



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:47 PM GMT

PDB ID : 1H38
Title : STRUCTURE OF A T7 RNA POLYMERASE ELONGATION COMPLEX
AT 2.9Å RESOLUTION
Authors : Tahirov, T.H.; Temyakov, D.; Anikin, M.; Patlan, V.; Mcallister, W.T.; Vasylyev, D.G.; Yokoyama, S.
Deposited on : 2002-08-24
Resolution : 2.90 Å(reported)

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

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

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

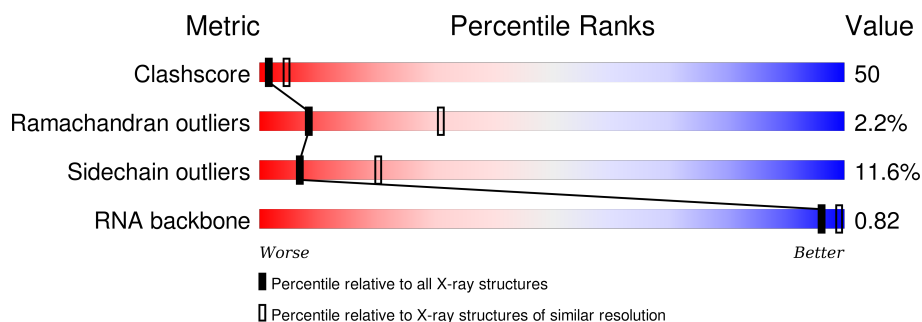
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)


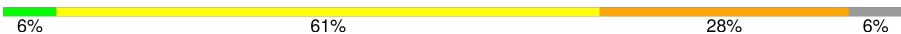


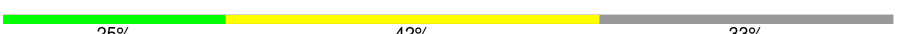
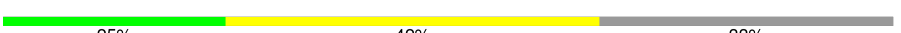
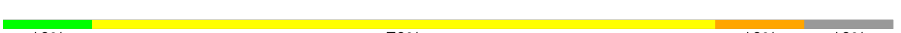



The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	883	
1	B	883	
1	C	883	
1	D	883	
2	E	18	
2	H	18	

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Mol	Chain	Length	Quality of chain
2	K	18	
2	N	18	
3	F	12	
3	I	12	
3	L	12	
3	O	12	
4	G	10	
4	J	10	
4	M	10	
4	P	10	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30948 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	B	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	C	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			
1	D	857	Total	C	N	O	S	0	0	0
			6746	4296	1173	1242	35			

- Molecule 2 is a DNA chain called 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			
2	H	18	Total	C	N	O	P	0	0	0
			367	174	72	104	17			
2	K	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			
2	N	17	Total	C	N	O	P	0	0	0
			345	164	67	98	16			

- Molecule 3 is a RNA chain called 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
3	I	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			
3	L	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	8	Total	C	N	O	P	0	0	0
			171	77	33	54	7			

- Molecule 4 is a DNA chain called 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	J	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	M	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			
4	P	9	Total	C	N	O	P	0	0	0
			179	87	30	54	8			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	310	Total	O	0	0
			310	310		
5	B	352	Total	O	0	0
			352	352		
5	C	185	Total	O	0	0
			185	185		
5	D	177	Total	O	0	0
			177	177		
5	E	13	Total	O	0	0
			13	13		
5	F	16	Total	O	0	0
			16	16		
5	G	12	Total	O	0	0
			12	12		
5	H	20	Total	O	0	0
			20	20		
5	I	11	Total	O	0	0
			11	11		
5	J	9	Total	O	0	0
			9	9		
5	K	17	Total	O	0	0
			17	17		
5	L	5	Total	O	0	0
			5	5		

