Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:01 PM GMT

PDB ID	:	1I3Q
Title	:	RNA POLYMERASE II CRYSTAL FORM I AT 3.1 A RESOLUTION
Authors	:	Cramer, P.; Bushnell, D.A.; Kornberg, R.D.
Deposited on	:	2001-02-15
Resolution	:	3.10 Å(reported)

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

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

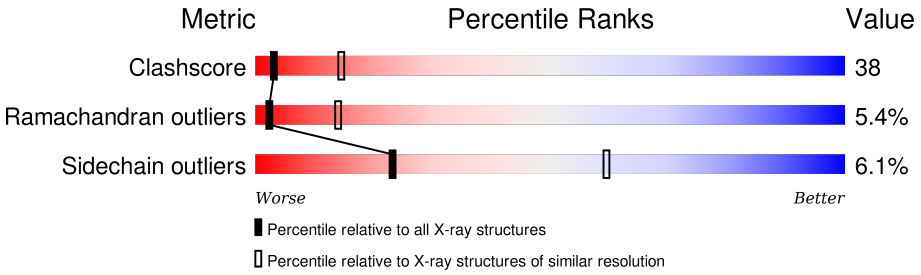
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 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	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1733	36% 40% 6% 18%
2	B	1224	37% 45% 6% 12%
3	C	318	34% 42% 8% 16%
4	E	215	52% 46%
5	F	155	21% 29% 5% 46%
6	H	146	34% 46% 9% 9%
7	I	122	45% 46% 9%

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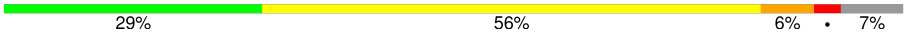
Mol	Chain	Length	Quality of chain
8	J	70	
9	K	120	
10	L	70	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28161 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1414	11114	7000	1947	2106	61	0	0	0

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1083	8624	5470	1501	1600	53	0	0	0

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE.

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

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	215	1760	1116	310	322	12	0	0	0

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE.

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

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEP-

TIDE.

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

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	122	Total	C	N	O	S	0	0	0
			997	613	182	191	11			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE.

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

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE.

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

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE.

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

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	J	1	Total	Zn	0	0
			1	1		
11	B	1	Total	Zn	0	0
			1	1		
11	I	2	Total	Zn	0	0
			2	2		
11	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	2	Total Zn 2 2	0	0
11	L	1	Total Zn 1 1	0	0

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	1	Total Mg 1 1	0	0

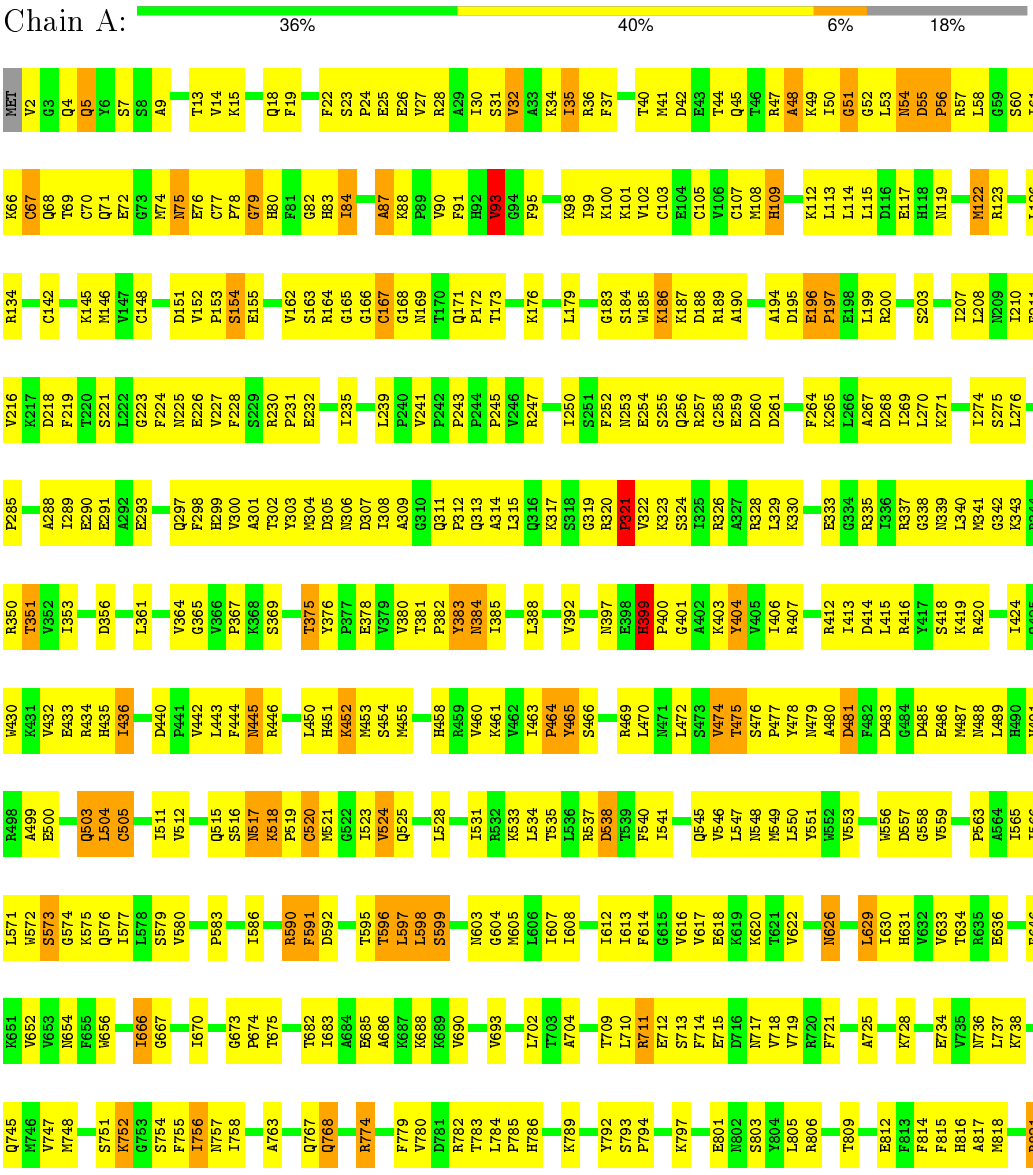
3 Residue-property plots (i)

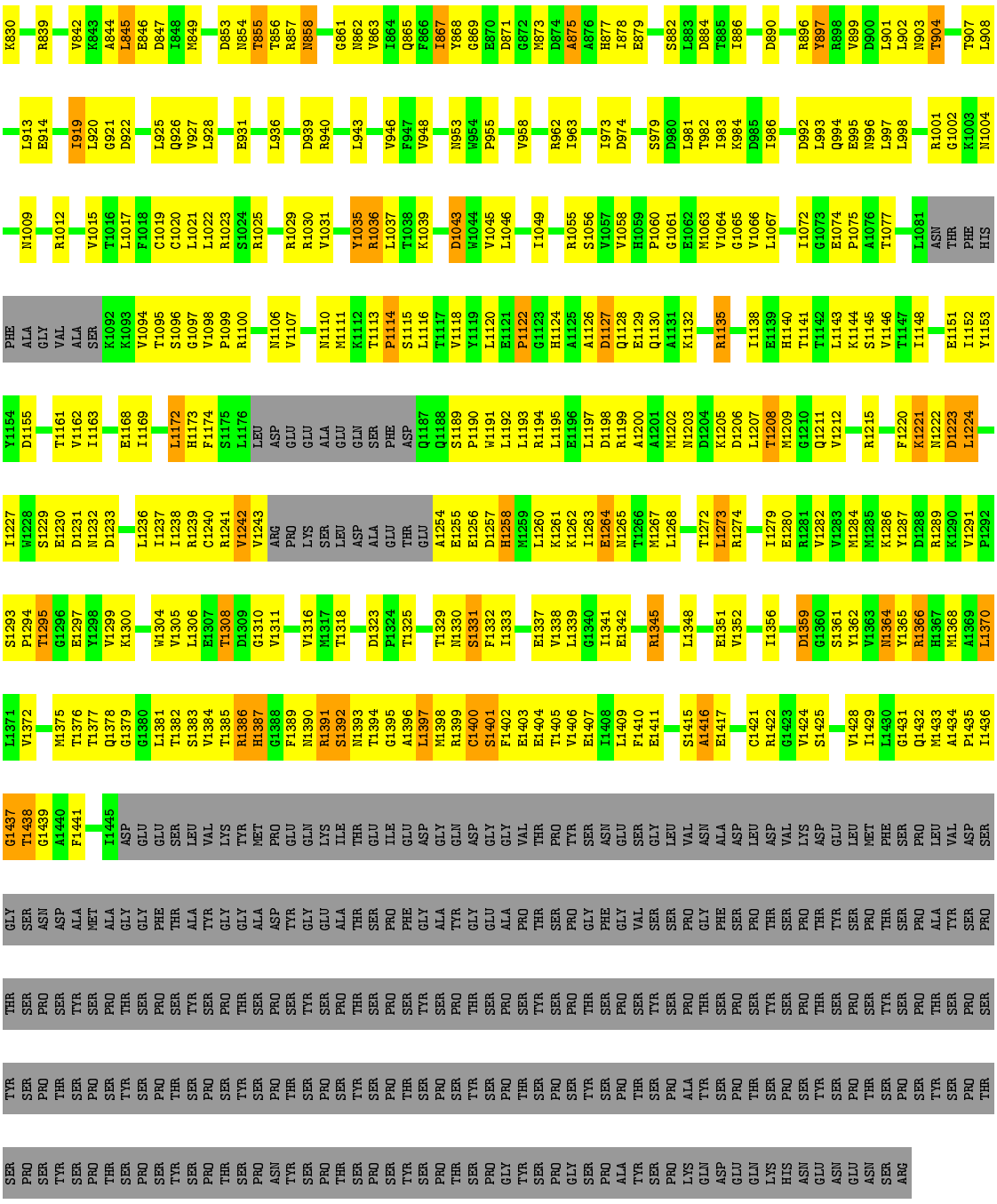
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: DNA-DIRECTED RNA POLYMERASE II LARGEST SUBUNIT

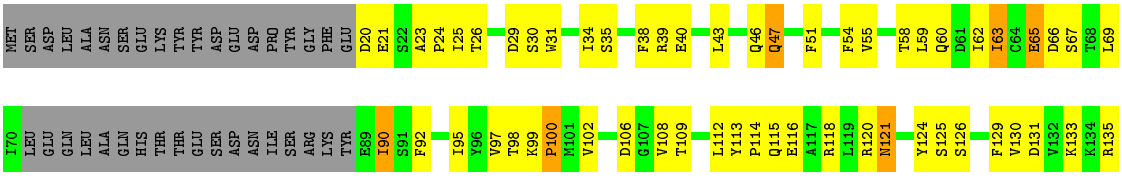
Chain A:

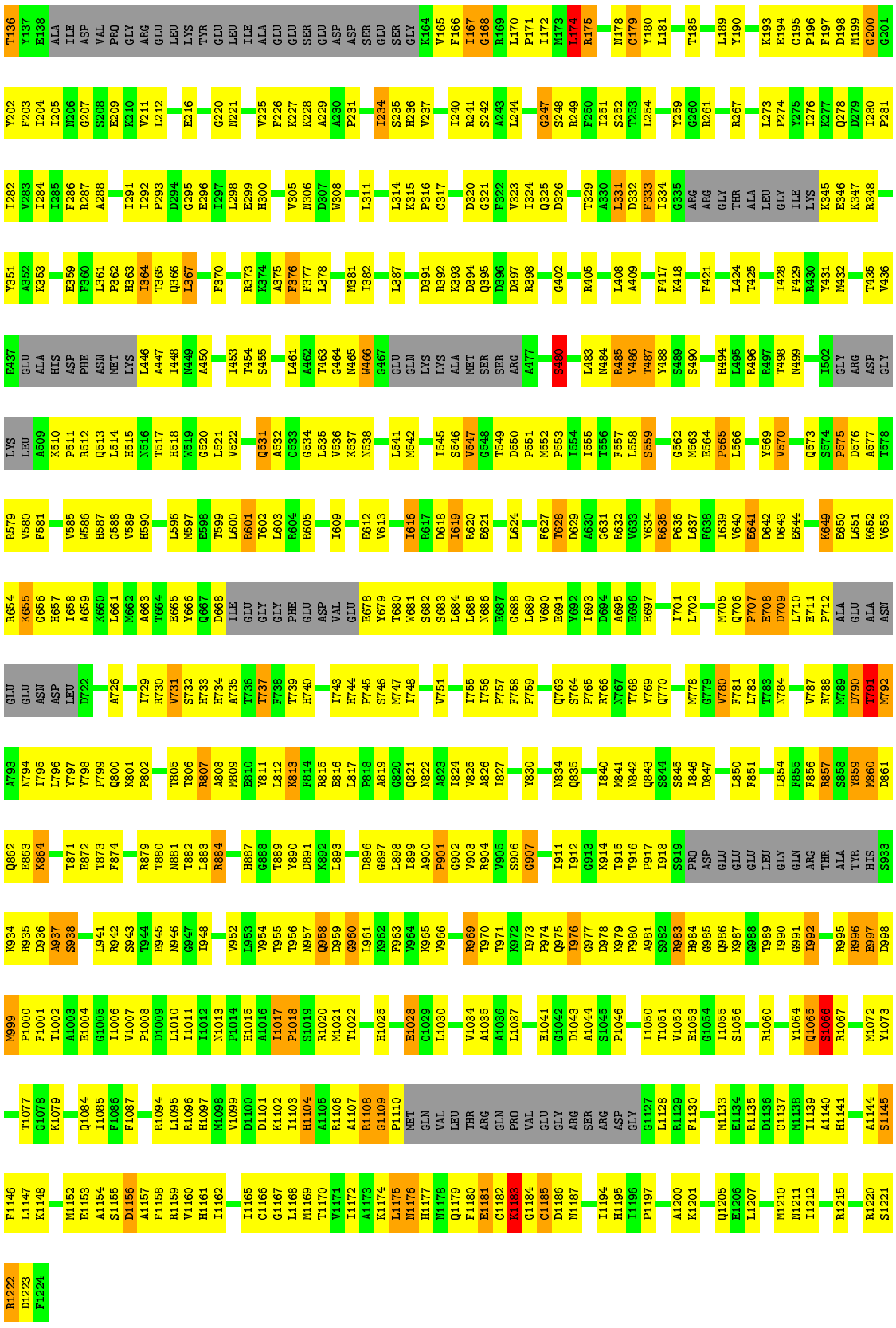




• Molecule 2: DNA-DIRECTED RNA POLYMERASE II 140KD POLYPEPTIDE

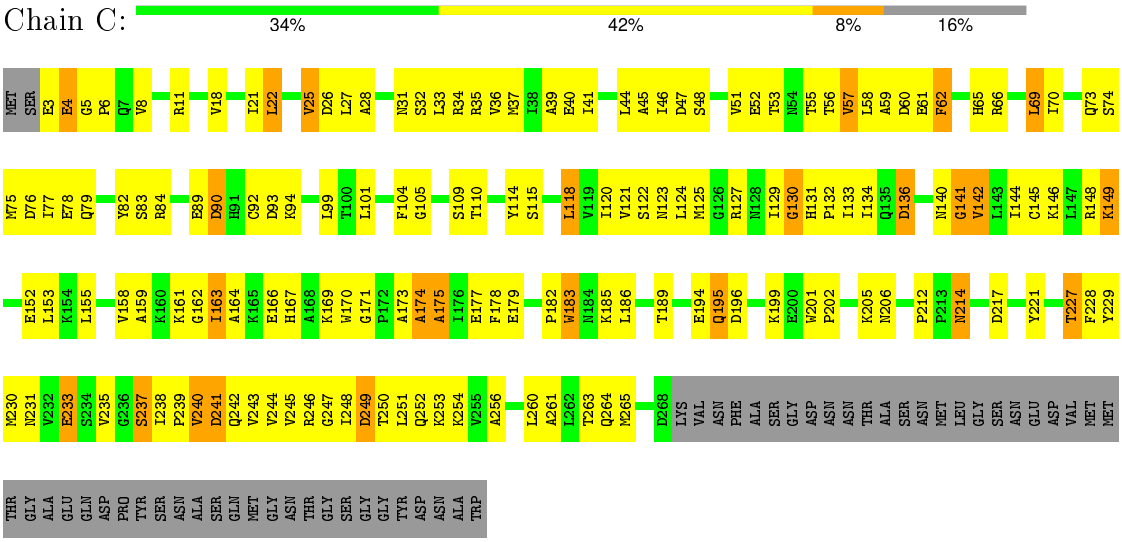
Chain B:





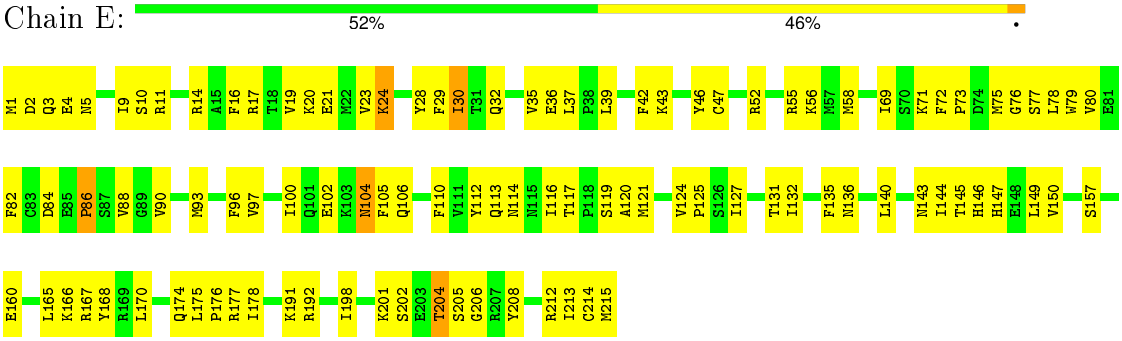
• Molecule 3: DNA-DIRECTED RNA POLYMERASE II 45KD POLYPEPTIDE

Chain C:



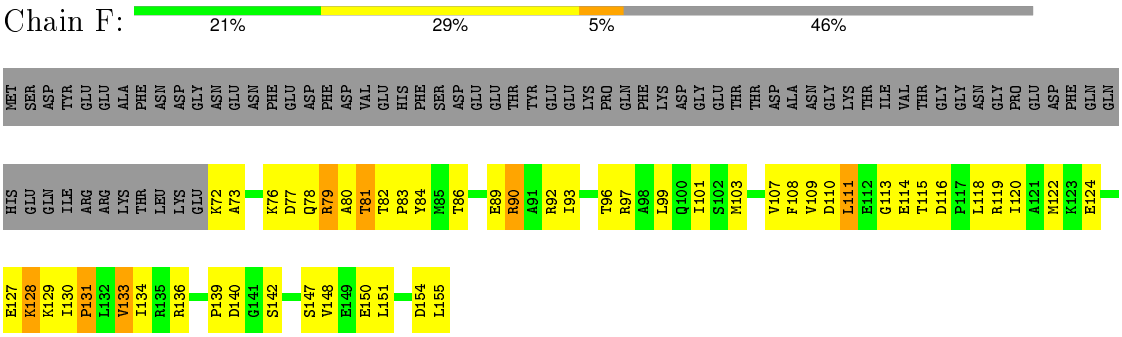
• Molecule 4: DNA-DIRECTED RNA POLYMERASE II 27KD POLYPEPTIDE

Chain E:



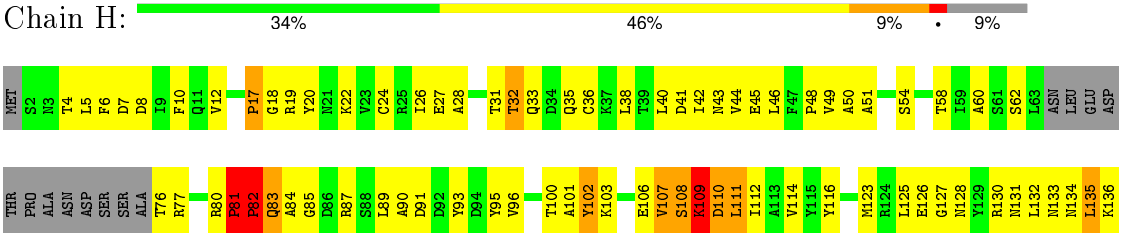
• Molecule 5: DNA-DIRECTED RNA POLYMERASE II 23KD POLYPEPTIDE

Chain F:



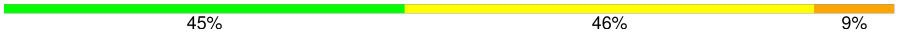
• Molecule 6: DNA-DIRECTED RNA POLYMERASE II 14.5KD POLYPEPTIDE

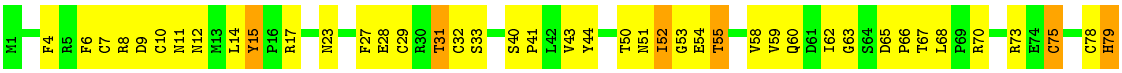
Chain H:



• Molecule 7: DNA-DIRECTED RNA POLYMERASE II 14.2KD POLYPEPTIDE

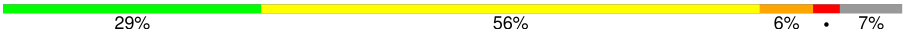
Chain I:





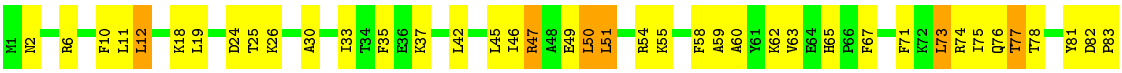
• Molecule 8: DNA-DIRECTED RNA POLYMERASE II 8.3KD POLYPEPTIDE

Chain J:



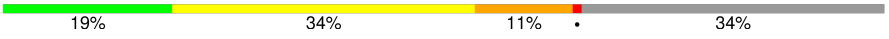
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II 13.6KD POLYPEPTIDE

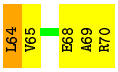
Chain K:



• Molecule 10: DNA-DIRECTED RNA POLYMERASE II 7.7KD POLYPEPTIDE

Chain L:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	130.70Å 224.80Å 369.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-3.10)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.283	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	28161	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.40	1/11312 (0.0%)	0.70	2/15298 (0.0%)
2	B	0.40	0/8793	0.68	3/11857 (0.0%)
3	C	0.42	0/2133	0.72	1/2891 (0.0%)
4	E	0.37	0/1796	0.63	0/2416
5	F	0.42	0/691	0.66	0/933
6	H	0.59	2/1086 (0.2%)	0.91	6/1470 (0.4%)
7	I	0.41	0/1016	0.70	0/1365
8	J	0.43	0/541	0.85	1/727 (0.1%)
9	K	0.42	0/937	0.61	0/1265
10	L	0.41	0/366	0.66	0/485
All	All	0.41	3/28671 (0.0%)	0.70	13/38707 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	109	LYS	CD-CE	7.54	1.70	1.51
6	H	109	LYS	CE-NZ	5.69	1.63	1.49
1	A	520	CYS	CB-SG	-5.67	1.72	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	109	LYS	N-CA-C	7.39	130.95	111.00
1	A	452	LYS	N-CA-C	-6.74	92.80	111.00
6	H	109	LYS	CA-CB-CG	6.68	128.09	113.40
6	H	80	ARG	NE-CZ-NH1	-6.09	117.25	120.30
6	H	80	ARG	NE-CZ-NH2	5.97	123.28	120.30
2	B	1066	SER	N-CA-C	5.54	125.97	111.00
1	A	399	HIS	N-CA-C	5.53	125.93	111.00
3	C	183	TRP	N-CA-C	-5.49	96.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	819	ALA	N-CA-C	-5.44	96.31	111.00
2	B	937	ALA	N-CA-C	-5.36	96.54	111.00
8	J	5	VAL	N-CA-C	-5.28	96.74	111.00
6	H	81	PRO	N-CA-C	5.21	125.65	112.10
6	H	108	SER	CB-CA-C	5.17	119.92	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11114	0	11193	945	0
2	B	8624	0	8642	736	1
3	C	2095	0	2051	177	0
4	E	1760	0	1788	103	0
5	F	679	0	701	56	0
6	H	1068	0	1040	93	0
7	I	997	0	955	71	0
8	J	532	0	542	78	0
9	K	919	0	929	62	0
10	L	364	0	388	47	0
11	A	2	0	0	0	0
11	B	1	0	0	0	0
11	C	1	0	0	0	0
11	I	2	0	0	1	0
11	J	1	0	0	0	0
11	L	1	0	0	0	0
12	A	1	0	0	0	0
All	All	28161	0	28229	2150	1

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 38.

