90
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.54	0.90
8:H:59:ILE:HG22	8:H:60:ALA:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:ALA:HB3	4:D:26:THR:HG23	1.53	0.90
8:H:84:ALA:HB2	8:H:87:ARG:HD2	1.54	0.89
3:C:112:ASN:CB	3:C:114:TYR:HE1	1.83	0.89
6:F:82:THR:HG22	6:F:84:TYR:H	1.34	0.89
2:B:615:MET:HB3	2:B:626:ILE:HG12	1.50	0.89
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.12	0.89
3:C:102:GLN:HG2	3:C:154:LYS:HG3	1.52	0.89
5:E:180:ARG:HB2	5:E:215:MET:OXT	1.70	0.89
1:A:1170:ILE:HD12	1:A:1170:ILE:H	1.35	0.89
1:A:567:LYS:HE3	1:A:568:PRO:CD	2.01	0.89
1:A:779:PHE:HE1	1:A:785:PRO:HD3	1.38	0.89
1:A:107:CYS:HA	1:A:171:GLN:HE22	1.37	0.89
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.54	0.88
4:D:220:LEU:HD23	4:D:221:TYR:H	1.36	0.88
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.08	0.88
2:B:364:ILE:HG13	2:B:585:VAL:HG22	1.54	0.88
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.37	0.88
1:A:185:TRP:H	1:A:185:TRP:HE3	1.18	0.88
11:K:21:ILE:HG23	11:K:33:ILE:HG12	1.56	0.88
5:E:23:VAL:O	5:E:28:TYR:HB2	1.73	0.88
6:F:103:MET:CE	7:G:66:GLY:H	1.86	0.88
8:H:89:LEU:C	8:H:91:ASP:H	1.74	0.88
7:G:88:ASP:HB3	7:G:144:ARG:HA	1.54	0.88
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.56	0.87
9:I:26:LEU:HD23	9:I:37:GLU:HA	1.57	0.87
2:B:707:PRO:HG2	2:B:708:GLU:H	1.39	0.87
2:B:882:THR:HG23	2:B:884:ARG:N	1.90	0.87
12:L:55:ILE:HG12	12:L:56:LEU:H	1.40	0.87
1:A:225:ASN:HD22	1:A:228:PHE:H	1.16	0.87
4:D:138:ASN:HD21	7:G:35:GLU:HB3	1.37	0.87
5:E:78:LEU:HA	5:E:107:THR:HB	1.56	0.87
2:B:603:LEU:HD13	2:B:608:ASP:HB2	1.55	0.87
1:A:55:ASP:C	1:A:57:ARG:H	1.75	0.87
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.10	0.87
1:A:34:LYS:NZ	1:A:57:ARG:NH2	2.23	0.86
9:I:105:SER:O	9:I:106:CYS:HB3	1.75	0.86
1:A:671:ALA:HB3	1:A:676:MET:HG3	1.57	0.86
3:C:73:GLN:HE21	3:C:75:MET:H	1.21	0.86
2:B:168:GLY:H	2:B:450:ALA:HB1	1.38	0.86
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.40	0.86
1:A:1308:THR:HG23	1:A:1309:ASP:N	1.90	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.58	0.86
5:E:16:PHE:CZ	5:E:20:LYS:HE2	2.11	0.85
1:A:1116:LEU:HB3	1:A:1308:THR:HG21	1.58	0.85
7:G:26:LEU:CD1	7:G:56:ILE:HD11	2.05	0.85
1:A:451:HIS:CD2	1:A:1074:GLU:HG3	2.12	0.85
1:A:1107:VAL:HG12	1:A:1107:VAL:O	1.76	0.85
2:B:278:GLN:HG2	2:B:279:ASP:H	1.40	0.85
4:D:154:PHE:CD1	4:D:163:VAL:HG21	2.10	0.85
1:A:901:LEU:H	1:A:926:GLN:NE2	1.74	0.85
14:T:10:DA:H2"	14:T:11:DA:N7	1.90	0.85
2:B:597:MET:SD	2:B:624:LEU:HD11	2.16	0.85
6:F:69:LEU:HB3	6:F:71:GLU:CD	1.97	0.85
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	1.59	0.85
6:F:99:LEU:O	6:F:103:MET:HG2	1.77	0.85
1:A:668:ASP:HB3	1:A:741:ASN:HD21	1.41	0.85
1:A:1100:ARG:NH2	1:A:1351:GLU:HG2	1.92	0.85
5:E:120:ALA:O	5:E:123:LEU:HG	1.77	0.84
1:A:335:ARG:HA	1:A:339:ASN:HD22	1.42	0.84
2:B:65:GLU:HG3	2:B:66:ASP:H	1.41	0.84
5:E:114:ASN:O	5:E:115:ASN:HB3	1.74	0.84
1:A:567:LYS:HB3	8:H:96:VAL:N	1.92	0.84
2:B:806:THR:HG22	2:B:808:ALA:N	1.92	0.84
2:B:664:THR:HA	2:B:667:GLN:HE21	1.41	0.84
2:B:345:LYS:HE2	2:B:349:ILE:HD11	1.60	0.83
2:B:579:ARG:HB2	2:B:586:TRP:NE1	1.93	0.83
2:B:911:ILE:HD11	2:B:941:LEU:HD13	1.59	0.83
2:B:841:MET:HG2	2:B:846:ILE:HD11	1.60	0.83
1:A:225:ASN:ND2	1:A:228:PHE:H	1.73	0.83
1:A:698:GLN:HA	9:I:97:MET:O	1.78	0.83
2:B:882:THR:HG23	2:B:884:ARG:HB2	1.59	0.83
8:H:130:ARG:NH1	8:H:130:ARG:HB2	1.93	0.83
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.60	0.83
4:D:23:ASN:H	4:D:23:ASN:HD22	1.24	0.83
1:A:503:GLN:HE21	6:F:90:ARG:NH2	1.76	0.83
1:A:1116:LEU:N	1:A:1308:THR:HG22	1.92	0.83
1:A:18:GLN:HG2	1:A:1418:LEU:HD13	1.58	0.83
2:B:805:THR:HG22	2:B:806:THR:H	1.43	0.83
7:G:138:THR:CG2	7:G:139:ILE:H	1.91	0.83
1:A:534:LEU:O	1:A:574:GLY:HA3	1.77	0.83
1:A:167:CYS:HB2	1:A:169:ASN:HD21	1.43	0.83
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:THR:HA	2:B:428:ILE:HD12	1.59	0.82
2:B:882:THR:HG21	2:B:935:ARG:HA	1.62	0.82
1:A:1293:SER:OG	1:A:1295:THR:HG23	1.79	0.82
7:G:122:ASN:ND2	7:G:125:SER:HB3	1.93	0.82
2:B:110:HIS:CB	12:L:54:ARG:HH22	1.92	0.82
2:B:559:SER:HA	2:B:563:MET:CB	2.07	0.82
1:A:40:THR:HG22	1:A:41:MET:HG3	1.62	0.82
1:A:14:VAL:H	1:A:1432:GLN:NE2	1.77	0.82
1:A:1348:LEU:O	1:A:1352:VAL:HG23	1.78	0.82
2:B:351:TYR:CE1	2:B:355:ILE:HD11	2.13	0.82
5:E:56:LYS:NZ	5:E:85:GLU:HG3	1.94	0.82
2:B:1065:GLN:HE21	2:B:1067:ARG:N	1.76	0.82
1:A:230:ARG:HG3	1:A:233:TRP:CZ3	2.13	0.82
1:A:591:PHE:HA	1:A:595:THR:HG21	1.59	0.82
11:K:47:ARG:HB3	11:K:47:ARG:HH11	1.44	0.82
3:C:120:ILE:HD13	3:C:124:LEU:HD11	1.61	0.82
3:C:128:ASN:O	3:C:129:ILE:HG13	1.77	0.82
1:A:1312:ASN:HD21	1:A:1315:GLU:HG3	1.45	0.82
8:H:65:LEU:HD23	8:H:65:LEU:N	1.95	0.82
2:B:583:ASN:ND2	2:B:628:THR:HG22	1.95	0.82
10:J:5:VAL:HG12	10:J:6:ARG:HG3	1.60	0.82
7:G:15:PRO:HA	7:G:18:PHE:CE1	2.15	0.82
2:B:1095:LEU:HD12	2:B:1095:LEU:H	1.45	0.81
2:B:798:TYR:HE2	3:C:62:PHE:CE2	1.97	0.81
1:A:831:THR:HG23	1:A:832:ALA:H	1.44	0.81
1:A:1420:ASP:HB2	1:A:1422:ARG:HG3	1.61	0.81
2:B:815:ARG:HD3	2:B:1041:GLU:OE2	1.79	0.81
1:A:646:PHE:O	1:A:650:GLN:HG3	1.80	0.81
2:B:1159:ARG:HB3	2:B:1159:ARG:HH11	1.46	0.81
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.15	0.81
1:A:390:GLN:HE21	1:A:394:ASN:HD22	1.27	0.81
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.44	0.81
1:A:332:LYS:HA	1:A:337:ARG:HB3	1.62	0.81
1:A:42:ASP:O	1:A:44:THR:N	2.13	0.81
10:J:53:HIS:CD2	10:J:54:VAL:N	2.47	0.81
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.60	0.81
1:A:56:PRO:O	1:A:57:ARG:HG3	1.81	0.81
5:E:207:ARG:HH11	5:E:207:ARG:HB3	1.45	0.81
2:B:642:ASP:HA	2:B:649:LYS:HA	1.62	0.81
1:A:903:ASN:HD22	1:A:904:THR:N	1.78	0.81
5:E:124:VAL:HG13	5:E:132:ILE:HG13	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:119:LEU:HD11	7:G:130:TYR:HB3	1.63	0.81
1:A:11:LEU:O	1:A:11:LEU:HD23	1.81	0.81
1:A:666:ILE:HD12	1:A:667:GLY:H	1.45	0.81
4:D:195:ILE:HG22	4:D:198:LEU:HG	1.62	0.81
1:A:1387:HIS:HA	1:A:1391:ARG:HH11	1.45	0.81
8:H:130:ARG:HH11	8:H:130:ARG:HB2	1.45	0.81
2:B:577:ALA:CB	2:B:589:VAL:HG11	2.10	0.80
1:A:666:ILE:H	2:B:1026:LEU:HD13	1.44	0.80
1:A:49:LYS:NZ	1:A:61:ILE:HG13	1.96	0.80
2:B:842:ASN:HD22	2:B:845:SER:H	1.27	0.80
2:B:975:GLN:HG2	2:B:976:ILE:H	1.45	0.80
9:I:93:LYS:H	9:I:93:LYS:HD3	1.46	0.80
2:B:579:ARG:HB2	2:B:586:TRP:HE1	1.45	0.80
1:A:754:SER:H	1:A:757:ASN:HD22	1.29	0.80
3:C:177:GLU:HG3	3:C:231:ASN:HD22	1.45	0.80
1:A:332:LYS:C	1:A:334:GLY:H	1.85	0.80
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.16	0.80
1:A:889:SER:HB3	1:A:1297:GLU:HG3	1.64	0.80
1:A:683:ILE:HD13	1:A:801:GLU:HG3	1.63	0.80
2:B:613:VAL:HG13	2:B:627:PHE:O	1.82	0.80
1:A:1186:ASP:O	1:A:1187:GLN:HB3	1.81	0.80
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.78	0.80
14:T:15:DG:H2'	14:T:16:DT:H71	1.63	0.80
14:T:16:DT:H2"	14:T:17:DT:H5'	1.62	0.80
9:I:6:PHE:HB3	9:I:12:ASN:O	1.82	0.80
2:B:278:GLN:CG	2:B:279:ASP:H	1.93	0.80
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.64	0.80
3:C:66:ARG:NH1	10:J:2:ILE:HG21	1.97	0.80
1:A:14:VAL:N	1:A:1432:GLN:HE22	1.79	0.80
1:A:831:THR:HG23	1:A:832:ALA:N	1.96	0.80
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.39	0.80
2:B:803:LEU:HD12	2:B:1032:SER:HB3	1.61	0.80
2:B:866:TYR:HB2	2:B:870:ILE:HB	1.63	0.79
7:G:30:LEU:HD22	7:G:72:VAL:HG11	1.63	0.79
5:E:22:MET:CE	5:E:26:ARG:HH21	1.94	0.79
2:B:172:ILE:HD13	2:B:178:ASN:HD22	1.46	0.79
5:E:44:ALA:O	5:E:45:LYS:HB2	1.81	0.79
1:A:697:ALA:HB2	1:A:702:LEU:HD12	1.64	0.79
1:A:571:LEU:HD22	8:H:46:LEU:HD11	1.65	0.79
2:B:165:VAL:HG11	2:B:448:ILE:HD13	1.64	0.79
6:F:119:ARG:HH11	6:F:119:ARG:HG3	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.18	0.79
1:A:567:LYS:CE	1:A:568:PRO:HD2	2.12	0.79
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.17	0.79
2:B:661:LEU:HD11	2:B:684:LEU:HD21	1.64	0.79
12:L:32:ALA:CB	12:L:55:ILE:HG13	2.12	0.79
12:L:60:ARG:HG2	12:L:61:THR:H	1.46	0.79
4:D:29:LEU:HD12	7:G:82:PHE:CZ	2.18	0.79
1:A:172:PRO:HB3	1:A:185:TRP:CD2	2.18	0.79
1:A:981:LEU:HD21	1:A:1039:LYS:HA	1.65	0.79
2:B:221:ASN:OD1	2:B:242:SER:HA	1.83	0.79
1:A:1241:ARG:O	1:A:1242:VAL:HG23	1.83	0.79
1:A:69:THR:O	1:A:71:GLN:N	2.16	0.79
5:E:117:THR:HG22	5:E:119:SER:N	1.96	0.78
7:G:9:LEU:HD12	7:G:10:ASN:H	1.48	0.78
2:B:942:ARG:HH22	14:T:23:BRU:H5”	1.47	0.78
5:E:117:THR:HB	5:E:120:ALA:HB2	1.65	0.78
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.65	0.78
1:A:535:THR:HG21	1:A:616:VAL:HA	1.66	0.78
7:G:14:HIS:CD2	7:G:16:SER:H	2.01	0.78
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.18	0.78
2:B:613:VAL:HG22	2:B:628:THR:HA	1.66	0.78
7:G:128:PRO:O	7:G:138:THR:HG23	1.84	0.78
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.65	0.78
2:B:126:SER:OG	2:B:172:ILE:HD11	1.84	0.78
1:A:710:LEU:HD12	1:A:710:LEU:H	1.47	0.78
8:H:59:ILE:HG22	8:H:60:ALA:N	1.97	0.78
2:B:294:ASP:H	9:I:12:ASN:ND2	1.81	0.78
4:D:203:SER:OG	4:D:206:GLU:HB2	1.83	0.78
7:G:106:MET:HG2	7:G:107:LYS:N	1.97	0.78
1:A:567:LYS:CB	1:A:568:PRO:HD2	2.14	0.78
2:B:583:ASN:HD21	2:B:628:THR:CG2	1.95	0.78
1:A:49:LYS:HZ1	1:A:61:ILE:N	1.81	0.78
1:A:665:GLY:O	1:A:667:GLY:N	2.16	0.78
1:A:53:LEU:CD2	1:A:54:ASN:H	1.89	0.78
1:A:265:LYS:HE3	1:A:265:LYS:CA	2.13	0.78
4:D:159:THR:O	4:D:163:VAL:HG23	1.83	0.78
1:A:1291:VAL:HG22	1:A:1292:PRO:HD2	1.66	0.78
2:B:542:MET:HG2	2:B:747:MET:HE3	1.64	0.77
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.18	0.77
4:D:130:LEU:HD13	4:D:142:LYS:HD3	1.65	0.77
5:E:90:VAL:HA	5:E:120:ALA:HB2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:129:SER:HB3	7:G:138:THR:OG1	1.84	0.77
2:B:167:ILE:HG22	2:B:453:ILE:HD12	1.67	0.77
2:B:516:ASN:N	2:B:516:ASN:HD22	1.81	0.77
4:D:14:ARG:HB3	4:D:14:ARG:NH1	1.98	0.77
2:B:955:THR:HG22	2:B:956:THR:O	1.83	0.77
4:D:71:LYS:HA	4:D:74:GLN:CG	2.14	0.77
2:B:465:ASN:HD22	2:B:465:ASN:N	1.81	0.77
2:B:547:VAL:HG12	2:B:612:GLU:OE2	1.85	0.77
5:E:117:THR:HB	5:E:120:ALA:CB	2.15	0.77
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.67	0.77
1:A:93:VAL:HG13	1:A:301:ALA:HB1	1.65	0.77
2:B:25:ILE:HD11	2:B:653:VAL:O	1.85	0.77
3:C:253:LYS:O	3:C:256:ALA:HB3	1.84	0.77
10:J:1:MET:N	10:J:57:ILE:H	1.82	0.77
5:E:124:VAL:HG13	5:E:132:ILE:CG1	2.14	0.77
4:D:202:ILE:HD13	4:D:207:LEU:HB2	1.65	0.77
1:A:1135:ARG:HG2	1:A:1136:SER:N	2.00	0.77
2:B:745:PRO:O	2:B:748:ILE:HG12	1.85	0.77
8:H:127:GLY:O	8:H:128:ASN:HB2	1.83	0.77
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.66	0.77
1:A:1227:ILE:HG22	1:A:1228:TRP:H	1.49	0.77
7:G:115:MET:HB3	7:G:116:PRO:HD2	1.65	0.76
1:A:1261:LYS:O	1:A:1264:GLU:HB3	1.85	0.76
2:B:589:VAL:HG12	2:B:590:HIS:H	1.50	0.76
2:B:987:LYS:HE3	15:P:11:G:O2'	1.85	0.76
1:A:1030:ARG:HG2	1:A:1034:GLU:OE2	1.86	0.76
1:A:666:ILE:N	2:B:1026:LEU:HD13	2.00	0.76
5:E:22:MET:HE1	5:E:26:ARG:NH2	2.01	0.76
2:B:193:LYS:NZ	12:L:32:ALA:HB1	1.99	0.76
2:B:824:ILE:HG12	10:J:48:ARG:NH1	2.01	0.76
14:T:27:DC:H42	15:P:2:A:H61	1.30	0.76
5:E:198:ILE:HD11	5:E:212:ARG:HG3	1.65	0.76
2:B:796:LEU:HD21	2:B:821:GLN:HE21	1.50	0.76
5:E:22:MET:HE3	5:E:26:ARG:HE	1.50	0.76
8:H:100:THR:HG23	8:H:138:GLU:HA	1.68	0.76
13:N:5:DC:H2"	13:N:6:DT:OP2	1.84	0.76
2:B:327:ARG:NH2	2:B:371:GLU:HG2	2.00	0.76
1:A:427:GLN:HG3	1:A:430:TRP:CE2	2.21	0.76
1:A:1214:GLU:O	1:A:1218:GLN:HG2	1.85	0.76
1:A:63:ARG:HA	1:A:74:MET:HE2	1.68	0.76
1:A:675:THR:O	1:A:679:ILE:HG13	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:LEU:HD12	2:B:272:THR:O	1.85	0.76
1:A:1409:LEU:HD13	2:B:1207:LEU:HD11	1.66	0.76
2:B:261:ARG:HB3	2:B:261:ARG:NH1	1.98	0.76
2:B:975:GLN:HG2	2:B:976:ILE:N	2.00	0.76
1:A:913:LEU:HD12	1:A:914:GLU:N	1.99	0.76
2:B:603:LEU:HD12	2:B:609:ILE:HG23	1.67	0.75
12:L:49:LYS:O	12:L:50:ASP:HB2	1.85	0.75
1:A:388:LEU:O	1:A:392:VAL:HG23	1.87	0.75
1:A:1206:ASP:HB3	1:A:1274:ARG:NH2	1.99	0.75
2:B:654:ARG:H	2:B:657:HIS:HD2	1.31	0.75
2:B:565:PRO:HB2	2:B:567:GLU:HG2	1.67	0.75
2:B:882:THR:CG2	2:B:884:ARG:H	2.00	0.75
4:D:167:LEU:HD21	4:D:214:LEU:HD21	1.69	0.75
1:A:1385:THR:HG22	1:A:1386:ARG:N	2.01	0.75
2:B:278:GLN:HG2	2:B:279:ASP:N	2.00	0.75
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.69	0.75
1:A:1158:PRO:HG2	1:A:1159:ARG:HE	1.49	0.75
1:A:372:LYS:HA	1:A:435:HIS:ND1	2.00	0.75
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.67	0.75
7:G:21:ARG:NH1	7:G:24:GLN:HB2	2.01	0.75
8:H:104:PHE:CZ	8:H:136:LYS:HA	2.20	0.75
2:B:351:TYR:O	2:B:355:ILE:HG13	1.86	0.75
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.68	0.75
1:A:524:VAL:HG12	1:A:525:GLN:H	1.49	0.75
2:B:272:THR:HG23	2:B:279:ASP:OD1	1.87	0.75
3:C:98:VAL:C	3:C:99:LEU:HD23	2.07	0.75
2:B:955:THR:HG22	2:B:956:THR:N	2.02	0.75
2:B:806:THR:H	2:B:809:MET:HE3	1.52	0.74
2:B:345:LYS:HG2	2:B:346:GLU:N	1.99	0.74
3:C:123:ASN:ND2	3:C:125:MET:HG2	2.01	0.74
2:B:112:LEU:HD12	2:B:113:TYR:H	1.52	0.74
3:C:259:LEU:HD21	11:K:91:CYS:HB3	1.69	0.74
2:B:593:PRO:HG2	2:B:617:ARG:NH2	2.02	0.74
2:B:408:LEU:O	2:B:412:LEU:HD12	1.87	0.74
1:A:1033:GLN:HA	1:A:1036:ARG:HH12	1.52	0.74
8:H:130:ARG:HD3	8:H:130:ARG:N	2.02	0.74
2:B:710:LEU:CA	2:B:733:HIS:HB3	2.18	0.74
5:E:144:ILE:HG13	5:E:145:THR:N	2.03	0.74
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.23	0.74
3:C:115:SER:HB3	3:C:141:GLY:O	1.86	0.74
1:A:886:ILE:HG23	1:A:887:GLY:N	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:HB	2:B:628:THR:OG1	1.87	0.74
1:A:709:THR:HG22	1:A:710:LEU:H	1.53	0.74
1:A:399:HIS:O	1:A:401:GLY:N	2.20	0.74
9:I:85:PHE:HD2	9:I:85:PHE:H	1.35	0.74
3:C:99:LEU:HD23	3:C:99:LEU:N	2.02	0.74
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.50	0.74
1:A:722:LEU:HD21	1:A:794:PRO:HB3	1.68	0.74
2:B:848:ARG:HH22	2:B:996:ARG:HD3	1.53	0.74
5:E:147:HIS:HB3	5:E:150:VAL:HG23	1.69	0.74
8:H:130:ARG:HH11	8:H:130:ARG:H	1.35	0.74
11:K:46:ILE:O	11:K:50:LEU:HB2	1.88	0.74
1:A:821:ARG:HB2	1:A:821:ARG:HH11	1.53	0.74
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.51	0.74
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.18	0.74
15:P:5:C:O2'	15:P:6:A:H5'	1.88	0.74
2:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.66	0.74
4:D:71:LYS:HA	4:D:74:GLN:HG3	1.70	0.74
2:B:68:THR:HG22	2:B:91:SER:HA	1.70	0.74
1:A:399:HIS:CB	1:A:400:PRO:HD3	2.18	0.73
7:G:125:SER:OG	7:G:128:PRO:HA	1.88	0.73
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.69	0.73
1:A:288:ALA:HA	1:A:291:GLU:OE1	1.89	0.73
2:B:637:LEU:HD12	2:B:693:ILE:HD11	1.69	0.73
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.23	0.73
2:B:114:PRO:HG2	2:B:115:GLN:H	1.54	0.73
2:B:508:LEU:HD13	2:B:510:LYS:CE	2.14	0.73
8:H:89:LEU:O	8:H:91:ASP:N	2.22	0.73
1:A:12:ARG:HB3	2:B:1218:THR:CG2	2.18	0.73
1:A:828:ALA:HB2	2:B:530:GLY:HA2	1.69	0.73
12:L:55:ILE:O	12:L:56:LEU:HB2	1.88	0.73
8:H:139:ASN:O	8:H:140:ALA:HB2	1.89	0.73
11:K:65:HIS:HD2	11:K:67:PHE:H	1.36	0.73
1:A:308:ILE:HG22	1:A:309:ALA:H	1.51	0.73
3:C:3:GLU:HG2	3:C:4:GLU:HG3	1.70	0.73
1:A:399:HIS:HB3	1:A:400:PRO:CD	2.18	0.73
2:B:918:ILE:HG21	2:B:935:ARG:NH2	2.03	0.73
2:B:622:LYS:HE2	9:I:59:VAL:CG2	2.19	0.73
2:B:110:HIS:HB3	12:L:54:ARG:HH22	1.51	0.73
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.17	0.73
3:C:183:TRP:O	3:C:185:LYS:N	2.21	0.73
1:A:49:LYS:HZ1	1:A:61:ILE:HG13	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:53:HIS:HB3	12:L:55:ILE:CD1	2.18	0.73
3:C:189:THR:HG22	3:C:190:ASP:N	2.01	0.73
2:B:557:PHE:HD2	2:B:557:PHE:O	1.72	0.73
1:A:549:MET:HE3	1:A:656:TRP:CD1	2.21	0.73
12:L:30:ILE:O	12:L:56:LEU:HD23	1.88	0.73
2:B:999:MET:HA	2:B:999:MET:CE	2.18	0.73
4:D:193:THR:HG21	7:G:167:TYR:CD1	2.24	0.73
2:B:219:ALA:HB2	2:B:405:ARG:NH1	2.03	0.73
1:A:898:ARG:HD2	1:A:899:VAL:N	2.04	0.73
4:D:7:THR:O	4:D:9:GLN:N	2.21	0.73
1:A:1329:THR:HG22	1:A:1331:SER:N	2.03	0.73
3:C:22:LEU:HG	3:C:25:VAL:HG21	1.71	0.73
4:D:23:ASN:N	4:D:23:ASN:ND2	2.33	0.73
4:D:4:SER:O	4:D:5:THR:HB	1.88	0.73
1:A:157:ASP:OD2	1:A:159:THR:HB	1.88	0.73
5:E:207:ARG:NH1	5:E:207:ARG:HB3	2.03	0.73
9:I:7:CYS:HB3	9:I:14:LEU:HD21	1.68	0.73
1:A:1121:GLU:HG2	1:A:1122:PRO:HD2	1.71	0.73
1:A:35:ILE:HA	1:A:52:GLY:O	1.89	0.73
2:B:800:GLN:HB3	10:J:52:THR:HG22	1.71	0.72
10:J:23:ASN:C	10:J:25:LEU:H	1.93	0.72
2:B:842:ASN:ND2	2:B:845:SER:H	1.86	0.72
2:B:186:GLU:HG3	10:J:62:ARG:HH22	1.52	0.72
14:T:16:DT:H2"	14:T:17:DT:C5'	2.20	0.72
11:K:12:LEU:HD12	11:K:37:LYS:HG2	1.71	0.72
2:B:1201:LYS:HE2	2:B:1205:GLN:OE1	1.89	0.72
2:B:865:LYS:NZ	2:B:869:SER:HA	2.04	0.72
6:F:103:MET:HE1	7:G:66:GLY:H	1.53	0.72
2:B:134:LYS:HE2	2:B:164:LYS:NZ	2.04	0.72
5:E:164:LEU:HD13	5:E:211:TYR:CE2	2.25	0.72
1:A:66:LYS:HD3	1:A:67:CYS:N	2.05	0.72
7:G:1:MET:SD	7:G:2:PHE:N	2.62	0.72
2:B:653:VAL:HG23	2:B:689:LEU:HB3	1.70	0.72
3:C:189:THR:HG22	3:C:190:ASP:H	1.53	0.72
3:C:167:HIS:CD2	12:L:70:ARG:HB3	2.24	0.72
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.20	0.72
1:A:236:LEU:HD11	1:A:304:MET:HE1	1.71	0.72
3:C:209:TYR:H	3:C:209:TYR:HD1	1.35	0.72
1:A:102:VAL:CG1	1:A:211:PHE:HE1	2.02	0.72
2:B:800:GLN:HB3	10:J:52:THR:HG21	1.69	0.72
4:D:23:ASN:ND2	4:D:23:ASN:H	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1149:ALA:HB2	9:I:47:GLU:HA	1.72	0.72
2:B:515:HIS:CD2	2:B:517:THR:HG23	2.25	0.72
11:K:45:LEU:HG	11:K:94:ILE:HD13	1.71	0.72
1:A:310:GLY:O	1:A:312:PRO:HD2	1.88	0.72
8:H:11:GLN:HA	8:H:53:ASP:O	1.89	0.72
2:B:705:MET:H	2:B:710:LEU:HD12	1.54	0.72
1:A:70:CYS:O	1:A:72:GLU:HG2	1.89	0.72
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.05	0.72
4:D:160:VAL:O	4:D:164:ILE:HG13	1.89	0.72
1:A:425:GLN:N	1:A:425:GLN:OE1	2.22	0.72
1:A:666:ILE:CD1	1:A:667:GLY:H	2.02	0.72
2:B:248:SER:H	2:B:418:LYS:HZ3	1.35	0.72
2:B:953:LEU:HD21	2:B:965:LYS:HB2	1.72	0.72
7:G:21:ARG:HD2	7:G:24:GLN:HB3	1.72	0.72
1:A:858:ASN:ND2	1:A:860:LEU:H	1.88	0.72
1:A:34:LYS:HZ1	1:A:57:ARG:NH2	1.87	0.72
12:L:55:ILE:HD13	12:L:55:ILE:H	1.55	0.72
1:A:1387:HIS:O	1:A:1391:ARG:HD3	1.90	0.72
2:B:824:ILE:HG12	10:J:48:ARG:HH12	1.53	0.72
3:C:7:GLN:HG3	11:K:104:ASN:HD22	1.53	0.72
1:A:1205:LYS:O	1:A:1207:LEU:HG	1.89	0.72
2:B:644:GLU:OE2	2:B:646:LEU:HB2	1.90	0.71
2:B:435:THR:C	2:B:437:GLU:H	1.93	0.71
2:B:44:VAL:HG21	2:B:199:MET:O	1.90	0.71
2:B:549:THR:HG22	2:B:550:ASP:N	2.05	0.71
3:C:79:GLN:HE21	3:C:127:ARG:HD3	1.55	0.71
5:E:124:VAL:HA	5:E:132:ILE:HD12	1.71	0.71
8:H:62:SER:O	8:H:63:LEU:HG	1.89	0.71
1:A:1438:THR:HB	2:B:1144:ALA:HB3	1.71	0.71
8:H:102:TYR:OH	8:H:122:LEU:HD22	1.89	0.71
7:G:111:THR:CG2	7:G:114:LEU:HD13	2.20	0.71
12:L:32:ALA:HB2	12:L:55:ILE:HG13	1.73	0.71
2:B:758:PHE:CE1	2:B:1027:ILE:HG22	2.25	0.71
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.72	0.71
1:A:305:ASP:OD2	1:A:326:ARG:HD3	1.90	0.71
1:A:135:PHE:CD1	1:A:222:LEU:HD22	2.24	0.71
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.20	0.71
10:J:64:ASN:HB3	10:J:65:PRO:HD2	1.73	0.71
3:C:76:ASP:OD2	3:C:128:ASN:N	2.24	0.71
1:A:960:ILE:O	1:A:963:ILE:HG22	1.90	0.71
2:B:1096:ARG:O	2:B:1097:HIS:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:345:LYS:CG	2:B:346:GLU:H	1.99	0.71
1:A:503:GLN:HE21	6:F:90:ARG:HH22	1.34	0.71
1:A:381:THR:HG22	1:A:383:TYR:N	2.03	0.71
3:C:56:THR:HG22	3:C:57:VAL:H	1.54	0.71
1:A:344:ARG:NH1	1:A:344:ARG:HB3	2.06	0.71
2:B:248:SER:H	2:B:418:LYS:NZ	1.88	0.71
2:B:1031:LEU:HD11	2:B:1042:GLY:HA3	1.73	0.71
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.72	0.71
1:A:821:ARG:HB2	1:A:821:ARG:NH1	2.06	0.71
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.73	0.71
1:A:335:ARG:NH1	2:B:1202:LEU:HD13	2.05	0.70
2:B:860:MET:HG3	2:B:965:LYS:HG2	1.72	0.70
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.72	0.70
3:C:66:ARG:NH2	10:J:3:VAL:O	2.24	0.70
1:A:670:ILE:HG23	1:A:805:LEU:HD21	1.73	0.70
4:D:24:ALA:CB	4:D:26:THR:HG23	2.21	0.70
2:B:424:LEU:O	2:B:428:ILE:HG13	1.90	0.70
11:K:68:PHE:HD1	11:K:70:ARG:HH12	1.39	0.70
5:E:197:LYS:HE2	5:E:199:ILE:HD11	1.73	0.70
9:I:71:SER:OG	9:I:83:ASN:HB2	1.92	0.70
3:C:220:ASP:CG	3:C:223:ALA:HB2	2.11	0.70
1:A:1424:VAL:HG11	2:B:1139:ILE:CD1	2.20	0.70
9:I:34:TYR:CD2	9:I:35:VAL:N	2.60	0.70
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.05	0.70
7:G:34:VAL:HG11	7:G:74:TYR:CE1	2.21	0.70
2:B:983:ARG:NH1	2:B:1028:GLU:OE1	2.24	0.70
2:B:243:ALA:HA	2:B:250:PHE:O	1.91	0.70
2:B:890:TYR:O	2:B:893:LEU:HB2	1.91	0.70
1:A:1244:ARG:HB2	1:A:1245:PRO:CD	2.22	0.70
2:B:842:ASN:ND2	2:B:845:SER:OG	2.24	0.70
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	1.74	0.70
1:A:444:PHE:HB3	1:A:458:HIS:HD2	1.56	0.70
2:B:705:MET:N	2:B:710:LEU:HD12	2.05	0.70
9:I:55:THR:HG23	9:I:86:PHE:HZ	1.55	0.70
2:B:980:PHE:HE1	2:B:990:ILE:HD11	1.56	0.70
1:A:763:ALA:O	1:A:803:SER:HB3	1.91	0.70
3:C:11:ARG:HH12	3:C:205:LYS:NZ	1.90	0.70
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.27	0.70
2:B:600:LEU:O	2:B:609:ILE:HD11	1.92	0.70
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.72	0.70
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:HD13	12:L:37:LYS:HD2	1.74	0.70
3:C:93:ASP:OD1	3:C:122:SER:HB2	1.92	0.70
1:A:1081:LEU:HD11	1:A:1098:VAL:H	1.55	0.70
1:A:244:PRO:HB2	1:A:245:PRO:CD	2.18	0.70
2:B:859:TYR:CZ	2:B:941:LEU:HD12	2.26	0.70
1:A:828:ALA:CB	2:B:530:GLY:HA2	2.21	0.70
2:B:681:TRP:HA	2:B:684:LEU:HD12	1.74	0.70
4:D:71:LYS:HG2	4:D:74:GLN:HG3	1.74	0.70
12:L:38:LEU:HD11	12:L:49:LYS:HE2	1.74	0.70
2:B:235:SER:C	2:B:236:HIS:HD2	1.95	0.70
1:A:1004:ASN:ND2	5:E:167:ARG:HD2	2.07	0.70
3:C:143:LEU:HD21	3:C:146:LYS:HE2	1.73	0.70
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.73	0.70
2:B:1122:ARG:HB3	14:T:22:DC:OP1	1.92	0.70
5:E:202:SER:OG	5:E:204:THR:HG22	1.90	0.70
4:D:190:GLU:O	4:D:193:THR:HG22	1.92	0.70
4:D:208:GLU:O	4:D:212:LYS:HG3	1.92	0.70
9:I:50:THR:HG23	9:I:52:ILE:HG12	1.73	0.70
1:A:866:PHE:O	1:A:867:ILE:HD12	1.91	0.70
2:B:345:LYS:O	2:B:347:LYS:HG2	1.92	0.69
1:A:567:LYS:HE3	1:A:568:PRO:CG	2.21	0.69
1:A:883:LEU:HD11	1:A:1017:LEU:HD11	1.73	0.69
8:H:4:THR:HA	8:H:60:ALA:CB	2.17	0.69
1:A:1436:ILE:O	1:A:1437:GLY:C	2.30	0.69
11:K:107:THR:O	11:K:111:LEU:HG	1.92	0.69
3:C:186:LEU:CD2	3:C:225:ALA:HB2	2.22	0.69
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.22	0.69
1:A:500:GLU:O	1:A:504:LEU:HB2	1.93	0.69
2:B:217:ARG:HE	2:B:405:ARG:HB2	1.57	0.69
1:A:982:THR:HB	1:A:985:ASP:H	1.56	0.69
1:A:53:LEU:CD2	1:A:54:ASN:N	2.50	0.69
1:A:1155:ASP:OD2	1:A:1161:THR:HA	1.93	0.69
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.57	0.69
5:E:90:VAL:HB	5:E:117:THR:HG21	1.73	0.69
5:E:23:VAL:HG13	5:E:78:LEU:HD13	1.74	0.69
7:G:51:TYR:O	7:G:54:ILE:HG13	1.91	0.69
3:C:89:GLU:O	3:C:90:ASP:HB3	1.93	0.69
2:B:882:THR:CG2	2:B:934:LYS:O	2.41	0.69
3:C:16:ASP:C	3:C:240:VAL:HG11	2.12	0.69
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.75	0.69
5:E:164:LEU:HD22	5:E:211:TYR:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:86:THR:HG23	6:F:89:GLU:OE1	1.92	0.69
9:I:102:VAL:HG22	9:I:109:ILE:HG12	1.73	0.69
8:H:130:ARG:HH11	8:H:130:ARG:CB	2.05	0.69
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.57	0.69
8:H:58:THR:HB	8:H:143:LEU:HD13	1.73	0.69
1:A:351:THR:HG22	2:B:1103:ILE:CA	2.23	0.69
1:A:1291:VAL:HG22	1:A:1292:PRO:CD	2.23	0.69
1:A:898:ARG:HD2	1:A:899:VAL:H	1.57	0.69
1:A:443:LEU:HD12	2:B:1146:PHE:CE2	2.28	0.69
1:A:916:GLY:O	1:A:919:ILE:HG22	1.93	0.69
12:L:30:ILE:HG22	12:L:31:CYS:N	2.07	0.69
4:D:23:ASN:N	4:D:23:ASN:HD22	1.91	0.69
3:C:186:LEU:HD21	3:C:225:ALA:HB2	1.74	0.69
1:A:105:CYS:SG	1:A:139:TRP:HA	2.32	0.69
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.75	0.69
1:A:7:SER:OG	2:B:1161:HIS:HE1	1.75	0.69
2:B:957:ASN:HD21	2:B:961:LEU:HB2	1.58	0.69
2:B:1002:THR:OG1	2:B:1006:ILE:HG13	1.93	0.69
3:C:133:ILE:HD12	3:C:237:SER:N	2.08	0.69
1:A:1420:ASP:O	1:A:1421:CYS:HB2	1.93	0.69
2:B:60:GLN:O	2:B:63:ILE:HG22	1.93	0.69
1:A:249:SER:O	1:A:250:ILE:HG13	1.91	0.69
1:A:1095:THR:HG21	1:A:1112:LYS:CB	2.23	0.68
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.28	0.68
2:B:405:ARG:NE	2:B:629:ASP:OD2	2.26	0.68
5:E:32:GLN:HG3	5:E:36:GLU:OE2	1.93	0.68
1:A:512:VAL:HA	1:A:519:PRO:HA	1.75	0.68
8:H:76:THR:O	8:H:77:ARG:HB2	1.92	0.68
2:B:805:THR:HG22	2:B:806:THR:N	2.07	0.68
1:A:1312:ASN:ND2	1:A:1315:GLU:HG3	2.08	0.68
7:G:21:ARG:HD2	7:G:24:GLN:CB	2.23	0.68
1:A:444:PHE:HB3	1:A:458:HIS:CD2	2.27	0.68
6:F:109:VAL:HG12	6:F:110:ASP:N	2.05	0.68
1:A:853:ASP:O	1:A:854:ASN:HB2	1.92	0.68
1:A:323:LYS:N	1:A:323:LYS:HD2	2.04	0.68
1:A:741:ASN:HD22	1:A:742:ASN:N	1.90	0.68
7:G:115:MET:HG2	7:G:163:ILE:HD11	1.74	0.68
10:J:12:LYS:O	10:J:14:VAL:HG23	1.93	0.68
1:A:567:LYS:CB	1:A:568:PRO:CD	2.69	0.68
1:A:567:LYS:HB3	8:H:95:TYR:HA	1.74	0.68