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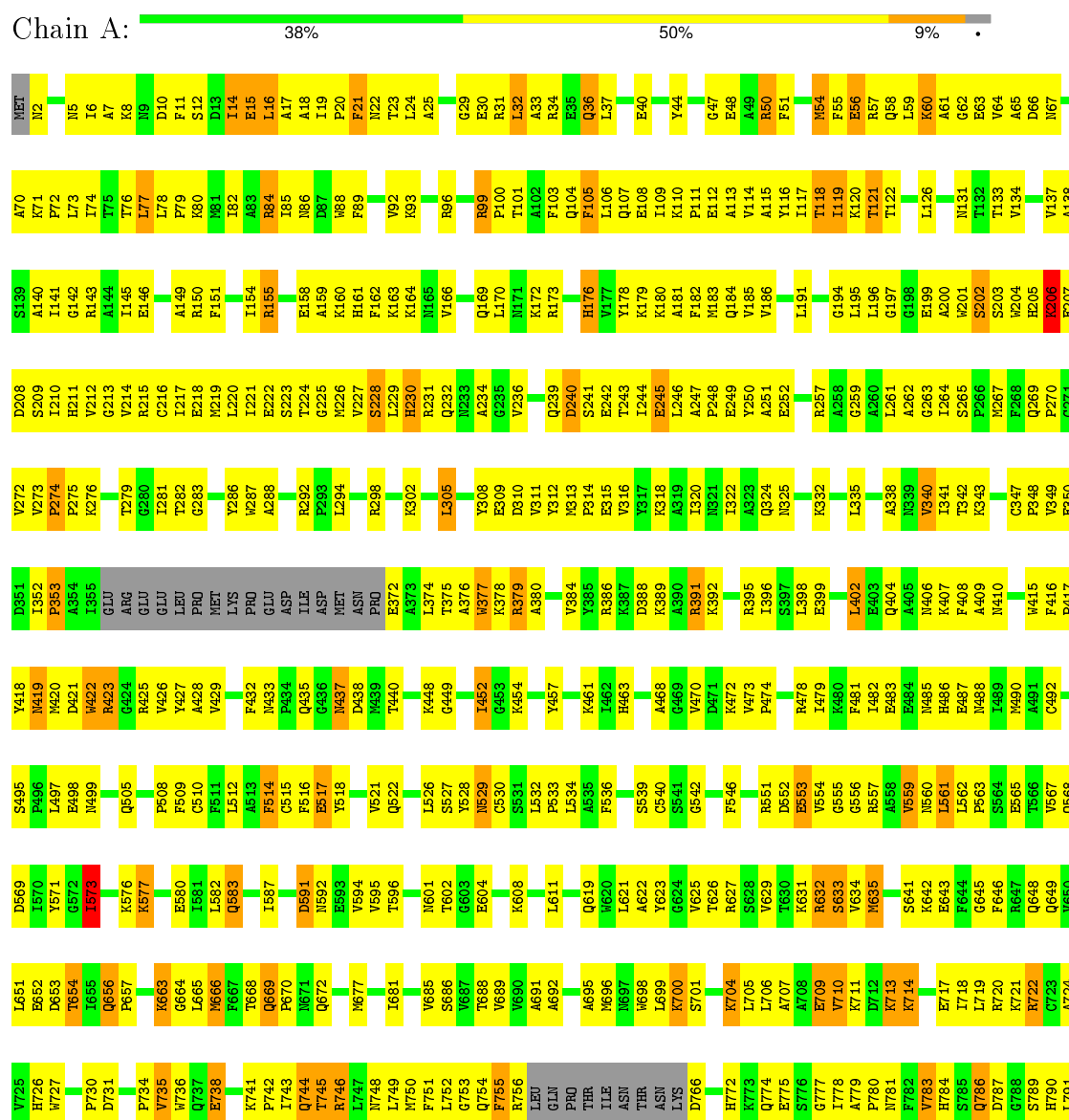
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	8	Total 8	O 8	0	0
5	N	12	Total 12	O 12	0	0
5	O	6	Total 6	O 6	0	0
5	P	9	Total 9	O 9	0	0

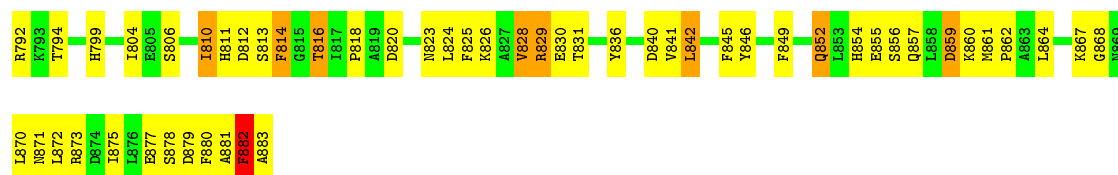
3 Residue-property plots

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

Note EDS was not executed.