All (2150) 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)
1:A:1364:ASN:ND2	1:A:1366:ARG:HG2	1.59	1.17
7:I:111:THR:HG22	7:I:113:ASP:H	1.05	1.17
10:L:60:ARG:HG3	10:L:61:THR:H	1.04	1.12
2:B:846:ILE:HG23	2:B:974:PRO:HG2	1.32	1.11
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.06	1.10
1:A:567:LYS:HB2	1:A:568:PRO:HD2	1.24	1.09
1:A:47:ARG:HH22	1:A:255:SER:HA	1.13	1.08
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.26	1.08
1:A:308:ILE:HG22	1:A:309:ALA:H	1.13	1.07
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.32	1.07
1:A:381:THR:HG22	1:A:383:TYR:H	1.21	1.06
3:C:44:LEU:HB2	3:C:77:ILE:HD11	1.38	1.04
2:B:1065:GLN:NE2	2:B:1067:ARG:H	1.55	1.04
2:B:955:THR:HG22	2:B:956:THR:H	0.88	1.04
1:A:535:THR:HG21	1:A:617:VAL:H	1.23	1.04
2:B:806:THR:HG22	2:B:808:ALA:H	1.24	1.03
2:B:955:THR:HG22	2:B:956:THR:N	1.72	1.02
2:B:120:ARG:HG2	2:B:955:THR:HG21	1.41	1.02
6:H:26:ILE:HD11	6:H:49:VAL:HG11	1.40	1.02
2:B:731:VAL:HG12	2:B:732:SER:H	1.26	1.01
10:L:60:ARG:CG	10:L:61:THR:H	1.72	1.01
1:A:313:GLN:HB2	1:A:320:ARG:HB3	1.42	1.01
2:B:637:LEU:HD12	2:B:693:ILE:HD12	1.42	1.01
2:B:955:THR:CG2	2:B:956:THR:H	1.70	1.00
2:B:405:ARG:NH1	2:B:632:ARG:HG2	1.75	1.00
1:A:40:THR:HG22	1:A:41:MET:HG3	1.40	1.00
2:B:708:GLU:HG3	2:B:709:ASP:H	1.27	0.99
1:A:868:TYR:CE1	1:A:1064:VAL:HG11	1.98	0.97
1:A:567:LYS:HZ1	6:H:46:LEU:HB2	1.27	0.97
2:B:871:THR:HG22	2:B:872:GLU:H	1.27	0.97
2:B:1165:ILE:HD12	2:B:1187:ASN:HD21	1.27	0.96
1:A:533:LYS:HE2	1:A:745:GLN:HE22	1.31	0.96
1:A:567:LYS:HB2	1:A:568:PRO:CD	1.96	0.95
1:A:1394:THR:HG22	1:A:1395:GLY:H	1.29	0.95
10:L:60:ARG:HG3	10:L:61:THR:N	1.79	0.95
1:A:869:GLY:O	4:E:204:THR:HG21	1.66	0.95
1:A:518:LYS:HB2	1:A:519:PRO:HD2	1.46	0.94
1:A:187:LYS:HB2	1:A:194:ALA:HB1	1.48	0.94
1:A:35:ILE:HD12	1:A:241:VAL:HG21	1.50	0.94
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.50	0.94
2:B:650:GLU:HG2	2:B:654:ARG:HH12	1.31	0.94
1:A:2:VAL:HG21	2:B:1157:ALA:HB3	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	1:A:568:PRO:HD2	1.96	0.93
1:A:49:LYS:HB3	1:A:55:ASP:HB2	1.49	0.93
2:B:642:ASP:HB3	2:B:649:LYS:HD3	1.51	0.93
1:A:849:MET:CE	1:A:1061:GLY:HA2	1.98	0.93
2:B:654:ARG:H	2:B:657:HIS:HD2	1.07	0.92
1:A:567:LYS:NZ	6:H:46:LEU:HB2	1.82	0.92
2:B:955:THR:HG23	10:L:54:ARG:O	1.68	0.92
2:B:680:THR:HG22	2:B:681:TRP:N	1.85	0.92
9:K:46:ILE:HG22	9:K:50:LEU:HD12	1.50	0.92
2:B:957:ASN:HD22	2:B:961:LEU:HD12	1.32	0.92
6:H:35:GLN:HB3	6:H:111:LEU:HD21	1.50	0.92
4:E:5:ASN:HD21	4:E:52:ARG:HG2	1.34	0.91
1:A:907:THR:HG22	1:A:908:LEU:H	1.36	0.91
1:A:15:LYS:HB3	2:B:1220:ARG:HG2	1.51	0.90
2:B:174:LEU:O	2:B:175:ARG:HB2	1.69	0.90
2:B:345:LYS:HA	2:B:348:ARG:HE	1.35	0.90
1:A:1116:LEU:HD13	1:A:1311:VAL:HG13	1.53	0.90
6:H:109:LYS:CG	6:H:110:ASP:H	1.83	0.90
2:B:884:ARG:O	2:B:936:ASP:HB3	1.72	0.90
2:B:882:THR:HG21	2:B:935:ARG:HA	1.54	0.89
2:B:65:GLU:HG3	2:B:66:ASP:H	1.35	0.89
1:A:47:ARG:NH2	1:A:255:SER:HA	1.88	0.89
2:B:680:THR:HG22	2:B:681:TRP:H	1.37	0.89
2:B:211:VAL:O	2:B:480:SER:HA	1.73	0.89
1:A:14:VAL:H	1:A:1432:GLN:HE22	1.21	0.89
2:B:801:LYS:O	8:J:52:THR:HG23	1.73	0.88
6:H:107:VAL:HG12	6:H:107:VAL:O	1.74	0.88
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.56	0.88
2:B:1072:MET:HE3	2:B:1085:ILE:HB	1.52	0.88
1:A:741:ASN:HD22	1:A:744:LYS:H	1.17	0.88
1:A:896:ARG:HD3	1:A:897:TYR:HE1	1.37	0.88
2:B:29:ASP:HB3	2:B:658:ILE:HD13	1.54	0.88
9:K:113:THR:O	9:K:114:LEU:HB2	1.73	0.87
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.55	0.87
2:B:311:LEU:HB3	7:I:4:PHE:HE2	1.40	0.87
2:B:569:TYR:CD1	2:B:589:VAL:HG21	2.09	0.87
5:F:111:LEU:H	5:F:111:LEU:HD12	1.38	0.87
6:H:4:THR:HA	6:H:60:ALA:HB2	1.57	0.87
1:A:1161:THR:HG22	1:A:1163:ILE:N	1.90	0.86
2:B:130:VAL:HG21	2:B:167:ILE:HD12	1.55	0.86
1:A:313:GLN:CB	1:A:320:ARG:HB3	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:LEU:O	1:A:475:THR:HB	1.76	0.86
7:I:111:THR:HG22	7:I:113:ASP:N	1.89	0.85
1:A:414:ASP:OD1	1:A:416:ARG:HG2	1.77	0.85
6:H:26:ILE:HD12	6:H:42:ILE:HD12	1.57	0.85
1:A:541:ILE:HG22	1:A:546:VAL:HG23	1.59	0.84
1:A:32:VAL:HG21	1:A:68:GLN:NE2	1.91	0.84
1:A:1404:GLU:C	1:A:1406:VAL:H	1.80	0.84
1:A:590:ARG:HB3	1:A:605:MET:H	1.42	0.84
4:E:143:ASN:HB3	4:E:146:HIS:HD2	1.43	0.84
2:B:744:HIS:HD2	2:B:746:SER:H	1.25	0.84
2:B:363:HIS:O	2:B:364:ILE:HB	1.77	0.83
1:A:590:ARG:NH1	1:A:590:ARG:HG3	1.92	0.83
1:A:13:THR:HG23	1:A:1432:GLN:NE2	1.93	0.83
3:C:123:ASN:HD22	3:C:125:MET:HG2	1.43	0.83
1:A:255:SER:O	1:A:256:GLN:HG3	1.78	0.83
2:B:559:SER:HA	2:B:563:MET:HB3	1.61	0.83
1:A:567:LYS:HD2	1:A:568:PRO:HD2	1.60	0.83
1:A:445:ASN:CB	1:A:455:MET:HG2	2.09	0.83
1:A:567:LYS:HD3	6:H:95:TYR:CD1	2.14	0.83
2:B:605:ARG:NH1	2:B:639:ILE:HD13	1.92	0.82
4:E:177:ARG:HD3	4:E:215:MET:SD	2.20	0.82
10:L:27:LEU:HD22	10:L:37:LYS:HD3	1.61	0.82
1:A:844:ALA:HB2	1:A:1384:VAL:HG13	1.59	0.82
1:A:84:ILE:HG23	1:A:239:LEU:HB3	1.61	0.82
3:C:214:ASN:HB2	3:C:217:ASP:OD2	1.80	0.82
2:B:200:GLY:HA2	2:B:202:TYR:CE2	2.15	0.82
1:A:32:VAL:HG21	1:A:68:GLN:HE22	1.42	0.82
1:A:1329:THR:HG22	1:A:1331:SER:H	1.45	0.82
2:B:956:THR:HA	2:B:961:LEU:O	1.80	0.81
3:C:123:ASN:ND2	3:C:125:MET:HG2	1.95	0.81
2:B:542:MET:HE3	2:B:747:MET:HG3	1.62	0.81
1:A:351:THR:HG23	2:B:1103:ILE:HA	1.60	0.81
1:A:48:ALA:O	1:A:49:LYS:HG3	1.80	0.81
1:A:412:ARG:NH2	2:B:1110:PRO:HD3	1.95	0.81
1:A:590:ARG:HB3	1:A:605:MET:N	1.95	0.81
1:A:315:LEU:HD12	1:A:321:PRO:HG2	1.60	0.81
6:H:89:LEU:C	6:H:91:ASP:H	1.82	0.81
10:L:54:ARG:HH11	10:L:54:ARG:HB2	1.46	0.80
3:C:174:ALA:O	8:J:10:CYS:HB2	1.81	0.80
1:A:308:ILE:HG22	1:A:309:ALA:N	1.95	0.80
1:A:590:ARG:HH11	1:A:590:ARG:HG3	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1094:VAL:HG13	1:A:1113:THR:HG21	1.61	0.80
8:J:32:GLU:CD	8:J:32:GLU:H	1.85	0.80
2:B:800:GLN:HB3	8:J:52:THR:CG2	2.11	0.80
1:A:453:MET:HB3	1:A:477:PRO:HB3	1.63	0.80
1:A:41:MET:HA	1:A:49:LYS:HA	1.64	0.80
2:B:680:THR:HG22	2:B:682:SER:H	1.45	0.80
3:C:134:ILE:HG12	3:C:141:GLY:HA3	1.64	0.80
7:I:17:ARG:HG3	7:I:28:GLU:HG2	1.64	0.80
1:A:650:GLN:O	1:A:654:ASN:HB2	1.82	0.80
2:B:29:ASP:HB3	2:B:658:ILE:CD1	2.11	0.79
10:L:55:ILE:HG13	10:L:56:LEU:H	1.47	0.79
1:A:913:LEU:HD12	1:A:914:GLU:H	1.46	0.79
2:B:1172:ILE:HD11	2:B:1183:LYS:HE2	1.65	0.79
2:B:871:THR:HG22	2:B:872:GLU:N	1.97	0.79
8:J:1:MET:N	8:J:56:LEU:HB2	1.97	0.79
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.63	0.79
1:A:107:CYS:SG	1:A:148:CYS:HB2	2.22	0.79
1:A:779:PHE:CE1	1:A:785:PRO:HD3	2.17	0.79
2:B:54:PHE:HA	2:B:58:THR:HB	1.64	0.79
1:A:896:ARG:HD3	1:A:897:TYR:CE1	2.16	0.79
2:B:807:ARG:HG3	2:B:807:ARG:HH11	1.45	0.79
1:A:1364:ASN:HD22	1:A:1366:ARG:HG2	1.45	0.79
1:A:567:LYS:HB3	6:H:96:VAL:H	1.48	0.79
4:E:147:HIS:CD2	4:E:149:LEU:H	2.00	0.79
7:I:54:GLU:OE2	7:I:118:ARG:NH1	2.15	0.79
3:C:99:LEU:HD22	3:C:120:ILE:HG12	1.64	0.78
6:H:109:LYS:HG2	6:H:110:ASP:H	1.48	0.78
1:A:704:ALA:HB2	1:A:710:LEU:HD12	1.63	0.78
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.48	0.78
1:A:805:LEU:O	1:A:805:LEU:HD12	1.83	0.78
1:A:675:THR:HG21	1:A:736:ASN:ND2	1.97	0.78
1:A:1390:ASN:O	1:A:1391:ARG:HB2	1.84	0.78
1:A:535:THR:HG21	1:A:617:VAL:N	1.98	0.78
6:H:123:MET:HE3	6:H:142:LEU:HD22	1.64	0.78
2:B:846:ILE:CG2	2:B:974:PRO:HG2	2.12	0.78
2:B:601:ARG:O	2:B:605:ARG:HG3	1.82	0.77
2:B:1002:THR:HG22	2:B:1006:ILE:N	1.99	0.77
1:A:524:VAL:HG12	1:A:525:GLN:H	1.48	0.77
2:B:991:GLY:O	2:B:992:ILE:HB	1.84	0.77
2:B:650:GLU:HG2	2:B:654:ARG:NH1	1.98	0.77
1:A:15:LYS:HD2	2:B:1220:ARG:HE	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LYS:HA	1:A:333:GLU:HG2	1.66	0.77
1:A:709:THR:HG22	1:A:711:ARG:H	1.48	0.77
3:C:242:GLN:HE21	3:C:246:ARG:HH21	1.31	0.77
2:B:1051:THR:HG22	2:B:1053:GLU:N	1.99	0.77
1:A:675:THR:CG2	1:A:736:ASN:HD21	1.97	0.77
2:B:429:PHE:HA	2:B:432:MET:HE3	1.66	0.77
4:E:124:VAL:HG13	4:E:132:ILE:HB	1.67	0.77
2:B:1065:GLN:HE21	2:B:1067:ARG:H	1.32	0.77
2:B:680:THR:CG2	2:B:681:TRP:H	1.97	0.76
1:A:563:PRO:HG3	1:A:572:TRP:CZ2	2.20	0.76
3:C:114:TYR:CD2	3:C:140:ASN:HB3	2.20	0.76
4:E:135:PHE:HB3	4:E:140:LEU:HD11	1.67	0.76
3:C:66:ARG:NH2	8:J:5:VAL:HG23	2.00	0.76
2:B:640:VAL:HG22	2:B:651:LEU:HD22	1.67	0.76
1:A:1017:LEU:HB2	4:E:206:GLY:H	1.50	0.76
2:B:702:LEU:CD2	2:B:737:THR:HG22	2.16	0.76
6:H:82:PRO:HG3	9:K:54:ARG:HG2	1.66	0.75
2:B:745:PRO:O	2:B:748:ILE:HG12	1.87	0.75
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.68	0.75
4:E:3:GLN:HG3	4:E:5:ASN:H	1.49	0.75
8:J:64:ASN:HB3	8:J:65:PRO:HD3	1.69	0.75
3:C:194:GLU:O	3:C:195:GLN:HG3	1.86	0.75
5:F:81:THR:HG21	5:F:136:ARG:HD3	1.68	0.75
1:A:1431:GLY:HA2	2:B:1152:MET:CE	2.16	0.75
1:A:1399:ARG:O	1:A:1401:SER:N	2.20	0.75
1:A:1431:GLY:HA2	2:B:1152:MET:HE2	1.69	0.75
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.68	0.75
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.52	0.75
4:E:90:VAL:HA	4:E:120:ALA:HB2	1.67	0.75
2:B:903:VAL:HG13	10:L:63:ARG:HH21	1.50	0.75
1:A:567:LYS:HB3	6:H:96:VAL:N	2.02	0.74
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.21	0.74
1:A:1400:CYS:HB3	1:A:1405:THR:HG1	1.53	0.74
2:B:654:ARG:H	2:B:657:HIS:CD2	1.98	0.74
3:C:73:GLN:NE2	3:C:75:MET:HB2	2.02	0.74
1:A:901:LEU:HD22	1:A:919:ILE:HG22	1.67	0.74
1:A:1114:PRO:HB2	1:A:1311:VAL:HG23	1.69	0.74
6:H:100:THR:HG23	6:H:138:GLU:HA	1.69	0.74
4:E:19:VAL:HG11	4:E:80:VAL:HG11	1.68	0.74
1:A:1242:VAL:HG12	1:A:1243:VAL:H	1.52	0.74
1:A:381:THR:HG21	1:A:383:TYR:CD1	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1072:MET:CE	2:B:1085:ILE:HB	2.17	0.74
1:A:210:ILE:O	1:A:214:ILE:HG13	1.87	0.74
1:A:1224:LEU:HD12	1:A:1241:ARG:O	1.88	0.74
1:A:308:ILE:CG2	1:A:309:ALA:H	1.98	0.74
3:C:77:ILE:HD13	3:C:129:ILE:HD11	1.70	0.74
10:L:32:ALA:HB3	10:L:55:ILE:HD12	1.69	0.74
5:F:76:LYS:HA	5:F:79:ARG:HD2	1.69	0.74
1:A:855:THR:HG21	1:A:857:ARG:HE	1.53	0.74
1:A:590:ARG:HB2	1:A:605:MET:HB3	1.69	0.74
1:A:219:PHE:HB3	1:A:224:PHE:HB2	1.69	0.73
1:A:1295:THR:HG23	1:A:1297:GLU:OE1	1.87	0.73
1:A:875:ALA:HA	1:A:878:ILE:HD12	1.69	0.73
2:B:737:THR:HG23	7:I:66:PRO:HB2	1.67	0.73
2:B:115:GLN:HG2	2:B:193:LYS:HB2	1.69	0.73
4:E:55:ARG:HB2	4:E:84:ASP:OD2	1.86	0.73
1:A:1173:HIS:NE2	1:A:1227:ILE:HG23	2.03	0.73
1:A:40:THR:HG23	1:A:54:ASN:OD1	1.89	0.73
2:B:487:THR:HG22	2:B:490:SER:H	1.53	0.73
4:E:17:ARG:O	4:E:21:GLU:HG3	1.88	0.73
2:B:120:ARG:CG	2:B:955:THR:HG21	2.18	0.73
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.70	0.73
2:B:35:SER:HA	2:B:811:TYR:HE2	1.53	0.73
2:B:702:LEU:HD22	2:B:737:THR:HG22	1.71	0.73
1:A:1168:GLU:O	1:A:1172:LEU:HG	1.87	0.73
1:A:270:LEU:O	1:A:274:ILE:HG13	1.88	0.73
2:B:642:ASP:HB3	2:B:649:LYS:CD	2.19	0.72
1:A:351:THR:CG2	2:B:1103:ILE:HA	2.18	0.72
2:B:879:ARG:HD2	2:B:883:LEU:HD22	1.68	0.72
1:A:523:ILE:HD12	1:A:622:VAL:HG21	1.71	0.72
1:A:1364:ASN:ND2	1:A:1366:ARG:H	1.87	0.72
1:A:317:LYS:HD2	1:A:321:PRO:HG3	1.72	0.72
2:B:705:MET:H	2:B:710:LEU:HD12	1.54	0.72
2:B:680:THR:CG2	2:B:681:TRP:N	2.53	0.72
6:H:109:LYS:CG	6:H:110:ASP:N	2.51	0.72
1:A:31:SER:CB	1:A:83:HIS:HB2	2.19	0.72
1:A:907:THR:HG22	1:A:908:LEU:N	2.05	0.72
2:B:98:THR:HG22	2:B:99:LYS:H	1.53	0.72
1:A:302:THR:OG1	1:A:312:PRO:HG3	1.90	0.72
1:A:590:ARG:HG2	1:A:604:GLY:HA2	1.72	0.72
2:B:737:THR:HG21	7:I:66:PRO:O	1.89	0.72
2:B:603:LEU:HB3	2:B:609:ILE:HG13	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:806:THR:HG22	2:B:808:ALA:N	2.02	0.72
3:C:167:HIS:HD2	3:C:169:LYS:H	1.38	0.72
9:K:55:LYS:HD3	9:K:78:THR:HB	1.72	0.71
1:A:1370:LEU:HD12	1:A:1370:LEU:O	1.89	0.71
1:A:1293:SER:HB2	1:A:1299:VAL:CG2	2.20	0.71
6:H:130:ARG:HB3	6:H:134:ASN:HD22	1.54	0.71
2:B:387:LEU:HD23	2:B:393:LYS:HD2	1.70	0.71
3:C:56:THR:HG22	3:C:58:LEU:H	1.54	0.71
2:B:254:LEU:HD23	2:B:381:MET:HE3	1.71	0.71
6:H:101:ALA:HB2	6:H:116:TYR:CE2	2.25	0.71
1:A:1341:ILE:HD12	1:A:1379:GLY:C	2.10	0.71
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.73	0.71
4:E:43:LYS:O	4:E:47:CYS:HB2	1.91	0.71
2:B:234:ILE:H	2:B:234:ILE:HD12	1.55	0.71
1:A:535:THR:HG22	1:A:616:VAL:HA	1.72	0.71
2:B:654:ARG:N	2:B:657:HIS:HD2	1.86	0.71
1:A:61:ILE:HG22	1:A:62:ASP:H	1.56	0.71
1:A:605:MET:HE2	1:A:607:ILE:HG13	1.73	0.71
1:A:901:LEU:HA	1:A:907:THR:HG23	1.72	0.71
1:A:1404:GLU:C	1:A:1406:VAL:N	2.40	0.71
2:B:709:ASP:O	2:B:710:LEU:HD23	1.89	0.71
2:B:25:ILE:HD11	2:B:653:VAL:O	1.91	0.71
2:B:642:ASP:O	2:B:644:GLU:N	2.24	0.71
2:B:824:ILE:HG12	8:J:48:ARG:NH1	2.05	0.71
1:A:1394:THR:HG22	1:A:1395:GLY:N	2.06	0.71
1:A:913:LEU:HD12	1:A:914:GLU:N	2.06	0.71
9:K:65:HIS:HD2	9:K:67:PHE:H	1.37	0.71
2:B:613:VAL:HG22	2:B:628:THR:HG23	1.72	0.70
1:A:57:ARG:HB3	1:A:68:GLN:HG3	1.72	0.70
10:L:27:LEU:HD13	10:L:37:LYS:HG2	1.71	0.70
5:F:81:THR:HG22	5:F:136:ARG:NH1	2.06	0.70
1:A:434:ARG:HG3	1:A:435:HIS:O	1.91	0.70
1:A:535:THR:CG2	1:A:616:VAL:HA	2.21	0.70
2:B:58:THR:O	2:B:62:ILE:HG13	1.91	0.70
1:A:114:LEU:HD22	1:A:171:GLN:NE2	2.06	0.70
2:B:821:GLN:OE1	2:B:850:LEU:HD12	1.91	0.70
3:C:76:ASP:O	3:C:79:GLN:HG2	1.91	0.70
2:B:118:ARG:HG3	2:B:204:ILE:HD13	1.73	0.70
2:B:92:PHE:HD2	2:B:130:VAL:HG11	1.57	0.70
1:A:1189:SER:HB2	1:A:1190:PRO:HD2	1.73	0.70
2:B:778:MET:HG2	2:B:794:ASN:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:LEU:HB2	4:E:206:GLY:N	2.05	0.70
9:K:55:LYS:HD3	9:K:78:THR:CB	2.22	0.70
1:A:608:ILE:HD12	1:A:613:ILE:HD13	1.72	0.70
2:B:63:ILE:HB	2:B:95:ILE:HD11	1.73	0.70
1:A:868:TYR:HE1	1:A:1064:VAL:HG11	1.52	0.70
1:A:994:GLN:HE22	1:A:1023:ARG:HE	1.40	0.70
2:B:311:LEU:HB3	7:I:4:PHE:CE2	2.25	0.70
3:C:70:ILE:HD11	3:C:144:ILE:HG12	1.73	0.69
1:A:353:ILE:HD13	1:A:487:MET:HE2	1.72	0.69
2:B:864:LYS:HD3	2:B:871:THR:HA	1.74	0.69
3:C:241:ASP:O	3:C:245:VAL:HG23	1.92	0.69
5:F:77:ASP:O	5:F:78:GLN:HB2	1.91	0.69
2:B:46:GLN:HG3	2:B:47:GLN:N	2.07	0.69
4:E:147:HIS:HD2	4:E:149:LEU:H	1.37	0.69
2:B:639:ILE:HD11	2:B:691:GLU:CG	2.16	0.69
1:A:711:ARG:HH12	7:I:95:THR:HG22	1.56	0.69
5:F:81:THR:CG2	5:F:136:ARG:HH11	2.05	0.69
1:A:853:ASP:OD1	1:A:855:THR:HB	1.92	0.69
2:B:46:GLN:HG3	2:B:47:GLN:H	1.57	0.69
2:B:889:THR:HG22	2:B:891:ASP:H	1.55	0.69
2:B:102:VAL:CG2	2:B:112:LEU:HB2	2.23	0.69
1:A:919:ILE:HD13	1:A:983:ILE:HD12	1.74	0.69
1:A:1111:MET:HE1	1:A:1114:PRO:HA	1.75	0.69
2:B:827:ILE:HD13	2:B:1017:ILE:HD11	1.73	0.69
1:A:367:PRO:HB3	1:A:466:SER:HA	1.75	0.69
2:B:963:PHE:HE2	2:B:965:LYS:HE3	1.58	0.69
1:A:751:SER:O	1:A:752:LYS:HB2	1.91	0.69
2:B:291:ILE:HD13	2:B:300:HIS:NE2	2.08	0.69
1:A:18:GLN:HB2	2:B:1215:ARG:HB2	1.75	0.69
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.22	0.69
1:A:757:ASN:OD1	2:B:1021:MET:HE2	1.94	0.68
1:A:57:ARG:HB3	1:A:68:GLN:CG	2.23	0.68
6:H:111:LEU:HA	6:H:127:GLY:O	1.93	0.68
2:B:130:VAL:CG2	2:B:167:ILE:HD12	2.23	0.68
1:A:436:ILE:HD11	1:A:491:VAL:HG21	1.76	0.68
1:A:115:LEU:HD12	1:A:142:CYS:HB3	1.76	0.68
1:A:567:LYS:CD	1:A:568:PRO:HD2	2.23	0.68
1:A:1400:CYS:HB3	1:A:1405:THR:OG1	1.93	0.68
8:J:16:ASP:OD1	8:J:17:LYS:HG3	1.93	0.68
1:A:541:ILE:HG22	1:A:546:VAL:CG2	2.23	0.68
2:B:102:VAL:HG22	2:B:112:LEU:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:ARG:NE	2:B:665:GLU:HG2	2.08	0.68
2:B:1162:ILE:HD11	2:B:1194:ILE:CD1	2.24	0.68
2:B:295:GLY:H	2:B:298:LEU:HG	1.58	0.68
1:A:579:SER:OG	1:A:612:ILE:HG22	1.94	0.68
1:A:4:GLN:O	1:A:5:GLN:HB2	1.94	0.68
1:A:82:GLY:HA3	1:A:241:VAL:HB	1.76	0.68
2:B:822:ASN:HD22	8:J:52:THR:HG21	1.59	0.68
1:A:1039:LYS:O	1:A:1043:ASP:HB2	1.94	0.68
2:B:39:ARG:HE	2:B:665:GLU:HG2	1.59	0.68
1:A:80:HIS:O	1:A:243:PRO:HB3	1.94	0.68
1:A:187:LYS:O	1:A:188:ASP:HB2	1.93	0.68
9:K:55:LYS:HB3	9:K:81:TYR:HD1	1.59	0.68
1:A:108:MET:O	1:A:109:HIS:HB2	1.93	0.67
1:A:1258:HIS:ND1	1:A:1262:LYS:HE3	2.09	0.67
3:C:66:ARG:CZ	8:J:5:VAL:HG23	2.24	0.67
1:A:741:ASN:ND2	1:A:744:LYS:H	1.92	0.67
1:A:913:LEU:HD11	1:A:981:LEU:O	1.95	0.67
1:A:185:TRP:O	1:A:186:LYS:HB2	1.93	0.67
1:A:783:THR:HG21	1:A:815:PHE:CZ	2.29	0.67
1:A:982:THR:HG22	1:A:984:LYS:H	1.58	0.67
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.94	0.67
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.23	0.67
2:B:707:PRO:HG2	2:B:708:GLU:H	1.58	0.67
1:A:32:VAL:HB	1:A:57:ARG:HD2	1.77	0.67
3:C:166:GLU:HG3	9:K:10:PHE:CZ	2.29	0.67
1:A:265:LYS:O	1:A:269:ILE:HG13	1.94	0.67
1:A:1193:LEU:HB2	1:A:1260:LEU:HD11	1.76	0.67
7:I:55:THR:HG23	7:I:58:VAL:HG21	1.75	0.67
2:B:871:THR:CG2	2:B:872:GLU:H	2.05	0.67
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.29	0.67
2:B:995:ARG:HB3	2:B:997:GLU:OE2	1.94	0.67
1:A:879:GLU:O	1:A:955:PRO:HA	1.94	0.67
1:A:474:VAL:HG13	1:A:478:TYR:CE1	2.29	0.67
1:A:1422:ARG:HG2	2:B:1220:ARG:NH1	2.10	0.67
3:C:148:ARG:NH1	8:J:64:ASN:HA	2.10	0.67
3:C:56:THR:HG22	3:C:57:VAL:N	2.09	0.67
4:E:29:PHE:O	4:E:30:ILE:HG13	1.94	0.67
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.75	0.67
1:A:31:SER:OG	1:A:83:HIS:HB2	1.94	0.67
6:H:12:VAL:HA	6:H:28:ALA:CB	2.25	0.67
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:882:THR:HG22	2:B:884:ARG:H	1.60	0.67
2:B:911:ILE:HD11	2:B:941:LEU:HD12	1.77	0.67
2:B:780:VAL:HG21	8:J:56:LEU:HD11	1.76	0.66
1:A:1342:GLU:OE2	4:E:212:ARG:NH1	2.25	0.66
7:I:111:THR:HG22	7:I:112:SER:N	2.10	0.66
2:B:392:ARG:NH2	7:I:52:ILE:HD11	2.10	0.66
1:A:711:ARG:NH1	7:I:95:THR:HG22	2.10	0.66
2:B:825:VAL:HG12	2:B:826:ALA:N	2.11	0.66
1:A:711:ARG:HH12	7:I:95:THR:CG2	2.07	0.66
1:A:1118:VAL:CG2	1:A:1306:LEU:HB2	2.24	0.66
2:B:731:VAL:HG12	2:B:732:SER:N	2.04	0.66
1:A:345:VAL:HG11	2:B:1128:LEU:O	1.95	0.66
2:B:345:LYS:HA	2:B:348:ARG:NE	2.10	0.66
2:B:1166:CYS:O	2:B:1168:LEU:N	2.27	0.66
1:A:32:VAL:HB	1:A:57:ARG:HB2	1.77	0.66
1:A:1114:PRO:O	1:A:1115:SER:HB3	1.94	0.66
1:A:896:ARG:NH2	1:A:1030:ARG:HH21	1.94	0.66
2:B:165:VAL:HG13	2:B:446:LEU:HD21	1.76	0.66
10:L:60:ARG:CG	10:L:61:THR:N	2.45	0.66
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.76	0.66
2:B:542:MET:CE	2:B:747:MET:HG3	2.24	0.66
1:A:709:THR:HB	1:A:712:GLU:HG3	1.77	0.66
2:B:240:ILE:HG22	2:B:254:LEU:HB3	1.76	0.66
1:A:1152:ILE:HG23	1:A:1260:LEU:HD23	1.76	0.66
1:A:540:PHE:C	1:A:541:ILE:HD12	2.16	0.66
2:B:293:PRO:HG2	2:B:296:GLU:HB2	1.77	0.66
2:B:293:PRO:HG2	2:B:296:GLU:CB	2.25	0.66
2:B:108:VAL:HG12	2:B:109:THR:H	1.60	0.66
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.11	0.66
2:B:1162:ILE:HD11	2:B:1194:ILE:HD13	1.78	0.66
3:C:124:LEU:O	3:C:127:ARG:HG2	1.94	0.66
1:A:806:ARG:HH12	2:B:729:ILE:HD11	1.61	0.66
2:B:712:PRO:HD3	2:B:733:HIS:CD2	2.31	0.66
2:B:515:HIS:CD2	2:B:517:THR:H	2.14	0.66
2:B:118:ARG:NH1	2:B:204:ILE:HD11	2.10	0.65
6:H:5:LEU:HB3	6:H:133:ASN:O	1.96	0.65
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.78	0.65
1:A:590:ARG:O	1:A:591:PHE:HB2	1.96	0.65
1:A:675:THR:CG2	1:A:736:ASN:ND2	2.59	0.65
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.79	0.65
1:A:783:THR:HG22	1:A:784:LEU:HG	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:147:SER:OG	5:F:150:GLU:HG3	1.96	0.65
1:A:24:PRO:HG2	1:A:25:GLU:OE2	1.96	0.65
5:F:97:ARG:NE	5:F:124:GLU:OE1	2.21	0.65
1:A:74:MET:O	1:A:75:ASN:HB2	1.95	0.65
2:B:378:LEU:O	2:B:382:ILE:HG13	1.97	0.65
1:A:515:GLN:HG3	1:A:516:SER:N	2.12	0.65
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.32	0.65
1:A:388:LEU:HD22	1:A:432:VAL:HB	1.78	0.65
1:A:1025:ARG:HD2	1:A:1030:ARG:HH12	1.61	0.65
1:A:868:TYR:CZ	1:A:1064:VAL:HG11	2.32	0.65
8:J:53:HIS:CD2	8:J:54:VAL:N	2.64	0.65
4:E:46:TYR:CD2	4:E:58:MET:HG2	2.31	0.65
3:C:47:ASP:HA	10:L:69:ALA:HB3	1.78	0.65
2:B:549:THR:HB	2:B:628:THR:HG22	1.78	0.65
2:B:800:GLN:HB3	8:J:52:THR:HG21	1.77	0.65
2:B:763:GLN:HB2	2:B:1021:MET:HB2	1.79	0.65
1:A:1195:LEU:HD11	1:A:1267:MET:HE3	1.77	0.65
4:E:69:ILE:HG23	4:E:73:PRO:HA	1.78	0.65
1:A:1364:ASN:HD21	1:A:1366:ARG:HH11	1.45	0.65
2:B:43:LEU:HD13	2:B:812:LEU:HD23	1.78	0.65
3:C:3:GLU:O	3:C:4:GLU:HB2	1.96	0.65
1:A:208:LEU:HD22	1:A:212:LYS:HE3	1.79	0.65
1:A:590:ARG:HH11	1:A:590:ARG:CG	2.10	0.64
1:A:901:LEU:HD23	1:A:907:THR:HG23	1.79	0.64
2:B:619:ILE:HD12	7:I:65:ASP:HB2	1.78	0.64
2:B:205:ILE:CD1	2:B:461:LEU:HB3	2.27	0.64
1:A:313:GLN:O	1:A:321:PRO:HD2	1.97	0.64
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.79	0.64
1:A:1410:PHE:HD2	2:B:1212:ILE:HD11	1.60	0.64
1:A:901:LEU:HD13	1:A:919:ILE:HG23	1.78	0.64
8:J:3:VAL:CG2	8:J:18:TRP:HB2	2.26	0.64
1:A:871:ASP:HB3	4:E:204:THR:CG2	2.28	0.64
1:A:399:HIS:HB3	1:A:400:PRO:HD3	1.79	0.64
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.80	0.64
1:A:1113:THR:HG22	1:A:1113:THR:O	1.97	0.64
1:A:737:LEU:HD11	1:A:758:ILE:HG21	1.78	0.64
2:B:1002:THR:CG2	2:B:1006:ILE:H	2.10	0.64
3:C:244:VAL:O	3:C:248:ILE:HG13	1.98	0.64
2:B:1065:GLN:NE2	2:B:1067:ARG:N	2.38	0.64
1:A:337:ARG:HH22	1:A:1403:GLU:HA	1.61	0.64
1:A:451:HIS:O	2:B:1137:CYS:SG	2.54	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:175:ALA:HB2	8:J:10:CYS:HB2	1.80	0.64
2:B:46:GLN:NE2	2:B:496:ARG:HD3	2.13	0.64
2:B:912:ILE:O	2:B:938:SER:HB2	1.97	0.64
1:A:65:LEU:O	1:A:71:GLN:HA	1.97	0.64
1:A:1293:SER:OG	1:A:1295:THR:HG22	1.98	0.64
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.33	0.63
2:B:446:LEU:O	2:B:447:ALA:HB3	1.97	0.63
9:K:47:ARG:HG3	9:K:60:ALA:HA	1.79	0.63
9:K:18:LYS:NZ	9:K:37:LYS:HB2	2.12	0.63
1:A:311:GLN:HG2	1:A:313:GLN:HG3	1.80	0.63
1:A:58:LEU:HD22	1:A:80:HIS:O	1.99	0.63
1:A:122:MET:O	1:A:126:LEU:HG	1.98	0.63
6:H:106:GLU:C	6:H:108:SER:H	2.02	0.63
1:A:305:ASP:OD1	1:A:306:ASN:N	2.32	0.63
1:A:49:LYS:CB	1:A:55:ASP:HB2	2.27	0.63
1:A:15:LYS:O	1:A:1421:CYS:HB2	1.98	0.63
1:A:100:LYS:HE2	1:A:176:LYS:HB2	1.79	0.63
2:B:1079:LYS:HA	3:C:27:LEU:HD21	1.80	0.63
1:A:1399:ARG:C	1:A:1401:SER:H	2.01	0.63
1:A:868:TYR:CD2	1:A:1058:VAL:HG21	2.34	0.63
1:A:1094:VAL:HG13	1:A:1113:THR:CG2	2.27	0.63
2:B:287:ARG:NH2	2:B:325:GLN:HE22	1.97	0.63
2:B:1077:THR:HG22	2:B:1079:LYS:H	1.62	0.63
3:C:92:CYS:SG	3:C:94:LYS:HB3	2.38	0.63
1:A:973:ILE:HG21	1:A:1036:ARG:O	1.97	0.63
2:B:35:SER:HA	2:B:811:TYR:CE2	2.32	0.63
6:H:36:CYS:HA	6:H:126:GLU:O	1.99	0.63
8:J:57:ILE:O	8:J:61:LEU:HG	1.98	0.63
3:C:33:LEU:HG	3:C:37:MET:CE	2.28	0.63
2:B:545:ILE:HG22	2:B:546:SER:O	1.98	0.63
5:F:111:LEU:H	5:F:111:LEU:CD1	2.11	0.63
6:H:81:PRO:HB2	6:H:82:PRO:HD3	1.80	0.63
2:B:90:ILE:HA	2:B:133:LYS:O	1.99	0.63
2:B:273:LEU:HB2	2:B:276:ILE:HD12	1.79	0.63
1:A:350:ARG:HD2	1:A:488:ASN:OD1	1.98	0.63
1:A:567:LYS:NZ	6:H:46:LEU:CB	2.61	0.63
1:A:1364:ASN:ND2	1:A:1366:ARG:HH11	1.97	0.63
1:A:470:LEU:HD13	1:A:474:VAL:HG12	1.79	0.63
1:A:399:HIS:O	1:A:401:GLY:N	2.30	0.63
1:A:340:LEU:HD22	1:A:1425:SER:HB2	1.79	0.63
3:C:45:ALA:HB3	3:C:170:TRP:NE1	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:O	1:A:226:GLU:HG2	1.99	0.63
1:A:434:ARG:NH2	1:A:440:ASP:OD1	2.31	0.63
2:B:834:ASN:O	2:B:1013:ASN:HB2	1.99	0.63
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.81	0.63
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.80	0.62
2:B:918:ILE:HD12	2:B:935:ARG:HD2	1.79	0.62
3:C:141:GLY:O	3:C:142:VAL:HB	1.98	0.62
3:C:66:ARG:NH2	8:J:3:VAL:O	2.32	0.62
1:A:98:LYS:NZ	1:A:1411:GLU:HG2	2.14	0.62
2:B:484:ASN:OD1	2:B:486:TYR:HE1	1.80	0.62
1:A:847:ASP:OD2	1:A:858:ASN:HB2	1.99	0.62
3:C:99:LEU:CD2	3:C:120:ILE:HG12	2.27	0.62
1:A:535:THR:O	1:A:575:LYS:HE3	1.99	0.62
2:B:541:LEU:CB	2:B:747:MET:HE3	2.26	0.62
2:B:515:HIS:HD2	2:B:517:THR:H	1.44	0.62
1:A:173:THR:O	1:A:183:GLY:HA2	2.00	0.62
3:C:73:GLN:HE21	3:C:75:MET:H	1.44	0.62
6:H:138:GLU:HG2	6:H:139:ASN:N	2.13	0.62
1:A:90:VAL:HG12	1:A:91:PHE:N	2.13	0.62
1:A:605:MET:HE3	1:A:612:ILE:HG13	1.80	0.62
1:A:100:LYS:NZ	1:A:176:LYS:HD2	2.13	0.62
1:A:927:VAL:O	1:A:931:GLU:HG3	2.00	0.62
2:B:288:ALA:HB1	2:B:331:LEU:HD12	1.82	0.62
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.28	0.62
1:A:1333:ILE:O	1:A:1337:GLU:HG3	1.99	0.62
2:B:1166:CYS:HB2	2:B:1215:ARG:NH1	2.14	0.62
1:A:908:LEU:HD12	1:A:983:ILE:HD11	1.80	0.62
2:B:1185:CYS:O	2:B:1186:ASP:HB2	1.98	0.62
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.64	0.62
2:B:778:MET:CE	2:B:1094:ARG:HD3	2.30	0.62
2:B:284:ILE:HD13	2:B:324:ILE:HD12	1.80	0.62
1:A:567:LYS:CG	1:A:568:PRO:HD2	2.29	0.62
1:A:337:ARG:HH22	1:A:1403:GLU:CA	2.12	0.62
2:B:708:GLU:HG3	2:B:709:ASP:N	2.08	0.62
8:J:1:MET:H1	8:J:56:LEU:HB2	1.64	0.62
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.82	0.62
4:E:113:GLN:C	4:E:114:ASN:HD22	2.02	0.62