1:A:1254:ALA:O	1:A:1255:GLU:HB2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1255:GLU:HG2	1:A:1258:HIS:HD2	1.58	0.68
4:D:50:LEU:HD11	7:G:4:ILE:HD11	1.74	0.68
3:C:147:LEU:HB2	3:C:151:GLN:HB2	1.74	0.68
2:B:737:THR:CG2	9:I:66:PRO:HA	2.23	0.68
2:B:987:LYS:HD3	2:B:987:LYS:H	1.57	0.68
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.08	0.68
2:B:891:ASP:C	2:B:893:LEU:H	1.97	0.68
2:B:873:THR:O	2:B:914:LYS:HA	1.93	0.68
14:T:11:DA:H2"	14:T:12:DG:H5'	1.75	0.68
5:E:124:VAL:N	5:E:125:PRO:HD2	2.09	0.68
1:A:55:ASP:CG	1:A:55:ASP:O	2.29	0.68
1:A:62:ASP:O	1:A:63:ARG:C	2.30	0.68
14:T:10:DA:H2"	14:T:11:DA:C8	2.29	0.68
1:A:1121:GLU:CG	1:A:1122:PRO:HD2	2.22	0.68
1:A:1188:GLN:OE1	1:A:1241:ARG:HD2	1.93	0.68
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.06	0.68
7:G:116:PRO:HG2	7:G:119:LEU:CB	2.24	0.68
11:K:65:HIS:CD2	11:K:67:PHE:H	2.11	0.68
1:A:1029:ARG:HG3	1:A:1029:ARG:HH11	1.59	0.68
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.75	0.68
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.74	0.68
6:F:96:THR:O	6:F:100:GLN:HG3	1.93	0.68
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.76	0.68
1:A:154:SER:HB3	1:A:162:VAL:CG2	2.24	0.68
12:L:48:CYS:HB3	12:L:51:CYS:O	1.93	0.68
4:D:24:ALA:HB3	4:D:26:THR:CG2	2.24	0.68
2:B:237:VAL:HG22	2:B:257:LYS:HA	1.75	0.68
1:A:709:THR:HG23	9:I:94:ASP:HA	1.75	0.68
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.34	0.68
1:A:1127:ASP:CG	1:A:1130:GLN:HB2	2.13	0.68
2:B:464:GLY:O	2:B:477:ALA:HA	1.94	0.68
1:A:117:GLU:H	1:A:117:GLU:CD	1.96	0.68
2:B:232:SER:HA	14:T:11:DA:OP1	1.93	0.67
2:B:43:LEU:HD11	2:B:811:TYR:O	1.94	0.67
1:A:709:THR:HB	1:A:712:GLU:H	1.59	0.67
1:A:1158:PRO:HG2	1:A:1159:ARG:NE	2.09	0.67
1:A:858:ASN:C	1:A:858:ASN:HD22	1.98	0.67
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.24	0.67
10:J:27:GLU:O	10:J:29:GLU:N	2.28	0.67
2:B:705:MET:H	2:B:710:LEU:CD1	2.07	0.67
4:D:59:ILE:HG21	4:D:145:MET:SD	2.35	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ALA:O	1:A:286:HIS:N	2.28	0.67
2:B:589:VAL:HG12	2:B:590:HIS:N	2.10	0.67
1:A:34:LYS:HZ2	1:A:57:ARG:NH2	1.90	0.67
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.22	0.67
1:A:369:SER:HB3	11:K:2:ASN:OD1	1.93	0.67
1:A:66:LYS:HZ3	1:A:68:GLN:N	1.83	0.67
2:B:863:GLU:O	2:B:961:LEU:HD13	1.94	0.67
8:H:81:PRO:CB	8:H:82:PRO:HD2	2.24	0.67
1:A:683:ILE:HD13	1:A:801:GLU:CG	2.24	0.67
1:A:886:ILE:HG23	1:A:887:GLY:H	1.58	0.67
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	1.94	0.67
3:C:254:LYS:O	3:C:258:ILE:HD13	1.94	0.67
1:A:1187:GLN:HA	1:A:1244:ARG:HB3	1.76	0.67
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.23	0.67
5:E:69:ILE:HD12	5:E:69:ILE:N	2.09	0.67
1:A:743:VAL:O	1:A:747:VAL:HG23	1.94	0.67
6:F:89:GLU:O	6:F:93:ILE:HD12	1.94	0.67
1:A:524:VAL:HG12	1:A:525:GLN:N	2.10	0.67
1:A:946:VAL:HG12	1:A:947:PHE:CD2	2.30	0.67
2:B:399:ASP:OD2	2:B:510:LYS:HB2	1.95	0.67
1:A:718:VAL:O	1:A:722:LEU:HD12	1.95	0.67
4:D:32:GLU:OE1	7:G:41:LYS:HE2	1.94	0.67
8:H:30:SER:HB2	8:H:36:CYS:HB3	1.77	0.67
2:B:863:GLU:OE2	2:B:873:THR:HA	1.94	0.67
9:I:55:THR:HG23	9:I:86:PHE:CZ	2.30	0.67
2:B:68:THR:HG22	2:B:91:SER:HB3	1.77	0.67
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.30	0.67
9:I:116:ASN:C	9:I:117:LYS:HD2	2.15	0.67
1:A:809:THR:OG1	1:A:812:GLU:HG3	1.94	0.67
2:B:899:ILE:HG22	2:B:900:ALA:O	1.95	0.67
4:D:119:ARG:HG3	4:D:119:ARG:HH11	1.60	0.66
5:E:94:LYS:O	5:E:98:ILE:HG13	1.95	0.66
9:I:80:SER:OG	9:I:105:SER:HB2	1.95	0.66
2:B:515:HIS:H	2:B:518:HIS:HD2	1.43	0.66
9:I:50:THR:HG22	9:I:51:ASN:N	2.10	0.66
1:A:567:LYS:CB	8:H:95:TYR:HA	2.24	0.66
1:A:382:PRO:CA	1:A:428:TYR:HE2	2.07	0.66
9:I:55:THR:O	9:I:55:THR:HG22	1.94	0.66
2:B:1187:ASN:O	2:B:1188:LYS:CB	2.42	0.66
1:A:925:LEU:HD13	1:A:983:ILE:CG2	2.24	0.66
1:A:332:LYS:O	1:A:333:GLU:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:ASP:HA	12:L:69:ALA:HB3	1.78	0.66
8:H:95:TYR:HE2	8:H:97:MET:CG	2.06	0.66
9:I:58:VAL:HG13	9:I:62:ILE:HD13	1.78	0.66
1:A:1223:ASP:HA	1:A:1243:VAL:HG11	1.76	0.66
2:B:917:PRO:O	2:B:918:ILE:HG13	1.95	0.66
1:A:684:ALA:O	1:A:687:LYS:HB2	1.94	0.66
1:A:688:LYS:HD2	1:A:691:LEU:HD23	1.77	0.66
2:B:251:ILE:HG22	2:B:251:ILE:O	1.96	0.66
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.24	0.66
9:I:8:ARG:HG3	9:I:34:TYR:CE1	2.30	0.66
1:A:122:MET:HA	1:A:141:LEU:CD1	2.25	0.66
1:A:55:ASP:N	1:A:56:PRO:HD3	2.10	0.66
3:C:124:LEU:HD21	3:C:129:ILE:O	1.95	0.66
4:D:185:CYS:O	4:D:211:LEU:HD22	1.94	0.66
9:I:76:PRO:HD2	9:I:108:HIS:CD2	2.29	0.66
3:C:161:LYS:O	3:C:170:TRP:NE1	2.27	0.66
8:H:89:LEU:C	8:H:91:ASP:N	2.47	0.66
4:D:29:LEU:HD22	4:D:29:LEU:N	2.10	0.66
6:F:82:THR:CG2	6:F:84:TYR:H	2.09	0.66
6:F:69:LEU:HD13	6:F:71:GLU:OE1	1.96	0.66
1:A:547:LEU:HD13	11:K:58:PHE:CD1	2.31	0.66
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.77	0.66
3:C:184:ASN:OD1	3:C:187:LYS:HA	1.94	0.66
1:A:866:PHE:C	1:A:867:ILE:HD12	2.15	0.66
1:A:446:ARG:HB3	1:A:478:TYR:HB3	1.77	0.66
8:H:58:THR:HG22	8:H:59:ILE:H	1.60	0.66
1:A:7:SER:HB3	2:B:1193:GLN:HE22	1.60	0.66
1:A:563:PRO:HD3	8:H:79:TRP:CD1	2.31	0.66
1:A:942:PHE:HE1	5:E:207:ARG:HD3	1.58	0.66
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.60	0.66
2:B:558:LEU:CD2	2:B:596:LEU:HD11	2.26	0.66
2:B:394:ASP:N	2:B:394:ASP:OD2	2.23	0.66
2:B:110:HIS:HB2	12:L:54:ARG:NH2	2.10	0.66
5:E:19:VAL:O	5:E:23:VAL:HG23	1.95	0.66
2:B:169:ARG:HB2	2:B:454:THR:HG23	1.78	0.66
5:E:48:ASP:HB3	5:E:54:GLN:NE2	2.10	0.66
2:B:69:LEU:HB3	2:B:429:PHE:HE1	1.61	0.66
1:A:50:ILE:C	1:A:52:GLY:H	1.98	0.66
2:B:1099:VAL:HG13	2:B:1100:ASP:N	2.11	0.66
1:A:1027:ALA:O	1:A:1031:VAL:HG23	1.96	0.66
1:A:503:GLN:NE2	6:F:90:ARG:HH22	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:HB3	1:A:265:LYS:HZ1	1.61	0.66
1:A:23:SER:HA	1:A:233:TRP:CD1	2.31	0.66
7:G:27:LYS:HD3	7:G:51:TYR:CE2	2.31	0.66
2:B:1060:ARG:CZ	3:C:202:PRO:HG3	2.25	0.66
4:D:54:GLU:O	4:D:58:VAL:HG23	1.95	0.66
2:B:882:THR:HG23	2:B:884:ARG:CB	2.24	0.65
1:A:914:GLU:HB2	1:A:979:SER:O	1.96	0.65
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.75	0.65
8:H:82:PRO:C	8:H:84:ALA:H	1.98	0.65
7:G:111:THR:HG23	7:G:114:LEU:HD13	1.77	0.65
9:I:4:PHE:HE2	9:I:14:LEU:O	1.79	0.65
3:C:35:ARG:NH1	11:K:41:THR:OG1	2.29	0.65
2:B:1115:THR:O	2:B:1116:ARG:HB2	1.94	0.65
2:B:37:PHE:CE1	2:B:41:LYS:HG3	2.31	0.65
4:D:156:ASP:O	4:D:158:GLU:N	2.30	0.65
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.77	0.65
12:L:30:ILE:O	12:L:56:LEU:HA	1.95	0.65
9:I:6:PHE:N	9:I:6:PHE:CD1	2.64	0.65
2:B:654:ARG:HH11	2:B:654:ARG:HG3	1.61	0.65
2:B:654:ARG:H	2:B:657:HIS:CD2	2.12	0.65
2:B:902:GLY:O	12:L:65:VAL:HG11	1.97	0.65
1:A:1152:ILE:HD13	1:A:1260:LEU:HD23	1.78	0.65
1:A:471:ASN:OD1	1:A:472:LEU:N	2.30	0.65
8:H:43:ASN:ND2	8:H:46:LEU:HD12	2.11	0.65
9:I:85:PHE:CD1	9:I:99:LEU:HD13	2.31	0.65
1:A:1313:LEU:O	1:A:1315:GLU:N	2.30	0.65
2:B:1124:ARG:HH11	2:B:1124:ARG:HB3	1.60	0.65
10:J:27:GLU:O	10:J:29:GLU:HG3	1.95	0.65
2:B:1001:PHE:CE2	3:C:34:ARG:NE	2.65	0.65
1:A:122:MET:HA	1:A:141:LEU:HD11	1.79	0.65
2:B:882:THR:HG21	2:B:934:LYS:O	1.95	0.65
3:C:172:PRO:O	3:C:235:VAL:HG23	1.95	0.65
10:J:3:VAL:HA	10:J:53:HIS:CE1	2.32	0.65
12:L:32:ALA:HB3	12:L:55:ILE:HG13	1.77	0.65
2:B:65:GLU:OE1	2:B:418:LYS:HE3	1.97	0.65
1:A:1255:GLU:HG2	1:A:1258:HIS:CD2	2.31	0.65
7:G:27:LYS:HG2	7:G:54:ILE:HD12	1.77	0.65
1:A:1149:ALA:CB	9:I:47:GLU:HA	2.26	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.27	0.65
5:E:56:LYS:HZ2	5:E:85:GLU:HG3	1.62	0.65
7:G:1:MET:SD	7:G:79:PHE:CD1	2.90	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:GLN:HE21	3:C:75:MET:N	1.93	0.65
2:B:189:LEU:O	2:B:192:LEU:N	2.29	0.65
1:A:709:THR:HG22	1:A:710:LEU:N	2.10	0.65
8:H:109:LYS:HG2	8:H:110:ASP:OD1	1.96	0.65
12:L:28:LYS:HB3	12:L:39:SER:HB2	1.79	0.65
3:C:34:ARG:NH1	3:C:35:ARG:HG2	2.12	0.65
1:A:66:LYS:O	1:A:67:CYS:HB2	1.96	0.65
2:B:243:ALA:CB	2:B:251:ILE:HD13	2.21	0.65
4:D:12:ARG:HH11	4:D:12:ARG:HG2	1.61	0.65
5:E:17:ARG:O	5:E:20:LYS:HB2	1.97	0.65
2:B:978:ASP:OD2	2:B:1098:MET:HG2	1.96	0.65
2:B:516:ASN:ND2	2:B:516:ASN:N	2.44	0.65
1:A:341:MET:HE1	2:B:1135:ARG:NH1	2.12	0.65
1:A:90:VAL:HG11	1:A:297:GLN:HA	1.77	0.65
4:D:66:ARG:HD2	4:D:133:THR:HB	1.78	0.65
1:A:102:VAL:HB	1:A:211:PHE:CE1	2.32	0.65
2:B:193:LYS:HZ2	12:L:32:ALA:HB1	1.60	0.65
6:F:82:THR:HG22	6:F:84:TYR:N	2.09	0.65
1:A:1313:LEU:HD23	1:A:1338:VAL:HG21	1.77	0.65
5:E:176:PRO:O	5:E:212:ARG:HA	1.97	0.65
11:K:63:VAL:O	11:K:63:VAL:HG23	1.95	0.65
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.31	0.65
1:A:67:CYS:C	1:A:68:GLN:HG3	2.17	0.65
4:D:124:GLU:CD	4:D:124:GLU:H	2.00	0.65
2:B:955:THR:CG2	2:B:956:THR:N	2.60	0.65
1:A:1130:GLN:O	1:A:1134:ILE:HG13	1.97	0.65
1:A:903:ASN:HD22	1:A:904:THR:H	1.45	0.65
7:G:27:LYS:HE2	7:G:54:ILE:HB	1.78	0.65
2:B:944:THR:HG21	2:B:1122:ARG:NH2	2.12	0.65
1:A:37:PHE:N	1:A:37:PHE:CD1	2.64	0.65
1:A:567:LYS:HZ3	8:H:46:LEU:HB2	1.61	0.65
1:A:7:SER:HB3	2:B:1193:GLN:NE2	2.11	0.65
2:B:879:ARG:CD	2:B:879:ARG:H	2.10	0.65
2:B:879:ARG:NH2	2:B:885:MET:CE	2.60	0.65
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.62	0.65
2:B:378:LEU:HD12	2:B:378:LEU:O	1.97	0.65
2:B:579:ARG:HA	2:B:589:VAL:HG13	1.78	0.65
6:F:118:LEU:O	6:F:122:MET:HG3	1.96	0.65
12:L:53:HIS:O	12:L:55:ILE:HD13	1.97	0.65
2:B:25:ILE:CG2	2:B:658:ILE:HD12	2.27	0.65
1:A:340:LEU:HD13	1:A:1429:ILE:HG23	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:ARG:HA	4:D:148:LEU:HD13	1.78	0.64
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.27	0.64
12:L:55:ILE:HG12	12:L:56:LEU:N	2.11	0.64
5:E:98:ILE:HA	5:E:101:GLN:HB3	1.79	0.64
1:A:1352:VAL:O	1:A:1355:VAL:HG12	1.96	0.64
7:G:116:PRO:HD2	7:G:119:LEU:HD23	1.79	0.64
2:B:90:ILE:HD11	2:B:432:MET:SD	2.38	0.64
1:A:250:ILE:HG22	1:A:250:ILE:O	1.96	0.64
1:A:977:LYS:HB3	1:A:978:PRO:HD2	1.78	0.64
3:C:244:VAL:O	3:C:248:ILE:HG13	1.98	0.64
1:A:904:THR:O	1:A:904:THR:HG22	1.97	0.64
2:B:294:ASP:O	2:B:296:GLU:N	2.30	0.64
8:H:25:ARG:HA	8:H:41:ASP:HA	1.79	0.64
9:I:55:THR:HG22	9:I:58:VAL:HG21	1.79	0.64
4:D:156:ASP:C	4:D:158:GLU:H	2.01	0.64
1:A:961:ARG:HG2	1:A:965:GLN:HE21	1.62	0.64
2:B:639:ILE:HG22	2:B:641:GLU:HG2	1.79	0.64
2:B:708:GLU:HG3	2:B:709:ASP:H	1.63	0.64
7:G:59:GLY:HA3	7:G:70:PHE:CD2	2.33	0.64
3:C:165:LYS:O	11:K:6:ARG:NH1	2.31	0.64
4:D:144:THR:O	4:D:148:LEU:HB2	1.97	0.64
1:A:390:GLN:NE2	1:A:394:ASN:HD22	1.95	0.64
3:C:31:ASN:OD1	3:C:34:ARG:HD3	1.97	0.64
1:A:55:ASP:C	1:A:57:ARG:N	2.47	0.64
4:D:119:ARG:NH1	4:D:119:ARG:HG3	2.12	0.64
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.79	0.64
8:H:84:ALA:CB	8:H:87:ARG:HD2	2.27	0.64
7:G:9:LEU:HD12	7:G:10:ASN:N	2.13	0.64
1:A:356:ASP:OD2	11:K:65:HIS:HE1	1.81	0.64
2:B:56:ASP:HB3	2:B:57:TYR:CD1	2.32	0.64
1:A:347:PHE:HE2	1:A:375:THR:HG23	1.61	0.64
1:A:573:SER:O	1:A:576:GLN:HB2	1.97	0.64
2:B:885:MET:HA	2:B:936:ASP:CB	2.26	0.64
2:B:98:THR:HG23	2:B:127:GLY:O	1.98	0.64
2:B:1159:ARG:NH1	2:B:1159:ARG:HB3	2.12	0.64
7:G:111:THR:O	7:G:114:LEU:N	2.28	0.64
1:A:535:THR:CG2	1:A:616:VAL:HA	2.27	0.64
1:A:35:ILE:O	1:A:35:ILE:HG22	1.96	0.64
14:T:18:DC:H2"	14:T:19:DT:OP2	1.97	0.64
5:E:127:ILE:O	5:E:127:ILE:HG13	1.96	0.64
2:B:597:MET:HA	2:B:597:MET:CE	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ILE:HD11	7:G:68:ALA:HB1	1.80	0.64
1:A:1444:MET:HG3	7:G:59:GLY:O	1.97	0.64
4:D:66:ARG:O	4:D:70:PHE:HB2	1.98	0.64
2:B:916:THR:HB	2:B:935:ARG:HD2	1.80	0.64
2:B:1181:GLU:HB2	2:B:1188:LYS:HG3	1.79	0.64
4:D:145:MET:O	4:D:149:THR:HB	1.96	0.64
5:E:144:ILE:HG13	5:E:145:THR:H	1.61	0.64
1:A:596:THR:O	1:A:598:LEU:N	2.31	0.64
1:A:153:PRO:HD3	1:A:161:LEU:HD13	1.77	0.64
5:E:128:PRO:HA	5:E:129:PRO:C	2.18	0.64
8:H:44:VAL:HG13	8:H:48:PRO:HA	1.78	0.64
10:J:1:MET:N	10:J:56:LEU:N	2.46	0.64
7:G:116:PRO:HG2	7:G:119:LEU:HB3	1.78	0.64
2:B:515:HIS:H	2:B:518:HIS:CD2	2.16	0.64
1:A:858:ASN:HD21	1:A:860:LEU:HB2	1.63	0.64
3:C:196:ASP:OD2	3:C:199:LYS:HE3	1.98	0.64
2:B:882:THR:C	2:B:884:ARG:H	2.00	0.64
5:E:78:LEU:HD21	5:E:80:VAL:HG23	1.80	0.64
1:A:1258:HIS:O	1:A:1262:LYS:HE3	1.97	0.64
2:B:408:LEU:O	2:B:411:PRO:HD2	1.97	0.64
2:B:521:LEU:HD22	2:B:633:VAL:HG12	1.79	0.64
2:B:426:LYS:O	2:B:426:LYS:HG3	1.97	0.64
2:B:364:ILE:O	2:B:365:THR:HB	1.97	0.63
1:A:794:PRO:HG2	1:A:795:GLU:OE2	1.98	0.63
3:C:120:ILE:CD1	3:C:124:LEU:HD11	2.27	0.63
7:G:112:LYS:HA	7:G:115:MET:CE	2.28	0.63
5:E:48:ASP:CG	5:E:49:SER:H	2.01	0.63
1:A:478:TYR:O	1:A:479:ASN:HB2	1.97	0.63
4:D:138:ASN:HB3	4:D:141:LEU:HB3	1.80	0.63
3:C:100:THR:HG21	3:C:102:GLN:HE21	1.64	0.63
5:E:28:TYR:C	5:E:65:THR:HG22	2.19	0.63
1:A:590:ARG:O	1:A:591:PHE:HB2	1.98	0.63
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.79	0.63
1:A:1341:ILE:HD12	1:A:1379:GLY:O	1.97	0.63
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.81	0.63
2:B:805:THR:HA	2:B:809:MET:HE1	1.80	0.63
2:B:221:ASN:O	2:B:222:ILE:HG13	1.99	0.63
4:D:35:LEU:HD11	4:D:173:HIS:CD2	2.33	0.63
2:B:879:ARG:NH2	2:B:885:MET:HE2	2.14	0.63
2:B:289:LEU:HD13	2:B:375:ALA:CB	2.25	0.63
2:B:996:ARG:HH12	3:C:175:ALA:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:236:GLY:O	3:C:238:ILE:N	2.31	0.63
2:B:95:ILE:CG1	2:B:130:VAL:HG22	2.29	0.63
2:B:95:ILE:HG13	2:B:130:VAL:HG22	1.78	0.63
1:A:984:LYS:HG2	1:A:988:LEU:HD11	1.80	0.63
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.33	0.63
7:G:87:VAL:HG23	7:G:103:VAL:HG21	1.79	0.63
4:D:179:GLN:OE1	4:D:179:GLN:HA	1.97	0.63
9:I:58:VAL:HG13	9:I:62:ILE:CD1	2.29	0.63
1:A:1107:VAL:CG1	1:A:1107:VAL:O	2.45	0.63
1:A:1387:HIS:CE1	13:N:4:DA:H5'	2.33	0.63
2:B:558:LEU:HD11	2:B:596:LEU:HD21	1.79	0.63
2:B:798:TYR:CE2	3:C:62:PHE:CE2	2.82	0.63
1:A:185:TRP:CE3	1:A:185:TRP:N	2.65	0.63
1:A:335:ARG:HH12	2:B:1206:GLU:CD	2.02	0.63
4:D:13:ARG:C	4:D:15:LEU:H	2.02	0.63
11:K:54:ARG:HG2	11:K:54:ARG:HH11	1.63	0.63
8:H:56:THR:HB	8:H:145:ARG:HG2	1.79	0.63
1:A:1223:ASP:HA	1:A:1243:VAL:CG1	2.28	0.63
1:A:1187:GLN:CB	1:A:1244:ARG:HG2	2.25	0.63
4:D:123:LEU:O	4:D:127:ASP:HB2	1.99	0.63
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.28	0.63
3:C:11:ARG:HH12	3:C:205:LYS:CE	2.11	0.63
2:B:579:ARG:HH11	2:B:579:ARG:HG2	1.64	0.63
1:A:710:LEU:HD12	1:A:710:LEU:N	2.14	0.63
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.14	0.63
4:D:190:GLU:C	4:D:193:THR:HG22	2.19	0.63
1:A:441:PRO:HD2	1:A:498:ARG:NH2	2.13	0.63
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.17	0.63
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.79	0.63
1:A:1313:LEU:C	1:A:1315:GLU:H	2.02	0.63
2:B:839:MET:CE	2:B:1010:LEU:HD21	2.28	0.63
1:A:37:PHE:HD1	1:A:37:PHE:N	1.97	0.63
2:B:56:ASP:HB3	2:B:57:TYR:HD1	1.63	0.63
2:B:259:TYR:HB2	2:B:268:THR:HG23	1.80	0.63
1:A:134:ARG:HD2	1:A:221:SER:O	1.98	0.63
5:E:84:ASP:O	5:E:86:PRO:HD3	1.97	0.63
2:B:999:MET:HE3	2:B:999:MET:HA	1.80	0.63
11:K:31:VAL:HG12	11:K:32:VAL:N	2.13	0.63
1:A:308:ILE:HG22	1:A:309:ALA:N	2.13	0.63
2:B:35:SER:HA	2:B:811:TYR:HE2	1.63	0.63
7:G:91:VAL:HG23	7:G:141:SER:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.81	0.62
3:C:163:ILE:HG13	3:C:165:LYS:H	1.64	0.62
2:B:995:ARG:NH1	3:C:165:LYS:HG2	2.14	0.62
12:L:53:HIS:HB3	12:L:55:ILE:HD11	1.80	0.62
1:A:390:GLN:O	1:A:394:ASN:HB2	1.99	0.62
3:C:179:GLU:HG2	3:C:180:TYR:N	2.14	0.62
1:A:347:PHE:H	2:B:1107:ALA:HA	1.63	0.62
5:E:213:ILE:HG12	5:E:214:CYS:H	1.64	0.62
7:G:20:PRO:HD2	7:G:21:ARG:H	1.64	0.62
2:B:891:ASP:O	2:B:893:LEU:N	2.32	0.62
2:B:1001:PHE:CE1	2:B:1073:TYR:HB2	2.34	0.62
2:B:756:ILE:O	2:B:759:PRO:HD3	1.98	0.62
11:K:82:ASP:OD1	11:K:84:LYS:N	2.32	0.62
1:A:714:PHE:O	1:A:718:VAL:HG23	2.00	0.62
1:A:754:SER:N	1:A:757:ASN:HD22	1.96	0.62
1:A:1018:PHE:O	1:A:1021:LEU:HB3	1.98	0.62
1:A:145:LYS:HE3	1:A:145:LYS:HA	1.81	0.62
1:A:11:LEU:HB2	2:B:1193:GLN:HG2	1.81	0.62
2:B:987:LYS:HG3	15:P:11:G:O2'	1.99	0.62
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.34	0.62
12:L:61:THR:HG22	12:L:62:LYS:N	2.15	0.62
1:A:443:LEU:HD12	2:B:1146:PHE:CZ	2.34	0.62
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.30	0.62
1:A:1239:ARG:HH22	1:A:1241:ARG:HH22	1.45	0.62
1:A:694:THR:O	1:A:698:GLN:HG3	1.98	0.62
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.00	0.62
1:A:831:THR:CG2	1:A:832:ALA:H	2.13	0.62
1:A:1420:ASP:OD2	1:A:1420:ASP:N	2.31	0.62
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.81	0.62
2:B:654:ARG:N	2:B:657:HIS:HD2	1.96	0.62
10:J:9:SER:HB2	10:J:45:CYS:HB2	1.82	0.62
8:H:77:ARG:HG2	8:H:78:SER:H	1.63	0.62
9:I:44:TYR:CD1	9:I:45:ARG:N	2.68	0.62
1:A:266:LEU:HD21	1:A:303:TYR:CE1	2.34	0.62
1:A:367:PRO:HG2	1:A:370:ILE:HD12	1.81	0.62
2:B:616:ILE:HD12	2:B:616:ILE:N	2.14	0.62
8:H:11:GLN:O	8:H:28:ALA:HB1	2.00	0.62
2:B:844:SER:O	2:B:847:ASP:HB2	2.00	0.62
10:J:3:VAL:HA	10:J:53:HIS:ND1	2.14	0.62
1:A:596:THR:C	1:A:598:LEU:H	2.03	0.62
12:L:26:THR:CG2	12:L:27:LEU:N	2.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:948:ILE:HG22	2:B:949:VAL:O	1.99	0.62
5:E:157:SER:O	5:E:159:ASP:N	2.33	0.62
2:B:345:LYS:N	2:B:347:LYS:HE2	2.15	0.62
1:A:41:MET:HB2	1:A:49:LYS:HA	1.81	0.62
2:B:957:ASN:O	2:B:959:ASP:N	2.33	0.62
2:B:954:VAL:O	12:L:55:ILE:O	2.16	0.62
1:A:1171:GLN:O	1:A:1174:PHE:HB2	2.00	0.62
9:I:93:LYS:HD3	9:I:93:LYS:N	2.15	0.62
3:C:34:ARG:HH11	3:C:35:ARG:HG2	1.64	0.62
4:D:192:LYS:HD2	4:D:199:ASN:HA	1.81	0.62
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.40	0.62
2:B:582:VAL:HG23	2:B:626:ILE:HB	1.80	0.62
1:A:718:VAL:HG12	1:A:722:LEU:HD11	1.81	0.62
1:A:106:VAL:HG12	1:A:107:CYS:N	2.15	0.62
1:A:590:ARG:HG2	1:A:604:GLY:HA2	1.80	0.62
2:B:466:TRP:O	2:B:468:GLU:N	2.33	0.62
1:A:984:LYS:HG2	1:A:988:LEU:CD1	2.30	0.62
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.35	0.62
1:A:1189:SER:O	1:A:1241:ARG:HD3	1.99	0.62
3:C:148:ARG:H	3:C:151:GLN:HG3	1.65	0.62
3:C:235:VAL:HG13	10:J:13:VAL:HG22	1.82	0.62
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.82	0.62
2:B:57:TYR:N	2:B:57:TYR:HD1	1.98	0.62
5:E:99:HIS:O	5:E:103:LYS:HG2	1.99	0.62
1:A:782:ARG:NH2	2:B:699:GLU:O	2.33	0.62
1:A:1218:GLN:O	1:A:1221:LYS:HG3	2.00	0.62
2:B:642:ASP:CA	2:B:649:LYS:HA	2.30	0.62
1:A:75:ASN:HD22	2:B:1116:ARG:NH1	1.97	0.62
1:A:873:MET:C	1:A:1058:VAL:HG23	2.19	0.61
2:B:615:MET:CB	2:B:626:ILE:HG12	2.29	0.61
2:B:707:PRO:HG2	2:B:708:GLU:N	2.13	0.61
1:A:1170:ILE:HD12	1:A:1170:ILE:N	2.13	0.61
7:G:112:LYS:HA	7:G:115:MET:HE3	1.80	0.61
9:I:84:VAL:O	9:I:84:VAL:HG13	2.00	0.61
7:G:132:SER:HB3	7:G:135:ASP:H	1.65	0.61
2:B:879:ARG:NE	2:B:879:ARG:H	1.97	0.61
2:B:996:ARG:NH2	3:C:38:ILE:HG23	2.15	0.61
3:C:205:LYS:HG2	3:C:205:LYS:O	2.00	0.61
2:B:1130:PHE:HZ	2:B:1138:MET:HG2	1.65	0.61
2:B:570:VAL:HG21	2:B:573:GLN:CD	2.20	0.61
1:A:69:THR:O	1:A:71:GLN:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:ARG:HB2	1:A:797:LYS:O	2.01	0.61
10:J:44:TYR:H	10:J:44:TYR:HD2	1.48	0.61
4:D:4:SER:O	4:D:5:THR:CB	2.47	0.61
2:B:305:VAL:HG12	2:B:305:VAL:O	1.99	0.61
2:B:617:ARG:HA	2:B:624:LEU:HD12	1.83	0.61
8:H:5:LEU:HG	8:H:60:ALA:HA	1.83	0.61
1:A:661:GLY:HA3	2:B:1081:LEU:HD22	1.81	0.61
2:B:953:LEU:CD2	2:B:965:LYS:HB2	2.30	0.61
1:A:23:SER:HB3	1:A:233:TRP:CZ2	2.35	0.61
4:D:195:ILE:CG2	4:D:198:LEU:HG	2.31	0.61
2:B:465:ASN:N	2:B:465:ASN:ND2	2.45	0.61
9:I:50:THR:CG2	9:I:52:ILE:HG12	2.30	0.61
9:I:44:TYR:HD1	9:I:45:ARG:N	1.98	0.61
1:A:150:THR:HG23	1:A:166:GLY:HA2	1.81	0.61
1:A:2:VAL:HG22	1:A:3:GLY:H	1.66	0.61
7:G:26:LEU:HD11	7:G:70:PHE:CD1	2.35	0.61
10:J:1:MET:H1	10:J:56:LEU:N	1.98	0.61
4:D:12:ARG:NH1	4:D:14:ARG:HA	2.15	0.61
1:A:768:GLN:CG	1:A:816:HIS:HA	2.28	0.61
1:A:288:ALA:HA	1:A:291:GLU:CG	2.30	0.61
1:A:1150:SER:HB3	1:A:1195:LEU:CD2	2.31	0.61
9:I:101:PHE:N	9:I:101:PHE:CD1	2.68	0.61
2:B:218:SER:CB	2:B:241:ARG:HH12	2.14	0.61
6:F:90:ARG:HD3	6:F:155:LEU:CD1	2.22	0.61
6:F:103:MET:O	6:F:104:ASN:HB2	2.01	0.61
1:A:898:ARG:HD3	1:A:933:TYR:CD1	2.36	0.61
1:A:482:PHE:CE1	2:B:836:GLU:HB2	2.35	0.61
2:B:906:SER:HA	2:B:946:ASN:HB2	1.82	0.61
4:D:207:LEU:O	4:D:207:LEU:HD12	2.00	0.61
2:B:290:GLY:O	2:B:292:ILE:HG13	2.01	0.61
3:C:11:ARG:HH12	3:C:205:LYS:HE2	1.66	0.61
6:F:109:VAL:HG11	6:F:123:LYS:HG2	1.81	0.61
3:C:50:GLU:OE1	12:L:64:LEU:HD13	2.00	0.61
2:B:637:LEU:HD11	2:B:703:ILE:HD13	1.81	0.61
8:H:38:LEU:HD12	8:H:124:ARG:O	2.01	0.61
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.13	0.61
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.83	0.61
2:B:283:VAL:HG21	2:B:317:CYS:O	2.00	0.61
2:B:39:ARG:CZ	2:B:665:GLU:HG2	2.30	0.61
1:A:517:ASN:HD22	1:A:1364:ASN:HD22	1.47	0.61
2:B:360:PHE:CD2	2:B:361:LEU:HB2	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1445:ILE:HD12	1:A:1445:ILE:N	2.08	0.61
1:A:691:LEU:O	1:A:694:THR:HB	2.01	0.61
3:C:123:ASN:HD21	3:C:125:MET:HA	1.64	0.61
1:A:16:GLU:OE1	4:D:13:ARG:NH2	2.32	0.61
1:A:1227:ILE:HG22	1:A:1228:TRP:N	2.15	0.61
1:A:1141:THR:CG2	1:A:1205:LYS:HD3	2.31	0.61
2:B:309:GLN:CD	9:I:52:ILE:HD11	2.21	0.61
10:J:14:VAL:HG12	10:J:14:VAL:O	2.01	0.61
2:B:123:THR:OG1	2:B:458:LYS:HE2	2.01	0.61
1:A:1241:ARG:O	1:A:1242:VAL:CG2	2.48	0.61
9:I:86:PHE:CE1	9:I:100:PHE:HB2	2.36	0.61
2:B:1096:ARG:O	2:B:1097:HIS:CB	2.48	0.61
2:B:57:TYR:CD1	2:B:57:TYR:N	2.68	0.61
3:C:147:LEU:HD23	3:C:147:LEU:N	2.16	0.60
2:B:847:ASP:C	2:B:849:GLY:H	2.02	0.60
3:C:166:GLU:C	11:K:6:ARG:NH1	2.54	0.60
3:C:66:ARG:NH1	10:J:2:ILE:CG2	2.63	0.60
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.82	0.60
1:A:353:ILE:HG21	1:A:487:MET:HG3	1.81	0.60
1:A:537:ARG:NH1	8:H:120:GLY:O	2.34	0.60
1:A:1244:ARG:HB2	1:A:1245:PRO:HD2	1.82	0.60
2:B:288:ALA:O	2:B:331:LEU:HD11	2.00	0.60
6:F:90:ARG:NH1	6:F:94:LEU:HD11	2.15	0.60
2:B:912:ILE:O	2:B:938:SER:HB3	2.01	0.60
8:H:58:THR:HG22	8:H:59:ILE:N	2.15	0.60
1:A:1308:THR:CG2	1:A:1309:ASP:N	2.62	0.60
1:A:733:ALA:O	1:A:737:LEU:HG	2.01	0.60
2:B:1124:ARG:NH1	2:B:1124:ARG:HB3	2.16	0.60
3:C:31:ASN:O	3:C:35:ARG:HG3	2.01	0.60
8:H:143:LEU:N	8:H:143:LEU:HD12	2.17	0.60
1:A:66:LYS:NZ	1:A:68:GLN:N	2.46	0.60
7:G:123:ALA:C	7:G:125:SER:H	2.04	0.60
1:A:1385:THR:HG22	1:A:1386:ARG:H	1.67	0.60
1:A:469:ARG:NH2	2:B:991:GLY:O	2.35	0.60
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.82	0.60
9:I:73:ARG:HD2	9:I:101:PHE:CE2	2.35	0.60
7:G:55:ASP:OD1	7:G:57:GLN:HG3	2.02	0.60
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.67	0.60
2:B:37:PHE:HE1	2:B:41:LYS:HG3	1.64	0.60
4:D:155:ARG:HD3	4:D:221:TYR:CE1	2.37	0.60
3:C:97:VAL:HG12	3:C:99:LEU:CD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:PRO:O	6:F:77:ASP:O	2.19	0.60
1:A:219:PHE:HE1	1:A:230:ARG:HE	1.48	0.60
1:A:289:ILE:HG22	1:A:290:GLU:N	2.16	0.60
2:B:235:SER:OG	2:B:236:HIS:CD2	2.54	0.60
1:A:869:GLY:O	5:E:204:THR:HG21	2.01	0.60
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.21	0.60
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.84	0.60
7:G:126:ASN:C	7:G:126:ASN:HD22	2.05	0.60
9:I:61:ASP:C	9:I:63:GLY:H	2.05	0.60
3:C:242:GLN:C	3:C:244:VAL:H	2.05	0.60
7:G:115:MET:HB3	7:G:116:PRO:CD	2.32	0.60
1:A:1342:GLU:CG	5:E:198:ILE:HD13	2.32	0.60
11:K:94:ILE:O	11:K:98:LEU:HG	2.00	0.60
9:I:46:HIS:CE1	9:I:48:LEU:HD23	2.37	0.60
2:B:205:ILE:N	2:B:205:ILE:HD12	2.17	0.60
4:D:130:LEU:HD13	4:D:142:LYS:CD	2.32	0.60
12:L:38:LEU:O	12:L:39:SER:HB3	2.02	0.60
6:F:130:ILE:HB	6:F:148:VAL:HG21	1.83	0.60
1:A:302:THR:HA	1:A:305:ASP:O	2.02	0.60
3:C:177:GLU:CG	3:C:231:ASN:HB3	2.29	0.60
1:A:870:GLU:HG2	5:E:208:TYR:CG	2.36	0.60
2:B:309:GLN:HG3	9:I:52:ILE:HD12	1.84	0.60
2:B:558:LEU:HD21	2:B:596:LEU:HD11	1.84	0.60
7:G:85:GLU:HG2	7:G:87:VAL:HG13	1.83	0.60
2:B:781:PHE:HE2	2:B:795:ILE:HD11	1.65	0.60
5:E:37:LEU:CD1	5:E:41:ASP:HB2	2.31	0.60
1:A:718:VAL:O	1:A:721:PHE:HB2	2.01	0.60
10:J:5:VAL:HG12	10:J:6:ARG:CG	2.32	0.60
1:A:351:THR:CG2	2:B:1103:ILE:HG13	2.32	0.60
8:H:84:ALA:O	8:H:85:GLY:C	2.41	0.60
5:E:192:ARG:HG3	5:E:192:ARG:HH11	1.67	0.60
1:A:1070:GLN:O	1:A:1074:GLU:HB2	2.02	0.60
1:A:23:SER:HA	1:A:233:TRP:NE1	2.16	0.60
8:H:65:LEU:H	8:H:65:LEU:HD23	1.66	0.60
2:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.32	0.60
10:J:21:TYR:HB2	10:J:39:LEU:CD1	2.32	0.60
1:A:100:LYS:HE2	1:A:104:GLU:OE2	2.01	0.60
3:C:33:LEU:O	3:C:33:LEU:HD12	2.01	0.60
1:A:1202:MET:CE	1:A:1212:VAL:HG21	2.31	0.60
2:B:557:PHE:O	2:B:557:PHE:CD2	2.53	0.60
1:A:1161:THR:HG21	1:A:1163:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:LEU:HD12	1:A:1194:ARG:N	2.17	0.60
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.37	0.60
2:B:126:SER:CB	2:B:172:ILE:HD11	2.32	0.60
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.01	0.60
1:A:1342:GLU:HG3	5:E:198:ILE:HG21	1.83	0.60
1:A:946:VAL:HG22	5:E:201:LYS:HD2	1.82	0.60
5:E:99:HIS:CE1	5:E:103:LYS:HG3	2.37	0.60
3:C:182:PRO:HD2	3:C:210:GLU:OE1	2.01	0.60
1:A:1144:LYS:HB2	1:A:1268:LEU:O	2.01	0.60