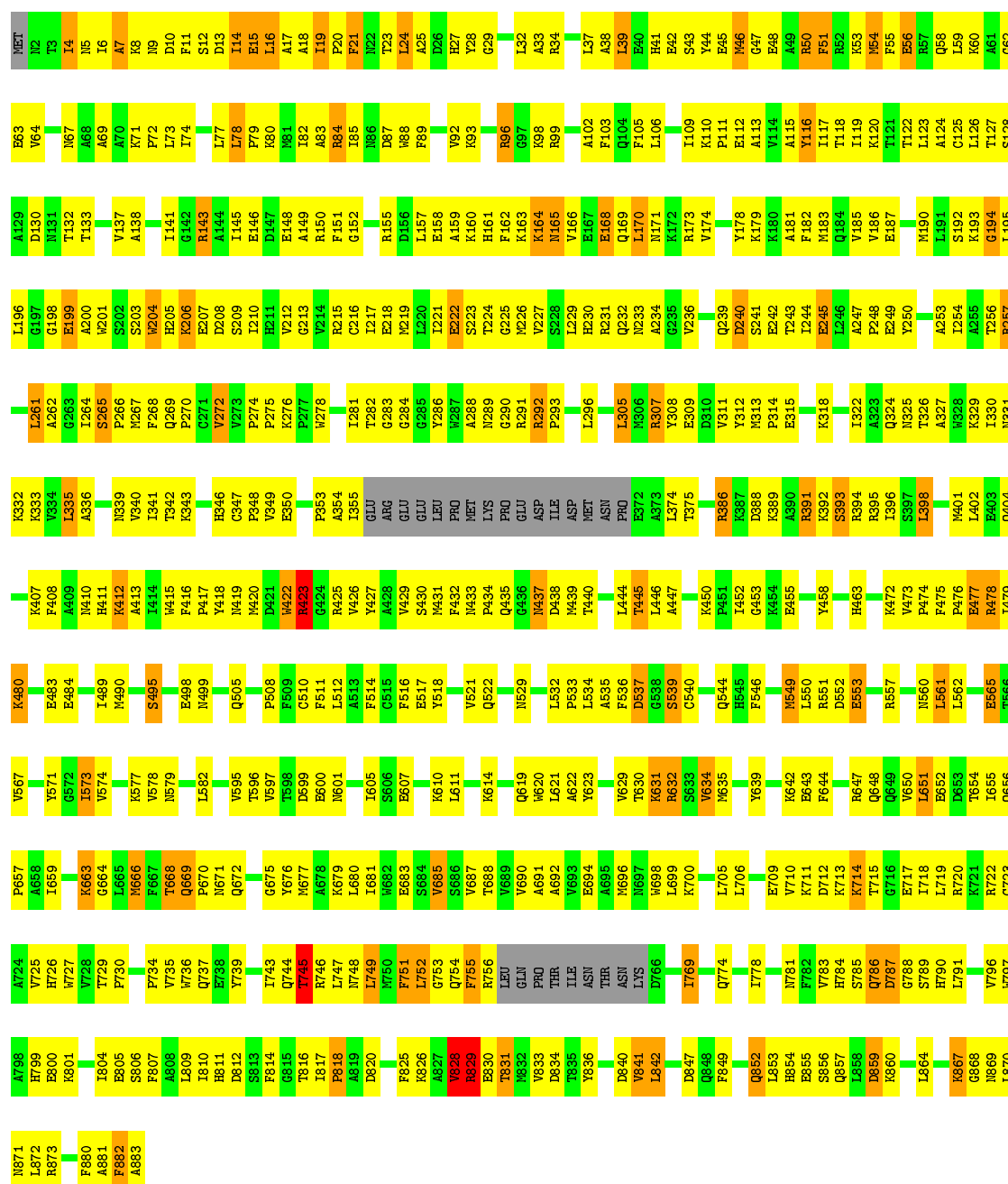
• Molecule 1: DNA-DIRECTED RNA POLYMERASE