2:B:636:PRO:HA	2:B:691:GLU:O	2.00	0.62
2:B:1056:SER:HB3	2:B:1066:SER:HB2	1.82	0.62
6:H:43:ASN:OD1	6:H:45:GLU:HB3	2.00	0.62
3:C:235:VAL:HG13	8:J:13:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:192:ARG:HB2	4:E:215:MET:O	1.99	0.62
7:I:32:CYS:HG	11:I:2003:ZN:ZN	1.14	0.62
1:A:1100:ARG:HH21	1:A:1351:GLU:CG	2.12	0.62
1:A:88:LYS:HD2	1:A:293:GLU:OE1	1.99	0.62
1:A:497:THR:HG23	2:B:1146:PHE:HD1	1.64	0.62
7:I:111:THR:CG2	7:I:112:SER:N	2.62	0.61
1:A:1341:ILE:HD11	1:A:1376:THR:HG23	1.82	0.61
3:C:175:ALA:HB3	8:J:43:ARG:CZ	2.29	0.61
3:C:93:ASP:O	3:C:127:ARG:NH2	2.32	0.61
2:B:952:VAL:HB	10:L:58:LYS:HB2	1.81	0.61
2:B:705:MET:H	2:B:710:LEU:CD1	2.13	0.61
1:A:743:VAL:O	1:A:747:VAL:HG23	2.01	0.61
1:A:367:PRO:HB3	1:A:465:TYR:O	2.00	0.61
1:A:675:THR:OG1	1:A:736:ASN:ND2	2.32	0.61
9:K:55:LYS:O	9:K:77:THR:HG22	2.00	0.61
1:A:381:THR:HG22	1:A:383:TYR:N	2.06	0.61
1:A:1025:ARG:HD2	1:A:1030:ARG:NH1	2.15	0.61
1:A:1410:PHE:CD2	2:B:1212:ILE:HD11	2.35	0.61
1:A:1438:THR:HG22	2:B:1144:ALA:HB3	1.81	0.61
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.82	0.61
2:B:787:VAL:O	2:B:787:VAL:HG12	2.00	0.61
1:A:596:THR:O	1:A:598:LEU:N	2.32	0.61
6:H:26:ILE:HD11	6:H:49:VAL:CG1	2.26	0.61
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.83	0.61
9:K:10:PHE:CD1	9:K:11:LEU:HD13	2.36	0.61
10:L:38:LEU:O	10:L:39:SER:HB3	2.00	0.61
1:A:709:THR:HG21	7:I:93:LYS:O	2.00	0.61
6:H:36:CYS:SG	6:H:130:ARG:NH2	2.73	0.61
2:B:860:MET:HG2	2:B:861:ASP:N	2.15	0.61
2:B:315:LYS:N	2:B:316:PRO:HD2	2.15	0.61
2:B:758:PHE:CE2	2:B:1044:ALA:HA	2.34	0.61
1:A:1120:LEU:HB3	1:A:1124:HIS:O	2.00	0.61
4:E:131:THR:HG21	4:E:191:LYS:HE2	1.82	0.61
10:L:43:THR:O	10:L:43:THR:HG22	2.01	0.61
1:A:252:PHE:HB2	1:A:256:GLN:OE1	2.00	0.61
2:B:1017:ILE:HB	2:B:1018:PRO:HD3	1.82	0.61
1:A:646:PHE:O	1:A:650:GLN:HG3	2.00	0.61
7:I:78:CYS:O	7:I:80:SER:N	2.33	0.61
6:H:26:ILE:CD1	6:H:49:VAL:HG11	2.22	0.61
1:A:1116:LEU:CD1	1:A:1311:VAL:HG13	2.29	0.61
1:A:786:HIS:CD2	1:A:786:HIS:N	2.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:242:GLN:OE1	3:C:242:GLN:HA	1.99	0.61
3:C:37:MET:HG2	3:C:243:VAL:HG12	1.83	0.61
1:A:19:PHE:O	1:A:1416:ALA:HA	2.00	0.61
4:E:79:TRP:HB2	4:E:105:PHE:CE1	2.36	0.61
1:A:725:ALA:HA	1:A:728:LYS:HE2	1.82	0.61
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.15	0.61
2:B:970:THR:HG22	2:B:971:THR:N	2.14	0.61
4:E:2:ASP:O	4:E:3:GLN:HG2	2.01	0.61
9:K:55:LYS:HB3	9:K:81:TYR:CD1	2.36	0.61
1:A:793:SER:HB2	1:A:794:PRO:HD2	1.83	0.61
6:H:4:THR:HA	6:H:60:ALA:CB	2.30	0.61
2:B:708:GLU:O	2:B:710:LEU:N	2.34	0.61
10:L:27:LEU:HD13	10:L:37:LYS:CG	2.30	0.61
2:B:1183:LYS:O	2:B:1185:CYS:N	2.29	0.61
6:H:139:ASN:O	6:H:140:ALA:HB2	2.01	0.61
3:C:133:ILE:HD12	3:C:237:SER:HA	1.83	0.61
1:A:50:ILE:C	1:A:52:GLY:H	2.04	0.60
1:A:151:ASP:HA	1:A:162:VAL:O	2.01	0.60
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.47	0.60
2:B:864:LYS:HG2	2:B:871:THR:HG23	1.83	0.60
6:H:82:PRO:O	6:H:84:ALA:N	2.34	0.60
9:K:55:LYS:HD3	9:K:78:THR:OG1	2.01	0.60
9:K:18:LYS:HZ1	9:K:37:LYS:HB2	1.66	0.60
1:A:470:LEU:HD21	1:A:487:MET:CE	2.31	0.60
1:A:313:GLN:HA	1:A:322:VAL:HG23	1.83	0.60
5:F:82:THR:HG22	5:F:84:TYR:H	1.66	0.60
2:B:292:ILE:HD13	2:B:326:ASP:HA	1.84	0.60
2:B:281:PRO:HG2	2:B:284:ILE:HD12	1.83	0.60
1:A:844:ALA:HB2	1:A:1384:VAL:CG1	2.31	0.60
1:A:537:ARG:HB2	6:H:20:TYR:CE2	2.36	0.60
1:A:285:PRO:HG2	1:A:288:ALA:HB3	1.82	0.60
1:A:875:ALA:HB2	1:A:1366:ARG:CD	2.31	0.60
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.36	0.60
1:A:35:ILE:HD11	1:A:241:VAL:HG11	1.82	0.60
2:B:807:ARG:NH1	2:B:807:ARG:HG3	2.17	0.60
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.83	0.60
2:B:1051:THR:CG2	2:B:1053:GLU:H	2.14	0.60
7:I:121:PHE:O	7:I:122:SER:HB3	2.01	0.60
1:A:1194:ARG:NH2	1:A:1237:ILE:HD13	2.16	0.60
1:A:353:ILE:HD13	1:A:487:MET:CE	2.30	0.60
8:J:48:ARG:HE	8:J:49:MET:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:840:ILE:HB	2:B:1011:ILE:HB	1.83	0.60
2:B:280:ILE:CD1	2:B:334:ILE:HG12	2.32	0.60
2:B:135:ARG:O	2:B:136:THR:CB	2.50	0.60
2:B:363:HIS:O	2:B:364:ILE:CB	2.49	0.60
2:B:97:VAL:HG12	2:B:178:ASN:HD21	1.67	0.60
1:A:857:ARG:HD3	1:A:861:GLY:O	2.02	0.60
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.83	0.60
4:E:32:GLN:HE21	4:E:36:GLU:HG3	1.67	0.60
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.66	0.60
6:H:18:GLY:O	6:H:19:ARG:HB2	2.02	0.60
9:K:46:ILE:HG22	9:K:50:LEU:CD1	2.29	0.60
8:J:45:CYS:O	8:J:48:ARG:HG3	2.01	0.60
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.84	0.60
3:C:75:MET:HG2	3:C:246:ARG:HH22	1.67	0.60
1:A:28:ARG:HG2	1:A:83:HIS:CE1	2.37	0.60
2:B:914:LYS:HB3	2:B:937:ALA:O	2.01	0.60
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.84	0.59
2:B:25:ILE:HD11	2:B:653:VAL:C	2.21	0.59
4:E:46:TYR:CE2	4:E:58:MET:HA	2.37	0.59
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.02	0.59
2:B:575:PRO:HG2	2:B:576:ASP:H	1.66	0.59
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.84	0.59
2:B:640:VAL:O	2:B:641:GLU:C	2.40	0.59
1:A:184:SER:HB3	1:A:199:LEU:CD2	2.32	0.59
5:F:109:VAL:CG2	5:F:124:GLU:HG2	2.32	0.59
1:A:190:ALA:HA	1:A:195:ASP:OD1	2.02	0.59
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.84	0.59
1:A:913:LEU:CD1	1:A:981:LEU:O	2.50	0.59
1:A:69:THR:HB	2:B:1174:LYS:HE2	1.84	0.59
3:C:260:LEU:O	3:C:263:THR:HB	2.01	0.59
1:A:32:VAL:HG11	1:A:68:GLN:OE1	2.02	0.59
1:A:1021:LEU:O	1:A:1025:ARG:HG2	2.01	0.59
5:F:81:THR:CG2	5:F:136:ARG:NH1	2.65	0.59
5:F:81:THR:HG22	5:F:82:THR:N	2.17	0.59
7:I:50:THR:HG22	7:I:51:ASN:N	2.17	0.59
1:A:230:ARG:HB3	1:A:232:GLU:HG2	1.85	0.59
2:B:1220:ARG:O	2:B:1222:ARG:N	2.34	0.59
1:A:465:TYR:CD1	1:A:465:TYR:N	2.71	0.59
2:B:733:HIS:O	2:B:735:ALA:N	2.35	0.59
1:A:34:LYS:HD2	1:A:36:ARG:NH2	2.17	0.59
1:A:353:ILE:HD11	1:A:485:ASP:HB2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1400:CYS:CB	1:A:1405:THR:HG1	2.16	0.59
3:C:166:GLU:HG3	9:K:10:PHE:CE2	2.37	0.59
1:A:741:ASN:HD22	1:A:744:LYS:N	1.96	0.59
2:B:569:TYR:CE1	2:B:589:VAL:HG21	2.38	0.59
2:B:129:PHE:CE2	2:B:166:PHE:HD1	2.20	0.59
2:B:429:PHE:HA	2:B:432:MET:CE	2.30	0.59
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.85	0.59
1:A:1004:ASN:CG	4:E:167:ARG:HD2	2.22	0.59
1:A:388:LEU:O	1:A:392:VAL:HG23	2.02	0.59
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.85	0.59
1:A:452:LYS:HB3	2:B:1141:HIS:CE1	2.37	0.59
6:H:38:LEU:HD13	6:H:125:LEU:CD1	2.31	0.59
2:B:847:ASP:O	3:C:65:HIS:HE1	1.85	0.59
8:J:1:MET:H3	8:J:56:LEU:HB2	1.68	0.59
9:K:47:ARG:HD2	9:K:51:LEU:HD22	1.83	0.59
1:A:862:ASN:HA	4:E:174:GLN:HB3	1.85	0.59
1:A:49:LYS:HD3	1:A:54:ASN:O	2.03	0.59
1:A:528:LEU:HD23	1:A:751:SER:HB3	1.85	0.59
1:A:548:ASN:OD1	9:K:60:ALA:HB1	2.03	0.59
2:B:770:GLN:HB2	2:B:985:GLY:H	1.66	0.59
2:B:555:ILE:HD13	2:B:587:HIS:NE2	2.18	0.59
5:F:118:LEU:O	5:F:122:MET:HG3	2.03	0.59
2:B:871:THR:O	2:B:917:PRO:HD2	2.02	0.59
5:F:111:LEU:N	5:F:111:LEU:HD12	2.14	0.59
2:B:280:ILE:HD13	2:B:334:ILE:HG12	1.85	0.59
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.85	0.59
10:L:47:ARG:HG2	10:L:52:GLY:HA2	1.85	0.59
6:H:24:CYS:SG	6:H:44:VAL:HG21	2.42	0.59
2:B:29:ASP:CB	2:B:658:ILE:HD13	2.31	0.58
1:A:533:LYS:HE2	1:A:745:GLN:NE2	2.13	0.58
5:F:81:THR:HG22	5:F:136:ARG:HH11	1.66	0.58
2:B:1148:LYS:HG2	2:B:1152:MET:HE3	1.85	0.58
2:B:1162:ILE:CD1	2:B:1194:ILE:HD13	2.32	0.58
1:A:1436:ILE:O	1:A:1437:GLY:C	2.41	0.58
3:C:32:SER:O	3:C:36:VAL:HG23	2.03	0.58
2:B:405:ARG:HH11	2:B:632:ARG:HG2	1.60	0.58
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.85	0.58
2:B:976:ILE:O	2:B:990:ILE:O	2.20	0.58
2:B:841:MET:HG3	2:B:1010:LEU:HD12	1.84	0.58
3:C:145:CYS:SG	3:C:146:LYS:N	2.76	0.58
2:B:1084:GLN:HG2	3:C:201:TRP:CZ2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:102:TYR:O	6:H:103:LYS:HG3	2.03	0.58
1:A:741:ASN:HD21	1:A:743:VAL:HB	1.69	0.58
2:B:484:ASN:OD1	2:B:486:TYR:CE1	2.56	0.58
1:A:337:ARG:NH2	1:A:1403:GLU:HA	2.18	0.58
1:A:68:GLN:HE22	1:A:80:HIS:CB	2.16	0.58
2:B:680:THR:HG22	2:B:682:SER:N	2.18	0.58
2:B:879:ARG:HH11	2:B:883:LEU:HB3	1.67	0.58
1:A:537:ARG:HB2	6:H:20:TYR:HE2	1.68	0.58
1:A:1144:LYS:HG3	1:A:1268:LEU:O	2.03	0.58
1:A:686:ALA:O	1:A:690:VAL:HG23	2.04	0.58
10:L:49:LYS:O	10:L:50:ASP:HB2	2.03	0.58
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.85	0.58
3:C:22:LEU:O	3:C:227:THR:HA	2.04	0.58
1:A:184:SER:HB3	1:A:199:LEU:HD21	1.85	0.58
7:I:40:SER:HB2	7:I:41:PRO:HD2	1.86	0.58
2:B:1139:ILE:HG13	2:B:1147:LEU:HD11	1.85	0.58
4:E:157:SER:OG	4:E:160:GLU:HG3	2.04	0.58
9:K:82:ASP:OD1	9:K:84:LYS:HG3	2.04	0.58
1:A:1383:SER:HB3	1:A:1387:HIS:NE2	2.19	0.58
2:B:100:PRO:HA	2:B:125:SER:O	2.03	0.58
1:A:474:VAL:O	1:A:477:PRO:HD2	2.03	0.58
2:B:234:ILE:N	2:B:234:ILE:HD12	2.19	0.58
8:J:7:CYS:SG	8:J:49:MET:HE3	2.44	0.58
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.69	0.58
2:B:1177:HIS:HB2	2:B:1179:GLN:HG3	1.86	0.58
1:A:1364:ASN:HD21	1:A:1366:ARG:NH1	2.01	0.58
1:A:567:LYS:HE3	6:H:46:LEU:CD1	2.34	0.58
1:A:1293:SER:OG	1:A:1294:PRO:HD2	2.04	0.58
1:A:225:ASN:HD22	1:A:228:PHE:HD1	1.51	0.58
2:B:542:MET:HG3	2:B:747:MET:HE1	1.86	0.57
1:A:1424:VAL:HA	1:A:1434:ALA:HB2	1.85	0.57
2:B:1060:ARG:O	2:B:1060:ARG:HD2	2.04	0.57
2:B:859:TYR:CD1	2:B:859:TYR:N	2.72	0.57
2:B:780:VAL:HG21	8:J:56:LEU:CD1	2.34	0.57
1:A:1376:THR:O	1:A:1378:GLN:N	2.37	0.57
1:A:1138:ILE:CG2	1:A:1279:ILE:HG21	2.34	0.57
1:A:886:ILE:HD11	1:A:943:LEU:HB3	1.85	0.57
2:B:780:VAL:CG2	2:B:799:PRO:HG2	2.34	0.57
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.04	0.57
3:C:51:VAL:HG11	3:C:60:ASP:OD2	2.03	0.57
1:A:1308:THR:CG2	1:A:1310:GLY:O	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:27:LEU:HD13	10:L:37:LYS:CB	2.34	0.57
4:E:16:PHE:CZ	4:E:20:LYS:HE2	2.40	0.57
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.35	0.57
1:A:444:PHE:HE2	1:A:470:LEU:CD2	2.18	0.57
2:B:43:LEU:HD11	2:B:811:TYR:O	2.05	0.57
5:F:77:ASP:O	5:F:78:GLN:CB	2.52	0.57
1:A:151:ASP:OD1	1:A:163:SER:HA	2.05	0.57
1:A:713:SER:O	1:A:717:ASN:ND2	2.38	0.57
2:B:282:ILE:HD11	2:B:317:CYS:SG	2.45	0.57
9:K:12:LEU:HD12	9:K:12:LEU:H	1.69	0.57
7:I:8:ARG:O	7:I:9:ASP:HB2	2.04	0.57
1:A:666:ILE:CD1	2:B:1030:LEU:HD22	2.34	0.57
1:A:575:LYS:HB3	1:A:612:ILE:CG2	2.34	0.57
1:A:518:LYS:HB2	1:A:519:PRO:CD	2.26	0.57
2:B:802:PRO:HA	2:B:822:ASN:HD21	1.70	0.57
10:L:36:SER:O	10:L:38:LEU:N	2.38	0.57
1:A:1169:ILE:O	1:A:1173:HIS:CD2	2.57	0.57
2:B:484:ASN:ND2	2:B:486:TYR:CD1	2.72	0.57
1:A:693:VAL:HG21	1:A:721:PHE:HE1	1.68	0.57
2:B:98:THR:O	2:B:126:SER:HB2	2.05	0.57
10:L:63:ARG:O	10:L:64:LEU:O	2.22	0.57
4:E:84:ASP:O	4:E:86:PRO:HD3	2.05	0.57
2:B:1177:HIS:HB2	2:B:1179:GLN:HE21	1.70	0.57
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.39	0.57
1:A:907:THR:CG2	1:A:908:LEU:H	2.15	0.57
2:B:882:THR:HB	2:B:934:LYS:O	2.05	0.57
3:C:148:ARG:CG	3:C:149:LYS:H	2.17	0.57
2:B:332:ASP:O	2:B:334:ILE:N	2.37	0.57
1:A:789:LYS:HE3	7:I:67:THR:OG1	2.05	0.57
1:A:474:VAL:HG13	1:A:478:TYR:CD1	2.40	0.57
2:B:693:ILE:HD11	2:B:740:HIS:NE2	2.19	0.57
2:B:737:THR:HG23	7:I:66:PRO:CB	2.35	0.57
6:H:12:VAL:HA	6:H:28:ALA:HB2	1.86	0.57
2:B:30:SER:HB2	2:B:743:ILE:O	2.05	0.57
1:A:1364:ASN:ND2	1:A:1366:ARG:CG	2.52	0.56
1:A:782:ARG:NH1	1:A:785:PRO:HA	2.20	0.56
6:H:89:LEU:C	6:H:91:ASP:N	2.52	0.56
2:B:726:ALA:HB1	2:B:1051:THR:HG21	1.87	0.56
1:A:172:PRO:HB3	1:A:185:TRP:CZ2	2.40	0.56
1:A:1293:SER:HB2	1:A:1299:VAL:HG23	1.87	0.56
9:K:73:LEU:HD22	9:K:75:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:VAL:O	1:A:846:GLU:HB2	2.05	0.56
1:A:979:SER:OG	1:A:981:LEU:HB2	2.05	0.56
2:B:69:LEU:HD21	2:B:425:THR:HG23	1.85	0.56
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.34	0.56
1:A:757:ASN:HA	2:B:1021:MET:HE1	1.87	0.56
1:A:1195:LEU:HD11	1:A:1267:MET:CE	2.35	0.56
5:F:93:ILE:HD11	5:F:134:ILE:HD11	1.87	0.56
1:A:1146:VAL:HG11	1:A:1202:MET:SD	2.45	0.56
9:K:63:VAL:O	9:K:63:VAL:CG2	2.53	0.56
1:A:347:PHE:CZ	2:B:1109:GLY:HA2	2.40	0.56
3:C:41:ILE:HD11	3:C:247:GLY:CA	2.35	0.56
2:B:463:THR:CG2	2:B:465:ASN:HD22	2.18	0.56
1:A:1074:GLU:N	1:A:1075:PRO:HD2	2.20	0.56
8:J:14:VAL:HG12	8:J:14:VAL:O	2.05	0.56
1:A:32:VAL:CB	1:A:57:ARG:HD2	2.35	0.56
2:B:521:LEU:HD21	2:B:635:ARG:HD3	1.88	0.56
2:B:764:SER:HB3	2:B:765:PRO:CD	2.36	0.56
1:A:49:LYS:HB3	1:A:55:ASP:CB	2.27	0.56
1:A:443:LEU:HD13	1:A:455:MET:CE	2.35	0.56
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.88	0.56
1:A:858:ASN:HD22	1:A:858:ASN:C	2.08	0.56
3:C:11:ARG:NH2	3:C:229:TYR:CD2	2.73	0.56
7:I:73:ARG:H	7:I:83:ASN:ND2	2.04	0.56
4:E:76:GLY:H	4:E:106:GLN:CD	2.08	0.56
1:A:442:VAL:CG2	1:A:489:LEU:HD11	2.36	0.56
2:B:984:HIS:CD2	2:B:1025:HIS:HA	2.40	0.56
2:B:120:ARG:CZ	10:L:54:ARG:HH12	2.18	0.56
1:A:108:MET:SD	1:A:210:ILE:HD13	2.46	0.56
4:E:46:TYR:HE2	4:E:58:MET:HA	1.69	0.56
1:A:276:LEU:HD11	1:A:293:GLU:HG3	1.87	0.56
1:A:567:LYS:HD2	1:A:568:PRO:CD	2.34	0.56
2:B:642:ASP:CB	2:B:649:LYS:HA	2.35	0.56
1:A:901:LEU:HA	1:A:907:THR:CG2	2.35	0.56
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.19	0.56
1:A:283:GLY:O	1:A:285:PRO:HD3	2.06	0.56
3:C:40:GLU:OE1	3:C:254:LYS:HE3	2.06	0.56
1:A:715:GLU:OE1	1:A:774:ARG:HD3	2.05	0.56
1:A:187:LYS:CB	1:A:194:ALA:HB1	2.29	0.56
2:B:69:LEU:HD13	2:B:432:MET:HE1	1.87	0.56
1:A:399:HIS:O	1:A:435:HIS:HD2	1.88	0.56
1:A:146:MET:HA	1:A:171:GLN:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:NZ	1:A:323:LYS:H	2.03	0.56
1:A:590:ARG:HH21	1:A:620:LYS:HD3	1.70	0.56
2:B:31:TRP:CD1	2:B:807:ARG:NH1	2.74	0.56
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.46	0.56
1:A:1035:TYR:O	1:A:1037:LEU:N	2.39	0.56
2:B:484:ASN:HB2	2:B:494:HIS:ND1	2.20	0.56
2:B:706:GLN:HE22	2:B:730:ARG:NH1	2.04	0.56
1:A:84:ILE:CG2	1:A:239:LEU:HB3	2.35	0.55
3:C:18:VAL:HG23	3:C:240:VAL:HG11	1.86	0.55
2:B:1148:LYS:CG	2:B:1152:MET:HE3	2.35	0.55
2:B:305:VAL:HG12	2:B:305:VAL:O	2.06	0.55
2:B:957:ASN:HD22	2:B:961:LEU:CD1	2.14	0.55
1:A:1431:GLY:HA2	2:B:1152:MET:HE1	1.89	0.55
1:A:768:GLN:CG	1:A:816:HIS:HA	2.36	0.55
2:B:770:GLN:HB2	2:B:985:GLY:N	2.21	0.55
2:B:616:ILE:N	2:B:616:ILE:HD12	2.20	0.55
1:A:1384:VAL:O	1:A:1386:ARG:N	2.40	0.55
2:B:1182:CYS:C	2:B:1183:LYS:HG3	2.27	0.55
1:A:1390:ASN:O	1:A:1391:ARG:CB	2.54	0.55
2:B:784:ASN:O	2:B:788:ARG:HG3	2.07	0.55
2:B:864:LYS:HD3	2:B:871:THR:CA	2.37	0.55
1:A:369:SER:HB3	9:K:2:ASN:OD1	2.06	0.55
2:B:999:MET:HA	2:B:999:MET:CE	2.37	0.55
2:B:54:PHE:HA	2:B:58:THR:CB	2.34	0.55
2:B:751:VAL:HG13	2:B:812:LEU:HD22	1.89	0.55
1:A:792:TYR:CE1	7:I:87:GLN:NE2	2.75	0.55
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.06	0.55
2:B:549:THR:CG2	2:B:550:ASP:N	2.69	0.55
1:A:445:ASN:HB2	1:A:454:SER:O	2.06	0.55
2:B:787:VAL:O	2:B:787:VAL:CG1	2.54	0.55
9:K:33:ILE:CD1	9:K:87:LEU:HD22	2.37	0.55
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.88	0.55
1:A:207:ILE:HG22	1:A:235:ILE:HD11	1.89	0.55
2:B:1166:CYS:HB2	2:B:1215:ARG:HH11	1.70	0.55
1:A:767:GLN:NE2	1:A:774:ARG:HB3	2.20	0.55
1:A:1264:GLU:HG3	1:A:1265:ASN:N	2.20	0.55
2:B:979:LYS:HE2	2:B:987:LYS:HD2	1.88	0.55
1:A:381:THR:CG2	1:A:383:TYR:CD1	2.89	0.55
2:B:393:LYS:HE2	2:B:621:GLU:CD	2.27	0.55
7:I:10:CYS:O	7:I:12:ASN:N	2.38	0.55
8:J:14:VAL:HG12	8:J:50:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:168:TYR:HB3	4:E:170:LEU:HD21	1.88	0.55
2:B:38:PHE:HZ	2:B:541:LEU:HB3	1.71	0.55
2:B:542:MET:HG3	2:B:747:MET:CE	2.37	0.55
1:A:630:ILE:HD13	1:A:646:PHE:CZ	2.42	0.55
1:A:483:ASP:HB2	2:B:987:LYS:HG3	1.89	0.55
3:C:73:GLN:HE21	3:C:75:MET:HB2	1.71	0.55
2:B:861:ASP:OD1	2:B:862:GLN:N	2.40	0.55
1:A:974:ASP:HB2	6:H:136:LYS:HZ1	1.72	0.55
4:E:71:LYS:HB3	4:E:72:PHE:CE1	2.41	0.55
2:B:168:GLY:HA2	2:B:454:THR:OG1	2.07	0.55
3:C:101:LEU:HD13	3:C:118:LEU:CD1	2.36	0.55
2:B:806:THR:CG2	2:B:808:ALA:H	2.08	0.55
2:B:693:ILE:HD11	2:B:740:HIS:CD2	2.42	0.55
2:B:903:VAL:CG1	10:L:63:ARG:HH21	2.18	0.55
1:A:690:VAL:HG13	1:A:718:VAL:HG13	1.89	0.55
2:B:220:GLY:HA2	2:B:241:ARG:HB3	1.89	0.55
5:F:90:ARG:HD3	5:F:155:LEU:CD1	2.37	0.55
1:A:381:THR:HG21	1:A:383:TYR:CE1	2.43	0.54
3:C:129:ILE:O	3:C:130:GLY:O	2.24	0.54
4:E:192:ARG:HH11	4:E:192:ARG:HG3	1.72	0.54
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.88	0.54
1:A:523:ILE:CD1	1:A:649:ILE:HG21	2.37	0.54
9:K:63:VAL:HG23	9:K:63:VAL:O	2.05	0.54
2:B:370:PHE:HD2	2:B:373:ARG:HD2	1.70	0.54
1:A:78:PRO:O	1:A:79:GLY:C	2.46	0.54
2:B:705:MET:N	2:B:710:LEU:HD12	2.22	0.54
2:B:165:VAL:CG1	2:B:446:LEU:HD21	2.37	0.54
1:A:1202:MET:O	1:A:1205:LYS:O	2.24	0.54
2:B:579:ARG:HG3	2:B:581:PHE:HE1	1.73	0.54
2:B:1197:PRO:HG2	2:B:1200:ALA:HB2	1.89	0.54
3:C:73:GLN:NE2	3:C:75:MET:H	2.04	0.54
2:B:108:VAL:HG12	2:B:109:THR:N	2.22	0.54
4:E:166:LYS:NZ	4:E:167:ARG:HH21	2.04	0.54
2:B:242:SER:OG	2:B:252:SER:O	2.25	0.54
2:B:1022:THR:HG23	2:B:1022:THR:O	2.08	0.54
2:B:654:ARG:C	2:B:656:GLY:H	2.11	0.54
3:C:36:VAL:HG21	3:C:251:LEU:HB2	1.88	0.54
2:B:597:MET:SD	2:B:624:LEU:HD11	2.48	0.54
1:A:557:ASP:HA	9:K:26:LYS:HD2	1.90	0.54
2:B:813:LYS:HA	2:B:816:GLU:OE1	2.07	0.54
1:A:25:GLU:CD	1:A:25:GLU:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:763:ALA:O	1:A:803:SER:HB3	2.08	0.54
2:B:1065:GLN:O	2:B:1065:GLN:HG3	2.06	0.54
1:A:845:LEU:O	1:A:1065:GLY:HA3	2.07	0.54
2:B:1182:CYS:O	2:B:1183:LYS:O	2.26	0.54
2:B:288:ALA:HB1	2:B:331:LEU:CD1	2.37	0.54
2:B:1177:HIS:CB	2:B:1179:GLN:HE21	2.21	0.54
2:B:551:PRO:O	2:B:555:ILE:HG13	2.08	0.54
8:J:14:VAL:CG1	8:J:50:ILE:HD11	2.38	0.54
1:A:1009:ASN:OD1	1:A:1012:ARG:NH1	2.41	0.54
4:E:93:MET:O	4:E:97:VAL:HG23	2.08	0.54
6:H:76:THR:HG22	6:H:76:THR:O	2.08	0.54
1:A:383:TYR:O	1:A:384:ASN:HB3	2.06	0.54
2:B:864:LYS:HB3	2:B:871:THR:HA	1.89	0.54
1:A:412:ARG:NE	2:B:1110:PRO:HG3	2.22	0.54
10:L:32:ALA:HB3	10:L:55:ILE:CD1	2.38	0.54
1:A:31:SER:HB2	1:A:83:HIS:HB2	1.88	0.54
1:A:1323:ASP:OD1	1:A:1325:THR:HB	2.08	0.54
1:A:1191:TRP:CD1	1:A:1256:GLU:HB2	2.42	0.54
3:C:253:LYS:O	3:C:256:ALA:HB3	2.08	0.54
1:A:268:ASP:HB3	1:A:299:HIS:ND1	2.23	0.54
3:C:84:ARG:CD	9:K:11:LEU:HD21	2.38	0.54
3:C:51:VAL:HG22	3:C:155:LEU:HD22	1.88	0.54
6:H:7:ASP:O	6:H:8:ASP:HB2	2.07	0.54
1:A:40:THR:HG21	1:A:259:GLU:OE2	2.07	0.54
1:A:626:ASN:O	1:A:631:HIS:CD2	2.61	0.54
3:C:173:ALA:O	3:C:175:ALA:N	2.40	0.54
2:B:954:VAL:O	10:L:55:ILE:O	2.26	0.54
5:F:81:THR:HG21	5:F:136:ARG:HH11	1.73	0.54
1:A:1220:PHE:O	1:A:1223:ASP:OD1	2.26	0.54
1:A:855:THR:CG2	1:A:857:ARG:HE	2.20	0.54
2:B:324:ILE:HG23	2:B:329:THR:HB	1.90	0.54
1:A:682:THR:CG2	1:A:728:LYS:HG3	2.38	0.54
1:A:963:ILE:HD12	1:A:1049:ILE:HG12	1.89	0.54
1:A:573:SER:O	1:A:576:GLN:HB2	2.07	0.54
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.89	0.54
2:B:642:ASP:HB2	2:B:649:LYS:HA	1.90	0.54
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.73	0.54
2:B:850:LEU:HG	2:B:851:PHE:HD1	1.71	0.54
7:I:10:CYS:SG	7:I:31:THR:HG21	2.48	0.54
1:A:460:VAL:HG12	1:A:461:LYS:N	2.22	0.54
1:A:383:TYR:HB2	5:F:115:THR:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:SER:OG	2:B:172:ILE:HD11	2.07	0.53
3:C:148:ARG:HG2	3:C:149:LYS:H	1.73	0.53
2:B:167:ILE:HD13	2:B:424:LEU:CD2	2.38	0.53
2:B:702:LEU:HD23	2:B:737:THR:HG22	1.89	0.53
8:J:64:ASN:HB3	8:J:65:PRO:CD	2.37	0.53
2:B:46:GLN:HE22	2:B:496:ARG:HD3	1.72	0.53
1:A:1284:MET:HG2	1:A:1306:LEU:CD2	2.38	0.53
1:A:882:SER:HB3	1:A:953:ASN:OD1	2.08	0.53
1:A:313:GLN:HB2	1:A:320:ARG:CB	2.27	0.53
1:A:13:THR:HG23	1:A:1432:GLN:CD	2.29	0.53
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.41	0.53
2:B:1172:ILE:O	2:B:1180:PHE:O	2.26	0.53
4:E:19:VAL:O	4:E:23:VAL:HG23	2.06	0.53
2:B:1079:LYS:CA	3:C:27:LEU:HD21	2.38	0.53
6:H:44:VAL:O	6:H:44:VAL:HG12	2.08	0.53
7:I:70:ARG:HG2	7:I:84:VAL:HG23	1.90	0.53
1:A:556:TRP:CH2	1:A:558:GLY:HA2	2.44	0.53
1:A:375:THR:HG23	1:A:376:TYR:N	2.22	0.53
1:A:575:LYS:HB3	1:A:612:ILE:HG23	1.91	0.53
2:B:800:GLN:CB	8:J:52:THR:HG22	2.38	0.53
6:H:31:THR:O	6:H:32:THR:CB	2.55	0.53
1:A:337:ARG:HG2	1:A:341:MET:HE2	1.91	0.53
1:A:896:ARG:HB3	1:A:897:TYR:HD1	1.72	0.53
1:A:1342:GLU:CD	4:E:212:ARG:HH12	2.11	0.53
2:B:737:THR:HG23	2:B:737:THR:O	2.09	0.53
1:A:528:LEU:O	1:A:531:ILE:HG22	2.08	0.53
3:C:31:ASN:O	3:C:35:ARG:HG3	2.07	0.53
2:B:957:ASN:O	2:B:959:ASP:N	2.42	0.53
1:A:326:ARG:CZ	1:A:1406:VAL:HG11	2.38	0.53
1:A:187:LYS:HB2	1:A:194:ALA:CB	2.32	0.53
1:A:2:VAL:HG21	2:B:1157:ALA:CB	2.31	0.53
8:J:7:CYS:CA	8:J:49:MET:HE3	2.39	0.53
2:B:178:ASN:O	2:B:179:CYS:C	2.46	0.53
2:B:135:ARG:O	2:B:136:THR:HB	2.09	0.53
1:A:1206:ASP:HB2	1:A:1274:ARG:NH1	2.24	0.53
2:B:244:LEU:O	2:B:249:ARG:HG2	2.09	0.53
1:A:568:PRO:HB2	3:C:221:TYR:CE1	2.44	0.53
2:B:1183:LYS:C	2:B:1185:CYS:H	2.09	0.53
3:C:242:GLN:NE2	3:C:246:ARG:HE	2.06	0.53
4:E:124:VAL:HA	4:E:132:ILE:HD12	1.90	0.53
1:A:622:VAL:HG22	1:A:622:VAL:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:83:GLN:C	6:H:85:GLY:H	2.12	0.53
2:B:893:LEU:HD22	2:B:897:GLY:C	2.29	0.53
2:B:185:THR:O	2:B:189:LEU:HG	2.09	0.53
1:A:878:ILE:HG21	1:A:955:PRO:HB2	1.91	0.53
2:B:1065:GLN:HE21	2:B:1067:ARG:N	2.01	0.53
2:B:25:ILE:HD11	2:B:653:VAL:HG12	1.91	0.53
8:J:18:TRP:O	8:J:21:TYR:HB3	2.08	0.53
3:C:66:ARG:CZ	8:J:2:ILE:HG21	2.39	0.53
3:C:22:LEU:HD12	3:C:230:MET:HE3	1.90	0.53
8:J:12:LYS:O	8:J:14:VAL:HG23	2.09	0.53
2:B:873:THR:HG22	2:B:874:PHE:N	2.23	0.53
1:A:517:ASN:O	1:A:517:ASN:OD1	2.27	0.53
2:B:512:ARG:NH2	2:B:535:LEU:HD11	2.24	0.53
1:A:337:ARG:HH22	1:A:1403:GLU:N	2.06	0.53
1:A:1394:THR:CG2	1:A:1395:GLY:H	2.12	0.53
1:A:779:PHE:CZ	1:A:785:PRO:HD3	2.44	0.53
3:C:241:ASP:HB3	9:K:109:TRP:CE2	2.44	0.53
2:B:897:GLY:O	2:B:898:LEU:HD23	2.09	0.53
1:A:55:ASP:N	1:A:56:PRO:HD2	2.24	0.52
1:A:751:SER:O	1:A:752:LYS:CB	2.56	0.52
5:F:109:VAL:HG23	5:F:124:GLU:HG2	1.91	0.52
2:B:970:THR:HG22	2:B:971:THR:H	1.72	0.52
1:A:685:GLU:HA	1:A:688:LYS:HD2	1.90	0.52
6:H:95:TYR:HB3	6:H:144:ILE:HB	1.91	0.52
8:J:7:CYS:CB	8:J:49:MET:HE3	2.38	0.52
1:A:451:HIS:NE2	1:A:1074:GLU:HG3	2.25	0.52
1:A:783:THR:HG21	1:A:815:PHE:HZ	1.74	0.52
1:A:996:ASN:O	1:A:997:LEU:C	2.47	0.52
3:C:89:GLU:O	3:C:90:ASP:CB	2.57	0.52
2:B:23:ALA:HB1	2:B:24:PRO:HD2	1.92	0.52
1:A:1208:THR:O	1:A:1212:VAL:HG23	2.09	0.52
1:A:1364:ASN:HD22	1:A:1366:ARG:N	2.07	0.52
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.43	0.52
2:B:650:GLU:HG3	2:B:651:LEU:N	2.24	0.52
2:B:547:VAL:N	2:B:612:GLU:OE2	2.41	0.52
1:A:902:LEU:HD23	1:A:921:GLY:HA2	1.91	0.52
1:A:855:THR:HG22	1:A:857:ARG:HG3	1.91	0.52
6:H:126:GLU:C	6:H:130:ARG:NH1	2.62	0.52
6:H:31:THR:O	6:H:32:THR:HB	2.10	0.52
3:C:109:SER:O	3:C:110:THR:HB	2.08	0.52
4:E:88:VAL:HG11	4:E:110:PHE:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:LYS:HG2	1:A:571:LEU:HD13	1.92	0.52
1:A:412:ARG:HH21	2:B:1110:PRO:HD3	1.73	0.52
2:B:914:LYS:O	2:B:937:ALA:O	2.27	0.52
2:B:1207:LEU:O	2:B:1212:ILE:HB	2.09	0.52
1:A:715:GLU:O	1:A:719:VAL:HG23	2.08	0.52
2:B:616:ILE:CG1	2:B:697:GLU:HA	2.39	0.52
2:B:616:ILE:HG12	2:B:697:GLU:HA	1.90	0.52
2:B:244:LEU:HD11	2:B:366:GLN:NE2	2.24	0.52
1:A:306:ASN:OD1	1:A:312:PRO:HD2	2.10	0.52
2:B:547:VAL:H	2:B:612:GLU:CD	2.12	0.52
1:A:148:CYS:HB3	1:A:167:CYS:O	2.09	0.52
5:F:76:LYS:O	5:F:79:ARG:HD3	2.08	0.52
2:B:63:ILE:HA	2:B:421:PHE:CE2	2.44	0.52
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.92	0.52
7:I:59:VAL:HG12	7:I:60:GLN:N	2.24	0.52
1:A:1161:THR:HG21	1:A:1163:ILE:HB	1.92	0.52
1:A:901:LEU:H	1:A:926:GLN:NE2	2.07	0.52
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.45	0.52
1:A:1375:MET:HG3	1:A:1382:THR:O	2.10	0.52
2:B:890:TYR:O	2:B:893:LEU:HB2	2.09	0.52
2:B:596:LEU:HD12	2:B:596:LEU:O	2.09	0.52
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.91	0.52
1:A:167:CYS:SG	1:A:167:CYS:O	2.68	0.52
2:B:1051:THR:CG2	2:B:1053:GLU:HB2	2.39	0.52
3:C:133:ILE:CD1	3:C:237:SER:HA	2.39	0.52
1:A:899:VAL:CG2	1:A:1029:ARG:HG2	2.40	0.52
10:L:48:CYS:HB3	10:L:51:CYS:O	2.10	0.52
8:J:31:ASP:OD1	8:J:34:THR:HB	2.10	0.52
2:B:60:GLN:HA	2:B:95:ILE:HD12	1.91	0.52
5:F:109:VAL:HG12	5:F:110:ASP:N	2.25	0.52
1:A:500:GLU:O	1:A:504:LEU:HB2	2.10	0.52
3:C:121:VAL:O	3:C:121:VAL:HG12	2.10	0.52
1:A:384:ASN:OD1	1:A:388:LEU:HD12	2.09	0.52
2:B:864:LYS:N	2:B:872:GLU:OE1	2.43	0.52
6:H:89:LEU:O	6:H:91:ASP:N	2.43	0.52
2:B:393:LYS:CE	2:B:621:GLU:OE1	2.58	0.52
2:B:392:ARG:HH21	7:I:52:ILE:HD11	1.74	0.52