2:B:559:SER:CA	2:B:563:MET:HB3	2.10	0.59
4:D:29:LEU:HD12	7:G:82:PHE:CE2	2.37	0.59
6:F:103:MET:HE2	7:G:66:GLY:H	1.66	0.59
1:A:754:SER:H	1:A:757:ASN:ND2	1.98	0.59
5:E:212:ARG:HH11	5:E:212:ARG:HG3	1.67	0.59
1:A:899:VAL:HB	1:A:929:LEU:HD12	1.83	0.59
2:B:260:GLY:O	2:B:267:ARG:NH1	2.34	0.59
8:H:59:ILE:O	8:H:60:ALA:HB3	2.01	0.59
1:A:385:ILE:HD11	1:A:426:LEU:HB2	1.82	0.59
2:B:872:GLU:CD	2:B:914:LYS:HE3	2.23	0.59
11:K:21:ILE:HG22	11:K:31:VAL:HG11	1.84	0.59
3:C:7:GLN:HG3	11:K:104:ASN:ND2	2.17	0.59
2:B:1177:HIS:HB3	2:B:1179:GLN:HE21	1.67	0.59
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.84	0.59
1:A:380:VAL:HG13	1:A:385:ILE:HG12	1.83	0.59
4:D:128:VAL:C	4:D:130:LEU:N	2.54	0.59
2:B:68:THR:HA	2:B:90:ILE:O	2.02	0.59
4:D:9:GLN:HG3	4:D:9:GLN:O	2.03	0.59
2:B:1031:LEU:HD11	2:B:1042:GLY:CA	2.32	0.59
1:A:1148:ILE:HG12	1:A:1198:ASP:HB2	1.83	0.59
3:C:35:ARG:NH1	11:K:41:THR:H	2.00	0.59
2:B:781:PHE:HD2	2:B:781:PHE:H	1.49	0.59
5:E:136:ASN:OD1	5:E:138:ALA:N	2.35	0.59
2:B:797:TYR:O	10:J:1:MET:HG2	2.02	0.59
4:D:153:ARG:C	4:D:154:PHE:CD2	2.76	0.59
4:D:156:ASP:C	4:D:158:GLU:N	2.54	0.59
4:D:56:ARG:HD3	4:D:149:THR:HA	1.84	0.59
1:A:186:LYS:O	1:A:187:LYS:HB2	2.01	0.59
8:H:30:SER:CB	8:H:36:CYS:HB3	2.32	0.59
2:B:347:LYS:HG3	2:B:348:ARG:H	1.67	0.59
2:B:868:MET:O	2:B:870:ILE:HG13	2.01	0.59
2:B:1007:VAL:CG2	2:B:1008:PRO:HD2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:258:ILE:HD11	11:K:42:LEU:HD21	1.83	0.59
1:A:353:ILE:HD12	1:A:470:LEU:HD21	1.85	0.59
4:D:51:ASN:O	4:D:52:LEU:O	2.20	0.59
3:C:208:GLU:O	3:C:210:GLU:N	2.36	0.59
2:B:745:PRO:O	2:B:747:MET:N	2.36	0.59
1:A:567:LYS:HD2	8:H:95:TYR:CG	2.38	0.59
1:A:87:ALA:CB	1:A:276:LEU:HD23	2.27	0.59
7:G:49:LEU:HG	7:G:76:ALA:HA	1.84	0.59
2:B:1102:LYS:O	2:B:1103:ILE:C	2.41	0.59
1:A:102:VAL:HG11	1:A:211:PHE:HE1	1.68	0.59
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.84	0.59
2:B:120:ARG:NH1	12:L:54:ARG:HH11	2.01	0.59
1:A:464:PRO:HG2	1:A:465:TYR:HD1	1.68	0.59
2:B:1031:LEU:O	2:B:1031:LEU:HD12	2.03	0.59
1:A:447:GLN:NE2	14:T:20:DG:H4'	2.17	0.59
2:B:549:THR:HG22	2:B:550:ASP:H	1.66	0.59
1:A:567:LYS:HD2	8:H:95:TYR:HA	1.84	0.59
1:A:666:ILE:HD11	2:B:1086:PHE:HE1	1.67	0.59
2:B:248:SER:N	2:B:418:LYS:HZ3	2.00	0.59
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.84	0.59
2:B:1084:GLN:NE2	2:B:1084:GLN:N	2.51	0.59
2:B:297:ILE:HG22	2:B:298:LEU:HD22	1.85	0.59
2:B:332:ASP:OD1	2:B:348:ARG:HD2	2.03	0.59
2:B:708:GLU:O	2:B:710:LEU:N	2.36	0.59
2:B:999:MET:HB3	2:B:1007:VAL:HG21	1.85	0.59
1:A:671:ALA:O	1:A:676:MET:HE2	2.02	0.59
1:A:981:LEU:CD2	1:A:1039:LYS:HA	2.32	0.59
1:A:964:ILE:O	1:A:967:ALA:HB3	2.03	0.59
1:A:1325:THR:HG22	1:A:1326:ARG:HG3	1.82	0.59
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.33	0.59
1:A:88:LYS:HG3	1:A:276:LEU:HD21	1.85	0.59
15:P:10:U:H5'	15:P:11:G:C3'	2.33	0.59
6:F:69:LEU:HB3	6:F:71:GLU:OE2	2.02	0.59
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.31	0.59
1:A:444:PHE:CB	1:A:458:HIS:HD2	2.16	0.59
2:B:732:SER:HB2	2:B:734:HIS:NE2	2.18	0.59
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.43	0.59
2:B:562:GLY:HA3	2:B:590:HIS:ND1	2.17	0.59
2:B:579:ARG:CB	2:B:586:TRP:HE1	2.16	0.59
5:E:135:PHE:HD2	5:E:140:LEU:HD21	1.67	0.59
2:B:1084:GLN:HE21	2:B:1084:GLN:N	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:SER:OG	1:A:477:PRO:HD3	2.03	0.59
7:G:90:THR:HG22	7:G:91:VAL:O	2.03	0.59
1:A:416:ARG:HH11	1:A:417:TYR:HE1	1.51	0.59
3:C:69:LEU:HD12	3:C:69:LEU:N	2.17	0.58
10:J:57:ILE:HA	10:J:60:PHE:HD2	1.66	0.58
1:A:925:LEU:HD13	1:A:983:ILE:HG21	1.83	0.58
2:B:975:GLN:O	2:B:990:ILE:HD12	2.02	0.58
2:B:429:PHE:HD1	2:B:432:MET:HE3	1.68	0.58
11:K:18:LYS:NZ	11:K:37:LYS:O	2.35	0.58
6:F:109:VAL:HG21	6:F:124:GLU:HA	1.84	0.58
2:B:360:PHE:HD2	2:B:361:LEU:HB2	1.68	0.58
3:C:40:GLU:HA	3:C:163:ILE:HD12	1.85	0.58
7:G:34:VAL:CG1	7:G:45:ILE:HG21	2.32	0.58
9:I:19:ASP:HB3	9:I:24:ARG:HG2	1.85	0.58
5:E:92:THR:O	5:E:95:THR:HB	2.03	0.58
1:A:1161:THR:C	1:A:1163:ILE:H	2.07	0.58
1:A:1239:ARG:HH12	1:A:1241:ARG:HH12	1.50	0.58
3:C:97:VAL:HG12	3:C:99:LEU:HD21	1.85	0.58
4:D:17:LYS:HD2	4:D:18:VAL:HG13	1.84	0.58
1:A:1259:MET:HA	1:A:1262:LYS:CD	2.33	0.58
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.85	0.58
9:I:116:ASN:O	9:I:117:LYS:HD2	2.03	0.58
2:B:246:LYS:HA	2:B:249:ARG:CZ	2.33	0.58
5:E:93:MET:CG	5:E:123:LEU:HD12	2.34	0.58
11:K:65:HIS:HD2	11:K:67:PHE:N	2.01	0.58
1:A:1286:LYS:HB2	1:A:1304:TRP:CZ3	2.39	0.58
1:A:186:LYS:NZ	1:A:197:PRO:HD3	2.18	0.58
2:B:353:LYS:O	2:B:357:GLN:HG2	2.03	0.58
8:H:42:ILE:HG23	8:H:95:TYR:CE1	2.39	0.58
4:D:120:GLU:OE1	4:D:120:GLU:O	2.22	0.58
1:A:1094:VAL:CG2	1:A:1113:THR:HG21	2.29	0.58
2:B:801:LYS:O	10:J:52:THR:CG2	2.51	0.58
1:A:1308:THR:HG23	1:A:1310:GLY:H	1.69	0.58
2:B:65:GLU:HG3	2:B:66:ASP:N	2.14	0.58
2:B:953:LEU:O	2:B:953:LEU:HD23	2.04	0.58
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.85	0.58
1:A:203:SER:O	1:A:206:GLU:HB3	2.03	0.58
1:A:288:ALA:HA	1:A:291:GLU:CD	2.24	0.58
2:B:235:SER:C	2:B:236:HIS:CD2	2.77	0.58
1:A:857:ARG:NH1	6:F:139:PRO:HB2	2.19	0.58
2:B:295:GLY:H	2:B:298:LEU:HD23	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:SER:O	3:C:36:VAL:HG23	2.03	0.58
1:A:1444:MET:CE	6:F:135:ARG:HB2	2.34	0.58
1:A:666:ILE:HD11	2:B:1067:ARG:O	2.03	0.58
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.85	0.58
1:A:332:LYS:HD3	1:A:333:GLU:HG2	1.85	0.58
5:E:213:ILE:HG12	5:E:214:CYS:N	2.18	0.58
1:A:1120:LEU:O	1:A:1323:ASP:HB2	2.03	0.58
7:G:58:ARG:HH11	7:G:58:ARG:HG3	1.68	0.58
1:A:503:GLN:NE2	6:F:90:ARG:NH2	2.48	0.58
1:A:256:GLN:NE2	2:B:935:ARG:HH12	2.01	0.58
2:B:1187:ASN:HD21	2:B:1190:ASP:HB3	1.69	0.58
3:C:177:GLU:HG3	3:C:231:ASN:ND2	2.18	0.58
8:H:81:PRO:HB3	8:H:82:PRO:HD2	1.85	0.58
9:I:80:SER:HB2	9:I:103:CYS:SG	2.43	0.58
1:A:1066:VAL:O	1:A:1070:GLN:HG3	2.04	0.58
1:A:710:LEU:CD1	1:A:710:LEU:H	2.15	0.58
3:C:114:TYR:CD2	3:C:140:ASN:CB	2.86	0.58
2:B:871:THR:HG22	2:B:872:GLU:O	2.04	0.58
2:B:955:THR:CG2	2:B:956:THR:H	2.17	0.58
9:I:78:CYS:SG	9:I:106:CYS:SG	3.01	0.58
2:B:468:GLU:OE1	2:B:470:LYS:HE3	2.04	0.58
2:B:217:ARG:C	2:B:217:ARG:HD2	2.24	0.58
1:A:1241:ARG:O	1:A:1242:VAL:CB	2.52	0.58
1:A:1438:THR:O	6:F:92:ARG:NH1	2.37	0.58
1:A:265:LYS:O	1:A:269:ILE:HG13	2.02	0.58
10:J:1:MET:H2	10:J:57:ILE:H	1.51	0.58
2:B:906:SER:O	2:B:941:LEU:HD23	2.04	0.58
9:I:8:ARG:HG3	9:I:34:TYR:HE1	1.66	0.58
5:E:198:ILE:CD1	5:E:212:ARG:HG3	2.34	0.58
1:A:119:ASN:O	1:A:122:MET:HB3	2.04	0.58
4:D:52:LEU:HD21	4:D:147:TYR:HE2	1.68	0.58
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.85	0.58
2:B:398:ARG:HB2	2:B:398:ARG:NH1	2.19	0.58
1:A:567:LYS:CB	8:H:96:VAL:H	2.05	0.57
4:D:35:LEU:H	4:D:35:LEU:HD12	1.68	0.57
3:C:124:LEU:O	3:C:127:ARG:HG2	2.03	0.57
2:B:758:PHE:HE1	2:B:1027:ILE:HG22	1.69	0.57
11:K:79:GLU:HG3	11:K:80:GLY:N	2.19	0.57
1:A:1340:GLY:HA2	5:E:183:PRO:HD2	1.86	0.57
1:A:1353:TYR:CD2	1:A:1353:TYR:C	2.77	0.57
1:A:1208:THR:HB	1:A:1211:GLN:CG	2.16	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:LEU:HD13	8:H:123:MET:CE	2.31	0.57
10:J:57:ILE:O	10:J:60:PHE:HB2	2.04	0.57
4:D:118:THR:O	4:D:121:LYS:N	2.29	0.57
4:D:163:VAL:O	4:D:167:LEU:HG	2.04	0.57
5:E:15:ALA:O	5:E:19:VAL:HG23	2.03	0.57
5:E:78:LEU:HD23	5:E:78:LEU:C	2.23	0.57
5:E:124:VAL:HA	5:E:132:ILE:CD1	2.33	0.57
3:C:226:ASP:O	3:C:227:THR:HB	2.04	0.57
1:A:129:LYS:O	1:A:130:ASP:HB2	2.04	0.57
2:B:254:LEU:HD11	2:B:273:LEU:HD23	1.85	0.57
1:A:63:ARG:HA	1:A:74:MET:CE	2.33	0.57
2:B:891:ASP:C	2:B:893:LEU:N	2.55	0.57
1:A:628:GLY:O	1:A:632:VAL:HG23	2.03	0.57
5:E:153:HIS:O	5:E:154:ILE:HG13	2.04	0.57
2:B:996:ARG:HH21	3:C:38:ILE:HG23	1.69	0.57
5:E:147:HIS:CD2	5:E:149:LEU:H	2.21	0.57
1:A:102:VAL:HB	1:A:211:PHE:CZ	2.39	0.57
4:D:123:LEU:CD1	4:D:149:THR:HG21	2.33	0.57
2:B:758:PHE:CE1	2:B:1027:ILE:CG2	2.87	0.57
1:A:851:HIS:O	1:A:853:ASP:N	2.37	0.57
1:A:855:THR:HG21	1:A:857:ARG:NE	2.20	0.57
1:A:833:GLU:O	1:A:837:ILE:HG13	2.04	0.57
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.26	0.57
1:A:265:LYS:HE3	1:A:265:LYS:HA	1.85	0.57
1:A:322:VAL:CG1	1:A:322:VAL:O	2.53	0.57
1:A:49:LYS:HE2	1:A:61:ILE:HD12	1.85	0.57
1:A:1339:LEU:HD13	5:E:147:HIS:CD2	2.40	0.57
3:C:101:LEU:HD13	3:C:118:LEU:HD23	1.86	0.57
12:L:30:ILE:HG22	12:L:31:CYS:H	1.69	0.57
2:B:1202:LEU:O	2:B:1206:GLU:HG3	2.04	0.57
14:T:16:DT:H1'	14:T:17:DT:H5"	1.86	0.57
2:B:25:ILE:HG21	2:B:658:ILE:HD12	1.86	0.57
2:B:483:LEU:HD11	2:B:491:THR:CG2	2.33	0.57
2:B:411:PRO:O	2:B:414:ALA:HB3	2.04	0.57
2:B:121:ASN:HA	2:B:207:GLY:HA2	1.85	0.57
1:A:196:GLU:HG2	1:A:197:PRO:HD2	1.87	0.57
1:A:317:LYS:O	1:A:318:SER:CB	2.52	0.57
1:A:399:HIS:O	1:A:400:PRO:C	2.40	0.57
2:B:914:LYS:HG2	2:B:937:ALA:HB3	1.87	0.57
1:A:1116:LEU:HB3	1:A:1308:THR:CG2	2.32	0.57
7:G:13:LEU:HD22	7:G:17:PHE:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1237:ILE:HG22	1:A:1238:ILE:N	2.19	0.57
2:B:707:PRO:CG	2:B:708:GLU:H	2.15	0.57
4:D:47:LEU:HD11	7:G:3:PHE:CD2	2.40	0.57
3:C:238:ILE:HG22	3:C:243:VAL:HG23	1.87	0.57
2:B:168:GLY:N	2:B:450:ALA:HB1	2.16	0.57
1:A:903:ASN:ND2	1:A:904:THR:N	2.52	0.57
1:A:446:ARG:HB2	1:A:487:MET:SD	2.44	0.57
1:A:438:ASP:O	1:A:439:ASN:HB2	2.05	0.57
5:E:67:GLU:O	5:E:70:SER:N	2.37	0.57
2:B:807:ARG:HG2	2:B:1045:SER:OG	2.05	0.57
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.34	0.57
10:J:2:ILE:HG12	10:J:57:ILE:HD12	1.86	0.57
3:C:238:ILE:HG23	3:C:242:GLN:HB2	1.85	0.57
2:B:129:PHE:HD2	2:B:166:PHE:HA	1.70	0.57
15:P:2:A:H2'	15:P:3:A:H8	1.70	0.57
2:B:326:ASP:OD2	2:B:328:GLU:HB3	2.05	0.57
7:G:21:ARG:CZ	7:G:24:GLN:HB2	2.35	0.57
1:A:853:ASP:OD1	1:A:855:THR:HB	2.04	0.57
2:B:222:ILE:H	2:B:240:ILE:CD1	2.17	0.57
2:B:865:LYS:HZ3	2:B:869:SER:HA	1.69	0.57
3:C:177:GLU:HG3	3:C:231:ASN:CB	2.32	0.57
3:C:99:LEU:HD12	3:C:118:LEU:HD13	1.87	0.57
8:H:130:ARG:HH11	8:H:130:ARG:N	2.00	0.57
2:B:992:ILE:HG12	2:B:993:THR:N	2.20	0.57
1:A:1037:LEU:HD22	1:A:1041:ALA:HB1	1.86	0.57
10:J:27:GLU:C	10:J:29:GLU:H	2.08	0.57
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.37	0.57
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.05	0.57
2:B:176:SER:O	2:B:182:SER:HB3	2.05	0.57
2:B:222:ILE:HD11	2:B:627:PHE:CZ	2.40	0.57
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.39	0.57
5:E:56:LYS:NZ	5:E:84:ASP:H	2.03	0.57
4:D:128:VAL:C	4:D:130:LEU:H	2.07	0.57
3:C:56:THR:HG21	3:C:145:CYS:SG	2.45	0.57
1:A:679:ILE:HG12	1:A:732:LEU:HD12	1.86	0.57
2:B:110:HIS:CB	12:L:54:ARG:NH2	2.64	0.57
8:H:130:ARG:H	8:H:130:ARG:NH1	2.01	0.57
2:B:810:GLU:HA	2:B:815:ARG:NH2	2.20	0.57
7:G:106:MET:HG3	7:G:157:ILE:O	2.04	0.57
4:D:7:THR:HG23	4:D:7:THR:O	2.03	0.57
1:A:1166:ASP:OD2	1:A:1239:ARG:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:47:LEU:HD13	4:D:48:ILE:N	2.19	0.56
2:B:865:LYS:O	2:B:866:TYR:HD1	1.88	0.56
14:T:15:DG:H2"	14:T:16:DT:H6	1.70	0.56
3:C:259:LEU:CD2	11:K:91:CYS:HB3	2.35	0.56
5:E:30:ILE:HG22	5:E:31:THR:O	2.05	0.56
4:D:52:LEU:O	4:D:54:GLU:N	2.35	0.56
2:B:431:TYR:CD1	2:B:447:ALA:HB2	2.40	0.56
2:B:916:THR:HB	2:B:935:ARG:CG	2.35	0.56
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.87	0.56
1:A:897:TYR:HB3	1:A:936:LEU:CD1	2.35	0.56
9:I:14:LEU:HA	9:I:28:GLU:O	2.06	0.56
2:B:68:THR:HG22	2:B:91:SER:CB	2.34	0.56
10:J:23:ASN:C	10:J:25:LEU:N	2.57	0.56
1:A:1045:VAL:O	1:A:1049:ILE:HG13	2.05	0.56
1:A:982:THR:C	1:A:984:LYS:H	2.07	0.56
1:A:457:ALA:HB3	1:A:506:ALA:HA	1.86	0.56
2:B:20:ASP:C	2:B:22:SER:H	2.09	0.56
9:I:10:CYS:SG	9:I:32:CYS:HB3	2.44	0.56
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.86	0.56
2:B:637:LEU:HB2	2:B:693:ILE:HD11	1.86	0.56
8:H:12:VAL:HG13	8:H:26:ILE:HD11	1.87	0.56
1:A:380:VAL:HG12	1:A:428:TYR:HA	1.86	0.56
7:G:139:ILE:CG2	7:G:140:LYS:N	2.68	0.56
9:I:118:ARG:NH1	9:I:120:GLN:HB2	2.20	0.56
3:C:124:LEU:O	3:C:126:GLY:N	2.38	0.56
5:E:145:THR:HG21	5:E:187:TYR:CE2	2.41	0.56
2:B:822:ASN:ND2	10:J:52:THR:HG21	2.20	0.56
2:B:859:TYR:OH	2:B:941:LEU:HD12	2.05	0.56
1:A:23:SER:HB3	1:A:233:TRP:CE2	2.40	0.56
1:A:596:THR:C	1:A:598:LEU:N	2.58	0.56
1:A:831:THR:CG2	1:A:832:ALA:N	2.65	0.56
9:I:7:CYS:SG	9:I:8:ARG:O	2.64	0.56
1:A:963:ILE:HD13	1:A:1049:ILE:HG12	1.87	0.56
3:C:254:LYS:HE2	11:K:42:LEU:HD13	1.86	0.56
1:A:477:PRO:HG2	1:A:521:MET:HG2	1.87	0.56
2:B:295:GLY:O	2:B:299:GLU:HG3	2.06	0.56
11:K:93:SER:OG	11:K:97:LYS:HE3	2.06	0.56
4:D:134:THR:HG22	4:D:135:GLY:N	2.20	0.56
1:A:875:ALA:HA	1:A:878:ILE:CD1	2.36	0.56
6:F:94:LEU:HD22	6:F:122:MET:HG2	1.87	0.56
1:A:57:ARG:O	1:A:68:GLN:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:850:LEU:HD12	2:B:851:PHE:N	2.20	0.56
2:B:885:MET:HA	2:B:936:ASP:HB3	1.87	0.56
1:A:698:GLN:NE2	9:I:99:LEU:HD11	2.21	0.56
10:J:1:MET:H1	10:J:57:ILE:H	1.53	0.56
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.36	0.56
7:G:20:PRO:CD	7:G:21:ARG:H	2.18	0.56
2:B:186:GLU:HG3	10:J:62:ARG:NH2	2.18	0.56
2:B:300:HIS:O	2:B:303:TYR:HE2	1.87	0.56
2:B:308:TRP:CH2	9:I:45:ARG:HG2	2.41	0.56
2:B:805:THR:HA	2:B:809:MET:CE	2.35	0.56
1:A:868:TYR:OH	1:A:1366:ARG:HD3	2.05	0.56
2:B:276:ILE:CG2	2:B:336:ARG:HB2	2.36	0.56
8:H:26:ILE:HG22	8:H:40:LEU:O	2.05	0.56
1:A:381:THR:HG23	1:A:382:PRO:CD	2.32	0.56
7:G:34:VAL:HG13	7:G:45:ILE:HG21	1.88	0.56
7:G:48:VAL:HG13	7:G:74:TYR:HD1	1.69	0.56
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.21	0.56
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.34	0.56
1:A:1317:MET:O	1:A:1322:ILE:HD11	2.04	0.56
11:K:88:LYS:O	11:K:91:CYS:HB2	2.04	0.56
2:B:1156:ASP:O	2:B:1157:ALA:O	2.23	0.56
2:B:459:TYR:CZ	2:B:469:GLN:HG2	2.41	0.56
3:C:33:LEU:O	3:C:37:MET:HG3	2.05	0.56
6:F:111:LEU:O	6:F:113:GLY:N	2.32	0.56
2:B:553:PRO:HG2	2:B:554:ILE:HD12	1.87	0.56
2:B:542:MET:HE3	2:B:747:MET:HG3	1.87	0.56
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.87	0.56
3:C:221:TYR:CE1	3:C:222:LYS:HG3	2.41	0.56
1:A:326:ARG:HG3	1:A:1406:VAL:HG21	1.86	0.56
1:A:69:THR:HG21	2:B:1174:LYS:HZ2	1.71	0.56
2:B:886:LYS:NZ	2:B:936:ASP:OD1	2.39	0.56
2:B:798:TYR:HE2	3:C:62:PHE:CZ	2.23	0.56
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.88	0.56
1:A:591:PHE:HA	1:A:595:THR:CG2	2.35	0.56
2:B:990:ILE:HG22	2:B:991:GLY:N	2.21	0.56
1:A:1159:ARG:HD2	1:A:1159:ARG:N	2.21	0.56
2:B:68:THR:HG22	2:B:91:SER:CA	2.35	0.56
1:A:1006:ILE:HD11	5:E:163:GLU:HG3	1.87	0.56
5:E:157:SER:C	5:E:159:ASP:H	2.09	0.56
2:B:39:ARG:NH2	2:B:665:GLU:HG2	2.20	0.56
1:A:129:LYS:O	1:A:130:ASP:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.87	0.56
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.88	0.56
7:G:138:THR:CG2	7:G:139:ILE:N	2.49	0.56
2:B:865:LYS:HZ2	2:B:869:SER:HA	1.69	0.56
10:J:53:HIS:CD2	10:J:53:HIS:C	2.77	0.56
4:D:14:ARG:NH1	4:D:16:LYS:HD2	2.21	0.56
2:B:120:ARG:NH1	12:L:54:ARG:HD2	2.20	0.56
1:A:1316:VAL:HG12	1:A:1316:VAL:O	2.05	0.56
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.88	0.56
1:A:973:ILE:HD13	1:A:1037:LEU:HA	1.88	0.56
3:C:73:GLN:NE2	3:C:75:MET:H	2.00	0.56
1:A:332:LYS:O	1:A:334:GLY:N	2.38	0.56
2:B:303:TYR:N	2:B:303:TYR:CD2	2.74	0.56
2:B:750:GLY:O	2:B:751:VAL:C	2.44	0.56
2:B:359:GLU:O	2:B:362:PRO:HD3	2.05	0.56
2:B:284:ILE:HD13	2:B:333:PHE:CD2	2.41	0.56
2:B:26:THR:HB	2:B:708:GLU:OE1	2.06	0.56
5:E:147:HIS:HB3	5:E:150:VAL:CG2	2.36	0.56
1:A:1033:GLN:HA	1:A:1036:ARG:NH1	2.19	0.56
2:B:204:ILE:C	2:B:205:ILE:HD12	2.26	0.56
2:B:254:LEU:HD23	2:B:381:MET:CE	2.36	0.56
2:B:615:MET:HB3	2:B:626:ILE:CG1	2.30	0.56
2:B:842:ASN:O	2:B:846:ILE:HG13	2.06	0.56
1:A:787:PHE:HE1	1:A:796:SER:HA	1.70	0.56
7:G:87:VAL:HB	7:G:103:VAL:HG11	1.87	0.56
5:E:179:GLN:HA	5:E:179:GLN:OE1	2.06	0.56
5:E:112:TYR:CE1	5:E:136:ASN:HA	2.41	0.55
2:B:1174:LYS:O	2:B:1176:ASN:N	2.39	0.55
3:C:235:VAL:HG21	10:J:6:ARG:NH2	2.21	0.55
2:B:129:PHE:CE2	2:B:166:PHE:CD1	2.94	0.55
5:E:164:LEU:CD2	5:E:211:TYR:CD2	2.88	0.55
5:E:171:LYS:HG2	5:E:174:GLN:CD	2.26	0.55
1:A:108:MET:HB3	1:A:210:ILE:CD1	2.36	0.55
8:H:12:VAL:CG1	8:H:26:ILE:HD11	2.36	0.55
2:B:705:MET:HA	2:B:705:MET:CE	2.35	0.55
1:A:34:LYS:HZ1	1:A:57:ARG:HH21	1.55	0.55
1:A:56:PRO:O	1:A:57:ARG:CG	2.52	0.55
2:B:847:ASP:C	2:B:849:GLY:N	2.59	0.55
1:A:427:GLN:HB2	1:A:430:TRP:CD1	2.41	0.55
3:C:243:VAL:HG12	3:C:243:VAL:O	2.06	0.55
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:7:CYS:HA	10:J:49:MET:HE3	1.88	0.55
2:B:186:GLU:CG	10:J:62:ARG:HH22	2.19	0.55
3:C:226:ASP:O	3:C:227:THR:CB	2.53	0.55
2:B:430:ARG:HB3	2:B:434:ARG:NH2	2.21	0.55
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.88	0.55
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.41	0.55
3:C:100:THR:CG2	3:C:102:GLN:HE21	2.18	0.55
1:A:1168:GLU:O	1:A:1171:GLN:OE1	2.24	0.55
1:A:590:ARG:HB3	1:A:605:MET:N	2.22	0.55
2:B:810:GLU:HA	2:B:815:ARG:HH22	1.71	0.55
12:L:61:THR:HG22	12:L:63:ARG:H	1.71	0.55
2:B:429:PHE:CD1	2:B:432:MET:HE3	2.41	0.55
4:D:50:LEU:HD21	7:G:4:ILE:HD12	1.87	0.55
2:B:1115:THR:HG22	2:B:1117:GLN:H	1.70	0.55
1:A:341:MET:CE	2:B:1135:ARG:NH1	2.70	0.55
7:G:101:VAL:HG12	7:G:102:GLN:N	2.21	0.55
5:E:169:ARG:HB3	6:F:140:ASP:OD2	2.07	0.55
8:H:12:VAL:CG1	8:H:51:ALA:HA	2.36	0.55
2:B:999:MET:HB3	2:B:1007:VAL:CG2	2.36	0.55
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.87	0.55
1:A:1348:LEU:HD23	1:A:1372:VAL:HG13	1.89	0.55
2:B:20:ASP:O	2:B:22:SER:N	2.35	0.55
2:B:1050:ILE:HG22	2:B:1051:THR:N	2.21	0.55
2:B:711:GLU:HB2	2:B:712:PRO:CD	2.36	0.55
1:A:571:LEU:CD2	8:H:46:LEU:HD11	2.36	0.55
2:B:1161:HIS:NE2	2:B:1175:LEU:HD21	2.22	0.55
2:B:842:ASN:HD21	2:B:844:SER:HB2	1.72	0.55
1:A:979:SER:OG	1:A:980:ASP:N	2.38	0.55
1:A:1308:THR:HG23	1:A:1309:ASP:H	1.69	0.55
1:A:616:VAL:HG12	1:A:617:VAL:N	2.21	0.55
2:B:315:LYS:N	2:B:316:PRO:HD2	2.22	0.55
6:F:128:LYS:HD3	6:F:149:GLU:O	2.06	0.55
1:A:780:VAL:O	1:A:782:ARG:HG2	2.07	0.55
1:A:567:LYS:HB3	8:H:95:TYR:CA	2.36	0.55
6:F:94:LEU:HD21	6:F:122:MET:HA	1.89	0.55
5:E:56:LYS:HZ3	5:E:84:ASP:H	1.54	0.55
1:A:598:LEU:HA	8:H:122:LEU:HD13	1.87	0.55
9:I:6:PHE:HA	9:I:14:LEU:HG	1.89	0.55
1:A:311:GLN:O	1:A:313:GLN:N	2.40	0.55
9:I:73:ARG:O	9:I:81:ARG:HA	2.07	0.55
2:B:360:PHE:CD2	2:B:360:PHE:C	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1174:LYS:O	2:B:1175:LEU:C	2.44	0.55
5:E:82:PHE:N	5:E:82:PHE:CD1	2.74	0.55
12:L:38:LEU:HG	12:L:39:SER:H	1.71	0.55
3:C:189:THR:CG2	3:C:190:ASP:N	2.70	0.55
3:C:10:ILE:HG13	11:K:108:GLU:HB3	1.87	0.55
1:A:870:GLU:HG2	5:E:208:TYR:CD2	2.41	0.55
1:A:853:ASP:OD1	1:A:855:THR:HG22	2.07	0.55
2:B:281:PRO:HB3	2:B:320:ASP:OD2	2.06	0.55
4:D:39:ASN:HD22	4:D:41:GLN:HB2	1.71	0.55
1:A:1076:ALA:HA	1:A:1079:MET:CE	2.37	0.55
2:B:704:ALA:HB2	2:B:738:PHE:CD2	2.42	0.55
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.88	0.55
2:B:549:THR:CG2	2:B:550:ASP:N	2.70	0.55
7:G:74:TYR:H	7:G:74:TYR:HD2	1.55	0.55
7:G:129:SER:CB	7:G:138:THR:OG1	2.55	0.55
2:B:916:THR:O	2:B:935:ARG:HG2	2.07	0.55
1:A:925:LEU:HD13	1:A:983:ILE:HG22	1.88	0.55
4:D:14:ARG:CZ	4:D:16:LYS:HD2	2.37	0.55
8:H:83:GLN:C	8:H:85:GLY:H	2.10	0.55
1:A:590:ARG:HG3	1:A:591:PHE:N	2.21	0.55
5:E:124:VAL:N	5:E:125:PRO:CD	2.70	0.55
1:A:1385:THR:CG2	1:A:1386:ARG:N	2.69	0.55
8:H:128:ASN:ND2	8:H:131:ASN:OD1	2.39	0.55
1:A:1029:ARG:CG	1:A:1029:ARG:HH11	2.20	0.55
1:A:266:LEU:HD21	1:A:303:TYR:CZ	2.41	0.55
2:B:1045:SER:O	2:B:1048:THR:HG23	2.06	0.55
1:A:1244:ARG:NE	1:A:1245:PRO:HD2	2.05	0.55
1:A:399:HIS:CB	1:A:400:PRO:CD	2.78	0.55
1:A:401:GLY:C	1:A:435:HIS:HD2	2.09	0.55
8:H:139:ASN:O	8:H:140:ALA:CB	2.54	0.55
1:A:1030:ARG:CG	1:A:1034:GLU:OE2	2.53	0.55
1:A:899:VAL:CG1	1:A:929:LEU:HD12	2.37	0.55
1:A:443:LEU:O	1:A:489:LEU:HD12	2.06	0.55
1:A:1120:LEU:HD23	1:A:1304:TRP:O	2.06	0.55
1:A:75:ASN:ND2	2:B:1116:ARG:NH1	2.54	0.55
1:A:940:ARG:O	1:A:944:ARG:HG3	2.06	0.55
10:J:16:ASP:OD1	10:J:16:ASP:N	2.34	0.55
3:C:91:HIS:ND1	3:C:158:VAL:HG11	2.21	0.55
9:I:22:ASN:O	9:I:23:ASN:HB2	2.07	0.55
1:A:1402:PHE:CE2	1:A:1403:GLU:HG3	2.42	0.55
2:B:857:ARG:HH21	2:B:942:ARG:CZ	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:31:ASP:OD1	10:J:34:THR:OG1	2.25	0.55
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.36	0.55
8:H:63:LEU:HD11	8:H:141:TYR:CD2	2.42	0.55
1:A:1105:LEU:HD22	1:A:1384:VAL:HG21	1.89	0.55
1:A:579:SER:HA	1:A:582:ILE:HG13	1.87	0.55
1:A:62:ASP:O	1:A:64:ASN:N	2.40	0.54
2:B:852:ARG:HH22	12:L:70:ARG:C	2.10	0.54
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.42	0.54
4:D:220:LEU:HD22	4:D:221:TYR:H	1.66	0.54
1:A:211:PHE:O	1:A:214:ILE:HG13	2.07	0.54
1:A:225:ASN:ND2	1:A:227:VAL:H	2.05	0.54
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.71	0.54
1:A:331:GLY:O	1:A:332:LYS:O	2.24	0.54
4:D:71:LYS:HA	4:D:74:GLN:CB	2.36	0.54
2:B:91:SER:OG	2:B:133:LYS:HB2	2.07	0.54
2:B:235:SER:O	2:B:236:HIS:HD2	1.88	0.54
3:C:91:HIS:HD2	3:C:91:HIS:O	1.90	0.54
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.42	0.54
1:A:738:LYS:HG3	1:A:740:LEU:HG	1.88	0.54
3:C:138:GLU:OE1	3:C:138:GLU:N	2.40	0.54
1:A:689:LYS:HE2	1:A:721:PHE:CE2	2.41	0.54
4:D:155:ARG:HD3	4:D:221:TYR:CZ	2.43	0.54
2:B:1068:GLY:O	2:B:1069:PHE:O	2.25	0.54
11:K:50:LEU:HD11	11:K:75:ILE:CD1	2.37	0.54
1:A:288:ALA:HA	1:A:291:GLU:HG3	1.88	0.54
1:A:1110:ASN:H	1:A:1110:ASN:HD22	1.55	0.54
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.90	0.54
1:A:264:PHE:C	1:A:265:LYS:HE3	2.27	0.54
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.90	0.54
1:A:962:ARG:O	1:A:964:ILE:N	2.41	0.54
2:B:90:ILE:CD1	2:B:432:MET:SD	2.94	0.54
11:K:108:GLU:O	11:K:112:GLN:HG2	2.07	0.54
10:J:14:VAL:CG1	10:J:50:ILE:HD11	2.37	0.54
11:K:52:ASN:O	11:K:54:ARG:N	2.40	0.54
6:F:111:LEU:C	6:F:113:GLY:H	2.08	0.54
5:E:21:GLU:O	5:E:24:LYS:HG2	2.08	0.54
8:H:33:GLN:C	8:H:35:GLN:H	2.10	0.54
1:A:744:LYS:HG2	1:A:748:MET:HE2	1.88	0.54
1:A:133:LYS:O	1:A:136:ALA:HB3	2.06	0.54
1:A:868:TYR:CZ	1:A:1366:ARG:HD3	2.42	0.54
2:B:222:ILE:HD11	2:B:627:PHE:HZ	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:CG2	3:C:44:LEU:N	2.70	0.54
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.88	0.54
7:G:119:LEU:HD12	7:G:120:THR:H	1.72	0.54
2:B:1182:CYS:SG	2:B:1185:CYS:HB2	2.47	0.54
1:A:311:GLN:O	1:A:312:PRO:C	2.45	0.54
1:A:1161:THR:C	1:A:1163:ILE:N	2.61	0.54
2:B:288:ALA:HA	2:B:331:LEU:HD12	1.90	0.54
1:A:668:ASP:HB3	1:A:741:ASN:ND2	2.17	0.54
15:P:2:A:H2'	15:P:3:A:C8	2.43	0.54
1:A:472:LEU:O	1:A:475:THR:HB	2.07	0.54
4:D:69:ALA:HB2	4:D:72:ARG:NH2	2.22	0.54
8:H:1:MET:O	8:H:1:MET:HG2	2.07	0.54
2:B:520:GLY:H	2:B:748:ILE:HG22	1.73	0.54
2:B:563:MET:SD	2:B:580:VAL:HG11	2.48	0.54
2:B:332:ASP:O	2:B:334:ILE:N	2.33	0.54
7:G:1:MET:SD	7:G:79:PHE:CE1	3.01	0.54
2:B:936:ASP:OD1	2:B:937:ALA:N	2.41	0.54
4:D:156:ASP:HB2	4:D:159:THR:OG1	2.08	0.54
1:A:1259:MET:HE3	1:A:1263:ILE:HG13	1.89	0.54
2:B:427:ASP:HA	2:B:430:ARG:HD2	1.87	0.54
2:B:345:LYS:HA	2:B:348:ARG:HE	1.72	0.54
3:C:143:LEU:HG	3:C:143:LEU:O	2.08	0.54
1:A:320:ARG:NE	1:A:323:LYS:NZ	2.55	0.54
7:G:126:ASN:C	7:G:126:ASN:ND2	2.60	0.54
10:J:1:MET:O	10:J:2:ILE:O	2.26	0.54
2:B:642:ASP:H	2:B:649:LYS:HE3	1.72	0.54
2:B:653:VAL:HA	2:B:657:HIS:CD2	2.43	0.54
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.42	0.54
2:B:313:MET:CE	2:B:386:LEU:HD22	2.37	0.54
1:A:75:ASN:O	1:A:76:GLU:CB	2.56	0.54
4:D:209:ARG:HG2	4:D:209:ARG:HH11	1.72	0.54
2:B:487:THR:HG22	2:B:490:SER:H	1.73	0.54
3:C:8:VAL:HG12	3:C:9:LYS:N	2.22	0.54
2:B:580:VAL:HG22	2:B:624:LEU:HB3	1.89	0.54
8:H:8:ASP:OD2	8:H:9:ILE:N	2.40	0.54
2:B:616:ILE:HG23	2:B:700:SER:OG	2.08	0.54
1:A:1236:LEU:C	1:A:1237:ILE:HG13	2.27	0.54
3:C:146:LYS:C	3:C:147:LEU:HD23	2.28	0.54
8:H:84:ALA:C	8:H:86:ASP:N	2.58	0.54
1:A:744:LYS:HG2	1:A:748:MET:CE	2.38	0.54
3:C:8:VAL:HG12	3:C:9:LYS:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:ILE:HD13	8:H:146:ARG:HH12	1.72	0.54
1:A:1244:ARG:HE	1:A:1245:PRO:CD	2.07	0.54
1:A:399:HIS:CG	1:A:400:PRO:N	2.74	0.54
4:D:130:LEU:O	4:D:132:GLN:N	2.37	0.54
4:D:35:LEU:HD12	4:D:35:LEU:N	2.23	0.54
2:B:866:TYR:CB	2:B:870:ILE:HB	2.36	0.54
2:B:914:LYS:HE2	2:B:937:ALA:HB1	1.90	0.54
1:A:541:ILE:HD11	1:A:656:TRP:CD1	2.42	0.54
11:K:31:VAL:HG12	11:K:32:VAL:H	1.72	0.54
8:H:130:ARG:HB3	8:H:134:ASN:H	1.73	0.54
2:B:69:LEU:HB3	2:B:429:PHE:CE1	2.40	0.54
1:A:833:GLU:HG3	1:A:1102:LYS:HE2	1.90	0.54
2:B:118:ARG:HH22	2:B:194:GLU:CD	2.11	0.54
2:B:637:LEU:HD22	2:B:741:CYS:O	2.07	0.54
1:A:1191:TRP:CZ3	9:I:43:VAL:HG21	2.43	0.54
2:B:644:GLU:HB3	2:B:648:HIS:O	2.07	0.54
1:A:1074:GLU:HB3	1:A:1075:PRO:CD	2.38	0.54
9:I:7:CYS:HB2	9:I:34:TYR:CG	2.43	0.54
8:H:127:GLY:O	8:H:128:ASN:CB	2.53	0.54
2:B:327:ARG:HH21	2:B:371:GLU:HG2	1.70	0.54
11:K:67:PHE:C	11:K:68:PHE:HD2	2.11	0.54
2:B:185:THR:O	2:B:186:GLU:C	2.46	0.54
2:B:398:ARG:NH1	2:B:398:ARG:CB	2.71	0.54
