



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:00 PM GMT

PDB ID : 1I6H
Title : RNA POLYMERASE II ELONGATION COMPLEX
Authors : Gnatt, A.L.; Cramer, P.; Kornberg, R.D.
Deposited on : 2001-03-02
Resolution : 3.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

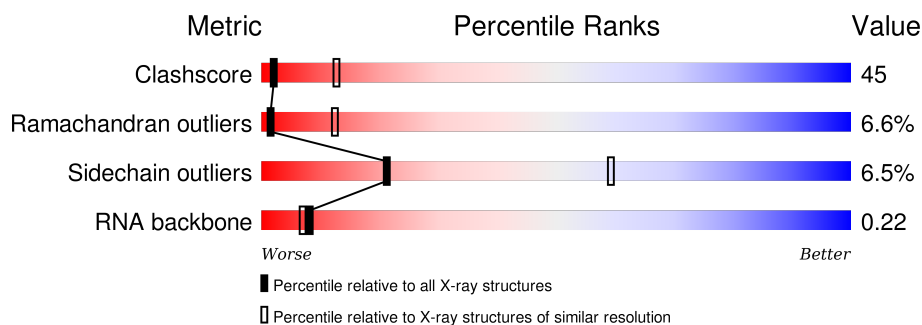
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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))
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RNA backbone	2183	1005 (3.82-2.78)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	13	
2	R	9	
3	A	1733	
4	B	1224	
5	C	318	
6	E	215	

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Mol	Chain	Length	Quality of chain
7	F	155	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 28430 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 DNA chain called 5'-D(P*AP*AP*AP*TP*GP*CP*CP*TP*GP*GP*TP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	13	Total	C	N	O	P	0	0	0
			267	127	47	80	13			

- Molecule 2 is a RNA chain called 5'-R(P*GP*AP*CP*CP*AP*GP*GP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	9	Total	C	N	O	P	0	0	0
			196	87	39	61	9			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	1381	Total	C	N	O	S	0	0	0
			10857	6851	1899	2046	61			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	1097	Total	C	N	O	S	0	0	0
			8721	5526	1523	1618	54			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

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

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

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 POLYMERASE II 8.3KD POLYPEPTIDE.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

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

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

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

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

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

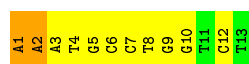
3 Residue-property plots

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

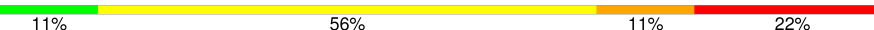
Note EDS was not executed.

- Molecule 1: 5'-D(P*AP*AP*AP*TP*GP*CP*CP*TP*GP*GP*TP*CP*T)-3'

Chain D: 



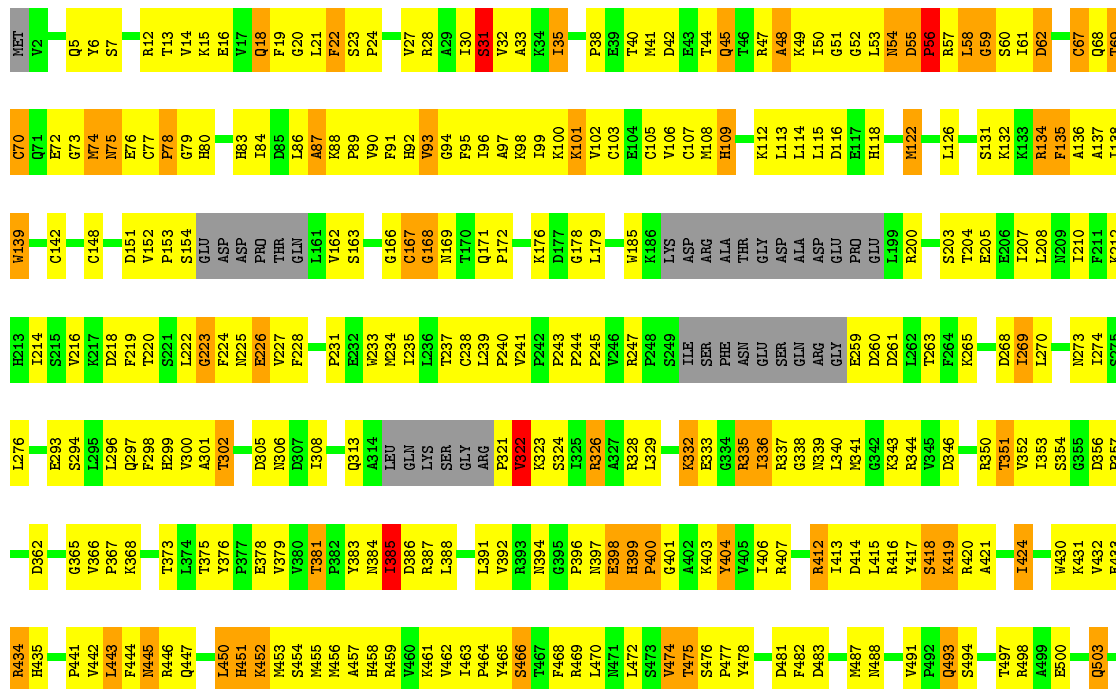
- Molecule 2: 5'-R(P*GP*AP*CP*CP*AP*GP*GP*CP*A)-3'

Chain R: 



- Molecule 3: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

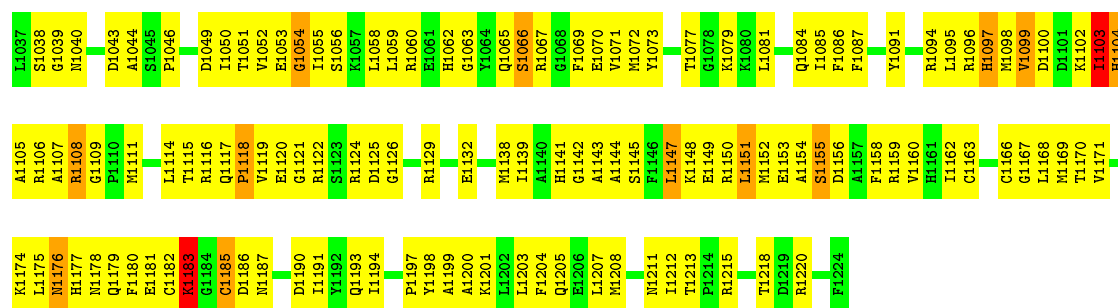
Chain A: 



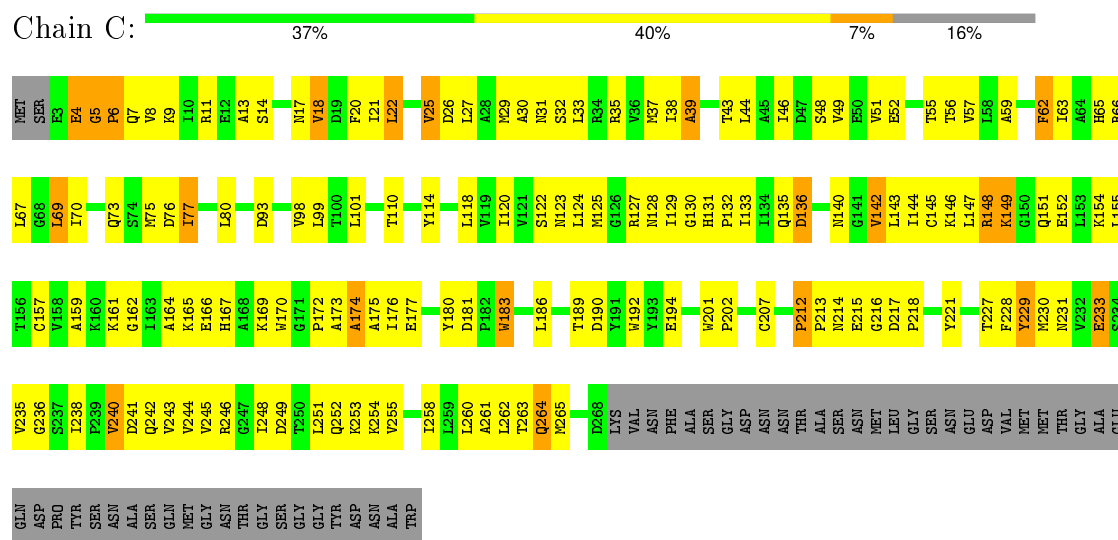


Chain B:

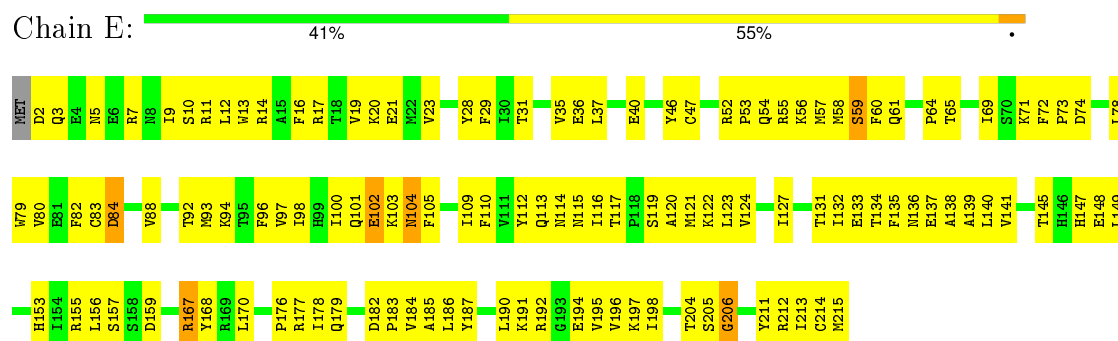




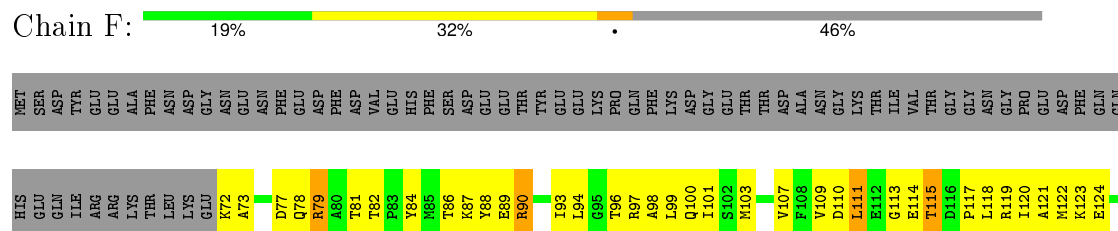
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE

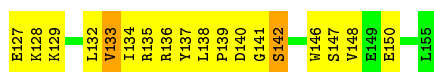


• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE





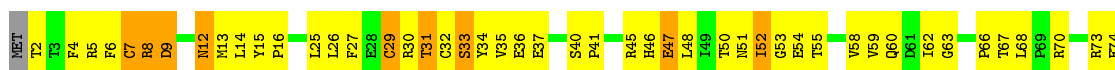
● Molecule 8: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

Chain H: 



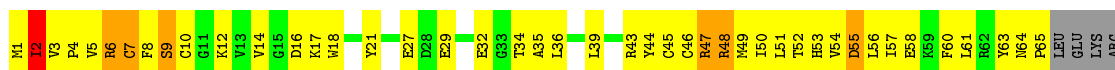
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

Chain I: 34% 51% 11% ..



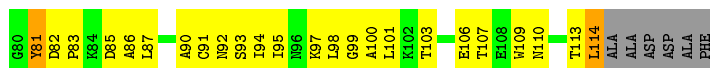
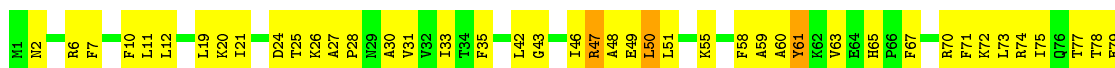
• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J:  30% 53% 9% • 7%

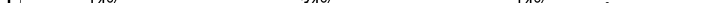


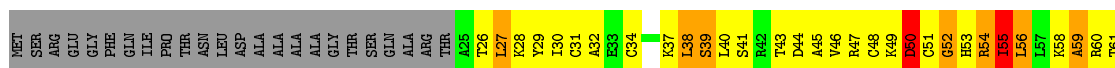
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

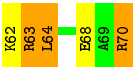
Chain K: 39% 52% • 5%



• Molecule 12: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE

Chain L:  14% 34% 14% 0 34%





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.30Å 220.70Å 191.30Å 90.00° 97.50° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.30)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28430	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	D	1.10	1/298 (0.3%)	1.03	0/456
2	R	1.70	4/219 (1.8%)	1.77	9/338 (2.7%)
3	A	0.41	0/11048	0.71	6/14936 (0.0%)
4	B	0.46	0/8891	0.71	2/11990 (0.0%)
5	C	0.48	0/2133	0.76	2/2891 (0.1%)
6	E	0.36	0/1788	0.65	0/2406
7	F	0.40	0/691	0.64	0/933
8	H	0.40	0/1086	0.73	0/1470
9	I	0.47	0/989	0.76	1/1331 (0.1%)
10	J	0.53	0/541	0.78	0/727
11	K	0.45	0/937	0.68	0/1265
12	L	0.48	0/366	0.78	0/485
All	All	0.47	5/28987 (0.0%)	0.73	20/39228 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	9	A	P-OP2	7.91	1.62	1.49
2	R	1	G	OP3-P	-7.91	1.51	1.61
1	D	1	DA	OP3-P	-6.84	1.52	1.61
2	R	9	A	P-OP1	6.39	1.59	1.49
2	R	9	A	C2'-O2'	5.17	1.48	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	9	A	N9-C1'-C2'	-14.41	95.27	114.00
2	R	3	C	O5'-P-OP2	12.38	125.55	110.70
3	A	1392	SER	N-CA-C	6.34	128.11	111.00
2	R	3	C	C5'-C4'-O4'	6.26	116.61	109.10
2	R	9	A	C1'-O4'-C4'	-6.17	104.97	109.90
5	C	39	ALA	N-CA-C	6.06	127.37	111.00
3	A	398	GLU	N-CA-C	-5.76	95.43	111.00
5	C	183	TRP	N-CA-C	-5.61	95.85	111.00
2	R	9	A	C5'-C4'-O4'	5.48	115.67	109.10
2	R	9	A	C5'-C4'-C3'	5.38	124.62	116.00
2	R	9	A	C2'-C3'-O3'	-5.27	97.91	109.50
4	B	647	GLY	N-CA-C	5.22	126.15	113.10
3	A	1403	GLU	N-CA-C	5.21	125.06	111.00
3	A	750	GLY	N-CA-C	-5.20	100.11	113.10
2	R	3	C	O4'-C4'-C3'	-5.16	98.84	104.00
9	I	75	CYS	N-CA-C	-5.15	97.10	111.00
3	A	452	LYS	N-CA-C	-5.08	97.29	111.00
2	R	9	A	C1'-C2'-O2'	-5.04	95.49	110.60
4	B	712	PRO	N-CA-C	-5.00	99.09	112.10
3	A	466	SER	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	2	DA	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	D	267	0	148	30	0
2	R	196	0	100	26	0
3	A	10857	0	10959	1050	0
4	B	8721	0	8746	897	0
5	C	2095	0	2052	167	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1752	0	1776	130	0
7	F	679	0	701	62	0
8	H	1068	0	1040	136	0
9	I	971	0	933	101	0
10	J	532	0	544	77	0
11	K	919	0	929	87	0
12	L	364	0	388	55	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	C	1	0	0	0	0
13	I	2	0	0	1	0
13	J	1	0	0	1	0
13	L	1	0	0	0	0
14	R	1	0	0	0	0
All	All	28430	0	28316	2555	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 45.