5:F:133:VAL:HG22	5:F:147:SER:HA	1.91	0.52
2:B:324:ILE:HD11	2:B:333:PHE:CD1	2.45	0.52
2:B:792:MET:HA	2:B:856:PHE:O	2.09	0.52
1:A:503:GLN:HE21	5:F:90:ARG:HH21	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:ALA:HA	3:C:264:GLN:OE1	2.09	0.52
1:A:313:GLN:HG2	1:A:322:VAL:HG23	1.92	0.52
1:A:519:PRO:HD3	1:A:631:HIS:CD2	2.45	0.52
2:B:167:ILE:HG12	2:B:448:ILE:HG21	1.92	0.52
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.92	0.52
2:B:115:GLN:HG2	2:B:193:LYS:CB	2.40	0.52
1:A:1242:VAL:HG12	1:A:1243:VAL:N	2.22	0.52
2:B:1013:ASN:OD1	2:B:1015:HIS:HB2	2.10	0.52
2:B:557:PHE:HZ	2:B:599:THR:HG21	1.74	0.52
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.39	0.52
3:C:205:LYS:O	3:C:205:LYS:HG2	2.10	0.52
1:A:801:GLU:HG3	1:A:801:GLU:O	2.10	0.52
1:A:493:GLN:HE21	1:A:493:GLN:CA	2.23	0.52
2:B:31:TRP:CE3	2:B:34:ILE:HD12	2.45	0.51
2:B:850:LEU:HG	2:B:851:PHE:CD1	2.46	0.51
1:A:517:ASN:HD22	1:A:1362:TYR:HE2	1.58	0.51
2:B:605:ARG:NH1	2:B:639:ILE:HG21	2.25	0.51
3:C:134:ILE:HG23	3:C:136:ASP:OD1	2.09	0.51
6:H:91:ASP:C	6:H:93:TYR:H	2.14	0.51
7:I:73:ARG:H	7:I:83:ASN:HD22	1.59	0.51
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.93	0.51
1:A:369:SER:CB	9:K:2:ASN:HD21	2.23	0.51
6:H:81:PRO:HB2	6:H:82:PRO:CD	2.41	0.51
2:B:914:LYS:H	2:B:938:SER:HB3	1.75	0.51
7:I:75:CYS:HB3	7:I:110:PHE:CE2	2.46	0.51
1:A:1286:LYS:HE3	1:A:1304:TRP:CE2	2.44	0.51
2:B:846:ILE:HG23	2:B:974:PRO:CG	2.22	0.51
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.40	0.51
3:C:52:GLU:HA	10:L:64:LEU:HD22	1.92	0.51
1:A:105:CYS:O	1:A:114:LEU:HG	2.11	0.51
7:I:55:THR:HG23	7:I:58:VAL:CG2	2.41	0.51
1:A:407:ARG:HG2	1:A:430:TRP:CE2	2.46	0.51
1:A:442:VAL:HB	1:A:489:LEU:HD11	1.93	0.51
2:B:1037:LEU:HD21	2:B:1064:TYR:HE1	1.74	0.51
1:A:1289:ARG:O	1:A:1291:VAL:HG23	2.10	0.51
1:A:1107:VAL:O	1:A:1107:VAL:HG12	2.10	0.51
2:B:955:THR:CG2	2:B:956:THR:N	2.45	0.51
1:A:849:MET:HE1	1:A:1061:GLY:HA2	1.91	0.51
1:A:1222:ASN:O	1:A:1223:ASP:HB3	2.09	0.51
1:A:98:LYS:CE	1:A:1411:GLU:HG2	2.41	0.51
3:C:55:THR:O	3:C:55:THR:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:THR:HB	2:B:628:THR:CG2	2.40	0.51
1:A:549:MET:SD	1:A:577:ILE:HD11	2.51	0.51
2:B:63:ILE:CB	2:B:95:ILE:HD11	2.41	0.51
2:B:46:GLN:HE22	2:B:496:ARG:HA	1.76	0.51
1:A:806:ARG:NH1	2:B:729:ILE:HD11	2.25	0.51
1:A:682:THR:HG21	1:A:728:LYS:HG3	1.91	0.51
7:I:7:CYS:SG	7:I:8:ARG:O	2.68	0.51
2:B:23:ALA:HB3	2:B:655:LYS:HE2	1.92	0.51
1:A:1143:LEU:HA	1:A:1273:LEU:CD2	2.41	0.51
5:F:72:LYS:N	5:F:142:SER:HA	2.25	0.51
4:E:144:ILE:HG13	4:E:145:THR:N	2.25	0.51
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.39	0.51
2:B:710:LEU:O	2:B:711:GLU:OE1	2.28	0.51
1:A:873:MET:O	1:A:1058:VAL:HG23	2.11	0.51
5:F:81:THR:HG21	5:F:136:ARG:CD	2.40	0.51
1:A:993:LEU:HD22	1:A:1046:LEU:CD2	2.40	0.51
1:A:1286:LYS:HE3	1:A:1304:TRP:CZ2	2.46	0.51
1:A:329:LEU:HD11	2:B:1210:MET:CE	2.41	0.51
1:A:567:LYS:HE3	6:H:46:LEU:HD12	1.93	0.51
2:B:707:PRO:HG2	2:B:708:GLU:N	2.26	0.51
3:C:174:ALA:O	3:C:175:ALA:HB2	2.11	0.51
1:A:108:MET:O	1:A:109:HIS:CB	2.59	0.51
1:A:596:THR:C	1:A:598:LEU:N	2.64	0.51
2:B:841:MET:CE	2:B:1010:LEU:HD11	2.41	0.51
6:H:6:PHE:O	6:H:58:THR:HA	2.10	0.51
1:A:1364:ASN:ND2	1:A:1366:ARG:N	2.56	0.51
1:A:326:ARG:CZ	1:A:1406:VAL:CG1	2.88	0.51
2:B:174:LEU:HD13	2:B:204:ILE:HG13	1.92	0.51
9:K:10:PHE:CE1	9:K:11:LEU:HD13	2.46	0.51
2:B:589:VAL:HG12	2:B:590:HIS:N	2.26	0.51
1:A:709:THR:HG22	1:A:710:LEU:N	2.26	0.51
1:A:185:TRP:CZ3	1:A:200:ARG:HG2	2.45	0.51
2:B:295:GLY:O	2:B:299:GLU:HG3	2.11	0.51
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.93	0.51
2:B:315:LYS:N	2:B:316:PRO:CD	2.74	0.51
1:A:1415:SER:O	1:A:1417:GLU:N	2.44	0.51
1:A:839:ARG:NE	2:B:1133:MET:HE1	2.26	0.51
1:A:1401:SER:O	1:A:1402:PHE:HB2	2.10	0.51
2:B:408:LEU:HD11	2:B:545:ILE:HD12	1.93	0.51
7:I:78:CYS:SG	7:I:106:CYS:HB3	2.51	0.51
1:A:1199:ARG:HG2	1:A:1203:ASN:HD21	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:GLN:HG2	2:B:983:ARG:O	2.11	0.51
2:B:579:ARG:HB2	2:B:586:TRP:NE1	2.26	0.51
9:K:91:CYS:O	9:K:95:ILE:HG13	2.11	0.51
1:A:412:ARG:NH2	1:A:433:GLU:OE1	2.44	0.50
3:C:175:ALA:HB3	8:J:43:ARG:NH1	2.26	0.50
1:A:857:ARG:HG2	1:A:863:VAL:HA	1.92	0.50
7:I:84:VAL:CG1	7:I:84:VAL:O	2.59	0.50
2:B:652:LYS:HE3	2:B:688:GLY:O	2.11	0.50
2:B:613:VAL:HG13	2:B:627:PHE:O	2.10	0.50
3:C:115:SER:OG	3:C:141:GLY:O	2.15	0.50
2:B:744:HIS:CD2	2:B:745:PRO:HD2	2.46	0.50
2:B:562:GLY:O	2:B:563:MET:C	2.50	0.50
6:H:126:GLU:C	6:H:130:ARG:HH12	2.14	0.50
8:J:53:HIS:CD2	8:J:54:VAL:H	2.28	0.50
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.46	0.50
2:B:1160:VAL:HG12	2:B:1161:HIS:N	2.25	0.50
1:A:648:ASN:O	1:A:652:VAL:HG23	2.11	0.50
1:A:1318:THR:OG1	4:E:11:ARG:NH1	2.44	0.50
6:H:112:ILE:HD12	6:H:131:ASN:HD21	1.76	0.50
1:A:337:ARG:HH22	1:A:1403:GLU:H	1.59	0.50
1:A:264:PHE:CD1	1:A:315:LEU:HD22	2.46	0.50
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.93	0.50
2:B:281:PRO:CG	2:B:284:ILE:HD12	2.41	0.50
1:A:285:PRO:CG	1:A:288:ALA:HB3	2.41	0.50
1:A:1206:ASP:HB2	1:A:1274:ARG:HH11	1.77	0.50
6:H:10:PHE:O	6:H:54:SER:HA	2.11	0.50
4:E:96:PHE:CZ	4:E:100:ILE:HD11	2.46	0.50
1:A:541:ILE:HG12	1:A:549:MET:HE1	1.92	0.50
2:B:446:LEU:O	2:B:447:ALA:CB	2.59	0.50
7:I:7:CYS:HB2	7:I:29:CYS:HB2	1.93	0.50
2:B:1107:ALA:O	2:B:1108:ARG:C	2.49	0.50
3:C:183:TRP:HB2	3:C:185:LYS:HG3	1.94	0.50
2:B:167:ILE:HD13	2:B:424:LEU:HD21	1.94	0.50
3:C:175:ALA:HB3	8:J:43:ARG:NH2	2.27	0.50
1:A:1169:ILE:HD11	1:A:1229:SER:HB3	1.92	0.50
7:I:31:THR:HG22	7:I:32:CYS:N	2.26	0.50
1:A:90:VAL:HG12	1:A:91:PHE:H	1.74	0.50
1:A:511:ILE:HG12	1:A:521:MET:HE2	1.92	0.50
8:J:36:LEU:HD12	8:J:47:ARG:NH1	2.25	0.50
1:A:381:THR:HG23	1:A:382:PRO:HD2	1.94	0.50
1:A:392:VAL:HG13	1:A:415:LEU:CD1	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:GLU:OE1	2:B:120:ARG:NH2	2.42	0.50
1:A:82:GLY:CA	1:A:241:VAL:HB	2.41	0.50
7:I:65:ASP:C	7:I:65:ASP:OD1	2.49	0.50
2:B:259:TYR:O	2:B:267:ARG:HG2	2.12	0.50
1:A:1329:THR:HG22	1:A:1330:ASN:N	2.26	0.50
1:A:1074:GLU:H	1:A:1075:PRO:HD2	1.75	0.50
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.94	0.50
6:H:130:ARG:O	6:H:133:ASN:N	2.45	0.50
1:A:994:GLN:HE21	1:A:1019:CYS:HB3	1.75	0.50
2:B:862:GLN:O	2:B:914:LYS:HE3	2.10	0.50
1:A:515:GLN:HG3	1:A:516:SER:H	1.76	0.50
1:A:1145:SER:HB2	1:A:1205:LYS:NZ	2.26	0.50
6:H:83:GLN:C	6:H:85:GLY:N	2.65	0.50
2:B:757:PRO:HG3	2:B:1028:GLU:OE2	2.12	0.50
1:A:260:ASP:OD2	1:A:328:ARG:NH2	2.45	0.50
2:B:558:LEU:HD13	2:B:580:VAL:HG11	1.94	0.50
2:B:986:GLN:OE1	2:B:986:GLN:HA	2.11	0.50
1:A:670:ILE:HD13	2:B:1067:ARG:CZ	2.42	0.50
2:B:179:CYS:SG	2:B:181:LEU:HB2	2.52	0.50
1:A:166:GLY:O	1:A:167:CYS:HB3	2.12	0.50
1:A:167:CYS:C	1:A:169:ASN:H	2.15	0.50
3:C:239:PRO:O	3:C:242:GLN:HB2	2.11	0.50
6:H:5:LEU:CD1	6:H:135:LEU:HG	2.41	0.50
1:A:503:GLN:HE21	5:F:90:ARG:NH2	2.10	0.50
2:B:25:ILE:CD1	2:B:653:VAL:HG12	2.41	0.50
1:A:35:ILE:HG12	1:A:52:GLY:O	2.11	0.50
2:B:361:LEU:N	2:B:362:PRO:CD	2.74	0.50
1:A:434:ARG:HH21	1:A:440:ASP:CG	2.14	0.50
3:C:101:LEU:HD13	3:C:118:LEU:HD12	1.94	0.49
1:A:406:ILE:HD11	1:A:412:ARG:NH1	2.27	0.49
6:H:123:MET:HE3	6:H:142:LEU:CD2	2.38	0.49
3:C:22:LEU:HD12	3:C:230:MET:CE	2.42	0.49
8:J:37:SER:OG	8:J:47:ARG:NH2	2.44	0.49
1:A:871:ASP:CG	4:E:204:THR:HG23	2.32	0.49
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.77	0.49
1:A:1116:LEU:H	1:A:1308:THR:HG22	1.77	0.49
1:A:1376:THR:CG2	4:E:212:ARG:HH21	2.25	0.49
10:L:38:LEU:O	10:L:39:SER:CB	2.59	0.49
1:A:856:THR:HB	1:A:865:GLN:HB2	1.93	0.49
2:B:484:ASN:HD21	2:B:486:TYR:HD1	1.57	0.49
5:F:96:THR:O	5:F:99:LEU:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:VAL:HG11	2:B:1140:ALA:HB2	1.94	0.49
1:A:385:ILE:HD11	1:A:428:TYR:CE2	2.46	0.49
1:A:590:ARG:CB	1:A:605:MET:N	2.73	0.49
1:A:902:LEU:HG	1:A:926:GLN:CG	2.43	0.49
1:A:505:CYS:HB3	2:B:1141:HIS:CE1	2.47	0.49
1:A:523:ILE:HD12	1:A:622:VAL:CG2	2.40	0.49
1:A:1015:VAL:CG1	1:A:1019:CYS:SG	3.00	0.49
9:K:90:ALA:O	9:K:94:ILE:HG13	2.12	0.49
1:A:442:VAL:HG21	1:A:489:LEU:HD11	1.94	0.49
2:B:220:GLY:O	2:B:221:ASN:HB2	2.12	0.49
1:A:1143:LEU:HA	1:A:1273:LEU:HD21	1.93	0.49
4:E:213:ILE:O	4:E:213:ILE:HG23	2.12	0.49
1:A:54:ASN:HA	1:A:58:LEU:HD12	1.94	0.49
2:B:1103:ILE:O	2:B:1103:ILE:HG22	2.13	0.49
3:C:56:THR:CG2	3:C:57:VAL:N	2.73	0.49
1:A:24:PRO:HG2	1:A:25:GLU:CD	2.33	0.49
3:C:248:ILE:CD1	9:K:101:LEU:HD22	2.43	0.49
1:A:427:GLN:HG3	1:A:430:TRP:CZ2	2.48	0.49
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.45	0.49
2:B:956:THR:HG21	2:B:960:GLY:HA2	1.95	0.49
1:A:243:PRO:C	1:A:245:PRO:HD2	2.33	0.49
1:A:1295:THR:CG2	1:A:1297:GLU:OE1	2.60	0.49
1:A:608:ILE:HD12	1:A:613:ILE:CD1	2.39	0.49
1:A:783:THR:CG2	1:A:815:PHE:CZ	2.96	0.49
1:A:1193:LEU:HD21	1:A:1267:MET:HE2	1.93	0.49
1:A:1118:VAL:O	1:A:1305:VAL:HG13	2.13	0.49
1:A:223:GLY:O	1:A:1415:SER:HA	2.12	0.49
1:A:1236:LEU:O	1:A:1237:ILE:HG13	2.13	0.49
2:B:1037:LEU:HD11	2:B:1064:TYR:CD1	2.47	0.49
1:A:275:SER:O	1:A:279:LEU:HG	2.13	0.49
1:A:636:GLU:OE2	1:A:962:ARG:HD2	2.13	0.49
1:A:1402:PHE:O	1:A:1404:GLU:HG3	2.13	0.49
1:A:901:LEU:H	1:A:926:GLN:HE21	1.60	0.49
1:A:1386:ARG:HG3	1:A:1386:ARG:O	2.12	0.49
2:B:1172:ILE:CD1	2:B:1183:LYS:HE2	2.41	0.49
1:A:469:ARG:HH21	2:B:976:ILE:HD13	1.78	0.49
2:B:228:LYS:HD3	2:B:234:ILE:HD13	1.95	0.49
1:A:757:ASN:HA	2:B:1021:MET:CE	2.43	0.49
2:B:969:ARG:HD3	3:C:61:GLU:OE2	2.12	0.49
2:B:365:THR:HG23	2:B:367:LEU:HG	1.94	0.49
2:B:65:GLU:HG3	2:B:66:ASP:N	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:O	1:A:103:CYS:N	2.46	0.49
2:B:981:ALA:HB2	2:B:987:LYS:HA	1.94	0.49
1:A:673:GLY:N	1:A:674:PRO:HD2	2.28	0.49
6:H:96:VAL:HG22	6:H:143:LEU:HD23	1.94	0.49
1:A:1406:VAL:HG12	1:A:1407:GLU:N	2.25	0.49
1:A:321:PRO:O	1:A:322:VAL:HG23	2.12	0.49
3:C:141:GLY:O	3:C:142:VAL:CB	2.60	0.49
1:A:464:PRO:O	9:K:2:ASN:HB3	2.13	0.49
3:C:174:ALA:HB3	3:C:233:GLU:HB3	1.95	0.49
1:A:1063:MET:SD	1:A:1436:ILE:HB	2.53	0.49
5:F:101:ILE:HD13	5:F:120:ILE:CG2	2.43	0.49
1:A:1396:ALA:O	1:A:1397:LEU:HG	2.12	0.49
2:B:778:MET:SD	2:B:1094:ARG:HD3	2.53	0.49
2:B:794:ASN:C	2:B:795:ILE:HD12	2.33	0.49
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.94	0.49
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.48	0.49
1:A:565:ILE:HG23	1:A:567:LYS:HG2	1.94	0.49
1:A:1400:CYS:O	1:A:1401:SER:O	2.31	0.49
1:A:305:ASP:OD2	1:A:326:ARG:HD2	2.12	0.49
2:B:650:GLU:CG	2:B:654:ARG:HH12	2.15	0.49
2:B:863:GLU:O	2:B:864:LYS:O	2.31	0.49
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.94	0.49
2:B:976:ILE:O	2:B:990:ILE:HB	2.13	0.49
4:E:71:LYS:HB3	4:E:72:PHE:CD1	2.47	0.49
2:B:957:ASN:O	2:B:958:GLN:C	2.51	0.48
2:B:397:ASP:OD2	2:B:515:HIS:HE1	1.96	0.48
4:E:88:VAL:HG21	4:E:110:PHE:CE2	2.48	0.48
10:L:48:CYS:HB3	10:L:51:CYS:HB2	1.95	0.48
3:C:53:THR:O	3:C:153:LEU:HA	2.12	0.48
1:A:566:ILE:O	1:A:566:ILE:HG22	2.13	0.48
2:B:959:ASP:O	2:B:961:LEU:HG	2.12	0.48
1:A:42:ASP:O	1:A:50:ILE:HD11	2.13	0.48
2:B:130:VAL:HG12	2:B:131:ASP:N	2.27	0.48
10:L:29:TYR:O	10:L:30:ILE:HG13	2.12	0.48
6:H:130:ARG:HB3	6:H:134:ASN:ND2	2.26	0.48
2:B:1166:CYS:O	2:B:1166:CYS:SG	2.71	0.48
2:B:1174:LYS:HD2	2:B:1179:GLN:HB2	1.95	0.48
2:B:635:ARG:HG3	2:B:635:ARG:HH11	1.77	0.48
1:A:203:SER:O	1:A:207:ILE:HG12	2.13	0.48
1:A:556:TRP:CZ3	1:A:558:GLY:HA2	2.48	0.48
7:I:15:TYR:N	7:I:15:TYR:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:CD1	3:C:129:ILE:HD11	2.40	0.48
2:B:65:GLU:CG	2:B:66:ASP:H	2.15	0.48
2:B:1051:THR:HG21	2:B:1053:GLU:HB2	1.95	0.48
5:F:81:THR:CG2	5:F:82:THR:N	2.75	0.48
1:A:939:ASP:OD2	1:A:1023:ARG:NH1	2.36	0.48
1:A:4:GLN:O	1:A:5:GLN:CB	2.61	0.48
1:A:95:PHE:O	1:A:98:LYS:HB2	2.14	0.48
2:B:484:ASN:ND2	2:B:486:TYR:CE1	2.82	0.48
2:B:635:ARG:HG3	2:B:635:ARG:NH1	2.28	0.48
1:A:1127:ASP:HB3	1:A:1130:GLN:H	1.78	0.48
9:K:113:THR:O	9:K:114:LEU:CB	2.52	0.48
2:B:1170:THR:O	2:B:1170:THR:HG22	2.14	0.48
2:B:896:ASP:OD2	10:L:58:LYS:HE3	2.13	0.48
2:B:784:ASN:HB3	8:J:63:TYR:OH	2.13	0.48
7:I:63:GLY:O	7:I:70:ARG:NH2	2.47	0.48
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.95	0.48
3:C:148:ARG:HH12	8:J:64:ASN:HA	1.78	0.48
2:B:618:ASP:HB3	2:B:621:GLU:HB3	1.94	0.48
1:A:493:GLN:HE21	1:A:493:GLN:HA	1.78	0.48
2:B:251:ILE:HG22	2:B:251:ILE:O	2.13	0.48
1:A:871:ASP:CB	4:E:204:THR:HG23	2.44	0.48
2:B:612:GLU:O	2:B:632:ARG:NH2	2.46	0.48
1:A:50:ILE:C	1:A:52:GLY:N	2.67	0.48
2:B:166:PHE:O	2:B:167:ILE:HG13	2.13	0.48
1:A:69:THR:O	2:B:1174:LYS:HG2	2.14	0.48
2:B:1037:LEU:HD21	2:B:1064:TYR:CE1	2.48	0.48
1:A:1338:VAL:O	4:E:144:ILE:HG21	2.13	0.48
8:J:43:ARG:HG3	8:J:46:CYS:SG	2.52	0.48
1:A:276:LEU:HD11	1:A:293:GLU:CG	2.43	0.48
1:A:1356:ILE:HD12	1:A:1368:MET:SD	2.53	0.48
10:L:51:CYS:C	10:L:53:HIS:H	2.17	0.48
1:A:326:ARG:NH1	1:A:1406:VAL:HG11	2.29	0.48
2:B:40:GLU:OE1	2:B:680:THR:CG2	2.61	0.48
1:A:505:CYS:HB3	2:B:1141:HIS:ND1	2.29	0.48
5:F:89:GLU:O	5:F:93:ILE:HG13	2.14	0.48
1:A:500:GLU:OE2	2:B:1145:SER:HB3	2.13	0.48
7:I:86:PHE:HD1	7:I:87:GLN:O	1.97	0.48
1:A:1264:GLU:OE2	7:I:44:TYR:HE2	1.97	0.48
4:E:102:GLU:C	4:E:104:ASN:H	2.17	0.48
2:B:690:VAL:HG12	2:B:691:GLU:N	2.28	0.48
2:B:25:ILE:HG22	2:B:26:THR:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:34:ILE:HG12	2:B:542:MET:CE	2.44	0.48
10:L:32:ALA:CB	10:L:55:ILE:HD12	2.41	0.48
1:A:1287:TYR:CD1	1:A:1305:VAL:HG21	2.49	0.48
5:F:109:VAL:CG1	5:F:110:ASP:N	2.77	0.48
1:A:492:PRO:CB	1:A:497:THR:HG22	2.44	0.48
7:I:121:PHE:O	7:I:122:SER:CB	2.61	0.48
2:B:463:THR:HG22	2:B:465:ASN:N	2.29	0.48
4:E:75:MET:HA	4:E:106:GLN:HE22	1.78	0.48
1:A:877:HIS:HB3	1:A:1056:SER:OG	2.13	0.48
1:A:814:PHE:O	1:A:817:ALA:HB3	2.14	0.48
7:I:14:LEU:HB3	7:I:27:PHE:HB3	1.96	0.48
1:A:849:MET:HE2	1:A:1061:GLY:HA2	1.87	0.48
1:A:451:HIS:HB3	1:A:452:LYS:H	1.50	0.48
1:A:549:MET:SD	1:A:577:ILE:CD1	3.02	0.48
2:B:563:MET:HG3	2:B:563:MET:O	2.14	0.48
10:L:27:LEU:HD23	10:L:27:LEU:N	2.29	0.48
1:A:1066:VAL:CG1	2:B:1140:ALA:HB2	2.43	0.48
2:B:498:THR:HG22	2:B:499:ASN:N	2.29	0.48
2:B:902:GLY:O	10:L:65:VAL:HG21	2.14	0.48
1:A:470:LEU:HD21	1:A:487:MET:HE1	1.96	0.47
1:A:745:GLN:HA	1:A:748:MET:HE3	1.96	0.47
2:B:824:ILE:HG12	8:J:48:ARG:HH12	1.74	0.47
2:B:796:LEU:O	2:B:799:PRO:HD3	2.14	0.47
3:C:171:GLY:O	8:J:6:ARG:NH2	2.47	0.47
4:E:177:ARG:O	4:E:212:ARG:HD3	2.14	0.47
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.95	0.47
1:A:1293:SER:HB2	1:A:1299:VAL:HG21	1.93	0.47
1:A:608:ILE:HB	1:A:613:ILE:CD1	2.44	0.47
1:A:88:LYS:HD2	1:A:293:GLU:CD	2.35	0.47
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.96	0.47
1:A:573:SER:H	1:A:576:GLN:HG3	1.78	0.47
1:A:329:LEU:HD11	2:B:1210:MET:HE1	1.95	0.47
3:C:166:GLU:OE1	10:L:70:ARG:NH2	2.43	0.47
2:B:393:LYS:HE2	2:B:621:GLU:OE2	2.14	0.47
1:A:399:HIS:O	1:A:435:HIS:CD2	2.67	0.47
2:B:825:VAL:CG1	2:B:826:ALA:N	2.77	0.47
1:A:1215:ARG:NH1	1:A:1272:THR:O	2.47	0.47
2:B:321:GLY:C	2:B:323:VAL:H	2.17	0.47
2:B:1043:ASP:O	2:B:1050:ILE:HD12	2.14	0.47
2:B:827:ILE:CD1	2:B:1017:ILE:HD11	2.43	0.47
2:B:999:MET:HB3	2:B:1007:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:124:VAL:HB	4:E:125:PRO:HD3	1.96	0.47
2:B:498:THR:CG2	2:B:499:ASN:N	2.77	0.47
2:B:653:VAL:CG2	2:B:689:LEU:HB3	2.44	0.47
5:F:111:LEU:C	5:F:113:GLY:H	2.17	0.47
1:A:90:VAL:HG13	1:A:297:GLN:HA	1.96	0.47
3:C:39:ALA:O	3:C:163:ILE:HG23	2.14	0.47
1:A:754:SER:O	1:A:755:PHE:C	2.53	0.47
2:B:957:ASN:ND2	2:B:961:LEU:HD12	2.15	0.47
1:A:535:THR:CG2	1:A:535:THR:O	2.63	0.47
3:C:169:LYS:C	3:C:171:GLY:H	2.17	0.47
9:K:49:GLU:HG3	9:K:94:ILE:CG1	2.44	0.47
5:F:127:GLU:O	5:F:129:LYS:HG3	2.15	0.47
3:C:33:LEU:HG	3:C:37:MET:HE2	1.96	0.47
2:B:984:HIS:NE2	2:B:1025:HIS:HA	2.29	0.47
3:C:254:LYS:HD3	9:K:42:LEU:HD13	1.96	0.47
1:A:568:PRO:HB2	3:C:221:TYR:CZ	2.49	0.47
2:B:680:THR:O	2:B:683:SER:OG	2.32	0.47
2:B:796:LEU:HB3	2:B:799:PRO:HG3	1.96	0.47
1:A:451:HIS:HB2	1:A:454:SER:OG	2.14	0.47
2:B:971:THR:OG1	3:C:61:GLU:HG3	2.14	0.47
1:A:1205:LYS:O	1:A:1207:LEU:N	2.47	0.47
1:A:365:GLY:HA3	1:A:463:ILE:HD13	1.96	0.47
4:E:204:THR:HG22	4:E:205:SER:N	2.30	0.47
1:A:337:ARG:NH2	1:A:1400:CYS:O	2.47	0.47
1:A:53:LEU:O	1:A:56:PRO:HD2	2.14	0.47
1:A:32:VAL:HB	1:A:57:ARG:CB	2.45	0.47
3:C:70:ILE:HG21	3:C:115:SER:HB2	1.96	0.47
2:B:424:LEU:O	2:B:428:ILE:HG13	2.15	0.47
1:A:844:ALA:C	1:A:845:LEU:HD23	2.34	0.47
1:A:785:PRO:HG2	1:A:786:HIS:CD2	2.50	0.47
3:C:75:MET:HG2	3:C:246:ARG:NH2	2.29	0.47
2:B:778:MET:HG2	2:B:794:ASN:CB	2.41	0.47
2:B:794:ASN:O	2:B:795:ILE:HD12	2.15	0.47
1:A:225:ASN:C	1:A:227:VAL:H	2.16	0.47
2:B:331:LEU:HD21	2:B:353:LYS:HG2	1.96	0.47
1:A:1415:SER:O	1:A:1416:ALA:C	2.52	0.47
1:A:1348:LEU:HD21	1:A:1375:MET:SD	2.55	0.47
2:B:463:THR:HG22	2:B:464:GLY:N	2.29	0.47
2:B:788:ARG:NH1	2:B:790:ASP:OD1	2.47	0.47
1:A:839:ARG:NE	2:B:1133:MET:CE	2.78	0.47
1:A:1155:ASP:CG	1:A:1162:VAL:HG23	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:77:ILE:C	3:C:79:GLN:H	2.17	0.47
2:B:959:ASP:O	2:B:961:LEU:N	2.48	0.47
1:A:535:THR:CG2	1:A:617:VAL:H	2.10	0.47
1:A:1402:PHE:C	1:A:1404:GLU:N	2.66	0.47
2:B:563:MET:HE1	2:B:588:GLY:N	2.30	0.47
1:A:1376:THR:CG2	4:E:212:ARG:NH2	2.78	0.47
2:B:189:LEU:HD13	2:B:196:PRO:HA	1.97	0.47
1:A:1433:MET:HE1	5:F:92:ARG:NH1	2.30	0.47
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.15	0.47
3:C:99:LEU:HD12	3:C:118:LEU:HD23	1.96	0.47
1:A:1402:PHE:C	1:A:1404:GLU:H	2.17	0.47
1:A:13:THR:HG23	1:A:1432:GLN:HE22	1.76	0.47
1:A:1431:GLY:O	2:B:1148:LYS:HE3	2.15	0.47
1:A:1223:ASP:HA	1:A:1243:VAL:HG13	1.97	0.47
5:F:76:LYS:CA	5:F:79:ARG:HD2	2.44	0.47
1:A:994:GLN:NE2	1:A:1019:CYS:HB3	2.30	0.47
1:A:1152:ILE:CG2	1:A:1260:LEU:HD23	2.44	0.47
1:A:71:GLN:O	1:A:72:GLU:HB2	2.15	0.47
1:A:974:ASP:HB2	6:H:136:LYS:NZ	2.29	0.47
1:A:460:VAL:CG1	1:A:461:LYS:N	2.78	0.47
4:E:117:THR:HG22	4:E:119:SER:H	1.79	0.47
1:A:1126:ALA:O	1:A:1128:GLN:N	2.48	0.47
1:A:565:ILE:O	1:A:570:PRO:HA	2.15	0.47
2:B:708:GLU:C	2:B:710:LEU:H	2.18	0.47
1:A:873:MET:C	1:A:1058:VAL:HG23	2.35	0.47
2:B:780:VAL:HG22	2:B:799:PRO:HG2	1.97	0.47
3:C:136:ASP:OD2	8:J:16:ASP:HB2	2.14	0.47
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.36	0.47
1:A:884:ASP:HB3	1:A:896:ARG:HH12	1.80	0.47
1:A:216:VAL:HA	1:A:219:PHE:CD1	2.50	0.47
1:A:1100:ARG:HH21	1:A:1351:GLU:HG3	1.79	0.47
1:A:77:CYS:O	1:A:79:GLY:N	2.48	0.47
9:K:24:ASP:HB3	9:K:30:ALA:HB3	1.97	0.47
2:B:904:ARG:NH2	2:B:948:ILE:HD11	2.30	0.47
1:A:534:LEU:HD13	1:A:656:TRP:CD1	2.50	0.47
1:A:1031:VAL:HG12	1:A:1031:VAL:O	2.14	0.47
2:B:25:ILE:HG22	2:B:26:THR:H	1.79	0.46
1:A:1441:PHE:HZ	5:F:89:GLU:HA	1.77	0.46
2:B:791:THR:O	2:B:792:MET:HB2	2.15	0.46
4:E:88:VAL:HG21	4:E:110:PHE:HE2	1.80	0.46
1:A:1198:ASP:OD1	1:A:1200:ALA:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:17:ARG:HG3	7:I:28:GLU:CG	2.40	0.46
2:B:1004:GLU:O	3:C:177:GLU:HG2	2.15	0.46
1:A:195:ASP:O	1:A:196:GLU:O	2.33	0.46
1:A:993:LEU:HD23	1:A:1022:LEU:HD21	1.98	0.46
2:B:815:ARG:NE	2:B:1041:GLU:OE2	2.48	0.46
1:A:364:VAL:HG13	1:A:364:VAL:O	2.15	0.46
7:I:99:LEU:O	7:I:111:THR:HG23	2.15	0.46
2:B:911:ILE:HD11	2:B:941:LEU:CD1	2.44	0.46
2:B:212:LEU:HD13	2:B:409:ALA:HA	1.96	0.46
2:B:946:ASN:CG	2:B:946:ASN:O	2.54	0.46
7:I:53:GLY:O	7:I:89:GLN:HB2	2.15	0.46
2:B:405:ARG:HA	2:B:631:GLY:O	2.15	0.46
2:B:167:ILE:CG2	2:B:453:ILE:HD12	2.46	0.46
1:A:783:THR:HG22	1:A:784:LEU:N	2.31	0.46
3:C:37:MET:HG2	3:C:243:VAL:CG1	2.45	0.46
2:B:969:ARG:HH21	3:C:59:ALA:HB1	1.81	0.46
9:K:73:LEU:HD22	9:K:75:ILE:CG1	2.46	0.46
1:A:670:ILE:HD13	2:B:1067:ARG:NH2	2.30	0.46
1:A:313:GLN:HB3	1:A:320:ARG:C	2.35	0.46
1:A:338:GLY:O	1:A:343:LYS:HB2	2.15	0.46
2:B:707:PRO:CG	2:B:708:GLU:H	2.26	0.46
2:B:549:THR:HG22	2:B:550:ASP:N	2.29	0.46
1:A:1111:MET:CE	1:A:1114:PRO:HA	2.45	0.46
1:A:897:TYR:CD1	1:A:897:TYR:N	2.84	0.46
1:A:577:ILE:O	1:A:580:VAL:HB	2.15	0.46
3:C:240:VAL:O	3:C:242:GLN:N	2.48	0.46
6:H:81:PRO:HD2	6:H:82:PRO:HD2	1.96	0.46
4:E:77:SER:HB2	4:E:105:PHE:HD2	1.81	0.46
1:A:346:ASP:HB3	1:A:347:PHE:CD1	2.51	0.46
5:F:154:ASP:O	5:F:155:LEU:HB2	2.15	0.46
1:A:99:ILE:HG23	1:A:211:PHE:CZ	2.50	0.46
1:A:821:ARG:HH21	2:B:534:GLY:HA2	1.80	0.46
3:C:134:ILE:HG23	3:C:141:GLY:H	1.80	0.46
2:B:172:ILE:HD13	2:B:178:ASN:CB	2.45	0.46
2:B:98:THR:HG22	2:B:99:LYS:N	2.26	0.46
6:H:40:LEU:HD12	6:H:41:ASP:H	1.80	0.46
3:C:105:GLY:O	3:C:149:LYS:O	2.34	0.46
1:A:1097:GLY:C	1:A:1099:PRO:HD2	2.35	0.46
2:B:552:MET:N	2:B:553:PRO:HD2	2.30	0.46
1:A:134:ARG:HD3	1:A:221:SER:O	2.16	0.46
3:C:131:HIS:O	3:C:132:PRO:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1201:LYS:HE2	2:B:1205:GLN:CD	2.36	0.46
1:A:595:THR:OG1	1:A:603:ASN:HB3	2.15	0.46
1:A:313:GLN:HB3	1:A:321:PRO:N	2.30	0.46
1:A:901:LEU:HD23	1:A:907:THR:CG2	2.44	0.46
8:J:48:ARG:O	8:J:52:THR:HB	2.16	0.46
1:A:709:THR:HB	1:A:712:GLU:H	1.81	0.46
1:A:857:ARG:CZ	5:F:139:PRO:HG3	2.45	0.46
2:B:618:ASP:CB	2:B:621:GLU:HB3	2.46	0.46
2:B:618:ASP:O	2:B:621:GLU:N	2.48	0.46
3:C:57:VAL:HG11	8:J:60:PHE:HB3	1.97	0.46
2:B:287:ARG:NH2	2:B:325:GLN:NE2	2.63	0.46
1:A:119:ASN:O	1:A:123:ARG:HG3	2.16	0.46
1:A:361:LEU:HD21	1:A:521:MET:CE	2.46	0.46
2:B:781:PHE:O	2:B:782:LEU:HG	2.16	0.46
3:C:104:PHE:HD1	3:C:152:GLU:HG3	1.80	0.46
1:A:1429:ILE:HG22	1:A:1429:ILE:O	2.16	0.46
1:A:1364:ASN:C	1:A:1364:ASN:HD22	2.19	0.46
1:A:41:MET:HB3	1:A:48:ALA:O	2.16	0.46
1:A:786:HIS:HD2	1:A:786:HIS:N	2.12	0.46
2:B:240:ILE:O	2:B:240:ILE:HG23	2.16	0.46
5:F:107:VAL:HG12	5:F:109:VAL:H	1.80	0.46
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.51	0.46
1:A:596:THR:C	1:A:598:LEU:H	2.18	0.46
1:A:839:ARG:HE	2:B:1133:MET:HE1	1.80	0.46
1:A:1017:LEU:O	1:A:1020:CYS:HB2	2.15	0.46
1:A:575:LYS:HG2	1:A:612:ILE:HD13	1.96	0.46
1:A:605:MET:CE	1:A:612:ILE:HG13	2.43	0.46
1:A:35:ILE:HD13	1:A:53:LEU:HD23	1.98	0.46
3:C:177:GLU:O	3:C:230:MET:HA	2.16	0.46
9:K:55:LYS:CD	9:K:78:THR:HB	2.43	0.46
6:H:126:GLU:N	6:H:130:ARG:HH12	2.14	0.46
3:C:6:PRO:HB2	9:K:101:LEU:HB2	1.98	0.46
10:L:45:ALA:O	10:L:46:VAL:CG2	2.64	0.46
1:A:774:ARG:HB2	1:A:797:LYS:O	2.15	0.46
2:B:121:ASN:HA	2:B:207:GLY:CA	2.46	0.46
1:A:534:LEU:HD13	1:A:656:TRP:CG	2.51	0.46
2:B:570:VAL:CG2	2:B:573:GLN:HB2	2.46	0.46
2:B:531:GLN:HG3	2:B:532:ALA:H	1.80	0.46
2:B:216:GLU:OE1	2:B:537:LYS:HE2	2.16	0.46
1:A:1153:TYR:CD1	1:A:1163:ILE:HD11	2.51	0.46
2:B:650:GLU:HG3	2:B:651:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:ASP:O	1:A:56:PRO:C	2.54	0.46
1:A:62:ASP:O	1:A:63:ARG:HB2	2.16	0.46
1:A:849:MET:HE3	1:A:1061:GLY:HA2	1.90	0.46
1:A:414:ASP:C	1:A:414:ASP:OD1	2.53	0.46
2:B:665:GLU:O	2:B:668:ASP:HB2	2.16	0.46
1:A:858:ASN:ND2	1:A:858:ASN:C	2.69	0.46
2:B:1034:VAL:HG12	2:B:1035:ALA:N	2.30	0.46
2:B:978:ASP:O	2:B:989:THR:HA	2.16	0.46
2:B:756:ILE:O	2:B:759:PRO:HD3	2.16	0.46
1:A:50:ILE:HG22	1:A:51:GLY:N	2.31	0.45
2:B:40:GLU:O	2:B:40:GLU:HG3	2.16	0.45
1:A:1114:PRO:O	1:A:1330:ASN:OD1	2.34	0.45
4:E:176:PRO:O	4:E:212:ARG:HA	2.16	0.45
6:H:40:LEU:HD13	6:H:123:MET:HB2	1.98	0.45
2:B:1152:MET:HG2	2:B:1153:GLU:N	2.32	0.45
1:A:1152:ILE:HD11	1:A:1260:LEU:O	2.16	0.45
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.81	0.45
2:B:314:LEU:C	2:B:316:PRO:HD2	2.36	0.45
2:B:859:TYR:H	2:B:859:TYR:HD1	1.64	0.45
1:A:128:ILE:HG21	1:A:133:LYS:HB3	1.98	0.45
2:B:235:SER:OG	2:B:236:HIS:HD2	1.99	0.45
2:B:843:GLN:HG3	9:K:6:ARG:NH2	2.31	0.45
1:A:44:THR:O	1:A:44:THR:HG22	2.17	0.45
2:B:1158:PHE:O	2:B:1195:HIS:HA	2.16	0.45
1:A:1161:THR:CG2	1:A:1163:ILE:HB	2.47	0.45
7:I:4:PHE:HE1	7:I:6:PHE:CZ	2.34	0.45
1:A:546:VAL:HG21	1:A:572:TRP:CE3	2.51	0.45
1:A:1342:GLU:CG	4:E:198:ILE:HD13	2.46	0.45
1:A:1220:PHE:O	1:A:1221:LYS:C	2.55	0.45
1:A:214:ILE:CG2	1:A:218:ASP:HB2	2.46	0.45
1:A:1118:VAL:HG22	1:A:1306:LEU:HB2	1.98	0.45
1:A:517:ASN:O	1:A:517:ASN:CG	2.54	0.45
1:A:289:ILE:O	1:A:291:GLU:N	2.49	0.45
1:A:922:ASP:HB3	1:A:925:LEU:HB2	1.97	0.45
1:A:412:ARG:CZ	2:B:1110:PRO:HD3	2.44	0.45
1:A:1339:LEU:HD13	4:E:147:HIS:CD2	2.51	0.45
1:A:1229:SER:HB2	1:A:1233:ASP:OD2	2.16	0.45
2:B:332:ASP:C	2:B:334:ILE:N	2.68	0.45
2:B:227:LYS:HB2	2:B:395:GLN:OE1	2.16	0.45
1:A:404:TYR:HA	1:A:413:ILE:O	2.16	0.45
2:B:463:THR:HG22	2:B:465:ASN:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:249:ASP:O	3:C:252:GLN:HB3	2.16	0.45
1:A:458:HIS:NE2	1:A:478:TYR:OH	2.46	0.45