2:B:794:ASN:ND2	2:B:794:ASN:N	2.56	0.54
2:B:590:HIS:NE2	2:B:592:ASN:O	2.40	0.53
3:C:137:LYS:HB3	3:C:138:GLU:OE1	2.07	0.53
2:B:557:PHE:CD2	2:B:557:PHE:C	2.81	0.53
5:E:192:ARG:NH1	5:E:192:ARG:HG3	2.23	0.53
1:A:464:PRO:HG2	1:A:465:TYR:CD1	2.43	0.53
12:L:61:THR:CG2	12:L:63:ARG:HG3	2.37	0.53
2:B:435:THR:C	2:B:437:GLU:N	2.60	0.53
9:I:101:PHE:H	9:I:101:PHE:HD1	1.56	0.53
1:A:416:ARG:HG3	1:A:417:TYR:CD1	2.43	0.53
3:C:251:LEU:O	3:C:255:VAL:HG23	2.08	0.53
4:D:117:GLU:HG2	4:D:122:GLU:OE2	2.08	0.53
4:D:130:LEU:C	4:D:132:GLN:H	2.11	0.53
10:J:53:HIS:NE2	10:J:55:ASP:HA	2.24	0.53
2:B:192:LEU:O	2:B:193:LYS:HB2	2.08	0.53
1:A:942:PHE:CE1	5:E:207:ARG:HD3	2.40	0.53
1:A:962:ARG:O	1:A:965:GLN:N	2.41	0.53
4:D:208:GLU:HA	4:D:211:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:GLU:OE2	2:B:485:ARG:NE	2.36	0.53
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.43	0.53
5:E:112:TYR:O	5:E:137:GLU:HG3	2.08	0.53
9:I:62:ILE:HG12	9:I:62:ILE:O	2.08	0.53
3:C:66:ARG:NH1	3:C:144:ILE:O	2.42	0.53
3:C:239:PRO:O	3:C:242:GLN:N	2.42	0.53
2:B:801:LYS:O	10:J:52:THR:HG23	2.08	0.53
2:B:831:SER:HB3	2:B:994:TYR:OH	2.09	0.53
1:A:335:ARG:O	1:A:339:ASN:HB2	2.08	0.53
5:E:108:GLY:O	5:E:132:ILE:HG22	2.09	0.53
1:A:1121:GLU:HB2	1:A:1321:GLY:O	2.08	0.53
1:A:1147:THR:HB	9:I:48:LEU:CD1	2.38	0.53
1:A:890:ASP:H	1:A:1296:GLY:HA3	1.73	0.53
8:H:37:LYS:HD2	8:H:126:GLU:OE2	2.09	0.53
1:A:205:GLU:CD	1:A:205:GLU:H	2.11	0.53
5:E:90:VAL:HA	5:E:120:ALA:CB	2.36	0.53
4:D:155:ARG:HD3	4:D:221:TYR:OH	2.07	0.53
3:C:100:THR:HG22	3:C:101:LEU:N	2.23	0.53
1:A:93:VAL:CG1	1:A:301:ALA:HB1	2.37	0.53
4:D:13:ARG:O	4:D:15:LEU:N	2.42	0.53
12:L:58:LYS:O	12:L:59:ALA:O	2.27	0.53
1:A:547:LEU:HD21	1:A:560:ILE:HD13	1.90	0.53
2:B:63:ILE:HD12	2:B:421:PHE:CE2	2.44	0.53
1:A:965:GLN:HA	1:A:968:GLN:HG3	1.89	0.53
1:A:50:ILE:O	1:A:52:GLY:N	2.40	0.53
11:K:12:LEU:HG	11:K:16:GLU:HB2	1.90	0.53
2:B:1180:PHE:HB3	2:B:1191:ILE:HD13	1.89	0.53
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.25	0.53
2:B:637:LEU:HD21	2:B:742:GLU:OE2	2.09	0.53
1:A:1186:ASP:O	1:A:1187:GLN:CB	2.53	0.53
2:B:871:THR:HG22	2:B:872:GLU:N	2.23	0.53
2:B:872:GLU:OE1	2:B:914:LYS:HE3	2.07	0.53
2:B:1065:GLN:HB3	2:B:1069:PHE:O	2.09	0.53
4:D:149:THR:CG2	4:D:150:ASN:N	2.72	0.53
12:L:34:CYS:SG	12:L:34:CYS:O	2.67	0.53
3:C:189:THR:CG2	3:C:190:ASP:H	2.21	0.53
1:A:853:ASP:OD1	1:A:855:THR:N	2.42	0.53
2:B:398:ARG:CB	2:B:398:ARG:HH11	2.21	0.53
6:F:111:LEU:C	6:F:113:GLY:N	2.62	0.53
9:I:82:GLU:HB3	9:I:104:LEU:HD12	1.91	0.53
1:A:1343:ALA:O	1:A:1346:ALA:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:MET:HE1	1:A:1212:VAL:HG21	1.89	0.53
2:B:864:LYS:HG3	2:B:872:GLU:OE1	2.09	0.53
2:B:770:GLN:CD	2:B:983:ARG:HA	2.27	0.53
3:C:177:GLU:O	3:C:230:MET:HA	2.09	0.53
1:A:665:GLY:C	1:A:666:ILE:HD12	2.28	0.53
1:A:549:MET:SD	1:A:577:ILE:CD1	2.96	0.53
1:A:93:VAL:HG21	1:A:301:ALA:O	2.08	0.53
1:A:356:ASP:OD1	1:A:358:ASN:N	2.42	0.53
1:A:50:ILE:C	1:A:52:GLY:N	2.62	0.53
1:A:458:HIS:CE1	1:A:507:VAL:HG21	2.43	0.53
9:I:50:THR:CG2	9:I:51:ASN:N	2.71	0.53
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.23	0.53
1:A:184:SER:CB	1:A:199:LEU:HD23	2.39	0.53
1:A:270:LEU:O	1:A:274:ILE:HG13	2.08	0.53
2:B:222:ILE:N	2:B:240:ILE:CD1	2.72	0.53
1:A:590:ARG:NH2	1:A:620:LYS:HB2	2.23	0.53
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	1.91	0.53
1:A:1341:ILE:HG23	1:A:1342:GLU:N	2.23	0.53
5:E:129:PRO:O	5:E:130:ALA:C	2.47	0.53
2:B:728:ARG:HH12	2:B:1047:PHE:HB3	1.73	0.53
1:A:350:ARG:HB2	2:B:1128:LEU:CD1	2.39	0.53
2:B:557:PHE:HD2	2:B:557:PHE:C	2.11	0.53
8:H:13:SER:HB3	8:H:27:GLU:O	2.09	0.53
3:C:241:ASP:O	3:C:245:VAL:HG23	2.09	0.53
1:A:666:ILE:CD1	1:A:667:GLY:N	2.72	0.53
2:B:1059:LEU:HD23	2:B:1065:GLN:O	2.09	0.53
1:A:1313:LEU:HD23	1:A:1338:VAL:CG2	2.39	0.53
5:E:161:LYS:HD2	5:E:195:VAL:HG23	1.91	0.53
4:D:193:THR:HG21	7:G:167:TYR:HD1	1.73	0.53
1:A:1325:THR:O	5:E:148:GLU:HB2	2.08	0.53
9:I:111:THR:OG1	9:I:112:SER:N	2.42	0.53
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.91	0.53
2:B:58:THR:O	2:B:62:ILE:HG13	2.08	0.53
2:B:755:ILE:HG22	2:B:755:ILE:O	2.09	0.53
2:B:376:PHE:CZ	2:B:569:TYR:HB3	2.44	0.53
2:B:363:HIS:O	2:B:364:ILE:HB	2.09	0.53
2:B:331:LEU:CD2	2:B:353:LYS:HG2	2.38	0.53
4:D:47:LEU:HD13	4:D:48:ILE:H	1.74	0.53
2:B:619:ILE:HG22	2:B:620:ARG:N	2.24	0.53
3:C:43:THR:HG22	3:C:44:LEU:N	2.24	0.53
2:B:102:VAL:HG23	2:B:112:LEU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:119:LEU:HD12	7:G:120:THR:N	2.24	0.53
2:B:292:ILE:HD11	2:B:327:ARG:H	1.74	0.53
10:J:23:ASN:O	10:J:25:LEU:N	2.42	0.53
2:B:558:LEU:HD22	2:B:596:LEU:HD11	1.91	0.53
8:H:133:ASN:O	8:H:135:LEU:N	2.41	0.53
1:A:786:HIS:CD2	1:A:786:HIS:N	2.74	0.53
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.89	0.53
3:C:148:ARG:N	3:C:151:GLN:HG3	2.23	0.53
1:A:719:VAL:HG13	1:A:723:ASN:ND2	2.24	0.53
3:C:123:ASN:C	3:C:125:MET:H	2.12	0.53
3:C:120:ILE:HD11	3:C:130:GLY:O	2.08	0.53
1:A:659:HIS:O	2:B:1081:LEU:HD23	2.09	0.53
2:B:763:GLN:HG2	2:B:765:PRO:CD	2.35	0.53
1:A:828:ALA:C	1:A:831:THR:HG22	2.30	0.53
2:B:185:THR:H	2:B:188:ASP:HB2	1.73	0.53
2:B:31:TRP:CZ2	2:B:807:ARG:HB2	2.44	0.52
2:B:806:THR:HA	2:B:1045:SER:OG	2.09	0.52
2:B:278:GLN:CG	2:B:279:ASP:N	2.58	0.52
1:A:1191:TRP:HZ3	9:I:43:VAL:HG21	1.73	0.52
2:B:244:LEU:O	2:B:249:ARG:HG3	2.08	0.52
1:A:385:ILE:CD1	1:A:426:LEU:HB2	2.39	0.52
2:B:882:THR:HG22	2:B:883:LEU:N	2.24	0.52
2:B:619:ILE:O	2:B:622:LYS:N	2.34	0.52
3:C:18:VAL:O	3:C:20:PHE:HD2	1.92	0.52
1:A:102:VAL:CB	1:A:211:PHE:HE1	2.22	0.52
1:A:337:ARG:HD3	1:A:839:ARG:NH2	2.24	0.52
5:E:178:ILE:HG22	5:E:213:ILE:O	2.08	0.52
12:L:26:THR:HG23	12:L:27:LEU:H	1.73	0.52
1:A:853:ASP:OD1	1:A:855:THR:CB	2.56	0.52
3:C:258:ILE:N	3:C:258:ILE:HD12	2.24	0.52
1:A:1009:ASN:CG	1:A:1012:ARG:HH12	2.13	0.52
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.08	0.52
2:B:875:GLU:O	2:B:877:PRO:HD3	2.08	0.52
3:C:123:ASN:ND2	3:C:125:MET:HA	2.24	0.52
1:A:154:SER:CB	1:A:162:VAL:CG2	2.87	0.52
7:G:115:MET:HA	7:G:163:ILE:HG13	1.91	0.52
1:A:710:LEU:HD22	9:I:96:SER:HA	1.90	0.52
6:F:109:VAL:CG1	6:F:110:ASP:N	2.72	0.52
2:B:816:GLU:O	2:B:817:LEU:HD23	2.09	0.52
8:H:91:ASP:O	8:H:93:TYR:N	2.39	0.52
8:H:27:GLU:HG2	8:H:39:THR:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:104:PHE:HD2	3:C:105:GLY:N	2.07	0.52
1:A:306:ASN:ND2	1:A:322:VAL:HG12	2.25	0.52
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.10	0.52
1:A:692:ASP:O	1:A:694:THR:N	2.42	0.52
1:A:168:GLY:O	1:A:169:ASN:C	2.47	0.52
1:A:897:TYR:HB3	1:A:936:LEU:HD12	1.92	0.52
2:B:294:ASP:C	2:B:296:GLU:H	2.12	0.52
2:B:874:PHE:HA	2:B:913:GLY:O	2.09	0.52
2:B:758:PHE:CZ	2:B:1044:ALA:HA	2.44	0.52
1:A:1006:ILE:CD1	5:E:163:GLU:HG3	2.39	0.52
1:A:851:HIS:HB2	1:A:855:THR:HG22	1.92	0.52
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.90	0.52
5:E:157:SER:C	5:E:159:ASP:N	2.62	0.52
1:A:1402:PHE:CG	1:A:1403:GLU:HG2	2.44	0.52
3:C:39:ALA:O	3:C:164:ALA:HB3	2.09	0.52
1:A:132:LYS:HE3	1:A:1411:GLU:HG3	1.90	0.52
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.43	0.52
8:H:106:GLU:O	8:H:108:SER:N	2.32	0.52
2:B:708:GLU:O	2:B:709:ASP:C	2.48	0.52
1:A:12:ARG:NH1	2:B:1218:THR:HB	2.25	0.52
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.74	0.52
5:E:61:GLN:NE2	5:E:105:PHE:CE2	2.78	0.52
2:B:1202:LEU:HD22	2:B:1206:GLU:CD	2.30	0.52
1:A:16:GLU:HB3	1:A:1418:LEU:HD11	1.91	0.52
12:L:60:ARG:HG2	12:L:61:THR:N	2.21	0.52
1:A:886:ILE:CG2	1:A:887:GLY:N	2.71	0.52
2:B:134:LYS:HE2	2:B:164:LYS:HZ3	1.72	0.52
1:A:851:HIS:HB2	1:A:855:THR:CG2	2.39	0.52
8:H:40:LEU:HB2	8:H:123:MET:HE2	1.91	0.52
3:C:148:ARG:NH1	10:J:64:ASN:HA	2.24	0.52
2:B:865:LYS:C	2:B:866:TYR:HD1	2.13	0.52
1:A:666:ILE:HD12	1:A:667:GLY:N	2.21	0.52
1:A:774:ARG:O	1:A:775:ILE:C	2.47	0.52
7:G:88:ASP:HB3	7:G:144:ARG:CA	2.32	0.52
7:G:106:MET:CG	7:G:107:LYS:N	2.72	0.52
1:A:356:ASP:OD1	1:A:358:ASN:HB2	2.09	0.52
2:B:1116:ARG:HD2	2:B:1198:TYR:CD1	2.44	0.52
1:A:626:ASN:O	1:A:631:HIS:CD2	2.62	0.52
1:A:555:ASP:O	1:A:556:TRP:C	2.48	0.52
1:A:864:ILE:HG22	1:A:865:GLN:HG3	1.91	0.52
2:B:373:ARG:NH2	2:B:587:HIS:HA	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:CG2	2:B:550:ASP:H	2.23	0.52
1:A:1161:THR:OG1	1:A:1239:ARG:NH2	2.43	0.52
1:A:13:THR:HB	1:A:1432:GLN:NE2	2.25	0.52
4:D:47:LEU:HD11	7:G:3:PHE:HD2	1.74	0.52
2:B:866:TYR:HB3	2:B:870:ILE:HD12	1.90	0.52
1:A:102:VAL:HG21	1:A:234:MET:HE1	1.91	0.52
2:B:193:LYS:HZ1	12:L:32:ALA:HB1	1.75	0.52
2:B:901:PRO:HD2	12:L:59:ALA:O	2.10	0.52
4:D:71:LYS:CG	4:D:74:GLN:HG3	2.40	0.52
2:B:383:ASN:O	2:B:387:LEU:HD12	2.10	0.52
1:A:1397:LEU:HB2	1:A:1426:GLU:OE1	2.10	0.52
15:P:1:C:H2'	15:P:1:C:O2	2.10	0.52
1:A:54:ASN:N	1:A:54:ASN:HD22	2.07	0.52
1:A:1218:GLN:O	1:A:1221:LYS:HE3	2.10	0.52
8:H:9:ILE:HG12	8:H:56:THR:HA	1.92	0.52
2:B:245:GLU:HG2	2:B:246:LYS:HG3	1.90	0.52
3:C:18:VAL:HG23	3:C:240:VAL:HB	1.89	0.52
1:A:598:LEU:O	1:A:599:SER:C	2.47	0.52
2:B:1095:LEU:HD12	2:B:1095:LEU:N	2.15	0.52
1:A:1385:THR:HG21	1:A:1387:HIS:CD2	2.45	0.52
3:C:184:ASN:OD1	3:C:187:LYS:CA	2.58	0.52
2:B:313:MET:O	2:B:316:PRO:HD2	2.09	0.52
2:B:1115:THR:HG22	2:B:1117:GLN:N	2.24	0.52
2:B:819:ALA:O	2:B:1093:GLN:HG2	2.09	0.52
1:A:1200:ALA:HA	1:A:1203:ASN:HD22	1.74	0.52
1:A:252:PHE:O	1:A:256:GLN:NE2	2.42	0.52
14:T:15:DG:H2"	14:T:16:DT:C6	2.45	0.52
2:B:282:ILE:CG2	2:B:382:ILE:HD11	2.40	0.52
2:B:282:ILE:HD12	2:B:382:ILE:HD13	1.91	0.52
7:G:87:VAL:O	7:G:87:VAL:HG23	2.08	0.52
1:A:92:HIS:O	1:A:94:GLY:N	2.42	0.52
1:A:305:ASP:OD1	1:A:306:ASN:N	2.43	0.52
3:C:242:GLN:C	3:C:244:VAL:N	2.63	0.52
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.40	0.52
1:A:963:ILE:HD11	1:A:1048:ASN:HB3	1.92	0.52
6:F:138:LEU:HB2	6:F:142:SER:HB2	1.90	0.52
3:C:249:ASP:O	3:C:252:GLN:HB3	2.09	0.52
1:A:1445:ILE:HD12	7:G:59:GLY:O	2.10	0.52
1:A:34:LYS:HB2	1:A:36:ARG:NH2	2.25	0.52
7:G:139:ILE:HG23	7:G:140:LYS:N	2.24	0.52
3:C:233:GLU:CG	3:C:234:SER:H	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:3:VAL:N	10:J:53:HIS:HE1	2.08	0.52
3:C:22:LEU:HD22	3:C:230:MET:CE	2.40	0.52
2:B:773:MET:CE	2:B:985:GLY:HA2	2.39	0.52
12:L:52:GLY:O	12:L:53:HIS:C	2.48	0.52
8:H:104:PHE:CD2	8:H:114:VAL:HG12	2.44	0.52
11:K:73:LEU:HD21	11:K:75:ILE:HD11	1.92	0.52
4:D:5:THR:O	4:D:5:THR:HG23	2.10	0.52
11:K:107:THR:HG22	11:K:108:GLU:N	2.24	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52
3:C:168:ALA:O	3:C:170:TRP:N	2.42	0.52
4:D:147:TYR:OH	7:G:103:VAL:HG13	2.10	0.52
2:B:498:THR:O	2:B:536:VAL:HA	2.09	0.52
1:A:440:ASP:O	1:A:460:VAL:HG23	2.11	0.52
2:B:787:VAL:HG12	2:B:787:VAL:O	2.10	0.52
2:B:276:ILE:HG23	2:B:336:ARG:HB2	1.91	0.51
2:B:519:TRP:C	2:B:519:TRP:CD1	2.83	0.51
1:A:64:ASN:O	1:A:65:LEU:C	2.48	0.51
9:I:53:GLY:O	9:I:89:GLN:HB2	2.10	0.51
5:E:147:HIS:HD2	5:E:149:LEU:H	1.58	0.51
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.10	0.51
7:G:116:PRO:HG2	7:G:119:LEU:HB2	1.92	0.51
2:B:429:PHE:HA	2:B:432:MET:CE	2.39	0.51
1:A:1230:GLU:O	1:A:1232:ASN:N	2.43	0.51
2:B:745:PRO:C	2:B:747:MET:N	2.63	0.51
2:B:806:THR:HB	2:B:809:MET:HG3	1.92	0.51
2:B:638:PHE:HB3	2:B:651:LEU:HD22	1.92	0.51
1:A:69:THR:C	1:A:71:GLN:N	2.60	0.51
2:B:1007:VAL:HG22	2:B:1008:PRO:CD	2.37	0.51
5:E:207:ARG:CB	5:E:207:ARG:NH1	2.71	0.51
1:A:697:ALA:HB2	1:A:702:LEU:CD1	2.39	0.51
1:A:988:LEU:O	1:A:992:ASP:HB2	2.10	0.51
6:F:127:GLU:O	6:F:128:LYS:C	2.48	0.51
9:I:44:TYR:CD1	9:I:44:TYR:C	2.83	0.51
1:A:1412:ALA:HA	1:A:1417:GLU:OE2	2.10	0.51
1:A:528:LEU:O	1:A:531:ILE:HG22	2.11	0.51
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.69	0.51
2:B:360:PHE:HE2	2:B:361:LEU:HD13	1.75	0.51
2:B:640:VAL:HG12	2:B:640:VAL:O	2.10	0.51
5:E:136:ASN:OD1	5:E:137:GLU:N	2.43	0.51
2:B:707:PRO:O	2:B:708:GLU:O	2.28	0.51
1:A:68:GLN:O	1:A:68:GLN:OE1	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:LEU:H	1:A:722:LEU:HD12	1.75	0.51
3:C:239:PRO:HB2	3:C:241:ASP:OD1	2.10	0.51
5:E:78:LEU:CA	5:E:107:THR:HB	2.34	0.51
7:G:51:TYR:C	7:G:51:TYR:CD2	2.84	0.51
1:A:999:VAL:HG12	1:A:1000:LEU:HD12	1.92	0.51
3:C:179:GLU:HG2	3:C:180:TYR:H	1.74	0.51
3:C:31:ASN:O	3:C:34:ARG:HB3	2.11	0.51
1:A:1268:LEU:O	1:A:1269:GLU:HG3	2.10	0.51
8:H:135:LEU:HB3	8:H:137:GLN:HG2	1.92	0.51
1:A:974:ASP:C	1:A:976:THR:H	2.14	0.51
2:B:745:PRO:C	2:B:747:MET:H	2.13	0.51
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.11	0.51
1:A:382:PRO:HD3	1:A:428:TYR:CD2	2.45	0.51
1:A:688:LYS:CD	1:A:691:LEU:HD23	2.41	0.51
9:I:53:GLY:O	9:I:55:THR:N	2.44	0.51
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.75	0.51
1:A:1435:PRO:O	1:A:1436:ILE:HG13	2.10	0.51
12:L:58:LYS:HG2	12:L:58:LYS:O	2.10	0.51
2:B:1031:LEU:HB2	2:B:1055:ILE:CD1	2.40	0.51
5:E:31:THR:HG1	5:E:34:GLU:H	1.57	0.51
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.93	0.51
2:B:398:ARG:HB3	2:B:398:ARG:HH11	1.76	0.51
12:L:66:GLN:HG2	12:L:67:PHE:N	2.25	0.51
8:H:10:PHE:CD1	8:H:10:PHE:N	2.78	0.51
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.11	0.51
2:B:708:GLU:HG3	2:B:709:ASP:N	2.25	0.51
1:A:688:LYS:HA	1:A:691:LEU:HB3	1.93	0.51
1:A:720:ARG:HG2	1:A:720:ARG:O	2.11	0.51
1:A:351:THR:HG22	2:B:1103:ILE:HG13	1.91	0.51
1:A:915:SER:O	1:A:919:ILE:HB	2.10	0.51
3:C:118:LEU:HB2	3:C:132:PRO:HG2	1.93	0.51
5:E:94:LYS:CE	5:E:98:ILE:HD11	2.33	0.51
2:B:976:ILE:O	2:B:990:ILE:HB	2.10	0.51
1:A:889:SER:CB	1:A:1297:GLU:HG3	2.38	0.51
1:A:696:GLU:OE2	1:A:702:LEU:HD21	2.09	0.51
1:A:982:THR:C	1:A:984:LYS:N	2.64	0.51
1:A:75:ASN:O	1:A:76:GLU:HB2	2.10	0.51
1:A:414:ASP:OD1	1:A:416:ARG:HG2	2.10	0.51
7:G:58:ARG:NH1	7:G:58:ARG:HG3	2.25	0.51
1:A:108:MET:HB3	1:A:210:ILE:HD11	1.91	0.51
1:A:1299:VAL:HG12	1:A:1300:LYS:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.76	0.51
1:A:247:ARG:NH1	1:A:263:THR:HG23	2.25	0.51
2:B:640:VAL:O	2:B:641:GLU:C	2.48	0.51
1:A:69:THR:C	1:A:71:GLN:H	2.13	0.51
2:B:1069:PHE:HA	2:B:1085:ILE:O	2.09	0.51
2:B:642:ASP:HB3	2:B:649:LYS:CG	2.39	0.51
1:A:332:LYS:O	1:A:333:GLU:CB	2.57	0.51
4:D:195:ILE:HG22	4:D:195:ILE:O	2.10	0.51
9:I:34:TYR:CE2	9:I:36:GLU:HB3	2.46	0.51
2:B:69:LEU:HD13	2:B:429:PHE:HD1	1.75	0.51
3:C:186:LEU:N	3:C:186:LEU:HD12	2.25	0.51
7:G:91:VAL:HG12	7:G:92:VAL:N	2.24	0.51
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.46	0.51
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.46	0.51
2:B:637:LEU:HD12	2:B:693:ILE:CD1	2.38	0.51
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.10	0.51
5:E:56:LYS:HZ3	5:E:84:ASP:N	2.09	0.51
1:A:33:ALA:HA	1:A:57:ARG:NH1	2.25	0.51
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
2:B:996:ARG:HH12	3:C:175:ALA:N	2.09	0.51
2:B:861:ASP:OD1	2:B:862:GLN:N	2.44	0.51
2:B:1095:LEU:CD1	2:B:1095:LEU:H	2.15	0.51
1:A:650:GLN:HB3	1:A:654:ASN:HD21	1.76	0.51
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.46	0.51
6:F:119:ARG:HG3	6:F:119:ARG:NH1	2.19	0.51
14:T:22:DC:H2"	14:T:23:BRU:OP2	2.10	0.51
2:B:130:VAL:HG23	2:B:167:ILE:HD13	1.92	0.51
11:K:68:PHE:N	11:K:68:PHE:CD2	2.75	0.51
1:A:445:ASN:HB2	1:A:454:SER:O	2.10	0.51
1:A:445:ASN:CB	1:A:455:MET:HG2	2.41	0.51
4:D:8:PHE:CD2	7:G:6:ASP:HB2	2.46	0.51
1:A:125:ALA:C	1:A:127:ALA:H	2.14	0.51
1:A:567:LYS:NZ	8:H:46:LEU:HB2	2.26	0.51
1:A:49:LYS:HD3	1:A:55:ASP:HB3	1.93	0.51
9:I:86:PHE:HE1	9:I:100:PHE:HB2	1.76	0.51
12:L:30:ILE:CG2	12:L:31:CYS:N	2.74	0.51
1:A:737:LEU:HD22	1:A:741:ASN:OD1	2.11	0.51
2:B:839:MET:CE	2:B:980:PHE:HB2	2.40	0.51
2:B:1182:CYS:O	2:B:1183:LYS:C	2.49	0.51
2:B:565:PRO:HB2	2:B:567:GLU:CG	2.40	0.51
2:B:46:GLN:HE21	2:B:539:LEU:HD12	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:68:PHE:HD1	11:K:70:ARG:NH1	2.05	0.51
3:C:183:TRP:CH2	3:C:203:GLN:NE2	2.78	0.51
1:A:1450:LEU:HG	7:G:19:GLY:O	2.11	0.51
1:A:447:GLN:HE22	14:T:20:DG:H4'	1.76	0.51
9:I:75:CYS:SG	9:I:79:HIS:N	2.84	0.51
1:A:483:ASP:O	2:B:979:LYS:HE3	2.11	0.51
2:B:555:ILE:HG22	2:B:556:THR:N	2.26	0.51
5:E:10:SER:O	5:E:13:TRP:HB3	2.11	0.51
5:E:168:TYR:HB3	5:E:170:LEU:HG	1.92	0.51
2:B:37:PHE:HD2	2:B:542:MET:SD	2.34	0.51
3:C:140:ASN:O	3:C:141:GLY:O	2.29	0.51
2:B:557:PHE:CE1	2:B:603:LEU:HD11	2.46	0.51
4:D:128:VAL:O	4:D:130:LEU:N	2.44	0.51
2:B:875:GLU:HG3	2:B:877:PRO:HD3	1.92	0.51
1:A:1054:LEU:HD13	6:F:84:TYR:OH	2.11	0.51
8:H:100:THR:HG22	8:H:101:ALA:N	2.26	0.51
1:A:332:LYS:C	1:A:334:GLY:N	2.52	0.51
1:A:1386:ARG:O	1:A:1391:ARG:HD2	2.10	0.51
2:B:307:ASP:OD2	2:B:310:MET:HB2	2.09	0.51
2:B:899:ILE:CG2	2:B:949:VAL:HG21	2.41	0.51
2:B:834:ASN:O	2:B:838:SER:O	2.29	0.51
3:C:70:ILE:HG12	3:C:142:VAL:HG11	1.93	0.51
1:A:583:PRO:O	1:A:610:GLY:HA3	2.11	0.51
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.46	0.51
2:B:593:PRO:O	2:B:595:ARG:N	2.43	0.51
2:B:361:LEU:O	2:B:363:HIS:O	2.29	0.51
1:A:88:LYS:HD3	1:A:293:GLU:CD	2.31	0.51
4:D:47:LEU:CD1	4:D:48:ILE:N	2.74	0.51
7:G:48:VAL:HA	7:G:76:ALA:HB2	1.93	0.51
1:A:691:LEU:O	1:A:691:LEU:HD12	2.11	0.51
2:B:1072:MET:HB2	2:B:1085:ILE:HD13	1.92	0.51
11:K:21:ILE:HG22	11:K:31:VAL:CG1	2.40	0.51
5:E:69:ILE:HD12	5:E:69:ILE:H	1.74	0.51
1:A:335:ARG:CZ	2:B:1202:LEU:HD13	2.41	0.51
8:H:62:SER:OG	8:H:63:LEU:N	2.43	0.51
1:A:1041:ALA:O	1:A:1045:VAL:HG23	2.11	0.51
2:B:1099:VAL:HG13	2:B:1100:ASP:H	1.76	0.51
2:B:1221:SER:O	2:B:1223:ASP:N	2.43	0.51
1:A:610:GLY:O	1:A:611:GLN:NE2	2.45	0.51
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.41	0.51
1:A:43:GLU:HG3	1:A:46:THR:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:606:LYS:HD2	2:B:608:ASP:OD2	2.10	0.50
3:C:104:PHE:HD2	3:C:105:GLY:H	1.57	0.50
1:A:7:SER:OG	2:B:1161:HIS:CE1	2.61	0.50
2:B:996:ARG:NH1	3:C:175:ALA:H	2.09	0.50
7:G:14:HIS:HD2	7:G:16:SER:OG	1.94	0.50
5:E:22:MET:HE3	5:E:26:ARG:NE	2.22	0.50
2:B:830:TYR:O	2:B:831:SER:C	2.49	0.50
1:A:1254:ALA:O	1:A:1255:GLU:CB	2.58	0.50
2:B:658:ILE:HG22	2:B:662:MET:HE2	1.93	0.50
2:B:326:ASP:OD1	2:B:329:THR:HB	2.10	0.50
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50
1:A:946:VAL:HG22	5:E:201:LYS:CD	2.41	0.50
2:B:39:ARG:HH21	2:B:665:GLU:CD	2.15	0.50
6:F:111:LEU:HD12	6:F:111:LEU:N	2.25	0.50
2:B:230:ALA:HB3	2:B:231:PRO:HD3	1.93	0.50
1:A:1453:TYR:O	1:A:1454:MET:HB3	2.12	0.50
2:B:393:LYS:HA	2:B:393:LYS:HE3	1.93	0.50
2:B:213:ILE:HD12	2:B:497:ARG:HB3	1.93	0.50
1:A:1444:MET:HE1	6:F:135:ARG:NE	2.26	0.50
2:B:879:ARG:HD2	2:B:879:ARG:H	1.76	0.50
2:B:983:ARG:HH11	2:B:1091:TYR:HB3	1.75	0.50
4:D:217:LEU:O	4:D:219:THR:N	2.44	0.50
4:D:220:LEU:CD2	4:D:221:TYR:N	2.63	0.50
4:D:53:SER:C	4:D:55:ALA:N	2.65	0.50
4:D:53:SER:H	4:D:148:LEU:CD2	2.24	0.50
2:B:504:ARG:NH2	14:T:15:DG:O6	2.43	0.50
2:B:661:LEU:HD23	2:B:679:TYR:O	2.11	0.50
11:K:53:ASP:OD1	11:K:55:LYS:HB2	2.12	0.50
4:D:52:LEU:HD12	4:D:182:SER:HB2	1.93	0.50
2:B:205:ILE:N	2:B:205:ILE:CD1	2.74	0.50
2:B:1197:PRO:O	2:B:1200:ALA:N	2.34	0.50
1:A:84:ILE:O	1:A:84:ILE:HG22	2.10	0.50
2:B:223:VAL:HG11	2:B:381:MET:HG2	1.93	0.50
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.40	0.50
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.46	0.50
4:D:46:GLU:HG2	4:D:47:LEU:N	2.26	0.50
4:D:60:LYS:HE3	4:D:126:ILE:CD1	2.33	0.50
2:B:642:ASP:O	2:B:644:GLU:N	2.38	0.50
5:E:65:THR:O	5:E:69:ILE:CD1	2.59	0.50
2:B:911:ILE:HG22	2:B:966:VAL:HG21	1.94	0.50
1:A:605:MET:HE1	1:A:612:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:LYS:H	1:A:337:ARG:HB2	1.77	0.50
1:A:1387:HIS:HA	1:A:1391:ARG:NH1	2.23	0.50
5:E:178:ILE:HB	5:E:212:ARG:HB3	1.94	0.50
2:B:212:LEU:HD23	2:B:480:SER:HB2	1.93	0.50
5:E:129:PRO:HG2	5:E:130:ALA:H	1.75	0.50
1:A:108:MET:SD	1:A:210:ILE:HD13	2.52	0.50
3:C:91:HIS:O	3:C:91:HIS:CD2	2.64	0.50
1:A:1220:PHE:O	1:A:1221:LYS:HB2	2.11	0.50
2:B:376:PHE:CZ	2:B:569:TYR:HD2	2.29	0.50
2:B:365:THR:OG1	2:B:367:LEU:HG	2.11	0.50
2:B:847:ASP:O	2:B:849:GLY:N	2.44	0.50
1:A:672:ASP:CG	1:A:674:PRO:HD2	2.32	0.50
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.11	0.50
1:A:1332:PHE:CE1	1:A:1348:LEU:HD13	2.46	0.50
2:B:687:GLU:O	2:B:689:LEU:HG	2.11	0.50
10:J:36:LEU:HB2	10:J:47:ARG:HH12	1.76	0.50
1:A:886:ILE:CG2	1:A:952:ALA:HB2	2.41	0.50
1:A:285:PRO:O	1:A:287:HIS:N	2.44	0.50
6:F:97:ARG:HD3	6:F:130:ILE:HG23	1.94	0.50
1:A:196:GLU:HG2	1:A:197:PRO:CD	2.41	0.50
5:E:182:ASP:HB3	5:E:185:ALA:CB	2.41	0.50
1:A:1211:GLN:O	1:A:1214:GLU:HB2	2.12	0.50
8:H:55:LEU:HD22	8:H:144:ILE:CG2	2.42	0.50
1:A:1187:GLN:HB2	1:A:1244:ARG:CG	2.30	0.50
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.46	0.50
1:A:51:GLY:C	1:A:56:PRO:HB3	2.32	0.50
2:B:622:LYS:CE	9:I:59:VAL:HG22	2.31	0.50
2:B:113:TYR:CD2	2:B:192:LEU:HD22	2.47	0.50
1:A:115:LEU:HD13	1:A:141:LEU:HD13	1.93	0.50
14:T:18:DC:H3'	14:T:18:DC:OP1	2.11	0.50
1:A:1208:THR:HG22	1:A:1210:GLY:H	1.76	0.50
1:A:298:PHE:O	1:A:302:THR:HB	2.12	0.50
2:B:882:THR:CG2	2:B:884:ARG:N	2.66	0.50
4:D:153:ARG:O	4:D:154:PHE:HD2	1.95	0.50
1:A:901:LEU:HA	1:A:907:THR:OG1	2.11	0.50
2:B:233:PRO:HG2	2:B:234:ILE:HD13	1.94	0.50
1:A:1138:ILE:HG21	1:A:1316:VAL:HG13	1.93	0.50
1:A:964:ILE:HD13	1:A:1035:TYR:CE1	2.46	0.50
1:A:836:TYR:CE2	1:A:840:ARG:HD2	2.47	0.50
2:B:259:TYR:HD1	2:B:259:TYR:H	1.59	0.50
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1017:ILE:H	2:B:1018:PRO:CD	2.24	0.50
2:B:59:LEU:HD12	2:B:417:PHE:CD2	2.47	0.50
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.42	0.50
10:J:24:LEU:O	10:J:30:LEU:HB2	2.11	0.50
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.11	0.50
3:C:138:GLU:HB2	3:C:140:ASN:ND2	2.26	0.50
1:A:1244:ARG:CB	1:A:1245:PRO:CD	2.88	0.50
1:A:12:ARG:NH2	2:B:1192:TYR:CZ	2.79	0.50
1:A:1111:MET:O	1:A:1112:LYS:O	2.30	0.50
2:B:678:GLU:HG2	2:B:679:TYR:N	2.26	0.50
1:A:886:ILE:CG2	1:A:887:GLY:H	2.23	0.50
3:C:213:PRO:HG2	3:C:214:ASN:H	1.76	0.50
1:A:858:ASN:ND2	1:A:858:ASN:C	2.65	0.50
1:A:460:VAL:HG12	1:A:461:LYS:N	2.26	0.50
2:B:258:LEU:HG	2:B:258:LEU:O	2.11	0.50
1:A:53:LEU:C	1:A:54:ASN:HD22	2.15	0.50
2:B:335:GLY:O	2:B:336:ARG:HG3	2.12	0.50
2:B:345:LYS:C	2:B:346:GLU:HG3	2.31	0.50
2:B:357:GLN:O	2:B:366:GLN:HA	2.11	0.50
1:A:269:ILE:HG23	1:A:300:VAL:HG23	1.94	0.50
2:B:705:MET:HB3	2:B:706:GLN:OE1	2.12	0.50
1:A:65:LEU:O	1:A:66:LYS:C	2.50	0.50
2:B:842:ASN:HD22	2:B:845:SER:N	2.04	0.50
7:G:3:PHE:HB2	7:G:78:VAL:HG23	1.94	0.50
1:A:690:VAL:HG12	1:A:691:LEU:N	2.26	0.50
3:C:242:GLN:O	3:C:244:VAL:N	2.45	0.50
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.93	0.50
5:E:211:TYR:CD1	5:E:211:TYR:N	2.79	0.50
1:A:475:THR:CG2	1:A:476:SER:N	2.75	0.50
5:E:37:LEU:HD11	5:E:41:ASP:HB2	1.93	0.50
1:A:1202:MET:HE1	1:A:1212:VAL:CG2	2.42	0.50
2:B:639:ILE:HD11	2:B:691:GLU:HB3	1.94	0.50
2:B:701:ILE:HD11	2:B:703:ILE:HD11	1.92	0.50
1:A:51:GLY:O	1:A:56:PRO:HB3	2.12	0.50
1:A:666:ILE:HD11	2:B:1086:PHE:CE1	2.46	0.50
5:E:27:GLY:O	5:E:65:THR:HG23	2.12	0.50
1:A:590:ARG:HH22	1:A:620:LYS:HB2	1.77	0.50
1:A:1313:LEU:C	1:A:1315:GLU:N	2.65	0.50
2:B:429:PHE:HA	2:B:432:MET:HE3	1.93	0.50
2:B:134:LYS:HE2	2:B:164:LYS:HZ1	1.77	0.50
1:A:115:LEU:HG	1:A:142:CYS:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:CD1	2:B:836:GLU:HB2	2.46	0.50
1:A:1214:GLU:C	1:A:1218:GLN:HE21	2.16	0.49
1:A:427:GLN:O	1:A:428:TYR:C	2.49	0.49
2:B:1187:ASN:OD1	2:B:1190:ASP:N	2.45	0.49
3:C:73:GLN:HB3	3:C:131:HIS:H	1.77	0.49
1:A:629:LEU:HD11	1:A:645:LEU:HD21	1.94	0.49
2:B:987:LYS:HE3	15:P:11:G:H1'	1.94	0.49
1:A:146:MET:HA	1:A:171:GLN:HB2	1.94	0.49
5:E:100:ILE:CG2	5:E:105:PHE:HB2	2.41	0.49
7:G:51:TYR:HD2	7:G:51:TYR:C	2.16	0.49
1:A:1003:LYS:O	1:A:1004:ASN:HB3	2.11	0.49
9:I:50:THR:HB	9:I:92:ARG:HH22	1.77	0.49
1:A:21:LEU:HD11	1:A:1414:ALA:HA	1.94	0.49
1:A:22:PHE:HB2	2:B:1211:ASN:OD1	2.12	0.49
1:A:1280:GLU:O	1:A:1281:ARG:O	2.30	0.49
9:I:119:THR:O	9:I:119:THR:HG22	2.11	0.49
1:A:40:THR:HB	1:A:41:MET:CE	2.41	0.49
4:D:29:LEU:N	4:D:29:LEU:CD2	2.74	0.49
2:B:882:THR:C	2:B:884:ARG:N	2.66	0.49
4:D:144:THR:HG21	7:G:46:LEU:HD13	1.92	0.49
4:D:12:ARG:NH1	4:D:12:ARG:HG2	2.26	0.49
8:H:82:PRO:C	8:H:84:ALA:N	2.64	0.49
2:B:839:MET:HE3	2:B:1010:LEU:CD2	2.39	0.49
5:E:48:ASP:CG	5:E:49:SER:N	2.64	0.49
6:F:109:VAL:HG12	6:F:110:ASP:H	1.75	0.49
1:A:108:MET:HA	1:A:210:ILE:HD13	1.93	0.49
1:A:40:THR:HB	1:A:41:MET:HE2	1.94	0.49
2:B:916:THR:HB	2:B:935:ARG:CD	2.41	0.49
9:I:118:ARG:HH12	9:I:120:GLN:HB2	1.77	0.49
3:C:97:VAL:HG21	3:C:129:ILE:HG22	1.93	0.49
2:B:654:ARG:O	2:B:656:GLY:N	2.46	0.49
3:C:46:ILE:HD13	3:C:157:CYS:SG	2.52	0.49
10:J:32:GLU:O	10:J:34:THR:N	2.45	0.49
10:J:48:ARG:HE	10:J:49:MET:HE2	1.78	0.49
2:B:211:VAL:HG23	2:B:483:LEU:HB2	1.93	0.49
1:A:153:PRO:CD	1:A:161:LEU:HD13	2.41	0.49
1:A:336:ILE:HD13	1:A:340:LEU:HD12	1.93	0.49
4:D:209:ARG:NH1	4:D:209:ARG:HG2	2.27	0.49
4:D:8:PHE:CE2	7:G:6:ASP:HB2	2.48	0.49
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.93	0.49