All (2555) 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)
3:A:567:LYS:HB2	3:A:568:PRO:HD2	1.18	1.17
12:L:60:ARG:HG3	12:L:61:THR:H	1.05	1.15
9:I:111:THR:HG22	9:I:113:ASP:H	1.05	1.13
4:B:345:LYS:HA	4:B:348:ARG:HE	1.11	1.13
3:A:1364:ASN:ND2	3:A:1366:ARG:HG2	1.65	1.11
6:E:124:VAL:HG13	6:E:132:ILE:HB	1.33	1.09
4:B:1051:THR:HG22	4:B:1053:GLU:H	1.00	1.09
1:D:1:DA:H1'	3:A:1386:ARG:HH12	1.02	1.09
3:A:855:THR:HG21	3:A:857:ARG:HE	1.12	1.09
3:A:93:VAL:HG13	3:A:301:ALA:HB1	1.33	1.08
3:A:704:ALA:HB2	3:A:710:LEU:HG	1.34	1.07
4:B:512:ARG:HH21	4:B:535:LEU:HD11	1.17	1.07
3:A:1329:THR:HG22	3:A:1331:SER:H	1.15	1.07
3:A:666:ILE:HD11	4:B:1030:LEU:HD13	1.27	1.05
4:B:287:ARG:HG2	4:B:292:ILE:HA	1.38	1.04
7:F:81:THR:HG21	7:F:136:ARG:HD3	1.38	1.04
4:B:570:VAL:HB	4:B:573:GLN:HB3	1.36	1.04
3:A:1161:THR:HG22	3:A:1163:ILE:H	1.18	1.04
4:B:708:GLU:HG3	4:B:709:ASP:H	1.17	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1159:ARG:HE	4:B:1193:GLN:NE2	1.56	1.03
3:A:902:LEU:HG	3:A:926:GLN:HG3	1.39	1.02
4:B:977:GLY:HA3	4:B:1099:VAL:HG21	1.41	1.02
5:C:80:LEU:HD22	5:C:129:ILE:HD11	1.41	1.02
4:B:120:ARG:HG2	4:B:955:THR:HG21	1.40	1.01
3:A:913:LEU:HD12	3:A:914:GLU:H	1.25	1.01
3:A:567:LYS:CB	3:A:568:PRO:HD2	1.91	1.01
3:A:567:LYS:HB3	8:H:96:VAL:H	1.26	1.01
4:B:1159:ARG:NE	4:B:1193:GLN:HE21	1.57	1.01
4:B:1002:THR:HG22	4:B:1006:ILE:H	1.22	1.01
5:C:57:VAL:HG11	10:J:60:PHE:HB3	1.44	0.99
12:L:32:ALA:HB3	12:L:55:ILE:HD12	1.39	0.98
4:B:1100:ASP:HA	4:B:1103:ILE:HD11	1.46	0.98
11:K:113:THR:O	11:K:114:LEU:HB2	1.60	0.97
3:A:244:PRO:HG2	3:A:245:PRO:HD3	1.46	0.97
1:D:1:DA:H1'	3:A:1386:ARG:NH1	1.80	0.96
4:B:842:ASN:ND2	4:B:845:SER:H	1.62	0.96
4:B:639:ILE:HD11	4:B:691:GLU:HG3	1.47	0.96
6:E:135:PHE:HB3	6:E:140:LEU:HD11	1.45	0.96
4:B:174:LEU:O	4:B:175:ARG:HB2	1.64	0.96
5:C:56:THR:HG22	5:C:57:VAL:H	1.28	0.95
9:I:75:CYS:HG	13:I:204:ZN:ZN	0.68	0.95
3:A:1116:LEU:HD12	3:A:1329:THR:OG1	1.67	0.95
5:C:167:HIS:CD2	5:C:169:LYS:H	1.83	0.95
4:B:955:THR:HG22	4:B:956:THR:H	1.31	0.95
4:B:1051:THR:HG22	4:B:1053:GLU:N	1.81	0.95
4:B:200:GLY:HA2	4:B:202:TYR:CE2	2.02	0.94
3:A:783:THR:HG22	3:A:784:LEU:HG	1.49	0.94
4:B:392:ARG:HH21	9:I:52:ILE:HD11	1.30	0.94
3:A:1281:ARG:HD2	3:A:1309:ASP:OD2	1.68	0.93
4:B:1159:ARG:HD3	4:B:1193:GLN:HG3	1.48	0.93
4:B:842:ASN:HD22	4:B:845:SER:H	1.17	0.93
4:B:737:THR:HG21	9:I:66:PRO:O	1.68	0.93
3:A:338:GLY:HA2	4:B:1129:ARG:HH22	1.33	0.93
4:B:824:ILE:HG12	10:J:48:ARG:HH12	1.32	0.92
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.47	0.92
3:A:1399:ARG:HB3	3:A:1408:ILE:HD13	1.50	0.92
12:L:60:ARG:HG3	12:L:61:THR:N	1.85	0.91
4:B:955:THR:HG22	4:B:956:THR:N	1.85	0.91
4:B:1002:THR:HG22	4:B:1006:ILE:N	1.84	0.91
3:A:1435:PRO:HA	3:A:1439:GLY:O	1.69	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:73:GLN:HE21	5:C:75:MET:H	1.14	0.91
9:I:111:THR:HG22	9:I:113:ASP:N	1.86	0.90
7:F:93:ILE:HD11	7:F:134:ILE:HD11	1.53	0.90
3:A:351:THR:HG23	4:B:1103:ILE:HA	1.53	0.90
5:C:22:LEU:HD22	5:C:25:VAL:HG21	1.53	0.90
6:E:5:ASN:HD21	6:E:52:ARG:HG2	1.34	0.90
3:A:15:LYS:HB3	4:B:1220:ARG:HG2	1.51	0.90
3:A:1194:ARG:NH2	3:A:1237:ILE:HD13	1.87	0.90
3:A:381:THR:HG22	3:A:383:TYR:H	1.35	0.90
4:B:956:THR:HA	4:B:961:LEU:O	1.71	0.89
3:A:590:ARG:NH1	3:A:590:ARG:HG3	1.86	0.89
3:A:868:TYR:HD2	3:A:1058:VAL:HG21	1.38	0.89
3:A:1105:LEU:HD22	3:A:1384:VAL:HG21	1.53	0.89
3:A:1410:PHE:CD2	4:B:1212:ILE:HD11	2.08	0.89
3:A:61:ILE:HG22	3:A:62:ASP:H	1.37	0.88
3:A:666:ILE:CD1	4:B:1030:LEU:HD13	2.04	0.88
5:C:57:VAL:HG11	10:J:60:PHE:CB	2.03	0.88
3:A:567:LYS:NZ	8:H:46:LEU:HB2	1.87	0.88
3:A:567:LYS:HB2	3:A:568:PRO:CD	2.01	0.88
4:B:955:THR:CG2	4:B:956:THR:H	1.87	0.88
4:B:800:GLN:HB3	10:J:52:THR:HG21	1.54	0.88
5:C:167:HIS:HD2	5:C:169:LYS:H	0.90	0.88
3:A:549:MET:SD	3:A:577:ILE:HD12	2.12	0.88
5:C:44:LEU:HB2	5:C:77:ILE:HD11	1.55	0.88
3:A:1192:LEU:HD11	3:A:1239:ARG:HB3	1.56	0.88
3:A:962:ARG:HA	3:A:965:GLN:HE21	1.37	0.88
4:B:512:ARG:HH21	4:B:535:LEU:CD1	1.88	0.87
3:A:667:GLY:HA2	3:A:670:ILE:HD12	1.56	0.87
4:B:345:LYS:CA	4:B:348:ARG:HE	1.87	0.87
3:A:605:MET:HE3	3:A:614:PHE:O	1.75	0.87
3:A:590:ARG:HH11	3:A:590:ARG:HG3	1.37	0.87
4:B:1077:THR:HG22	4:B:1079:LYS:H	1.35	0.87
4:B:1065:GLN:HE21	4:B:1067:ARG:N	1.72	0.87
4:B:1159:ARG:HE	4:B:1193:GLN:HE21	0.93	0.87
4:B:1072:MET:HE3	4:B:1085:ILE:HB	1.56	0.86
3:A:337:ARG:NH1	3:A:839:ARG:HH12	1.72	0.86
4:B:228:LYS:HD3	4:B:234:ILE:HD13	1.57	0.86
3:A:886:ILE:HD11	3:A:943:LEU:HB3	1.56	0.86
4:B:977:GLY:HA3	4:B:1099:VAL:CG2	2.04	0.86
4:B:130:VAL:HG21	4:B:167:ILE:HD12	1.56	0.86
3:A:269:ILE:HD11	3:A:300:VAL:HA	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:801:LYS:O	10:J:52:THR:HG23	1.76	0.86
3:A:1039:LYS:O	3:A:1043:ASP:HB2	1.76	0.86
1:D:1:DA:C1'	3:A:1386:ARG:HH12	1.87	0.85
11:K:10:PHE:CD1	11:K:11:LEU:HD13	2.11	0.85
4:B:912:ILE:O	4:B:938:SER:HB2	1.76	0.85
4:B:744:HIS:HD2	4:B:746:SER:H	1.23	0.85
3:A:417:TYR:O	3:A:418:SER:HB2	1.75	0.85
8:H:125:LEU:HG	8:H:130:ARG:NH1	1.92	0.85
3:A:1242:VAL:HG12	3:A:1243:VAL:H	1.40	0.85
3:A:1348:LEU:HD23	3:A:1372:VAL:HG13	1.59	0.84
6:E:177:ARG:HD3	6:E:215:MET:SD	2.18	0.84
3:A:535:THR:HG21	3:A:617:VAL:H	1.43	0.84
4:B:1106:ARG:NH1	4:B:1118:PRO:HB3	1.91	0.84
10:J:46:CYS:HG	13:J:101:ZN:ZN	0.90	0.84
3:A:709:THR:HG21	9:I:93:LYS:O	1.77	0.84
7:F:147:SER:OG	7:F:150:GLU:HG3	1.78	0.84
2:R:2:A:C2'	2:R:3:C:H5'	2.07	0.83
3:A:683:ILE:HD11	3:A:764:CYS:HB2	1.60	0.83
4:B:345:LYS:HA	4:B:348:ARG:NE	1.91	0.83
4:B:1106:ARG:HH21	4:B:1109:GLY:H	1.23	0.83
3:A:1390:ASN:ND2	3:A:1399:ARG:HA	1.93	0.83
3:A:1118:VAL:CG2	3:A:1306:LEU:HB2	2.08	0.83
11:K:12:LEU:H	11:K:12:LEU:HD12	1.42	0.83
4:B:763:GLN:HG2	4:B:765:PRO:HD2	1.61	0.83
4:B:108:VAL:HG12	4:B:109:THR:H	1.42	0.83
4:B:999:MET:HG3	4:B:1000:PRO:HD2	1.61	0.83
5:C:11:ARG:NH2	5:C:229:TYR:HD2	1.77	0.83
6:E:2:ASP:O	6:E:3:GLN:HG2	1.78	0.82
4:B:1002:THR:CG2	4:B:1006:ILE:H	1.91	0.82
3:A:1017:LEU:HB2	6:E:206:GLY:H	1.44	0.82
3:A:565:ILE:HG23	3:A:567:LYS:HG2	1.62	0.82
5:C:37:MET:HG2	5:C:243:VAL:HG12	1.62	0.81
10:J:3:VAL:HG21	10:J:18:TRP:HB2	1.61	0.81
4:B:1106:ARG:HE	4:B:1109:GLY:N	1.79	0.81
3:A:885:THR:HG23	3:A:893:PHE:HE1	1.43	0.81
8:H:93:TYR:HB3	8:H:144:ILE:O	1.80	0.81
3:A:406:ILE:HB	3:A:431:LYS:HB2	1.61	0.81
3:A:563:PRO:HG3	3:A:572:TRP:CZ2	2.15	0.81
9:I:50:THR:CG2	9:I:52:ILE:HG23	2.11	0.81
4:B:269:ILE:HD11	4:B:386:LEU:HD21	1.62	0.81
4:B:519:TRP:HZ2	4:B:705:MET:HE1	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:742:ASN:HA	3:A:745:GLN:HB2	1.63	0.81
4:B:244:LEU:O	4:B:249:ARG:HG2	1.81	0.81
3:A:337:ARG:NH1	3:A:839:ARG:NH1	2.29	0.81
4:B:637:LEU:HD12	4:B:693:ILE:HD12	1.60	0.81
8:H:5:LEU:HD11	8:H:135:LEU:HG	1.63	0.80
8:H:81:PRO:HB2	8:H:82:PRO:CD	2.11	0.80
4:B:800:GLN:HB3	10:J:52:THR:CG2	2.11	0.80
4:B:899:ILE:HD11	4:B:911:ILE:HA	1.63	0.80
4:B:121:ASN:HD22	4:B:121:ASN:N	1.79	0.80
3:A:93:VAL:CG1	3:A:301:ALA:HB1	2.11	0.80
4:B:1106:ARG:HH21	4:B:1109:GLY:N	1.78	0.80
3:A:208:LEU:HD22	3:A:212:LYS:HE3	1.62	0.80
4:B:834:ASN:HB3	4:B:840:ILE:HG13	1.63	0.80
3:A:472:LEU:O	3:A:475:THR:HB	1.81	0.80
4:B:293:PRO:HG2	4:B:296:GLU:CB	2.12	0.80
4:B:200:GLY:HA2	4:B:202:TYR:HE2	1.43	0.80
4:B:1100:ASP:HA	4:B:1103:ILE:CD1	2.12	0.80
5:C:148:ARG:NH1	10:J:64:ASN:HA	1.96	0.80
3:A:679:ILE:HG23	3:A:729:ALA:HB1	1.63	0.80
9:I:75:CYS:SG	9:I:78:CYS:SG	2.80	0.80
3:A:868:TYR:CE1	3:A:1064:VAL:HG11	2.17	0.80
10:J:64:ASN:HB3	10:J:65:PRO:HD3	1.63	0.80
4:B:1065:GLN:HE21	4:B:1067:ARG:H	1.28	0.80
3:A:313:GLN:HB2	3:A:322:VAL:HG23	1.64	0.80
10:J:3:VAL:HG21	10:J:18:TRP:CB	2.12	0.79
3:A:32:VAL:HG21	3:A:68:GLN:NE2	1.97	0.79
3:A:523:ILE:HD12	3:A:622:VAL:CG2	2.12	0.79
3:A:567:LYS:HZ1	8:H:46:LEU:HB2	1.46	0.79
4:B:313:MET:HE3	4:B:386:LEU:HD22	1.63	0.79
4:B:1106:ARG:NH2	4:B:1109:GLY:H	1.79	0.79
8:H:81:PRO:HB2	8:H:82:PRO:HD3	1.62	0.79
5:C:56:THR:HG22	5:C:57:VAL:N	1.97	0.79
4:B:842:ASN:ND2	4:B:845:SER:N	2.31	0.79
3:A:666:ILE:HD13	4:B:1030:LEU:HD22	1.65	0.79
4:B:487:THR:HG22	4:B:489:SER:H	1.48	0.79
3:A:913:LEU:HD12	3:A:914:GLU:N	1.99	0.78
4:B:102:VAL:CG2	4:B:112:LEU:HB2	2.13	0.78
3:A:40:THR:HG22	3:A:41:MET:HG3	1.64	0.78
3:A:353:ILE:HD13	3:A:487:MET:CE	2.14	0.78
3:A:783:THR:HG21	3:A:815:PHE:CZ	2.19	0.78
4:B:796:LEU:HB3	4:B:799:PRO:HG3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1438:THR:HB	4:B:1144:ALA:HB3	1.66	0.78
3:A:341:MET:HE1	3:A:1401:SER:HB2	1.66	0.78
8:H:40:LEU:HD23	8:H:42:ILE:HD11	1.66	0.78
1:D:1:DA:H2'	1:D:2:DA:C8	2.18	0.78
3:A:768:GLN:CG	3:A:816:HIS:HA	2.13	0.78
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.48	0.78
3:A:298:PHE:O	3:A:302:THR:HB	1.83	0.78
3:A:399:HIS:O	3:A:401:GLY:N	2.17	0.78
3:A:901:LEU:H	3:A:926:GLN:NE2	1.82	0.78
3:A:1118:VAL:HG22	3:A:1306:LEU:HB2	1.64	0.78
3:A:1281:ARG:O	3:A:1282:VAL:HG23	1.83	0.78
3:A:23:SER:HB3	3:A:233:TRP:CZ2	2.19	0.78
3:A:1299:VAL:HG12	3:A:1300:LYS:H	1.47	0.78
4:B:1100:ASP:OD1	4:B:1103:ILE:HD11	1.84	0.78
4:B:392:ARG:NH2	9:I:52:ILE:HD11	1.98	0.78
3:A:855:THR:HG21	3:A:857:ARG:NE	1.95	0.77
3:A:58:LEU:HD22	3:A:80:HIS:O	1.83	0.77
5:C:165:LYS:O	11:K:6:ARG:NH1	2.17	0.77
4:B:855:PHE:HZ	4:B:857:ARG:NH1	1.81	0.77
3:A:313:GLN:HB2	3:A:322:VAL:CG2	2.14	0.77
4:B:708:GLU:HG3	4:B:709:ASP:N	1.98	0.77
3:A:1094:VAL:HG13	3:A:1113:THR:HG21	1.66	0.77
2:R:3:C:H2'	2:R:4:C:C6	2.19	0.77
4:B:542:MET:HG3	4:B:747:MET:HE3	1.66	0.77
4:B:542:MET:HE3	4:B:747:MET:HG3	1.64	0.77
3:A:1345:ARG:HD2	3:A:1373:ASP:OD1	1.84	0.77
4:B:496:ARG:NH1	4:B:539:LEU:HB2	1.99	0.77
3:A:70:CYS:O	3:A:72:GLU:HG2	1.84	0.77
4:B:519:TRP:CZ2	4:B:705:MET:HE1	2.19	0.77
3:A:549:MET:HE1	3:A:656:TRP:HD1	1.49	0.77
3:A:24:PRO:HB3	3:A:237:THR:HB	1.67	0.77
12:L:38:LEU:O	12:L:39:SER:HB3	1.85	0.77
4:B:211:VAL:HG21	4:B:483:LEU:HD13	1.68	0.77
4:B:102:VAL:HG23	4:B:112:LEU:HB2	1.65	0.76
11:K:47:ARG:HH11	11:K:47:ARG:HB3	1.49	0.76
10:J:10:CYS:SG	10:J:46:CYS:SG	2.83	0.76
4:B:232:SER:OG	4:B:234:ILE:HD12	1.84	0.76
4:B:707:PRO:HG2	4:B:708:GLU:H	1.49	0.76
5:C:166:GLU:HG3	11:K:10:PHE:HZ	1.51	0.76
11:K:55:LYS:HB3	11:K:81:TYR:HD1	1.50	0.76
4:B:996:ARG:NH2	5:C:174:ALA:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:336:ILE:HD12	3:A:1405:THR:HG21	1.68	0.76
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.68	0.76
3:A:896:ARG:HD3	3:A:897:TYR:CE1	2.21	0.76
4:B:882:THR:HG22	4:B:884:ARG:H	1.50	0.76
3:A:541:ILE:HG21	3:A:549:MET:HE3	1.67	0.76
5:C:124:LEU:O	5:C:127:ARG:HG2	1.85	0.76
10:J:12:LYS:O	10:J:14:VAL:HG23	1.85	0.76
1:D:3:DA:H5'	3:A:836:TYR:CE1	2.21	0.76
4:B:1106:ARG:HE	4:B:1109:GLY:H	1.29	0.76
3:A:265:LYS:NZ	3:A:323:LYS:H	1.84	0.76
3:A:1323:ASP:OD1	3:A:1325:THR:HB	1.86	0.76
3:A:31:SER:CB	3:A:83:HIS:HB2	2.15	0.76
4:B:1166:CYS:O	4:B:1168:LEU:N	2.18	0.76
4:B:1096:ARG:O	4:B:1097:HIS:HB2	1.85	0.76
3:A:223:GLY:O	3:A:1415:SER:HA	1.86	0.76
4:B:583:ASN:HD21	4:B:628:THR:HB	1.49	0.76
3:A:469:ARG:HH21	4:B:976:ILE:HD13	1.51	0.75
3:A:95:PHE:O	3:A:99:ILE:HG13	1.85	0.75
3:A:41:MET:HA	3:A:49:LYS:HA	1.68	0.75
5:C:57:VAL:CG1	10:J:60:PHE:HB3	2.15	0.75
4:B:899:ILE:CD1	4:B:911:ILE:HA	2.16	0.75
4:B:423:LYS:HA	4:B:426:LYS:HE2	1.68	0.75
4:B:842:ASN:HD22	4:B:845:SER:N	1.83	0.75
4:B:62:ILE:HG23	4:B:418:LYS:HG2	1.69	0.75
6:E:69:ILE:HG23	6:E:73:PRO:HA	1.67	0.75
3:A:353:ILE:HD13	3:A:487:MET:HE1	1.69	0.75
3:A:326:ARG:HG2	3:A:1406:VAL:HG21	1.67	0.75
4:B:770:GLN:HG2	4:B:983:ARG:O	1.86	0.75
2:R:8:C:O2'	2:R:9:A:H5'	1.87	0.75
4:B:118:ARG:HH22	4:B:194:GLU:CD	1.90	0.75
3:A:575:LYS:HB3	3:A:612:ILE:CG2	2.17	0.74
3:A:1146:VAL:HG11	3:A:1202:MET:SD	2.27	0.74
4:B:711:GLU:N	4:B:712:PRO:HD3	2.02	0.74
3:A:535:THR:CG2	3:A:616:VAL:HA	2.18	0.74
2:R:1:G:H2'	2:R:2:A:C8	2.22	0.74
11:K:65:HIS:HD2	11:K:67:PHE:H	1.35	0.74
4:B:651:LEU:HD11	4:B:707:PRO:HB3	1.69	0.74
7:F:111:LEU:N	7:F:111:LEU:HD12	2.02	0.74
3:A:321:PRO:O	3:A:322:VAL:HB	1.87	0.74
6:E:61:GLN:HE21	6:E:105:PHE:HE2	1.33	0.74
3:A:268:ASP:HB3	3:A:299:HIS:CE1	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1436:ILE:HG22	3:A:1437:GLY:H	1.52	0.74
3:A:1436:ILE:HG22	3:A:1437:GLY:N	2.03	0.74
3:A:1299:VAL:HG12	3:A:1300:LYS:N	2.02	0.74
4:B:570:VAL:HB	4:B:573:GLN:CB	2.17	0.74
4:B:1106:ARG:NE	4:B:1109:GLY:H	1.85	0.74
3:A:458:HIS:CE1	3:A:507:VAL:HG21	2.22	0.74
3:A:857:ARG:HD3	3:A:861:GLY:O	1.88	0.74
8:H:5:LEU:HB3	8:H:133:ASN:O	1.88	0.74
8:H:89:LEU:C	8:H:91:ASP:H	1.90	0.74
3:A:853:ASP:OD1	3:A:855:THR:HB	1.88	0.74
4:B:118:ARG:HG3	4:B:204:ILE:HD13	1.68	0.73
3:A:925:LEU:O	3:A:929:LEU:HD23	1.88	0.73
3:A:500:GLU:OE2	4:B:1145:SER:HB2	1.88	0.73
4:B:172:ILE:HD13	4:B:178:ASN:HB3	1.70	0.73
3:A:567:LYS:HB3	8:H:96:VAL:N	2.02	0.73
6:E:61:GLN:NE2	6:E:105:PHE:HE2	1.86	0.73
3:A:693:VAL:HG21	3:A:721:PHE:HE1	1.51	0.73
3:A:399:HIS:HB3	3:A:400:PRO:HD3	1.69	0.73
3:A:691:LEU:HD11	3:A:695:LYS:HE3	1.71	0.73
3:A:1436:ILE:CG2	4:B:1142:GLY:HA2	2.17	0.73
3:A:828:ALA:HB2	4:B:530:GLY:HA2	1.70	0.73
4:B:363:HIS:O	4:B:364:ILE:HB	1.88	0.73
3:A:1441:PHE:CZ	7:F:89:GLU:HA	2.23	0.73
3:A:443:LEU:HD21	3:A:455:MET:HB3	1.70	0.73
6:E:124:VAL:HA	6:E:132:ILE:HD12	1.70	0.73
3:A:445:ASN:CB	3:A:455:MET:HG2	2.19	0.73
3:A:75:ASN:O	3:A:76:GLU:HB3	1.88	0.73
11:K:65:HIS:CD2	11:K:67:PHE:H	2.06	0.73
4:B:745:PRO:O	4:B:748:ILE:HG12	1.88	0.73
4:B:58:THR:O	4:B:62:ILE:HG13	1.89	0.73
3:A:445:ASN:HB2	3:A:455:MET:HG2	1.70	0.73
3:A:154:SER:HB3	3:A:162:VAL:CG2	2.17	0.73
4:B:879:ARG:HB3	4:B:883:LEU:HD23	1.70	0.73
8:H:89:LEU:HB3	8:H:91:ASP:OD1	1.88	0.73
4:B:313:MET:CE	4:B:386:LEU:HD22	2.19	0.72
4:B:839:MET:HE3	4:B:1010:LEU:HD11	1.71	0.72
4:B:1007:VAL:HG22	4:B:1008:PRO:HD2	1.71	0.72
3:A:710:LEU:H	3:A:710:LEU:HD12	1.52	0.72
3:A:598:LEU:HD22	8:H:25:ARG:NH1	2.05	0.72
9:I:74:GLU:HB3	9:I:79:HIS:HA	1.70	0.72
4:B:521:LEU:HD22	4:B:633:VAL:HG12	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:234:ILE:H	4:B:234:ILE:HD12	1.54	0.72
3:A:417:TYR:O	3:A:418:SER:CB	2.36	0.72
4:B:980:PHE:CE2	4:B:1094:ARG:HG3	2.23	0.72
3:A:48:ALA:O	3:A:49:LYS:HG3	1.89	0.72
5:C:167:HIS:HD2	5:C:169:LYS:N	1.76	0.72
3:A:868:TYR:CD2	3:A:1058:VAL:HG21	2.23	0.72
3:A:567:LYS:HD3	8:H:95:TYR:CD1	2.25	0.72
3:A:337:ARG:NE	3:A:839:ARG:HH22	1.88	0.72
3:A:1258:HIS:ND1	3:A:1262:LYS:HE3	2.04	0.72
4:B:570:VAL:HG21	4:B:573:GLN:NE2	2.04	0.72
3:A:351:THR:HG21	4:B:1103:ILE:HG23	1.71	0.72
3:A:534:LEU:O	3:A:574:GLY:HA3	1.88	0.72
4:B:542:MET:HE1	4:B:743:ILE:HG21	1.69	0.72
4:B:193:LYS:HD3	4:B:787:VAL:HG11	1.70	0.72
8:H:35:GLN:HB3	8:H:111:LEU:HD21	1.70	0.72
3:A:32:VAL:HB	3:A:57:ARG:HD2	1.71	0.72
3:A:1397:LEU:O	3:A:1400:CYS:HB2	1.89	0.72
4:B:1066:SER:O	4:B:1067:ARG:HD3	1.90	0.72
3:A:901:LEU:HG	3:A:926:GLN:HE21	1.54	0.72
2:R:1:G:H2'	2:R:2:A:H8	1.54	0.72
8:H:123:MET:HE3	8:H:142:LEU:HD22	1.70	0.71
4:B:708:GLU:O	4:B:710:LEU:N	2.22	0.71
4:B:737:THR:HG23	9:I:66:PRO:CB	2.20	0.71
1:D:12:DC:N3	2:R:1:G:N2	2.32	0.71
3:A:899:VAL:HB	3:A:929:LEU:HD12	1.71	0.71
3:A:1399:ARG:HB2	3:A:1408:ILE:HG21	1.70	0.71
3:A:575:LYS:HB3	3:A:612:ILE:HG23	1.71	0.71
3:A:1152:ILE:HG23	3:A:1260:LEU:HD23	1.71	0.71
4:B:637:LEU:CD1	4:B:693:ILE:HD12	2.20	0.71
3:A:1332:PHE:H	3:A:1332:PHE:HD2	1.38	0.71
6:E:168:TYR:HB3	6:E:170:LEU:HD21	1.72	0.71
4:B:46:GLN:HG3	4:B:47:GLN:N	2.03	0.71
11:K:55:LYS:HD3	11:K:78:THR:CB	2.20	0.71
3:A:1209:MET:SD	3:A:1236:LEU:HB3	2.30	0.71
3:A:900:ASP:OD2	3:A:903:ASN:HB2	1.90	0.71
3:A:340:LEU:HD21	4:B:1200:ALA:HB2	1.72	0.71
3:A:675:THR:CB	3:A:736:ASN:HD21	2.04	0.71
4:B:555:ILE:HD13	4:B:587:HIS:CE1	2.26	0.71
7:F:81:THR:HG21	7:F:136:ARG:CD	2.20	0.71
11:K:55:LYS:HD3	11:K:78:THR:HB	1.72	0.71
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:47:ARG:HG2	12:L:52:GLY:HA2	1.72	0.70
4:B:309:GLN:HG3	9:I:52:ILE:HD13	1.72	0.70
3:A:451:HIS:NE2	3:A:1074:GLU:HG3	2.06	0.70
3:A:1015:VAL:HG12	3:A:1019:CYS:SG	2.31	0.70
4:B:108:VAL:HG12	4:B:109:THR:N	2.06	0.70
3:A:675:THR:HG21	3:A:736:ASN:ND2	2.06	0.70
3:A:672:ASP:HB2	3:A:736:ASN:OD1	1.90	0.70
4:B:1056:SER:HB3	4:B:1066:SER:HB2	1.74	0.70
4:B:792:MET:HA	4:B:856:PHE:O	1.91	0.70
3:A:503:GLN:HE21	7:F:90:ARG:NH2	1.88	0.70
3:A:567:LYS:HE3	8:H:46:LEU:HD12	1.71	0.70
3:A:383:TYR:HB3	7:F:115:THR:HG22	1.73	0.70
3:A:335:ARG:HA	3:A:339:ASN:HD22	1.57	0.70
3:A:343:LYS:HE3	4:B:1151:LEU:O	1.92	0.70
5:C:18:VAL:HG23	5:C:240:VAL:HG11	1.72	0.70
3:A:855:THR:HG23	3:A:857:ARG:HG3	1.72	0.70
4:B:955:THR:HG23	12:L:54:ARG:O	1.91	0.70
3:A:463:ILE:HB	3:A:464:PRO:HD2	1.74	0.70
4:B:638:PHE:CE1	4:B:743:ILE:HA	2.26	0.70
6:E:56:LYS:HG3	6:E:84:ASP:HB2	1.73	0.70
4:B:636:PRO:O	4:B:637:LEU:HG	1.90	0.70
3:A:225:ASN:O	3:A:227:VAL:N	2.21	0.70
8:H:49:VAL:HG12	8:H:50:ALA:N	2.07	0.70
3:A:1095:THR:HG22	3:A:1100:ARG:HB2	1.74	0.70
4:B:293:PRO:HG2	4:B:296:GLU:HB3	1.74	0.70
3:A:367:PRO:HB3	3:A:466:SER:HA	1.73	0.70
3:A:584:ASN:O	3:A:637:LYS:HE3	1.92	0.69
4:B:130:VAL:HG12	4:B:131:ASP:N	2.07	0.69
8:H:36:CYS:SG	8:H:130:ARG:NH2	2.65	0.69
6:E:83:CYS:SG	6:E:88:VAL:HG22	2.32	0.69
4:B:463:THR:CG2	4:B:465:ASN:HD22	2.05	0.69
4:B:314:LEU:O	4:B:317:CYS:HB2	1.92	0.69
1:D:4:DT:H2'	1:D:5:DG:C8	2.27	0.69
4:B:378:LEU:O	4:B:382:ILE:HG13	1.92	0.69
3:A:1208:THR:HB	3:A:1211:GLN:HG3	1.74	0.69
4:B:957:ASN:HD22	4:B:961:LEU:HD12	1.57	0.69
3:A:472:LEU:HD11	4:B:835:GLN:NE2	2.07	0.69
4:B:281:PRO:HG2	4:B:284:ILE:HD12	1.73	0.69
3:A:392:VAL:HG13	3:A:415:LEU:HD11	1.74	0.69
5:C:39:ALA:HA	5:C:164:ALA:HB3	1.75	0.69
3:A:786:HIS:HE1	4:B:742:GLU:OE1	1.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:954:VAL:O	12:L:55:ILE:O	2.11	0.69
3:A:414:ASP:OD1	3:A:416:ARG:HG2	1.93	0.69
3:A:340:LEU:HD13	3:A:1429:ILE:HG23	1.74	0.69
3:A:763:ALA:O	3:A:803:SER:HB3	1.92	0.69
3:A:858:ASN:HD22	3:A:858:ASN:C	1.96	0.69
3:A:391:LEU:HD22	3:A:400:PRO:O	1.93	0.68
4:B:280:ILE:CD1	4:B:334:ILE:HG12	2.23	0.68
3:A:567:LYS:HE3	8:H:46:LEU:CD1	2.22	0.68
4:B:22:SER:O	4:B:654:ARG:HD2	1.94	0.68
2:R:2:A:H2'	2:R:3:C:O4'	1.93	0.68
3:A:693:VAL:CG2	3:A:721:PHE:HE1	2.07	0.68
9:I:75:CYS:SG	9:I:103:CYS:SG	2.91	0.68
4:B:46:GLN:HG3	4:B:47:GLN:H	1.58	0.68
4:B:884:ARG:O	4:B:936:ASP:HB3	1.93	0.68
4:B:65:GLU:HG3	4:B:66:ASP:H	1.56	0.68
4:B:986:GLN:OE1	4:B:986:GLN:HA	1.92	0.68
5:C:51:VAL:HG22	5:C:155:LEU:HD22	1.76	0.68
12:L:46:VAL:HG13	12:L:56:LEU:HD12	1.76	0.68
3:A:768:GLN:HG2	3:A:816:HIS:HA	1.75	0.68
4:B:976:ILE:O	4:B:990:ILE:HB	1.94	0.68
8:H:7:ASP:O	8:H:8:ASP:HB2	1.92	0.68
3:A:72:GLU:OE2	4:B:1175:LEU:HD12	1.92	0.68
3:A:535:THR:HG21	3:A:617:VAL:N	2.08	0.68
4:B:542:MET:CE	4:B:747:MET:HG3	2.22	0.68
3:A:44:THR:O	3:A:45:GLN:HB2	1.91	0.68
3:A:563:PRO:HB2	3:A:565:ILE:O	1.94	0.68
3:A:599:SER:HB2	3:A:603:ASN:H	1.58	0.68
4:B:562:GLY:HA3	4:B:590:HIS:CE1	2.29	0.68
2:R:2:A:O2'	2:R:3:C:H5'	1.93	0.68
3:A:453:MET:HB3	3:A:477:PRO:HB3	1.76	0.68
9:I:55:THR:HG23	9:I:58:VAL:HG21	1.76	0.68
4:B:864:LYS:HB3	4:B:872:GLU:H	1.59	0.68
3:A:446:ARG:HH11	3:A:446:ARG:HG2	1.59	0.68
4:B:709:ASP:O	4:B:710:LEU:HD23	1.94	0.67
3:A:1390:ASN:HD22	3:A:1399:ARG:HA	1.57	0.67
5:C:166:GLU:HG3	11:K:10:PHE:CZ	2.29	0.67
5:C:93:ASP:O	5:C:127:ARG:NH2	2.27	0.67
4:B:54:PHE:HA	4:B:58:THR:HB	1.74	0.67
3:A:994:GLN:HE22	3:A:1023:ARG:HE	1.38	0.67
4:B:514:LEU:HD12	4:B:515:HIS:N	2.09	0.67
6:E:93:MET:HE2	6:E:120:ALA:HB1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:535:THR:HG21	3:A:616:VAL:HA	1.75	0.67
3:A:694:THR:O	3:A:698:GLN:HG3	1.94	0.67
9:I:53:GLY:O	9:I:89:GLN:HB2	1.94	0.67
5:C:56:THR:HG21	5:C:145:CYS:SG	2.35	0.67
12:L:60:ARG:CG	12:L:61:THR:H	1.94	0.67
4:B:842:ASN:ND2	4:B:844:SER:HB2	2.09	0.67
10:J:58:GLU:HA	10:J:61:LEU:HD12	1.76	0.67
3:A:450:LEU:HD13	3:A:1074:GLU:HG2	1.77	0.67
4:B:288:ALA:HB1	4:B:331:LEU:HD12	1.75	0.67
6:E:127:ILE:O	6:E:127:ILE:HG13	1.93	0.67
5:C:80:LEU:HD22	5:C:129:ILE:CD1	2.21	0.67
4:B:955:THR:CG2	4:B:956:THR:N	2.49	0.67
5:C:5:GLY:O	5:C:7:GLN:HG3	1.95	0.67
5:C:8:VAL:HG12	5:C:9:LYS:N	2.09	0.67
4:B:280:ILE:HG22	4:B:285:ILE:HG13	1.76	0.67
4:B:121:ASN:HA	4:B:207:GLY:HA3	1.77	0.67
4:B:1147:LEU:HD22	4:B:1151:LEU:HD22	1.77	0.67
3:A:76:GLU:OE2	4:B:1159:ARG:NH1	2.28	0.67
3:A:994:GLN:HE21	3:A:1019:CYS:HB3	1.59	0.67
3:A:16:GLU:HB3	3:A:1418:LEU:HD11	1.77	0.67
3:A:351:THR:CG2	4:B:1103:ILE:HG23	2.24	0.67
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.76	0.67
12:L:45:ALA:O	12:L:46:VAL:HG23	1.95	0.67
4:B:128:LEU:HB3	4:B:167:ILE:O	1.95	0.67
3:A:1348:LEU:HD21	3:A:1375:MET:SD	2.35	0.67
12:L:51:CYS:O	12:L:53:HIS:N	2.28	0.67
3:A:828:ALA:CB	4:B:530:GLY:HA2	2.25	0.67
7:F:109:VAL:HG12	7:F:110:ASP:N	2.10	0.67
3:A:1364:ASN:ND2	3:A:1365:TYR:N	2.43	0.66
4:B:957:ASN:O	4:B:959:ASP:N	2.28	0.66
4:B:882:THR:HG21	4:B:935:ARG:HA	1.75	0.66
4:B:566:LEU:HD13	4:B:588:GLY:HA2	1.77	0.66
8:H:115:TYR:CE2	8:H:124:ARG:HG3	2.30	0.66
5:C:98:VAL:C	5:C:99:LEU:HD23	2.16	0.66
4:B:363:HIS:O	4:B:364:ILE:CB	2.44	0.66
3:A:897:TYR:CD2	3:A:936:LEU:HD13	2.30	0.66
4:B:711:GLU:N	4:B:712:PRO:CD	2.57	0.66
4:B:986:GLN:HE22	4:B:1020:ARG:CZ	2.08	0.66
5:C:254:LYS:HB3	11:K:42:LEU:HD11	1.76	0.66
3:A:381:THR:HG22	3:A:383:TYR:N	2.09	0.66
3:A:306:ASN:HD21	3:A:324:SER:H	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:260:LEU:O	5:C:264:GLN:HG3	1.95	0.66
3:A:305:ASP:HB3	3:A:308:ILE:HD11	1.77	0.66
4:B:1002:THR:HG23	4:B:1004:GLU:N	2.10	0.66
3:A:590:ARG:HH11	3:A:590:ARG:CG	2.06	0.66
3:A:751:SER:O	3:A:752:LYS:HG2	1.96	0.66
3:A:525:GLN:CB	4:B:835:GLN:HG2	2.25	0.66
11:K:47:ARG:NH1	11:K:47:ARG:HB3	2.09	0.66
3:A:1267:MET:HA	3:A:1271:ILE:HD12	1.77	0.66
3:A:90:VAL:CG1	3:A:297:GLN:HA	2.26	0.66
3:A:1333:ILE:O	3:A:1336:MET:HB3	1.96	0.66
4:B:603:LEU:HB3	4:B:609:ILE:HG13	1.76	0.66
4:B:429:PHE:HA	4:B:432:MET:HE2	1.76	0.66
9:I:32:CYS:SG	9:I:33:SER:N	2.69	0.66
4:B:349:ILE:O	4:B:352:ALA:HB3	1.96	0.66
4:B:287:ARG:NH2	4:B:294:ASP:OD2	2.28	0.66
3:A:914:GLU:HB2	3:A:979:SER:O	1.95	0.66
2:R:1:G:O2'	2:R:2:A:H5'	1.95	0.66
2:R:3:C:H2'	2:R:4:C:H6	1.59	0.66
4:B:1039:GLY:HA2	10:J:51:LEU:HD21	1.77	0.66
4:B:1106:ARG:CZ	4:B:1109:GLY:H	2.07	0.66
3:A:1115:SER:HA	3:A:1308:THR:HG22	1.77	0.66
3:A:816:HIS:CE1	4:B:764:SER:HB2	2.31	0.66
3:A:590:ARG:HB3	3:A:605:MET:N	2.10	0.66
4:B:311:LEU:HB3	9:I:4:PHE:CZ	2.30	0.66
3:A:715:GLU:O	3:A:719:VAL:HG23	1.96	0.66
4:B:1162:ILE:HD11	4:B:1194:ILE:HD13	1.77	0.66
3:A:1111:MET:HE1	3:A:1114:PRO:HA	1.76	0.66
3:A:1042:PHE:CE2	3:A:1046:LEU:HD11	2.31	0.66
4:B:1001:PHE:CZ	4:B:1073:TYR:HB2	2.30	0.66
3:A:741:ASN:HD22	3:A:741:ASN:C	1.99	0.66
4:B:911:ILE:CG2	4:B:966:VAL:HG11	2.26	0.65
8:H:38:LEU:HD13	8:H:125:LEU:HD13	1.77	0.65
3:A:95:PHE:HE2	3:A:1414:ALA:HB2	1.62	0.65
3:A:1193:LEU:HB2	3:A:1260:LEU:HD11	1.78	0.65
4:B:751:VAL:O	4:B:754:SER:HB2	1.95	0.65
4:B:824:ILE:CG1	10:J:48:ARG:HH12	2.08	0.65
3:A:814:PHE:O	3:A:817:ALA:HB3	1.95	0.65
3:A:1342:GLU:OE2	6:E:212:ARG:NH1	2.28	0.65
5:C:8:VAL:HG12	5:C:9:LYS:H	1.60	0.65
3:A:1319:VAL:HG13	3:A:1320:PRO:HD2	1.79	0.65
8:H:95:TYR:CE2	8:H:97:MET:HG3	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:22:LEU:HD22	5:C:25:VAL:CG2	2.25	0.65
4:B:649:LYS:HE2	4:B:738:PHE:O	1.96	0.65
4:B:711:GLU:H	4:B:712:PRO:HD3	1.60	0.65
3:A:87:ALA:HB3	3:A:276:LEU:HD23	1.79	0.65
4:B:293:PRO:HG2	4:B:296:GLU:HB2	1.78	0.65
4:B:120:ARG:CG	4:B:955:THR:HG21	2.23	0.65
4:B:114:PRO:HG3	4:B:181:LEU:HD11	1.79	0.65
6:E:176:PRO:O	6:E:212:ARG:HA	1.95	0.65
4:B:211:VAL:HG23	4:B:483:LEU:HB2	1.78	0.65
8:H:24:CYS:HB2	8:H:44:VAL:CG2	2.27	0.65
3:A:1161:THR:HG22	3:A:1163:ILE:N	2.03	0.65
3:A:381:THR:CG2	3:A:383:TYR:H	2.09	0.65
4:B:1197:PRO:HG2	4:B:1200:ALA:HB2	1.79	0.65
4:B:805:THR:HG21	4:B:815:ARG:HE	1.62	0.65
3:A:381:THR:HG21	3:A:383:TYR:CD1	2.31	0.65
8:H:107:VAL:HG21	8:H:126:GLU:HG3	1.79	0.65
4:B:879:ARG:HB3	4:B:883:LEU:CD2	2.26	0.65
10:J:9:SER:OG	10:J:48:ARG:NH2	2.30	0.65
7:F:111:LEU:H	7:F:111:LEU:HD12	1.61	0.65
3:A:512:VAL:HA	3:A:519:PRO:HA	1.79	0.65
3:A:1394:THR:CG2	3:A:1395:GLY:N	2.60	0.65
3:A:1224:LEU:HD12	3:A:1241:ARG:O	1.97	0.65
9:I:111:THR:HG21	9:I:113:ASP:HB2	1.78	0.64
6:E:124:VAL:HG22	6:E:132:ILE:HG21	1.79	0.64
7:F:96:THR:O	7:F:100:GLN:HG3	1.97	0.64
4:B:1051:THR:CG2	4:B:1053:GLU:H	1.93	0.64
5:C:11:ARG:HH21	5:C:229:TYR:HD2	1.44	0.64
6:E:96:PHE:CZ	6:E:100:ILE:HD11	2.32	0.64
3:A:329:LEU:HD23	3:A:335:ARG:HG3	1.78	0.64
3:A:1035:TYR:O	3:A:1037:LEU:N	2.30	0.64
5:C:114:TYR:CD2	5:C:140:ASN:HB3	2.32	0.64
4:B:788:ARG:NH1	4:B:790:ASP:OD1	2.31	0.64
3:A:579:SER:OG	3:A:612:ILE:HG22	1.97	0.64
4:B:46:GLN:HE22	4:B:496:ARG:HA	1.62	0.64
4:B:446:LEU:O	4:B:447:ALA:HB3	1.97	0.64
4:B:1170:THR:O	4:B:1170:THR:HG22	1.97	0.64
3:A:901:LEU:HA	3:A:907:THR:HG23	1.80	0.64
3:A:994:GLN:HE22	3:A:1023:ARG:NE	1.95	0.64
4:B:577:ALA:HB1	4:B:589:VAL:CG1	2.27	0.64
3:A:523:ILE:HD12	3:A:622:VAL:HG21	1.80	0.64
3:A:629:LEU:HD13	3:A:645:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:604:ARG:HG2	4:B:604:ARG:O	1.98	0.64
4:B:25:ILE:HG22	4:B:29:ASP:HB2	1.79	0.64
3:A:1436:ILE:HB	4:B:1144:ALA:HB2	1.80	0.64
4:B:1034:VAL:HG23	4:B:1059:LEU:HB2	1.80	0.64
3:A:1242:VAL:HG12	3:A:1243:VAL:N	2.12	0.64
3:A:475:THR:HG22	3:A:476:SER:N	2.12	0.64
3:A:1402:PHE:CD2	3:A:1403:GLU:HG3	2.33	0.64
3:A:523:ILE:HD12	3:A:622:VAL:HG22	1.79	0.64
7:F:109:VAL:HG21	7:F:124:GLU:HA	1.79	0.64
4:B:1001:PHE:CE1	4:B:1073:TYR:HB2	2.33	0.64
5:C:241:ASP:HB3	11:K:109:TRP:CE2	2.32	0.64
4:B:1104:HIS:HB2	4:B:1122:ARG:HD2	1.80	0.63
4:B:515:HIS:HD2	4:B:517:THR:OG1	1.81	0.63
3:A:84:ILE:HG23	3:A:239:LEU:HB3	1.80	0.63
3:A:225:ASN:O	3:A:226:GLU:HG2	1.99	0.63
8:H:101:ALA:HB2	8:H:116:TYR:CE2	2.33	0.63
12:L:48:CYS:SG	12:L:49:LYS:N	2.70	0.63
4:B:914:LYS:HB3	4:B:937:ALA:O	1.98	0.63
7:F:86:THR:OG1	7:F:89:GLU:HG3	1.98	0.63
4:B:373:ARG:NE	4:B:567:GLU:OE2	2.29	0.63
3:A:1444:MET:HE1	7:F:135:ARG:NE	2.13	0.63
12:L:55:ILE:HG13	12:L:56:LEU:H	1.63	0.63
3:A:33:ALA:O	3:A:83:HIS:HB3	1.99	0.63
3:A:268:ASP:HB3	3:A:299:HIS:ND1	2.14	0.63
3:A:1074:GLU:HB3	3:A:1075:PRO:CD	2.29	0.63
3:A:328:ARG:O	3:A:335:ARG:HG2	1.99	0.63
3:A:354:SER:HA	3:A:482:PHE:CD2	2.34	0.63
8:H:12:VAL:HA	8:H:28:ALA:CB	2.28	0.63
3:A:418:SER:O	3:A:420:ARG:N	2.32	0.63
6:E:100:ILE:HG23	6:E:105:PHE:HB2	1.80	0.63
4:B:221:ASN:OD1	4:B:242:SER:HA	1.98	0.63
4:B:525:ALA:O	4:B:527:THR:HG22	1.98	0.63
8:H:31:THR:O	8:H:32:THR:CB	2.47	0.63
4:B:512:ARG:NH2	4:B:535:LEU:HD11	2.02	0.63
4:B:780:VAL:HG21	10:J:56:LEU:CD1	2.29	0.63
8:H:106:GLU:C	8:H:108:SER:H	2.02	0.63
4:B:1201:LYS:O	4:B:1205:GLN:HG3	1.97	0.63
12:L:40:LEU:HD13	12:L:44:ASP:CG	2.19	0.63
3:A:244:PRO:CG	3:A:245:PRO:HD3	2.27	0.63
3:A:1212:VAL:O	3:A:1216:ILE:HG13	1.99	0.63
3:A:1317:MET:HA	3:A:1322:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:173:ALA:O	5:C:174:ALA:HB3	2.00	0.62
4:B:496:ARG:HH11	4:B:539:LEU:HB2	1.62	0.62
7:F:111:LEU:H	7:F:111:LEU:CD1	2.12	0.62
6:E:156:LEU:HD12	6:E:195:VAL:HG12	1.81	0.62
6:E:178:ILE:HG23	6:E:214:CYS:HA	1.81	0.62
4:B:913:GLY:HA2	4:B:938:SER:HB3	1.81	0.62
4:B:1106:ARG:HD2	4:B:1126:GLY:O	1.99	0.62
6:E:78:LEU:C	6:E:78:LEU:HD23	2.20	0.62
3:A:689:LYS:O	3:A:693:VAL:HG23	2.00	0.62
3:A:1054:LEU:O	3:A:1057:VAL:HG23	1.99	0.62
3:A:821:ARG:HG3	3:A:825:ILE:HD11	1.81	0.62
4:B:1187:ASN:OD1	4:B:1190:ASP:HB3	1.99	0.62
3:A:1336:MET:HE1	3:A:1381:LEU:HG	1.82	0.62
3:A:590:ARG:HB3	3:A:605:MET:H	1.64	0.62
3:A:736:ASN:O	3:A:737:LEU:C	2.38	0.62
3:A:915:SER:O	3:A:919:ILE:HG13	2.00	0.62
3:A:871:ASP:HB3	6:E:204:THR:CG2	2.30	0.62
3:A:672:ASP:OD1	3:A:674:PRO:HD2	2.00	0.62
3:A:778:GLY:HA3	4:B:516:ASN:HB2	1.80	0.62
3:A:108:MET:O	3:A:109:HIS:HB2	1.99	0.62
4:B:1002:THR:HG23	4:B:1004:GLU:H	1.64	0.62
4:B:208:SER:OG	4:B:210:LYS:HD3	1.99	0.62
8:H:49:VAL:HG12	8:H:50:ALA:H	1.62	0.62
3:A:1021:LEU:O	3:A:1025:ARG:HG2	2.00	0.62
3:A:871:ASP:HB3	6:E:204:THR:HG22	1.82	0.62
7:F:109:VAL:HG23	7:F:124:GLU:HG2	1.82	0.62
4:B:195:CYS:HB3	4:B:782:LEU:HD22	1.81	0.62
5:C:46:ILE:HA	5:C:159:ALA:HA	1.82	0.62
3:A:871:ASP:OD2	6:E:204:THR:HG23	1.99	0.62
5:C:166:GLU:HA	11:K:6:ARG:HB3	1.82	0.62
3:A:709:THR:HB	3:A:712:GLU:H	1.64	0.62
7:F:97:ARG:O	7:F:101:ILE:HG13	1.99	0.62
3:A:148:CYS:O	3:A:168:GLY:HA2	1.99	0.62
3:A:88:LYS:HD2	3:A:293:GLU:CD	2.20	0.62
4:B:25:ILE:HG22	4:B:26:THR:H	1.65	0.61
4:B:842:ASN:HD21	4:B:844:SER:HB2	1.63	0.61
11:K:63:VAL:O	11:K:63:VAL:CG2	2.48	0.61
4:B:29:ASP:HB3	4:B:658:ILE:CD1	2.30	0.61
10:J:3:VAL:HG21	10:J:18:TRP:CG	2.34	0.61
4:B:114:PRO:HB3	4:B:174:LEU:HD11	1.82	0.61