1:A:50:ILE:O	1:A:52:GLY:N	2.49	0.45
1:A:1115:SER:O	1:A:1329:THR:HG23	2.16	0.45
4:E:192:ARG:NH1	4:E:192:ARG:HG3	2.31	0.45
1:A:1189:SER:HB2	1:A:1190:PRO:CD	2.44	0.45
1:A:1254:ALA:O	1:A:1255:GLU:HB2	2.16	0.45
2:B:805:THR:HA	2:B:809:MET:HE1	1.98	0.45
1:A:185:TRP:O	1:A:197:PRO:HA	2.16	0.45
2:B:273:LEU:CB	2:B:276:ILE:HD12	2.46	0.45
1:A:1424:VAL:O	1:A:1428:VAL:HG23	2.16	0.45
1:A:598:LEU:O	1:A:599:SER:C	2.54	0.45
7:I:84:VAL:O	7:I:84:VAL:HG13	2.16	0.45
1:A:329:LEU:CD1	2:B:1210:MET:HE1	2.46	0.45
4:E:205:SER:O	4:E:206:GLY:C	2.54	0.45
2:B:654:ARG:O	2:B:656:GLY:N	2.49	0.45
1:A:736:ASN:O	1:A:737:LEU:C	2.54	0.45
3:C:33:LEU:HD11	3:C:248:ILE:HG12	1.99	0.45
1:A:225:ASN:ND2	1:A:228:PHE:CD1	2.84	0.45
1:A:1261:LYS:C	1:A:1263:ILE:N	2.69	0.45
2:B:906:SER:O	2:B:907:GLY:C	2.54	0.45
1:A:49:LYS:NZ	1:A:60:SER:HA	2.31	0.45
1:A:896:ARG:HB3	1:A:897:TYR:CD1	2.50	0.45
2:B:577:ALA:HB1	2:B:589:VAL:CG1	2.46	0.45
2:B:1103:ILE:O	2:B:1104:HIS:C	2.55	0.45
1:A:1370:LEU:C	1:A:1370:LEU:HD12	2.35	0.45
2:B:666:TYR:C	2:B:668:ASP:H	2.19	0.45
5:F:127:GLU:O	5:F:129:LYS:N	2.50	0.45
1:A:1383:SER:HB3	1:A:1387:HIS:CD2	2.51	0.45
2:B:212:LEU:HD12	2:B:409:ALA:CB	2.46	0.45
1:A:466:SER:HB2	2:B:1103:ILE:HD13	1.98	0.45
2:B:282:ILE:O	2:B:286:PHE:HD1	2.00	0.45
1:A:1208:THR:N	1:A:1211:GLN:OE1	2.50	0.45
2:B:1155:SER:O	2:B:1156:ASP:O	2.34	0.45
2:B:564:GLU:HA	2:B:565:PRO:HD2	1.70	0.45
1:A:474:VAL:HG13	1:A:478:TYR:HE1	1.77	0.45
1:A:343:LYS:O	1:A:345:VAL:HG22	2.17	0.45
6:H:109:LYS:HG3	6:H:110:ASP:N	2.30	0.45
2:B:172:ILE:HD13	2:B:178:ASN:HB2	1.99	0.45
6:H:5:LEU:O	6:H:133:ASN:HB3	2.17	0.45
7:I:50:THR:HG22	7:I:52:ILE:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:826:ALA:HB2	2:B:1087:PHE:CE1	2.51	0.45
1:A:1199:ARG:HA	1:A:1236:LEU:CD1	2.47	0.45
1:A:1106:ASN:OD1	1:A:1385:THR:HB	2.16	0.45
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.52	0.45
1:A:380:VAL:HG12	1:A:381:THR:N	2.32	0.45
1:A:605:MET:HE2	1:A:607:ILE:CG1	2.45	0.45
2:B:640:VAL:HG23	2:B:740:HIS:HA	1.99	0.45
1:A:49:LYS:NZ	1:A:61:ILE:HG13	2.31	0.45
4:E:177:ARG:HD3	4:E:215:MET:CE	2.46	0.45
1:A:709:THR:HG23	7:I:94:ASP:HA	1.99	0.45
1:A:886:ILE:CG1	1:A:943:LEU:HB3	2.47	0.45
1:A:886:ILE:CD1	1:A:943:LEU:HB3	2.47	0.45
1:A:553:VAL:HG22	1:A:652:VAL:HG22	1.99	0.45
2:B:229:ALA:HB1	2:B:231:PRO:HD2	1.98	0.45
1:A:826:ASP:O	1:A:830:LYS:N	2.45	0.45
10:L:55:ILE:HG13	10:L:56:LEU:N	2.24	0.44
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.57	0.44
1:A:34:LYS:CD	1:A:36:ARG:NH2	2.79	0.44
8:J:30:LEU:HD13	8:J:34:THR:HG22	1.99	0.44
8:J:19:GLU:O	8:J:20:SER:C	2.54	0.44
1:A:867:ILE:HG13	4:E:208:TYR:HE1	1.81	0.44
3:C:48:SER:HB3	3:C:158:VAL:HB	1.99	0.44
2:B:915:THR:HG22	2:B:916:THR:N	2.33	0.44
1:A:1389:PHE:N	1:A:1389:PHE:CD1	2.84	0.44
1:A:32:VAL:HG11	1:A:68:GLN:CD	2.38	0.44
2:B:1099:VAL:C	2:B:1101:ASP:H	2.20	0.44
6:H:91:ASP:C	6:H:93:TYR:N	2.70	0.44
8:J:32:GLU:CD	8:J:32:GLU:N	2.62	0.44
2:B:1148:LYS:O	2:B:1152:MET:HB2	2.17	0.44
1:A:114:LEU:HD22	1:A:171:GLN:HE22	1.80	0.44
3:C:8:VAL:HG21	9:K:105:PHE:HB2	1.99	0.44
1:A:583:PRO:HG2	1:A:586:ILE:HG13	1.99	0.44
6:H:42:ILE:CG2	6:H:43:ASN:N	2.80	0.44
2:B:864:LYS:CG	2:B:871:THR:HG23	2.47	0.44
2:B:990:ILE:HG22	2:B:992:ILE:H	1.82	0.44
1:A:1066:VAL:O	1:A:1067:LEU:C	2.54	0.44
1:A:1197:LEU:HD12	1:A:1209:MET:SD	2.57	0.44
4:E:10:SER:O	4:E:14:ARG:HG3	2.17	0.44
1:A:591:PHE:HA	1:A:595:THR:CB	2.48	0.44
1:A:167:CYS:HB2	1:A:169:ASN:ND2	2.32	0.44
3:C:238:ILE:HG23	3:C:242:GLN:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:43:LYS:HA	4:E:47:CYS:SG	2.57	0.44
1:A:783:THR:CG2	1:A:815:PHE:CE2	3.00	0.44
1:A:269:ILE:HD11	1:A:303:TYR:CB	2.48	0.44
1:A:1279:ILE:HD11	1:A:1316:VAL:HG21	1.99	0.44
1:A:903:ASN:O	1:A:904:THR:C	2.55	0.44
1:A:66:LYS:O	1:A:67:CYS:HB2	2.17	0.44
1:A:1364:ASN:ND2	1:A:1364:ASN:C	2.70	0.44
2:B:657:HIS:CE1	2:B:689:LEU:HD11	2.52	0.44
2:B:627:PHE:CB	2:B:632:ARG:HH11	2.30	0.44
2:B:864:LYS:HD3	2:B:871:THR:OG1	2.18	0.44
3:C:166:GLU:HG3	9:K:10:PHE:HZ	1.79	0.44
6:H:139:ASN:O	6:H:140:ALA:CB	2.65	0.44
4:E:56:LYS:HG3	4:E:84:ASP:HB2	1.99	0.44
2:B:603:LEU:O	2:B:609:ILE:N	2.49	0.44
4:E:39:LEU:HG	4:E:43:LYS:HE3	1.99	0.44
1:A:91:PHE:HB2	1:A:297:GLN:HE22	1.83	0.44
1:A:90:VAL:CG1	1:A:91:PHE:N	2.79	0.44
2:B:969:ARG:NH2	3:C:59:ALA:HB1	2.32	0.44
2:B:575:PRO:HG2	2:B:576:ASP:N	2.32	0.44
1:A:591:PHE:HA	1:A:595:THR:HB	1.99	0.44
1:A:341:MET:CE	1:A:343:LYS:HE3	2.48	0.44
8:J:7:CYS:HA	8:J:49:MET:HE3	2.00	0.44
1:A:465:TYR:HA	9:K:2:ASN:O	2.17	0.44
4:E:35:VAL:C	4:E:37:LEU:H	2.20	0.44
1:A:446:ARG:HD3	1:A:480:ALA:HB2	1.98	0.44
2:B:857:ARG:HD2	2:B:945:GLU:OE1	2.17	0.44
10:L:54:ARG:NH1	10:L:54:ARG:HB2	2.23	0.44
1:A:317:LYS:HD2	1:A:321:PRO:CG	2.45	0.44
2:B:175:ARG:HH11	2:B:175:ARG:HG2	1.83	0.44
2:B:200:GLY:HA2	2:B:202:TYR:CD2	2.53	0.44
7:I:28:GLU:O	7:I:28:GLU:HG3	2.17	0.44
7:I:94:ASP:OD1	7:I:94:ASP:N	2.50	0.44
6:H:138:GLU:O	6:H:139:ASN:C	2.56	0.44
2:B:240:ILE:CG2	2:B:254:LEU:HB3	2.45	0.44
2:B:226:PHE:CE2	2:B:398:ARG:HG2	2.53	0.44
2:B:1135:ARG:HG3	2:B:1147:LEU:HD22	2.00	0.44
3:C:196:ASP:OD2	3:C:199:LYS:HG3	2.18	0.44
6:H:43:ASN:C	6:H:45:GLU:H	2.21	0.44
2:B:364:ILE:HG12	2:B:585:VAL:HG13	1.99	0.44
1:A:780:VAL:O	1:A:782:ARG:HG2	2.17	0.44
2:B:377:PHE:O	2:B:378:LEU:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:VAL:CB	1:A:489:LEU:HD11	2.48	0.44
1:A:825:ILE:HD11	2:B:512:ARG:O	2.18	0.44
2:B:306:ASN:O	2:B:308:TRP:N	2.48	0.44
2:B:247:GLY:O	2:B:248:SER:HB3	2.18	0.44
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.33	0.44
3:C:74:SER:HB3	3:C:77:ILE:HG13	1.99	0.44
8:J:17:LYS:O	8:J:18:TRP:C	2.55	0.44
2:B:618:ASP:HB3	2:B:621:GLU:CB	2.48	0.44
2:B:979:LYS:HB3	2:B:1095:LEU:HB2	1.99	0.44
1:A:567:LYS:HZ3	6:H:95:TYR:HE1	1.62	0.43
2:B:864:LYS:CB	2:B:871:THR:HA	2.48	0.43
4:E:3:GLN:HG3	4:E:4:GLU:N	2.33	0.43
8:J:6:ARG:HD2	8:J:13:VAL:HG22	1.99	0.43
3:C:56:THR:HG21	3:C:145:CYS:SG	2.57	0.43
1:A:1425:SER:HA	1:A:1428:VAL:HG23	1.98	0.43
1:A:154:SER:HB3	1:A:162:VAL:HG23	2.00	0.43
1:A:1106:ASN:HA	1:A:1383:SER:OG	2.18	0.43
1:A:403:LYS:O	1:A:404:TYR:O	2.35	0.43
2:B:766:ARG:HD3	2:B:766:ARG:HA	1.86	0.43
1:A:499:ALA:O	1:A:503:GLN:HB2	2.18	0.43
1:A:534:LEU:O	1:A:574:GLY:HA3	2.18	0.43
3:C:62:PHE:C	3:C:62:PHE:HD2	2.21	0.43
1:A:1365:TYR:HD2	4:E:204:THR:HG1	1.65	0.43
1:A:1161:THR:HG23	1:A:1239:ARG:HH21	1.82	0.43
1:A:443:LEU:HD13	1:A:455:MET:HE2	1.99	0.43
10:L:29:TYR:HD1	10:L:39:SER:HA	1.82	0.43
2:B:446:LEU:O	2:B:446:LEU:HG	2.18	0.43
1:A:90:VAL:CG1	1:A:297:GLN:HA	2.47	0.43
2:B:1020:ARG:HB2	2:B:1022:THR:HG22	1.98	0.43
3:C:110:THR:O	3:C:110:THR:HG22	2.18	0.43
4:E:88:VAL:HG11	4:E:110:PHE:CE2	2.54	0.43
4:E:116:ILE:HG22	4:E:121:MET:HG2	2.00	0.43
1:A:1401:SER:O	1:A:1402:PHE:CB	2.65	0.43
1:A:849:MET:HE2	1:A:1061:GLY:CA	2.49	0.43
10:L:39:SER:O	10:L:40:LEU:HD23	2.18	0.43
1:A:172:PRO:HA	1:A:184:SER:O	2.19	0.43
7:I:78:CYS:SG	7:I:103:CYS:SG	3.15	0.43
2:B:168:GLY:H	2:B:450:ALA:HB1	1.83	0.43
2:B:634:TYR:CD1	2:B:634:TYR:C	2.92	0.43
2:B:956:THR:CG2	2:B:960:GLY:HA2	2.48	0.43
2:B:25:ILE:HG22	2:B:29:ASP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:69:LEU:HB3	8:J:5:VAL:HG11	1.99	0.43
2:B:130:VAL:HG12	2:B:131:ASP:H	1.83	0.43
3:C:56:THR:HG22	3:C:57:VAL:H	1.79	0.43
1:A:119:ASN:HB3	1:A:122:MET:HB3	2.01	0.43
1:A:1230:GLU:O	1:A:1232:ASN:N	2.51	0.43
2:B:659:ALA:O	2:B:663:ALA:HB2	2.19	0.43
1:A:756:ILE:HD13	1:A:756:ILE:HA	1.90	0.43
1:A:179:LEU:HD21	1:A:308:ILE:HD13	2.01	0.43
3:C:77:ILE:HG22	3:C:161:LYS:HE3	1.99	0.43
1:A:1143:LEU:N	1:A:1273:LEU:HD22	2.33	0.43
1:A:300:VAL:O	1:A:304:MET:HG3	2.18	0.43
2:B:198:ASP:OD1	2:B:485:ARG:NH2	2.50	0.43
1:A:392:VAL:HG21	1:A:426:LEU:HD11	2.00	0.43
2:B:1128:LEU:O	2:B:1128:LEU:HG	2.18	0.43
4:E:29:PHE:C	4:E:30:ILE:HG13	2.38	0.43
1:A:123:ARG:NH2	1:A:155:GLU:OE2	2.50	0.43
1:A:537:ARG:NH2	1:A:599:SER:O	2.51	0.43
2:B:765:PRO:O	2:B:766:ARG:C	2.56	0.43
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.59	0.43
3:C:62:PHE:CD2	3:C:62:PHE:C	2.91	0.43
1:A:1135:ARG:HG3	1:A:1282:VAL:CG1	2.48	0.43
2:B:1175:LEU:O	2:B:1176:ASN:ND2	2.52	0.43
1:A:474:VAL:O	1:A:478:TYR:HD1	2.02	0.43
2:B:654:ARG:C	2:B:656:GLY:N	2.70	0.43
8:J:3:VAL:O	8:J:4:PRO:C	2.55	0.43
8:J:6:ARG:HG3	8:J:11:GLY:O	2.18	0.43
2:B:566:LEU:HB2	2:B:588:GLY:HA2	2.00	0.43
2:B:999:MET:CG	2:B:1008:PRO:HG2	2.48	0.43
2:B:51:PHE:O	2:B:54:PHE:HB3	2.19	0.43
1:A:805:LEU:C	1:A:805:LEU:HD12	2.39	0.43
1:A:675:THR:CB	1:A:736:ASN:HD21	2.31	0.43
1:A:855:THR:HG21	1:A:857:ARG:NE	2.28	0.43
1:A:219:PHE:CD2	1:A:231:PRO:HG2	2.54	0.43
2:B:293:PRO:HA	7:I:12:ASN:HD21	1.84	0.43
7:I:32:CYS:SG	7:I:33:SER:N	2.92	0.43
1:A:492:PRO:HB3	1:A:497:THR:HG22	2.00	0.43
2:B:856:PHE:CD2	2:B:969:ARG:HB2	2.53	0.43
3:C:11:ARG:NH2	3:C:229:TYR:HD2	2.13	0.43
2:B:522:VAL:HG13	2:B:537:LYS:HB3	2.01	0.43
2:B:880:THR:O	2:B:881:ASN:HB2	2.19	0.43
1:A:299:HIS:HA	1:A:302:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:577:ALA:HB1	2:B:589:VAL:HG12	2.00	0.43
1:A:704:ALA:CB	1:A:710:LEU:HD12	2.42	0.43
1:A:1222:ASN:O	1:A:1223:ASP:CB	2.67	0.43
2:B:63:ILE:CG1	2:B:95:ILE:HD11	2.48	0.43
1:A:265:LYS:HZ2	1:A:323:LYS:H	1.65	0.43
2:B:842:ASN:HD22	2:B:845:SER:HB3	1.83	0.43
2:B:973:ILE:HA	2:B:974:PRO:HD2	1.87	0.43
3:C:120:ILE:HD11	3:C:130:GLY:O	2.18	0.43
1:A:592:ASP:N	1:A:595:THR:OG1	2.50	0.43
1:A:298:PHE:CZ	1:A:312:PRO:HB3	2.54	0.43
2:B:640:VAL:HG12	2:B:640:VAL:O	2.18	0.43
10:L:30:ILE:O	10:L:56:LEU:HA	2.18	0.43
10:L:28:LYS:H	10:L:39:SER:HB2	1.83	0.43
2:B:193:LYS:HZ3	8:J:65:PRO:HG2	1.84	0.43
1:A:356:ASP:OD2	9:K:65:HIS:HE1	2.02	0.43
5:F:150:GLU:O	5:F:151:LEU:C	2.57	0.43
1:A:72:GLU:OE2	1:A:76:GLU:HB3	2.19	0.43
4:E:127:ILE:O	4:E:127:ILE:HG13	2.19	0.43
1:A:1398:MET:O	1:A:1399:ARG:C	2.57	0.43
1:A:1404:GLU:O	1:A:1406:VAL:N	2.52	0.43
1:A:57:ARG:O	1:A:68:GLN:HG3	2.18	0.43
3:C:136:ASP:OD1	3:C:141:GLY:HA2	2.19	0.43
2:B:393:LYS:HE2	2:B:621:GLU:OE1	2.19	0.43
2:B:291:ILE:HD12	2:B:375:ALA:HB1	2.00	0.43
1:A:115:LEU:HD21	1:A:145:LYS:CE	2.49	0.43
2:B:397:ASP:OD2	2:B:515:HIS:CE1	2.72	0.43
1:A:1151:GLU:HA	7:I:44:TYR:O	2.19	0.43
1:A:1060:PRO:HD2	5:F:86:THR:HG21	2.01	0.43
7:I:111:THR:CG2	7:I:112:SER:H	2.32	0.42
1:A:345:VAL:CG2	2:B:1106:ARG:HH11	2.31	0.42
4:E:1:MET:C	4:E:3:GLN:H	2.21	0.42
1:A:399:HIS:HE1	1:A:436:ILE:O	2.01	0.42
7:I:50:THR:HG22	7:I:51:ASN:H	1.84	0.42
3:C:33:LEU:HG	3:C:37:MET:HE3	2.00	0.42
1:A:1198:ASP:OD1	1:A:1200:ALA:HB3	2.19	0.42
1:A:512:VAL:HG23	1:A:634:THR:HG21	2.01	0.42
2:B:195:CYS:SG	2:B:197:PHE:HB2	2.59	0.42
2:B:690:VAL:CG1	2:B:691:GLU:N	2.82	0.42
1:A:378:GLU:HG2	1:A:388:LEU:HD11	2.00	0.42
2:B:651:LEU:HD11	2:B:707:PRO:HB3	2.01	0.42
1:A:68:GLN:HE22	1:A:80:HIS:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ILE:N	1:A:541:ILE:HD12	2.34	0.42
1:A:75:ASN:O	1:A:76:GLU:HB2	2.18	0.42
1:A:774:ARG:H	1:A:774:ARG:HG2	1.62	0.42
2:B:376:PHE:O	2:B:586:TRP:HZ3	2.01	0.42
1:A:1127:ASP:C	1:A:1129:GLU:N	2.72	0.42
4:E:102:GLU:C	4:E:104:ASN:N	2.72	0.42
1:A:1148:ILE:HD11	1:A:1198:ASP:HA	2.00	0.42
1:A:128:ILE:HG21	1:A:133:LYS:CB	2.49	0.42
1:A:44:THR:O	1:A:45:GLN:HB2	2.18	0.42
1:A:342:GLY:HA3	2:B:1130:PHE:HB3	2.01	0.42
2:B:488:TYR:CD1	2:B:817:LEU:HD12	2.54	0.42
3:C:179:GLU:CD	3:C:206:ASN:HD22	2.22	0.42
2:B:203:PHE:O	2:B:209:GLU:HA	2.19	0.42
2:B:193:LYS:NZ	8:J:65:PRO:HG2	2.35	0.42
2:B:841:MET:HE2	2:B:1010:LEU:HD11	2.00	0.42
1:A:335:ARG:O	1:A:339:ASN:ND2	2.52	0.42
1:A:250:ILE:N	1:A:258:GLY:O	2.53	0.42
1:A:547:LEU:HD22	9:K:58:PHE:CE1	2.54	0.42
9:K:35:PHE:N	9:K:35:PHE:CD1	2.87	0.42
1:A:453:MET:HG2	1:A:520:CYS:SG	2.60	0.42
2:B:822:ASN:O	8:J:48:ARG:NH1	2.53	0.42
1:A:472:LEU:HD13	2:B:835:GLN:OE1	2.20	0.42
2:B:179:CYS:C	2:B:181:LEU:H	2.23	0.42
6:H:40:LEU:HD21	6:H:142:LEU:HD21	2.00	0.42
2:B:63:ILE:HD13	2:B:95:ILE:HD11	2.01	0.42
2:B:291:ILE:HD13	2:B:300:HIS:CD2	2.53	0.42
9:K:101:LEU:HD23	9:K:101:LEU:O	2.19	0.42
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.54	0.42
2:B:332:ASP:O	2:B:333:PHE:C	2.58	0.42
1:A:1004:ASN:OD1	4:E:167:ARG:HD2	2.19	0.42
1:A:557:ASP:OD2	1:A:559:VAL:HB	2.19	0.42
8:J:36:LEU:HD22	8:J:41:LEU:HD12	2.01	0.42
1:A:1130:GLN:HG3	1:A:1130:GLN:O	2.20	0.42
2:B:435:THR:O	2:B:435:THR:HG22	2.19	0.42
1:A:928:LEU:HD23	1:A:928:LEU:HA	1.93	0.42
1:A:252:PHE:O	1:A:253:ASN:C	2.58	0.42
2:B:345:LYS:CA	2:B:348:ARG:HE	2.18	0.42
3:C:136:ASP:OD1	3:C:136:ASP:N	2.50	0.42
1:A:1094:VAL:HG12	1:A:1095:THR:N	2.35	0.42
1:A:436:ILE:CD1	1:A:491:VAL:HG21	2.47	0.42
2:B:446:LEU:HD23	2:B:446:LEU:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:596:LEU:O	2:B:599:THR:HB	2.20	0.42
2:B:170:LEU:O	2:B:171:PRO:C	2.55	0.42
2:B:806:THR:C	2:B:808:ALA:N	2.72	0.42
10:L:28:LYS:N	10:L:39:SER:HB2	2.34	0.42
2:B:1051:THR:CG2	2:B:1052:VAL:N	2.83	0.42
4:E:166:LYS:CE	4:E:167:ARG:HH21	2.31	0.42
2:B:1084:GLN:OE1	3:C:189:THR:HG22	2.19	0.42
2:B:365:THR:CG2	2:B:367:LEU:H	2.33	0.42
5:F:101:ILE:HD13	5:F:120:ILE:HG21	2.02	0.42
1:A:586:ILE:HD12	1:A:633:VAL:HG22	2.02	0.42
9:K:83:PRO:O	9:K:86:ALA:HB3	2.20	0.42
5:F:116:ASP:HB3	5:F:119:ARG:HB2	2.00	0.42
1:A:1077:THR:HG22	1:A:1077:THR:O	2.20	0.42
6:H:42:ILE:HG22	6:H:43:ASN:N	2.35	0.42
6:H:49:VAL:HG12	6:H:50:ALA:N	2.34	0.42
1:A:849:MET:CE	1:A:1061:GLY:CA	2.84	0.42
8:J:5:VAL:O	8:J:6:ARG:CB	2.66	0.42
1:A:855:THR:CG2	1:A:856:THR:N	2.82	0.42
7:I:50:THR:CG2	7:I:51:ASN:N	2.82	0.42
1:A:100:LYS:O	1:A:102:VAL:N	2.53	0.42
2:B:284:ILE:CD1	2:B:324:ILE:HD12	2.48	0.42
4:E:77:SER:HB2	4:E:105:PHE:CD2	2.54	0.42
1:A:1098:VAL:N	1:A:1099:PRO:CD	2.83	0.42
10:L:45:ALA:C	10:L:46:VAL:HG23	2.40	0.42
2:B:765:PRO:O	2:B:768:THR:N	2.51	0.42
8:J:30:LEU:HD22	8:J:34:THR:HG21	2.01	0.42
2:B:570:VAL:HB	2:B:573:GLN:HB2	2.01	0.42
2:B:899:ILE:HG22	2:B:900:ALA:N	2.34	0.42
1:A:575:LYS:HB3	1:A:612:ILE:HG21	2.01	0.42
2:B:864:LYS:HD3	2:B:871:THR:CB	2.50	0.42
3:C:239:PRO:HD2	3:C:242:GLN:HG3	2.02	0.42
1:A:569:LYS:HG2	1:A:571:LEU:CD1	2.49	0.42
3:C:264:GLN:H	3:C:264:GLN:HG3	1.64	0.42
2:B:274:PRO:HG3	2:B:359:GLU:O	2.19	0.42
2:B:956:THR:HG23	2:B:961:LEU:N	2.35	0.42
1:A:261:ASP:OD1	1:A:315:LEU:HD13	2.19	0.42
2:B:682:SER:O	2:B:686:ASN:ND2	2.53	0.42
2:B:744:HIS:CD2	2:B:746:SER:H	2.17	0.42
4:E:39:LEU:O	4:E:42:PHE:HB3	2.20	0.42
1:A:815:PHE:O	1:A:818:MET:HB2	2.20	0.42
5:F:109:VAL:HG13	5:F:127:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1425:SER:HA	1:A:1428:VAL:CG2	2.50	0.42
1:A:1096:SER:O	1:A:1099:PRO:HG2	2.20	0.42
1:A:551:TYR:CE2	9:K:62:LYS:HE2	2.54	0.42
1:A:1001:ARG:O	1:A:1002:GLY:C	2.58	0.42
2:B:755:ILE:HG22	2:B:755:ILE:O	2.20	0.42
1:A:306:ASN:ND2	1:A:322:VAL:CG1	2.83	0.42
3:C:31:ASN:O	3:C:34:ARG:HB3	2.20	0.42
1:A:100:LYS:CE	1:A:176:LYS:HB2	2.48	0.42
2:B:486:TYR:CD2	2:B:1096:ARG:CZ	3.03	0.42
1:A:714:PHE:O	1:A:718:VAL:HG23	2.20	0.42
1:A:1191:TRP:HZ3	7:I:43:VAL:HG21	1.84	0.42
1:A:418:SER:O	1:A:420:ARG:N	2.53	0.42
3:C:265:MET:HE1	9:K:19:LEU:O	2.19	0.42
1:A:388:LEU:HD22	1:A:432:VAL:CB	2.46	0.41
2:B:627:PHE:HB3	2:B:632:ARG:HH11	1.84	0.41
8:J:1:MET:O	8:J:2:ILE:O	2.38	0.41
2:B:1183:LYS:C	2:B:1185:CYS:N	2.72	0.41
3:C:146:LYS:HB2	8:J:57:ILE:CD1	2.50	0.41
2:B:1177:HIS:O	2:B:1179:GLN:HG3	2.20	0.41
10:L:46:VAL:O	10:L:47:ARG:HG3	2.19	0.41
1:A:992:ASP:O	1:A:995:GLU:HB2	2.20	0.41
2:B:514:LEU:HD12	2:B:518:HIS:HD2	1.84	0.41
1:A:1359:ASP:C	1:A:1361:SER:H	2.23	0.41
1:A:7:SER:C	1:A:9:ALA:H	2.24	0.41
1:A:112:LYS:NZ	1:A:165:GLY:H	2.18	0.41
1:A:113:LEU:HA	1:A:113:LEU:HD23	1.87	0.41
1:A:179:LEU:HD21	1:A:308:ILE:CD1	2.50	0.41
4:E:5:ASN:O	4:E:9:ILE:HG13	2.19	0.41
8:J:9:SER:OG	8:J:48:ARG:NH2	2.53	0.41
5:F:147:SER:O	5:F:148:VAL:C	2.58	0.41
1:A:1045:VAL:O	1:A:1046:LEU:C	2.56	0.41
1:A:1436:ILE:O	1:A:1436:ILE:HG13	2.20	0.41
2:B:1197:PRO:O	2:B:1200:ALA:HB3	2.19	0.41
1:A:289:ILE:C	1:A:291:GLU:H	2.24	0.41
2:B:857:ARG:NH1	2:B:945:GLU:OE2	2.53	0.41
2:B:225:VAL:HA	2:B:237:VAL:O	2.20	0.41
1:A:23:SER:O	1:A:27:VAL:HG23	2.20	0.41
3:C:46:ILE:HA	3:C:159:ALA:HA	2.02	0.41
1:A:252:PHE:CD1	1:A:252:PHE:N	2.88	0.41
1:A:1064:VAL:HG12	1:A:1064:VAL:O	2.21	0.41
8:J:52:THR:O	8:J:52:THR:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:N	1:A:845:LEU:HD23	2.35	0.41
2:B:1007:VAL:HG22	2:B:1008:PRO:HD2	2.01	0.41
1:A:805:LEU:CD1	2:B:1052:VAL:HG21	2.50	0.41
3:C:75:MET:CG	3:C:246:ARG:HH22	2.30	0.41
2:B:914:LYS:N	2:B:938:SER:HB3	2.35	0.41
2:B:515:HIS:HD2	2:B:517:THR:OG1	2.02	0.41
9:K:18:LYS:HA	9:K:18:LYS:HD3	1.85	0.41
1:A:225:ASN:ND2	1:A:228:PHE:HD1	2.16	0.41
1:A:768:GLN:HG2	1:A:816:HIS:CA	2.50	0.41
2:B:784:ASN:HB3	8:J:63:TYR:CZ	2.56	0.41
2:B:532:ALA:HB1	2:B:536:VAL:HG23	2.02	0.41
4:E:165:LEU:HD21	4:E:175:LEU:HD11	2.02	0.41
1:A:267:ALA:O	1:A:271:LYS:HG3	2.19	0.41
4:E:178:ILE:HG23	4:E:214:CYS:HA	2.03	0.41
1:A:1364:ASN:HD21	1:A:1366:ARG:H	1.64	0.41
1:A:1364:ASN:CG	1:A:1366:ARG:HH11	2.24	0.41
1:A:311:GLN:HA	1:A:312:PRO:HD2	1.90	0.41
1:A:319:GLY:O	1:A:321:PRO:HD3	2.19	0.41
2:B:871:THR:CG2	2:B:872:GLU:N	2.68	0.41
3:C:66:ARG:CZ	8:J:2:ILE:CG2	2.98	0.41
2:B:827:ILE:O	2:B:1085:ILE:HG23	2.21	0.41
8:J:43:ARG:HG2	8:J:43:ARG:H	1.67	0.41
2:B:737:THR:CG2	2:B:737:THR:O	2.69	0.41
6:H:82:PRO:HG3	9:K:54:ARG:CG	2.43	0.41
2:B:879:ARG:HD2	2:B:883:LEU:CD2	2.47	0.41
1:A:399:HIS:C	1:A:401:GLY:N	2.73	0.41
9:K:49:GLU:HG3	9:K:94:ILE:HG12	2.01	0.41
2:B:873:THR:CG2	2:B:874:PHE:N	2.84	0.41
3:C:77:ILE:C	3:C:79:GLN:N	2.73	0.41
1:A:315:LEU:HD12	1:A:321:PRO:CG	2.41	0.41
2:B:996:ARG:NH2	3:C:175:ALA:HA	2.35	0.41
2:B:43:LEU:CD1	2:B:812:LEU:HD23	2.49	0.41
2:B:825:VAL:HG12	2:B:826:ALA:H	1.83	0.41
2:B:205:ILE:HD11	2:B:461:LEU:HD23	2.02	0.41
2:B:551:PRO:HG2	2:B:552:MET:SD	2.60	0.41
1:A:503:GLN:HG3	5:F:90:ARG:HH21	1.84	0.41
1:A:1009:ASN:HA	1:A:1012:ARG:NH1	2.36	0.41
4:E:78:LEU:C	4:E:78:LEU:HD23	2.41	0.41
1:A:481:ASP:OD1	1:A:485:ASP:OD2	2.39	0.41
1:A:1391:ARG:HB3	1:A:1392:SER:H	1.61	0.41
6:H:84:ALA:HA	6:H:87:ARG:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1173:HIS:O	1:A:1174:PHE:CG	2.74	0.41
5:F:127:GLU:O	5:F:128:LYS:C	2.59	0.41
3:C:248:ILE:HG23	9:K:98:LEU:HD22	2.03	0.41
1:A:1141:THR:HG21	1:A:1207:LEU:HD11	2.03	0.41
2:B:1001:PHE:HE1	3:C:178:PHE:HB3	1.86	0.41
3:C:82:TYR:O	3:C:83:SER:C	2.59	0.41
1:A:702:LEU:HD23	1:A:702:LEU:HA	1.87	0.41
1:A:550:LEU:HD23	1:A:550:LEU:HA	1.88	0.41
1:A:535:THR:HG23	1:A:575:LYS:HE3	2.03	0.41
1:A:1111:MET:HE1	1:A:1330:ASN:OD1	2.21	0.41
3:C:69:LEU:HA	3:C:69:LEU:HD12	1.83	0.41
1:A:505:CYS:HB3	2:B:1141:HIS:CG	2.56	0.41
5:F:111:LEU:HD23	5:F:114:GLU:O	2.20	0.41
4:E:191:LYS:O	4:E:192:ARG:C	2.59	0.41
5:F:82:THR:HA	5:F:83:PRO:HD3	1.75	0.41
1:A:853:ASP:OD2	1:A:857:ARG:NH2	2.49	0.41
3:C:56:THR:CG2	3:C:57:VAL:H	2.34	0.41
1:A:1193:LEU:HB2	1:A:1260:LEU:CD1	2.45	0.41
2:B:100:PRO:HG2	2:B:124:TYR:CZ	2.55	0.41
1:A:974:ASP:HB3	6:H:136:LYS:HZ3	1.85	0.41
1:A:152:VAL:HG23	1:A:164:ARG:HD3	2.01	0.41
1:A:1140:HIS:CE1	1:A:1272:THR:HG23	2.55	0.41
1:A:1215:ARG:NH1	1:A:1273:LEU:O	2.53	0.41
1:A:511:ILE:HG12	1:A:521:MET:CE	2.51	0.41
5:F:130:ILE:HA	5:F:131:PRO:HD2	1.83	0.41
1:A:1300:LYS:NZ	1:A:1300:LYS:HB3	2.36	0.41
4:E:82:PHE:N	4:E:82:PHE:CD1	2.89	0.41
1:A:486:GLU:OE1	2:B:1102:LYS:HD3	2.20	0.41
2:B:797:TYR:HE1	2:B:854:LEU:CD2	2.33	0.41
1:A:254:GLU:O	1:A:255:SER:OG	2.35	0.41
2:B:31:TRP:CZ3	2:B:34:ILE:HD12	2.56	0.41
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.56	0.41
3:C:127:ARG:HG2	3:C:127:ARG:H	1.70	0.41
2:B:484:ASN:CG	2:B:486:TYR:CE1	2.94	0.41
1:A:67:CYS:O	1:A:70:CYS:SG	2.79	0.41
2:B:806:THR:N	2:B:809:MET:HE3	2.35	0.41
2:B:653:VAL:HG22	2:B:689:LEU:HB3	2.02	0.41
2:B:707:PRO:CG	2:B:708:GLU:N	2.84	0.41
1:A:868:TYR:CE2	1:A:1058:VAL:HG21	2.56	0.41
2:B:345:LYS:HB3	2:B:346:GLU:H	1.57	0.41
2:B:798:TYR:CD2	8:J:4:PRO:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:TYR:CD2	1:A:936:LEU:HD13	2.56	0.41
2:B:1099:VAL:O	2:B:1103:ILE:HG13	2.20	0.41
1:A:148:CYS:O	1:A:168:GLY:HA2	2.21	0.41
1:A:734:GLU:HA	1:A:737:LEU:HD12	2.03	0.41
1:A:214:ILE:HG22	1:A:218:ASP:HB2	2.02	0.41
2:B:254:LEU:HD22	2:B:361:LEU:HD13	2.03	0.41
2:B:112:LEU:HD12	2:B:113:TYR:H	1.86	0.41
1:A:751:SER:OG	2:B:1015:HIS:HE1	2.04	0.41
4:E:24:LYS:HE3	4:E:30:ILE:O	2.21	0.41
1:A:100:LYS:CE	1:A:176:LYS:HD2	2.50	0.41
1:A:1035:TYR:O	1:A:1036:ARG:C	2.59	0.41
7:I:78:CYS:O	7:I:79:HIS:C	2.59	0.41
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.86	0.41
2:B:23:ALA:HB3	2:B:655:LYS:CE	2.51	0.41
2:B:59:LEU:HD11	2:B:417:PHE:CZ	2.56	0.41
7:I:96:SER:OG	7:I:98:VAL:HG23	2.20	0.41
1:A:22:PHE:HD2	1:A:26:GLU:HG2	1.86	0.41
2:B:806:THR:C	2:B:808:ALA:H	2.24	0.41
1:A:519:PRO:HD3	1:A:631:HIS:CG	2.56	0.41
2:B:1222:ARG:HG2	2:B:1223:ASP:N	2.36	0.41
2:B:520:GLY:HA2	2:B:748:ILE:HG22	2.02	0.41
2:B:1182:CYS:C	2:B:1183:LYS:O	2.59	0.41
1:A:608:ILE:HB	1:A:613:ILE:HD11	2.03	0.41
2:B:997:GLU:HB2	3:C:35:ARG:HH21	1.86	0.41
7:I:10:CYS:SG	7:I:31:THR:CG2	3.09	0.41
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.21	0.41
1:A:1438:THR:CG2	2:B:1144:ALA:HB3	2.50	0.41
1:A:1199:ARG:HG2	1:A:1203:ASN:ND2	2.36	0.41
2:B:782:LEU:HD23	2:B:782:LEU:HA	1.85	0.41
3:C:182:PRO:HB3	3:C:206:ASN:HB2	2.01	0.41
2:B:514:LEU:HD12	2:B:518:HIS:CD2	2.56	0.41
1:A:1364:ASN:ND2	1:A:1365:TYR:N	2.70	0.40
2:B:605:ARG:CZ	2:B:639:ILE:HD13	2.50	0.40
1:A:1116:LEU:HD12	1:A:1329:THR:OG1	2.21	0.40
2:B:1152:MET:HG2	2:B:1153:GLU:H	1.86	0.40
6:H:130:ARG:C	6:H:132:LEU:N	2.72	0.40
1:A:1152:ILE:HA	1:A:1192:LEU:O	2.21	0.40
2:B:431:TYR:CZ	2:B:447:ALA:HB2	2.56	0.40
2:B:575:PRO:CG	2:B:576:ASP:H	2.34	0.40
9:K:63:VAL:HG12	9:K:71:PHE:HB3	2.03	0.40
2:B:984:HIS:CD2	2:B:1025:HIS:CA	3.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:40:GLU:O	3:C:250:THR:HG21	2.21	0.40
1:A:629:LEU:O	1:A:633:VAL:HG23	2.21	0.40
2:B:510:LYS:N	2:B:511:PRO:CD	2.84	0.40
1:A:538:ASP:OD1	6:H:22:LYS:HG3	2.22	0.40
1:A:890:ASP:OD1	1:A:940:ARG:NH1	2.54	0.40
1:A:948:VAL:HG12	1:A:948:VAL:O	2.20	0.40
2:B:202:TYR:CD2	2:B:483:LEU:HD22	2.56	0.40
1:A:107:CYS:SG	1:A:148:CYS:CB	3.04	0.40
2:B:597:MET:HE3	2:B:600:LEU:HD12	2.03	0.40
2:B:1037:LEU:HD11	2:B:1064:TYR:CE1	2.56	0.40
1:A:547:LEU:HD22	9:K:58:PHE:CD1	2.56	0.40
2:B:959:ASP:O	2:B:960:GLY:C	2.59	0.40
1:A:326:ARG:HD3	1:A:1406:VAL:HG11	2.03	0.40
2:B:701:ILE:HB	2:B:739:THR:OG1	2.21	0.40
1:A:61:ILE:HG22	1:A:62:ASP:N	2.30	0.40
1:A:475:THR:CG2	1:A:476:SER:N	2.85	0.40
6:H:84:ALA:HA	6:H:87:ARG:CB	2.51	0.40
2:B:377:PHE:CD2	2:B:381:MET:HE2	2.57	0.40
1:A:613:ILE:O	1:A:614:PHE:HB3	2.22	0.40
1:A:1237:ILE:CG2	1:A:1238:ILE:N	2.84	0.40
2:B:859:TYR:CE2	2:B:942:ARG:HG3	2.56	0.40
4:E:72:PHE:CD1	4:E:72:PHE:N	2.89	0.40
2:B:23:ALA:HB3	2:B:655:LYS:CD	2.51	0.40
4:E:116:ILE:CG2	4:E:121:MET:HG2	2.52	0.40
2:B:842:ASN:HD22	2:B:845:SER:CB	2.34	0.40
9:K:58:PHE:HB3	9:K:76:GLN:HB3	2.03	0.40
1:A:1001:ARG:HB2	5:F:80:ALA:O	2.21	0.40
7:I:101:PHE:CD1	7:I:101:PHE:N	2.89	0.40
7:I:85:PHE:HB3	7:I:101:PHE:CD2	2.56	0.40
1:A:809:THR:H	1:A:812:GLU:HB2	1.86	0.40
1:A:567:LYS:NZ	6:H:95:TYR:CE1	2.88	0.40
1:A:666:ILE:O	1:A:667:GLY:C	2.59	0.40
2:B:693:ILE:HD13	2:B:701:ILE:HD13	2.04	0.40
2:B:348:ARG:O	2:B:351:TYR:HB3	2.21	0.40
2:B:918:ILE:HD12	2:B:935:ARG:NH1	2.36	0.40
1:A:545:GLN:O	1:A:549:MET:HG3	2.21	0.40
3:C:175:ALA:CB	8:J:43:ARG:NH1	2.84	0.40
2:B:1180:PHE:O	2:B:1181:GLU:O	2.39	0.40
1:A:1391:ARG:O	1:A:1392:SER:HB3	2.22	0.40
2:B:603:LEU:HD23	2:B:603:LEU:HA	1.86	0.40
1:A:189:ARG:O	1:A:190:ALA:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:ILE:O	1:A:686:ALA:HB3	2.21	0.40
2:B:893:LEU:HA	2:B:893:LEU:HD23	1.91	0.40
2:B:121:ASN:HD22	2:B:121:ASN:N	2.19	0.40
2:B:1050:ILE:CG2	2:B:1055:ILE:HD11	2.52	0.40
1:A:1332:PHE:CD1	1:A:1381:LEU:HD13	2.56	0.40
3:C:77:ILE:O	3:C:79:GLN:N	2.54	0.40
1:A:341:MET:HE3	1:A:343:LYS:HE3	2.04	0.40
3:C:167:HIS:HE1	10:L:70:ARG:O	2.05	0.40
1:A:1015:VAL:O	1:A:1015:VAL:HG12	2.22	0.40
1:A:269:ILE:HD11	1:A:303:TYR:HB3	2.03	0.40
2:B:292:ILE:N	2:B:293:PRO:HD2	2.36	0.40
3:C:92:CYS:C	3:C:94:LYS:H	2.24	0.40
6:H:44:VAL:HG13	6:H:48:PRO:HA	2.03	0.40
1:A:1129:GLU:O	1:A:1132:LYS:HB2	2.21	0.40
3:C:62:PHE:HD2	3:C:62:PHE:O	2.05	0.40
1:A:946:VAL:HG22	4:E:201:LYS:HD2	2.04	0.40
4:E:112:TYR:CZ	4:E:136:ASN:HB2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:ASP:OD1	2:B:106:ASP:OD1[2_655]	2.08	0.12