1:A:1206:ASP:O	1:A:1274:ARG:NH2	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:105:GLY:O	3:C:149:LYS:O	2.31	0.49
1:A:382:PRO:N	1:A:428:TYR:HE2	2.10	0.49
2:B:996:ARG:HH22	3:C:175:ALA:H	1.60	0.49
2:B:167:ILE:HD12	2:B:167:ILE:N	2.27	0.49
1:A:287:HIS:ND1	1:A:290:GLU:HG2	2.28	0.49
1:A:809:THR:H	1:A:812:GLU:HB2	1.77	0.49
1:A:1349:TYR:CD2	1:A:1349:TYR:C	2.86	0.49
2:B:363:HIS:O	2:B:364:ILE:CB	2.61	0.49
1:A:55:ASP:OD2	1:A:55:ASP:O	2.31	0.49
4:D:35:LEU:HA	4:D:47:LEU:HB2	1.92	0.49
3:C:239:PRO:O	3:C:241:ASP:N	2.45	0.49
1:A:670:ILE:HD12	2:B:1067:ARG:NH2	2.27	0.49
5:E:61:GLN:HG3	5:E:78:LEU:O	2.11	0.49
9:I:88:SER:C	9:I:90:GLN:H	2.15	0.49
2:B:910:VAL:HG11	2:B:938:SER:HB3	1.94	0.49
4:D:71:LYS:HA	4:D:74:GLN:HB2	1.93	0.49
2:B:287:ARG:HG3	2:B:292:ILE:HA	1.93	0.49
3:C:215:GLU:O	3:C:217:ASP:N	2.46	0.49
1:A:946:VAL:CG2	5:E:201:LYS:HD2	2.42	0.49
4:D:20:GLU:H	4:D:20:GLU:CD	2.16	0.49
1:A:1129:GLU:OE2	1:A:1132:LYS:HD2	2.12	0.49
2:B:254:LEU:HD22	2:B:361:LEU:HD12	1.94	0.49
1:A:49:LYS:HZ1	1:A:61:ILE:H	1.57	0.49
1:A:56:PRO:O	1:A:57:ARG:NH1	2.45	0.49
2:B:995:ARG:HH12	3:C:165:LYS:HG2	1.77	0.49
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.42	0.49
2:B:575:PRO:HG2	2:B:576:ASP:H	1.76	0.49
4:D:153:ARG:HB3	4:D:154:PHE:CE2	2.48	0.49
6:F:69:LEU:HB2	6:F:72:LYS:HD2	1.95	0.49
2:B:25:ILE:CD1	2:B:653:VAL:O	2.60	0.49
2:B:185:THR:O	2:B:188:ASP:N	2.46	0.49
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.42	0.49
1:A:888:GLY:O	1:A:940:ARG:NH2	2.45	0.49
5:E:168:TYR:CB	5:E:170:LEU:HG	2.42	0.49
7:G:165:GLU:HB2	7:G:168:LEU:HD12	1.94	0.49
1:A:343:LYS:HZ2	2:B:1151:LEU:HG	1.76	0.49
2:B:240:ILE:HG23	2:B:254:LEU:HB3	1.94	0.49
2:B:603:LEU:HD13	2:B:608:ASP:CB	2.35	0.49
2:B:849:GLY:O	2:B:850:LEU:C	2.51	0.49
2:B:1065:GLN:NE2	2:B:1066:SER:N	2.61	0.49
4:D:149:THR:HG22	4:D:150:ASN:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:874:PHE:HB3	2:B:896:ASP:O	2.12	0.49
12:L:61:THR:HG22	12:L:62:LYS:H	1.78	0.49
3:C:33:LEU:HD12	3:C:37:MET:HG3	1.95	0.49
8:H:135:LEU:CB	8:H:137:GLN:HG2	2.43	0.49
2:B:579:ARG:N	2:B:589:VAL:HG13	2.28	0.49
2:B:579:ARG:CA	2:B:589:VAL:HG13	2.42	0.49
2:B:603:LEU:HD12	2:B:609:ILE:CG2	2.41	0.49
8:H:12:VAL:HG11	8:H:51:ALA:HA	1.95	0.49
1:A:265:LYS:CA	1:A:265:LYS:CE	2.86	0.49
1:A:382:PRO:HD3	1:A:428:TYR:CE2	2.47	0.49
1:A:774:ARG:NH1	1:A:797:LYS:HG3	2.27	0.49
2:B:129:PHE:HA	2:B:165:VAL:O	2.13	0.49
11:K:50:LEU:HD11	11:K:75:ILE:HD13	1.94	0.49
1:A:820:GLY:O	1:A:822:GLU:N	2.45	0.49
2:B:217:ARG:NE	2:B:405:ARG:HB2	2.26	0.49
1:A:846:GLU:OE1	1:A:1425:SER:OG	2.29	0.49
1:A:2:VAL:HG22	1:A:3:GLY:N	2.26	0.49
2:B:281:PRO:O	2:B:283:VAL:N	2.45	0.49
2:B:711:GLU:HB2	2:B:712:PRO:HD2	1.94	0.49
15:P:9:C:OP2	15:P:9:C:H6	1.96	0.49
2:B:542:MET:CE	2:B:747:MET:HG3	2.43	0.49
8:H:93:TYR:HB3	8:H:144:ILE:O	2.12	0.49
8:H:44:VAL:CG1	8:H:48:PRO:HA	2.41	0.49
3:C:167:HIS:N	11:K:6:ARG:NH1	2.61	0.49
1:A:256:GLN:HE21	2:B:935:ARG:HH12	1.60	0.49
3:C:144:ILE:HG22	3:C:145:CYS:N	2.28	0.49
10:J:53:HIS:CD2	10:J:54:VAL:C	2.86	0.49
4:D:118:THR:CB	4:D:121:LYS:HB3	2.43	0.49
1:A:337:ARG:HD2	2:B:1132:GLU:OE1	2.13	0.49
9:I:7:CYS:C	9:I:8:ARG:O	2.51	0.49
1:A:993:LEU:HD22	1:A:1046:LEU:CD2	2.42	0.49
2:B:59:LEU:HD12	2:B:417:PHE:CE2	2.48	0.49
2:B:277:LYS:HG2	2:B:336:ARG:HB3	1.94	0.49
1:A:1187:GLN:HG2	1:A:1188:GLN:N	2.28	0.49
5:E:119:SER:O	5:E:123:LEU:HD21	2.13	0.49
1:A:306:ASN:HD22	1:A:322:VAL:HG12	1.78	0.49
1:A:70:CYS:HA	2:B:1174:LYS:HG2	1.94	0.49
1:A:919:ILE:HG12	1:A:925:LEU:HD12	1.95	0.49
4:D:120:GLU:HA	4:D:123:LEU:HD23	1.95	0.49
1:A:1436:ILE:O	1:A:1439:GLY:N	2.27	0.49
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.53	0.49
8:H:82:PRO:HG2	8:H:83:GLN:H	1.78	0.49
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.13	0.49
2:B:815:ARG:HB2	2:B:815:ARG:NH1	2.28	0.49
13:N:4:DA:H2"	13:N:5:DC:C6	2.48	0.49
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.31	0.49
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.46	0.49
1:A:853:ASP:C	1:A:853:ASP:OD1	2.51	0.49
1:A:639:PRO:HG2	1:A:640:GLN:HE21	1.77	0.49
3:C:15:LYS:HG2	3:C:15:LYS:O	2.12	0.49
1:A:321:PRO:O	1:A:322:VAL:CB	2.60	0.48
1:A:12:ARG:CB	2:B:1218:THR:HG22	2.29	0.48
3:C:166:GLU:C	11:K:6:ARG:HH11	2.16	0.48
2:B:866:TYR:O	2:B:867:GLY:C	2.50	0.48
2:B:879:ARG:N	2:B:879:ARG:CD	2.75	0.48
4:D:14:ARG:NH2	4:D:16:LYS:HD2	2.28	0.48
5:E:79:TRP:HB2	5:E:105:PHE:CE1	2.47	0.48
2:B:1094:ARG:HH21	2:B:1098:MET:HG2	1.78	0.48
2:B:753:ALA:O	2:B:756:ILE:HG13	2.13	0.48
1:A:482:PHE:HB2	2:B:838:SER:OG	2.13	0.48
3:C:82:TYR:O	3:C:83:SER:C	2.50	0.48
9:I:2:THR:HG23	9:I:2:THR:O	2.13	0.48
2:B:641:GLU:C	2:B:643:ASP:H	2.16	0.48
2:B:247:GLY:H	2:B:249:ARG:HH21	1.61	0.48
5:E:112:TYR:CD1	5:E:112:TYR:C	2.86	0.48
8:H:44:VAL:HG12	8:H:44:VAL:O	2.13	0.48
4:D:136:GLY:HA2	4:D:142:LYS:NZ	2.28	0.48
10:J:53:HIS:HD2	10:J:54:VAL:C	2.17	0.48
5:E:22:MET:CE	5:E:26:ARG:NH2	2.67	0.48
1:A:774:ARG:CZ	1:A:797:LYS:HB2	2.43	0.48
12:L:34:CYS:SG	12:L:51:CYS:SG	3.11	0.48
2:B:839:MET:HG3	2:B:1010:LEU:HD23	1.94	0.48
2:B:405:ARG:NE	2:B:632:ARG:HG2	2.27	0.48
5:E:157:SER:OG	5:E:160:GLU:HG3	2.13	0.48
1:A:482:PHE:HD1	2:B:838:SER:HG	1.61	0.48
1:A:1280:GLU:O	1:A:1281:ARG:C	2.51	0.48
2:B:183:GLU:O	2:B:184:ALA:O	2.30	0.48
2:B:218:SER:HB3	2:B:241:ARG:HH12	1.77	0.48
9:I:61:ASP:O	9:I:63:GLY:N	2.47	0.48
3:C:238:ILE:HD11	3:C:246:ARG:NH1	2.28	0.48
1:A:666:ILE:HG23	2:B:1026:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:642:ASP:CB	2:B:649:LYS:HA	2.44	0.48
1:A:144:THR:O	1:A:146:MET:HG3	2.12	0.48
1:A:463:ILE:CD1	1:A:469:ARG:HG3	2.43	0.48
2:B:976:ILE:HD13	2:B:992:ILE:HA	1.95	0.48
9:I:17:ARG:HG3	9:I:28:GLU:HG2	1.95	0.48
7:G:30:LEU:HD23	7:G:54:ILE:HD13	1.95	0.48
12:L:61:THR:HG22	12:L:63:ARG:HG3	1.93	0.48
12:L:27:LEU:HD13	12:L:37:LYS:CD	2.43	0.48
11:K:45:LEU:HG	11:K:94:ILE:CD1	2.41	0.48
1:A:883:LEU:CD1	1:A:1017:LEU:HD11	2.40	0.48
3:C:89:GLU:O	3:C:90:ASP:CB	2.60	0.48
2:B:1001:PHE:CD2	3:C:34:ARG:NH2	2.81	0.48
7:G:87:VAL:CG2	7:G:103:VAL:HG21	2.44	0.48
1:A:336:ILE:HD11	2:B:1203:LEU:HD22	1.94	0.48
3:C:167:HIS:N	11:K:6:ARG:HH12	2.11	0.48
1:A:901:LEU:HD23	1:A:907:THR:OG1	2.12	0.48
1:A:925:LEU:C	1:A:927:VAL:N	2.66	0.48
3:C:177:GLU:CG	3:C:231:ASN:HD22	2.20	0.48
2:B:766:ARG:HH11	2:B:769:TYR:HD1	1.61	0.48
2:B:120:ARG:NH1	12:L:54:ARG:NH1	2.60	0.48
1:A:1315:GLU:C	1:A:1317:MET:H	2.17	0.48
12:L:36:SER:O	12:L:37:LYS:C	2.51	0.48
2:B:282:ILE:HG21	2:B:382:ILE:HD11	1.95	0.48
2:B:384:ARG:HA	2:B:387:LEU:HD13	1.96	0.48
11:K:54:ARG:HG2	11:K:54:ARG:NH1	2.27	0.48
8:H:56:THR:O	8:H:144:ILE:HA	2.14	0.48
8:H:4:THR:CA	8:H:60:ALA:HB2	2.23	0.48
1:A:381:THR:CG2	1:A:382:PRO:HD2	2.35	0.48
1:A:255:SER:OG	2:B:918:ILE:CG2	2.61	0.48
1:A:720:ARG:O	1:A:724:GLU:HB2	2.12	0.48
2:B:797:TYR:C	2:B:798:TYR:HD2	2.17	0.48
1:A:200:ARG:HG2	1:A:201:VAL:N	2.28	0.48
12:L:31:CYS:SG	12:L:34:CYS:N	2.86	0.48
2:B:416:LEU:HD12	2:B:466:TRP:CE2	2.49	0.48
3:C:35:ARG:NH1	11:K:41:THR:N	2.60	0.48
2:B:521:LEU:HB3	2:B:633:VAL:HG11	1.95	0.48
1:A:1057:VAL:HG12	1:A:1058:VAL:N	2.29	0.48
1:A:264:PHE:HB3	1:A:265:LYS:NZ	2.28	0.48
1:A:320:ARG:NE	1:A:323:LYS:HZ2	2.12	0.48
1:A:34:LYS:HZ2	1:A:57:ARG:HH22	1.59	0.48
1:A:65:LEU:O	1:A:71:GLN:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:7:LEU:HB2	7:G:74:TYR:CE2	2.49	0.48
2:B:882:THR:HG23	2:B:884:ARG:CA	2.44	0.48
3:C:56:THR:HG22	3:C:57:VAL:N	2.26	0.48
3:C:133:ILE:CD1	3:C:236:GLY:C	2.82	0.48
1:A:1094:VAL:HG13	1:A:1113:THR:HB	1.96	0.48
2:B:644:GLU:C	2:B:646:LEU:H	2.17	0.48
2:B:831:SER:CB	2:B:994:TYR:OH	2.61	0.48
2:B:860:MET:CG	2:B:965:LYS:HG2	2.42	0.48
7:G:115:MET:O	7:G:164:LYS:HD3	2.14	0.48
9:I:12:ASN:HA	9:I:12:ASN:HD22	1.53	0.48
2:B:412:LEU:HB3	2:B:466:TRP:NE1	2.28	0.48
1:A:1029:ARG:NH1	1:A:1029:ARG:CG	2.77	0.48
1:A:20:GLY:O	1:A:21:LEU:HD23	2.13	0.48
5:E:7:ARG:HG3	5:E:8:ASN:H	1.77	0.48
1:A:663:SER:OG	1:A:664:THR:N	2.43	0.48
1:A:49:LYS:CD	1:A:55:ASP:HB3	2.44	0.48
4:D:40:HIS:CE1	7:G:7:LEU:O	2.65	0.48
4:D:126:ILE:HD13	4:D:145:MET:HE2	1.95	0.48
4:D:17:LYS:C	4:D:17:LYS:HD2	2.33	0.48
2:B:190:TYR:CE1	2:B:196:PRO:HG3	2.49	0.48
2:B:1000:PRO:O	2:B:1007:VAL:HG23	2.14	0.48
7:G:88:ASP:CB	7:G:144:ARG:HA	2.34	0.48
2:B:896:ASP:OD2	12:L:58:LYS:HE3	2.14	0.48
8:H:61:SER:O	8:H:62:SER:HB2	2.14	0.48
2:B:1115:THR:O	2:B:1116:ARG:CB	2.59	0.48
2:B:360:PHE:CE2	2:B:361:LEU:HD13	2.49	0.48
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.79	0.48
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.43	0.48
2:B:957:ASN:O	2:B:958:GLN:C	2.52	0.48
4:D:155:ARG:HB3	4:D:155:ARG:HH11	1.79	0.48
1:A:593:GLU:C	1:A:595:THR:H	2.15	0.48
1:A:1127:ASP:HB3	1:A:1130:GLN:HB3	1.94	0.48
1:A:1134:ILE:O	1:A:1138:ILE:HG12	2.13	0.48
2:B:515:HIS:HD2	2:B:517:THR:OG1	1.97	0.48
11:K:111:LEU:N	11:K:111:LEU:HD23	2.29	0.48
1:A:477:PRO:CG	1:A:521:MET:HG2	2.44	0.48
2:B:434:ARG:O	2:B:436:VAL:HG23	2.13	0.48
4:D:39:ASN:ND2	4:D:41:GLN:HB2	2.28	0.48
1:A:526:ASP:HB2	2:B:835:GLN:OE1	2.14	0.48
1:A:26:GLU:O	1:A:29:ALA:HB3	2.14	0.48
2:B:1170:THR:O	2:B:1172:ILE:HD13	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:46:VAL:O	12:L:46:VAL:HG12	2.14	0.48
1:A:396:PRO:HB3	1:A:402:ALA:O	2.13	0.48
8:H:5:LEU:CG	8:H:60:ALA:HA	2.44	0.48
8:H:9:ILE:HG23	8:H:55:LEU:C	2.34	0.48
1:A:9:ALA:O	1:A:10:PRO:C	2.52	0.48
2:B:1072:MET:HB2	2:B:1085:ILE:CD1	2.44	0.48
4:D:123:LEU:CD2	4:D:149:THR:HG21	2.44	0.48
11:K:21:ILE:CG2	11:K:33:ILE:HG12	2.37	0.48
1:A:896:ARG:HD3	1:A:897:TYR:CZ	2.48	0.48
3:C:213:PRO:O	3:C:214:ASN:HB3	2.14	0.48
2:B:405:ARG:HD2	2:B:631:GLY:O	2.14	0.48
3:C:186:LEU:N	3:C:186:LEU:CD1	2.77	0.48
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.59	0.48
10:J:24:LEU:HA	10:J:28:ASP:HB2	1.96	0.48
2:B:1154:ALA:O	2:B:1155:SER:HB2	2.13	0.48
2:B:360:PHE:HD2	2:B:360:PHE:C	2.16	0.48
2:B:701:ILE:HG13	2:B:702:LEU:N	2.29	0.48
3:C:105:GLY:HA3	3:C:149:LYS:O	2.14	0.48
1:A:49:LYS:NZ	1:A:61:ILE:N	2.58	0.48
7:G:31:LEU:HD13	7:G:35:GLU:HG3	1.96	0.48
4:D:154:PHE:CE2	4:D:218:GLU:HA	2.49	0.48
3:C:236:GLY:C	3:C:238:ILE:N	2.66	0.48
11:K:101:LEU:HD23	11:K:101:LEU:O	2.13	0.48
2:B:100:PRO:HG3	2:B:172:ILE:HD12	1.96	0.48
7:G:111:THR:O	7:G:112:LYS:C	2.52	0.48
7:G:111:THR:O	7:G:113:HIS:N	2.47	0.48
1:A:821:ARG:HD2	1:A:825:ILE:HD11	1.96	0.48
11:K:8:GLU:O	11:K:37:LYS:HD2	2.14	0.48
11:K:53:ASP:C	11:K:55:LYS:H	2.18	0.48
9:I:82:GLU:HB3	9:I:104:LEU:CG	2.44	0.48
8:H:135:LEU:HD13	8:H:137:GLN:NE2	2.29	0.48
4:D:27:LEU:HD11	4:D:197:SER:HB3	1.96	0.48
3:C:84:ARG:HG3	3:C:85:ASP:OD1	2.14	0.48
2:B:1219:ASP:C	2:B:1219:ASP:OD1	2.51	0.48
1:A:1025:ARG:HG3	1:A:1025:ARG:HH11	1.79	0.48
8:H:47:PHE:HB3	8:H:95:TYR:HD1	1.78	0.47
2:B:935:ARG:HG3	2:B:935:ARG:O	2.12	0.47
1:A:208:LEU:HD22	1:A:212:LYS:HD2	1.96	0.47
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.14	0.47
2:B:425:THR:HA	2:B:428:ILE:CD1	2.39	0.47
1:A:595:THR:C	1:A:596:THR:HG23	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1319:VAL:HG12	1:A:1320:PRO:O	2.14	0.47
2:B:975:GLN:CG	2:B:976:ILE:N	2.74	0.47
1:A:899:VAL:CB	1:A:929:LEU:HD12	2.44	0.47
1:A:443:LEU:HD21	1:A:455:MET:HB3	1.96	0.47
3:C:35:ARG:HH12	11:K:41:THR:H	1.62	0.47
2:B:1223:ASP:O	2:B:1224:PHE:CB	2.60	0.47
1:A:1169:ILE:O	1:A:1169:ILE:HG22	2.15	0.47
5:E:138:ALA:HA	5:E:141:VAL:HG23	1.95	0.47
1:A:7:SER:C	1:A:9:ALA:H	2.17	0.47
2:B:875:GLU:O	2:B:877:PRO:CD	2.62	0.47
9:I:55:THR:HG22	9:I:58:VAL:CG2	2.44	0.47
1:A:645:LEU:HG	1:A:649:ILE:CD1	2.44	0.47
1:A:1278:ASN:O	1:A:1310:GLY:HA3	2.13	0.47
5:E:49:SER:OG	5:E:50:MET:N	2.47	0.47
6:F:119:ARG:HH11	6:F:119:ARG:CG	2.21	0.47
12:L:26:THR:CG2	12:L:27:LEU:H	2.27	0.47
7:G:21:ARG:HD2	7:G:24:GLN:HB2	1.93	0.47
2:B:313:MET:HE2	2:B:390:LEU:HD11	1.95	0.47
14:T:19:DT:OP1	14:T:19:DT:H3'	2.14	0.47
1:A:195:ASP:O	1:A:196:GLU:HB3	2.14	0.47
2:B:431:TYR:CG	2:B:447:ALA:HB2	2.49	0.47
2:B:434:ARG:O	2:B:436:VAL:N	2.46	0.47
10:J:16:ASP:OD1	10:J:17:LYS:HD2	2.14	0.47
1:A:1285:MET:O	1:A:1305:VAL:N	2.39	0.47
8:H:11:GLN:O	8:H:28:ALA:CB	2.61	0.47
8:H:41:ASP:O	8:H:42:ILE:HG13	2.15	0.47
10:J:2:ILE:HG12	10:J:57:ILE:CD1	2.44	0.47
4:D:17:LYS:CD	4:D:18:VAL:HG13	2.43	0.47
2:B:1097:HIS:H	2:B:1098:MET:HE2	1.80	0.47
1:A:90:VAL:HG12	1:A:91:PHE:N	2.29	0.47
1:A:537:ARG:HB2	8:H:20:TYR:CE2	2.50	0.47
1:A:186:LYS:HZ1	1:A:197:PRO:HD3	1.77	0.47
14:T:13:DT:H2"	14:T:14:DA:C8	2.48	0.47
1:A:1394:THR:HG21	1:A:1398:MET:SD	2.53	0.47
7:G:45:ILE:HA	7:G:78:VAL:HG12	1.95	0.47
2:B:882:THR:CG2	2:B:883:LEU:N	2.78	0.47
3:C:235:VAL:CG1	10:J:13:VAL:HG13	2.44	0.47
3:C:66:ARG:NH2	10:J:5:VAL:HG23	2.28	0.47
4:D:220:LEU:HD23	4:D:221:TYR:N	2.17	0.47
1:A:106:VAL:CG1	1:A:107:CYS:N	2.77	0.47
5:E:61:GLN:HG2	5:E:62:ALA:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:MET:HB3	2:B:109:THR:CG2	2.45	0.47
2:B:47:GLN:O	2:B:173:MET:HE1	2.14	0.47
1:A:963:ILE:HD11	1:A:1048:ASN:CB	2.44	0.47
6:F:109:VAL:HG13	6:F:127:GLU:OE1	2.14	0.47
1:A:494:SER:O	1:A:498:ARG:HG2	2.14	0.47
1:A:262:LEU:O	1:A:266:LEU:HG	2.14	0.47
1:A:350:ARG:CB	2:B:1128:LEU:HD11	2.45	0.47
5:E:182:ASP:HB3	5:E:185:ALA:HB2	1.96	0.47
2:B:55:VAL:HG13	2:B:97:VAL:HG21	1.97	0.47
2:B:635:ARG:HB2	2:B:636:PRO:HD2	1.95	0.47
2:B:638:PHE:HD2	2:B:690:VAL:HG22	1.79	0.47
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.48	0.47
1:A:500:GLU:OE1	2:B:1145:SER:N	2.48	0.47
2:B:997:GLU:H	2:B:997:GLU:HG3	1.41	0.47
2:B:878:GLN:O	2:B:879:ARG:C	2.53	0.47
2:B:918:ILE:CG2	2:B:935:ARG:NH2	2.74	0.47
1:A:719:VAL:HG12	1:A:720:ARG:N	2.29	0.47
1:A:698:GLN:HE21	9:I:99:LEU:HD21	1.78	0.47
5:E:145:THR:HG21	5:E:187:TYR:CD2	2.50	0.47
2:B:642:ASP:CA	2:B:649:LYS:HG3	2.43	0.47
2:B:113:TYR:CE2	2:B:192:LEU:HD21	2.50	0.47
2:B:167:ILE:HG22	2:B:453:ILE:CD1	2.41	0.47
12:L:26:THR:HG22	12:L:27:LEU:N	2.30	0.47
2:B:291:ILE:CD1	2:B:300:HIS:NE2	2.77	0.47
1:A:843:LYS:HD3	1:A:846:GLU:OE2	2.14	0.47
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.42	0.47
1:A:38:PRO:HA	1:A:270:LEU:HD23	1.96	0.47
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.96	0.47
3:C:193:TYR:HD1	3:C:193:TYR:O	1.97	0.47
7:G:136:VAL:O	7:G:136:VAL:HG12	2.14	0.47
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.49	0.47
2:B:849:GLY:O	2:B:852:ARG:HG3	2.14	0.47
7:G:123:ALA:O	7:G:125:SER:N	2.48	0.47
2:B:798:TYR:CE2	3:C:62:PHE:HE2	2.30	0.47
3:C:22:LEU:CD2	3:C:230:MET:HE2	2.45	0.47
1:A:1332:PHE:H	1:A:1332:PHE:HD2	1.63	0.47
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.44	0.47
1:A:1341:ILE:CG2	1:A:1342:GLU:N	2.78	0.47
1:A:960:ILE:HA	1:A:963:ILE:HG22	1.97	0.47
1:A:456:MET:HE3	1:A:474:VAL:CG2	2.45	0.47
1:A:316:GLN:O	1:A:317:LYS:C	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:GLU:O	2:B:561:TRP:CD1	2.68	0.47
2:B:34:ILE:HG12	2:B:542:MET:HE1	1.97	0.47
1:A:1166:ASP:O	1:A:1167:GLU:C	2.52	0.47
2:B:331:LEU:HD23	2:B:353:LYS:HG2	1.97	0.47
5:E:112:TYR:CE1	5:E:136:ASN:HB2	2.50	0.47
1:A:1441:PHE:HE1	6:F:92:ARG:HG2	1.79	0.47
1:A:269:ILE:HG12	1:A:299:HIS:HB3	1.97	0.47
1:A:69:THR:HB	2:B:1174:LYS:HZ3	1.79	0.47
1:A:795:GLU:CD	1:A:795:GLU:H	2.17	0.47
3:C:59:ALA:O	3:C:62:PHE:HB3	2.13	0.47
2:B:996:ARG:HH12	3:C:174:ALA:HA	1.80	0.47
3:C:44:LEU:HD21	3:C:159:ALA:CB	2.44	0.47
3:C:73:GLN:NE2	3:C:75:MET:N	2.62	0.47
3:C:131:HIS:O	3:C:133:ILE:N	2.48	0.47
1:A:1424:VAL:HG13	1:A:1436:ILE:CD1	2.45	0.47
8:H:81:PRO:CB	8:H:82:PRO:CD	2.92	0.47
8:H:82:PRO:O	8:H:84:ALA:N	2.33	0.47
2:B:126:SER:HA	2:B:169:ARG:HH12	1.79	0.47
2:B:789:MET:HE2	2:B:965:LYS:HB2	1.96	0.47
2:B:952:VAL:HG12	2:B:953:LEU:N	2.30	0.47
2:B:860:MET:SD	2:B:963:PHE:HE1	2.37	0.47
1:A:233:TRP:C	1:A:235:ILE:H	2.16	0.47
9:I:95:THR:HG22	9:I:96:SER:O	2.15	0.47
2:B:129:PHE:CD2	2:B:166:PHE:HA	2.49	0.47
2:B:654:ARG:O	2:B:657:HIS:N	2.47	0.47
2:B:654:ARG:NH1	2:B:654:ARG:HG3	2.29	0.47
12:L:27:LEU:O	12:L:28:LYS:HB2	2.13	0.47
1:A:898:ARG:HD3	1:A:933:TYR:CE1	2.50	0.47
1:A:79:GLY:H	2:B:1205:GLN:HE22	1.63	0.47
2:B:515:HIS:NE2	2:B:517:THR:HG23	2.30	0.47
1:A:1048:ASN:HD22	1:A:1048:ASN:N	2.12	0.47
2:B:1073:TYR:HE2	3:C:180:TYR:CE2	2.32	0.47
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.96	0.47
1:A:993:LEU:CD2	1:A:1022:LEU:HD11	2.45	0.47
1:A:1353:TYR:HD2	1:A:1353:TYR:C	2.17	0.47
8:H:98:TYR:C	8:H:118:PHE:HD2	2.16	0.47
1:A:551:TYR:CE2	11:K:62:LYS:HE2	2.50	0.47
2:B:526:GLU:HG3	2:B:771:SER:HB3	1.96	0.47
1:A:953:ASN:C	1:A:954:TRP:CD1	2.88	0.47
1:A:814:PHE:O	1:A:814:PHE:CD2	2.67	0.47
2:B:37:PHE:HE1	2:B:41:LYS:CG	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:GLU:O	2:B:643:ASP:N	2.46	0.47
2:B:706:GLN:NE2	2:B:730:ARG:HD3	2.29	0.47
1:A:385:ILE:HG22	1:A:386:ASP:N	2.30	0.47
2:B:878:GLN:HA	2:B:885:MET:HE1	1.97	0.47
9:I:100:PHE:CD1	9:I:100:PHE:N	2.83	0.47
12:L:53:HIS:C	12:L:55:ILE:HD13	2.34	0.47
2:B:98:THR:O	2:B:126:SER:HB2	2.14	0.47
1:A:23:SER:CB	1:A:233:TRP:NE1	2.78	0.47
1:A:904:THR:O	1:A:904:THR:CG2	2.62	0.47
2:B:1183:LYS:HE3	2:B:1183:LYS:O	2.14	0.47
12:L:60:ARG:HH21	12:L:65:VAL:CG2	2.28	0.47
10:J:7:CYS:SG	10:J:49:MET:HE3	2.55	0.47
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.45	0.47
2:B:735:ALA:HB3	2:B:738:PHE:CE1	2.50	0.47
2:B:376:PHE:HB3	2:B:566:LEU:HD21	1.96	0.47
1:A:1166:ASP:OD2	1:A:1239:ARG:CD	2.62	0.47
2:B:848:ARG:HD3	10:J:11:GLY:HA2	1.97	0.47
2:B:1181:GLU:H	2:B:1188:LYS:HA	1.80	0.47
12:L:30:ILE:CG2	12:L:31:CYS:H	2.28	0.47
2:B:126:SER:HB3	2:B:172:ILE:HD11	1.97	0.47
2:B:992:ILE:HG12	2:B:993:THR:H	1.79	0.47
2:B:412:LEU:HB3	2:B:466:TRP:CZ2	2.50	0.47
2:B:1167:GLY:O	2:B:1215:ARG:HA	2.15	0.47
1:A:180:LYS:NZ	1:A:294:SER:HB3	2.30	0.47
1:A:1283:VAL:HG12	1:A:1284:MET:N	2.29	0.47
5:E:162:ARG:HB3	5:E:162:ARG:CZ	2.45	0.47
2:B:562:GLY:HA3	2:B:590:HIS:CE1	2.50	0.47
8:H:15:VAL:HG22	8:H:26:ILE:CD1	2.45	0.47
4:D:139:LYS:HG3	4:D:140:ASP:OD1	2.15	0.47
3:C:101:LEU:HD13	3:C:118:LEU:CD2	2.45	0.47
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.96	0.47
14:T:15:DG:C8	14:T:16:DT:C7	2.98	0.47
2:B:63:ILE:HD12	2:B:421:PHE:CD2	2.49	0.47
1:A:960:ILE:HA	1:A:963:ILE:CG2	2.45	0.47
2:B:307:ASP:OD1	2:B:309:GLN:HB2	2.15	0.47
1:A:90:VAL:HG12	1:A:297:GLN:NE2	2.30	0.47
10:J:21:TYR:HB2	10:J:39:LEU:HD11	1.96	0.47
2:B:430:ARG:HB3	2:B:434:ARG:CZ	2.45	0.47
4:D:39:ASN:ND2	4:D:41:GLN:H	2.13	0.47
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.96	0.47
1:A:1410:PHE:HD2	2:B:1212:ILE:HD12	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:LEU:HD11	3:C:95:CYS:C	2.35	0.47
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.51	0.46
2:B:360:PHE:O	2:B:361:LEU:C	2.53	0.46
1:A:71:GLN:C	1:A:73:GLY:H	2.17	0.46
9:I:58:VAL:HG12	9:I:58:VAL:O	2.15	0.46
2:B:797:TYR:HE1	2:B:854:LEU:HD21	1.80	0.46
4:D:155:ARG:NE	4:D:221:TYR:CE1	2.83	0.46
4:D:15:LEU:O	4:D:15:LEU:HD12	2.15	0.46
1:A:590:ARG:NH1	1:A:590:ARG:HG2	2.29	0.46
1:A:1315:GLU:C	1:A:1317:MET:N	2.68	0.46
2:B:528:PRO:HG2	2:B:532:ALA:O	2.15	0.46
2:B:466:TRP:N	2:B:475:SER:OG	2.48	0.46
3:C:196:ASP:HB3	3:C:199:LYS:HD2	1.96	0.46
1:A:1208:THR:HG22	1:A:1210:GLY:N	2.29	0.46
2:B:706:GLN:HB2	2:B:709:ASP:HB2	1.97	0.46
7:G:126:ASN:HD22	7:G:127:PRO:N	2.13	0.46
2:B:649:LYS:HD3	2:B:736:THR:O	2.14	0.46
2:B:189:LEU:CD1	2:B:196:PRO:HA	2.45	0.46
5:E:78:LEU:HD21	5:E:80:VAL:CG2	2.45	0.46
2:B:777:ALA:HA	2:B:1095:LEU:HA	1.97	0.46
11:K:12:LEU:HD12	11:K:37:LYS:CG	2.44	0.46
2:B:269:ILE:O	2:B:282:ILE:HG12	2.15	0.46
1:A:1081:LEU:HD21	1:A:1097:GLY:HA3	1.96	0.46
11:K:79:GLU:C	11:K:81:TYR:H	2.19	0.46
11:K:55:LYS:HB2	11:K:81:TYR:CE1	2.49	0.46
10:J:41:LEU:HD11	10:J:50:ILE:HG13	1.97	0.46
2:B:1130:PHE:CE1	2:B:1134:GLU:HB3	2.51	0.46
1:A:1349:TYR:O	1:A:1350:LYS:C	2.52	0.46
2:B:970:THR:HG22	2:B:971:THR:N	2.30	0.46
1:A:934:LYS:O	1:A:937:VAL:HG12	2.16	0.46
5:E:12:LEU:HD22	5:E:55:ARG:CZ	2.46	0.46
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.97	0.46
8:H:94:ASP:O	8:H:95:TYR:HB2	2.15	0.46
1:A:504:LEU:HD13	6:F:91:ALA:CB	2.44	0.46
1:A:398:GLU:O	1:A:399:HIS:O	2.34	0.46
1:A:49:LYS:HZ3	1:A:61:ILE:HG13	1.78	0.46
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.40	0.46
4:D:154:PHE:N	4:D:154:PHE:CD2	2.82	0.46
4:D:219:THR:HG23	4:D:220:LEU:O	2.16	0.46
2:B:952:VAL:HG22	2:B:966:VAL:HG13	1.96	0.46
6:F:116:ASP:OD1	6:F:117:PRO:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HD13	2:B:653:VAL:HG12	1.96	0.46
12:L:59:ALA:O	12:L:60:ARG:O	2.34	0.46
2:B:944:THR:HG21	2:B:1122:ARG:CZ	2.45	0.46
8:H:109:LYS:HD3	8:H:111:LEU:HD11	1.96	0.46
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.50	0.46
2:B:696:GLU:O	2:B:699:GLU:HB2	2.15	0.46
1:A:196:GLU:HG2	1:A:197:PRO:N	2.31	0.46
6:F:111:LEU:HD12	6:F:111:LEU:H	1.80	0.46
8:H:9:ILE:HG23	8:H:55:LEU:O	2.15	0.46
2:B:604:ARG:C	2:B:606:LYS:H	2.19	0.46
3:C:221:TYR:CD1	3:C:222:LYS:HG3	2.50	0.46
1:A:690:VAL:CG1	1:A:691:LEU:N	2.78	0.46
9:I:62:ILE:HD11	9:I:86:PHE:CE2	2.50	0.46
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.96	0.46
1:A:1420:ASP:CB	1:A:1422:ARG:HG3	2.41	0.46
2:B:96:TYR:N	2:B:129:PHE:O	2.38	0.46
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.44	0.46
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.51	0.46
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.46
11:K:85:ASP:O	11:K:88:LYS:HB2	2.15	0.46
3:C:10:ILE:HG22	3:C:11:ARG:O	2.16	0.46
2:B:236:HIS:CE1	2:B:389:ALA:HA	2.50	0.46
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.97	0.46
1:A:1076:ALA:HA	1:A:1079:MET:HG3	1.96	0.46
1:A:350:ARG:HB2	2:B:1128:LEU:HD11	1.97	0.46
2:B:602:THR:HA	2:B:605:ARG:HB2	1.97	0.46
1:A:1166:ASP:HA	1:A:1169:ILE:HD12	1.97	0.46
1:A:1197:LEU:HD11	1:A:1238:ILE:HD11	1.96	0.46
1:A:401:GLY:C	1:A:435:HIS:CD2	2.89	0.46
1:A:244:PRO:CB	1:A:245:PRO:CD	2.91	0.46
2:B:293:PRO:C	2:B:294:ASP:O	2.51	0.46
2:B:792:MET:H	2:B:857:ARG:HA	1.79	0.46
3:C:209:TYR:N	3:C:209:TYR:CD1	2.75	0.46
11:K:53:ASP:HB3	11:K:56:VAL:HG23	1.97	0.46
1:A:1289:ARG:NH1	1:A:1326:ARG:NH1	2.63	0.46
1:A:100:LYS:O	1:A:104:GLU:HG3	2.16	0.46
1:A:108:MET:O	1:A:109:HIS:HB3	2.15	0.46
2:B:427:ASP:OD1	2:B:430:ARG:HD2	2.16	0.46
1:A:751:SER:O	1:A:752:LYS:HG2	2.16	0.46
1:A:699:ALA:HB3	1:A:701:LEU:HG	1.96	0.46
2:B:254:LEU:CD1	2:B:273:LEU:HD23	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:LYS:CG	2:B:348:ARG:H	2.29	0.46
1:A:295:LEU:O	1:A:298:PHE:HB3	2.16	0.46
4:D:138:ASN:C	4:D:140:ASP:N	2.67	0.46
9:I:61:ASP:C	9:I:63:GLY:N	2.67	0.46
10:J:3:VAL:N	10:J:53:HIS:CE1	2.84	0.46
4:D:155:ARG:NE	4:D:221:TYR:HE1	2.14	0.46
1:A:728:LYS:O	1:A:732:LEU:HG	2.15	0.46
1:A:767:GLN:NE2	1:A:774:ARG:CB	2.77	0.46
6:F:103:MET:HE1	7:G:66:GLY:N	2.24	0.46
2:B:294:ASP:H	9:I:12:ASN:HD22	1.57	0.46
2:B:910:VAL:CG1	2:B:938:SER:HB3	2.46	0.46
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.50	0.46
1:A:121:LEU:O	1:A:121:LEU:HD23	2.16	0.46
3:C:196:ASP:CB	3:C:199:LYS:HD2	2.45	0.46
2:B:430:ARG:NH1	2:B:430:ARG:HG2	2.31	0.46
2:B:417:PHE:O	2:B:420:LEU:HB2	2.16	0.46
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.49	0.46
1:A:1155:ASP:OD2	1:A:1162:VAL:N	2.48	0.46
2:B:918:ILE:HD12	2:B:935:ARG:CZ	2.45	0.46
2:B:914:LYS:HE2	2:B:937:ALA:CB	2.45	0.46
1:A:675:THR:HB	1:A:736:ASN:OD1	2.15	0.46
1:A:577:ILE:HA	1:A:580:VAL:HG23	1.98	0.46
2:B:860:MET:HE2	2:B:965:LYS:HE2	1.98	0.46
2:B:527:THR:OG1	2:B:528:PRO:HD2	2.15	0.46
9:I:8:ARG:H	9:I:8:ARG:HG3	1.59	0.46
1:A:284:ALA:HB1	1:A:289:ILE:HD12	1.97	0.46
2:B:282:ILE:CD1	2:B:382:ILE:HD13	2.46	0.46
1:A:492:PRO:HB2	1:A:497:THR:HG22	1.96	0.46
2:B:311:LEU:O	2:B:314:LEU:N	2.49	0.46
2:B:265:SER:O	2:B:266:ALA:HB3	2.16	0.46
2:B:37:PHE:CD2	2:B:542:MET:SD	3.09	0.46
6:F:90:ARG:O	6:F:91:ALA:C	2.55	0.46
10:J:3:VAL:HA	10:J:53:HIS:HD1	1.80	0.46
7:G:14:HIS:HD2	7:G:16:SER:CB	2.29	0.46
1:A:1423:GLY:O	1:A:1424:VAL:C	2.54	0.46
1:A:592:ASP:N	1:A:595:THR:OG1	2.49	0.46
1:A:1420:ASP:O	1:A:1421:CYS:CB	2.62	0.46
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.48	0.46
1:A:80:HIS:H	1:A:243:PRO:CB	2.28	0.46
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.98	0.46
1:A:851:HIS:C	1:A:853:ASP:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:ASP:OD1	1:A:855:THR:CG2	2.63	0.46
2:B:1116:ARG:NE	2:B:1198:TYR:CE1	2.84	0.46
1:A:1394:THR:CG2	1:A:1398:MET:SD	3.04	0.46
7:G:154:VAL:HG12	7:G:155:SER:N	2.30	0.46
2:B:593:PRO:O	2:B:594:ALA:C	2.54	0.46
1:A:871:ASP:OD2	1:A:873:MET:HB2	2.16	0.46
2:B:582:VAL:HG22	2:B:626:ILE:HG22	1.98	0.46
5:E:56:LYS:NZ	5:E:84:ASP:N	2.63	0.46
4:D:123:LEU:HD13	4:D:149:THR:HG21	1.97	0.46
4:D:14:ARG:O	4:D:16:LYS:N	2.40	0.46
1:A:185:TRP:HE3	1:A:185:TRP:N	1.98	0.46
6:F:69:LEU:HD22	6:F:71:GLU:OE2	2.15	0.46
7:G:112:LYS:HA	7:G:115:MET:HE2	1.98	0.46
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.51	0.46
10:J:32:GLU:CD	10:J:32:GLU:H	2.18	0.46