9:I:8:ARG:HG3	9:I:9:ASP:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:49:VAL:HG21	5:C:67:LEU:HD12	1.83	0.61
5:C:123:ASN:HD22	5:C:125:MET:HG2	1.65	0.61
5:C:235:VAL:HG21	10:J:6:ARG:HH21	1.65	0.61
12:L:51:CYS:HB2	12:L:53:HIS:CD2	2.35	0.61
3:A:898:ARG:HB2	3:A:933:TYR:CE1	2.34	0.61
3:A:855:THR:CG2	3:A:857:ARG:HG3	2.30	0.61
9:I:7:CYS:HB2	9:I:29:CYS:HB2	1.81	0.61
4:B:616:ILE:N	4:B:616:ILE:HD12	2.15	0.61
4:B:39:ARG:HE	4:B:665:GLU:HG2	1.64	0.61
3:A:1437:GLY:HA3	7:F:88:TYR:CD2	2.36	0.61
4:B:549:THR:HB	4:B:628:THR:CG2	2.30	0.61
4:B:787:VAL:O	4:B:787:VAL:HG12	2.00	0.61
3:A:503:GLN:HE21	7:F:90:ARG:HH21	1.47	0.61
3:A:1111:MET:HE1	3:A:1330:ASN:OD1	1.99	0.61
6:E:96:PHE:O	6:E:100:ILE:HG13	1.99	0.61
8:H:15:VAL:HG22	8:H:26:ILE:HG12	1.83	0.61
3:A:961:ARG:O	3:A:965:GLN:HG3	2.00	0.61
4:B:839:MET:HE3	4:B:1010:LEU:CD1	2.30	0.61
6:E:93:MET:O	6:E:97:VAL:HG23	2.00	0.61
7:F:135:ARG:HG2	7:F:137:TYR:CE1	2.34	0.61
3:A:567:LYS:CG	3:A:568:PRO:HD2	2.31	0.61
3:A:506:ALA:HB1	3:A:508:PRO:HD2	1.83	0.61
4:B:299:GLU:OE1	4:B:571:PRO:HG2	2.01	0.61
3:A:1293:SER:OG	3:A:1294:PRO:HD2	2.01	0.61
7:F:138:LEU:HB3	7:F:139:PRO:HD2	1.83	0.61
3:A:73:GLY:O	3:A:75:ASN:N	2.32	0.61
1:D:6:DC:H4'	3:A:447:GLN:NE2	2.16	0.61
3:A:709:THR:OG1	3:A:712:GLU:HG3	2.00	0.61
12:L:34:CYS:SG	12:L:51:CYS:SG	2.98	0.61
12:L:26:THR:O	12:L:27:LEU:HB3	2.01	0.61
3:A:443:LEU:HD22	3:A:455:MET:HE2	1.83	0.61
3:A:789:LYS:HG3	9:I:67:THR:HB	1.83	0.61
3:A:1364:ASN:HD22	3:A:1364:ASN:C	2.04	0.60
4:B:1072:MET:CE	4:B:1085:ILE:HB	2.28	0.60
3:A:1208:THR:O	3:A:1212:VAL:HG23	2.01	0.60
4:B:446:LEU:O	4:B:447:ALA:CB	2.48	0.60
3:A:982:THR:HG22	3:A:984:LYS:H	1.64	0.60
3:A:1132:LYS:O	3:A:1135:ARG:HB3	2.01	0.60
3:A:338:GLY:HA2	4:B:1129:ARG:NH2	2.10	0.60
4:B:57:TYR:CD1	4:B:57:TYR:N	2.68	0.60
3:A:445:ASN:HB2	3:A:454:SER:O	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F:101:ILE:HD12	7:F:121:ALA:HB2	1.82	0.60
3:A:528:LEU:O	3:A:531:ILE:HG22	2.01	0.60
4:B:211:VAL:O	4:B:480:SER:HA	2.01	0.60
3:A:1115:SER:O	3:A:1329:THR:HG23	2.02	0.60
4:B:913:GLY:HA2	4:B:938:SER:CB	2.32	0.60
3:A:824:LEU:O	3:A:827:THR:HB	2.00	0.60
11:K:90:ALA:O	11:K:94:ILE:HG13	2.01	0.60
4:B:582:VAL:HG22	4:B:626:ILE:HB	1.82	0.60
3:A:567:LYS:O	3:A:569:LYS:N	2.35	0.60
3:A:1402:PHE:CE2	3:A:1403:GLU:HG3	2.37	0.60
1:D:2:DA:H2'	1:D:3:DA:C8	2.37	0.60
3:A:337:ARG:CZ	3:A:839:ARG:NH1	2.64	0.60
3:A:86:LEU:HA	3:A:273:ASN:OD1	2.02	0.60
4:B:90:ILE:HD12	4:B:432:MET:SD	2.42	0.60
6:E:47:CYS:HA	6:E:53:PRO:HA	1.83	0.60
3:A:322:VAL:O	3:A:323:LYS:HG3	2.01	0.60
2:R:8:C:H2'	2:R:9:A:O4'	2.02	0.60
4:B:1039:GLY:HA2	10:J:51:LEU:CD2	2.31	0.60
3:A:231:PRO:HA	3:A:234:MET:HE2	1.83	0.60
9:I:85:PHE:CD1	9:I:99:LEU:HD22	2.37	0.60
3:A:306:ASN:OD1	3:A:324:SER:HB3	2.01	0.60
3:A:896:ARG:NH2	3:A:1030:ARG:HH21	2.00	0.60
4:B:686:ASN:C	4:B:688:GLY:H	2.04	0.60
4:B:185:THR:HG23	4:B:188:ASP:OD2	2.01	0.60
3:A:1192:LEU:HD22	3:A:1239:ARG:NH2	2.16	0.60
8:H:89:LEU:C	8:H:91:ASP:N	2.55	0.60
4:B:1117:GLN:HG3	4:B:1156:ASP:OD1	2.02	0.60
3:A:76:GLU:O	3:A:76:GLU:HG3	2.02	0.60
4:B:463:THR:HG22	4:B:465:ASN:HD22	1.66	0.60
3:A:756:ILE:HG22	3:A:757:ASN:N	2.17	0.60
9:I:15:TYR:O	9:I:27:PHE:HA	2.02	0.60
10:J:1:MET:N	10:J:56:LEU:HB2	2.17	0.59
4:B:778:MET:CE	4:B:1094:ARG:HD3	2.32	0.59
4:B:1169:MET:HE1	4:B:1201:LYS:O	2.01	0.59
3:A:1394:THR:HG22	3:A:1395:GLY:N	2.17	0.59
4:B:217:ARG:NH1	4:B:407:ASP:OD1	2.35	0.59
12:L:70:ARG:HG2	12:L:70:ARG:HH11	1.66	0.59
3:A:68:GLN:HE22	3:A:80:HIS:HB3	1.67	0.59
4:B:803:LEU:H	4:B:822:ASN:HD21	1.48	0.59
5:C:244:VAL:O	5:C:248:ILE:HG13	2.03	0.59
3:A:704:ALA:HB2	3:A:710:LEU:CG	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:901:LEU:N	3:A:926:GLN:NE2	2.50	0.59
4:B:1102:LYS:O	4:B:1104:HIS:N	2.32	0.59
3:A:549:MET:SD	3:A:577:ILE:CD1	2.87	0.59
4:B:912:ILE:HD11	4:B:966:VAL:HG23	1.84	0.59
4:B:121:ASN:ND2	4:B:121:ASN:N	2.50	0.59
3:A:151:ASP:HA	3:A:162:VAL:O	2.02	0.59
3:A:44:THR:HG22	3:A:44:THR:O	2.02	0.59
3:A:107:CYS:HB2	3:A:114:LEU:CD2	2.33	0.59
4:B:1159:ARG:CD	4:B:1193:GLN:HE21	2.15	0.59
2:R:8:C:HO2'	2:R:9:A:H5'	1.67	0.59
4:B:666:TYR:C	4:B:668:ASP:H	2.06	0.59
4:B:1174:LYS:HB2	4:B:1179:GLN:O	2.02	0.59
4:B:1171:VAL:CG1	4:B:1191:ILE:HD13	2.32	0.59
9:I:5:ARG:HD3	9:I:36:GLU:OE2	2.01	0.59
4:B:708:GLU:CG	4:B:709:ASP:H	1.97	0.59
3:A:1018:PHE:O	3:A:1021:LEU:HB3	2.03	0.59
5:C:166:GLU:CG	11:K:10:PHE:HZ	2.14	0.59
4:B:975:GLN:HG2	4:B:976:ILE:H	1.67	0.59
3:A:1158:PRO:HB3	3:A:1241:ARG:NH1	2.17	0.59
10:J:64:ASN:HB3	10:J:65:PRO:CD	2.29	0.59
5:C:18:VAL:HG23	5:C:240:VAL:CG1	2.33	0.59
3:A:1042:PHE:HE2	3:A:1046:LEU:HD11	1.66	0.59
6:E:29:PHE:HB2	6:E:65:THR:HG22	1.83	0.59
6:E:5:ASN:ND2	6:E:52:ARG:HG2	2.12	0.59
3:A:1223:ASP:HA	3:A:1243:VAL:CG1	2.32	0.59
4:B:860:MET:HG2	4:B:861:ASP:N	2.18	0.59
3:A:239:LEU:HD12	3:A:240:PRO:HD2	1.84	0.59
4:B:198:ASP:OD1	4:B:485:ARG:NH2	2.33	0.59
4:B:995:ARG:NH1	4:B:995:ARG:HB2	2.16	0.59
4:B:512:ARG:NH2	4:B:535:LEU:CD1	2.62	0.59
4:B:642:ASP:O	4:B:644:GLU:N	2.36	0.59
3:A:225:ASN:ND2	3:A:227:VAL:HB	2.18	0.59
3:A:779:PHE:CZ	4:B:517:THR:HA	2.37	0.59
8:H:139:ASN:O	8:H:140:ALA:HB2	2.02	0.59
4:B:405:ARG:NH1	4:B:632:ARG:HG2	2.17	0.59
5:C:148:ARG:HG3	10:J:61:LEU:O	2.03	0.59
4:B:779:GLY:HA2	4:B:796:LEU:HB2	1.85	0.59
4:B:479:VAL:HG12	4:B:480:SER:N	2.17	0.59
3:A:31:SER:OG	3:A:83:HIS:HB2	2.02	0.59
6:E:78:LEU:HD23	6:E:79:TRP:N	2.16	0.59
3:A:90:VAL:HG11	3:A:297:GLN:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:49:GLU:HG3	11:K:94:ILE:CG1	2.33	0.59
11:K:49:GLU:HG3	11:K:94:ILE:HG12	1.83	0.59
8:H:109:LYS:NZ	8:H:109:LYS:HB2	2.18	0.59
3:A:840:ARG:HB3	3:A:1384:VAL:HG12	1.85	0.59
6:E:61:GLN:HB2	6:E:79:TRP:CE3	2.38	0.59
8:H:84:ALA:HA	8:H:87:ARG:CG	2.32	0.59
9:I:111:THR:CG2	9:I:113:ASP:HB2	2.33	0.58
4:B:642:ASP:HB3	4:B:649:LYS:HD2	1.85	0.58
3:A:596:THR:O	3:A:598:LEU:N	2.36	0.58
4:B:744:HIS:CD2	4:B:746:SER:H	2.14	0.58
3:A:511:ILE:HA	3:A:521:MET:HE3	1.84	0.58
3:A:1295:THR:HG23	3:A:1297:GLU:OE1	2.03	0.58
4:B:519:TRP:C	4:B:519:TRP:CD1	2.76	0.58
3:A:68:GLN:HE22	3:A:80:HIS:CB	2.15	0.58
3:A:469:ARG:NH2	4:B:976:ILE:HD13	2.18	0.58
4:B:46:GLN:O	4:B:408:LEU:HD23	2.03	0.58
7:F:127:GLU:O	7:F:129:LYS:HG3	2.03	0.58
3:A:1004:ASN:ND2	6:E:167:ARG:HD2	2.18	0.58
4:B:589:VAL:HG12	4:B:590:HIS:N	2.18	0.58
3:A:1336:MET:CE	3:A:1381:LEU:HG	2.33	0.58
4:B:806:THR:HB	4:B:809:MET:HG3	1.85	0.58
6:E:156:LEU:HD12	6:E:195:VAL:CG1	2.33	0.58
4:B:653:VAL:HG22	4:B:689:LEU:HB3	1.85	0.58
3:A:418:SER:O	3:A:419:LYS:C	2.39	0.58
3:A:443:LEU:HD13	3:A:455:MET:HE1	1.86	0.58
3:A:97:ALA:HA	3:A:100:LYS:HE3	1.84	0.58
3:A:567:LYS:CB	3:A:568:PRO:CD	2.67	0.58
3:A:93:VAL:HG11	3:A:308:ILE:CD1	2.33	0.58
3:A:1308:THR:HG21	3:A:1310:GLY:O	2.04	0.58
3:A:896:ARG:HD3	3:A:897:TYR:HE1	1.67	0.58
6:E:157:SER:C	6:E:159:ASP:H	2.07	0.58
3:A:57:ARG:O	3:A:68:GLN:HG3	2.03	0.58
9:I:47:GLU:OE1	9:I:50:THR:HG23	2.04	0.58
4:B:803:LEU:N	4:B:822:ASN:HD21	2.02	0.58
3:A:524:VAL:HG12	3:A:525:GLN:H	1.69	0.58
7:F:111:LEU:N	7:F:111:LEU:CD1	2.67	0.58
3:A:1332:PHE:N	3:A:1332:PHE:CD2	2.72	0.58
4:B:1201:LYS:HE2	4:B:1205:GLN:NE2	2.18	0.58
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.85	0.58
3:A:1385:THR:HG22	3:A:1386:ARG:H	1.68	0.58
4:B:23:ALA:HB1	4:B:24:PRO:HD2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:23:ALA:O	4:B:654:ARG:HB3	2.04	0.58
4:B:855:PHE:HZ	4:B:857:ARG:HH11	1.52	0.58
3:A:444:PHE:HB3	3:A:458:HIS:HD2	1.68	0.58
3:A:219:PHE:O	3:A:222:LEU:N	2.33	0.58
4:B:101:MET:HB2	4:B:169:ARG:HH12	1.69	0.58
3:A:567:LYS:HZ3	8:H:95:TYR:HE1	1.50	0.58
3:A:1364:ASN:ND2	3:A:1364:ASN:C	2.56	0.58
4:B:25:ILE:HG22	4:B:29:ASP:CB	2.34	0.58
3:A:1149:ALA:HB2	9:I:47:GLU:HA	1.84	0.58
3:A:260:ASP:OD1	3:A:261:ASP:N	2.37	0.58
3:A:1325:THR:O	6:E:148:GLU:HB2	2.04	0.58
3:A:28:ARG:HG2	3:A:83:HIS:CE1	2.39	0.58
6:E:61:GLN:HB2	6:E:79:TRP:HE3	1.69	0.58
3:A:1074:GLU:O	3:A:1076:ALA:N	2.37	0.58
3:A:166:GLY:O	3:A:167:CYS:HB3	2.03	0.58
3:A:101:LYS:O	3:A:105:CYS:HB2	2.04	0.58
4:B:701:ILE:HD11	4:B:703:ILE:HD11	1.86	0.58
7:F:81:THR:HG22	7:F:82:THR:N	2.18	0.58
10:J:48:ARG:HE	10:J:49:MET:CE	2.16	0.58
3:A:1281:ARG:HB2	3:A:1309:ASP:HB2	1.86	0.58
3:A:385:ILE:HG22	3:A:386:ASP:N	2.18	0.58
4:B:1077:THR:CG2	4:B:1079:LYS:HB2	2.34	0.58
3:A:1400:CYS:SG	3:A:1409:LEU:HG	2.44	0.58
3:A:1143:LEU:HD23	3:A:1267:MET:HB3	1.86	0.58
3:A:1155:ASP:OD2	3:A:1161:THR:HG23	2.04	0.57
3:A:41:MET:HB3	3:A:48:ALA:O	2.04	0.57
4:B:130:VAL:HG12	4:B:131:ASP:H	1.68	0.57
3:A:742:ASN:CA	3:A:745:GLN:HB2	2.33	0.57
4:B:980:PHE:CE1	4:B:990:ILE:HD11	2.39	0.57
11:K:47:ARG:HD3	11:K:59:ALA:O	2.03	0.57
11:K:65:HIS:CD2	11:K:67:PHE:HB2	2.39	0.57
12:L:49:LYS:O	12:L:50:ASP:HB2	2.03	0.57
3:A:482:PHE:CD1	4:B:836:GLU:HB2	2.38	0.57
5:C:175:ALA:HB3	10:J:43:ARG:NH2	2.19	0.57
8:H:12:VAL:HA	8:H:28:ALA:HB2	1.85	0.57
3:A:40:THR:HG21	3:A:259:GLU:OE2	2.04	0.57
4:B:1077:THR:HG22	4:B:1079:LYS:N	2.13	0.57
6:E:213:ILE:O	6:E:213:ILE:HG23	2.04	0.57
3:A:93:VAL:HG22	3:A:301:ALA:HA	1.86	0.57
3:A:337:ARG:CD	3:A:839:ARG:HH22	2.17	0.57
3:A:414:ASP:O	3:A:417:TYR:O	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:24:CYS:HB2	8:H:44:VAL:HG21	1.84	0.57
4:B:205:ILE:N	4:B:205:ILE:HD12	2.19	0.57
9:I:16:PRO:HB3	9:I:27:PHE:CE2	2.38	0.57
4:B:287:ARG:NH1	4:B:324:ILE:O	2.37	0.57
3:A:886:ILE:CD1	3:A:943:LEU:HB3	2.31	0.57
8:H:81:PRO:CB	8:H:82:PRO:CD	2.81	0.57
5:C:251:LEU:O	5:C:255:VAL:HG23	2.04	0.57
3:A:901:LEU:H	3:A:926:GLN:HE21	1.50	0.57
3:A:879:GLU:OE2	3:A:962:ARG:NH2	2.37	0.57
4:B:1079:LYS:HA	5:C:27:LEU:HD21	1.87	0.57
7:F:87:LYS:HE2	7:F:88:TYR:CZ	2.39	0.57
3:A:98:LYS:O	3:A:102:VAL:HG23	2.05	0.57
3:A:225:ASN:HD22	3:A:227:VAL:HB	1.68	0.57
4:B:756:ILE:O	4:B:759:PRO:HD3	2.04	0.57
3:A:663:SER:OG	3:A:664:THR:N	2.34	0.57
3:A:1315:GLU:O	3:A:1318:THR:HG23	2.04	0.57
8:H:97:MET:CE	8:H:142:LEU:HD23	2.35	0.57
3:A:577:ILE:O	3:A:580:VAL:HG23	2.04	0.57
3:A:353:ILE:HD13	3:A:487:MET:HE3	1.87	0.57
6:E:46:TYR:HA	6:E:57:MET:SD	2.43	0.57
5:C:56:THR:CG2	5:C:57:VAL:H	2.09	0.57
4:B:130:VAL:CG2	4:B:167:ILE:HD12	2.34	0.57
5:C:37:MET:HG2	5:C:243:VAL:CG1	2.34	0.57
3:A:353:ILE:HG22	3:A:468:PHE:HB2	1.85	0.57
3:A:1300:LYS:NZ	3:A:1300:LYS:HB3	2.20	0.57
11:K:51:LEU:HD13	11:K:59:ALA:HB3	1.86	0.57
11:K:55:LYS:HB3	11:K:81:TYR:CD1	2.36	0.57
4:B:983:ARG:HD2	4:B:1091:TYR:HB3	1.86	0.57
7:F:111:LEU:C	7:F:113:GLY:H	2.07	0.57
8:H:24:CYS:SG	8:H:44:VAL:HG21	2.45	0.57
3:A:619:LYS:O	3:A:623:GLY:N	2.38	0.57
11:K:50:LEU:CD1	11:K:73:LEU:HD21	2.35	0.57
3:A:567:LYS:NZ	8:H:95:TYR:CE1	2.71	0.57
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.69	0.57
8:H:89:LEU:HD22	8:H:91:ASP:CG	2.25	0.57
4:B:1051:THR:HG22	4:B:1052:VAL:N	2.17	0.57
3:A:1342:GLU:HG3	6:E:198:ILE:HG21	1.86	0.57
4:B:1106:ARG:HH12	4:B:1118:PRO:HB3	1.67	0.57
3:A:401:GLY:C	3:A:435:HIS:CD2	2.79	0.57
4:B:211:VAL:CG2	4:B:483:LEU:HD13	2.32	0.57
3:A:69:THR:HB	4:B:1174:LYS:HE2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:973:ILE:HG23	4:B:974:PRO:HD2	1.87	0.57
3:A:565:ILE:CG2	3:A:567:LYS:HG2	2.31	0.57
4:B:704:ALA:HB1	4:B:710:LEU:HD12	1.87	0.57
3:A:399:HIS:O	3:A:435:HIS:HD2	1.87	0.57
4:B:1147:LEU:HD22	4:B:1151:LEU:CD2	2.34	0.57
3:A:1420:ASP:O	3:A:1421:CYS:HB2	2.04	0.57
4:B:955:THR:OG1	12:L:55:ILE:HA	2.04	0.56
3:A:1436:ILE:HG22	4:B:1142:GLY:HA2	1.87	0.56
5:C:258:ILE:O	5:C:261:ALA:HB3	2.04	0.56
11:K:46:ILE:HG22	11:K:50:LEU:HD12	1.86	0.56
4:B:984:HIS:HB3	4:B:1022:THR:OG1	2.05	0.56
8:H:123:MET:HE1	8:H:142:LEU:CD1	2.35	0.56
3:A:401:GLY:O	3:A:435:HIS:CD2	2.58	0.56
4:B:429:PHE:HA	4:B:432:MET:CE	2.35	0.56
3:A:537:ARG:HB2	8:H:20:TYR:CE2	2.39	0.56
3:A:185:TRP:CZ3	3:A:200:ARG:HG2	2.40	0.56
8:H:97:MET:HE2	8:H:142:LEU:HD23	1.87	0.56
3:A:1364:ASN:HD21	3:A:1366:ARG:HG2	1.68	0.56
3:A:1364:ASN:ND2	3:A:1366:ARG:N	2.53	0.56
9:I:78:CYS:SG	9:I:106:CYS:SG	3.02	0.56
9:I:7:CYS:O	9:I:8:ARG:O	2.24	0.56
8:H:89:LEU:HD22	8:H:91:ASP:OD2	2.05	0.56
3:A:672:ASP:HB3	3:A:675:THR:OG1	2.05	0.56
3:A:882:SER:HA	3:A:952:ALA:O	2.04	0.56
3:A:1111:MET:CE	3:A:1114:PRO:HA	2.35	0.56
8:H:6:PHE:HE1	8:H:130:ARG:HE	1.53	0.56
4:B:57:TYR:HD1	4:B:57:TYR:N	2.03	0.56
4:B:566:LEU:HD22	4:B:586:TRP:O	2.06	0.56
4:B:311:LEU:HB3	9:I:4:PHE:CE2	2.40	0.56
4:B:522:VAL:HG11	4:B:537:LYS:HB3	1.86	0.56
4:B:979:LYS:HG2	4:B:1095:LEU:HD12	1.86	0.56
3:A:35:ILE:HG12	3:A:52:GLY:O	2.06	0.56
3:A:1342:GLU:HG2	6:E:212:ARG:NH1	2.20	0.56
1:D:8:DT:H2'	1:D:9:DG:O4'	2.04	0.56
3:A:1193:LEU:HD21	3:A:1267:MET:HE2	1.86	0.56
8:H:106:GLU:C	8:H:108:SER:N	2.57	0.56
4:B:243:ALA:HA	4:B:250:PHE:O	2.05	0.56
3:A:547:LEU:HD22	11:K:58:PHE:CD1	2.41	0.56
3:A:1017:LEU:HD23	6:E:204:THR:O	2.05	0.56
6:E:46:TYR:CE2	6:E:58:MET:HA	2.40	0.56
4:B:1022:THR:HG23	4:B:1022:THR:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:131:HIS:O	5:C:132:PRO:C	2.43	0.56
3:A:452:LYS:HB3	4:B:1141:HIS:CE1	2.40	0.56
3:A:76:GLU:O	3:A:76:GLU:CG	2.52	0.56
8:H:82:PRO:O	8:H:83:GLN:HB2	2.04	0.56
11:K:65:HIS:HD2	11:K:67:PHE:N	2.02	0.56
5:C:99:LEU:HD23	5:C:99:LEU:N	2.20	0.56
5:C:55:THR:HB	5:C:152:GLU:H	1.70	0.56
8:H:59:ILE:HG22	8:H:60:ALA:N	2.21	0.56
4:B:120:ARG:NH1	12:L:54:ARG:NH1	2.54	0.56
2:R:3:C:H2'	2:R:4:C:O4'	2.06	0.56
4:B:1116:ARG:HD2	4:B:1198:TYR:CG	2.40	0.56
4:B:806:THR:OG1	4:B:809:MET:HE3	2.05	0.56
4:B:1180:PHE:O	4:B:1181:GLU:HB2	2.05	0.56
3:A:838:GLN:O	3:A:842:VAL:HG23	2.06	0.56
5:C:145:CYS:SG	5:C:146:LYS:N	2.79	0.56
8:H:84:ALA:HA	8:H:87:ARG:HG3	1.88	0.56
3:A:92:HIS:HD2	3:A:94:GLY:H	1.53	0.56
3:A:1261:LYS:HA	3:A:1264:GLU:HB3	1.88	0.56
3:A:1096:SER:O	3:A:1099:PRO:HG2	2.05	0.56
4:B:958:GLN:O	4:B:960:GLY:N	2.33	0.56
3:A:216:VAL:O	3:A:219:PHE:HB2	2.06	0.56
5:C:248:ILE:CD1	11:K:101:LEU:HD22	2.35	0.56
4:B:1171:VAL:HG11	4:B:1191:ILE:HD13	1.88	0.56
3:A:1399:ARG:CB	3:A:1408:ILE:HD13	2.28	0.55
3:A:1300:LYS:HB3	3:A:1300:LYS:HZ2	1.71	0.55
12:L:26:THR:HG22	12:L:27:LEU:N	2.21	0.55
3:A:974:ASP:HB2	8:H:136:LYS:NZ	2.20	0.55
4:B:556:THR:HG22	4:B:557:PHE:N	2.20	0.55
7:F:99:LEU:HD12	7:F:99:LEU:O	2.05	0.55
3:A:1389:PHE:O	3:A:1392:SER:HB3	2.05	0.55
3:A:1308:THR:CG2	3:A:1310:GLY:O	2.55	0.55
3:A:1329:THR:HG22	3:A:1331:SER:N	2.01	0.55
5:C:242:GLN:NE2	5:C:246:ARG:HE	2.02	0.55
4:B:361:LEU:N	4:B:362:PRO:CD	2.69	0.55
5:C:70:ILE:HD11	5:C:144:ILE:HG12	1.88	0.55
3:A:849:MET:CE	3:A:1061:GLY:HA2	2.36	0.55
5:C:242:GLN:HE21	5:C:246:ARG:HE	1.54	0.55
1:D:4:DT:H2'	1:D:5:DG:H8	1.72	0.55
4:B:864:LYS:HD3	4:B:871:THR:OG1	2.05	0.55
6:E:195:VAL:HG22	6:E:213:ILE:HB	1.88	0.55
5:C:101:LEU:HD13	5:C:118:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:898:LEU:HD22	4:B:964:VAL:HG11	1.89	0.55
10:J:21:TYR:HA	10:J:39:LEU:HD11	1.89	0.55
4:B:120:ARG:HE	4:B:955:THR:CG2	2.20	0.55
4:B:839:MET:CE	4:B:980:PHE:HB2	2.35	0.55
3:A:825:ILE:HD12	4:B:513:GLN:NE2	2.21	0.55
4:B:1051:THR:CG2	4:B:1052:VAL:N	2.70	0.55
4:B:801:LYS:O	10:J:52:THR:CG2	2.52	0.55
5:C:229:TYR:N	5:C:229:TYR:CD1	2.74	0.55
4:B:980:PHE:HE1	4:B:990:ILE:HD11	1.70	0.55
4:B:479:VAL:HG12	4:B:480:SER:H	1.72	0.55
4:B:794:ASN:C	4:B:795:ILE:HD12	2.26	0.55
11:K:61:TYR:HA	11:K:72:LYS:O	2.06	0.55
3:A:548:ASN:HA	11:K:60:ALA:HB1	1.87	0.55
3:A:517:ASN:ND2	3:A:1362:TYR:HE2	2.05	0.55
4:B:25:ILE:HD11	4:B:653:VAL:HB	1.89	0.55
3:A:463:ILE:HD11	3:A:469:ARG:HG3	1.89	0.55
3:A:233:TRP:C	3:A:235:ILE:N	2.60	0.55
4:B:172:ILE:HD13	4:B:178:ASN:CB	2.37	0.55
4:B:864:LYS:HG3	4:B:865:LYS:N	2.21	0.55
3:A:1116:LEU:O	3:A:1308:THR:HB	2.07	0.55
3:A:683:ILE:HD11	3:A:764:CYS:CB	2.35	0.55
6:E:195:VAL:HG22	6:E:213:ILE:CB	2.36	0.55
3:A:556:TRP:CE3	3:A:558:GLY:HA2	2.41	0.55
8:H:123:MET:HE3	8:H:142:LEU:CD2	2.36	0.55
3:A:875:ALA:HB2	3:A:1366:ARG:HD2	1.88	0.55
3:A:337:ARG:NE	3:A:839:ARG:NH2	2.55	0.55
3:A:885:THR:O	3:A:885:THR:HG22	2.05	0.55
4:B:515:HIS:H	4:B:518:HIS:CD2	2.24	0.55
3:A:738:LYS:HB2	3:A:740:LEU:HG	1.89	0.55
7:F:72:LYS:N	7:F:142:SER:HA	2.22	0.55
7:F:94:LEU:HD21	7:F:122:MET:HA	1.89	0.55
9:I:111:THR:HG22	9:I:112:SER:N	2.19	0.55
3:A:885:THR:O	3:A:940:ARG:HG3	2.07	0.55
6:E:61:GLN:NE2	6:E:105:PHE:CE2	2.71	0.55
3:A:693:VAL:HG21	3:A:721:PHE:CE1	2.39	0.55
3:A:1073:GLY:O	3:A:1076:ALA:HB3	2.07	0.55
4:B:864:LYS:N	4:B:872:GLU:OE1	2.39	0.55
7:F:109:VAL:HG13	7:F:127:GLU:OE1	2.07	0.55
12:L:70:ARG:HG2	12:L:70:ARG:NH1	2.22	0.55
3:A:809:THR:O	3:A:810:PRO:C	2.46	0.55
3:A:867:ILE:HG22	3:A:872:GLY:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:63:ARG:O	12:L:64:LEU:O	2.24	0.55
9:I:111:THR:CG2	9:I:112:SER:N	2.69	0.55
3:A:1328:TYR:CG	3:A:1329:THR:N	2.74	0.55
3:A:665:GLY:HA3	4:B:1086:PHE:CD1	2.41	0.55
5:C:238:ILE:HG23	5:C:242:GLN:HB2	1.89	0.55
3:A:1222:ASN:O	3:A:1223:ASP:HB3	2.06	0.55
6:E:176:PRO:HD2	6:E:211:TYR:O	2.07	0.55
3:A:533:LYS:O	3:A:535:THR:N	2.40	0.55
4:B:549:THR:HB	4:B:628:THR:HG23	1.89	0.55
6:E:46:TYR:CD2	6:E:58:MET:HG2	2.42	0.55
3:A:1341:ILE:HD12	3:A:1379:GLY:O	2.07	0.55
9:I:2:THR:HG22	9:I:2:THR:O	2.07	0.55
3:A:710:LEU:N	3:A:710:LEU:HD12	2.20	0.54
4:B:783:THR:HA	10:J:60:PHE:HE1	1.72	0.54
4:B:911:ILE:HD11	4:B:941:LEU:CD1	2.37	0.54
4:B:566:LEU:HD13	4:B:588:GLY:CA	2.37	0.54
5:C:162:GLY:HA3	5:C:170:TRP:CE2	2.41	0.54
3:A:843:LYS:HG3	3:A:1402:PHE:HD1	1.72	0.54
4:B:287:ARG:HG2	4:B:292:ILE:CA	2.27	0.54
3:A:23:SER:HB3	3:A:233:TRP:CE2	2.41	0.54
4:B:515:HIS:H	4:B:518:HIS:HD2	1.55	0.54
3:A:50:ILE:C	3:A:52:GLY:H	2.09	0.54
3:A:1341:ILE:HD12	3:A:1379:GLY:C	2.28	0.54
12:L:32:ALA:HB3	12:L:55:ILE:CD1	2.26	0.54
4:B:955:THR:HG1	12:L:55:ILE:HA	1.72	0.54
4:B:780:VAL:HG21	10:J:56:LEU:HD13	1.88	0.54
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.47	0.54
4:B:308:TRP:CH2	9:I:45:ARG:HG2	2.43	0.54
4:B:680:THR:HG22	4:B:681:TRP:H	1.72	0.54
4:B:63:ILE:HA	4:B:421:PHE:CE2	2.42	0.54
3:A:1339:LEU:HD13	6:E:147:HIS:CD2	2.41	0.54
10:J:32:GLU:O	10:J:36:LEU:HG	2.07	0.54
3:A:1365:TYR:O	3:A:1366:ARG:C	2.43	0.54
4:B:93:GLY:N	4:B:131:ASP:O	2.37	0.54
4:B:108:VAL:CG1	4:B:109:THR:H	2.18	0.54
9:I:62:ILE:HG23	9:I:63:GLY:N	2.22	0.54
3:A:646:PHE:O	3:A:650:GLN:HG3	2.08	0.54
3:A:845:LEU:N	3:A:845:LEU:HD23	2.22	0.54
3:A:1116:LEU:H	3:A:1308:THR:HG22	1.72	0.54
3:A:399:HIS:O	3:A:435:HIS:CD2	2.60	0.54
3:A:451:HIS:CE1	3:A:1074:GLU:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:837:ASP:OD1	4:B:1020:ARG:NH2	2.41	0.54
7:F:107:VAL:HG12	7:F:109:VAL:H	1.72	0.54
3:A:741:ASN:ND2	3:A:743:VAL:H	2.05	0.54
4:B:784:ASN:ND2	4:B:788:ARG:HD2	2.23	0.54
4:B:756:ILE:HG21	4:B:759:PRO:HB3	1.90	0.54
3:A:1366:ARG:O	3:A:1369:ALA:HB3	2.08	0.54
3:A:902:LEU:HD21	3:A:923:LEU:HD23	1.90	0.54
3:A:15:LYS:HD2	4:B:1220:ARG:HE	1.72	0.54
3:A:356:ASP:OD2	11:K:65:HIS:HE1	1.90	0.54
3:A:1205:LYS:O	3:A:1207:LEU:N	2.41	0.54
12:L:27:LEU:HD13	12:L:37:LYS:HB3	1.90	0.54
4:B:406:LEU:HD12	4:B:545:ILE:HD11	1.89	0.54
3:A:350:ARG:HB2	3:A:488:ASN:OD1	2.08	0.54
6:E:153:HIS:CE1	6:E:184:VAL:HG11	2.43	0.54
4:B:758:PHE:C	4:B:760:ASP:H	2.11	0.54
3:A:563:PRO:HG3	3:A:572:TRP:CE2	2.42	0.54
3:A:515:GLN:HG3	3:A:516:SER:N	2.22	0.54
5:C:13:ALA:O	11:K:114:LEU:HD13	2.08	0.54
4:B:179:CYS:SG	4:B:181:LEU:HB2	2.47	0.54
4:B:28:GLU:CD	4:B:807:ARG:HH22	2.10	0.54
4:B:195:CYS:CB	4:B:782:LEU:HD22	2.37	0.54
4:B:292:ILE:H	4:B:293:PRO:HD2	1.73	0.54
4:B:640:VAL:O	4:B:641:GLU:C	2.46	0.54
3:A:89:PRO:O	3:A:204:THR:HG21	2.07	0.54
12:L:51:CYS:C	12:L:53:HIS:H	2.12	0.54
4:B:34:ILE:O	4:B:37:PHE:HB3	2.06	0.54
4:B:484:ASN:ND2	4:B:486:TYR:CD1	2.76	0.54
9:I:75:CYS:C	9:I:77:LYS:N	2.59	0.54
3:A:768:GLN:HG2	3:A:816:HIS:CA	2.38	0.54
3:A:1194:ARG:HH22	3:A:1237:ILE:HD13	1.73	0.54
3:A:399:HIS:C	3:A:401:GLY:H	2.10	0.54
4:B:118:ARG:NH2	4:B:194:GLU:CD	2.60	0.54
3:A:339:ASN:O	3:A:343:LYS:HG2	2.07	0.54
4:B:205:ILE:HD11	4:B:461:LEU:HD23	1.90	0.54
3:A:556:TRP:CD2	3:A:558:GLY:HA2	2.42	0.54
3:A:738:LYS:HZ1	5:C:194:GLU:C	2.12	0.54
3:A:122:MET:O	3:A:126:LEU:HG	2.07	0.54
4:B:755:ILE:CG2	4:B:755:ILE:O	2.55	0.54
3:A:1094:VAL:HG13	3:A:1113:THR:CG2	2.37	0.54
9:I:7:CYS:C	9:I:8:ARG:O	2.43	0.54
5:C:11:ARG:NH2	5:C:229:TYR:CD2	2.68	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:168:TYR:HB3	6:E:170:LEU:CD2	2.36	0.54
3:A:226:GLU:HG2	3:A:227:VAL:HG23	1.90	0.54
4:B:288:ALA:HB1	4:B:331:LEU:CD1	2.38	0.54
5:C:183:TRP:CZ2	5:C:207:CYS:HB3	2.42	0.54
3:A:444:PHE:HB3	3:A:458:HIS:CD2	2.43	0.53
3:A:898:ARG:HD2	3:A:899:VAL:H	1.73	0.53
3:A:367:PRO:HB3	3:A:465:TYR:O	2.08	0.53
5:C:241:ASP:O	5:C:245:VAL:HG23	2.08	0.53
3:A:92:HIS:CD2	3:A:94:GLY:H	2.26	0.53
3:A:608:ILE:HD12	3:A:613:ILE:CD1	2.38	0.53
4:B:644:GLU:HG3	4:B:654:ARG:HH22	1.74	0.53
10:J:48:ARG:HE	10:J:49:MET:HE2	1.73	0.53
10:J:52:THR:O	10:J:52:THR:HG22	2.08	0.53
4:B:102:VAL:HG22	4:B:112:LEU:HD22	1.88	0.53
6:E:23:VAL:HG12	6:E:28:TYR:HB2	1.89	0.53
3:A:821:ARG:O	3:A:822:GLU:C	2.46	0.53
3:A:38:PRO:N	3:A:270:LEU:HD23	2.22	0.53
3:A:557:ASP:OD2	3:A:559:VAL:HB	2.08	0.53
4:B:916:THR:HG22	4:B:918:ILE:HG13	1.90	0.53
4:B:899:ILE:HD11	4:B:910:VAL:O	2.09	0.53
8:H:6:PHE:O	8:H:58:THR:HA	2.08	0.53
3:A:1220:PHE:O	3:A:1222:ASN:N	2.42	0.53
4:B:542:MET:HE1	4:B:743:ILE:CG2	2.38	0.53
3:A:225:ASN:O	3:A:227:VAL:HG23	2.09	0.53
3:A:1225:PHE:CE2	3:A:1227:ILE:HD11	2.43	0.53
4:B:235:SER:OG	4:B:236:HIS:HD2	1.91	0.53
3:A:1147:THR:HA	3:A:1197:LEU:HD23	1.90	0.53
4:B:842:ASN:HD22	4:B:845:SER:CB	2.21	0.53
4:B:848:ARG:NH1	10:J:8:PHE:O	2.35	0.53
3:A:963:ILE:HD12	3:A:1049:ILE:HG12	1.88	0.53
8:H:5:LEU:CD1	8:H:135:LEU:HG	2.34	0.53
12:L:38:LEU:O	12:L:39:SER:CB	2.56	0.53
8:H:32:THR:HG22	8:H:33:GLN:HG3	1.90	0.53
4:B:405:ARG:HA	4:B:631:GLY:O	2.09	0.53
3:A:696:GLU:OE2	3:A:702:LEU:HD23	2.08	0.53
5:C:189:THR:HG22	5:C:190:ASP:N	2.24	0.53
4:B:43:LEU:HD13	4:B:812:LEU:CD2	2.38	0.53
3:A:1116:LEU:HD12	3:A:1329:THR:HG1	1.72	0.53
4:B:287:ARG:CG	4:B:292:ILE:HA	2.26	0.53
3:A:852:TYR:CE2	7:F:136:ARG:HG2	2.42	0.53
3:A:1410:PHE:HD2	4:B:1212:ILE:HD11	1.70	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1375:MET:HG2	3:A:1382:THR:O	2.08	0.53
6:E:197:LYS:HG3	6:E:211:TYR:CE2	2.42	0.53
6:E:28:TYR:CE1	6:E:78:LEU:HD12	2.44	0.53
3:A:511:ILE:HG12	3:A:521:MET:HE3	1.90	0.53
3:A:154:SER:HB3	3:A:162:VAL:HG23	1.89	0.53
5:C:248:ILE:HD13	11:K:101:LEU:HD22	1.89	0.53
6:E:17:ARG:O	6:E:21:GLU:HG3	2.09	0.53
3:A:337:ARG:CZ	3:A:839:ARG:HH12	2.22	0.53
3:A:90:VAL:HG13	3:A:297:GLN:HA	1.90	0.53
5:C:46:ILE:HD13	5:C:157:CYS:CB	2.38	0.53
4:B:43:LEU:HD13	4:B:812:LEU:HD23	1.90	0.53
4:B:911:ILE:HD11	4:B:941:LEU:HD12	1.91	0.53
4:B:542:MET:CG	4:B:747:MET:HE3	2.36	0.53
8:H:89:LEU:O	8:H:91:ASP:N	2.37	0.53
4:B:463:THR:HG21	4:B:465:ASN:HD22	1.74	0.53
10:J:36:LEU:HD12	10:J:47:ARG:NH1	2.23	0.53
3:A:134:ARG:HH12	3:A:220:THR:HG22	1.74	0.53
3:A:552:TRP:NE1	3:A:655:PHE:CD1	2.77	0.53
7:F:114:GLU:OE1	7:F:119:ARG:HG3	2.08	0.53
4:B:1065:GLN:NE2	4:B:1067:ARG:HG2	2.24	0.53
3:A:384:ASN:OD1	3:A:385:ILE:N	2.42	0.53
11:K:10:PHE:HD1	11:K:11:LEU:HD13	1.67	0.53
6:E:78:LEU:HD21	6:E:109:ILE:HD12	1.90	0.53
4:B:90:ILE:CD1	4:B:432:MET:SD	2.97	0.53
4:B:1034:VAL:HG12	4:B:1035:ALA:N	2.23	0.53
9:I:46:HIS:CD2	9:I:48:LEU:HD21	2.44	0.53
8:H:38:LEU:CD1	8:H:125:LEU:HD13	2.38	0.53
8:H:40:LEU:CD2	8:H:42:ILE:HD11	2.39	0.53
4:B:284:ILE:HD13	4:B:324:ILE:HD12	1.91	0.53
4:B:844:SER:OG	4:B:996:ARG:N	2.33	0.53
3:A:596:THR:O	3:A:597:LEU:C	2.47	0.53
4:B:234:ILE:HG21	4:B:257:LYS:HB3	1.91	0.53
3:A:529:CYS:HB2	4:B:1015:HIS:CE1	2.43	0.53
3:A:675:THR:CG2	3:A:736:ASN:HD21	2.22	0.53
4:B:898:LEU:CD2	4:B:964:VAL:HG11	2.38	0.53
7:F:118:LEU:O	7:F:122:MET:HG3	2.08	0.53
3:A:134:ARG:NH1	3:A:220:THR:O	2.42	0.53
6:E:35:VAL:C	6:E:37:LEU:H	2.12	0.53
4:B:875:GLU:O	4:B:877:PRO:HD3	2.09	0.53
7:F:77:ASP:O	7:F:78:GLN:HB2	2.09	0.53
4:B:547:VAL:H	4:B:612:GLU:CD	2.13	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:124:VAL:HG22	6:E:132:ILE:CG2	2.39	0.52
3:A:710:LEU:H	3:A:710:LEU:CD1	2.19	0.52
4:B:293:PRO:HA	9:I:12:ASN:HD21	1.74	0.52
3:A:852:TYR:CZ	7:F:136:ARG:HG2	2.44	0.52
4:B:956:THR:CG2	4:B:960:GLY:HA2	2.38	0.52
3:A:261:ASP:OD2	3:A:323:LYS:HD2	2.09	0.52
3:A:1299:VAL:CG1	3:A:1300:LYS:N	2.72	0.52
3:A:114:LEU:HD22	3:A:171:GLN:NE2	2.23	0.52
11:K:46:ILE:O	11:K:50:LEU:HB2	2.09	0.52
4:B:271:ALA:HB3	4:B:285:ILE:CD1	2.40	0.52
5:C:80:LEU:CD2	5:C:129:ILE:HD11	2.28	0.52
4:B:857:ARG:HD2	4:B:945:GLU:OE1	2.08	0.52
3:A:741:ASN:ND2	3:A:741:ASN:C	2.62	0.52
3:A:219:PHE:O	3:A:222:LEU:O	2.28	0.52
7:F:132:LEU:O	7:F:148:VAL:HG23	2.09	0.52
12:L:62:LYS:C	12:L:64:LEU:H	2.13	0.52
3:A:1111:MET:CE	3:A:1330:ASN:OD1	2.57	0.52
3:A:670:ILE:HD13	4:B:1067:ARG:CZ	2.39	0.52
4:B:287:ARG:HA	4:B:291:ILE:O	2.09	0.52
9:I:29:CYS:C	9:I:31:THR:H	2.13	0.52
3:A:590:ARG:O	3:A:591:PHE:HB2	2.08	0.52
7:F:109:VAL:CG1	7:F:110:ASP:N	2.73	0.52
3:A:1365:TYR:O	3:A:1367:HIS:N	2.42	0.52
3:A:1161:THR:HG22	3:A:1162:VAL:N	2.24	0.52
4:B:120:ARG:NH2	12:L:54:ARG:HD2	2.24	0.52
12:L:47:ARG:HG2	12:L:52:GLY:CA	2.39	0.52
5:C:57:VAL:HG11	10:J:60:PHE:HB2	1.88	0.52
5:C:164:ALA:HA	5:C:167:HIS:O	2.10	0.52
9:I:29:CYS:O	9:I:29:CYS:SG	2.66	0.52
4:B:31:TRP:CD1	4:B:807:ARG:NH1	2.78	0.52
3:A:442:VAL:O	3:A:457:ALA:HA	2.09	0.52
3:A:225:ASN:C	3:A:227:VAL:H	2.10	0.52
4:B:559:SER:HA	4:B:563:MET:HB3	1.91	0.52
11:K:63:VAL:HG23	11:K:63:VAL:O	2.08	0.52
3:A:849:MET:HE1	3:A:1061:GLY:HA2	1.90	0.52
6:E:12:LEU:HD22	6:E:55:ARG:CZ	2.39	0.52
3:A:568:PRO:HB2	5:C:221:TYR:CE1	2.45	0.52
3:A:1116:LEU:N	3:A:1308:THR:HG22	2.25	0.52
3:A:907:THR:HG22	3:A:908:LEU:N	2.25	0.52
11:K:65:HIS:HD2	11:K:67:PHE:HB2	1.74	0.52
7:F:97:ARG:NE	7:F:124:GLU:OE1	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:91:PHE:HB2	3:A:297:GLN:OE1	2.09	0.52
4:B:1177:HIS:HB3	4:B:1179:GLN:HE21	1.74	0.52
3:A:50:ILE:HG22	3:A:51:GLY:N	2.24	0.52
4:B:484:ASN:ND2	4:B:486:TYR:CE1	2.77	0.52
3:A:722:LEU:HD11	3:A:794:PRO:HB3	1.91	0.52
4:B:240:ILE:HG23	4:B:240:ILE:O	2.09	0.52
3:A:32:VAL:HG21	3:A:68:GLN:HE22	1.74	0.52
4:B:1069:PHE:HA	4:B:1085:ILE:O	2.08	0.52
7:F:101:ILE:HD13	7:F:120:ILE:HG22	1.91	0.52
9:I:73:ARG:O	9:I:81:ARG:HA	2.09	0.52
6:E:155:ARG:HD2	6:E:194:GLU:OE2	2.09	0.52
3:A:357:PRO:HG2	4:B:833:TYR:CE1	2.45	0.52
3:A:1029:ARG:HG3	3:A:1029:ARG:HH11	1.74	0.52
3:A:1392:SER:O	3:A:1393:ASN:CB	2.58	0.52
4:B:248:SER:O	4:B:249:ARG:HB2	2.09	0.52
3:A:387:ARG:O	3:A:391:LEU:HG	2.09	0.52
12:L:38:LEU:HG	12:L:39:SER:N	2.24	0.52
3:A:451:HIS:CD2	3:A:1074:GLU:HG3	2.45	0.52
3:A:1152:ILE:CG2	3:A:1260:LEU:HD23	2.38	0.52
3:A:27:VAL:HG13	3:A:240:PRO:HB3	1.91	0.52
4:B:614:SER:OG	4:B:627:PHE:HB2	2.09	0.52
3:A:808:LEU:O	4:B:728:ARG:NH1	2.43	0.52
3:A:928:LEU:O	3:A:931:GLU:N	2.42	0.52
4:B:737:THR:CG2	9:I:66:PRO:HB2	2.40	0.52
4:B:120:ARG:HB2	4:B:122:LEU:HG	1.91	0.52
10:J:7:CYS:SG	10:J:9:SER:HB2	2.50	0.52
3:A:365:GLY:HA3	3:A:469:ARG:HB2	1.91	0.52
3:A:507:VAL:N	3:A:508:PRO:CD	2.72	0.52
3:A:847:ASP:OD2	3:A:858:ASN:HB2	2.10	0.52
4:B:864:LYS:HD3	4:B:871:THR:HA	1.91	0.52
4:B:806:THR:C	4:B:808:ALA:H	2.12	0.52
4:B:825:VAL:HG12	4:B:826:ALA:N	2.24	0.52
4:B:292:ILE:N	4:B:293:PRO:HD2	2.25	0.52
3:A:817:ALA:HA	4:B:764:SER:OG	2.10	0.52
3:A:96:ILE:O	3:A:100:LYS:HG3	2.10	0.52
4:B:552:MET:N	4:B:553:PRO:HD2	2.24	0.52
3:A:567:LYS:HZ2	8:H:46:LEU:HB2	1.73	0.52
3:A:836:TYR:CE2	3:A:840:ARG:HD2	2.45	0.52
10:J:1:MET:H1	10:J:56:LEU:HB2	1.75	0.52
4:B:1197:PRO:HG2	4:B:1200:ALA:CB	2.40	0.52
3:A:167:CYS:HB2	3:A:169:ASN:ND2	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1084:GLN:HG2	5:C:201:TRP:CZ2	2.45	0.52
1:D:2:DA:OP1	3:A:1403:GLU:O	2.29	0.51
10:J:9:SER:CB	10:J:45:CYS:HB2	2.40	0.51
3:A:384:ASN:O	3:A:385:ILE:C	2.48	0.51
4:B:834:ASN:O	4:B:1013:ASN:HB2	2.10	0.51
4:B:542:MET:HE2	4:B:747:MET:HE2	1.93	0.51
5:C:93:ASP:OD1	5:C:122:SER:HB2	2.09	0.51
6:E:23:VAL:HG13	6:E:28:TYR:CD1	2.45	0.51
3:A:929:LEU:H	3:A:929:LEU:CD2	2.23	0.51
4:B:577:ALA:HB1	4:B:589:VAL:HG11	1.91	0.51
4:B:98:THR:OG1	4:B:127:GLY:HA3	2.09	0.51
3:A:1269:GLU:OE2	4:B:263:GLY:HA3	2.10	0.51
1:D:1:DA:H2'	1:D:2:DA:H8	1.70	0.51
3:A:49:LYS:HB3	3:A:55:ASP:HB2	1.92	0.51
10:J:54:VAL:O	10:J:56:LEU:N	2.43	0.51
6:E:5:ASN:O	6:E:9:ILE:HG13	2.10	0.51
3:A:407:ARG:HD2	3:A:413:ILE:HD11	1.91	0.51
4:B:846:ILE:HD13	4:B:974:PRO:HG2	1.91	0.51
4:B:25:ILE:HG22	4:B:26:THR:N	2.24	0.51
7:F:109:VAL:CG2	7:F:124:GLU:HG2	2.40	0.51
3:A:753:GLY:HA2	3:A:757:ASN:HD22	1.74	0.51
4:B:271:ALA:O	4:B:279:ASP:HA	2.11	0.51
3:A:384:ASN:OD1	3:A:388:LEU:HD12	2.10	0.51
3:A:1299:VAL:CG1	3:A:1300:LYS:H	2.20	0.51
3:A:737:LEU:HD11	3:A:758:ILE:HG21	1.92	0.51