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1406/1733 (81%)	1138 (81%)	203 (14%)	65 (5%)	3 17
2	B	1061/1224 (87%)	868 (82%)	128 (12%)	65 (6%)	2 11
3	C	264/318 (83%)	210 (80%)	35 (13%)	19 (7%)	1 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	E	213/215 (99%)	184 (86%)	27 (13%)	2 (1%)	21 61
5	F	82/155 (53%)	63 (77%)	15 (18%)	4 (5%)	3 16
6	H	129/146 (88%)	91 (70%)	22 (17%)	16 (12%)	0 1
7	I	120/122 (98%)	97 (81%)	17 (14%)	6 (5%)	3 16
8	J	63/70 (90%)	53 (84%)	7 (11%)	3 (5%)	3 17
9	K	112/120 (93%)	106 (95%)	5 (4%)	1 (1%)	21 61
10	L	44/70 (63%)	28 (64%)	9 (20%)	7 (16%)	0 0
All	All	3494/4173 (84%)	2838 (81%)	468 (13%)	188 (5%)	2 14

All (188) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	35	ILE
1	A	48	ALA
1	A	55	ASP
1	A	56	PRO
1	A	87	ALA
1	A	167	CYS
1	A	196	GLU
1	A	257	ARG
1	A	314	ALA
1	A	384	ASN
1	A	404	TYR
1	A	465	TYR
1	A	567	LYS
1	A	597	LEU
1	A	904	THR
1	A	998	LEU
1	A	1036	ARG
1	A	1114	PRO
1	A	1122	PRO
1	A	1127	ASP
1	A	1223	ASP
1	A	1377	THR
1	A	1386	ARG
1	A	1391	ARG
1	A	1393	ASN
1	A	1400	CYS
1	A	1401	SER