10:J:9:SER:OG	10:J:48:ARG:NH2	2.48	0.46
1:A:1195:LEU:HD11	1:A:1267:MET:HE1	1.95	0.46
2:B:525:ALA:O	2:B:768:THR:HG23	2.16	0.46
6:F:79:ARG:NH2	6:F:150:GLU:OE1	2.35	0.46
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.97	0.46
3:C:23:SER:O	3:C:24:ASN:HB3	2.16	0.46
5:E:186:LEU:HA	5:E:186:LEU:HD23	1.71	0.46
2:B:356:LEU:HD23	2:B:360:PHE:CD1	2.51	0.46
2:B:582:VAL:O	2:B:582:VAL:HG12	2.14	0.46
8:H:15:VAL:HG13	8:H:26:ILE:HD12	1.98	0.46
8:H:11:GLN:C	8:H:28:ALA:HB1	2.35	0.46
2:B:710:LEU:HA	2:B:733:HIS:CB	2.29	0.46
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.81	0.46
2:B:878:GLN:HB2	2:B:879:ARG:NH1	2.30	0.46
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.98	0.46
3:C:100:THR:CG2	3:C:101:LEU:N	2.79	0.46
1:A:648:ASN:O	1:A:649:ILE:C	2.55	0.46
1:A:645:LEU:HG	1:A:649:ILE:HD11	1.98	0.46
2:B:773:MET:HE1	2:B:985:GLY:HA2	1.98	0.46
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.96	0.46
5:E:19:VAL:HG11	5:E:80:VAL:HG11	1.98	0.46
2:B:169:ARG:CB	2:B:454:THR:HG23	2.45	0.46
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.46	0.46
5:E:108:GLY:HA3	5:E:132:ILE:HG23	1.98	0.46
2:B:980:PHE:HD2	2:B:1094:ARG:HA	1.81	0.46
2:B:1034:VAL:O	2:B:1037:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1033:LYS:HA	2:B:1089:PRO:HD2	1.98	0.46
2:B:792:MET:O	2:B:793:ALA:HB2	2.16	0.46
1:A:356:ASP:OD2	11:K:65:HIS:CE1	2.65	0.46
1:A:898:ARG:HA	1:A:933:TYR:CD1	2.51	0.46
2:B:295:GLY:N	2:B:298:LEU:HD23	2.29	0.46
1:A:738:LYS:NZ	3:C:194:GLU:O	2.48	0.46
4:D:8:PHE:CG	4:D:38:ILE:O	2.69	0.46
1:A:1362:TYR:CD1	1:A:1363:VAL:N	2.84	0.46
2:B:1045:SER:HB3	2:B:1046:PRO:HD2	1.98	0.45
2:B:582:VAL:O	2:B:582:VAL:CG1	2.63	0.45
8:H:123:MET:HE3	8:H:142:LEU:HD21	1.98	0.45
1:A:321:PRO:O	1:A:322:VAL:HG12	2.16	0.45
4:D:64:VAL:C	4:D:66:ARG:N	2.68	0.45
2:B:866:TYR:CB	2:B:870:ILE:HD12	2.47	0.45
1:A:698:GLN:O	9:I:98:VAL:HA	2.16	0.45
2:B:797:TYR:HE1	2:B:854:LEU:HD23	1.81	0.45
2:B:112:LEU:HD12	2:B:113:TYR:N	2.27	0.45
1:A:741:ASN:C	1:A:741:ASN:HD22	2.16	0.45
1:A:233:TRP:C	1:A:235:ILE:N	2.69	0.45
11:K:47:ARG:HH11	11:K:47:ARG:CB	2.23	0.45
12:L:38:LEU:O	12:L:39:SER:CB	2.63	0.45
1:A:282:ASN:O	1:A:284:ALA:N	2.48	0.45
1:A:153:PRO:HD3	1:A:161:LEU:CD1	2.46	0.45
1:A:474:VAL:HG22	1:A:478:TYR:HE1	1.81	0.45
1:A:138:ILE:HD12	1:A:221:SER:O	2.16	0.45
1:A:639:PRO:HG2	1:A:640:GLN:N	2.31	0.45
2:B:210:LYS:HD3	2:B:482:VAL:HG22	1.98	0.45
3:C:134:ILE:HG21	3:C:139:GLY:HA2	1.97	0.45
2:B:1106:ARG:HD3	2:B:1126:GLY:C	2.36	0.45
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.47	0.45
10:J:3:VAL:CA	10:J:53:HIS:CE1	2.98	0.45
1:A:329:LEU:HD21	2:B:1206:GLU:OE1	2.16	0.45
1:A:332:LYS:HB3	1:A:337:ARG:NE	2.31	0.45
1:A:806:ARG:O	2:B:761:HIS:HE1	1.99	0.45
2:B:567:GLU:HA	2:B:567:GLU:OE1	2.16	0.45
1:A:1081:LEU:CD2	1:A:1097:GLY:HA3	2.46	0.45
3:C:34:ARG:HG2	3:C:35:ARG:N	2.31	0.45
4:D:146:GLN:O	4:D:147:TYR:C	2.55	0.45
2:B:1180:PHE:HB3	2:B:1191:ILE:CD1	2.47	0.45
7:G:12:THR:HG23	7:G:67:SER:HB3	1.98	0.45
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:244:LEU:HD13	2:B:366:GLN:HE22	1.81	0.45
1:A:61:ILE:HG22	1:A:62:ASP:N	2.31	0.45
7:G:123:ALA:C	7:G:125:SER:N	2.70	0.45
7:G:129:SER:CB	7:G:138:THR:HG1	2.29	0.45
9:I:55:THR:OG1	9:I:100:PHE:HD2	1.99	0.45
3:C:75:MET:HB3	3:C:128:ASN:HB3	1.98	0.45
1:A:207:ILE:O	1:A:208:LEU:C	2.55	0.45
9:I:105:SER:O	9:I:106:CYS:CB	2.52	0.45
1:A:858:ASN:HD22	1:A:860:LEU:H	1.62	0.45
1:A:867:ILE:HD11	1:A:1000:LEU:HD21	1.97	0.45
2:B:1130:PHE:CD2	2:B:1150:ARG:HG2	2.52	0.45
1:A:856:THR:HG22	1:A:856:THR:O	2.16	0.45
1:A:492:PRO:O	1:A:493:GLN:NE2	2.49	0.45
2:B:314:LEU:O	2:B:318:VAL:HG23	2.16	0.45
2:B:722:ASP:HB3	2:B:723:VAL:H	1.62	0.45
1:A:41:MET:O	1:A:42:ASP:C	2.55	0.45
7:G:1:MET:SD	7:G:1:MET:C	2.95	0.45
9:I:85:PHE:HD1	9:I:99:LEU:HD13	1.75	0.45
1:A:768:GLN:NE2	1:A:816:HIS:ND1	2.64	0.45
5:E:135:PHE:HD2	5:E:140:LEU:CD2	2.28	0.45
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.52	0.45
1:A:335:ARG:HH12	2:B:1202:LEU:HD22	1.81	0.45
1:A:1141:THR:HG21	1:A:1205:LYS:HD3	1.98	0.45
1:A:1048:ASN:O	1:A:1049:ILE:C	2.53	0.45
2:B:1099:VAL:CG1	2:B:1100:ASP:N	2.78	0.45
1:A:164:ARG:HG3	1:A:165:GLY:N	2.32	0.45
1:A:1203:ASN:O	1:A:1204:ASP:C	2.55	0.45
1:A:608:ILE:HG13	1:A:613:ILE:HD12	1.99	0.45
2:B:500:THR:HA	2:B:501:PRO:HD2	1.75	0.45
2:B:591:ARG:O	2:B:592:ASN:C	2.55	0.45
1:A:1187:GLN:CA	1:A:1244:ARG:HB3	2.45	0.45
2:B:345:LYS:C	2:B:347:LYS:H	2.20	0.45
1:A:1444:MET:O	6:F:133:VAL:N	2.47	0.45
1:A:255:SER:OG	2:B:918:ILE:HG21	2.16	0.45
1:A:211:PHE:HA	1:A:214:ILE:HG13	1.98	0.45
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.17	0.45
1:A:774:ARG:NH2	1:A:797:LYS:HB2	2.31	0.45
2:B:120:ARG:HH11	12:L:54:ARG:HH11	1.63	0.45
12:L:52:GLY:O	12:L:54:ARG:N	2.50	0.45
1:A:146:MET:CA	1:A:171:GLN:HB2	2.47	0.45
2:B:66:ASP:OD1	2:B:422:LYS:HE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:100:THR:OG1	8:H:138:GLU:HG2	2.16	0.45
2:B:412:LEU:CD2	2:B:479:VAL:HG11	2.45	0.45
1:A:35:ILE:HD13	1:A:241:VAL:HG11	1.98	0.45
3:C:204:SER:C	3:C:206:ASN:N	2.69	0.45
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.99	0.45
1:A:447:GLN:HA	1:A:448:PRO:C	2.37	0.45
1:A:1110:ASN:HD22	1:A:1110:ASN:N	2.14	0.45
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.81	0.45
1:A:95:PHE:O	1:A:96:ILE:C	2.55	0.45
2:B:27:ALA:O	2:B:28:GLU:C	2.55	0.45
2:B:604:ARG:CA	2:B:609:ILE:HG13	2.47	0.45
2:B:288:ALA:HA	2:B:331:LEU:CD1	2.46	0.45
4:D:35:LEU:H	4:D:35:LEU:CD1	2.29	0.45
2:B:848:ARG:HA	3:C:69:LEU:HD21	1.98	0.45
3:C:99:LEU:HD22	3:C:120:ILE:HG12	1.98	0.45
1:A:549:MET:SD	1:A:577:ILE:HD12	2.57	0.45
2:B:642:ASP:C	2:B:644:GLU:H	2.18	0.45
2:B:120:ARG:CG	2:B:955:THR:HG21	2.46	0.45
5:E:69:ILE:CD1	5:E:69:ILE:N	2.79	0.45
2:B:101:MET:HB2	2:B:169:ARG:HH22	1.82	0.45
1:A:332:LYS:CD	1:A:333:GLU:HG2	2.47	0.45
1:A:1173:HIS:CD2	1:A:1227:ILE:HG23	2.52	0.45
2:B:46:GLN:HB2	2:B:408:LEU:HD21	1.98	0.45
7:G:17:PHE:C	7:G:19:GLY:H	2.20	0.45
1:A:1454:MET:HG3	1:A:1454:MET:O	2.17	0.45
1:A:96:ILE:HG22	1:A:97:ALA:N	2.32	0.45
1:A:1395:GLY:HA3	1:A:1419:ASP:OD2	2.16	0.45
1:A:1266:THR:O	1:A:1270:ASN:HB2	2.17	0.45
2:B:1214:PRO:HG2	2:B:1214:PRO:O	2.16	0.45
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.31	0.45
1:A:1242:VAL:CG1	1:A:1243:VAL:N	2.43	0.45
5:E:90:VAL:CA	5:E:120:ALA:HB2	2.40	0.45
1:A:1062:GLU:HG2	6:F:88:TYR:OH	2.17	0.45
5:E:56:LYS:CE	5:E:84:ASP:H	2.29	0.45
6:F:77:ASP:O	6:F:78:GLN:CB	2.49	0.45
5:E:145:THR:HG21	5:E:187:TYR:CZ	2.51	0.45
8:H:138:GLU:O	8:H:139:ASN:C	2.55	0.45
2:B:679:TYR:HE1	2:B:687:GLU:OE2	1.98	0.45
2:B:729:ILE:HG22	2:B:729:ILE:O	2.16	0.45
1:A:860:LEU:HA	1:A:860:LEU:HD23	1.81	0.45
5:E:204:THR:HG23	5:E:205:SER:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:129:PRO:O	5:E:130:ALA:O	2.35	0.45
8:H:20:TYR:O	8:H:22:LYS:N	2.50	0.45
5:E:92:THR:HG22	5:E:92:THR:O	2.15	0.45
2:B:431:TYR:CE1	2:B:447:ALA:HB2	2.52	0.45
1:A:492:PRO:CB	1:A:497:THR:HG22	2.47	0.45
3:C:249:ASP:O	3:C:250:THR:C	2.55	0.45
1:A:125:ALA:O	1:A:127:ALA:N	2.50	0.45
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.98	0.45
2:B:856:PHE:N	2:B:856:PHE:CD1	2.84	0.45
3:C:229:TYR:CD1	3:C:229:TYR:N	2.84	0.45
8:H:7:ASP:O	8:H:8:ASP:HB2	2.17	0.45
5:E:112:TYR:HB3	5:E:116:ILE:HD11	1.99	0.45
4:D:138:ASN:ND2	7:G:35:GLU:HB3	2.19	0.45
1:A:709:THR:HG21	9:I:93:LYS:O	2.16	0.45
3:C:185:LYS:HE2	3:C:213:PRO:HA	1.99	0.45
11:K:17:SER:O	11:K:18:LYS:C	2.50	0.45
11:K:37:LYS:HA	11:K:37:LYS:HD3	1.88	0.45
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.29	0.45
3:C:193:TYR:C	3:C:193:TYR:CD1	2.89	0.45
2:B:1119:VAL:O	2:B:1126:GLY:HA3	2.15	0.45
2:B:880:THR:O	2:B:880:THR:HG22	2.17	0.45
1:A:1277:GLU:C	1:A:1279:ILE:H	2.20	0.45
1:A:565:ILE:HG22	1:A:565:ILE:O	2.17	0.45
2:B:621:GLU:HG3	2:B:621:GLU:O	2.17	0.45
1:A:785:PRO:HG2	1:A:786:HIS:HD2	1.81	0.45
2:B:349:ILE:O	2:B:353:LYS:HG3	2.17	0.45
1:A:55:ASP:N	1:A:56:PRO:CD	2.78	0.45
1:A:687:LYS:O	1:A:690:VAL:HG12	2.16	0.45
1:A:692:ASP:O	1:A:693:VAL:C	2.55	0.45
3:C:20:PHE:C	3:C:20:PHE:CD1	2.90	0.45
2:B:769:TYR:HB3	2:B:987:LYS:NZ	2.31	0.45
1:A:1116:LEU:N	1:A:1308:THR:CG2	2.73	0.45
1:A:1115:SER:C	1:A:1308:THR:HG22	2.38	0.45
2:B:531:GLN:HG3	2:B:532:ALA:H	1.82	0.45
1:A:1387:HIS:NE2	13:N:4:DA:H5'	2.32	0.45
1:A:50:ILE:HG22	1:A:52:GLY:N	2.32	0.45
11:K:12:LEU:HD21	11:K:17:SER:C	2.37	0.45
10:J:27:GLU:C	10:J:29:GLU:N	2.67	0.45
1:A:416:ARG:HG3	1:A:417:TYR:CE1	2.52	0.45
5:E:154:ILE:HG22	5:E:155:ARG:O	2.17	0.45
1:A:108:MET:O	1:A:109:HIS:CB	2.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:370:PHE:CD2	2:B:373:ARG:HD2	2.52	0.45
10:J:30:LEU:HD11	10:J:38:ARG:NH1	2.32	0.45
3:C:193:TYR:HD1	3:C:193:TYR:C	2.21	0.45
8:H:55:LEU:HD22	8:H:144:ILE:HG22	1.99	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:HD12	2.46	0.45
12:L:54:ARG:HG3	12:L:54:ARG:H	1.43	0.45
2:B:100:PRO:HB2	2:B:180:TYR:HE1	1.82	0.45
7:G:113:HIS:CD2	7:G:113:HIS:H	2.34	0.45
2:B:69:LEU:HD13	2:B:429:PHE:CD1	2.52	0.45
2:B:889:THR:HG23	2:B:891:ASP:N	2.32	0.45
1:A:1081:LEU:HD11	1:A:1097:GLY:HA3	1.98	0.45
2:B:811:TYR:N	2:B:811:TYR:CD1	2.84	0.45
1:A:1199:ARG:O	1:A:1203:ASN:ND2	2.50	0.45
1:A:1072:ILE:HG23	1:A:1356:ILE:HD11	1.99	0.45
1:A:798:GLY:HA2	1:A:815:PHE:HD1	1.81	0.45
2:B:203:PHE:N	2:B:203:PHE:CD1	2.85	0.45
2:B:805:THR:CG2	2:B:806:THR:H	2.20	0.44
6:F:89:GLU:OE2	6:F:134:ILE:HG21	2.16	0.44
4:D:29:LEU:HB3	7:G:82:PHE:CE2	2.52	0.44
1:A:692:ASP:C	1:A:694:THR:N	2.68	0.44
10:J:53:HIS:CD2	10:J:55:ASP:N	2.85	0.44
2:B:1072:MET:O	2:B:1081:LEU:HB2	2.17	0.44
2:B:486:TYR:HD1	2:B:775:LYS:O	2.00	0.44
1:A:451:HIS:HA	1:A:1070:GLN:OE1	2.16	0.44
4:D:13:ARG:C	4:D:15:LEU:N	2.68	0.44
1:A:605:MET:HE1	1:A:607:ILE:HG12	1.98	0.44
1:A:330:LYS:O	1:A:334:GLY:HA3	2.17	0.44
7:G:111:THR:O	7:G:111:THR:HG23	2.17	0.44
2:B:294:ASP:H	9:I:12:ASN:HD21	1.60	0.44
10:J:62:ARG:HG2	10:J:62:ARG:O	2.17	0.44
2:B:458:LYS:O	2:B:459:TYR:C	2.55	0.44
9:I:40:SER:OG	9:I:41:PRO:HD2	2.17	0.44
1:A:1208:THR:HA	1:A:1231:ASP:OD1	2.17	0.44
8:H:2:SER:OG	8:H:3:ASN:N	2.50	0.44
2:B:958:GLN:C	2:B:960:GLY:H	2.20	0.44
9:I:100:PHE:N	9:I:100:PHE:HD1	2.15	0.44
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.98	0.44
3:C:79:GLN:HE21	3:C:127:ARG:CD	2.27	0.44
2:B:1072:MET:HE3	2:B:1085:ILE:CB	2.44	0.44
1:A:335:ARG:NH1	2:B:1206:GLU:CD	2.68	0.44
2:B:412:LEU:HB3	2:B:466:TRP:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:55:LYS:HB2	11:K:81:TYR:HE1	1.82	0.44
6:F:97:ARG:NH2	6:F:108:PHE:CE1	2.86	0.44
5:E:128:PRO:HA	5:E:129:PRO:O	2.17	0.44
3:C:67:LEU:HA	3:C:70:ILE:CD1	2.48	0.44
2:B:1106:ARG:HD2	2:B:1125:ASP:O	2.17	0.44
3:C:68:GLY:O	3:C:169:LYS:HB2	2.17	0.44
1:A:352:VAL:O	1:A:467:THR:HB	2.17	0.44
2:B:806:THR:CG2	2:B:808:ALA:HB3	2.47	0.44
2:B:579:ARG:HG2	2:B:579:ARG:NH1	2.30	0.44
8:H:4:THR:O	8:H:5:LEU:HD23	2.17	0.44
4:D:173:HIS:ND1	4:D:174:PRO:HD2	2.33	0.44
2:B:1002:THR:HG23	2:B:1087:PHE:HE1	1.81	0.44
3:C:124:LEU:O	3:C:125:MET:C	2.55	0.44
1:A:102:VAL:HB	1:A:211:PHE:HE1	1.77	0.44
1:A:1111:MET:HG3	1:A:1114:PRO:HB3	2.00	0.44
2:B:987:LYS:HE3	15:P:11:G:C2'	2.46	0.44
1:A:1170:ILE:HG22	1:A:1174:PHE:CZ	2.52	0.44
2:B:234:ILE:HG21	2:B:237:VAL:HG23	1.98	0.44
4:D:51:ASN:OD1	4:D:54:GLU:HB2	2.17	0.44
1:A:1147:THR:HB	9:I:48:LEU:HD12	1.98	0.44
5:E:33:GLU:C	5:E:35:VAL:N	2.71	0.44
1:A:224:PHE:CD2	1:A:231:PRO:HG3	2.52	0.44
2:B:263:GLY:O	2:B:264:SER:C	2.55	0.44
2:B:593:PRO:C	2:B:595:ARG:N	2.71	0.44
2:B:637:LEU:HD22	2:B:742:GLU:HA	2.00	0.44
1:A:1161:THR:HG22	1:A:1163:ILE:HG13	1.98	0.44
1:A:264:PHE:CB	1:A:265:LYS:NZ	2.81	0.44
1:A:12:ARG:NH2	2:B:1192:TYR:CE2	2.85	0.44
7:G:1:MET:SD	7:G:79:PHE:HD1	2.39	0.44
3:C:69:LEU:HB3	10:J:6:ARG:HD3	1.99	0.44
2:B:1003:ALA:HA	3:C:178:PHE:O	2.17	0.44
1:A:1094:VAL:HG13	1:A:1113:THR:CB	2.48	0.44
5:E:100:ILE:HG23	5:E:105:PHE:CD1	2.53	0.44
8:H:100:THR:CG2	8:H:101:ALA:N	2.81	0.44
1:A:939:ASP:O	1:A:942:PHE:HB3	2.18	0.44
1:A:121:LEU:HD22	1:A:141:LEU:HD21	2.00	0.44
2:B:485:ARG:HG3	2:B:781:PHE:HD1	1.83	0.44
1:A:833:GLU:OE2	1:A:1102:LYS:HE3	2.17	0.44
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.52	0.44
9:I:74:GLU:O	9:I:74:GLU:HG3	2.17	0.44
5:E:74:ASP:N	5:E:74:ASP:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:135:ARG:HG2	6:F:137:TYR:CE1	2.52	0.44
1:A:49:LYS:HZ1	1:A:61:ILE:CG1	2.26	0.44
2:B:879:ARG:N	2:B:879:ARG:HD2	2.33	0.44
9:I:59:VAL:C	9:I:61:ASP:H	2.21	0.44
1:A:1424:VAL:HG11	2:B:1139:ILE:HD11	1.98	0.44
2:B:114:PRO:O	2:B:115:GLN:C	2.55	0.44
1:A:1100:ARG:O	1:A:1100:ARG:HD2	2.17	0.44
7:G:114:LEU:HD23	7:G:161:GLY:O	2.16	0.44
1:A:755:PHE:O	1:A:757:ASN:N	2.51	0.44
2:B:650:GLU:HG3	2:B:654:ARG:HH21	1.83	0.44
1:A:378:GLU:CD	1:A:387:ARG:HH22	2.21	0.44
2:B:408:LEU:HB3	2:B:409:ALA:H	1.69	0.44
1:A:858:ASN:ND2	1:A:860:LEU:HB2	2.32	0.44
1:A:1037:LEU:HD13	1:A:1042:PHE:HA	2.00	0.44
1:A:336:ILE:CD1	2:B:1203:LEU:HD22	2.47	0.44
1:A:1019:CYS:O	1:A:1020:CYS:C	2.56	0.44
1:A:377:PRO:O	1:A:377:PRO:HG2	2.18	0.44
5:E:89:GLY:C	5:E:91:LYS:H	2.20	0.44
8:H:99:GLY:HA3	8:H:117:SER:O	2.17	0.44
2:B:273:LEU:HD22	2:B:360:PHE:CD1	2.52	0.44
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.79	0.44
5:E:111:VAL:HG12	5:E:137:GLU:HG2	1.99	0.44
1:A:384:ASN:O	1:A:385:ILE:C	2.55	0.44
3:C:174:ALA:O	3:C:175:ALA:HB3	2.18	0.44
4:D:155:ARG:CD	4:D:221:TYR:CE1	3.00	0.44
1:A:1311:VAL:HG21	1:A:1329:THR:HG23	2.00	0.44
6:F:82:THR:HA	6:F:83:PRO:HD3	1.71	0.44
8:H:102:TYR:N	8:H:102:TYR:CD2	2.86	0.44
5:E:124:VAL:HG13	5:E:132:ILE:CB	2.47	0.44
9:I:88:SER:HB3	9:I:95:THR:HG21	2.00	0.44
6:F:119:ARG:CG	6:F:119:ARG:NH1	2.78	0.44
1:A:388:LEU:HD13	1:A:432:VAL:CG2	2.48	0.44
1:A:821:ARG:HG2	2:B:514:LEU:H	1.82	0.44
3:C:183:TRP:CZ3	3:C:203:GLN:NE2	2.86	0.44
1:A:1081:LEU:CD1	1:A:1098:VAL:H	2.29	0.44
7:G:91:VAL:CG1	7:G:92:VAL:N	2.80	0.44
2:B:781:PHE:N	2:B:781:PHE:CD2	2.83	0.44
5:E:33:GLU:C	5:E:35:VAL:H	2.19	0.44
1:A:317:LYS:O	1:A:318:SER:HB3	2.18	0.44
3:C:91:HIS:C	3:C:91:HIS:CD2	2.91	0.44
1:A:730:GLY:O	1:A:731:ARG:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:VAL:HG11	2:B:385:LEU:HA	1.99	0.44
4:D:180:LEU:HD23	4:D:180:LEU:HA	1.89	0.44
1:A:1166:ASP:CG	1:A:1194:ARG:HE	2.21	0.44
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.52	0.44
1:A:321:PRO:O	1:A:322:VAL:HB	2.16	0.44
5:E:56:LYS:CE	5:E:84:ASP:HB2	2.29	0.44
7:G:1:MET:HE2	7:G:3:PHE:CE1	2.53	0.44
5:E:78:LEU:HD11	5:E:109:ILE:HD12	1.99	0.44
2:B:860:MET:HG2	2:B:861:ASP:N	2.32	0.44
8:H:65:LEU:CD2	8:H:65:LEU:N	2.64	0.44
1:A:378:GLU:OE1	1:A:388:LEU:HD21	2.17	0.44
1:A:1118:VAL:HG23	1:A:1118:VAL:O	2.18	0.44
1:A:973:ILE:CD1	1:A:1037:LEU:HA	2.47	0.44
3:C:208:GLU:C	3:C:210:GLU:H	2.20	0.44
1:A:173:THR:HG22	1:A:184:SER:OG	2.18	0.44
1:A:818:MET:HB3	1:A:818:MET:HE2	1.89	0.44
1:A:935:GLN:NE2	1:A:938:LYS:HD2	2.32	0.44
3:C:114:TYR:HB3	3:C:140:ASN:O	2.18	0.44
2:B:599:THR:O	2:B:603:LEU:HB2	2.18	0.44
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.48	0.44
1:A:722:LEU:HD23	1:A:799:PHE:CD1	2.53	0.44
1:A:666:ILE:HD12	1:A:666:ILE:N	2.33	0.44
5:E:78:LEU:HD23	5:E:79:TRP:N	2.33	0.44
2:B:860:MET:HG3	2:B:965:LYS:CG	2.44	0.44
2:B:906:SER:O	2:B:907:GLY:C	2.56	0.44
1:A:337:ARG:HD2	2:B:1132:GLU:CD	2.38	0.44
5:E:46:TYR:O	5:E:54:GLN:HB2	2.18	0.44
2:B:758:PHE:HB3	2:B:761:HIS:HD2	1.82	0.44
1:A:117:GLU:N	1:A:117:GLU:CD	2.68	0.44
1:A:836:TYR:N	14:T:18:DC:H5'	2.33	0.44
11:K:83:PRO:O	11:K:84:LYS:C	2.56	0.44
1:A:482:PHE:C	1:A:484:GLY:H	2.20	0.44
1:A:1410:PHE:HD2	2:B:1212:ILE:CD1	2.30	0.44
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.17	0.44
1:A:817:ALA:O	1:A:818:MET:C	2.54	0.44
2:B:33:VAL:O	2:B:36:ALA:HB3	2.17	0.44
2:B:597:MET:SD	2:B:617:ARG:HB2	2.57	0.44
2:B:603:LEU:CD1	2:B:609:ILE:HG23	2.43	0.44
1:A:1161:THR:O	1:A:1163:ILE:N	2.51	0.44
1:A:382:PRO:HB3	1:A:428:TYR:CE2	2.53	0.44
9:I:55:THR:OG1	9:I:100:PHE:CD2	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:OE1	2:B:983:ARG:CA	2.53	0.44
3:C:233:GLU:CG	3:C:234:SER:N	2.80	0.44
4:D:216:ASN:C	4:D:218:GLU:N	2.68	0.44
5:E:114:ASN:O	5:E:115:ASN:CB	2.54	0.44
2:B:351:TYR:CD1	2:B:355:ILE:HD11	2.52	0.44
1:A:889:SER:C	1:A:891:ALA:N	2.69	0.44
14:T:16:DT:C2'	14:T:17:DT:C5'	2.94	0.44
6:F:116:ASP:C	6:F:116:ASP:OD1	2.56	0.44
2:B:661:LEU:C	2:B:663:ALA:N	2.70	0.44
1:A:884:ASP:HB2	1:A:1024:SER:OG	2.18	0.44
3:C:3:GLU:N	11:K:104:ASN:HD21	2.15	0.44
2:B:309:GLN:OE1	9:I:52:ILE:HD11	2.18	0.44
6:F:120:ILE:O	6:F:124:GLU:HG3	2.18	0.44
4:D:51:ASN:C	4:D:52:LEU:O	2.55	0.44
1:A:1144:LYS:HA	1:A:1268:LEU:HD22	2.00	0.44
1:A:277:GLU:HG2	1:A:277:GLU:O	2.18	0.44
8:H:6:PHE:CD2	8:H:6:PHE:C	2.91	0.44
2:B:376:PHE:CE2	2:B:569:TYR:HD2	2.35	0.43
8:H:143:LEU:C	8:H:144:ILE:HG13	2.38	0.43
1:A:1241:ARG:O	1:A:1242:VAL:HB	2.17	0.43
8:H:123:MET:CE	8:H:142:LEU:HD21	2.47	0.43
1:A:265:LYS:HA	1:A:265:LYS:CE	2.48	0.43
7:G:138:THR:HG22	7:G:139:ILE:HB	2.00	0.43
9:I:69:PRO:HG2	9:I:85:PHE:CD2	2.52	0.43
7:G:18:PHE:HA	7:G:22:MET:CE	2.48	0.43
8:H:130:ARG:HH11	8:H:130:ARG:CA	2.31	0.43
1:A:1259:MET:CE	1:A:1263:ILE:HG13	2.48	0.43
1:A:683:ILE:HG21	1:A:801:GLU:CG	2.48	0.43
1:A:844:ALA:O	1:A:845:LEU:HD23	2.18	0.43
3:C:33:LEU:C	3:C:33:LEU:HD12	2.37	0.43
2:B:526:GLU:OE1	2:B:752:ALA:CB	2.66	0.43
8:H:92:ASP:C	8:H:93:TYR:CD1	2.91	0.43
2:B:240:ILE:HD12	2:B:241:ARG:N	2.33	0.43
2:B:273:LEU:HD12	2:B:280:ILE:HD12	2.00	0.43
2:B:604:ARG:NH1	2:B:691:GLU:OE2	2.42	0.43
1:A:571:LEU:HD22	8:H:46:LEU:CD1	2.41	0.43
1:A:306:ASN:O	1:A:306:ASN:OD1	2.36	0.43
1:A:34:LYS:NZ	1:A:57:ARG:HH21	2.10	0.43
7:G:138:THR:O	7:G:140:LYS:N	2.51	0.43
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.82	0.43
10:J:57:ILE:HA	10:J:60:PHE:CD2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:60:PHE:O	10:J:63:TYR:HD1	2.01	0.43
2:B:1002:THR:O	2:B:1004:GLU:N	2.50	0.43
3:C:44:LEU:HD21	3:C:159:ALA:HB1	2.00	0.43
7:G:14:HIS:CE1	7:G:15:PRO:HD2	2.53	0.43
1:A:1319:VAL:O	1:A:1322:ILE:HG12	2.17	0.43
2:B:235:SER:O	2:B:236:HIS:CD2	2.69	0.43
1:A:347:PHE:CD1	1:A:347:PHE:N	2.87	0.43
1:A:495:GLU:O	1:A:498:ARG:HG3	2.17	0.43
1:A:528:LEU:HD23	1:A:751:SER:HA	2.01	0.43
2:B:880:THR:O	2:B:881:ASN:HB2	2.17	0.43
5:E:42:PHE:O	5:E:43:LYS:C	2.57	0.43
2:B:604:ARG:O	2:B:606:LYS:N	2.51	0.43
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.48	0.43
5:E:111:VAL:O	5:E:111:VAL:HG12	2.18	0.43
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.48	0.43
2:B:885:MET:HA	2:B:936:ASP:HB2	1.98	0.43
5:E:82:PHE:N	5:E:82:PHE:HD1	2.17	0.43
6:F:69:LEU:O	6:F:70:LYS:HB2	2.19	0.43
2:B:1033:LYS:O	2:B:1037:LEU:HG	2.18	0.43
10:J:47:ARG:C	10:J:49:MET:N	2.69	0.43
2:B:50:SER:OG	2:B:411:PRO:HD3	2.17	0.43
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.99	0.43
1:A:857:ARG:CZ	6:F:139:PRO:HG3	2.48	0.43
1:A:341:MET:CE	1:A:843:LYS:NZ	2.82	0.43
1:A:184:SER:HB3	1:A:199:LEU:HD23	1.99	0.43
1:A:184:SER:HB2	1:A:199:LEU:HD23	2.00	0.43
1:A:528:LEU:HD23	1:A:751:SER:CA	2.48	0.43
6:F:76:LYS:O	6:F:79:ARG:HD3	2.17	0.43
2:B:604:ARG:HA	2:B:609:ILE:HG13	1.99	0.43
2:B:604:ARG:O	2:B:607:GLY:N	2.51	0.43
7:G:26:LEU:HA	7:G:26:LEU:HD23	1.73	0.43
1:A:717:ASN:O	1:A:718:VAL:C	2.56	0.43
1:A:787:PHE:CE1	1:A:796:SER:HA	2.50	0.43
3:C:52:GLU:OE2	3:C:154:LYS:HD2	2.18	0.43
2:B:1004:GLU:HG3	10:J:42:LYS:HZ1	1.82	0.43
3:C:22:LEU:HD11	11:K:101:LEU:HD21	2.00	0.43
1:A:207:ILE:CG2	1:A:211:PHE:CE2	3.02	0.43
2:B:778:MET:HE3	2:B:1094:ARG:HD3	2.00	0.43
1:A:709:THR:CG2	1:A:710:LEU:H	2.28	0.43
2:B:69:LEU:HD22	2:B:429:PHE:CE1	2.53	0.43
2:B:546:SER:OG	2:B:631:GLY:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:7:THR:HG21	4:D:32:GLU:CD	2.38	0.43
1:A:973:ILE:HD11	1:A:1041:ALA:CB	2.48	0.43
2:B:1001:PHE:CE2	3:C:34:ARG:CZ	3.02	0.43
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.00	0.43
5:E:35:VAL:C	5:E:37:LEU:H	2.22	0.43
1:A:1230:GLU:C	1:A:1232:ASN:N	2.72	0.43
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.64	0.43
1:A:1399:ARG:HB3	1:A:1408:ILE:HD13	2.00	0.43
3:C:58:LEU:N	3:C:58:LEU:HD23	2.33	0.43
10:J:8:PHE:CD2	10:J:8:PHE:N	2.86	0.43
2:B:887:HIS:N	2:B:887:HIS:CD2	2.85	0.43
1:A:1193:LEU:HD12	1:A:1193:LEU:C	2.38	0.43
2:B:261:ARG:HH11	2:B:261:ARG:CB	2.09	0.43
5:E:116:ILE:HG22	5:E:120:ALA:HB3	2.00	0.43
8:H:40:LEU:HG	8:H:42:ILE:HG13	2.00	0.43
1:A:298:PHE:HD2	1:A:299:HIS:HD2	1.67	0.43
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.31	0.43
4:D:33:PHE:CE1	7:G:80:LYS:HD3	2.52	0.43
4:D:219:THR:CG2	4:D:220:LEU:O	2.67	0.43
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.18	0.43
1:A:1389:PHE:C	1:A:1391:ARG:H	2.22	0.43
1:A:709:THR:OG1	1:A:712:GLU:HG3	2.17	0.43
5:E:46:TYR:CD2	5:E:58:MET:HG3	2.54	0.43
2:B:95:ILE:CB	2:B:130:VAL:HG22	2.48	0.43
10:J:7:CYS:CA	10:J:49:MET:HE3	2.47	0.43
5:E:161:LYS:HD2	5:E:195:VAL:CG2	2.49	0.43
12:L:38:LEU:HG	12:L:39:SER:N	2.33	0.43
4:D:187:THR:C	4:D:189:ASP:N	2.70	0.43
2:B:269:ILE:CG2	2:B:282:ILE:HD13	2.49	0.43
2:B:312:GLU:O	2:B:315:LYS:HB2	2.19	0.43
3:C:31:ASN:HA	3:C:34:ARG:HB3	1.99	0.43
11:K:40:HIS:O	11:K:41:THR:C	2.57	0.43
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.06	0.43
5:E:153:HIS:C	5:E:154:ILE:HG13	2.39	0.43
1:A:1336:MET:CE	1:A:1381:LEU:HG	2.49	0.43
1:A:1077:THR:HB	1:A:1078:GLN:HE21	1.84	0.43
2:B:218:SER:HA	2:B:404:LYS:HA	2.00	0.43
1:A:11:LEU:CD2	1:A:11:LEU:O	2.61	0.43
1:A:47:ARG:NH1	1:A:254:GLU:HG2	2.34	0.43
1:A:794:PRO:C	1:A:796:SER:H	2.22	0.43
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:220:ASP:OD1	3:C:223:ALA:HB2	2.18	0.43
9:I:50:THR:CG2	9:I:51:ASN:H	2.32	0.43
1:A:836:TYR:CD2	1:A:840:ARG:HD2	2.54	0.43
1:A:2:VAL:CG1	2:B:1157:ALA:O	2.67	0.43
9:I:82:GLU:HB3	9:I:104:LEU:HG	2.01	0.43
1:A:343:LYS:NZ	2:B:1151:LEU:O	2.51	0.43
1:A:1376:THR:O	1:A:1377:THR:C	2.56	0.43
3:C:136:ASP:OD2	3:C:137:LYS:N	2.52	0.43
2:B:222:ILE:C	2:B:240:ILE:HD13	2.39	0.43
2:B:605:ARG:NE	2:B:639:ILE:HD13	2.33	0.43
8:H:15:VAL:HG22	8:H:26:ILE:HD11	2.00	0.43
4:D:29:LEU:HD12	7:G:82:PHE:CE1	2.52	0.43
4:D:35:LEU:HD11	4:D:173:HIS:NE2	2.33	0.43
2:B:883:LEU:O	2:B:885:MET:N	2.52	0.43
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.54	0.43
10:J:1:MET:HB2	10:J:56:LEU:HD12	1.99	0.43
4:D:119:ARG:HD2	4:D:221:TYR:CG	2.53	0.43
4:D:155:ARG:NH1	4:D:155:ARG:CB	2.82	0.43
1:A:351:THR:HG21	2:B:1103:ILE:HG13	2.00	0.43
4:D:53:SER:H	4:D:148:LEU:HD22	1.84	0.43
1:A:774:ARG:HG3	1:A:797:LYS:HB3	2.01	0.43
1:A:804:TYR:OH	2:B:763:GLN:HA	2.19	0.43
1:A:1308:THR:HG21	1:A:1310:GLY:O	2.19	0.43
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.34	0.43
8:H:130:ARG:HD3	8:H:130:ARG:H	1.79	0.43
1:A:1124:HIS:HB2	1:A:1130:GLN:HG2	2.01	0.43
7:G:20:PRO:CD	7:G:21:ARG:N	2.82	0.43
2:B:46:GLN:HB2	2:B:408:LEU:CD2	2.48	0.43
2:B:46:GLN:OE1	2:B:47:GLN:N	2.50	0.43
1:A:289:ILE:CG2	1:A:290:GLU:N	2.80	0.43
11:K:55:LYS:CB	11:K:81:TYR:CD1	3.01	0.43
1:A:833:GLU:CG	1:A:1102:LYS:HE2	2.48	0.43
4:D:38:ILE:HG12	4:D:38:ILE:H	1.47	0.43
1:A:396:PRO:HG2	1:A:397:ASN:OD1	2.19	0.43
2:B:821:GLN:OE1	2:B:850:LEU:CD1	2.67	0.43
1:A:382:PRO:CB	1:A:428:TYR:HE2	2.32	0.43
2:B:1023:VAL:O	2:B:1026:LEU:HB2	2.18	0.43
4:D:53:SER:HA	4:D:56:ARG:HB3	2.00	0.43
2:B:766:ARG:NH1	2:B:769:TYR:CE1	2.87	0.43
1:A:218:ASP:O	1:A:219:PHE:C	2.56	0.43
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1198:TYR:O	2:B:1198:TYR:CD2	2.72	0.43
2:B:259:TYR:N	2:B:259:TYR:CD1	2.87	0.43
2:B:570:VAL:HG21	2:B:573:GLN:NE2	2.34	0.43
2:B:317:CYS:O	2:B:320:ASP:HB3	2.19	0.43
1:A:239:LEU:HA	1:A:240:PRO:HD2	1.82	0.43
1:A:108:MET:CB	1:A:210:ILE:HD13	2.49	0.43
3:C:142:VAL:H	10:J:16:ASP:HB3	1.83	0.43
1:A:565:ILE:O	1:A:570:PRO:HA	2.19	0.43
1:A:360:GLU:HB2	1:A:363:GLN:HG3	2.01	0.43
1:A:785:PRO:O	2:B:702:LEU:HD12	2.18	0.43
1:A:1189:SER:HB2	1:A:1256:GLU:OE1	2.18	0.43
1:A:69:THR:HG22	2:B:1174:LYS:HD3	2.01	0.43
7:G:1:MET:HE1	7:G:80:LYS:H	1.83	0.43
3:C:22:LEU:HD22	3:C:230:MET:HE2	1.99	0.43
3:C:99:LEU:CD2	3:C:99:LEU:N	2.74	0.43
1:A:889:SER:HA	1:A:1297:GLU:N	2.33	0.43
3:C:184:ASN:ND2	3:C:189:THR:HB	2.34	0.43
11:K:12:LEU:HD12	11:K:12:LEU:HA	1.88	0.43
1:A:1450:LEU:CD1	6:F:108:PHE:CZ	3.02	0.43
11:K:41:THR:HG22	11:K:42:LEU:N	2.33	0.43
2:B:308:TRP:CZ3	9:I:45:ARG:HG2	2.54	0.43
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.90	0.43
2:B:460:ALA:O	2:B:462:ALA:N	2.52	0.43
2:B:376:PHE:CE1	2:B:569:TYR:HB3	2.53	0.43
5:E:112:TYR:C	5:E:112:TYR:HD1	2.21	0.43
4:D:138:ASN:O	4:D:142:LYS:HG2	2.19	0.43
4:D:173:HIS:CG	4:D:174:PRO:HD2	2.54	0.43
7:G:49:LEU:HD21	7:G:77:VAL:HG23	2.00	0.43
4:D:118:THR:O	4:D:119:ARG:C	2.57	0.43
1:A:919:ILE:CG1	1:A:925:LEU:HD12	2.49	0.43
4:D:12:ARG:HH12	4:D:14:ARG:HA	1.81	0.43
1:A:151:ASP:HA	1:A:162:VAL:O	2.19	0.43
1:A:1115:SER:OG	1:A:1116:LEU:N	2.51	0.43
2:B:479:VAL:O	2:B:480:SER:HB3	2.17	0.43