11:K:49:GLU:OE2	11:K:97:LYS:HE3	2.10	0.51
8:H:84:ALA:C	8:H:86:ASP:N	2.64	0.51
4:B:755:ILE:HG22	4:B:755:ILE:O	2.09	0.51
3:A:1364:ASN:ND2	3:A:1366:ARG:HH11	2.09	0.51
4:B:737:THR:CG2	9:I:66:PRO:CB	2.89	0.51
3:A:470:LEU:HD21	3:A:487:MET:HE1	1.92	0.51
3:A:233:TRP:C	3:A:235:ILE:H	2.13	0.51
4:B:59:LEU:HD11	4:B:417:PHE:CZ	2.44	0.51
3:A:1319:VAL:CG1	3:A:1320:PRO:HD2	2.39	0.51
3:A:1359:ASP:C	3:A:1361:SER:H	2.13	0.51
4:B:271:ALA:HB3	4:B:285:ILE:HD11	1.93	0.51
4:B:648:HIS:NE2	4:B:650:GLU:OE1	2.43	0.51
3:A:901:LEU:HD23	3:A:907:THR:HG23	1.92	0.51
3:A:13:THR:HG23	3:A:1432:GLN:NE2	2.24	0.51
3:A:1376:THR:HG23	6:E:212:ARG:NH2	2.26	0.51
4:B:46:GLN:NE2	4:B:496:ARG:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:898:ARG:HD2	3:A:899:VAL:N	2.26	0.51
3:A:443:LEU:HD11	4:B:1138:MET:SD	2.50	0.51
3:A:715:GLU:OE2	3:A:774:ARG:NH1	2.43	0.51
4:B:827:ILE:HG12	4:B:1012:ILE:HD11	1.93	0.51
5:C:177:GLU:HG3	5:C:231:ASN:HB3	1.93	0.51
8:H:95:TYR:HE2	8:H:97:MET:HG3	1.73	0.51
4:B:707:PRO:CG	4:B:708:GLU:H	2.21	0.51
9:I:50:THR:HG22	9:I:52:ILE:H	1.75	0.51
4:B:130:VAL:CG1	4:B:131:ASP:N	2.74	0.51
1:D:10:DG:OP1	4:B:857:ARG:NH2	2.44	0.51
1:D:12:DC:C2	2:R:1:G:N2	2.75	0.51
4:B:563:MET:HG3	4:B:563:MET:O	2.10	0.51
4:B:1162:ILE:HD11	4:B:1194:ILE:CD1	2.41	0.51
3:A:795:GLU:HG2	4:B:731:VAL:HG21	1.93	0.51
4:B:25:ILE:CG2	4:B:29:ASP:HB3	2.40	0.51
3:A:535:THR:HG23	3:A:575:LYS:HE2	1.93	0.51
4:B:1106:ARG:HH12	4:B:1118:PRO:CB	2.24	0.51
10:J:14:VAL:HG12	10:J:50:ILE:HD11	1.92	0.51
3:A:340:LEU:HD21	4:B:1200:ALA:CB	2.40	0.51
4:B:1035:ALA:HB1	4:B:1040:ASN:O	2.10	0.51
3:A:821:ARG:HG3	3:A:825:ILE:CD1	2.40	0.51
9:I:25:LEU:HD12	9:I:26:LEU:H	1.76	0.51
8:H:84:ALA:C	8:H:86:ASP:H	2.13	0.51
3:A:346:ASP:CG	4:B:1108:ARG:HA	2.31	0.51
3:A:1349:TYR:CD2	3:A:1349:TYR:C	2.84	0.51
3:A:1351:GLU:O	3:A:1352:VAL:C	2.49	0.51
4:B:283:VAL:HG13	4:B:297:ILE:CD1	2.41	0.51
3:A:587:HIS:HA	3:A:607:ILE:O	2.11	0.51
3:A:1362:TYR:OH	3:A:1364:ASN:HA	2.11	0.51
4:B:642:ASP:HB3	4:B:649:LYS:CD	2.41	0.51
5:C:66:ARG:NH2	10:J:2:ILE:CG2	2.74	0.51
3:A:326:ARG:HG2	3:A:1406:VAL:CG2	2.39	0.51
4:B:1163:CYS:SG	4:B:1182:CYS:SG	3.08	0.51
4:B:101:MET:HE2	4:B:169:ARG:HH12	1.76	0.51
4:B:428:ILE:O	4:B:431:TYR:HB3	2.10	0.51
4:B:1159:ARG:CD	4:B:1193:GLN:HG3	2.31	0.51
3:A:751:SER:O	3:A:752:LYS:CG	2.59	0.51
5:C:33:LEU:HG	5:C:37:MET:CE	2.41	0.51
3:A:888:GLY:O	3:A:940:ARG:NH2	2.44	0.51
3:A:893:PHE:CE1	3:A:940:ARG:HD2	2.46	0.51
11:K:24:ASP:HB3	11:K:30:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:810:PRO:O	3:A:813:PHE:HB3	2.11	0.51
4:B:283:VAL:O	4:B:286:PHE:HB2	2.11	0.51
3:A:1214:GLU:O	3:A:1218:GLN:HG2	2.10	0.51
6:E:121:MET:C	6:E:123:LEU:H	2.13	0.51
3:A:41:MET:HG2	3:A:49:LYS:HG2	1.92	0.50
3:A:1410:PHE:CE2	4:B:1212:ILE:HD11	2.45	0.50
8:H:83:GLN:C	8:H:85:GLY:H	2.14	0.50
11:K:55:LYS:CD	11:K:78:THR:HB	2.41	0.50
3:A:329:LEU:HD22	4:B:1203:LEU:CD1	2.41	0.50
3:A:135:PHE:HD1	3:A:222:LEU:HD22	1.76	0.50
3:A:185:TRP:HZ3	3:A:200:ARG:HG2	1.74	0.50
3:A:115:LEU:HB2	3:A:122:MET:CE	2.41	0.50
3:A:567:LYS:NZ	8:H:46:LEU:CB	2.67	0.50
3:A:1384:VAL:HG12	3:A:1384:VAL:O	2.11	0.50
3:A:15:LYS:CB	4:B:1220:ARG:HG2	2.33	0.50
4:B:100:PRO:HG3	4:B:172:ILE:HD12	1.92	0.50
5:C:18:VAL:HG12	5:C:20:PHE:HD2	1.76	0.50
12:L:27:LEU:HD13	12:L:37:LYS:CG	2.41	0.50
3:A:754:SER:O	3:A:755:PHE:C	2.48	0.50
3:A:376:TYR:OH	3:A:498:ARG:HD2	2.11	0.50
12:L:62:LYS:O	12:L:64:LEU:HG	2.11	0.50
3:A:1312:ASN:O	3:A:1316:VAL:HG23	2.11	0.50
3:A:394:ASN:OD1	3:A:398:GLU:OE1	2.30	0.50
4:B:514:LEU:HD12	4:B:515:HIS:H	1.74	0.50
5:C:254:LYS:HE2	11:K:42:LEU:HD13	1.94	0.50
4:B:195:CYS:SG	4:B:197:PHE:HB2	2.51	0.50
11:K:91:CYS:O	11:K:95:ILE:HG13	2.11	0.50
9:I:29:CYS:SG	9:I:31:THR:HG22	2.52	0.50
4:B:542:MET:HG3	4:B:747:MET:CE	2.38	0.50
3:A:500:GLU:OE1	4:B:1143:ALA:HB1	2.11	0.50
4:B:1084:GLN:CD	4:B:1084:GLN:H	2.14	0.50
9:I:68:LEU:HB3	9:I:84:VAL:HG22	1.94	0.50
3:A:573:SER:O	3:A:576:GLN:HB2	2.11	0.50
9:I:75:CYS:O	9:I:77:LYS:N	2.44	0.50
3:A:341:MET:CE	3:A:1401:SER:HB2	2.41	0.50
6:E:168:TYR:HB3	6:E:170:LEU:CG	2.41	0.50
4:B:864:LYS:HG2	4:B:871:THR:HG23	1.93	0.50
8:H:31:THR:O	8:H:32:THR:HB	2.11	0.50
4:B:485:ARG:NH2	4:B:782:LEU:HD11	2.27	0.50
11:K:101:LEU:HD23	11:K:101:LEU:O	2.11	0.50
3:A:1326:ARG:O	3:A:1327:ILE:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1376:THR:HG23	3:A:1376:THR:O	2.12	0.50
4:B:751:VAL:HG12	4:B:752:ALA:N	2.26	0.50
3:A:649:ILE:O	3:A:653:VAL:HG23	2.11	0.50
3:A:107:CYS:HB2	3:A:114:LEU:HD23	1.93	0.50
3:A:105:CYS:SG	3:A:138:ILE:HG22	2.52	0.50
4:B:240:ILE:O	4:B:253:THR:HG23	2.11	0.50
8:H:128:ASN:O	8:H:131:ASN:ND2	2.45	0.50
4:B:35:SER:O	4:B:36:ALA:C	2.50	0.50
4:B:653:VAL:CG2	4:B:689:LEU:HB3	2.42	0.50
5:C:77:ILE:HG23	5:C:161:LYS:HE3	1.94	0.50
4:B:906:SER:O	4:B:907:GLY:C	2.50	0.50
3:A:612:ILE:O	3:A:612:ILE:HG23	2.12	0.50
4:B:1119:VAL:O	4:B:1126:GLY:HA3	2.11	0.50
4:B:975:GLN:O	4:B:990:ILE:HD12	2.12	0.50
3:A:31:SER:HB2	3:A:83:HIS:HB2	1.91	0.50
3:A:444:PHE:CB	3:A:458:HIS:HD2	2.24	0.50
6:E:157:SER:C	6:E:159:ASP:N	2.64	0.50
10:J:36:LEU:HD13	10:J:47:ARG:HG2	1.92	0.50
3:A:1189:SER:OG	3:A:1190:PRO:HD2	2.12	0.50
6:E:177:ARG:O	6:E:212:ARG:HD3	2.11	0.50
4:B:579:ARG:HB2	4:B:586:TRP:NE1	2.27	0.50
8:H:44:VAL:O	8:H:44:VAL:HG12	2.12	0.50
12:L:40:LEU:HD13	12:L:44:ASP:OD1	2.11	0.50
9:I:15:TYR:CD1	9:I:15:TYR:N	2.79	0.50
3:A:100:LYS:NZ	3:A:176:LYS:HD2	2.27	0.50
8:H:59:ILE:O	8:H:60:ALA:HB3	2.12	0.50
3:A:545:GLN:O	3:A:548:ASN:N	2.44	0.50
3:A:567:LYS:HD2	3:A:568:PRO:HD2	1.92	0.50
5:C:43:THR:CG2	5:C:44:LEU:N	2.75	0.50
3:A:332:LYS:HG3	3:A:333:GLU:HG2	1.94	0.50
3:A:1436:ILE:CG2	3:A:1437:GLY:N	2.72	0.50
3:A:167:CYS:O	3:A:169:ASN:N	2.45	0.50
4:B:581:PHE:HB2	4:B:625:LYS:HG2	1.93	0.50
7:F:82:THR:HG22	7:F:84:TYR:H	1.77	0.49
12:L:52:GLY:O	12:L:54:ARG:HG3	2.12	0.49
3:A:306:ASN:HD21	3:A:324:SER:N	2.08	0.49
3:A:821:ARG:CG	3:A:825:ILE:HD11	2.41	0.49
6:E:98:ILE:O	6:E:102:GLU:HG3	2.12	0.49
10:J:16:ASP:OD1	10:J:17:LYS:HE3	2.12	0.49
3:A:1001:ARG:HG2	3:A:1001:ARG:HH11	1.77	0.49
3:A:857:ARG:HG2	3:A:863:VAL:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:666:ILE:CD1	4:B:1030:LEU:HD22	2.41	0.49
4:B:635:ARG:NH1	4:B:742:GLU:OE2	2.45	0.49
3:A:54:ASN:HA	3:A:58:LEU:HD12	1.95	0.49
4:B:911:ILE:HD11	4:B:941:LEU:HB2	1.94	0.49
4:B:858:SER:HA	4:B:966:VAL:O	2.11	0.49
6:E:54:GLN:O	6:E:57:MET:HB3	2.11	0.49
8:H:88:SER:O	8:H:89:LEU:HG	2.12	0.49
3:A:466:SER:HB3	11:K:2:ASN:ND2	2.28	0.49
3:A:1134:ILE:O	3:A:1138:ILE:HG13	2.12	0.49
6:E:191:LYS:O	6:E:192:ARG:C	2.50	0.49
8:H:76:THR:HG22	8:H:76:THR:O	2.11	0.49
8:H:49:VAL:CG1	8:H:50:ALA:N	2.74	0.49
1:D:2:DA:H4'	3:A:1403:GLU:OE2	2.12	0.49
4:B:734:HIS:O	4:B:735:ALA:HB2	2.12	0.49
3:A:709:THR:CB	3:A:712:GLU:HG3	2.41	0.49
4:B:269:ILE:CD1	4:B:386:LEU:HD21	2.39	0.49
11:K:97:LYS:O	11:K:100:ALA:HB3	2.12	0.49
3:A:1142:THR:O	3:A:1273:LEU:HD22	2.12	0.49
4:B:260:GLY:O	4:B:267:ARG:HD3	2.12	0.49
3:A:1153:TYR:HA	9:I:41:PRO:O	2.12	0.49
4:B:351:TYR:O	4:B:355:ILE:HG13	2.13	0.49
3:A:61:ILE:HA	3:A:74:MET:SD	2.53	0.49
3:A:74:MET:O	3:A:75:ASN:HB2	2.13	0.49
4:B:873:THR:O	4:B:914:LYS:HA	2.12	0.49
4:B:763:GLN:CG	4:B:765:PRO:HD2	2.40	0.49
3:A:738:LYS:NZ	5:C:194:GLU:HA	2.26	0.49
3:A:819:GLY:O	3:A:820:GLY:C	2.49	0.49
4:B:365:THR:HG23	4:B:367:LEU:HG	1.93	0.49
8:H:47:PHE:HB2	8:H:95:TYR:HD1	1.76	0.49
4:B:570:VAL:HG11	4:B:573:GLN:OE1	2.13	0.49
3:A:606:LEU:HB2	3:A:614:PHE:CE2	2.47	0.49
3:A:332:LYS:H	3:A:337:ARG:HD2	1.76	0.49
7:F:133:VAL:HG22	7:F:147:SER:HA	1.95	0.49
6:E:46:TYR:HE2	6:E:58:MET:HA	1.76	0.49
9:I:101:PHE:O	9:I:109:ILE:HA	2.12	0.49
5:C:4:GLU:O	5:C:5:GLY:O	2.31	0.49
3:A:741:ASN:ND2	3:A:743:VAL:N	2.60	0.49
4:B:660:LYS:O	4:B:663:ALA:HB3	2.13	0.49
4:B:1043:ASP:O	4:B:1050:ILE:HD12	2.12	0.49
3:A:834:THR:HG21	3:A:1077:THR:CA	2.43	0.49
1:D:2:DA:H5'	3:A:1403:GLU:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:291:ILE:HD13	4:B:300:HIS:CD2	2.48	0.49
4:B:1208:MET:HA	4:B:1212:ILE:O	2.12	0.49
4:B:55:VAL:HG12	4:B:56:ASP:N	2.27	0.49
4:B:756:ILE:CG2	4:B:759:PRO:HB3	2.42	0.49
4:B:896:ASP:OD2	12:L:58:LYS:HE3	2.13	0.49
3:A:1364:ASN:HD21	3:A:1366:ARG:HH11	1.60	0.49
4:B:708:GLU:C	4:B:710:LEU:H	2.16	0.49
4:B:800:GLN:OE1	4:B:822:ASN:HB2	2.12	0.49
4:B:999:MET:HE2	4:B:1011:ILE:HD11	1.94	0.49
3:A:511:ILE:HG12	3:A:521:MET:CE	2.42	0.49
4:B:805:THR:HA	4:B:809:MET:HE1	1.95	0.49
4:B:488:TYR:CE2	4:B:813:LYS:HB2	2.48	0.49
3:A:918:GLU:O	3:A:918:GLU:HG3	2.12	0.49
4:B:1054:GLY:O	4:B:1058:LEU:HG	2.13	0.49
1:D:2:DA:C5'	3:A:1403:GLU:HB3	2.43	0.49
3:A:378:GLU:HG2	3:A:388:LEU:HD11	1.95	0.49
3:A:874:ASP:HA	3:A:1058:VAL:HG22	1.95	0.49
8:H:36:CYS:HA	8:H:126:GLU:O	2.13	0.49
5:C:254:LYS:O	5:C:258:ILE:HD13	2.13	0.49
4:B:185:THR:O	4:B:189:LEU:HG	2.11	0.49
6:E:102:GLU:O	6:E:104:ASN:N	2.46	0.49
3:A:890:ASP:H	3:A:1296:GLY:HA3	1.77	0.49
3:A:1066:VAL:O	3:A:1068:ALA:N	2.46	0.49
5:C:212:PRO:HB3	5:C:213:PRO:HD2	1.95	0.49
8:H:118:PHE:HB2	8:H:121:LEU:HB2	1.95	0.49
4:B:1053:GLU:O	4:B:1054:GLY:C	2.50	0.49
7:F:82:THR:HG22	7:F:84:TYR:N	2.27	0.49
4:B:977:GLY:CA	4:B:1099:VAL:CG2	2.86	0.49
1:D:6:DC:H4'	3:A:447:GLN:HE22	1.78	0.49
8:H:6:PHE:HE1	8:H:130:ARG:NE	2.10	0.49
4:B:1118:PRO:HD3	4:B:1155:SER:HA	1.94	0.49
3:A:475:THR:CG2	3:A:476:SER:N	2.76	0.49
6:E:80:VAL:HG22	6:E:109:ILE:HD12	1.94	0.49
3:A:1150:SER:HB2	3:A:1195:LEU:HD23	1.93	0.49
9:I:55:THR:HG21	9:I:109:ILE:HD13	1.93	0.49
4:B:1182:CYS:O	4:B:1183:LYS:O	2.31	0.49
4:B:781:PHE:O	4:B:782:LEU:HG	2.12	0.49
3:A:69:THR:HG22	3:A:69:THR:O	2.12	0.49
4:B:821:GLN:OE1	4:B:850:LEU:HD12	2.13	0.49
4:B:171:PRO:HD2	4:B:457:LEU:CD1	2.43	0.49
9:I:85:PHE:O	9:I:86:PHE:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1348:LEU:CD2	3:A:1372:VAL:HG13	2.39	0.49
4:B:1160:VAL:HG11	4:B:1169:MET:SD	2.53	0.49
11:K:83:PRO:HA	11:K:86:ALA:HB3	1.95	0.49
5:C:142:VAL:H	10:J:16:ASP:HB3	1.77	0.49
4:B:1053:GLU:O	4:B:1055:ILE:N	2.46	0.48
3:A:5:GLN:O	4:B:1159:ARG:NH2	2.46	0.48
10:J:7:CYS:O	10:J:8:PHE:C	2.50	0.48
9:I:7:CYS:CB	9:I:14:LEU:HD21	2.32	0.48
3:A:994:GLN:NE2	3:A:1019:CYS:HB3	2.27	0.48
4:B:1177:HIS:CB	4:B:1179:GLN:HE21	2.24	0.48
3:A:1099:PRO:O	3:A:1102:LYS:HB3	2.13	0.48
3:A:538:ASP:OD1	8:H:22:LYS:HB2	2.12	0.48
3:A:474:VAL:HG13	3:A:478:TYR:CE1	2.48	0.48
3:A:491:VAL:O	3:A:493:GLN:NE2	2.46	0.48
8:H:39:THR:O	8:H:123:MET:HA	2.14	0.48
3:A:1386:ARG:HE	3:A:1387:HIS:CE1	2.32	0.48
3:A:1392:SER:O	3:A:1393:ASN:CG	2.52	0.48
4:B:737:THR:HG23	9:I:66:PRO:HB2	1.93	0.48
3:A:589:GLN:OE1	3:A:591:PHE:HE1	1.96	0.48
4:B:1106:ARG:HH21	4:B:1109:GLY:C	2.16	0.48
3:A:1284:MET:HG2	3:A:1306:LEU:CD2	2.43	0.48
4:B:487:THR:HG22	4:B:489:SER:N	2.24	0.48
10:J:44:TYR:HA	10:J:47:ARG:HB2	1.94	0.48
6:E:102:GLU:C	6:E:104:ASN:N	2.67	0.48
4:B:1060:ARG:O	4:B:1063:GLY:N	2.45	0.48
9:I:99:LEU:HB2	9:I:112:SER:HB3	1.94	0.48
4:B:25:ILE:CG2	4:B:29:ASP:CB	2.90	0.48
3:A:783:THR:HG21	3:A:815:PHE:CE2	2.48	0.48
3:A:1406:VAL:CG1	3:A:1410:PHE:HE1	2.26	0.48
12:L:31:CYS:SG	12:L:34:CYS:SG	3.11	0.48
3:A:365:GLY:O	3:A:468:PHE:HA	2.14	0.48
2:R:9:A:C3'	2:R:9:A:C8	2.96	0.48
3:A:226:GLU:CG	3:A:227:VAL:N	2.75	0.48
8:H:84:ALA:HB1	8:H:87:ARG:HB2	1.94	0.48
5:C:142:VAL:H	10:J:16:ASP:CB	2.26	0.48
2:R:6:G:O2'	2:R:7:G:H5'	2.13	0.48
3:A:954:TRP:O	3:A:956:LEU:HG	2.14	0.48
4:B:227:LYS:HB2	4:B:395:GLN:OE1	2.14	0.48
4:B:726:ALA:HB1	4:B:1051:THR:CG2	2.43	0.48
4:B:653:VAL:HG12	4:B:654:ARG:N	2.28	0.48
3:A:154:SER:HB3	3:A:162:VAL:HG21	1.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:674:PRO:O	3:A:677:ARG:HB3	2.14	0.48
3:A:178:GLY:O	3:A:179:LEU:HD23	2.13	0.48
3:A:829:VAL:C	3:A:831:THR:H	2.15	0.48
4:B:380:TYR:CE1	4:B:384:ARG:HD3	2.48	0.48
3:A:61:ILE:HG22	3:A:62:ASP:N	2.16	0.48
3:A:418:SER:HB3	3:A:421:ALA:HB2	1.94	0.48
3:A:1152:ILE:HG23	3:A:1260:LEU:CD2	2.43	0.48
3:A:226:GLU:HG2	3:A:227:VAL:N	2.29	0.48
3:A:1100:ARG:NH2	3:A:1330:ASN:HB2	2.28	0.48
4:B:284:ILE:CD1	4:B:324:ILE:HD12	2.43	0.48
5:C:62:PHE:O	5:C:66:ARG:HG3	2.13	0.48
5:C:75:MET:HG3	5:C:246:ARG:NH2	2.28	0.48
3:A:381:THR:O	3:A:384:ASN:N	2.41	0.48
5:C:43:THR:HG22	5:C:44:LEU:N	2.29	0.48
10:J:57:ILE:HG12	10:J:61:LEU:HD11	1.94	0.48
7:F:87:LYS:HE2	7:F:88:TYR:CE1	2.48	0.48
6:E:78:LEU:HD21	6:E:80:VAL:HG22	1.95	0.48
3:A:1074:GLU:C	3:A:1076:ALA:N	2.67	0.48
3:A:994:GLN:HE21	3:A:1019:CYS:CB	2.26	0.48
4:B:806:THR:HG22	4:B:808:ALA:H	1.79	0.48
4:B:280:ILE:HD13	4:B:334:ILE:HG12	1.95	0.48
7:F:81:THR:HG22	7:F:82:THR:H	1.78	0.48
4:B:845:SER:HB2	10:J:8:PHE:HB3	1.96	0.48
3:A:89:PRO:C	3:A:204:THR:HG21	2.33	0.48
3:A:352:VAL:HG12	3:A:353:ILE:N	2.29	0.48
3:A:391:LEU:O	3:A:394:ASN:N	2.46	0.48
1:D:5:DG:N2	2:R:8:C:N3	2.61	0.48
9:I:62:ILE:CG2	9:I:63:GLY:N	2.77	0.48
4:B:890:TYR:O	4:B:892:LYS:N	2.46	0.48
6:E:135:PHE:HD2	6:E:140:LEU:HD21	1.79	0.48
3:A:817:ALA:HA	4:B:764:SER:HG	1.79	0.48
9:I:50:THR:HG22	9:I:51:ASN:N	2.28	0.48
3:A:89:PRO:HG3	3:A:208:LEU:CD1	2.44	0.48
4:B:51:PHE:CD2	4:B:173:MET:HB3	2.49	0.48
11:K:83:PRO:O	11:K:87:LEU:N	2.46	0.48
3:A:112:LYS:HG2	3:A:113:LEU:H	1.79	0.48
3:A:376:TYR:CD2	3:A:376:TYR:C	2.87	0.48
3:A:1412:ALA:HA	3:A:1417:GLU:OE2	2.14	0.48
3:A:869:GLY:O	6:E:204:THR:HG21	2.14	0.48
11:K:10:PHE:CE1	11:K:11:LEU:HD13	2.49	0.48
3:A:418:SER:C	3:A:420:ARG:N	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:363:HIS:CD2	4:B:585:VAL:HG22	2.49	0.48
5:C:67:LEU:HD11	5:C:155:LEU:HD13	1.95	0.48
4:B:750:GLY:O	4:B:751:VAL:C	2.53	0.48
3:A:18:GLN:O	4:B:1215:ARG:CG	2.62	0.48
4:B:1065:GLN:HE22	4:B:1067:ARG:HG2	1.79	0.48
4:B:956:THR:HG21	4:B:960:GLY:HA2	1.96	0.48
3:A:913:LEU:HD11	3:A:981:LEU:O	2.13	0.48
3:A:14:VAL:H	3:A:1432:GLN:HE22	1.61	0.48
8:H:93:TYR:HA	8:H:145:ARG:CB	2.41	0.48
4:B:839:MET:HE2	4:B:980:PHE:CD1	2.49	0.48
4:B:46:GLN:HE21	4:B:496:ARG:HG2	1.78	0.48
6:E:100:ILE:CG2	6:E:105:PHE:HB2	2.42	0.48
9:I:54:GLU:O	9:I:89:GLN:HG2	2.14	0.48
3:A:90:VAL:HG21	3:A:296:LEU:HG	1.95	0.48
3:A:1356:ILE:HD12	3:A:1368:MET:SD	2.54	0.48
4:B:291:ILE:HD13	4:B:300:HIS:NE2	2.29	0.47
4:B:284:ILE:HD13	4:B:333:PHE:CD2	2.49	0.47
3:A:68:GLN:NE2	3:A:80:HIS:CB	2.76	0.47
1:D:9:DG:H1	2:R:4:C:H42	1.62	0.47
3:A:265:LYS:HZ1	3:A:323:LYS:H	1.62	0.47
3:A:929:LEU:HD21	3:A:983:ILE:HG21	1.94	0.47
3:A:443:LEU:CD2	3:A:455:MET:HB3	2.42	0.47
8:H:33:GLN:OE1	8:H:129:TYR:CE2	2.67	0.47
4:B:210:LYS:HE2	4:B:461:LEU:O	2.14	0.47
4:B:236:HIS:CE1	4:B:389:ALA:HA	2.49	0.47
5:C:35:ARG:O	5:C:38:ILE:N	2.47	0.47
3:A:786:HIS:CE1	4:B:742:GLU:OE1	2.64	0.47
3:A:1017:LEU:O	3:A:1018:PHE:C	2.53	0.47
4:B:864:LYS:HB3	4:B:871:THR:HA	1.96	0.47
7:F:109:VAL:HG11	7:F:123:LYS:HG2	1.96	0.47
4:B:825:VAL:CG1	4:B:826:ALA:N	2.76	0.47
3:A:1134:ILE:HD11	3:A:1321:GLY:HA3	1.96	0.47
4:B:726:ALA:HB1	4:B:1051:THR:HG21	1.95	0.47
4:B:294:ASP:H	9:I:12:ASN:ND2	2.13	0.47
5:C:66:ARG:CZ	10:J:2:ILE:HG21	2.44	0.47
6:E:7:ARG:C	6:E:9:ILE:H	2.17	0.47
3:A:1237:ILE:HG22	3:A:1238:ILE:N	2.29	0.47
3:A:742:ASN:O	3:A:745:GLN:HB2	2.13	0.47
11:K:59:ALA:HA	11:K:74:ARG:O	2.15	0.47
4:B:773:MET:SD	4:B:987:LYS:HD2	2.54	0.47
4:B:321:GLY:C	4:B:323:VAL:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:300:HIS:ND1	4:B:376:PHE:CD2	2.81	0.47
3:A:783:THR:CG2	3:A:815:PHE:CE2	2.97	0.47
4:B:1077:THR:HG22	4:B:1079:LYS:HB2	1.95	0.47
3:A:332:LYS:N	3:A:337:ARG:HD2	2.28	0.47
3:A:885:THR:HG23	3:A:893:PHE:CE1	2.36	0.47
4:B:1156:ASP:HB3	4:B:1197:PRO:HA	1.95	0.47
4:B:1020:ARG:H	4:B:1020:ARG:HG2	1.51	0.47
4:B:821:GLN:HB2	4:B:851:PHE:CE2	2.49	0.47
11:K:27:ALA:HB1	11:K:28:PRO:HD2	1.95	0.47
4:B:1124:ARG:O	4:B:1125:ASP:HB3	2.14	0.47
11:K:43:GLY:HA2	11:K:71:PHE:CZ	2.49	0.47
7:F:79:ARG:HG2	7:F:146:TRP:CZ2	2.49	0.47
4:B:332:ASP:C	4:B:334:ILE:H	2.17	0.47
4:B:1106:ARG:NH2	4:B:1109:GLY:C	2.67	0.47
4:B:408:LEU:HA	4:B:408:LEU:HD12	1.71	0.47
3:A:1074:GLU:HB3	3:A:1075:PRO:HD3	1.97	0.47
6:E:56:LYS:HG3	6:E:84:ASP:CB	2.42	0.47
5:C:258:ILE:N	5:C:258:ILE:HD12	2.30	0.47
3:A:829:VAL:O	3:A:831:THR:N	2.48	0.47
4:B:798:TYR:CD2	10:J:4:PRO:HG3	2.49	0.47
3:A:1364:ASN:HD22	3:A:1365:TYR:N	2.13	0.47
4:B:123:THR:O	4:B:125:SER:N	2.47	0.47
3:A:804:TYR:HE1	4:B:1021:MET:CE	2.28	0.47
10:J:5:VAL:O	10:J:6:ARG:HB2	2.15	0.47
3:A:20:GLY:HA2	3:A:1413:GLY:O	2.14	0.47
9:I:100:PHE:HZ	9:I:118:ARG:HH12	1.62	0.47
12:L:62:LYS:O	12:L:64:LEU:N	2.37	0.47
4:B:726:ALA:CB	4:B:1051:THR:HG21	2.45	0.47
1:D:3:DA:H5'	3:A:836:TYR:HE1	1.77	0.47
4:B:1098:MET:O	4:B:1099:VAL:C	2.53	0.47
4:B:1104:HIS:HB2	4:B:1122:ARG:CD	2.44	0.47
3:A:383:TYR:HB3	7:F:115:THR:CG2	2.44	0.47
3:A:1410:PHE:C	3:A:1412:ALA:N	2.68	0.47
8:H:125:LEU:HG	8:H:130:ARG:CZ	2.43	0.47
4:B:1013:ASN:OD1	4:B:1015:HIS:HB2	2.15	0.47
3:A:1436:ILE:CG2	3:A:1437:GLY:H	2.22	0.47
6:E:58:MET:O	6:E:59:SER:C	2.53	0.47
4:B:100:PRO:HD2	4:B:180:TYR:CE1	2.50	0.47
4:B:1158:PHE:HE2	4:B:1201:LYS:HE3	1.80	0.47
4:B:566:LEU:CD1	4:B:588:GLY:HA2	2.44	0.47
4:B:298:LEU:N	4:B:298:LEU:HD23	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:738:LYS:HB3	8:H:19:ARG:HH22	1.78	0.47
3:A:1327:ILE:O	6:E:147:HIS:HE1	1.98	0.47
3:A:12:ARG:HD3	4:B:1218:THR:HB	1.97	0.47
3:A:515:GLN:HA	3:A:1367:HIS:NE2	2.29	0.47
5:C:75:MET:HG3	5:C:246:ARG:HH22	1.77	0.47
4:B:230:ALA:C	4:B:232:SER:H	2.17	0.47
4:B:830:TYR:CE2	4:B:1000:PRO:HD3	2.50	0.47
3:A:679:ILE:HG23	3:A:729:ALA:CB	2.39	0.47
4:B:1116:ARG:NH1	4:B:1198:TYR:CD1	2.83	0.47
7:F:101:ILE:HD13	7:F:120:ILE:CG2	2.45	0.47
7:F:101:ILE:HD11	7:F:124:GLU:OE1	2.15	0.47
3:A:1225:PHE:O	3:A:1240:CYS:HA	2.14	0.47
8:H:138:GLU:O	8:H:139:ASN:C	2.53	0.47
4:B:851:PHE:O	4:B:974:PRO:HD3	2.15	0.47
3:A:890:ASP:N	3:A:1296:GLY:HA3	2.30	0.47
12:L:30:ILE:CD1	12:L:59:ALA:HA	2.44	0.47
3:A:22:PHE:HB2	4:B:1211:ASN:CG	2.35	0.47
4:B:1033:LYS:NZ	4:B:1070:GLU:OE1	2.46	0.47
3:A:568:PRO:HB2	5:C:221:TYR:CZ	2.50	0.47
3:A:567:LYS:NZ	8:H:95:TYR:CD1	2.80	0.47
3:A:666:ILE:O	3:A:667:GLY:C	2.53	0.47
4:B:842:ASN:HD22	4:B:845:SER:HB3	1.80	0.47
3:A:540:PHE:C	3:A:541:ILE:HD12	2.35	0.47
4:B:1117:GLN:NE2	4:B:1156:ASP:OD2	2.48	0.47
7:F:98:ALA:O	7:F:117:PRO:HB2	2.14	0.47
3:A:881:GLN:OE1	3:A:959:ASN:HA	2.15	0.47
3:A:116:ASP:HB2	3:A:118:HIS:CD2	2.49	0.47
3:A:1392:SER:O	3:A:1393:ASN:ND2	2.48	0.47
3:A:381:THR:CG2	3:A:383:TYR:CD1	2.98	0.47
1:D:6:DC:H2'	1:D:7:DC:C6	2.50	0.47
4:B:167:ILE:HG22	4:B:167:ILE:O	2.14	0.47
3:A:530:GLY:O	3:A:531:ILE:C	2.54	0.47
3:A:83:HIS:CE1	3:A:238:CYS:SG	3.08	0.47
3:A:1074:GLU:C	3:A:1076:ALA:H	2.18	0.47
3:A:1227:ILE:HG22	3:A:1228:TRP:N	2.30	0.47
3:A:573:SER:OG	3:A:576:GLN:HG3	2.15	0.47
4:B:96:TYR:CD1	4:B:96:TYR:N	2.83	0.47
4:B:332:ASP:C	4:B:334:ILE:N	2.68	0.46
4:B:780:VAL:HG21	10:J:56:LEU:HD11	1.97	0.46
3:A:351:THR:CG2	4:B:1103:ILE:HA	2.36	0.46
4:B:800:GLN:CB	10:J:52:THR:CG2	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:906:SER:CB	4:B:946:ASN:HB2	2.46	0.46
8:H:113:ALA:HA	8:H:125:LEU:O	2.15	0.46
6:E:96:PHE:CE2	6:E:110:PHE:HB2	2.50	0.46
9:I:74:GLU:OE1	9:I:79:HIS:ND1	2.47	0.46
3:A:1209:MET:CG	3:A:1236:LEU:HD22	2.45	0.46
4:B:1169:MET:SD	4:B:1201:LYS:HG2	2.54	0.46
4:B:1169:MET:HE3	4:B:1205:GLN:HG2	1.98	0.46
5:C:18:VAL:O	5:C:18:VAL:HG12	2.15	0.46
4:B:1182:CYS:O	4:B:1183:LYS:HD2	2.15	0.46
3:A:849:MET:HB2	3:A:1063:MET:SD	2.55	0.46
4:B:758:PHE:C	4:B:760:ASP:N	2.68	0.46
5:C:263:THR:C	5:C:265:MET:H	2.18	0.46
5:C:180:TYR:O	5:C:181:ASP:HB3	2.15	0.46
4:B:300:HIS:ND1	4:B:376:PHE:CE2	2.83	0.46
3:A:1149:ALA:CB	9:I:47:GLU:HA	2.45	0.46
4:B:31:TRP:CE3	4:B:34:ILE:HD12	2.50	0.46
4:B:1200:ALA:O	4:B:1201:LYS:C	2.54	0.46
4:B:871:THR:HG22	4:B:872:GLU:O	2.14	0.46
4:B:225:VAL:HG11	4:B:388:CYS:HB3	1.95	0.46
9:I:34:TYR:O	9:I:35:VAL:HG23	2.16	0.46
4:B:324:ILE:HG23	4:B:329:THR:HB	1.96	0.46
4:B:640:VAL:HG12	4:B:640:VAL:O	2.15	0.46
10:J:48:ARG:HH21	10:J:49:MET:CE	2.24	0.46
3:A:531:ILE:CD1	3:A:617:VAL:HG11	2.44	0.46
3:A:893:PHE:CD1	3:A:940:ARG:HD2	2.50	0.46
5:C:258:ILE:HG23	11:K:19:LEU:HD11	1.96	0.46
3:A:964:ILE:HD13	3:A:1035:TYR:CZ	2.50	0.46
3:A:848:ILE:CD1	3:A:1374:VAL:HG21	2.45	0.46
3:A:1277:GLU:O	3:A:1278:ASN:HB2	2.14	0.46
3:A:975:HIS:ND1	3:A:1036:ARG:HG3	2.30	0.46
3:A:563:PRO:HG3	3:A:572:TRP:CH2	2.48	0.46
4:B:1072:MET:O	4:B:1081:LEU:HB2	2.15	0.46
4:B:802:PRO:HA	4:B:822:ASN:HD21	1.79	0.46
3:A:897:TYR:HD2	3:A:936:LEU:HD13	1.78	0.46
6:E:96:PHE:CE1	6:E:100:ILE:HD11	2.50	0.46
5:C:5:GLY:O	5:C:6:PRO:C	2.54	0.46
3:A:1394:THR:HG21	3:A:1398:MET:SD	2.56	0.46
3:A:167:CYS:C	3:A:169:ASN:H	2.18	0.46
4:B:890:TYR:C	4:B:892:LYS:H	2.19	0.46
6:E:179:GLN:OE1	6:E:179:GLN:HA	2.16	0.46
5:C:62:PHE:C	5:C:62:PHE:CD2	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1237:ILE:CG2	3:A:1238:ILE:N	2.78	0.46
4:B:800:GLN:HB3	10:J:52:THR:HG22	1.97	0.46
5:C:252:GLN:CG	11:K:95:ILE:HG23	2.46	0.46
4:B:1177:HIS:C	4:B:1179:GLN:N	2.68	0.46
9:I:2:THR:OG1	9:I:45:ARG:HB3	2.15	0.46
4:B:282:ILE:HG13	4:B:283:VAL:N	2.31	0.46
4:B:1120:GLU:HG2	4:B:1121:GLY:N	2.31	0.46
3:A:152:VAL:CG1	3:A:153:PRO:HD2	2.45	0.46
3:A:1140:HIS:HB2	3:A:1276:VAL:O	2.16	0.46
3:A:542:GLU:C	3:A:546:VAL:HG23	2.36	0.46
8:H:26:ILE:HD13	8:H:49:VAL:HG11	1.97	0.46
3:A:517:ASN:OD1	3:A:517:ASN:O	2.34	0.46
12:L:55:ILE:H	12:L:55:ILE:HG12	1.53	0.46
3:A:535:THR:HG21	3:A:616:VAL:CA	2.43	0.46
4:B:860:MET:HB2	4:B:965:LYS:HG2	1.97	0.46
4:B:62:ILE:HG21	4:B:417:PHE:HD2	1.80	0.46
3:A:67:CYS:SG	3:A:77:CYS:SG	3.11	0.46
4:B:199:MET:N	4:B:199:MET:SD	2.87	0.46
4:B:519:TRP:HE1	4:B:635:ARG:HH22	1.64	0.46
2:R:2:A:H2'	2:R:3:C:H5'	1.91	0.46
3:A:294:SER:HA	3:A:297:GLN:HB3	1.96	0.46
3:A:645:LEU:O	3:A:649:ILE:HG13	2.15	0.46
3:A:222:LEU:O	3:A:224:PHE:N	2.46	0.46
4:B:1060:ARG:C	4:B:1062:HIS:N	2.69	0.46
4:B:1017:ILE:HB	4:B:1018:PRO:HD3	1.98	0.46
8:H:47:PHE:CD1	8:H:95:TYR:HB2	2.50	0.46
3:A:1405:THR:O	3:A:1406:VAL:C	2.54	0.46
3:A:418:SER:O	3:A:421:ALA:N	2.49	0.46
4:B:361:LEU:N	4:B:362:PRO:HD2	2.31	0.46
4:B:574:SER:HB3	4:B:577:ALA:HB2	1.98	0.46
5:C:249:ASP:O	5:C:252:GLN:HB3	2.16	0.46
3:A:50:ILE:HG22	3:A:51:GLY:H	1.81	0.46
3:A:53:LEU:HD13	3:A:263:THR:HG23	1.97	0.46
3:A:556:TRP:CZ3	3:A:558:GLY:HA2	2.51	0.46
5:C:38:ILE:HG13	5:C:176:ILE:HD12	1.97	0.46
4:B:238:ALA:HB3	4:B:256:VAL:HB	1.98	0.46
3:A:1041:ALA:O	3:A:1044:TRP:HB3	2.15	0.46
4:B:704:ALA:HB2	4:B:738:PHE:CE1	2.51	0.46
5:C:242:GLN:OE1	5:C:242:GLN:HA	2.16	0.46
3:A:1166:ASP:CG	3:A:1194:ARG:HH21	2.19	0.46
3:A:549:MET:HE1	3:A:656:TRP:CD1	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:477:PRO:HG2	3:A:521:MET:HG2	1.97	0.46
3:A:1208:THR:HG22	3:A:1210:GLY:H	1.81	0.46
3:A:1173:HIS:CD2	3:A:1227:ILE:HG23	2.51	0.46
3:A:35:ILE:HD12	3:A:241:VAL:HG21	1.98	0.46
3:A:50:ILE:C	3:A:52:GLY:N	2.69	0.46
4:B:345:LYS:O	4:B:347:LYS:N	2.49	0.46
3:A:517:ASN:ND2	3:A:1362:TYR:CE2	2.83	0.46
4:B:276:ILE:HD13	4:B:334:ILE:CG2	2.47	0.46
4:B:25:ILE:HD11	4:B:653:VAL:CB	2.46	0.46
4:B:1100:ASP:HA	4:B:1103:ILE:CG1	2.46	0.46
4:B:914:LYS:H	4:B:938:SER:HB3	1.81	0.46
4:B:589:VAL:HG12	4:B:590:HIS:H	1.81	0.46
4:B:864:LYS:H	4:B:872:GLU:CG	2.28	0.46
3:A:446:ARG:HG2	3:A:446:ARG:NH1	2.28	0.46
4:B:185:THR:H	4:B:188:ASP:HB2	1.81	0.46
11:K:73:LEU:CD2	11:K:75:ILE:HD11	2.46	0.46
3:A:738:LYS:NZ	5:C:194:GLU:CA	2.79	0.46
4:B:892:LYS:NZ	4:B:909:ASP:OD2	2.47	0.46
3:A:923:LEU:O	3:A:927:VAL:HG23	2.14	0.45
4:B:605:ARG:CZ	4:B:639:ILE:HD13	2.46	0.45
4:B:230:ALA:N	4:B:231:PRO:HD2	2.31	0.45
4:B:1154:ALA:O	4:B:1155:SER:CB	2.64	0.45
4:B:215:GLN:HB2	4:B:407:ASP:HB2	1.97	0.45
4:B:995:ARG:NH1	4:B:997:GLU:OE1	2.49	0.45
3:A:112:LYS:HG2	3:A:113:LEU:N	2.31	0.45
4:B:322:PHE:O	4:B:322:PHE:CG	2.69	0.45
6:E:10:SER:O	6:E:14:ARG:HG3	2.16	0.45
3:A:1317:MET:CA	3:A:1322:ILE:HD11	2.46	0.45
4:B:640:VAL:HG23	4:B:740:HIS:HA	1.97	0.45
4:B:653:VAL:C	4:B:654:ARG:HG2	2.36	0.45
4:B:201:GLY:H	4:B:202:TYR:HD2	1.63	0.45
4:B:1106:ARG:CD	4:B:1126:GLY:O	2.62	0.45
3:A:223:GLY:HA3	3:A:1415:SER:HB3	1.98	0.45
4:B:1198:TYR:HE1	4:B:1201:LYS:HZ2	1.64	0.45
5:C:262:LEU:O	5:C:265:MET:HB3	2.15	0.45
8:H:49:VAL:CG1	8:H:50:ALA:H	2.27	0.45
4:B:708:GLU:CG	4:B:709:ASP:N	2.69	0.45
3:A:47:ARG:O	3:A:48:ALA:HB2	2.16	0.45
10:J:1:MET:O	10:J:2:ILE:O	2.33	0.45
4:B:1085:ILE:CG2	4:B:1086:PHE:N	2.78	0.45
3:A:658:LEU:HD13	4:B:831:SER:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1208:THR:HG22	3:A:1210:GLY:N	2.31	0.45
8:H:114:VAL:O	8:H:124:ARG:HA	2.16	0.45
3:A:1336:MET:SD	3:A:1381:LEU:HG	2.56	0.45
3:A:1037:LEU:HD13	3:A:1042:PHE:HA	1.98	0.45
4:B:295:GLY:O	4:B:299:GLU:HG3	2.16	0.45
3:A:889:SER:HB3	3:A:1297:GLU:HG3	1.97	0.45
8:H:26:ILE:CD1	8:H:49:VAL:HG11	2.46	0.45
3:A:1155:ASP:OD1	3:A:1162:VAL:HG23	2.17	0.45
4:B:229:ALA:HB1	4:B:231:PRO:HD2	1.98	0.45
3:A:1208:THR:N	3:A:1211:GLN:OE1	2.49	0.45
8:H:101:ALA:HB2	8:H:116:TYR:CD2	2.51	0.45
3:A:573:SER:H	3:A:576:GLN:HG3	1.81	0.45
3:A:701:LEU:HA	9:I:115:LYS:HE3	1.98	0.45
4:B:371:GLU:N	4:B:371:GLU:OE1	2.49	0.45
3:A:567:LYS:CD	3:A:568:PRO:HD2	2.45	0.45
8:H:123:MET:HE1	8:H:142:LEU:HD13	1.97	0.45
4:B:1085:ILE:HG22	4:B:1086:PHE:N	2.31	0.45
9:I:75:CYS:C	9:I:77:LYS:H	2.20	0.45
4:B:314:LEU:O	4:B:315:LYS:C	2.53	0.45
4:B:980:PHE:HE1	4:B:990:ILE:CD1	2.30	0.45
4:B:549:THR:H	4:B:628:THR:HG22	1.81	0.45
3:A:1209:MET:CE	3:A:1236:LEU:HB3	2.47	0.45
4:B:1158:PHE:CD2	4:B:1198:TYR:HD1	2.35	0.45
8:H:116:TYR:HE2	8:H:140:ALA:CB	2.30	0.45
11:K:91:CYS:O	11:K:94:ILE:HB	2.16	0.45
4:B:370:PHE:N	4:B:371:GLU:OE1	2.50	0.45
4:B:893:LEU:HD22	4:B:897:GLY:O	2.16	0.45
4:B:707:PRO:O	4:B:708:GLU:O	2.35	0.45
4:B:824:ILE:CG2	4:B:1087:PHE:CE2	3.00	0.45
9:I:75:CYS:O	9:I:76:PRO:C	2.52	0.45
9:I:8:ARG:HG3	9:I:9:ASP:CG	2.37	0.45
3:A:420:ARG:O	3:A:424:ILE:HG13	2.16	0.45
4:B:994:TYR:HD1	4:B:999:MET:HE3	1.81	0.45
3:A:329:LEU:HA	3:A:335:ARG:HB2	1.98	0.45
5:C:8:VAL:CG1	5:C:9:LYS:N	2.80	0.45
3:A:644:LYS:O	3:A:645:LEU:C	2.55	0.45
6:E:147:HIS:CD2	6:E:149:LEU:H	2.35	0.45
9:I:34:TYR:O	9:I:35:VAL:CG2	2.65	0.45
5:C:120:ILE:HD11	5:C:130:GLY:O	2.17	0.45
5:C:17:ASN:OD1	5:C:233:GLU:HG2	2.16	0.45
3:A:958:VAL:HG22	3:A:1052:GLN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:377:PHE:C	4:B:379:GLY:N	2.68	0.45
9:I:99:LEU:HB2	9:I:112:SER:CB	2.46	0.45
4:B:1051:THR:HG21	4:B:1053:GLU:HB2	1.97	0.45
4:B:977:GLY:C	4:B:1099:VAL:HG23	2.37	0.45
3:A:388:LEU:O	3:A:392:VAL:HG23	2.17	0.45
8:H:111:LEU:HA	8:H:127:GLY:O	2.17	0.45
5:C:9:LYS:HB2	5:C:21:ILE:HB	1.98	0.45
7:F:117:PRO:O	7:F:120:ILE:HB	2.16	0.45
3:A:69:THR:O	4:B:1174:LYS:HG2	2.17	0.45
8:H:84:ALA:HA	8:H:87:ARG:HB2	1.98	0.45
4:B:50:SER:O	4:B:53:GLN:HB3	2.16	0.45
4:B:365:THR:CG2	4:B:367:LEU:H	2.30	0.45
6:E:112:TYR:CE2	6:E:134:THR:HB	2.51	0.45
8:H:40:LEU:HG	8:H:42:ILE:HG13	1.98	0.45
3:A:666:ILE:H	3:A:666:ILE:HG13	1.33	0.45
4:B:702:LEU:HD21	4:B:735:ALA:HB1	1.98	0.45
3:A:55:ASP:HB3	3:A:56:PRO:HD3	1.98	0.45
12:L:45:ALA:O	12:L:46:VAL:CG2	2.64	0.45
3:A:1192:LEU:HD11	3:A:1239:ARG:CB	2.37	0.45
4:B:168:GLY:H	4:B:450:ALA:HB1	1.82	0.45
4:B:744:HIS:CD2	4:B:746:SER:OG	2.70	0.45
11:K:12:LEU:CD1	11:K:12:LEU:H	2.23	0.45
12:L:34:CYS:HG	12:L:51:CYS:HG	1.57	0.45
4:B:864:LYS:HD3	4:B:871:THR:CA	2.47	0.45
3:A:778:GLY:HA3	4:B:516:ASN:CB	2.46	0.45
11:K:61:TYR:CD1	11:K:61:TYR:C	2.89	0.45
4:B:276:ILE:HD13	4:B:334:ILE:HG23	1.99	0.45
3:A:78:PRO:O	3:A:79:GLY:C	2.56	0.45
5:C:166:GLU:CG	11:K:10:PHE:CZ	2.96	0.45
8:H:57:VAL:HG12	8:H:58:THR:N	2.32	0.45
4:B:1106:ARG:HG2	4:B:1107:ALA:N	2.31	0.45
8:H:81:PRO:HD2	8:H:82:PRO:HD2	1.98	0.45
4:B:963:PHE:HE2	4:B:965:LYS:HE3	1.81	0.45
3:A:233:TRP:O	3:A:235:ILE:N	2.50	0.45
12:L:38:LEU:HG	12:L:39:SER:H	1.82	0.45
4:B:56:ASP:HB3	4:B:57:TYR:CD1	2.52	0.45
3:A:340:LEU:HD21	4:B:1200:ALA:CA	2.47	0.45
4:B:515:HIS:CD2	4:B:517:THR:OG1	2.66	0.45
4:B:680:THR:O	4:B:683:SER:OG	2.34	0.45
3:A:456:MET:HB2	3:A:478:TYR:OH	2.17	0.45
6:E:190:LEU:HD11	6:E:196:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:186:LEU:HD12	5:C:186:LEU:HA	1.86	0.45
8:H:40:LEU:HD13	8:H:123:MET:HB2	1.99	0.45
4:B:200:GLY:HA2	4:B:202:TYR:CD2	2.50	0.45
9:I:7:CYS:HB2	9:I:14:LEU:CD2	2.34	0.45
5:C:236:GLY:C	5:C:238:ILE:N	2.69	0.45
3:A:1410:PHE:C	3:A:1412:ALA:H	2.19	0.45
6:E:205:SER:O	6:E:206:GLY:C	2.54	0.45
9:I:92:ARG:CG	9:I:93:LYS:H	2.30	0.45
4:B:426:LYS:O	4:B:430:ARG:HG3	2.17	0.45
3:A:858:ASN:ND2	3:A:858:ASN:C	2.68	0.45
3:A:974:ASP:CB	8:H:136:LYS:NZ	2.80	0.45
3:A:152:VAL:HG13	3:A:153:PRO:HD2	1.99	0.45
3:A:1155:ASP:CG	3:A:1162:VAL:HG23	2.37	0.44
4:B:958:GLN:C	4:B:960:GLY:H	2.20	0.44
6:E:7:ARG:C	6:E:9:ILE:N	2.71	0.44