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Mol	Chain	Res	Type
1	A	1416	ALA
2	B	65	GLU
2	B	136	THR
2	B	175	ARG
2	B	367	LEU
2	B	436	VAL
2	B	480	SER
2	B	531	GLN
2	B	643	ASP
2	B	708	GLU
2	B	709	ASP
2	B	734	HIS
2	B	864	LYS
2	B	884	ARG
2	B	943	SER
2	B	958	GLN
2	B	992	ILE
2	B	1108	ARG
2	B	1156	ASP
2	B	1167	GLY
2	B	1176	ASN
2	B	1181	GLU
2	B	1183	LYS
2	B	1221	SER
2	B	1222	ARG
3	C	90	ASP
3	C	141	GLY
3	C	174	ALA
5	F	73	ALA
5	F	128	LYS
6	H	81	PRO
6	H	83	GLN
6	H	140	ALA
7	I	11	ASN
7	I	79	HIS
8	J	2	ILE
10	L	38	LEU
10	L	64	LEU
1	A	54	ASN
1	A	67	CYS
1	A	75	ASN
1	A	109	HIS

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Mol	Chain	Res	Type
1	A	154	SER
1	A	186	LYS
1	A	290	GLU
1	A	920	LEU
1	A	986	ILE
1	A	1224	LEU
1	A	1231	ASP
1	A	1392	SER
2	B	55	VAL
2	B	174	LEU
2	B	200	GLY
2	B	247	GLY
2	B	333	PHE
2	B	347	LYS
2	B	364	ILE
2	B	575	PRO
2	B	649	LYS
2	B	887	HIS
2	B	901	PRO
2	B	907	GLY
2	B	960	GLY
2	B	996	ARG
2	B	1066	SER
2	B	1104	HIS
2	B	1154	ALA
3	C	4	GLU
3	C	5	GLY
3	C	130	GLY
3	C	142	VAL
3	C	195	GLN
3	C	241	ASP
6	H	17	PRO
6	H	32	THR
6	H	82	PRO
6	H	128	ASN
6	H	139	ASN
7	I	116	ASN
8	J	26	GLN
10	L	37	LYS
10	L	39	SER
1	A	79	GLY
1	A	101	LYS