• Molecule 1: DNA-DIRECTED RNA POLYMERASE

Chain B: 38% 49% 9%



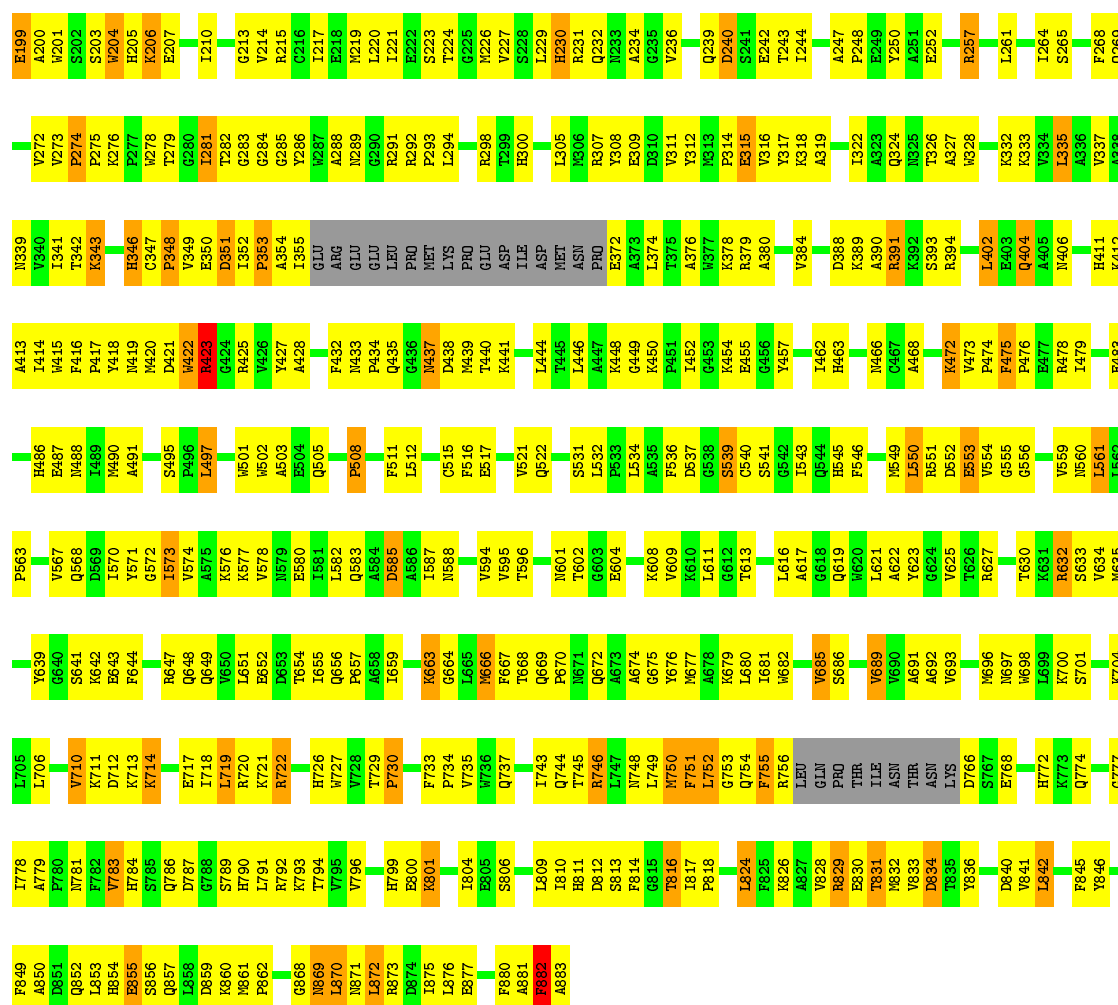
• Molecule 1: DNA-DIRECTED RNA POLYMERASE

Chain C: 39% 49% 8%



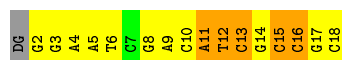
Chain D:  38% 51% 8% .



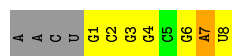




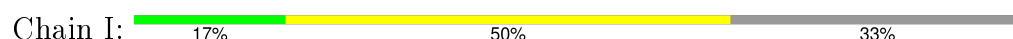
- Molecule 2: 5'-D(*GP*GP*GP*AP*AP*TP*CP*GP*AP*CP *AP*TP*CP*GP*CP*CP*GP*C)-3'



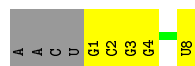
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



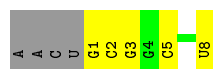
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



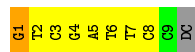
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'



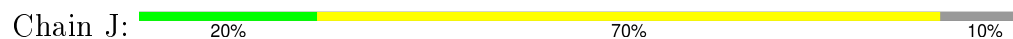
- Molecule 3: 5'-R(*AP*AP*CP*UP*GP*CP*GP*GP*CP*GP *AP*U)-3'




- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'



- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'




- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'

Chain M:  90% 10%

G1 T2 C3 G4 A5 T6 T7 C8 C9 DC

- Molecule 4: 5'-D(*GP*TP*CP*GP*AP*TP*TP*CP*CP*CP)-3'

Chain P:  80% 10% 10%

G1 T2 C3 G4 A5 T6 T7 C8 C9 DC

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.91 Å 84.97 Å 202.00 Å 90.36° 92.97° 109.94°	Depositor
Resolution (Å)	39.93 – 2.90	Depositor
% Data completeness (in resolution range)	98.0 (39.93-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	30948	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.89	9/6897 (0.1%)	0.85	5/9329 (0.1%)
1	B	0.93	2/6897 (0.0%)	0.87	9/9329 (0.1%)
1	C	0.64	0/6897	0.73	0/9329
1	D	0.58	0/6897	0.70	2/9329 (0.0%)
2	E	0.89	0/387	1.06	1/595 (0.2%)
2	H	0.94	0/412	1.03	1/634 (0.2%)
2	K	0.90	0/387	0.97	0/595
2	N	0.80	0/387	0.95	0/595
3	F	1.09	1/191 (0.5%)	0.85	0/297
3	I	0.94	0/191	0.81	0/297
3	L	0.81	0/191	0.79	0/297
3	O	0.61	0/191	0.74	0/297
4	G	0.88	0/199	0.84	0/305
4	J	0.77	0/199	0.93	0/305
4	M	0.68	0/199	0.85	0/305
4	P	0.74	0/199	1.05	0/305
All	All	0.78	12/30721 (0.0%)	0.81	18/42143 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	6
2	H	0	8
2	K	0	7
2	N	0	6
4	G	0	1
4	J	0	1
4	P	0	1
All	All	0	30

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	CYS	CB-SG	-8.42	1.68	1.82
1	A	573	ILE	CA-CB	7.10	1.71	1.54
1	A	654	THR	CA-CB	5.53	1.67	1.53
1	A	783	VAL	CA-CB	-5.40	1.43	1.54
3	F	7	A	C5-C6	-5.31	1.36	1.41
1	B	828	VAL	CB-CG2	-5.30	1.41	1.52
1	B	805	GLU	CB-CG	-5.28	1.42	1.52
1	A	340	VAL	CB-CG2	-5.16	1.42	1.52
1	A	492	CYS	CB-SG	-5.12	1.73	1.81
1	A	783	VAL	CB-CG2	-5.09	1.42	1.52
1	A	709	GLU	CG-CD	5.01	1.59	1.51
1	A	426	VAL	CB-CG2	-5.00	1.42	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	ASP	CB-CG-OD1	-8.22	110.90	118.30
1	A	557	ARG	NE-CZ-NH2	-8.21	116.20	120.30
1	A	829	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	B	549	MET	CB-CG-SD	-6.86	91.82	112.40
1	A	787	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	B	478	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	D	550	LEU	CA-CB-CG	-6.00	101.51	115.30
1	B	829	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	419	ASN	CB-CA-C	-5.92	98.56	110.40
1	A	510	CYS	CA-CB-SG	-5.90	103.38	114.00
2	H	11	DA	N9-C1'-C2'	-5.88	101.42	112.60
1	B	423	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	828	VAL	CB-CA-C	-5.44	101.07	111.40
1	B	24	LEU	CA-CB-CG	5.39	127.70	115.30
1	D	423	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	B	537	ASP	CB-CG-OD2	5.18	122.96	118.30
2	E	11	DA	N9-C1'-C2'	-5.13	102.86	112.60
1	B	78	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (30) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	11	DA	Sidechain
2	E	12	DT	Sidechain

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Mol	Chain	Res	Type	Group
2	E	13	DC	Sidechain
2	E	14	DG	Sidechain
2	E	15	DC	Sidechain
2	E	16	DC	Sidechain
4	G	1	DG	Sidechain
2	H	10	DC	Sidechain
2	H	11	DA	Sidechain
2	H	12	DT	Sidechain
2	H	13	DC	Sidechain
2	H	14	DG	Sidechain
2	H	15	DC	Sidechain
2	H	16	DC	Sidechain
2	H	9	DA	Sidechain
4	J	7	DT	Sidechain
2	K	10	DC	Sidechain
2	K	11	DA	Sidechain
2	K	12	DT	Sidechain
2	K	13	DC	Sidechain
2	K	14	DG	Sidechain
2	K	15	DC	Sidechain
2	K	16	DC	Sidechain
2	N	11	DA	Sidechain
2	N	12	DT	Sidechain
2	N	13	DC	Sidechain
2	N	14	DG	Sidechain
2	N	15	DC	Sidechain
2	N	16	DC	Sidechain
4	P	7	DT	Sidechain