4:B:912:ILE:O	4:B:938:SER:CB	2.59	0.44
4:B:316:PRO:HA	4:B:319:GLU:HG2	1.98	0.44
4:B:526:GLU:CD	4:B:752:ALA:HB3	2.38	0.44
8:H:24:CYS:CB	8:H:44:VAL:HG21	2.47	0.44
4:B:973:ILE:CG2	4:B:974:PRO:HD2	2.47	0.44
4:B:216:GLU:OE1	4:B:537:LYS:CE	2.66	0.44
6:E:94:LYS:O	6:E:98:ILE:HG13	2.16	0.44
4:B:260:GLY:HA3	4:B:267:ARG:HG2	1.98	0.44
3:A:210:ILE:O	3:A:214:ILE:HG13	2.17	0.44
6:E:82:PHE:N	6:E:82:PHE:CD1	2.85	0.44
4:B:640:VAL:HG23	4:B:740:HIS:CA	2.48	0.44
3:A:243:PRO:HB2	3:A:245:PRO:HD2	1.99	0.44
5:C:39:ALA:HA	5:C:164:ALA:CB	2.46	0.44
3:A:1441:PHE:HB2	7:F:134:ILE:CG2	2.47	0.44
3:A:1436:ILE:O	3:A:1437:GLY:C	2.56	0.44
11:K:78:THR:O	11:K:79:GLU:C	2.56	0.44
3:A:1409:LEU:HD23	3:A:1409:LEU:HA	1.83	0.44
4:B:1185:CYS:O	4:B:1186:ASP:HB2	2.17	0.44
5:C:31:ASN:O	5:C:32:SER:C	2.56	0.44
4:B:847:ASP:O	5:C:65:HIS:HE1	2.01	0.44
4:B:709:ASP:C	4:B:710:LEU:HD23	2.38	0.44
3:A:54:ASN:O	3:A:55:ASP:HB2	2.18	0.44
3:A:901:LEU:HD13	3:A:919:ILE:CG2	2.48	0.44
5:C:62:PHE:C	5:C:62:PHE:HD2	2.20	0.44
4:B:800:GLN:CB	10:J:52:THR:HG22	2.47	0.44
3:A:709:THR:C	3:A:711:ARG:N	2.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:247:GLY:O	4:B:248:SER:HB3	2.17	0.44
11:K:24:ASP:HB3	11:K:30:ALA:CB	2.47	0.44
3:A:466:SER:HB3	11:K:2:ASN:HD22	1.82	0.44
3:A:1046:LEU:O	3:A:1047:SER:C	2.55	0.44
5:C:123:ASN:ND2	5:C:125:MET:HG2	2.31	0.44
3:A:848:ILE:HD13	3:A:864:ILE:HD13	1.98	0.44
10:J:16:ASP:OD1	10:J:17:LYS:HG3	2.17	0.44
5:C:31:ASN:O	5:C:35:ARG:HG3	2.17	0.44
3:A:494:SER:HB2	3:A:497:THR:OG1	2.18	0.44
12:L:43:THR:O	12:L:43:THR:HG22	2.18	0.44
4:B:664:THR:HG1	4:B:678:GLU:N	2.14	0.44
9:I:98:VAL:CG1	9:I:99:LEU:N	2.81	0.44
4:B:332:ASP:O	4:B:334:ILE:N	2.50	0.44
4:B:957:ASN:O	4:B:958:GLN:C	2.55	0.44
5:C:173:ALA:O	5:C:174:ALA:CB	2.64	0.44
4:B:690:VAL:HG12	4:B:691:GLU:N	2.33	0.44
8:H:5:LEU:O	8:H:133:ASN:HB3	2.17	0.44
3:A:458:HIS:ND1	3:A:507:VAL:HG21	2.33	0.44
4:B:100:PRO:HA	4:B:125:SER:O	2.16	0.44
4:B:65:GLU:HG3	4:B:66:ASP:N	2.27	0.44
4:B:864:LYS:HD3	4:B:871:THR:CB	2.47	0.44
7:F:109:VAL:HG12	7:F:110:ASP:H	1.82	0.44
4:B:806:THR:C	4:B:808:ALA:N	2.70	0.44
3:A:825:ILE:C	3:A:827:THR:N	2.70	0.44
4:B:205:ILE:HG12	4:B:461:LEU:HB3	1.99	0.44
4:B:1038:SER:HB3	4:B:1062:HIS:NE2	2.32	0.44
5:C:52:GLU:HB3	5:C:154:LYS:HB3	1.99	0.44
3:A:103:CYS:O	3:A:106:VAL:O	2.35	0.44
3:A:571:LEU:HD22	8:H:46:LEU:HD11	1.99	0.44
3:A:1114:PRO:O	3:A:1330:ASN:OD1	2.35	0.44
6:E:133:GLU:HB3	6:E:135:PHE:HE1	1.83	0.44
3:A:525:GLN:HB2	4:B:835:GLN:HG2	2.00	0.44
2:R:8:C:H2'	2:R:9:A:C8	2.52	0.44
4:B:100:PRO:O	4:B:180:TYR:OH	2.31	0.44
3:A:968:GLN:NE2	3:A:1035:TYR:HB2	2.33	0.44
3:A:84:ILE:HG23	3:A:84:ILE:O	2.17	0.44
3:A:219:PHE:CE2	3:A:231:PRO:HD2	2.52	0.44
10:J:32:GLU:CD	10:J:32:GLU:H	2.20	0.44
3:A:829:VAL:C	3:A:831:THR:N	2.70	0.44
3:A:1121:GLU:O	3:A:1122:PRO:C	2.56	0.44
4:B:904:ARG:CZ	4:B:948:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:123:MET:HE1	8:H:142:LEU:HD11	1.99	0.44
4:B:650:GLU:HG2	4:B:654:ARG:NH1	2.33	0.44
3:A:783:THR:CG2	3:A:815:PHE:CZ	2.98	0.44
3:A:1118:VAL:O	3:A:1305:VAL:HG13	2.17	0.44
4:B:315:LYS:O	4:B:318:VAL:N	2.46	0.44
4:B:214:ALA:HB2	4:B:408:LEU:CD1	2.48	0.44
11:K:47:ARG:CB	11:K:47:ARG:HH11	2.23	0.44
6:E:28:TYR:CE2	6:E:64:PRO:HG3	2.53	0.44
4:B:686:ASN:C	4:B:688:GLY:N	2.70	0.44
4:B:1171:VAL:HG13	4:B:1191:ILE:HD13	1.99	0.44
6:E:185:ALA:CB	6:E:190:LEU:HD12	2.47	0.44
9:I:106:CYS:O	9:I:107:SER:HB2	2.18	0.44
3:A:13:THR:HG23	3:A:1432:GLN:CD	2.38	0.44
3:A:591:PHE:HD2	3:A:595:THR:HB	1.83	0.44
5:C:77:ILE:CG2	5:C:161:LYS:HE3	2.48	0.44
5:C:148:ARG:HD3	5:C:149:LYS:H	1.83	0.44
3:A:21:LEU:HD21	3:A:95:PHE:CZ	2.53	0.44
4:B:194:GLU:HA	4:B:194:GLU:OE1	2.18	0.44
3:A:1195:LEU:HD11	3:A:1267:MET:HE3	1.99	0.44
3:A:1207:LEU:HA	3:A:1211:GLN:OE1	2.17	0.44
4:B:986:GLN:OE1	4:B:986:GLN:CA	2.64	0.44
3:A:756:ILE:CG2	3:A:757:ASN:N	2.80	0.44
4:B:101:MET:HE2	4:B:169:ARG:NH1	2.33	0.44
3:A:845:LEU:O	3:A:848:ILE:HG13	2.17	0.44
3:A:1349:TYR:O	3:A:1350:LYS:C	2.56	0.44
3:A:1066:VAL:O	3:A:1067:LEU:C	2.55	0.44
5:C:228:PHE:HB2	5:C:230:MET:HE2	2.00	0.44
5:C:69:LEU:HA	5:C:69:LEU:HD12	1.76	0.44
3:A:373:THR:HG21	4:B:1105:ALA:O	2.18	0.44
3:A:1384:VAL:O	3:A:1389:PHE:HE2	2.01	0.44
4:B:1002:THR:CG2	4:B:1004:GLU:HB2	2.47	0.44
6:E:138:ALA:C	6:E:140:LEU:H	2.21	0.44
3:A:595:THR:HG22	3:A:596:THR:N	2.33	0.44
3:A:1347:ALA:O	3:A:1348:LEU:C	2.56	0.44
3:A:679:ILE:O	3:A:682:THR:HB	2.18	0.44
3:A:1415:SER:O	3:A:1416:ALA:C	2.56	0.44
4:B:56:ASP:HB3	4:B:57:TYR:CE1	2.53	0.44
4:B:126:SER:OG	4:B:172:ILE:HD11	2.18	0.44
3:A:741:ASN:HD22	3:A:743:VAL:N	2.16	0.44
11:K:92:ASN:O	11:K:93:SER:C	2.56	0.44
8:H:84:ALA:CA	8:H:87:ARG:HB2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:115:LEU:HB2	3:A:122:MET:HE2	1.99	0.44
8:H:98:TYR:O	8:H:118:PHE:HD2	1.99	0.44
1:D:1:DA:C1'	3:A:1386:ARG:NH1	2.62	0.44
5:C:143:LEU:HD21	5:C:146:LYS:HE3	1.99	0.44
9:I:46:HIS:O	9:I:47:GLU:HB2	2.18	0.44
3:A:1049:ILE:O	3:A:1050:GLU:C	2.56	0.44
3:A:709:THR:HG23	9:I:94:ASP:HA	2.00	0.44
3:A:742:ASN:C	3:A:745:GLN:HB2	2.38	0.44
11:K:24:ASP:OD1	11:K:26:LYS:N	2.51	0.44
4:B:515:HIS:O	4:B:516:ASN:C	2.54	0.44
9:I:84:VAL:CG1	9:I:84:VAL:O	2.65	0.44
6:E:113:GLN:HG2	6:E:137:GLU:OE1	2.19	0.43
3:A:815:PHE:O	3:A:818:MET:N	2.50	0.43
3:A:592:ASP:N	3:A:595:THR:OG1	2.48	0.43
8:H:5:LEU:O	8:H:6:PHE:HB2	2.18	0.43
3:A:533:LYS:C	3:A:535:THR:N	2.72	0.43
5:C:46:ILE:HG23	5:C:157:CYS:HB3	2.00	0.43
3:A:845:LEU:O	3:A:846:GLU:C	2.57	0.43
3:A:1068:ALA:O	3:A:1069:ALA:C	2.55	0.43
4:B:345:LYS:N	4:B:348:ARG:HE	2.16	0.43
4:B:274:PRO:O	4:B:276:ILE:N	2.51	0.43
4:B:1175:LEU:O	4:B:1176:ASN:CG	2.56	0.43
9:I:50:THR:HG22	9:I:52:ILE:N	2.33	0.43
3:A:1166:ASP:OD1	3:A:1194:ARG:NH2	2.49	0.43
3:A:404:TYR:HA	3:A:413:ILE:O	2.18	0.43
4:B:315:LYS:N	4:B:316:PRO:HD2	2.32	0.43
3:A:399:HIS:CB	3:A:400:PRO:HD3	2.45	0.43
4:B:1116:ARG:CZ	4:B:1198:TYR:CE1	3.01	0.43
4:B:781:PHE:CE2	4:B:795:ILE:HD11	2.53	0.43
5:C:135:GLN:C	5:C:136:ASP:O	2.56	0.43
3:A:362:ASP:OD1	3:A:459:ARG:HD3	2.18	0.43
12:L:61:THR:HG22	12:L:62:LYS:N	2.33	0.43
9:I:29:CYS:O	9:I:31:THR:N	2.49	0.43
5:C:73:GLN:NE2	5:C:75:MET:H	1.97	0.43
3:A:326:ARG:HE	3:A:1406:VAL:HG11	1.82	0.43
3:A:960:ILE:HD12	3:A:1021:LEU:HD21	1.99	0.43
3:A:344:ARG:O	4:B:1118:PRO:HG2	2.19	0.43
3:A:751:SER:OG	4:B:1015:HIS:CE1	2.71	0.43
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.51	0.43
3:A:457:ALA:O	3:A:507:VAL:HG23	2.19	0.43
3:A:1428:VAL:HG13	4:B:1151:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:446:LEU:HD23	4:B:446:LEU:N	2.33	0.43
5:C:249:ASP:OD1	5:C:253:LYS:HE3	2.19	0.43
8:H:84:ALA:CB	8:H:87:ARG:HB2	2.49	0.43
3:A:547:LEU:HD22	11:K:58:PHE:HD1	1.84	0.43
3:A:1094:VAL:HG12	3:A:1095:THR:N	2.32	0.43
4:B:642:ASP:O	4:B:643:ASP:C	2.56	0.43
4:B:1002:THR:HG21	4:B:1006:ILE:HB	2.00	0.43
3:A:541:ILE:HG12	3:A:549:MET:HE3	2.01	0.43
3:A:306:ASN:OD1	3:A:313:GLN:NE2	2.51	0.43
3:A:1015:VAL:O	3:A:1015:VAL:HG12	2.18	0.43
3:A:774:ARG:O	3:A:775:ILE:C	2.57	0.43
3:A:1004:ASN:O	3:A:1008:GLN:HB2	2.19	0.43
4:B:758:PHE:CZ	4:B:1044:ALA:HA	2.52	0.43
6:E:145:THR:HG21	6:E:187:TYR:CE2	2.54	0.43
4:B:969:ARG:HG2	4:B:970:THR:N	2.33	0.43
3:A:850:VAL:O	3:A:1060:PRO:HA	2.18	0.43
4:B:212:LEU:HD13	4:B:409:ALA:HA	2.00	0.43
4:B:705:MET:H	4:B:710:LEU:CD1	2.32	0.43
4:B:708:GLU:C	4:B:710:LEU:N	2.72	0.43
3:A:80:HIS:O	3:A:243:PRO:HB3	2.17	0.43
3:A:7:SER:OG	4:B:1193:GLN:NE2	2.51	0.43
3:A:907:THR:HG22	3:A:908:LEU:H	1.82	0.43
4:B:977:GLY:CA	4:B:1099:VAL:HG21	2.30	0.43
4:B:1103:ILE:O	4:B:1104:HIS:C	2.56	0.43
3:A:815:PHE:C	3:A:817:ALA:N	2.72	0.43
4:B:130:VAL:CG1	4:B:131:ASP:H	2.29	0.43
4:B:288:ALA:HA	4:B:331:LEU:HD13	1.99	0.43
3:A:87:ALA:HB3	3:A:276:LEU:CD2	2.45	0.43
11:K:98:LEU:HD23	11:K:98:LEU:HA	1.89	0.43
4:B:850:LEU:CD2	4:B:1009:ASP:HB3	2.48	0.43
3:A:35:ILE:HD13	3:A:53:LEU:HD23	2.00	0.43
3:A:1097:GLY:C	3:A:1099:PRO:HD2	2.39	0.43
4:B:758:PHE:CE2	4:B:1044:ALA:HA	2.53	0.43
4:B:358:LYS:O	4:B:359:GLU:OE1	2.36	0.43
10:J:9:SER:HB2	10:J:45:CYS:HB2	2.01	0.43
11:K:55:LYS:HD3	11:K:78:THR:OG1	2.18	0.43
6:E:69:ILE:O	6:E:73:PRO:HG3	2.19	0.43
4:B:361:LEU:O	4:B:363:HIS:O	2.35	0.43
4:B:1152:MET:SD	4:B:1197:PRO:HD3	2.59	0.43
3:A:367:PRO:CB	3:A:466:SER:HA	2.47	0.43
5:C:8:VAL:HA	5:C:21:ILE:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:27:LEU:HD13	12:L:37:LYS:CB	2.48	0.43
5:C:135:GLN:O	5:C:136:ASP:O	2.37	0.43
7:F:140:ASP:OD1	7:F:141:GLY:N	2.52	0.43
4:B:329:THR:O	4:B:333:PHE:N	2.48	0.43
4:B:705:MET:N	4:B:710:LEU:HD12	2.34	0.43
3:A:68:GLN:O	3:A:70:CYS:N	2.52	0.43
3:A:534:LEU:HD13	3:A:656:TRP:CD1	2.54	0.43
4:B:121:ASN:HA	4:B:207:GLY:CA	2.46	0.43
5:C:148:ARG:H	5:C:151:GLN:HG3	1.84	0.43
1:D:5:DG:H1	2:R:8:C:N4	2.16	0.43
8:H:111:LEU:HD23	8:H:127:GLY:O	2.18	0.43
3:A:672:ASP:O	3:A:675:THR:HB	2.19	0.43
4:B:562:GLY:O	4:B:563:MET:C	2.56	0.43
4:B:784:ASN:HD21	4:B:788:ARG:HD2	1.84	0.43
4:B:295:GLY:H	4:B:298:LEU:HG	1.84	0.43
5:C:76:ASP:OD2	5:C:128:ASN:N	2.47	0.43
3:A:545:GLN:O	3:A:546:VAL:C	2.55	0.43
3:A:1364:ASN:HD22	3:A:1366:ARG:N	2.16	0.43
4:B:310:MET:O	4:B:313:MET:HB2	2.18	0.43
4:B:102:VAL:HG21	4:B:112:LEU:HD13	1.99	0.43
4:B:1197:PRO:O	4:B:1200:ALA:HB3	2.19	0.43
3:A:760:GLN:HB2	4:B:1021:MET:HE1	2.01	0.43
3:A:42:ASP:OD1	3:A:45:GLN:O	2.36	0.43
3:A:645:LEU:HD11	3:A:649:ILE:HD11	2.01	0.43
4:B:203:PHE:HE1	4:B:212:LEU:CD1	2.31	0.43
4:B:329:THR:O	4:B:332:ASP:HB3	2.19	0.43
3:A:852:TYR:CE2	7:F:136:ARG:NE	2.86	0.43
4:B:640:VAL:HG22	4:B:651:LEU:HD23	2.01	0.43
4:B:702:LEU:HA	4:B:702:LEU:HD12	1.76	0.43
4:B:601:ARG:O	4:B:605:ARG:HG3	2.19	0.43
6:E:138:ALA:O	6:E:140:LEU:N	2.50	0.43
3:A:396:PRO:HG3	3:A:416:ARG:HB3	2.00	0.43
3:A:401:GLY:H	3:A:435:HIS:HD2	1.66	0.43
3:A:366:VAL:HA	3:A:367:PRO:HD2	1.81	0.43
3:A:86:LEU:HB3	3:A:296:LEU:HD21	1.99	0.43
4:B:1073:TYR:N	4:B:1073:TYR:CD1	2.87	0.43
3:A:108:MET:O	3:A:109:HIS:CB	2.66	0.43
3:A:148:CYS:HB3	3:A:167:CYS:O	2.18	0.43
5:C:251:LEU:HG	11:K:98:LEU:HD11	2.01	0.43
8:H:47:PHE:CB	8:H:95:TYR:HD1	2.31	0.43
3:A:1366:ARG:HG2	3:A:1366:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1155:ASP:O	3:A:1190:PRO:O	2.37	0.43
4:B:702:LEU:HD22	4:B:737:THR:CG2	2.49	0.43
3:A:1390:ASN:HD22	3:A:1399:ARG:CA	2.30	0.43
3:A:1441:PHE:HB2	7:F:134:ILE:HG23	2.00	0.43
3:A:337:ARG:CZ	3:A:839:ARG:CZ	2.97	0.43
2:R:2:A:C3'	2:R:3:C:H5'	2.43	0.43
3:A:675:THR:HG21	3:A:736:ASN:HD21	1.77	0.43
3:A:114:LEU:HD12	3:A:142:CYS:O	2.18	0.43
3:A:412:ARG:CZ	4:B:1108:ARG:NH2	2.81	0.43
3:A:639:PRO:HG2	3:A:640:GLN:H	1.84	0.43
4:B:915:THR:HG21	4:B:934:LYS:HG2	2.00	0.43
4:B:1204:PHE:O	4:B:1207:LEU:HB2	2.19	0.43
9:I:59:VAL:HG12	9:I:60:GLN:N	2.34	0.43
3:A:1385:THR:HG22	3:A:1386:ARG:N	2.34	0.42
10:J:53:HIS:CE1	10:J:55:ASP:HA	2.54	0.42
3:A:614:PHE:C	3:A:614:PHE:CD1	2.92	0.42
3:A:1342:GLU:HG2	6:E:212:ARG:HH11	1.83	0.42
6:E:168:TYR:O	6:E:170:LEU:HD23	2.19	0.42
4:B:1148:LYS:O	4:B:1152:MET:HB2	2.19	0.42
3:A:1394:THR:HG22	3:A:1395:GLY:O	2.19	0.42
4:B:189:LEU:O	4:B:190:TYR:C	2.57	0.42
3:A:753:GLY:HA2	3:A:757:ASN:ND2	2.34	0.42
4:B:666:TYR:C	4:B:668:ASP:N	2.72	0.42
6:E:102:GLU:C	6:E:104:ASN:H	2.20	0.42
4:B:366:GLN:O	4:B:367:LEU:O	2.36	0.42
3:A:834:THR:HG21	3:A:1077:THR:HA	2.00	0.42
3:A:1424:VAL:HG11	4:B:1139:ILE:HD13	2.00	0.42
3:A:567:LYS:HZ2	8:H:46:LEU:CB	2.29	0.42
3:A:666:ILE:HD11	4:B:1030:LEU:CD1	2.20	0.42
4:B:280:ILE:CG2	4:B:285:ILE:HG13	2.47	0.42
4:B:955:THR:HA	12:L:54:ARG:O	2.19	0.42
10:J:48:ARG:NE	10:J:49:MET:HE2	2.33	0.42
6:E:137:GLU:O	6:E:138:ALA:C	2.57	0.42
3:A:407:ARG:HG2	3:A:430:TRP:CE2	2.54	0.42
4:B:834:ASN:HB2	4:B:838:SER:O	2.19	0.42
8:H:83:GLN:C	8:H:85:GLY:N	2.73	0.42
3:A:1027:ALA:O	3:A:1030:ARG:HB2	2.19	0.42
3:A:30:ILE:O	3:A:31:SER:O	2.37	0.42
3:A:99:ILE:O	3:A:102:VAL:HB	2.19	0.42
4:B:115:GLN:HG2	4:B:193:LYS:HB2	2.01	0.42
3:A:673:GLY:N	3:A:674:PRO:HD2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:55:THR:HG21	9:I:109:ILE:CD1	2.48	0.42
4:B:757:PRO:HG2	4:B:984:HIS:CE1	2.55	0.42
3:A:1161:THR:OG1	3:A:1170:ILE:HD11	2.20	0.42
8:H:4:THR:O	8:H:5:LEU:HD23	2.20	0.42
3:A:533:LYS:C	3:A:535:THR:H	2.23	0.42
4:B:778:MET:HE3	4:B:1094:ARG:HD3	2.01	0.42
4:B:745:PRO:C	4:B:747:MET:N	2.70	0.42
6:E:117:THR:C	6:E:119:SER:N	2.73	0.42
5:C:5:GLY:O	5:C:6:PRO:O	2.37	0.42
4:B:806:THR:O	4:B:808:ALA:N	2.53	0.42
4:B:113:TYR:CD2	4:B:192:LEU:HD22	2.53	0.42
4:B:1177:HIS:C	4:B:1179:GLN:H	2.22	0.42
4:B:1177:HIS:O	4:B:1179:GLN:HG3	2.19	0.42
3:A:974:ASP:HB2	8:H:136:LYS:HZ1	1.82	0.42
3:A:738:LYS:HZ1	5:C:194:GLU:CA	2.32	0.42
3:A:113:LEU:HG	3:A:218:ASP:OD1	2.19	0.42
3:A:134:ARG:O	3:A:137:ALA:N	2.52	0.42
6:E:114:ASN:O	6:E:115:ASN:HB3	2.18	0.42
3:A:1148:ILE:HD12	3:A:1196:GLU:HG2	2.01	0.42
3:A:1215:ARG:HD2	3:A:1215:ARG:HA	1.88	0.42
3:A:565:ILE:HD13	3:A:567:LYS:HE2	2.01	0.42
8:H:143:LEU:N	8:H:143:LEU:HD12	2.34	0.42
10:J:53:HIS:CD2	10:J:54:VAL:N	2.88	0.42
1:D:8:DT:H2'	1:D:9:DG:C8	2.55	0.42
3:A:751:SER:O	3:A:752:LYS:CB	2.67	0.42
3:A:89:PRO:HG3	3:A:208:LEU:HD12	2.00	0.42
4:B:34:ILE:HG12	4:B:542:MET:CE	2.49	0.42
3:A:443:LEU:HD22	3:A:455:MET:CE	2.48	0.42
3:A:760:GLN:OE1	4:B:1021:MET:HE2	2.19	0.42
3:A:166:GLY:O	3:A:167:CYS:CB	2.67	0.42
11:K:95:ILE:O	11:K:98:LEU:HB2	2.19	0.42
4:B:1177:HIS:O	4:B:1179:GLN:N	2.52	0.42
4:B:1108:ARG:O	4:B:1108:ARG:CG	2.67	0.42
4:B:749:LEU:HD22	4:B:753:ALA:CB	2.50	0.42
3:A:1168:GLU:O	3:A:1172:LEU:HG	2.19	0.42
9:I:91:ARG:HD3	9:I:91:ARG:HA	1.75	0.42
6:E:16:PHE:CZ	6:E:20:LYS:HE2	2.54	0.42
3:A:1329:THR:HG22	3:A:1330:ASN:N	2.34	0.42
5:C:242:GLN:O	5:C:246:ARG:N	2.52	0.42
8:H:57:VAL:CG1	8:H:58:THR:N	2.83	0.42
1:D:9:DG:O3'	4:B:792:MET:HE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:3:C:C2'	2:R:4:C:O4'	2.67	0.42
4:B:831:SER:CB	4:B:994:TYR:OH	2.67	0.42
2:R:9:A:OP1	3:A:483:ASP:OD1	2.38	0.42
3:A:151:ASP:OD1	3:A:163:SER:HA	2.19	0.42
4:B:880:THR:O	4:B:881:ASN:HB2	2.20	0.42
4:B:1020:ARG:O	4:B:1021:MET:C	2.58	0.42
4:B:784:ASN:HB3	10:J:63:TYR:OH	2.18	0.42
4:B:781:PHE:HE2	4:B:795:ILE:HD11	1.83	0.42
3:A:984:LYS:O	3:A:988:LEU:HB2	2.19	0.42
4:B:280:ILE:HA	4:B:281:PRO:HD2	1.85	0.42
3:A:80:HIS:N	3:A:243:PRO:HB3	2.34	0.42
3:A:68:GLN:C	3:A:70:CYS:N	2.73	0.42
4:B:202:TYR:CD2	4:B:202:TYR:N	2.87	0.42
3:A:336:ILE:CD1	3:A:1405:THR:HG21	2.45	0.42
3:A:541:ILE:N	3:A:541:ILE:HD12	2.34	0.42
3:A:960:ILE:O	3:A:961:ARG:C	2.57	0.42
3:A:1187:GLN:HA	3:A:1243:VAL:HG23	2.02	0.42
3:A:709:THR:O	3:A:712:GLU:N	2.52	0.42
4:B:778:MET:HE1	4:B:1094:ARG:HD3	2.01	0.42
3:A:1150:SER:HB2	3:A:1195:LEU:CD2	2.49	0.42
3:A:760:GLN:CB	4:B:1021:MET:HE1	2.50	0.42
4:B:794:ASN:O	4:B:795:ILE:HD12	2.19	0.42
4:B:203:PHE:HE1	4:B:212:LEU:HD12	1.85	0.42
5:C:214:ASN:CB	5:C:217:ASP:OD2	2.68	0.42
3:A:441:PRO:HG2	3:A:441:PRO:O	2.20	0.42
3:A:131:SER:OG	3:A:132:LYS:N	2.51	0.42
4:B:1072:MET:HE2	4:B:1087:PHE:HD1	1.85	0.42
7:F:89:GLU:HB3	7:F:134:ILE:HD13	2.01	0.42
4:B:1106:ARG:HH12	4:B:1118:PRO:CA	2.33	0.42
6:E:168:TYR:CB	6:E:170:LEU:HG	2.49	0.42
3:A:629:LEU:CD1	3:A:645:LEU:HD21	2.48	0.42
3:A:38:PRO:CA	3:A:270:LEU:HD23	2.49	0.42
9:I:84:VAL:O	9:I:84:VAL:HG13	2.19	0.42
11:K:71:PHE:CD1	11:K:71:PHE:C	2.93	0.42
4:B:797:TYR:HB3	4:B:798:TYR:CD1	2.55	0.42
3:A:514:PRO:HB2	3:A:875:ALA:HB3	2.01	0.42
5:C:39:ALA:CA	5:C:164:ALA:HB3	2.46	0.42
3:A:683:ILE:O	3:A:686:ALA:N	2.53	0.42
3:A:683:ILE:CD1	3:A:764:CYS:HB2	2.42	0.42
4:B:269:ILE:HB	4:B:317:CYS:SG	2.60	0.42
4:B:879:ARG:O	4:B:880:THR:HB	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1162:ILE:HG22	4:B:1163:CYS:N	2.34	0.42
3:A:782:ARG:NH2	9:I:67:THR:HG22	2.34	0.42
4:B:995:ARG:HH11	4:B:995:ARG:HB2	1.81	0.42
10:J:21:TYR:CA	10:J:39:LEU:HD11	2.49	0.42
4:B:877:PRO:O	4:B:878:GLN:HG2	2.19	0.42
6:E:131:THR:HG21	6:E:191:LYS:HE2	2.02	0.42
3:A:1126:ALA:O	3:A:1128:GLN:N	2.53	0.42
4:B:346:GLU:O	4:B:347:LYS:C	2.58	0.42
3:A:1402:PHE:O	3:A:1404:GLU:N	2.51	0.42
4:B:640:VAL:HG22	4:B:651:LEU:CD2	2.50	0.42
4:B:955:THR:CG2	12:L:54:ARG:O	2.65	0.42
10:J:3:VAL:CG2	10:J:18:TRP:CG	3.02	0.42
6:E:9:ILE:C	6:E:11:ARG:N	2.71	0.42
4:B:167:ILE:O	4:B:168:GLY:O	2.38	0.42
6:E:28:TYR:CE1	6:E:78:LEU:CD1	3.03	0.42
3:A:339:ASN:HB3	4:B:1117:GLN:HE22	1.85	0.42
4:B:1182:CYS:SG	4:B:1185:CYS:HB2	2.60	0.42
3:A:633:VAL:HG11	3:A:645:LEU:HD22	2.00	0.42
8:H:31:THR:O	8:H:32:THR:OG1	2.37	0.42
3:A:567:LYS:CD	8:H:95:TYR:CD1	3.00	0.42
3:A:49:LYS:NZ	3:A:60:SER:HA	2.34	0.42
3:A:598:LEU:HD22	8:H:25:ARG:CZ	2.50	0.42
3:A:962:ARG:O	3:A:963:ILE:C	2.57	0.42
1:D:5:DG:H1	2:R:8:C:H42	1.67	0.42
6:E:59:SER:HA	6:E:80:VAL:O	2.19	0.42
4:B:1197:PRO:O	4:B:1200:ALA:N	2.52	0.42
3:A:637:LYS:HA	3:A:637:LYS:HD3	1.93	0.42
12:L:40:LEU:HD23	12:L:40:LEU:HA	1.78	0.42
3:A:568:PRO:CB	5:C:221:TYR:CZ	3.03	0.41
4:B:1096:ARG:O	4:B:1097:HIS:CB	2.59	0.41
6:E:71:LYS:C	6:E:73:PRO:HD3	2.41	0.41
4:B:995:ARG:CB	4:B:995:ARG:HH11	2.33	0.41
9:I:63:GLY:O	9:I:70:ARG:NH2	2.53	0.41
3:A:650:GLN:O	3:A:651:LYS:C	2.58	0.41
3:A:59:GLY:HA2	3:A:67:CYS:SG	2.60	0.41
4:B:105:SER:O	4:B:106:ASP:HB2	2.19	0.41
4:B:499:ASN:OD1	4:B:500:THR:N	2.53	0.41
4:B:1149:GLU:HG3	4:B:1153:GLU:OE1	2.20	0.41
3:A:725:ALA:HA	3:A:728:LYS:HE2	2.02	0.41
8:H:12:VAL:HG13	8:H:26:ILE:HG23	2.01	0.41
3:A:843:LYS:HG3	3:A:1402:PHE:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:383:TYR:O	7:F:115:THR:HG22	2.20	0.41
4:B:1106:ARG:HH12	4:B:1118:PRO:HA	1.85	0.41
4:B:315:LYS:O	4:B:317:CYS:N	2.53	0.41
4:B:55:VAL:O	4:B:59:LEU:HB3	2.19	0.41
3:A:675:THR:CG2	3:A:736:ASN:ND2	2.78	0.41
11:K:98:LEU:O	11:K:99:GLY:C	2.58	0.41
5:C:59:ALA:O	5:C:63:ILE:HG13	2.19	0.41
3:A:1254:ALA:O	3:A:1255:GLU:HB2	2.19	0.41
11:K:82:ASP:O	11:K:85:ASP:HB2	2.20	0.41
3:A:481:ASP:C	3:A:481:ASP:OD1	2.58	0.41
8:H:96:VAL:HG13	8:H:143:LEU:HG	2.02	0.41
5:C:56:THR:CG2	5:C:57:VAL:N	2.69	0.41
3:A:14:VAL:HB	3:A:1430:LEU:HD13	2.02	0.41
5:C:27:LEU:HD12	5:C:27:LEU:O	2.20	0.41
4:B:92:PHE:HD2	4:B:130:VAL:HG11	1.85	0.41
4:B:941:LEU:HD21	4:B:946:ASN:HA	2.02	0.41
3:A:530:GLY:O	3:A:532:ARG:N	2.53	0.41
3:A:321:PRO:O	3:A:322:VAL:CB	2.63	0.41
4:B:579:ARG:HB2	4:B:586:TRP:HE1	1.84	0.41
3:A:1158:PRO:HB3	3:A:1241:ARG:HH12	1.83	0.41
4:B:205:ILE:CD1	4:B:205:ILE:N	2.84	0.41
5:C:252:GLN:NE2	11:K:99:GLY:N	2.68	0.41
4:B:546:SER:OG	4:B:631:GLY:N	2.52	0.41
3:A:134:ARG:O	3:A:136:ALA:N	2.53	0.41
3:A:1364:ASN:HD21	3:A:1366:ARG:NH1	2.19	0.41
3:A:515:GLN:CG	3:A:516:SER:N	2.84	0.41
4:B:350:GLN:O	4:B:351:TYR:C	2.59	0.41
4:B:276:ILE:HD11	4:B:355:ILE:CD1	2.50	0.41
4:B:519:TRP:HZ2	4:B:705:MET:CE	2.24	0.41
9:I:103:CYS:SG	9:I:106:CYS:SG	2.99	0.41
3:A:598:LEU:O	3:A:599:SER:C	2.59	0.41
3:A:531:ILE:CG2	3:A:532:ARG:N	2.84	0.41
3:A:463:ILE:CD1	3:A:469:ARG:HG3	2.50	0.41
3:A:401:GLY:N	3:A:435:HIS:HD2	2.18	0.41
11:K:65:HIS:HD2	11:K:67:PHE:CB	2.33	0.41
6:E:79:TRP:HD1	6:E:96:PHE:HE1	1.67	0.41
3:A:451:HIS:HB2	3:A:454:SER:OG	2.19	0.41
4:B:53:GLN:HG2	4:B:547:VAL:HG13	2.02	0.41
3:A:474:VAL:HG13	3:A:478:TYR:HE1	1.85	0.41
4:B:368:GLU:O	4:B:371:GLU:OE1	2.37	0.41
4:B:901:PRO:O	4:B:949:VAL:O	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:648:HIS:HB2	4:B:649:LYS:H	1.61	0.41
3:A:407:ARG:HG2	3:A:430:TRP:CZ2	2.56	0.41
6:E:116:ILE:CG2	6:E:117:THR:N	2.84	0.41
5:C:8:VAL:CG1	5:C:9:LYS:H	2.32	0.41
3:A:518:LYS:HB2	3:A:519:PRO:HD2	2.01	0.41
3:A:1173:HIS:NE2	3:A:1227:ILE:HG23	2.35	0.41
3:A:88:LYS:HD2	3:A:293:GLU:OE1	2.19	0.41
4:B:39:ARG:HG2	4:B:39:ARG:HH11	1.85	0.41
5:C:252:GLN:HG3	11:K:95:ILE:HG23	2.03	0.41
8:H:84:ALA:HA	8:H:87:ARG:CB	2.50	0.41
10:J:43:ARG:HG2	10:J:43:ARG:H	1.68	0.41
8:H:117:SER:HA	8:H:122:LEU:HD23	2.02	0.41
12:L:28:LYS:O	12:L:29:TYR:CG	2.74	0.41
11:K:103:THR:O	11:K:106:GLU:N	2.53	0.41
11:K:35:PHE:O	11:K:70:ARG:HB2	2.21	0.41
3:A:1006:ILE:HG22	3:A:1007:ILE:N	2.36	0.41
4:B:707:PRO:HG2	4:B:708:GLU:N	2.27	0.41
4:B:175:ARG:CG	4:B:175:ARG:HH11	2.34	0.41
3:A:1406:VAL:CG1	3:A:1410:PHE:CE1	3.03	0.41
4:B:855:PHE:HZ	4:B:857:ARG:HH12	1.64	0.41
3:A:751:SER:OG	4:B:1015:HIS:HE1	2.03	0.41
5:C:124:LEU:O	5:C:127:ARG:CG	2.65	0.41
4:B:577:ALA:HB1	4:B:589:VAL:HG12	2.00	0.41
5:C:235:VAL:HG21	10:J:6:ARG:NH2	2.35	0.41
3:A:101:LYS:HG2	3:A:139:TRP:CZ2	2.55	0.41
4:B:846:ILE:CG2	4:B:974:PRO:HG2	2.51	0.41
4:B:843:GLN:HB2	4:B:993:THR:OG1	2.20	0.41
3:A:542:GLU:OE1	3:A:569:LYS:HE2	2.20	0.41
4:B:707:PRO:O	4:B:708:GLU:C	2.59	0.41
3:A:76:GLU:O	3:A:78:PRO:CD	2.68	0.41
3:A:79:GLY:C	3:A:243:PRO:HG3	2.41	0.41
3:A:908:LEU:O	3:A:909:ASP:C	2.58	0.41
4:B:120:ARG:HH22	12:L:54:ARG:HD2	1.86	0.41
3:A:332:LYS:H	3:A:337:ARG:CB	2.33	0.41
4:B:911:ILE:HD11	4:B:941:LEU:CB	2.50	0.41
4:B:840:ILE:HB	4:B:1011:ILE:HB	2.03	0.41
9:I:101:PHE:HD1	9:I:110:PHE:O	2.02	0.41
5:C:264:GLN:H	5:C:264:GLN:HG3	1.61	0.41
12:L:41:SER:O	12:L:44:ASP:HB2	2.21	0.41
4:B:188:ASP:O	4:B:192:LEU:HG	2.21	0.41
4:B:405:ARG:CZ	4:B:632:ARG:HG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:866:PHE:C	3:A:867:ILE:HG13	2.40	0.41
6:E:13:TRP:O	6:E:16:PHE:HB3	2.21	0.41
10:J:27:GLU:C	10:J:29:GLU:H	2.23	0.41
3:A:1107:VAL:CG2	3:A:1383:SER:HA	2.51	0.41
3:A:765:VAL:HG12	3:A:766:GLY:N	2.35	0.41
3:A:568:PRO:HB3	5:C:221:TYR:OH	2.21	0.41
5:C:146:LYS:O	5:C:147:LEU:HD23	2.20	0.41
3:A:960:ILE:HD12	3:A:1021:LEU:CD2	2.50	0.41
3:A:530:GLY:O	3:A:533:LYS:N	2.53	0.41
9:I:92:ARG:CG	9:I:93:LYS:N	2.84	0.41
4:B:244:LEU:HB2	4:B:249:ARG:HA	2.03	0.41
3:A:525:GLN:HB3	4:B:835:GLN:HG2	2.01	0.41
6:E:100:ILE:O	6:E:101:GLN:C	2.58	0.41
3:A:84:ILE:HG21	3:A:239:LEU:HD23	2.01	0.41
4:B:616:ILE:HG12	4:B:696:GLU:HG3	2.03	0.41
3:A:556:TRP:CE2	3:A:558:GLY:HA2	2.56	0.41
4:B:1120:GLU:CG	4:B:1121:GLY:N	2.84	0.41
3:A:553:VAL:HG22	3:A:652:VAL:CG2	2.51	0.41
5:C:29:MET:O	5:C:30:ALA:C	2.58	0.41
4:B:435:THR:O	4:B:435:THR:HG22	2.20	0.41
9:I:98:VAL:HG12	9:I:99:LEU:N	2.36	0.41
9:I:99:LEU:O	9:I:111:THR:HG23	2.21	0.41
9:I:99:LEU:HB2	9:I:112:SER:OG	2.21	0.41
4:B:348:ARG:O	4:B:349:ILE:C	2.60	0.41
4:B:519:TRP:CZ2	4:B:705:MET:CE	2.99	0.41
4:B:120:ARG:HH12	12:L:54:ARG:NH1	2.18	0.41
5:C:14:SER:HA	11:K:114:LEU:HD22	2.02	0.41
6:E:3:GLN:HG3	6:E:5:ASN:H	1.85	0.41
3:A:873:MET:C	3:A:1058:VAL:HG23	2.40	0.41
3:A:574:GLY:O	3:A:577:ILE:HG12	2.21	0.41
3:A:942:PHE:HZ	6:E:206:GLY:HA3	1.86	0.41
4:B:234:ILE:H	4:B:234:ILE:CD1	2.16	0.41
4:B:913:GLY:HA2	4:B:938:SER:HB2	2.02	0.41
3:A:403:LYS:O	3:A:404:TYR:O	2.39	0.41
4:B:121:ASN:HD21	4:B:965:LYS:HE3	1.86	0.41
3:A:399:HIS:NE2	3:A:462:VAL:HG21	2.36	0.41
11:K:47:ARG:HH11	11:K:48:ALA:N	2.19	0.41
3:A:894:GLU:C	3:A:896:ARG:N	2.74	0.41
4:B:1114:LEU:O	4:B:1198:TYR:HE2	2.03	0.41
3:A:343:LYS:NZ	4:B:1156:ASP:OD2	2.49	0.41
3:A:1381:LEU:HD23	3:A:1381:LEU:HA	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:982:THR:HB	3:A:985:ASP:CG	2.40	0.41
11:K:93:SER:O	11:K:97:LYS:HG3	2.20	0.41
9:I:25:LEU:HD12	9:I:26:LEU:N	2.35	0.41
3:A:1264:GLU:HG3	3:A:1265:ASN:N	2.36	0.41
3:A:974:ASP:CB	8:H:136:LYS:HZ3	2.34	0.41
3:A:113:LEU:C	3:A:115:LEU:H	2.23	0.41
3:A:19:PHE:HB3	3:A:1413:GLY:HA2	2.03	0.41
4:B:1070:GLU:O	4:B:1071:VAL:C	2.59	0.41
11:K:106:GLU:O	11:K:110:ASN:ND2	2.54	0.41
4:B:634:TYR:CD1	4:B:692:TYR:HB3	2.55	0.41
6:E:72:PHE:CD1	6:E:72:PHE:N	2.89	0.41
4:B:724:ASP:HA	4:B:725:PRO:HD2	1.95	0.41
9:I:85:PHE:HD1	9:I:99:LEU:HD22	1.83	0.41
3:A:1116:LEU:H	3:A:1308:THR:CG2	2.34	0.41
4:B:707:PRO:CG	4:B:708:GLU:N	2.84	0.41
4:B:1104:HIS:HB2	4:B:1122:ARG:CB	2.51	0.41
3:A:396:PRO:HB3	3:A:403:LYS:HG2	2.03	0.41
4:B:992:ILE:CD1	4:B:994:TYR:CE2	3.04	0.41
3:A:399:HIS:C	3:A:401:GLY:N	2.71	0.41
4:B:34:ILE:HG12	4:B:542:MET:HE1	2.03	0.41
4:B:549:THR:HG22	4:B:550:ASP:N	2.36	0.41
5:C:51:VAL:HG22	5:C:155:LEU:CD2	2.47	0.41
6:E:117:THR:O	6:E:120:ALA:N	2.54	0.41
9:I:26:LEU:HD23	9:I:37:GLU:HA	2.03	0.41
4:B:850:LEU:HD22	4:B:1009:ASP:HB3	2.02	0.41
3:A:172:PRO:HB3	3:A:185:TRP:CZ2	2.56	0.41
3:A:1098:VAL:O	3:A:1099:PRO:C	2.59	0.41
3:A:1102:LYS:HG2	3:A:1106:ASN:ND2	2.36	0.41
3:A:848:ILE:HG23	3:A:864:ILE:HD12	2.03	0.41
9:I:40:SER:HB2	9:I:41:PRO:HD2	2.03	0.41
4:B:380:TYR:O	4:B:384:ARG:HG2	2.21	0.41
3:A:1107:VAL:HG23	3:A:1383:SER:HA	2.03	0.41
4:B:593:PRO:HG2	4:B:617:ARG:NH2	2.36	0.41
3:A:1026:LEU:HA	3:A:1026:LEU:HD23	1.90	0.41
4:B:284:ILE:HG12	4:B:324:ILE:HD12	2.03	0.40
4:B:739:THR:HG1	4:B:740:HIS:CE1	2.36	0.40
5:C:66:ARG:NH2	10:J:3:VAL:O	2.54	0.40
3:A:871:ASP:CB	6:E:204:THR:CG2	2.98	0.40
3:A:332:LYS:H	3:A:337:ARG:CD	2.34	0.40
8:H:126:GLU:N	8:H:130:ARG:HH12	2.19	0.40
3:A:302:THR:O	3:A:313:GLN:NE2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:127:ARG:HG2	5:C:127:ARG:H	1.73	0.40
4:B:418:LYS:O	4:B:420:LEU:N	2.54	0.40
4:B:56:ASP:CB	4:B:57:TYR:HD1	2.34	0.40
4:B:56:ASP:CB	4:B:57:TYR:CD1	3.04	0.40
5:C:5:GLY:HA3	5:C:6:PRO:HD2	1.78	0.40
7:F:109:VAL:CG1	7:F:110:ASP:H	2.34	0.40
3:A:719:VAL:HG22	3:A:774:ARG:HD2	2.03	0.40
5:C:46:ILE:CG2	5:C:157:CYS:HB3	2.51	0.40
4:B:1177:HIS:HB2	4:B:1179:GLN:HG3	2.03	0.40
3:A:738:LYS:HA	8:H:19:ARG:NH2	2.37	0.40
4:B:283:VAL:HG13	4:B:297:ILE:HD12	2.03	0.40
3:A:1139:GLU:HG3	3:A:1280:GLU:O	2.20	0.40
3:A:1343:ALA:O	3:A:1346:ALA:HB3	2.20	0.40
10:J:34:THR:O	10:J:35:ALA:C	2.58	0.40
3:A:1116:LEU:CD2	3:A:1316:VAL:HG21	2.51	0.40
3:A:909:ASP:OD1	3:A:910:PRO:HD2	2.21	0.40
3:A:901:LEU:CG	3:A:926:GLN:HE21	2.30	0.40
4:B:818:PRO:HG3	10:J:54:VAL:HG21	2.03	0.40
6:E:137:GLU:O	6:E:140:LEU:N	2.43	0.40
3:A:14:VAL:O	3:A:15:LYS:HD3	2.20	0.40
1:D:6:DC:OP2	3:A:332:LYS:NZ	2.45	0.40
2:R:2:A:H2'	2:R:3:C:C5'	2.50	0.40
3:A:1224:LEU:HD11	3:A:1240:CYS:HB3	2.04	0.40
3:A:648:ASN:O	3:A:649:ILE:C	2.59	0.40
8:H:138:GLU:HG2	8:H:139:ASN:N	2.35	0.40
9:I:16:PRO:HA	9:I:26:LEU:O	2.21	0.40
3:A:270:LEU:O	3:A:274:ILE:HG13	2.21	0.40
3:A:474:VAL:HG13	3:A:474:VAL:O	2.20	0.40
6:E:182:ASP:O	6:E:186:LEU:HG	2.21	0.40
3:A:913:LEU:CD1	3:A:981:LEU:O	2.69	0.40
6:E:11:ARG:NH2	6:E:141:VAL:HG21	2.37	0.40
4:B:952:VAL:HG13	4:B:966:VAL:HG22	2.03	0.40
1:D:10:DG:H5'	4:B:792:MET:HE3	2.04	0.40
3:A:379:VAL:HG22	3:A:431:LYS:HG2	2.03	0.40
6:E:116:ILE:HG22	6:E:117:THR:N	2.36	0.40
4:B:446:LEU:HG	4:B:446:LEU:O	2.21	0.40
3:A:354:SER:CA	3:A:482:PHE:CD2	3.03	0.40
4:B:627:PHE:O	4:B:632:ARG:NH1	2.54	0.40
4:B:101:MET:HE3	4:B:169:ARG:HH22	1.86	0.40
4:B:484:ASN:CG	4:B:486:TYR:HE1	2.23	0.40
4:B:240:ILE:C	4:B:253:THR:HG23	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1084:GLN:NE2	5:C:192:TRP:HB2	2.37	0.40
3:A:18:GLN:O	4:B:1215:ARG:HG3	2.21	0.40
3:A:19:PHE:HA	4:B:1213:THR:O	2.22	0.40
3:A:432:VAL:O	3:A:434:ARG:N	2.54	0.40
4:B:578:THR:HG23	4:B:622:LYS:C	2.42	0.40
6:E:136:ASN:OD1	6:E:136:ASN:C	2.60	0.40
3:A:1316:VAL:O	3:A:1322:ILE:HD13	2.21	0.40
4:B:281:PRO:HG2	4:B:284:ILE:CD1	2.45	0.40
4:B:702:LEU:CD2	4:B:735:ALA:HB1	2.51	0.40
3:A:541:ILE:HG12	3:A:549:MET:CE	2.52	0.40
3:A:1220:PHE:O	3:A:1221:LYS:C	2.60	0.40
3:A:205:GLU:O	3:A:208:LEU:HB2	2.22	0.40
4:B:1156:ASP:HB3	4:B:1197:PRO:CA	2.52	0.40
3:A:225:ASN:ND2	3:A:228:PHE:CD1	2.90	0.40
4:B:288:ALA:O	4:B:331:LEU:CD1	2.70	0.40
8:H:33:GLN:OE1	8:H:129:TYR:HE2	2.05	0.40
3:A:738:LYS:CB	8:H:19:ARG:HH22	2.34	0.40
3:A:808:LEU:HD12	3:A:808:LEU:N	2.35	0.40
4:B:171:PRO:HD2	4:B:457:LEU:HD12	2.03	0.40
4:B:387:LEU:HD23	4:B:393:LYS:HD2	2.03	0.40
3:A:578:LEU:O	3:A:581:ALA:N	2.51	0.40
3:A:203:SER:O	3:A:207:ILE:HG12	2.21	0.40
4:B:61:ASP:N	4:B:61:ASP:OD1	2.54	0.40
4:B:1115:THR:CG2	4:B:1199:ALA:HB2	2.50	0.40
9:I:6:PHE:HD2	9:I:13:MET:HA	1.86	0.40
4:B:737:THR:O	4:B:738:PHE:C	2.60	0.40
3:A:48:ALA:O	3:A:49:LYS:CG	2.65	0.40
3:A:13:THR:HB	3:A:15:LYS:HE2	2.04	0.40
4:B:803:LEU:HD13	4:B:1036:ALA:HB2	2.03	0.40
4:B:51:PHE:O	4:B:54:PHE:N	2.54	0.40
3:A:508:PRO:O	3:A:511:ILE:HG13	2.21	0.40
4:B:185:THR:N	4:B:188:ASP:HB2	2.36	0.40
11:K:21:ILE:HG12	11:K:33:ILE:HG12	2.03	0.40
5:C:214:ASN:HB2	5:C:217:ASP:OD2	2.22	0.40
6:E:19:VAL:O	6:E:19:VAL:HG12	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	1365/1733 (79%)	1021 (75%)	253 (18%)	91 (7%)	1	12
4	B	1077/1224 (88%)	839 (78%)	169 (16%)	69 (6%)	2	13
5	C	264/318 (83%)	208 (79%)	39 (15%)	17 (6%)	2	13
6	E	212/215 (99%)	170 (80%)	33 (16%)	9 (4%)	3	23
7	F	82/155 (53%)	64 (78%)	15 (18%)	3 (4%)	4	27
8	H	129/146 (88%)	93 (72%)	21 (16%)	15 (12%)	0	3
9	I	117/122 (96%)	93 (80%)	15 (13%)	9 (8%)	1	9
10	J	63/70 (90%)	48 (76%)	11 (18%)	4 (6%)	2	13
11	K	112/120 (93%)	96 (86%)	15 (13%)	1 (1%)	21	60
12	L	44/70 (63%)	22 (50%)	12 (27%)	10 (23%)	0	0
All	All	3465/4173 (83%)	2654 (77%)	583 (17%)	228 (7%)	1	12