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Mol	Chain	Res	Type
1	A	324	SER
1	A	419	LYS
1	A	464	PRO
1	A	1221	LYS
1	A	1280	GLU
2	B	21	GLU
2	B	47	GLN
2	B	641	GLU
2	B	1109	GLY
3	C	175	ALA
3	C	202	PRO
3	C	212	PRO
3	C	227	THR
3	C	237	SER
6	H	51	ALA
6	H	62	SER
6	H	90	ALA
6	H	138	GLU
7	I	121	PHE
1	A	197	PRO
1	A	307	ASP
1	A	321	PRO
1	A	399	HIS
1	A	591	PHE
1	A	958	VAL
1	A	1172	LEU
2	B	466	TRP
2	B	619	ILE
2	B	655	LYS
2	B	731	VAL
2	B	791	THR
2	B	792	MET
2	B	813	LYS
2	B	1046	PRO
3	C	78	GLU
3	C	149	LYS
6	H	77	ARG
6	H	111	LEU
6	H	135	LEU
7	I	23	ASN
8	J	6	ARG
9	K	107	THR

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Mol	Chain	Res	Type
10	L	56	LEU
1	A	51	GLY
1	A	84	ILE
1	A	424	ILE
1	A	599	SER
1	A	752	LYS
1	A	875	ALA
1	A	1397	LEU
1	A	1437	GLY
2	B	90	ILE
2	B	179	CYS
2	B	180	TYR
2	B	707	PRO
2	B	938	SER
2	B	1017	ILE
3	C	28	ALA
3	C	214	ASN
5	F	81	THR
10	L	26	THR
2	B	168	GLY
2	B	1018	PRO
4	E	86	PRO
5	F	131	PRO
6	H	107	VAL
10	L	45	ALA
2	B	565	PRO
7	I	62	ILE
2	B	1184	GLY
4	E	30	ILE
2	B	167	ILE
3	C	240	VAL
1	A	1242	VAL
2	B	100	PRO
1	A	93	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1234/1520 (81%)	1165 (94%)	69 (6%)	26 62
2	B	942/1061 (89%)	884 (94%)	58 (6%)	23 59
3	C	234/274 (85%)	221 (94%)	13 (6%)	26 62
4	E	197/197 (100%)	193 (98%)	4 (2%)	63 86
5	F	74/137 (54%)	67 (90%)	7 (10%)	11 38
6	H	117/128 (91%)	108 (92%)	9 (8%)	16 50
7	I	116/116 (100%)	107 (92%)	9 (8%)	16 49
8	J	60/65 (92%)	54 (90%)	6 (10%)	9 34
9	K	99/102 (97%)	90 (91%)	9 (9%)	12 40
10	L	40/57 (70%)	35 (88%)	5 (12%)	6 22
All	All	3113/3657 (85%)	2924 (94%)	189 (6%)	23 59

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	93	VAL
1	A	117	GLU
1	A	122	MET
1	A	247	ARG
1	A	321	PRO
1	A	345	VAL
1	A	351	THR
1	A	375	THR
1	A	383	TYR
1	A	397	ASN
1	A	436	ILE
1	A	445	ASN
1	A	450	LEU
1	A	474	VAL
1	A	475	THR
1	A	479	ASN
1	A	481	ASP
1	A	493	GLN
1	A	503	GLN
1	A	504	LEU
1	A	505	CYS
1	A	517	ASN
1	A	518	LYS

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Mol	Chain	Res	Type
1	A	524	VAL
1	A	538	ASP
1	A	573	SER
1	A	590	ARG
1	A	596	THR
1	A	597	LEU
1	A	598	LEU
1	A	618	GLU
1	A	626	ASN
1	A	629	LEU
1	A	666	ILE
1	A	711	ARG
1	A	756	ILE
1	A	768	GLN
1	A	774	ARG
1	A	821	ARG
1	A	826	ASP
1	A	845	LEU
1	A	854	ASN
1	A	855	THR
1	A	858	ASN
1	A	867	ILE
1	A	897	TYR
1	A	919	ILE
1	A	1035	TYR
1	A	1043	ASP
1	A	1055	ARG
1	A	1110	ASN
1	A	1122	PRO
1	A	1135	ARG
1	A	1208	THR
1	A	1257	ASP
1	A	1258	HIS
1	A	1264	GLU
1	A	1273	LEU
1	A	1295	THR
1	A	1308	THR
1	A	1331	SER
1	A	1345	ARG
1	A	1359	ASP
1	A	1364	ASN
1	A	1366	ARG

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Mol	Chain	Res	Type
1	A	1370	LEU
1	A	1387	HIS
1	A	1438	THR
2	B	20	ASP
2	B	63	ILE
2	B	121	ASN
2	B	174	LEU
2	B	194	GLU
2	B	199	MET
2	B	234	ILE
2	B	261	ARG
2	B	278	GLN
2	B	320	ASP
2	B	331	LEU
2	B	376	PHE
2	B	391	ASP
2	B	394	ASP
2	B	455	SER
2	B	466	TRP
2	B	480	SER
2	B	485	ARG
2	B	486	TYR
2	B	487	THR
2	B	513	GLN
2	B	538	ASN
2	B	547	VAL
2	B	559	SER
2	B	570	VAL
2	B	601	ARG
2	B	602	THR
2	B	616	ILE
2	B	628	THR
2	B	629	ASP
2	B	635	ARG
2	B	678	GLU
2	B	679	TYR
2	B	685	LEU
2	B	737	THR
2	B	769	TYR
2	B	780	VAL
2	B	790	ASP
2	B	791	THR

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Mol	Chain	Res	Type
2	B	807	ARG
2	B	857	ARG
2	B	859	TYR
2	B	860	MET
2	B	901	PRO
2	B	969	ARG
2	B	975	GLN
2	B	976	ILE
2	B	983	ARG
2	B	997	GLU
2	B	999	MET
2	B	1028	GLU
2	B	1065	GLN
2	B	1145	SER
2	B	1159	ARG
2	B	1175	LEU
2	B	1183	LYS
2	B	1185	CYS
2	B	1211	ASN
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	57	VAL
3	C	62	PHE
3	C	69	LEU
3	C	118	LEU
3	C	122	SER
3	C	136	ASP
3	C	163	ILE
3	C	186	LEU
3	C	233	GLU
3	C	249	ASP
4	E	24	LYS
4	E	104	ASN
4	E	202	SER
4	E	204	THR
5	F	79	ARG
5	F	90	ARG
5	F	103	MET
5	F	108	PHE
5	F	111	LEU
5	F	133	VAL

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Mol	Chain	Res	Type
5	F	140	ASP
6	H	17	PRO
6	H	27	GLU
6	H	33	GLN
6	H	82	PRO
6	H	102	TYR
6	H	109	LYS
6	H	110	ASP
6	H	114	VAL
6	H	143	LEU
7	I	15	TYR
7	I	31	THR
7	I	52	ILE
7	I	55	THR
7	I	75	CYS
7	I	84	VAL
7	I	94	ASP
7	I	95	THR
7	I	118	ARG
8	J	2	ILE
8	J	6	ARG
8	J	7	CYS
8	J	43	ARG
8	J	48	ARG
8	J	55	ASP
9	K	12	LEU
9	K	25	THR
9	K	47	ARG
9	K	50	LEU
9	K	51	LEU
9	K	73	LEU
9	K	74	ARG
9	K	77	THR
9	K	101	LEU
10	L	38	LEU
10	L	50	ASP
10	L	54	ARG
10	L	58	LYS
10	L	68	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	92	HIS
1	A	169	ASN
1	A	225	ASN
1	A	281	HIS
1	A	297	GLN
1	A	399	HIS
1	A	435	HIS
1	A	445	ASN
1	A	479	ASN
1	A	493	GLN
1	A	631	HIS
1	A	654	ASN
1	A	698	GLN
1	A	736	ASN
1	A	741	ASN
1	A	745	GLN
1	A	768	GLN
1	A	786	HIS
1	A	858	ASN
1	A	926	GLN
1	A	935	GLN
1	A	994	GLN
1	A	1078	GLN
1	A	1140	HIS
1	A	1203	ASN
1	A	1270	ASN
1	A	1364	ASN
1	A	1432	GLN
2	B	46	GLN
2	B	115	GLN
2	B	178	ASN
2	B	215	GLN
2	B	236	HIS
2	B	325	GLN
2	B	366	GLN
2	B	465	ASN
2	B	513	GLN
2	B	515	HIS
2	B	516	ASN
2	B	518	HIS
2	B	538	ASN
2	B	657	HIS

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Mol	Chain	Res	Type
2	B	686	ASN
2	B	706	GLN
2	B	744	HIS
2	B	822	ASN
2	B	842	ASN
2	B	957	ASN
2	B	984	HIS
2	B	1015	HIS
2	B	1040	ASN
2	B	1065	GLN
2	B	1179	GLN
2	B	1187	ASN
3	C	65	HIS
3	C	73	GLN
3	C	102	GLN
3	C	112	ASN
3	C	123	ASN
3	C	167	HIS
3	C	242	GLN
4	E	5	ASN
4	E	32	GLN
4	E	61	GLN
4	E	101	GLN
4	E	104	ASN
4	E	113	GLN
4	E	114	ASN
4	E	146	HIS
4	E	147	HIS
6	H	11	GLN
6	H	128	ASN
6	H	131	ASN
6	H	134	ASN
7	I	12	ASN
7	I	83	ASN
8	J	53	HIS
9	K	29	ASN
9	K	65	HIS
9	K	76	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 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.