11:K:79:GLU:HG3	11:K:80:GLY:H	1.83	0.43
2:B:1224:PHE:CE1	5:E:171:LYS:HG3	2.54	0.43
1:A:1110:ASN:ND2	1:A:1110:ASN:N	2.66	0.43
5:E:24:LYS:HB2	5:E:24:LYS:HE3	1.88	0.43
3:C:24:ASN:O	3:C:24:ASN:CG	2.55	0.43
1:A:423:ASP:OD1	1:A:424:ILE:N	2.52	0.43
8:H:42:ILE:O	8:H:44:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:94:ASP:N	8:H:94:ASP:OD1	2.51	0.42
1:A:504:LEU:HD21	6:F:88:TYR:HD2	1.83	0.42
1:A:71:GLN:O	1:A:73:GLY:N	2.45	0.42
3:C:167:HIS:CA	11:K:6:ARG:HH12	2.32	0.42
2:B:576:ASP:HB3	2:B:622:LYS:NZ	2.34	0.42
3:C:235:VAL:HG21	10:J:6:ARG:HH22	1.83	0.42
2:B:822:ASN:HD22	10:J:52:THR:HG21	1.83	0.42
5:E:135:PHE:CD2	5:E:140:LEU:HD21	2.52	0.42
1:A:1035:TYR:N	1:A:1035:TYR:CD2	2.85	0.42
3:C:214:ASN:O	3:C:217:ASP:OD2	2.36	0.42
1:A:78:PRO:CB	2:B:1201:LYS:HE3	2.49	0.42
1:A:114:LEU:HB2	1:A:142:CYS:HB2	2.01	0.42
4:D:51:ASN:O	4:D:52:LEU:C	2.55	0.42
9:I:82:GLU:HB3	9:I:104:LEU:CD1	2.49	0.42
1:A:1153:TYR:HA	9:I:41:PRO:O	2.19	0.42
2:B:604:ARG:NH2	2:B:613:VAL:O	2.41	0.42
10:J:64:ASN:CB	10:J:65:PRO:CD	2.78	0.42
1:A:67:CYS:O	1:A:68:GLN:HG3	2.19	0.42
1:A:690:VAL:CG2	1:A:718:VAL:HG13	2.48	0.42
3:C:101:LEU:CD1	3:C:118:LEU:HD23	2.47	0.42
1:A:463:ILE:HD11	1:A:469:ARG:HG3	2.01	0.42
1:A:754:SER:O	1:A:757:ASN:HB2	2.19	0.42
1:A:636:GLU:OE2	1:A:962:ARG:NH1	2.52	0.42
2:B:1207:LEU:HD23	2:B:1207:LEU:HA	1.73	0.42
2:B:405:ARG:CD	2:B:631:GLY:O	2.67	0.42
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.34	0.42
10:J:14:VAL:CG1	10:J:14:VAL:O	2.66	0.42
1:A:353:ILE:HG21	1:A:487:MET:HE3	2.01	0.42
1:A:1152:ILE:HG23	1:A:1260:LEU:CD2	2.49	0.42
1:A:482:PHE:CB	2:B:838:SER:OG	2.66	0.42
1:A:583:PRO:HG2	1:A:586:ILE:HG13	2.01	0.42
1:A:26:GLU:O	1:A:27:VAL:C	2.57	0.42
1:A:849:MET:CE	1:A:1061:GLY:HA2	2.49	0.42
2:B:785:TYR:CD1	2:B:786:ASN:N	2.87	0.42
2:B:522:VAL:CG1	2:B:537:LYS:HB3	2.50	0.42
2:B:522:VAL:HG11	2:B:537:LYS:HB3	2.01	0.42
11:K:27:ALA:HB1	11:K:28:PRO:HD2	2.02	0.42
1:A:874:ASP:N	1:A:1058:VAL:HG23	2.34	0.42
2:B:636:PRO:O	2:B:636:PRO:HG2	2.20	0.42
1:A:264:PHE:CB	1:A:265:LYS:HZ1	2.31	0.42
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:125:SER:O	7:G:126:ASN:HB2	2.20	0.42
3:C:97:VAL:CG1	3:C:99:LEU:HD21	2.48	0.42
2:B:233:PRO:HD3	14:T:11:DA:OP1	2.18	0.42
1:A:806:ARG:HH12	2:B:729:ILE:CD1	2.33	0.42
7:G:21:ARG:HH11	7:G:24:GLN:HB2	1.81	0.42
2:B:473:MET:C	2:B:475:SER:H	2.23	0.42
3:C:183:TRP:CZ2	3:C:212:PRO:HG3	2.54	0.42
1:A:829:VAL:O	1:A:830:LYS:C	2.57	0.42
1:A:443:LEU:CD1	2:B:1146:PHE:CE2	3.01	0.42
11:K:63:VAL:O	11:K:63:VAL:CG2	2.66	0.42
7:G:101:VAL:CG1	7:G:102:GLN:N	2.83	0.42
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.83	0.42
2:B:1220:ARG:NH1	2:B:1220:ARG:HB3	2.34	0.42
8:H:59:ILE:CG2	8:H:60:ALA:N	2.70	0.42
8:H:89:LEU:CD1	8:H:91:ASP:OD1	2.68	0.42
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.54	0.42
1:A:722:LEU:HB3	1:A:799:PHE:CD1	2.54	0.42
3:C:66:ARG:HH21	10:J:5:VAL:HG23	1.85	0.42
2:B:172:ILE:HD13	2:B:178:ASN:ND2	2.24	0.42
1:A:1332:PHE:N	1:A:1332:PHE:CD2	2.86	0.42
10:J:34:THR:O	10:J:35:ALA:C	2.57	0.42
10:J:46:CYS:O	10:J:49:MET:HB3	2.20	0.42
2:B:412:LEU:HD21	2:B:479:VAL:HG11	2.02	0.42
1:A:1081:LEU:CD1	1:A:1097:GLY:HA3	2.49	0.42
4:D:8:PHE:HZ	4:D:37:GLN:CD	2.23	0.42
2:B:788:ARG:O	2:B:967:ARG:NH1	2.53	0.42
2:B:1079:LYS:HA	3:C:27:LEU:HD21	2.01	0.42
1:A:1001:ARG:O	1:A:1002:GLY:C	2.57	0.42
1:A:116:ASP:C	1:A:118:HIS:N	2.71	0.42
5:E:5:ASN:ND2	5:E:5:ASN:O	2.52	0.42
2:B:700:SER:O	2:B:701:ILE:HG22	2.20	0.42
2:B:244:LEU:CD2	2:B:366:GLN:NE2	2.82	0.42
6:F:88:TYR:O	6:F:89:GLU:C	2.58	0.42
4:D:138:ASN:C	4:D:140:ASP:H	2.23	0.42
4:D:213:GLU:O	4:D:217:LEU:HG	2.18	0.42
1:A:674:PRO:HG2	1:A:675:THR:H	1.84	0.42
1:A:548:ASN:O	1:A:549:MET:C	2.57	0.42
1:A:1263:ILE:O	1:A:1263:ILE:HG22	2.19	0.42
2:B:530:GLY:O	2:B:531:GLN:C	2.57	0.42
1:A:1385:THR:CG2	1:A:1386:ARG:H	2.29	0.42
12:L:61:THR:CG2	12:L:62:LYS:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:ARG:HB3	2:B:384:ARG:HE	1.34	0.42
2:B:431:TYR:CG	2:B:447:ALA:CB	3.02	0.42
5:E:13:TRP:CZ3	5:E:39:LEU:HB2	2.54	0.42
1:A:364:VAL:O	1:A:364:VAL:HG13	2.17	0.42
1:A:517:ASN:ND2	1:A:1364:ASN:HD22	2.16	0.42
2:B:600:LEU:HD13	2:B:626:ILE:HD11	2.02	0.42
2:B:604:ARG:HG3	2:B:611:PRO:HA	2.01	0.42
2:B:345:LYS:HA	2:B:348:ARG:NE	2.33	0.42
2:B:244:LEU:CD1	2:B:366:GLN:HE22	2.32	0.42
1:A:66:LYS:HD3	1:A:67:CYS:H	1.84	0.42
4:D:138:ASN:O	4:D:140:ASP:N	2.52	0.42
2:B:1065:GLN:CD	2:B:1066:SER:N	2.73	0.42
5:E:22:MET:HG3	5:E:187:TYR:CD1	2.55	0.42
1:A:774:ARG:CZ	1:A:797:LYS:CB	2.98	0.42
1:A:816:HIS:HE2	2:B:764:SER:H	1.68	0.42
2:B:831:SER:HB2	2:B:833:TYR:CD1	2.54	0.42
2:B:1202:LEU:HD22	2:B:1206:GLU:OE2	2.19	0.42
9:I:93:LYS:H	9:I:93:LYS:CD	2.12	0.42
1:A:889:SER:OG	1:A:891:ALA:HB3	2.20	0.42
3:C:46:ILE:HG13	3:C:72:LEU:HD11	2.02	0.42
2:B:51:PHE:CD2	2:B:173:MET:HB3	2.55	0.42
1:A:283:GLY:O	1:A:285:PRO:CD	2.67	0.42
3:C:11:ARG:NH2	3:C:206:ASN:OD1	2.52	0.42
3:C:204:SER:C	3:C:206:ASN:H	2.23	0.42
1:A:993:LEU:CD2	1:A:1022:LEU:HD21	2.49	0.42
1:A:555:ASP:O	1:A:556:TRP:O	2.36	0.42
1:A:639:PRO:CD	1:A:640:GLN:H	2.32	0.42
5:E:89:GLY:C	5:E:91:LYS:N	2.72	0.42
6:F:132:LEU:HD23	6:F:132:LEU:HA	1.82	0.42
2:B:597:MET:CE	2:B:624:LEU:HD21	2.49	0.42
8:H:39:THR:O	8:H:123:MET:HG3	2.19	0.42
6:F:133:VAL:HG13	6:F:146:TRP:O	2.19	0.42
2:B:995:ARG:CB	2:B:997:GLU:OE2	2.67	0.42
1:A:385:ILE:CG2	1:A:386:ASP:N	2.82	0.42
7:G:35:GLU:HG2	7:G:48:VAL:HG23	2.02	0.42
9:I:99:LEU:C	9:I:100:PHE:HD1	2.23	0.42
11:K:47:ARG:O	11:K:47:ARG:HD2	2.19	0.42
2:B:1082:MET:HA	3:C:189:THR:HA	2.02	0.42
2:B:386:LEU:O	2:B:387:LEU:C	2.55	0.42
2:B:889:THR:CG2	2:B:891:ASP:HB2	2.50	0.42
2:B:56:ASP:CB	2:B:57:TYR:HD1	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:THR:HA	2:B:204:ILE:O	2.19	0.42
1:A:130:ASP:O	1:A:131:SER:C	2.58	0.42
2:B:1050:ILE:CG2	2:B:1051:THR:N	2.82	0.42
1:A:626:ASN:O	1:A:631:HIS:HD2	2.02	0.42
2:B:526:GLU:OE1	2:B:752:ALA:HB3	2.20	0.42
1:A:1371:LEU:HD12	1:A:1375:MET:HG3	2.00	0.42
3:C:136:ASP:CB	3:C:141:GLY:H	2.33	0.42
2:B:637:LEU:HA	2:B:637:LEU:HD23	1.80	0.42
8:H:27:GLU:HG2	8:H:38:LEU:O	2.20	0.42
1:A:244:PRO:CB	1:A:245:PRO:HD3	2.31	0.42
1:A:719:VAL:O	1:A:721:PHE:N	2.53	0.42
1:A:1339:LEU:HD13	5:E:147:HIS:CG	2.55	0.42
3:C:44:LEU:HD13	3:C:129:ILE:HG23	2.01	0.42
12:L:34:CYS:O	12:L:35:SER:C	2.58	0.42
12:L:34:CYS:CB	12:L:51:CYS:HG	2.32	0.42
8:H:83:GLN:CD	8:H:87:ARG:NH2	2.73	0.42
5:E:180:ARG:HH21	5:E:192:ARG:HB2	1.85	0.42
5:E:61:GLN:HB2	5:E:79:TRP:HE3	1.85	0.42
5:E:78:LEU:HB2	5:E:107:THR:HG21	2.02	0.42
2:B:100:PRO:HG2	2:B:124:TYR:CE1	2.55	0.42
1:A:219:PHE:O	1:A:222:LEU:N	2.51	0.42
2:B:992:ILE:HD11	11:K:66:PRO:HB2	2.00	0.42
1:A:709:THR:CG2	1:A:710:LEU:N	2.80	0.42
2:B:1182:CYS:C	2:B:1183:LYS:HE3	2.40	0.42
2:B:44:VAL:HG11	2:B:495:LEU:HD13	2.02	0.42
5:E:167:ARG:HD3	5:E:167:ARG:HA	1.78	0.42
11:K:78:THR:HG22	11:K:79:GLU:N	2.35	0.42
6:F:97:ARG:NH2	6:F:108:PHE:HE1	2.17	0.42
2:B:558:LEU:HD11	2:B:596:LEU:CD2	2.48	0.42
9:I:25:LEU:HG	9:I:38:ALA:HB2	2.02	0.42
7:G:53:ASN:HD22	7:G:53:ASN:N	2.15	0.42
1:A:758:ILE:H	1:A:758:ILE:HG13	1.72	0.42
2:B:597:MET:HE2	2:B:597:MET:HA	2.01	0.42
2:B:638:PHE:CD2	2:B:690:VAL:HG22	2.54	0.42
2:B:973:ILE:HG23	2:B:974:PRO:HD2	2.02	0.42
2:B:885:MET:HG2	2:B:936:ASP:HB2	2.02	0.42
1:A:692:ASP:O	1:A:695:LYS:N	2.53	0.42
4:D:155:ARG:HB3	4:D:155:ARG:NH1	2.34	0.42
3:C:248:ILE:CD1	11:K:101:LEU:HD22	2.49	0.42
1:A:913:LEU:CD1	1:A:914:GLU:N	2.78	0.42
2:B:859:TYR:CD1	2:B:859:TYR:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:138:GLU:OE1	8:H:138:GLU:C	2.58	0.42
1:A:903:ASN:ND2	1:A:903:ASN:C	2.73	0.42
5:E:124:VAL:H	5:E:125:PRO:HD2	1.82	0.42
1:A:1297:GLU:OE1	1:A:1297:GLU:N	2.53	0.42
1:A:683:ILE:HG21	1:A:801:GLU:CD	2.40	0.42
4:D:71:LYS:C	4:D:74:GLN:H	2.23	0.42
1:A:1225:PHE:CE2	1:A:1227:ILE:HD11	2.55	0.42
10:J:32:GLU:O	10:J:33:GLY:C	2.57	0.42
1:A:870:GLU:CB	5:E:204:THR:HG21	2.49	0.42
1:A:845:LEU:O	1:A:846:GLU:C	2.58	0.42
7:G:132:SER:HB3	7:G:135:ASP:N	2.32	0.42
2:B:39:ARG:NH2	2:B:665:GLU:CD	2.73	0.42
2:B:779:GLY:O	2:B:795:ILE:HA	2.20	0.42
4:D:8:PHE:HZ	4:D:37:GLN:NE2	2.17	0.42
1:A:923:LEU:HD23	1:A:923:LEU:HA	1.88	0.42
2:B:580:VAL:CG2	2:B:624:LEU:HB3	2.49	0.42
1:A:850:VAL:HG21	1:A:1058:VAL:HG11	2.01	0.42
8:H:3:ASN:CG	8:H:4:THR:H	2.24	0.42
2:B:365:THR:O	2:B:365:THR:HG23	2.20	0.42
8:H:40:LEU:HD22	8:H:123:MET:CE	2.50	0.42
8:H:12:VAL:HB	8:H:52:GLN:N	2.34	0.42
1:A:65:LEU:O	1:A:66:LYS:O	2.38	0.42
1:A:10:PRO:HG2	2:B:1192:TYR:HD2	1.85	0.42
3:C:38:ILE:H	3:C:38:ILE:HG13	1.61	0.42
3:C:22:LEU:HB2	3:C:230:MET:CE	2.50	0.42
4:D:16:LYS:O	4:D:18:VAL:N	2.50	0.42
5:E:22:MET:O	5:E:26:ARG:HG2	2.20	0.42
2:B:642:ASP:N	2:B:649:LYS:HG3	2.35	0.42
2:B:644:GLU:C	2:B:646:LEU:N	2.73	0.42
1:A:148:CYS:HB3	1:A:167:CYS:O	2.19	0.42
1:A:547:LEU:HD21	1:A:560:ILE:CD1	2.50	0.42
2:B:1124:ARG:NH2	15:P:2:A:OP2	2.52	0.42
11:K:53:ASP:HB3	11:K:56:VAL:CG2	2.50	0.42
1:A:442:VAL:HB	1:A:489:LEU:HD11	2.01	0.42
1:A:700:ASN:C	1:A:701:LEU:HD23	2.40	0.42
2:B:512:ARG:HG2	2:B:512:ARG:HH11	1.83	0.42
2:B:594:ALA:HA	2:B:617:ARG:NH1	2.35	0.41
8:H:9:ILE:HA	8:H:55:LEU:O	2.20	0.41
2:B:377:PHE:C	2:B:379:GLY:N	2.72	0.41
1:A:1189:SER:OG	1:A:1191:TRP:HB2	2.20	0.41
2:B:865:LYS:HD3	2:B:866:TYR:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:VAL:HG12	1:A:722:LEU:CD1	2.50	0.41
4:D:218:GLU:O	4:D:219:THR:C	2.58	0.41
4:D:124:GLU:N	4:D:124:GLU:CD	2.71	0.41
5:E:19:VAL:HG22	5:E:140:LEU:HD12	2.00	0.41
8:H:110:ASP:O	8:H:128:ASN:OD1	2.38	0.41
1:A:884:ASP:OD2	1:A:1030:ARG:NH2	2.53	0.41
10:J:47:ARG:NH1	10:J:47:ARG:HG2	2.34	0.41
3:C:215:GLU:O	3:C:216:GLY:C	2.57	0.41
2:B:44:VAL:O	2:B:45:SER:C	2.59	0.41
1:A:740:LEU:HD12	1:A:740:LEU:C	2.41	0.41
1:A:1451:VAL:C	1:A:1453:TYR:N	2.73	0.41
4:D:27:LEU:CD1	4:D:197:SER:HB3	2.50	0.41
1:A:1025:ARG:HG3	1:A:1025:ARG:NH1	2.33	0.41
2:B:557:PHE:HE1	2:B:603:LEU:HD11	1.84	0.41
3:C:113:VAL:HG23	3:C:147:LEU:HD21	2.01	0.41
5:E:56:LYS:HZ1	5:E:85:GLU:HG3	1.82	0.41
7:G:122:ASN:HB2	7:G:131:GLN:NE2	2.35	0.41
3:C:69:LEU:O	10:J:6:ARG:HD2	2.20	0.41
3:C:22:LEU:HD22	3:C:230:MET:HE1	2.01	0.41
1:A:821:ARG:CB	1:A:821:ARG:HH11	2.27	0.41
1:A:150:THR:O	1:A:150:THR:HG22	2.20	0.41
1:A:1102:LYS:O	1:A:1106:ASN:ND2	2.53	0.41
3:C:88:CYS:SG	3:C:91:HIS:HA	2.61	0.41
1:A:877:HIS:C	1:A:878:ILE:HG13	2.40	0.41
1:A:41:MET:O	1:A:42:ASP:O	2.38	0.41
2:B:850:LEU:HD12	2:B:850:LEU:C	2.39	0.41
1:A:253:ASN:HB3	1:A:254:GLU:H	1.70	0.41
1:A:1127:ASP:O	1:A:1128:GLN:C	2.58	0.41
1:A:1314:SER:C	1:A:1315:GLU:HG2	2.41	0.41
4:D:7:THR:HG21	4:D:32:GLU:OE2	2.20	0.41
1:A:77:CYS:C	1:A:78:PRO:O	2.58	0.41
1:A:1037:LEU:HD11	1:A:1045:VAL:HG21	2.00	0.41
11:K:79:GLU:O	11:K:81:TYR:N	2.54	0.41
4:D:50:LEU:HD21	7:G:4:ILE:CD1	2.49	0.41
1:A:347:PHE:HE2	1:A:375:THR:CG2	2.32	0.41
2:B:570:VAL:HA	2:B:571:PRO:HD2	1.82	0.41
1:A:150:THR:HA	1:A:165:GLY:O	2.20	0.41
2:B:430:ARG:HG2	2:B:430:ARG:HH11	1.84	0.41
1:A:481:ASP:O	1:A:485:ASP:HB2	2.21	0.41
5:E:7:ARG:HG3	5:E:8:ASN:N	2.35	0.41
1:A:260:ASP:OD1	1:A:261:ASP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:VAL:HA	1:A:554:PRO:HD2	1.90	0.41
1:A:54:ASN:HB3	1:A:247:ARG:NH2	2.33	0.41
7:G:26:LEU:O	7:G:28:THR:N	2.52	0.41
4:D:29:LEU:H	4:D:29:LEU:CD2	2.33	0.41
7:G:126:ASN:HA	7:G:127:PRO:HA	1.95	0.41
3:C:234:SER:OG	3:C:235:VAL:N	2.54	0.41
4:D:118:THR:HB	4:D:121:LYS:HB3	2.00	0.41
3:C:44:LEU:CD2	3:C:159:ALA:HB1	2.50	0.41
6:F:105:ALA:HB1	6:F:106:PRO:CD	2.50	0.41
2:B:766:ARG:NH1	2:B:769:TYR:CD1	2.87	0.41
2:B:114:PRO:HG2	2:B:115:GLN:N	2.30	0.41
1:A:332:LYS:HB3	1:A:337:ARG:CZ	2.50	0.41
1:A:697:ALA:CB	1:A:702:LEU:HD12	2.41	0.41
10:J:34:THR:O	10:J:37:SER:N	2.54	0.41
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.35	0.41
5:E:195:VAL:HG22	5:E:213:ILE:HG13	2.01	0.41
11:K:68:PHE:CD1	11:K:70:ARG:NH1	2.81	0.41
1:A:348:SER:HA	1:A:489:LEU:O	2.21	0.41
1:A:855:THR:HG21	1:A:857:ARG:HE	1.85	0.41
2:B:615:MET:C	2:B:616:ILE:HD12	2.41	0.41
8:H:38:LEU:HD12	8:H:38:LEU:HA	1.84	0.41
1:A:382:PRO:N	1:A:428:TYR:CE2	2.89	0.41
1:A:382:PRO:CD	1:A:428:TYR:CE2	3.04	0.41
2:B:877:PRO:O	2:B:878:GLN:HB3	2.20	0.41
2:B:936:ASP:CG	2:B:937:ALA:N	2.74	0.41
2:B:1002:THR:OG1	2:B:1006:ILE:CG1	2.66	0.41
6:F:106:PRO:HG2	7:G:18:PHE:C	2.41	0.41
4:D:124:GLU:HA	4:D:127:ASP:HB2	2.01	0.41
1:A:767:GLN:NE2	1:A:768:GLN:O	2.53	0.41
1:A:774:ARG:CZ	1:A:797:LYS:HG3	2.51	0.41
8:H:84:ALA:O	8:H:86:ASP:N	2.53	0.41
9:I:78:CYS:O	9:I:80:SER:N	2.53	0.41
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.23	0.41
10:J:37:SER:OG	10:J:47:ARG:NH2	2.53	0.41
12:L:27:LEU:N	12:L:27:LEU:HD23	2.36	0.41
2:B:313:MET:CE	2:B:386:LEU:HB3	2.50	0.41
1:A:830:LYS:HG3	1:A:1098:VAL:HG21	2.02	0.41
9:I:60:GLN:OE1	9:I:107:SER:OG	2.35	0.41
1:A:557:ASP:O	1:A:559:VAL:HG23	2.20	0.41
2:B:1175:LEU:O	2:B:1176:ASN:CB	2.66	0.41
1:A:255:SER:OG	2:B:918:ILE:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:62:ILE:HD11	9:I:86:PHE:HE2	1.86	0.41
4:D:153:ARG:C	4:D:154:PHE:HD2	2.24	0.41
3:C:124:LEU:C	3:C:126:GLY:N	2.74	0.41
3:C:73:GLN:CB	3:C:131:HIS:H	2.34	0.41
1:A:665:GLY:O	1:A:666:ILE:C	2.59	0.41
2:B:113:TYR:CE2	2:B:192:LEU:CD2	3.03	0.41
8:H:83:GLN:O	8:H:85:GLY:N	2.54	0.41
2:B:94:LYS:HZ3	2:B:96:TYR:HE2	1.66	0.41
2:B:63:ILE:HG12	2:B:130:VAL:HG21	2.03	0.41
1:A:392:VAL:HG13	1:A:415:LEU:HD11	2.03	0.41
2:B:515:HIS:O	2:B:518:HIS:HB2	2.20	0.41
1:A:425:GLN:HG2	1:A:425:GLN:O	2.20	0.41
3:C:258:ILE:N	3:C:258:ILE:CD1	2.83	0.41
9:I:46:HIS:CE1	9:I:48:LEU:CD2	3.03	0.41
1:A:1147:THR:O	9:I:48:LEU:HD12	2.20	0.41
9:I:73:ARG:NH1	9:I:101:PHE:CZ	2.89	0.41
1:A:1454:MET:HA	1:A:1455:PRO:HD2	1.94	0.41
2:B:54:PHE:CZ	2:B:59:LEU:HD13	2.56	0.41
4:D:170:THR:HB	4:D:172:LEU:HG	2.02	0.41
1:A:516:SER:O	1:A:517:ASN:C	2.59	0.41
3:C:138:GLU:HB2	3:C:140:ASN:HD21	1.86	0.41
2:B:361:LEU:N	2:B:362:PRO:CD	2.84	0.41
2:B:618:ASP:O	2:B:622:LYS:N	2.53	0.41
4:D:154:PHE:HE1	4:D:163:VAL:HG11	1.85	0.41
4:D:156:ASP:HB2	4:D:159:THR:HG1	1.84	0.41
2:B:1002:THR:O	2:B:1003:ALA:C	2.59	0.41
2:B:1003:ALA:O	3:C:177:GLU:HA	2.21	0.41
1:A:219:PHE:HB2	1:A:220:THR:H	1.46	0.41
1:A:593:GLU:HB3	1:A:594:GLY:H	1.48	0.41
4:D:198:LEU:O	4:D:200:ASN:N	2.54	0.41
11:K:85:ASP:O	11:K:88:LYS:N	2.54	0.41
1:A:820:GLY:O	1:A:823:GLY:N	2.54	0.41
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.51	0.41
2:B:1001:PHE:CD1	2:B:1001:PHE:C	2.94	0.41
1:A:946:VAL:HG12	1:A:947:PHE:CE2	2.56	0.41
9:I:45:ARG:HG3	9:I:46:HIS:N	2.36	0.41
1:A:396:PRO:HB3	1:A:403:LYS:HA	2.02	0.41
7:G:104:GLY:HA3	7:G:105:PRO:HD2	1.93	0.41
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.56	0.41
2:B:707:PRO:CG	2:B:708:GLU:N	2.75	0.41
9:I:54:GLU:HB3	9:I:100:PHE:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ILE:C	10:J:53:HIS:CE1	2.94	0.41
4:D:150:ASN:HB3	7:G:142:ARG:NH2	2.36	0.41
4:D:24:ALA:C	4:D:26:THR:H	2.24	0.41
1:A:93:VAL:HG21	1:A:301:ALA:HA	2.01	0.41
1:A:451:HIS:O	1:A:452:LYS:C	2.58	0.41
2:B:976:ILE:CD1	2:B:992:ILE:HA	2.51	0.41
9:I:88:SER:C	9:I:90:GLN:N	2.74	0.41
5:E:45:LYS:HD3	5:E:46:TYR:CE1	2.56	0.41
5:E:175:LEU:HA	5:E:176:PRO:HD3	1.81	0.41
2:B:1084:GLN:OE1	3:C:189:THR:CG2	2.69	0.41
6:F:97:ARG:NE	6:F:124:GLU:OE1	2.54	0.41
1:A:800:VAL:HA	1:A:812:GLU:OE2	2.20	0.41
1:A:120:GLU:C	1:A:122:MET:N	2.73	0.41
1:A:473:SER:O	1:A:521:MET:HB3	2.21	0.41
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	2.01	0.41
2:B:259:TYR:O	2:B:260:GLY:O	2.39	0.41
2:B:205:ILE:O	2:B:207:GLY:N	2.54	0.41
1:A:460:VAL:CG1	1:A:461:LYS:N	2.83	0.41
1:A:343:LYS:NZ	2:B:1151:LEU:HG	2.35	0.41
1:A:639:PRO:CG	1:A:640:GLN:N	2.83	0.41
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.60	0.41
1:A:1273:LEU:CD1	1:A:1273:LEU:N	2.84	0.41
6:F:152:ILE:HG22	6:F:153:VAL:N	2.35	0.41
2:B:593:PRO:HG2	2:B:617:ARG:CZ	2.50	0.41
1:A:298:PHE:CD2	1:A:299:HIS:HD2	2.38	0.41
1:A:40:THR:C	1:A:41:MET:HG3	2.41	0.41
4:D:66:ARG:NH2	7:G:31:LEU:HD11	2.35	0.41
2:B:918:ILE:HG21	2:B:935:ARG:HH22	1.83	0.41
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.03	0.41
9:I:54:GLU:OE1	9:I:118:ARG:NH2	2.53	0.41
10:J:57:ILE:HG23	10:J:58:GLU:N	2.35	0.41
3:C:133:ILE:CD1	3:C:237:SER:N	2.82	0.41
3:C:154:LYS:HE3	3:C:154:LYS:HB2	1.85	0.41
3:C:177:GLU:HB2	3:C:231:ASN:HB3	2.02	0.41
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.51	0.41
11:K:31:VAL:CG1	11:K:32:VAL:N	2.81	0.41
2:B:789:MET:HE2	2:B:965:LYS:CB	2.51	0.41
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.49	0.41
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.01	0.41
6:F:116:ASP:HB3	6:F:119:ARG:HB2	2.02	0.41
2:B:25:ILE:HG21	2:B:658:ILE:CD1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:912:ILE:O	2:B:938:SER:CB	2.67	0.41
2:B:913:GLY:HA2	2:B:938:SER:OG	2.20	0.41
8:H:128:ASN:C	8:H:128:ASN:HD22	2.23	0.41
2:B:326:ASP:OD1	2:B:329:THR:CB	2.68	0.41
2:B:467:GLY:N	2:B:475:SER:OG	2.54	0.41
1:A:820:GLY:O	1:A:821:ARG:C	2.58	0.41
2:B:1084:GLN:HE21	2:B:1084:GLN:H	1.67	0.41
2:B:401:PHE:HB2	2:B:517:THR:OG1	2.20	0.41
2:B:435:THR:HG22	2:B:437:GLU:C	2.41	0.41
1:A:1038:THR:H	1:A:1041:ALA:HB3	1.85	0.41
6:F:138:LEU:HA	6:F:138:LEU:HD23	1.84	0.41
2:B:1073:TYR:CE2	2:B:1080:LYS:HG3	2.56	0.41
1:A:479:ASN:HA	1:A:479:ASN:HD22	1.62	0.41
5:E:99:HIS:ND1	5:E:103:LYS:HG3	2.36	0.41
2:B:571:PRO:HG2	2:B:572:HIS:H	1.86	0.41
4:D:122:GLU:HA	4:D:125:SER:HB3	2.02	0.41
1:A:526:ASP:OD1	2:B:1013:ASN:ND2	2.52	0.41
2:B:969:ARG:HD2	3:C:61:GLU:OE2	2.21	0.41
1:A:1279:ILE:O	1:A:1279:ILE:HG22	2.21	0.41
1:A:559:VAL:O	1:A:561:PRO:HD3	2.20	0.41
7:G:145:VAL:HG12	7:G:146:LYS:N	2.36	0.41
7:G:44:TYR:OH	7:G:156:SER:HB2	2.20	0.41
9:I:15:TYR:CD1	9:I:30:ARG:HD2	2.56	0.41
1:A:542:GLU:HG2	1:A:542:GLU:H	1.63	0.41
2:B:333:PHE:O	2:B:334:ILE:HG13	2.20	0.41
7:G:59:GLY:CA	7:G:70:PHE:CD2	3.04	0.41
1:A:64:ASN:O	1:A:66:LYS:N	2.54	0.41
7:G:1:MET:CE	7:G:80:LYS:O	2.69	0.41
1:A:722:LEU:HD23	1:A:799:PHE:CG	2.56	0.41
2:B:798:TYR:CE2	3:C:62:PHE:CZ	3.07	0.41
2:B:251:ILE:O	2:B:251:ILE:CG2	2.67	0.41
3:C:22:LEU:HD11	11:K:101:LEU:HD11	2.03	0.41
1:A:1116:LEU:HG	1:A:1308:THR:HB	2.03	0.41
8:H:130:ARG:N	8:H:130:ARG:CD	2.80	0.41
1:A:1138:ILE:HG13	1:A:1139:GLU:N	2.36	0.41
1:A:650:GLN:HB3	1:A:654:ASN:ND2	2.36	0.41
2:B:1032:SER:HB3	2:B:1089:PRO:HG2	2.03	0.41
12:L:49:LYS:O	12:L:50:ASP:CB	2.58	0.41
2:B:186:GLU:OE2	2:B:186:GLU:HA	2.21	0.41
5:E:164:LEU:HD22	5:E:211:TYR:HD2	1.77	0.41
2:B:205:ILE:HG12	2:B:461:LEU:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:PHE:O	1:A:1056:SER:N	2.54	0.41
1:A:996:ASN:O	1:A:998:LEU:N	2.49	0.41
1:A:371:ALA:HB2	1:A:462:VAL:HG13	2.03	0.41
7:G:61:ILE:HG22	7:G:62:LEU:O	2.21	0.41
2:B:806:THR:HG21	2:B:808:ALA:HB3	2.03	0.40
8:H:8:ASP:OD1	8:H:30:SER:OG	2.31	0.40
2:B:333:PHE:O	2:B:334:ILE:CG1	2.69	0.40
3:C:239:PRO:O	3:C:240:VAL:C	2.59	0.40
2:B:1026:LEU:HA	2:B:1026:LEU:HD23	1.86	0.40
4:D:53:SER:HA	4:D:56:ARG:CB	2.51	0.40
5:E:98:ILE:HG22	5:E:102:GLU:HG3	2.03	0.40
1:A:683:ILE:HG21	1:A:801:GLU:OE1	2.21	0.40
12:L:38:LEU:CG	12:L:39:SER:N	2.83	0.40
2:B:390:LEU:O	2:B:391:ASP:C	2.59	0.40
5:E:29:PHE:HD1	5:E:30:ILE:N	2.19	0.40
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.51	0.40
1:A:347:PHE:CE2	2:B:1107:ALA:HB1	2.56	0.40
4:D:134:THR:CG2	4:D:135:GLY:N	2.84	0.40
5:E:11:ARG:C	5:E:13:TRP:N	2.74	0.40
1:A:909:ASP:OD1	1:A:911:SER:N	2.46	0.40
1:A:786:HIS:HE1	2:B:519:TRP:CZ2	2.39	0.40
2:B:276:ILE:HG22	2:B:336:ARG:HB2	2.02	0.40
1:A:34:LYS:CB	1:A:36:ARG:NH2	2.85	0.40
2:B:854:LEU:HD23	2:B:854:LEU:HA	1.91	0.40
10:J:53:HIS:HD2	10:J:54:VAL:H	1.58	0.40
4:D:154:PHE:HA	4:D:219:THR:HB	2.02	0.40
3:C:44:LEU:HD23	3:C:44:LEU:C	2.42	0.40
1:A:546:VAL:HG21	1:A:572:TRP:HB2	2.03	0.40
2:B:769:TYR:HA	15:P:11:G:H22	1.87	0.40
12:L:44:ASP:O	12:L:45:ALA:HB3	2.21	0.40
2:B:955:THR:HG23	12:L:54:ARG:O	2.21	0.40
6:F:84:TYR:N	6:F:84:TYR:CD1	2.90	0.40
1:A:598:LEU:HA	8:H:122:LEU:CD1	2.48	0.40
1:A:897:TYR:CD1	1:A:897:TYR:N	2.89	0.40
9:I:8:ARG:O	9:I:9:ASP:HB2	2.21	0.40
2:B:473:MET:HE3	2:B:474:SER:N	2.37	0.40
3:C:3:GLU:HB3	11:K:104:ASN:OD1	2.21	0.40
4:D:190:GLU:O	4:D:193:THR:CG2	2.67	0.40
2:B:186:GLU:HB3	2:B:187:SER:H	1.71	0.40
11:K:49:GLU:C	11:K:51:LEU:N	2.75	0.40
2:B:1031:LEU:HB2	2:B:1055:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:857:ARG:NH1	6:F:139:PRO:CB	2.84	0.40
1:A:101:LYS:HA	1:A:104:GLU:OE1	2.22	0.40
1:A:752:LYS:HD3	1:A:752:LYS:HA	1.77	0.40
7:G:62:LEU:HD13	7:G:62:LEU:HA	1.89	0.40
2:B:104:GLU:OE2	12:L:47:ARG:NH2	2.55	0.40
1:A:589:GLN:HG3	1:A:606:LEU:HD13	2.04	0.40
2:B:224:GLN:HA	2:B:396:ASP:OD2	2.20	0.40
2:B:624:LEU:HA	2:B:624:LEU:HD12	1.57	0.40
8:H:43:ASN:C	8:H:45:GLU:H	2.24	0.40
1:A:47:ARG:CZ	1:A:254:GLU:HG2	2.51	0.40
1:A:665:GLY:HA2	2:B:1026:LEU:CD2	2.50	0.40
4:D:126:ILE:HD13	4:D:145:MET:CE	2.50	0.40
1:A:1170:ILE:CD1	1:A:1170:ILE:H	2.16	0.40
1:A:604:GLY:O	1:A:605:MET:HB2	2.21	0.40
1:A:1134:ILE:HG13	1:A:1134:ILE:H	1.66	0.40
9:I:5:ARG:CZ	9:I:36:GLU:OE1	2.69	0.40
2:B:687:GLU:O	2:B:688:GLY:C	2.59	0.40
1:A:1030:ARG:NH1	1:A:1035:TYR:OH	2.54	0.40
1:A:524:VAL:CG1	1:A:525:GLN:H	2.25	0.40
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.86	0.40
2:B:282:ILE:HG21	2:B:382:ILE:CD1	2.51	0.40
1:A:1006:ILE:HD12	5:E:167:ARG:CG	2.50	0.40
1:A:984:LYS:HG2	1:A:988:LEU:HD12	2.02	0.40
6:F:109:VAL:CG2	6:F:124:GLU:HA	2.51	0.40
3:C:77:ILE:HG23	3:C:161:LYS:HE3	2.03	0.40
11:K:92:ASN:O	11:K:93:SER:C	2.60	0.40
2:B:1221:SER:C	2:B:1223:ASP:H	2.25	0.40
1:A:738:LYS:H	1:A:738:LYS:HD3	1.85	0.40
8:H:37:LYS:H	8:H:126:GLU:HB2	1.87	0.40
2:B:58:THR:HG22	2:B:62:ILE:HD11	2.02	0.40
2:B:969:ARG:HG2	2:B:970:THR:N	2.36	0.40
2:B:970:THR:CG2	2:B:971:THR:N	2.84	0.40
4:D:176:GLU:O	4:D:178:ALA:N	2.54	0.40
1:A:600:PRO:HG2	1:A:601:LYS:H	1.87	0.40
1:A:1333:ILE:H	1:A:1333:ILE:HG12	1.48	0.40
1:A:409:SER:O	1:A:410:GLY:C	2.59	0.40
2:B:345:LYS:CG	2:B:346:GLU:N	2.70	0.40
3:C:148:ARG:CG	3:C:149:LYS:H	2.34	0.40
1:A:276:LEU:HD13	1:A:293:GLU:HA	2.03	0.40
1:A:381:THR:C	1:A:383:TYR:N	2.73	0.40
4:D:173:HIS:O	4:D:177:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:80:LYS:O	7:G:82:PHE:CE1	2.75	0.40
2:B:871:THR:CG2	2:B:872:GLU:N	2.85	0.40
1:A:253:ASN:ND2	2:B:884:ARG:HD2	2.35	0.40
2:B:620:ARG:NH1	9:I:68:LEU:HD21	2.37	0.40
1:A:154:SER:C	1:A:156:ASP:H	2.25	0.40
1:A:135:PHE:HD1	1:A:222:LEU:HD22	1.79	0.40
1:A:588:LEU:HD23	1:A:607:ILE:HD12	2.02	0.40
2:B:129:PHE:HE2	2:B:166:PHE:CD1	2.38	0.40
2:B:327:ARG:HH22	2:B:371:GLU:HG2	1.79	0.40
4:D:187:THR:HB	4:D:190:GLU:H	1.86	0.40
2:B:185:THR:N	2:B:188:ASP:OD2	2.55	0.40
1:A:1120:LEU:HD12	1:A:1120:LEU:C	2.42	0.40
1:A:1104:ILE:O	1:A:1106:ASN:N	2.55	0.40
11:K:93:SER:O	11:K:97:LYS:HG3	2.21	0.40
2:B:231:PRO:HG2	2:B:231:PRO:O	2.21	0.40
1:A:1334:ASP:O	1:A:1336:MET:N	2.54	0.40
2:B:950:ASP:HB3	2:B:967:ARG:O	2.21	0.40
1:A:89:PRO:HG2	1:A:204:THR:HB	2.04	0.40
5:E:60:PHE:CD1	5:E:60:PHE:C	2.95	0.40
2:B:655:LYS:HA	2:B:655:LYS:HD2	1.90	0.40
2:B:273:LEU:HA	2:B:274:PRO:HD2	1.95	0.40
2:B:557:PHE:CZ	2:B:603:LEU:HG	2.56	0.40
8:H:12:VAL:HG11	8:H:15:VAL:HG22	2.03	0.40
2:B:796:LEU:HD12	2:B:852:ARG:O	2.21	0.40
2:B:878:GLN:HB2	2:B:879:ARG:HH11	1.87	0.40
3:C:238:ILE:CG2	3:C:242:GLN:HB2	2.50	0.40
1:A:208:LEU:C	1:A:208:LEU:CD2	2.90	0.40
2:B:1030:LEU:HD11	2:B:1059:LEU:HD22	2.04	0.40
2:B:773:MET:C	2:B:775:LYS:N	2.74	0.40
5:E:80:VAL:HG12	5:E:82:PHE:CE1	2.57	0.40
1:A:671:ALA:CB	1:A:676:MET:HG3	2.40	0.40
1:A:599:SER:HB2	1:A:603:ASN:H	1.87	0.40
2:B:515:HIS:CD2	2:B:517:THR:CG2	3.02	0.40
2:B:390:LEU:O	2:B:392:ARG:HG3	2.21	0.40
9:I:50:THR:H	9:I:92:ARG:HH12	1.69	0.40
1:A:249:SER:O	1:A:250:ILE:CG1	2.66	0.40
6:F:138:LEU:HB3	6:F:139:PRO:HD2	2.03	0.40
2:B:570:VAL:HB	2:B:573:GLN:HB3	2.02	0.40
2:B:286:PHE:HB3	2:B:297:ILE:HG12	2.02	0.40
1:A:856:THR:HG21	1:A:1370:LEU:HD21	2.04	0.40
2:B:1017:ILE:H	2:B:1018:PRO:HD2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:118:PHE:O	8:H:119:GLY:C	2.60	0.40
1:A:699:ALA:O	1:A:700:ASN:HB3	2.22	0.40
2:B:825:VAL:HG21	2:B:1092:TYR:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1408/1733 (81%)	1012 (72%)	262 (19%)	134 (10%)	1 14
2	B	1089/1224 (89%)	779 (72%)	201 (18%)	109 (10%)	1 12
3	C	264/347 (76%)	186 (70%)	51 (19%)	27 (10%)	1 12
4	D	175/221 (79%)	121 (69%)	39 (22%)	15 (9%)	1 16
5	E	212/215 (99%)	154 (73%)	42 (20%)	16 (8%)	1 20
6	F	85/155 (55%)	69 (81%)	14 (16%)	2 (2%)	7 51
7	G	169/171 (99%)	145 (86%)	13 (8%)	11 (6%)	1 25
8	H	132/146 (90%)	85 (64%)	23 (17%)	24 (18%)	0 3
9	I	117/122 (96%)	79 (68%)	29 (25%)	9 (8%)	1 19
10	J	63/70 (90%)	39 (62%)	11 (18%)	13 (21%)	0 2
11	K	113/120 (94%)	87 (77%)	22 (20%)	4 (4%)	4 43
12	L	44/70 (63%)	23 (52%)	9 (20%)	12 (27%)	0 0
All	All	3871/4594 (84%)	2779 (72%)	716 (18%)	376 (10%)	1 13