All (228) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	31	SER
3	A	48	ALA
3	A	55	ASP
3	A	56	PRO
3	A	74	MET
3	A	75	ASN
3	A	167	CYS
3	A	322	VAL
3	A	404	TYR
3	A	418	SER
3	A	543	LEU
3	A	567	LYS
3	A	597	LEU
3	A	598	LEU

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Mol	Chain	Res	Type
3	A	628	GLY
3	A	752	LYS
3	A	846	GLU
3	A	998	LEU
3	A	1036	ARG
3	A	1127	ASP
3	A	1206	ASP
3	A	1221	LYS
3	A	1223	ASP
3	A	1392	SER
3	A	1393	ASN
3	A	1403	GLU
3	A	1406	VAL
3	A	1416	ALA
4	B	65	GLU
4	B	124	TYR
4	B	174	LEU
4	B	175	ARG
4	B	200	GLY
4	B	229	ALA
4	B	364	ILE
4	B	367	LEU
4	B	531	GLN
4	B	708	GLU
4	B	709	ASP
4	B	731	VAL
4	B	751	VAL
4	B	958	GLN
4	B	959	ASP
4	B	1046	PRO
4	B	1103	ILE
4	B	1167	GLY
4	B	1176	ASN
4	B	1183	LYS
5	C	4	GLU
5	C	5	GLY
5	C	6	PRO
5	C	110	THR
5	C	142	VAL
5	C	215	GLU
7	F	73	ALA
8	H	32	THR

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Mol	Chain	Res	Type
8	H	81	PRO
8	H	140	ALA
9	I	8	ARG
10	J	2	ILE
10	J	55	ASP
12	L	27	LEU
12	L	38	LEU
12	L	64	LEU
3	A	35	ILE
3	A	54	ASN
3	A	62	ASP
3	A	87	ALA
3	A	109	HIS
3	A	135	PHE
3	A	168	GLY
3	A	332	LYS
3	A	385	ILE
3	A	419	LYS
3	A	534	LEU
3	A	568	PRO
3	A	790	ASP
3	A	986	ILE
3	A	1114	PRO
3	A	1365	TYR
3	A	1366	ARG
3	A	1379	GLY
4	B	55	VAL
4	B	168	GLY
4	B	275	TYR
4	B	346	GLU
4	B	410	GLY
4	B	480	SER
4	B	641	GLU
4	B	643	ASP
4	B	792	MET
4	B	864	LYS
4	B	866	TYR
4	B	884	ARG
4	B	891	ASP
4	B	992	ILE
4	B	1066	SER
4	B	1155	SER

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Mol	Chain	Res	Type
5	C	136	ASP
7	F	142	SER
8	H	61	SER
8	H	77	ARG
8	H	88	SER
8	H	128	ASN
9	I	30	ARG
9	I	79	HIS
12	L	39	SER
12	L	52	GLY
3	A	6	TYR
3	A	45	GLN
3	A	59	GLY
3	A	67	CYS
3	A	69	THR
3	A	335	ARG
3	A	433	GLU
3	A	596	THR
3	A	737	LEU
3	A	775	ILE
3	A	830	LYS
3	A	920	LEU
4	B	28	GLU
4	B	249	ARG
4	B	277	LYS
4	B	447	ALA
4	B	629	ASP
4	B	735	ALA
4	B	807	ARG
4	B	880	THR
4	B	1017	ILE
4	B	1099	VAL
4	B	1104	HIS
5	C	48	SER
5	C	212	PRO
5	C	227	THR
6	E	31	THR
6	E	102	GLU
6	E	103	LYS
6	E	122	LYS
6	E	139	ALA
6	E	206	GLY