All (376) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN

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Mol	Chain	Res	Type
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	54	ASN
1	A	57	ARG
1	A	58	LEU
1	A	62	ASP
1	A	63	ARG
1	A	67	CYS
1	A	70	CYS
1	A	128	ILE
1	A	130	ASP
1	A	154	SER
1	A	167	CYS
1	A	250	ILE
1	A	286	HIS
1	A	311	GLN
1	A	312	PRO
1	A	332	LYS
1	A	399	HIS
1	A	423	ASP
1	A	567	LYS
1	A	666	ILE
1	A	1112	LYS
1	A	1114	PRO
1	A	1120	LEU
1	A	1124	HIS
1	A	1223	ASP
1	A	1233	ASP
1	A	1242	VAL
1	A	1255	GLU
1	A	1281	ARG
1	A	1314	SER
1	A	1405	THR
2	B	21	GLU
2	B	67	SER
2	B	68	THR
2	B	108	VAL
2	B	184	ALA
2	B	186	GLU
2	B	282	ILE
2	B	365	THR

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Mol	Chain	Res	Type
2	B	367	LEU
2	B	435	THR
2	B	467	GLY
2	B	619	ILE
2	B	708	GLU
2	B	709	ASP
2	B	731	VAL
2	B	850	LEU
2	B	879	ARG
2	B	907	GLY
2	B	958	GLN
2	B	1041	GLU
2	B	1046	PRO
2	B	1069	PHE
2	B	1097	HIS
2	B	1103	ILE
2	B	1108	ARG
2	B	1155	SER
2	B	1157	ALA
2	B	1181	GLU
2	B	1188	LYS
2	B	1222	ARG
3	C	56	THR
3	C	90	ASP
3	C	110	THR
3	C	125	MET
3	C	141	GLY
3	C	149	LYS
3	C	161	LYS
3	C	184	ASN
3	C	209	TYR
3	C	215	GLU
3	C	216	GLY
3	C	237	SER
4	D	5	THR
4	D	8	PHE
4	D	17	LYS
4	D	52	LEU
4	D	198	LEU
4	D	218	GLU
5	E	45	LYS
5	E	74	ASP

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Mol	Chain	Res	Type
5	E	106	GLN
5	E	115	ASN
7	G	112	LYS
7	G	139	ILE
8	H	62	SER
8	H	77	ARG
8	H	82	PRO
8	H	108	SER
8	H	128	ASN
8	H	134	ASN
8	H	140	ALA
9	I	11	ASN
9	I	79	HIS
10	J	2	ILE
10	J	28	ASP
10	J	42	LYS
10	J	55	ASP
10	J	64	ASN
12	L	50	ASP
12	L	53	HIS
12	L	59	ALA
12	L	60	ARG
1	A	5	GLN
1	A	76	GLU
1	A	93	VAL
1	A	126	LEU
1	A	249	SER
1	A	253	ASN
1	A	318	SER
1	A	400	PRO
1	A	410	GLY
1	A	424	ILE
1	A	556	TRP
1	A	576	GLN
1	A	591	PHE
1	A	592	ASP
1	A	597	LEU
1	A	628	GLY
1	A	718	VAL
1	A	821	ARG
1	A	846	GLU
1	A	852	TYR

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Mol	Chain	Res	Type
1	A	884	ASP
1	A	885	THR
1	A	891	ALA
1	A	963	ILE
1	A	968	GLN
1	A	986	ILE
1	A	1002	GLY
1	A	1123	GLY
1	A	1127	ASP
1	A	1139	GLU
1	A	1187	GLN
1	A	1231	ASP
1	A	1280	GLU
1	A	1309	ASP
1	A	1438	THR
2	B	58	THR
2	B	65	GLU
2	B	100	PRO
2	B	221	ASN
2	B	249	ARG
2	B	258	LEU
2	B	259	TYR
2	B	260	GLY
2	B	295	GLY
2	B	333	PHE
2	B	334	ILE
2	B	448	ILE
2	B	461	LEU
2	B	466	TRP
2	B	468	GLU
2	B	474	SER
2	B	501	PRO
2	B	575	PRO
2	B	591	ARG
2	B	642	ASP
2	B	643	ASP
2	B	655	LYS
2	B	746	SER
2	B	751	VAL
2	B	792	MET
2	B	869	SER
2	B	943	SER

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Mol	Chain	Res	Type
2	B	1175	LEU
2	B	1176	ASN
2	B	1214	PRO
3	C	60	ASP
3	C	173	ALA
3	C	240	VAL
4	D	14	ARG
4	D	19	GLU
4	D	119	ARG
4	D	131	GLU
4	D	199	ASN
5	E	36	GLU
5	E	130	ALA
5	E	158	SER
7	G	63	PRO
7	G	154	VAL
8	H	12	VAL
8	H	17	PRO
8	H	21	ASN
8	H	32	THR
8	H	51	ALA
8	H	59	ILE
8	H	84	ALA
8	H	90	ALA
8	H	92	ASP
8	H	95	TYR
8	H	107	VAL
9	I	54	GLU
9	I	57	GLY
9	I	106	CYS
10	J	6	ARG
10	J	17	LYS
10	J	33	GLY
10	J	62	ARG
11	K	53	ASP
11	K	80	GLY
12	L	28	LYS
12	L	40	LEU
12	L	54	ARG
1	A	51	GLY
1	A	61	ILE
1	A	66	LYS

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Mol	Chain	Res	Type
1	A	74	MET
1	A	131	SER
1	A	169	ASN
1	A	219	PHE
1	A	283	GLY
1	A	313	GLN
1	A	322	VAL
1	A	426	LEU
1	A	517	ASN
1	A	755	PHE
1	A	975	HIS
1	A	1122	PRO
1	A	1206	ASP
1	A	1221	LYS
1	A	1308	THR
1	A	1378	GLN
1	A	1390	ASN
2	B	24	PRO
2	B	27	ALA
2	B	206	ASN
2	B	309	GLN
2	B	531	GLN
2	B	561	TRP
2	B	594	ALA
2	B	605	ARG
2	B	641	GLU
2	B	711	GLU
2	B	728	ARG
2	B	734	HIS
2	B	752	ALA
2	B	881	ASN
2	B	892	LYS
2	B	906	SER
2	B	959	ASP
2	B	1003	ALA
2	B	1100	ASP
3	C	132	PRO
3	C	169	LYS
3	C	172	PRO
3	C	208	GLU
4	D	157	GLN
5	E	76	GLY

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Mol	Chain	Res	Type
6	F	128	LYS
7	G	2	PHE
7	G	20	PRO
8	H	44	VAL
8	H	63	LEU
9	I	8	ARG
9	I	9	ASP
10	J	14	VAL
10	J	24	LEU
12	L	27	LEU
12	L	35	SER
1	A	69	THR
1	A	159	THR
1	A	294	SER
1	A	331	GLY
1	A	466	SER
1	A	510	GLN
1	A	526	ASP
1	A	789	LYS
1	A	875	ALA
1	A	1278	ASN
2	B	114	PRO
2	B	257	LYS
2	B	264	SER
2	B	277	LYS
2	B	294	ASP
2	B	509	ALA
2	B	680	THR
2	B	810	GLU
2	B	848	ARG
2	B	937	ALA
2	B	1017	ILE
2	B	1082	MET
3	C	11	ARG
3	C	142	VAL
3	C	213	PRO
3	C	227	THR
3	C	243	VAL
4	D	118	THR
5	E	95	THR
5	E	129	PRO
7	G	27	LYS

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Mol	Chain	Res	Type
7	G	136	VAL
8	H	81	PRO
8	H	139	ASN
9	I	62	ILE
11	K	54	ARG
11	K	79	GLU
12	L	39	SER
1	A	35	ILE
1	A	42	ASP
1	A	244	PRO
1	A	465	TYR
1	A	543	LEU
1	A	619	LYS
1	A	673	GLY
1	A	693	VAL
1	A	704	ALA
1	A	720	ARG
1	A	958	VAL
1	A	995	GLU
1	A	1067	LEU
1	A	1105	LEU
1	A	1158	PRO
1	A	1244	ARG
1	A	1270	ASN
1	A	1365	TYR
1	A	1454	MET
2	B	45	SER
2	B	245	GLU
2	B	291	ILE
2	B	449	ASN
2	B	460	ALA
2	B	738	PHE
2	B	878	GLN
2	B	1075	GLY
2	B	1171	VAL
2	B	1183	LYS
3	C	12	GLU
4	D	30	GLY
4	D	53	SER
5	E	66	GLU
5	E	73	PRO
5	E	92	THR

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Mol	Chain	Res	Type
6	F	150	GLU
8	H	8	ASP
9	I	95	THR
10	J	27	GLU
12	L	45	ALA
12	L	56	LEU
1	A	599	SER
1	A	605	MET
1	A	922	ASP
1	A	1211	GLN
2	B	793	ALA
3	C	78	GLU
5	E	38	PRO
5	E	44	ALA
10	J	13	VAL
1	A	1437	GLY
2	B	818	PRO
2	B	1167	GLY
5	E	183	PRO
8	H	47	PHE
1	A	719	VAL
1	A	1335	ILE
2	B	593	PRO
7	G	126	ASN
1	A	775	ILE
2	B	707	PRO
2	B	764	SER
2	B	867	GLY
7	G	163	ILE
1	A	84	ILE
1	A	568	PRO
1	A	583	PRO
1	A	756	ILE
1	A	973	ILE
2	B	364	ILE
3	C	18	VAL
7	G	128	PRO
1	A	96	ILE
1	A	1006	ILE

5.3.2 Protein sidechains (i)

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	1241/1520 (82%)	1109 (89%)	132 (11%)	8 42
2	B	963/1061 (91%)	841 (87%)	122 (13%)	5 32
3	C	234/299 (78%)	206 (88%)	28 (12%)	6 35
4	D	161/200 (80%)	139 (86%)	22 (14%)	4 30
5	E	196/197 (100%)	180 (92%)	16 (8%)	14 54
6	F	77/137 (56%)	73 (95%)	4 (5%)	29 70
7	G	152/152 (100%)	137 (90%)	15 (10%)	10 45
8	H	120/128 (94%)	104 (87%)	16 (13%)	5 31
9	I	113/116 (97%)	97 (86%)	16 (14%)	4 28
10	J	60/65 (92%)	55 (92%)	5 (8%)	14 53
11	K	99/102 (97%)	92 (93%)	7 (7%)	18 60
12	L	40/57 (70%)	36 (90%)	4 (10%)	9 44
All	All	3456/4034 (86%)	3069 (89%)	387 (11%)	7 39

All (387) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	18	GLN
1	A	32	VAL
1	A	34	LYS
1	A	37	PHE
1	A	41	MET
1	A	42	ASP
1	A	46	THR
1	A	54	ASN
1	A	68	GLN
1	A	70	CYS
1	A	83	HIS
1	A	93	VAL
1	A	141	LEU

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Mol	Chain	Res	Type
1	A	145	LYS
1	A	160	GLN
1	A	161	LEU
1	A	162	VAL
1	A	169	ASN
1	A	185	TRP
1	A	196	GLU
1	A	203	SER
1	A	208	LEU
1	A	221	SER
1	A	244	PRO
1	A	245	PRO
1	A	265	LYS
1	A	289	ILE
1	A	290	GLU
1	A	302	THR
1	A	312	PRO
1	A	320	ARG
1	A	321	PRO
1	A	322	VAL
1	A	324	SER
1	A	332	LYS
1	A	337	ARG
1	A	344	ARG
1	A	385	ILE
1	A	396	PRO
1	A	408	ASP
1	A	416	ARG
1	A	443	LEU
1	A	445	ASN
1	A	451	HIS
1	A	454	SER
1	A	462	VAL
1	A	470	LEU
1	A	475	THR
1	A	479	ASN
1	A	481	ASP
1	A	483	ASP
1	A	505	CYS
1	A	513	SER
1	A	518	LYS
1	A	539	THR

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Mol	Chain	Res	Type
1	A	547	LEU
1	A	549	MET
1	A	562	THR
1	A	565	ILE
1	A	571	LEU
1	A	582	ILE
1	A	593	GLU
1	A	618	GLU
1	A	664	THR
1	A	666	ILE
1	A	680	THR
1	A	690	VAL
1	A	701	LEU
1	A	710	LEU
1	A	735	VAL
1	A	738	LYS
1	A	741	ASN
1	A	768	GLN
1	A	774	ARG
1	A	810	PRO
1	A	821	ARG
1	A	822	GLU
1	A	827	THR
1	A	838	GLN
1	A	858	ASN
1	A	871	ASP
1	A	882	SER
1	A	903	ASN
1	A	906	HIS
1	A	920	LEU
1	A	923	LEU
1	A	941	LYS
1	A	961	ARG
1	A	978	PRO
1	A	983	ILE
1	A	992	ASP
1	A	1009	ASN
1	A	1029	ARG
1	A	1048	ASN
1	A	1067	LEU
1	A	1096	SER
1	A	1116	LEU

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Mol	Chain	Res	Type
1	A	1120	LEU
1	A	1122	PRO
1	A	1124	HIS
1	A	1135	ARG
1	A	1146	VAL
1	A	1170	ILE
1	A	1171	GLN
1	A	1193	LEU
1	A	1217	LYS
1	A	1222	ASN
1	A	1257	ASP
1	A	1265	ASN
1	A	1276	VAL
1	A	1280	GLU
1	A	1288	ASP
1	A	1291	VAL
1	A	1295	THR
1	A	1297	GLU
1	A	1308	THR
1	A	1315	GLU
1	A	1325	THR
1	A	1333	ILE
1	A	1349	TYR
1	A	1353	TYR
1	A	1359	ASP
1	A	1368	MET
1	A	1370	LEU
1	A	1371	LEU
1	A	1393	ASN
1	A	1394	THR
1	A	1400	CYS
1	A	1420	ASP
1	A	1442	ASP
1	A	1445	ILE
2	B	21	GLU
2	B	25	ILE
2	B	37	PHE
2	B	46	GLN
2	B	57	TYR
2	B	91	SER
2	B	98	THR
2	B	128	LEU

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Mol	Chain	Res	Type
2	B	167	ILE
2	B	194	GLU
2	B	217	ARG
2	B	222	ILE
2	B	225	VAL
2	B	249	ARG
2	B	261	ARG
2	B	262	GLU
2	B	272	THR
2	B	297	ILE
2	B	298	LEU
2	B	303	TYR
2	B	323	VAL
2	B	348	ARG
2	B	360	PHE
2	B	361	LEU
2	B	364	ILE
2	B	371	GLU
2	B	376	PHE
2	B	378	LEU
2	B	393	LYS
2	B	394	ASP
2	B	401	PHE
2	B	416	LEU
2	B	425	THR
2	B	427	ASP
2	B	429	PHE
2	B	446	LEU
2	B	455	SER
2	B	465	ASN
2	B	466	TRP
2	B	473	MET
2	B	476	ARG
2	B	485	ARG
2	B	487	THR
2	B	493	SER
2	B	502	ILE
2	B	513	GLN
2	B	516	ASN
2	B	529	GLU
2	B	557	PHE
2	B	558	LEU

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Mol	Chain	Res	Type
2	B	568	ASP
2	B	570	VAL
2	B	576	ASP
2	B	582	VAL
2	B	597	MET
2	B	603	LEU
2	B	615	MET
2	B	635	ARG
2	B	636	PRO
2	B	682	SER
2	B	691	GLU
2	B	693	ILE
2	B	705	MET
2	B	730	ARG
2	B	737	THR
2	B	742	GLU
2	B	748	ILE
2	B	776	GLN
2	B	781	PHE
2	B	786	ASN
2	B	790	ASP
2	B	794	ASN
2	B	797	TYR
2	B	805	THR
2	B	830	TYR
2	B	835	GLN
2	B	839	MET
2	B	859	TYR
2	B	878	GLN
2	B	879	ARG
2	B	882	THR
2	B	883	LEU
2	B	884	ARG
2	B	889	THR
2	B	909	ASP
2	B	939	THR
2	B	944	THR
2	B	953	LEU
2	B	956	THR
2	B	959	ASP
2	B	966	VAL
2	B	987	LYS

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Mol	Chain	Res	Type
2	B	997	GLU
2	B	999	MET
2	B	1010	LEU
2	B	1031	LEU
2	B	1046	PRO
2	B	1047	PHE
2	B	1049	ASP
2	B	1060	ARG
2	B	1077	THR
2	B	1084	GLN
2	B	1087	PHE
2	B	1095	LEU
2	B	1097	HIS
2	B	1098	MET
2	B	1122	ARG
2	B	1124	ARG
2	B	1129	ARG
2	B	1147	LEU
2	B	1148	LYS
2	B	1150	ARG
2	B	1159	ARG
2	B	1160	VAL
2	B	1175	LEU
2	B	1176	ASN
2	B	1182	CYS
2	B	1183	LYS
2	B	1185	CYS
2	B	1202	LEU
2	B	1218	THR
2	B	1220	ARG
3	C	7	GLN
3	C	11	ARG
3	C	16	ASP
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	53	THR
3	C	55	THR
3	C	62	PHE
3	C	77	ILE
3	C	78	GLU
3	C	91	HIS

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Mol	Chain	Res	Type
3	C	99	LEU
3	C	104	PHE
3	C	108	GLU
3	C	115	SER
3	C	124	LEU
3	C	138	GLU
3	C	145	CYS
3	C	147	LEU
3	C	155	LEU
3	C	156	THR
3	C	166	GLU
3	C	193	TYR
3	C	209	TYR
3	C	238	ILE
3	C	262	LEU
3	C	266	ASP
4	D	11	ARG
4	D	14	ARG
4	D	16	LYS
4	D	17	LYS
4	D	20	GLU
4	D	22	GLU
4	D	23	ASN
4	D	29	LEU
4	D	38	ILE
4	D	41	GLN
4	D	47	LEU
4	D	70	PHE
4	D	118	THR
4	D	120	GLU
4	D	124	GLU
4	D	138	ASN
4	D	149	THR
4	D	187	THR
4	D	213	GLU
4	D	214	LEU
4	D	219	THR
4	D	221	TYR
5	E	5	ASN
5	E	8	ASN
5	E	29	PHE
5	E	31	THR

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Mol	Chain	Res	Type
5	E	41	ASP
5	E	65	THR
5	E	72	PHE
5	E	78	LEU
5	E	82	PHE
5	E	110	PHE
5	E	112	TYR
5	E	123	LEU
5	E	131	THR
5	E	132	ILE
5	E	134	THR
5	E	150	VAL
6	F	79	ARG
6	F	103	MET
6	F	112	GLU
6	F	119	ARG
7	G	1	MET
7	G	13	LEU
7	G	21	ARG
7	G	31	LEU
7	G	51	TYR
7	G	58	ARG
7	G	62	LEU
7	G	74	TYR
7	G	120	THR
7	G	126	ASN
7	G	128	PRO
7	G	133	SER
7	G	134	GLU
7	G	139	ILE
7	G	165	GLU
8	H	10	PHE
8	H	14	GLU
8	H	17	PRO
8	H	53	ASP
8	H	65	LEU
8	H	88	SER
8	H	89	LEU
8	H	91	ASP
8	H	94	ASP
8	H	102	TYR
8	H	128	ASN

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Mol	Chain	Res	Type
8	H	129	TYR
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
8	H	143	LEU
9	I	2	THR
9	I	4	PHE
9	I	6	PHE
9	I	8	ARG
9	I	9	ASP
9	I	12	ASN
9	I	31	THR
9	I	44	TYR
9	I	59	VAL
9	I	72	ASP
9	I	85	PHE
9	I	86	PHE
9	I	93	LYS
9	I	94	ASP
9	I	100	PHE
9	I	101	PHE
10	J	13	VAL
10	J	28	ASP
10	J	43	ARG
10	J	44	TYR
10	J	48	ARG
11	K	21	ILE
11	K	25	THR
11	K	47	ARG
11	K	50	LEU
11	K	81	TYR
11	K	103	THR
11	K	111	LEU
12	L	27	LEU
12	L	55	ILE
12	L	68	GLU
12	L	70	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN

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Mol	Chain	Res	Type
1	A	68	GLN
1	A	71	GLN
1	A	75	ASN
1	A	169	ASN
1	A	171	GLN
1	A	225	ASN
1	A	253	ASN
1	A	256	GLN
1	A	282	ASN
1	A	306	ASN
1	A	316	GLN
1	A	339	ASN
1	A	390	GLN
1	A	435	HIS
1	A	447	GLN
1	A	451	HIS
1	A	479	ASN
1	A	493	GLN
1	A	503	GLN
1	A	517	ASN
1	A	611	GLN
1	A	640	GLN
1	A	654	ASN
1	A	723	ASN
1	A	741	ASN
1	A	745	GLN
1	A	757	ASN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	903	ASN
1	A	926	GLN
1	A	935	GLN
1	A	965	GLN
1	A	994	GLN
1	A	1048	ASN
1	A	1078	GLN
1	A	1110	ASN
1	A	1140	HIS
1	A	1203	ASN
1	A	1211	GLN
1	A	1218	GLN

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Mol	Chain	Res	Type
1	A	1258	HIS
1	A	1265	ASN
1	A	1312	ASN
1	A	1393	ASN
1	A	1432	GLN
2	B	53	GLN
2	B	60	GLN
2	B	115	GLN
2	B	178	ASN
2	B	236	HIS
2	B	366	GLN
2	B	383	ASN
2	B	465	ASN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	657	HIS
2	B	667	GLN
2	B	794	ASN
2	B	842	ASN
2	B	862	GLN
2	B	887	HIS
2	B	957	ASN
2	B	1065	GLN
2	B	1076	HIS
2	B	1161	HIS
2	B	1179	GLN
2	B	1193	GLN
3	C	7	GLN
3	C	65	HIS
3	C	73	GLN
3	C	79	GLN
3	C	91	HIS
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	135	GLN
3	C	140	ASN
3	C	231	ASN
4	D	23	ASN
4	D	39	ASN
4	D	40	HIS

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Mol	Chain	Res	Type
4	D	41	GLN
4	D	138	ASN
5	E	54	GLN
5	E	61	GLN
5	E	101	GLN
5	E	104	ASN
5	E	147	HIS
7	G	14	HIS
7	G	53	ASN
7	G	113	HIS
7	G	122	ASN
7	G	126	ASN
7	G	131	GLN
8	H	128	ASN
8	H	131	ASN
9	I	12	ASN
9	I	46	HIS
9	I	108	HIS
10	J	53	HIS
11	K	65	HIS
11	K	89	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	10/18 (55%)	2 (20%)	1 (10%)

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	3	A
15	P	11	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
15	P	2	A

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
14	BRU	T	23	15,14	13,21,22	4.60	4 (30%)	16,30,33	3.98	2 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BRU	T	23	15,14	-	0/3/21/22	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	T	23	BRU	BR-C5	-15.07	1.50	1.90
14	T	23	BRU	C6-N1	2.52	1.38	1.35
14	T	23	BRU	C4-N3	3.21	1.39	1.33
14	T	23	BRU	C4-C5	5.32	1.45	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	T	23	BRU	C5-C4-N3	-7.91	115.55	124.00
14	T	23	BRU	C4-N3-C2	13.47	126.89	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	T	23	BRU	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 9 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, 95^{th} 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	1418/1733 (81%)	-0.11	16 (1%) 82 68	23, 70, 112, 141	0
2	B	1109/1224 (90%)	-0.09	15 (1%) 78 62	23, 81, 123, 141	0
3	C	266/347 (76%)	-0.14	1 (0%) 93 88	34, 69, 105, 119	0
4	D	179/221 (80%)	-0.02	1 (0%) 90 82	37, 79, 118, 131	0
5	E	214/215 (99%)	0.13	1 (0%) 91 85	41, 97, 129, 137	0
6	F	87/155 (56%)	-0.38	0 100 100	19, 46, 77, 86	0
7	G	171/171 (100%)	-0.06	1 (0%) 90 82	48, 64, 104, 113	0
8	H	136/146 (93%)	0.48	4 (2%) 55 37	80, 106, 127, 135	0
9	I	119/122 (97%)	0.31	7 (5%) 26 14	65, 100, 125, 143	0
10	J	65/70 (92%)	-0.34	0 100 100	49, 65, 92, 105	0
11	K	115/120 (95%)	-0.08	1 (0%) 85 74	34, 73, 93, 122	0
12	L	46/70 (65%)	0.22	0 100 100	48, 108, 125, 132	0
13	N	7/12 (58%)	1.66	1 (14%) 4 2	135, 140, 151, 157	0
14	T	18/26 (69%)	1.48	7 (38%) 0 1	117, 144, 155, 155	0
15	P	11/18 (61%)	1.70	3 (27%) 1 1	125, 133, 152, 156	0
All	All	3961/4650 (85%)	-0.04	58 (1%) 76 61	19, 76, 121, 157	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1455	PRO	3.9
15	P	1	C	3.9
14	T	28	DA	3.8
2	B	733	HIS	3.7
1	A	255	SER	3.6
1	A	253	ASN	3.4
1	A	155	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	256	GLN	3.2
1	A	1257	ASP	2.9
1	A	158	PRO	2.9
4	D	19	GLU	2.9
14	T	13	DT	2.9
2	B	919	SER	2.8
2	B	868	MET	2.8
9	I	76	PRO	2.8
1	A	154	SER	2.7
9	I	83	ASN	2.6
8	H	139	ASN	2.5
2	B	918	ILE	2.5
15	P	4	C	2.5
14	T	27	DC	2.5
5	E	126	SER	2.5
9	I	116	ASN	2.4
13	N	3	DT	2.4
1	A	1188	GLN	2.4
9	I	120	GLN	2.4
1	A	156	ASP	2.4
1	A	195	ASP	2.3
2	B	470	LYS	2.3
7	G	122	ASN	2.3
2	B	349	ILE	2.3
8	H	36	CYS	2.3
14	T	14	DA	2.3
14	T	11	DA	2.3
14	T	12	DG	2.3
1	A	159	THR	2.3
1	A	153	PRO	2.3
2	B	433	GLN	2.2
2	B	250	PHE	2.2
2	B	871	THR	2.2
15	P	11	G	2.2
1	A	161	LEU	2.2
14	T	15	DG	2.2
2	B	715	ALA	2.2
1	A	251	SER	2.2
9	I	80	SER	2.2
1	A	149	GLU	2.1
3	C	139	GLY	2.1
2	B	346	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
11	K	114	LEU	2.1
2	B	882	THR	2.1
2	B	249	ARG	2.1
9	I	105	SER	2.1
2	B	265	SER	2.1
8	H	133	ASN	2.1
9	I	77	LYS	2.0
8	H	86	ASP	2.0
2	B	883	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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(Å^2)	Q<0.9
14	BRU	T	23	20/21	0.67	0.36	-	136,142,145,146	0

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, 95^{th} 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(Å^2)	Q<0.9
17	MG	P	2458	1/1	0.84	0.32	0.18	180,180,180,180	0
16	ZN	J	1066	1/1	1.00	0.20	-0.36	53,53,53,53	0
16	ZN	B	2225	1/1	0.99	0.17	-0.71	30,30,30,30	0
16	ZN	C	1269	1/1	1.00	0.10	-1.57	40,40,40,40	0
16	ZN	A	2457	1/1	1.00	0.13	-1.69	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
16	ZN	L	1071	1/1	0.98	0.05	-1.92	100,100,100,100	0
16	ZN	I	1121	1/1	0.99	0.08	-2.33	76,76,76,76	0
16	ZN	I	1122	1/1	0.95	0.14	-2.63	135,135,135,135	0
16	ZN	A	2456	1/1	0.97	0.07	-4.04	88,88,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.