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Mol	Chain	Res	Type
7	F	128	LYS
8	H	8	ASP
8	H	17	PRO
8	H	82	PRO
8	H	135	LEU
8	H	139	ASN
9	I	9	ASP
9	I	33	SER
9	I	86	PHE
10	J	9	SER
12	L	63	ARG
3	A	101	LYS
3	A	134	ARG
3	A	139	TRP
3	A	424	ILE
3	A	599	SER
3	A	1067	LEU
3	A	1097	GLY
3	A	1115	SER
3	A	1122	PRO
3	A	1405	THR
4	B	304	ASP
4	B	436	VAL
4	B	501	PRO
4	B	667	GLN
4	B	791	THR
4	B	1054	GLY
4	B	1097	HIS
4	B	1178	ASN
5	C	18	VAL
5	C	149	LYS
5	C	174	ALA
6	E	59	SER
10	J	6	ARG
12	L	50	ASP
12	L	56	LEU
3	A	58	LEU
3	A	223	GLY
3	A	400	PRO
3	A	958	VAL
3	A	972	HIS
3	A	1098	VAL

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Mol	Chain	Res	Type
3	A	1130	GLN
3	A	1282	VAL
3	A	1351	GLU
3	A	1378	GLN
4	B	248	SER
4	B	419	THR
4	B	619	ILE
4	B	648	HIS
4	B	687	GLU
4	B	707	PRO
4	B	712	PRO
4	B	764	SER
4	B	907	GLY
4	B	982	SER
4	B	1108	ARG
6	E	36	GLU
8	H	62	SER
8	H	89	LEU
9	I	47	GLU
9	I	88	SER
3	A	226	GLU
3	A	368	LYS
3	A	399	HIS
3	A	531	ILE
3	A	1014	ALA
3	A	1314	SER
3	A	1352	VAL
4	B	27	ALA
6	E	167	ARG
8	H	138	GLU
9	I	98	VAL
11	K	107	THR
12	L	59	ALA
4	B	247	GLY
3	A	336	ILE
3	A	1104	ILE
12	L	55	ILE
3	A	810	PRO
3	A	1075	PRO
3	A	1242	VAL
5	C	172	PRO
5	C	216	GLY

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Mol	Chain	Res	Type
3	A	78	PRO
4	B	511	PRO
5	C	202	PRO
5	C	218	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	1206/1520 (79%)	1129 (94%)	77 (6%)	22	60
4	B	952/1061 (90%)	886 (93%)	66 (7%)	19	57
5	C	234/274 (85%)	222 (95%)	12 (5%)	29	68
6	E	196/197 (100%)	189 (96%)	7 (4%)	42	76
7	F	74/137 (54%)	68 (92%)	6 (8%)	15	48
8	H	117/128 (91%)	112 (96%)	5 (4%)	35	72
9	I	113/116 (97%)	104 (92%)	9 (8%)	15	49
10	J	60/65 (92%)	56 (93%)	4 (7%)	20	58
11	K	99/102 (97%)	90 (91%)	9 (9%)	12	41
12	L	40/57 (70%)	35 (88%)	5 (12%)	6	24
All	All	3091/3657 (84%)	2891 (94%)	200 (6%)	21	59

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	18	GLN
3	A	22	PHE
3	A	31	SER
3	A	56	PRO
3	A	70	CYS
3	A	93	VAL
3	A	122	MET
3	A	247	ARG
3	A	269	ILE

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Mol	Chain	Res	Type
3	A	302	THR
3	A	322	VAL
3	A	326	ARG
3	A	351	THR
3	A	375	THR
3	A	381	THR
3	A	385	ILE
3	A	397	ASN
3	A	412	ARG
3	A	434	ARG
3	A	443	LEU
3	A	445	ASN
3	A	450	LEU
3	A	451	HIS
3	A	461	LYS
3	A	474	VAL
3	A	475	THR
3	A	493	GLN
3	A	503	GLN
3	A	524	VAL
3	A	538	ASP
3	A	590	ARG
3	A	596	THR
3	A	597	LEU
3	A	598	LEU
3	A	618	GLU
3	A	629	LEU
3	A	666	ILE
3	A	682	THR
3	A	740	LEU
3	A	741	ASN
3	A	745	GLN
3	A	756	ILE
3	A	768	GLN
3	A	774	ARG
3	A	821	ARG
3	A	845	LEU
3	A	849	MET
3	A	855	THR
3	A	858	ASN
3	A	920	LEU
3	A	929	LEU

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Mol	Chain	Res	Type
3	A	948	VAL
3	A	949	ASP
3	A	979	SER
3	A	1029	ARG
3	A	1035	TYR
3	A	1043	ASP
3	A	1057	VAL
3	A	1077	THR
3	A	1128	GLN
3	A	1222	ASN
3	A	1232	ASN
3	A	1258	HIS
3	A	1264	GLU
3	A	1295	THR
3	A	1308	THR
3	A	1318	THR
3	A	1332	PHE
3	A	1335	ILE
3	A	1351	GLU
3	A	1359	ASP
3	A	1364	ASN
3	A	1366	ARG
3	A	1375	MET
3	A	1376	THR
3	A	1425	SER
3	A	1442	ASP
4	B	20	ASP
4	B	43	LEU
4	B	57	TYR
4	B	61	ASP
4	B	63	ILE
4	B	98	THR
4	B	109	THR
4	B	121	ASN
4	B	175	ARG
4	B	194	GLU
4	B	232	SER
4	B	234	ILE
4	B	261	ARG
4	B	268	THR
4	B	278	GLN
4	B	309	GLN

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Mol	Chain	Res	Type
4	B	313	MET
4	B	317	CYS
4	B	320	ASP
4	B	331	LEU
4	B	376	PHE
4	B	387	LEU
4	B	396	ASP
4	B	408	LEU
4	B	466	TRP
4	B	485	ARG
4	B	513	GLN
4	B	514	LEU
4	B	538	ASN
4	B	547	VAL
4	B	570	VAL
4	B	576	ASP
4	B	624	LEU
4	B	629	ASP
4	B	644	GLU
4	B	680	THR
4	B	723	VAL
4	B	732	SER
4	B	762	ASN
4	B	764	SER
4	B	780	VAL
4	B	791	THR
4	B	835	GLN
4	B	901	PRO
4	B	909	ASP
4	B	915	THR
4	B	944	THR
4	B	951	GLN
4	B	953	LEU
4	B	976	ILE
4	B	986	GLN
4	B	987	LYS
4	B	996	ARG
4	B	999	MET
4	B	1007	VAL
4	B	1021	MET
4	B	1049	ASP
4	B	1103	ILE

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Mol	Chain	Res	Type
4	B	1111	MET
4	B	1118	PRO
4	B	1132	GLU
4	B	1147	LEU
4	B	1150	ARG
4	B	1151	LEU
4	B	1183	LYS
4	B	1185	CYS
5	C	22	LEU
5	C	25	VAL
5	C	26	ASP
5	C	62	PHE
5	C	69	LEU
5	C	77	ILE
5	C	133	ILE
5	C	148	ARG
5	C	229	TYR
5	C	233	GLU
5	C	240	VAL
5	C	264	GLN
6	E	40	GLU
6	E	60	PHE
6	E	74	ASP
6	E	84	ASP
6	E	92	THR
6	E	104	ASN
6	E	183	PRO
7	F	79	ARG
7	F	90	ARG
7	F	103	MET
7	F	111	LEU
7	F	115	THR
7	F	133	VAL
8	H	21	ASN
8	H	27	GLU
8	H	109	LYS
8	H	110	ASP
8	H	134	ASN
9	I	7	CYS
9	I	12	ASN
9	I	29	CYS
9	I	31	THR

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Mol	Chain	Res	Type
9	I	52	ILE
9	I	75	CYS
9	I	76	PRO
9	I	87	GLN
9	I	103	CYS
10	J	2	ILE
10	J	7	CYS
10	J	47	ARG
10	J	48	ARG
11	K	20	LYS
11	K	25	THR
11	K	31	VAL
11	K	47	ARG
11	K	50	LEU
11	K	61	TYR
11	K	77	THR
11	K	81	TYR
11	K	114	LEU
12	L	50	ASP
12	L	54	ARG
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 (75) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	68	GLN
3	A	92	HIS
3	A	118	HIS
3	A	169	ASN
3	A	225	ASN
3	A	281	HIS
3	A	339	ASN
3	A	358	ASN
3	A	435	HIS
3	A	445	ASN
3	A	447	GLN
3	A	493	GLN
3	A	503	GLN
3	A	517	ASN
3	A	631	HIS

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Mol	Chain	Res	Type
3	A	736	ASN
3	A	741	ASN
3	A	757	ASN
3	A	768	GLN
3	A	786	HIS
3	A	858	ASN
3	A	926	GLN
3	A	965	GLN
3	A	968	GLN
3	A	994	GLN
3	A	1364	ASN
3	A	1387	HIS
3	A	1390	ASN
3	A	1432	GLN
4	B	46	GLN
4	B	178	ASN
4	B	215	GLN
4	B	236	HIS
4	B	325	GLN
4	B	363	HIS
4	B	465	ASN
4	B	484	ASN
4	B	513	GLN
4	B	515	HIS
4	B	516	ASN
4	B	518	HIS
4	B	538	ASN
4	B	587	HIS
4	B	657	HIS
4	B	744	HIS
4	B	822	ASN
4	B	842	ASN
4	B	862	GLN
4	B	957	ASN
4	B	975	GLN
4	B	1015	HIS
4	B	1065	GLN
4	B	1117	GLN
4	B	1179	GLN
4	B	1193	GLN
5	C	65	HIS
5	C	73	GLN

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Mol	Chain	Res	Type
5	C	112	ASN
5	C	123	ASN
5	C	167	HIS
5	C	242	GLN
5	C	252	GLN
6	E	5	ASN
6	E	32	GLN
6	E	101	GLN
6	E	104	ASN
6	E	114	ASN
6	E	147	HIS
8	H	33	GLN
9	I	12	ASN
10	J	53	HIS
11	K	52	ASN
11	K	65	HIS
11	K	76	GLN
11	K	110	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	3	C
2	R	9	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.