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	6746	0	6708	722	0
1	B	6746	0	6708	733	0
1	C	6746	0	6708	680	0
1	D	6746	0	6708	653	0
2	E	345	0	191	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	367	0	202	28	0
2	K	345	0	191	38	0
2	N	345	0	191	21	0
3	F	171	0	89	7	0
3	I	171	0	89	11	0
3	L	171	0	89	9	0
3	O	171	0	89	5	0
4	G	179	0	104	14	0
4	J	179	0	104	8	0
4	M	179	0	104	18	0
4	P	179	0	104	11	0
5	A	310	0	0	102	0
5	B	352	0	0	133	0
5	C	185	0	0	79	0
5	D	177	0	0	105	0
5	E	13	0	0	2	0
5	F	16	0	0	2	0
5	G	12	0	0	5	0
5	H	20	0	0	6	0
5	I	11	0	0	4	0
5	J	9	0	0	4	0
5	K	17	0	0	7	0
5	L	5	0	0	2	0
5	M	8	0	0	1	0
5	N	12	0	0	4	0
5	O	6	0	0	0	0
5	P	9	0	0	3	0
All	All	30948	0	28379	2933	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 50.

All (2933) 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:668:THR:HG22	1:A:669:GLN:NE2	1.51	1.24
1:C:428:ALA:H	1:C:435:GLN:NE2	1.44	1.15
1:B:50:ARG:HG2	1:B:50:ARG:HH11	1.01	1.14
1:C:133:THR:HA	1:C:243:THR:HG22	1.28	1.10
1:A:120:LYS:HE3	1:A:752:LEU:HD21	1.31	1.10
1:B:806:SER:O	1:B:816:THR:HG22	1.51	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:839:CYS:HB3	5:C:2179:HOH:O	1.49	1.09
1:A:562:LEU:HD21	1:A:870:LEU:HD11	1.11	1.08
1:B:663:LYS:HG2	1:B:664:GLY:H	1.15	1.07
1:B:647:ARG:HH22	1:B:671:ASN:ND2	1.53	1.06
1:A:669:GLN:HG2	1:A:672:GLN:HE21	1.14	1.06
1:B:330:ILE:HG22	5:B:2150:HOH:O	1.54	1.06
1:B:194:GLY:HA3	5:B:2099:HOH:O	1.55	1.06
1:A:269:GLN:HE22	1:A:407:LYS:NZ	1.54	1.05
4:G:5:DA:H2''	4:G:6:DT:H71	1.34	1.05
1:B:157:LEU:HB3	5:B:2089:HOH:O	1.55	1.04
1:C:536:PHE:HB3	1:C:882:PHE:HB3	1.36	1.04
1:B:291:ARG:HB2	5:B:2136:HOH:O	1.56	1.04
1:C:333:LYS:HB3	1:C:516:PHE:CE2	1.93	1.04
1:B:5:ASN:HB3	5:B:2024:HOH:O	1.59	1.03
1:A:562:LEU:HD21	1:A:870:LEU:CD1	1.89	1.02
1:A:669:GLN:HG2	1:A:672:GLN:NE2	1.74	1.02
1:C:347:CYS:SG	1:C:350:GLU:HG2	2.00	1.01
1:D:536:PHE:HB3	1:D:882:PHE:HB3	1.42	1.01
1:A:668:THR:HG22	1:A:669:GLN:HE22	1.04	1.01
1:D:351:ASP:HB2	5:D:2099:HOH:O	1.58	1.01
1:B:720:ARG:HH11	1:B:720:ARG:HG2	1.26	1.01
1:A:536:PHE:HB3	1:A:882:PHE:HB3	1.43	1.00
1:D:281:ILE:HG22	1:D:282:THR:HG23	1.42	1.00
1:A:594:VAL:HB	5:A:2236:HOH:O	1.60	0.99
1:B:80:LYS:HD2	1:B:224:THR:HG22	1.45	0.98
1:C:307:ARG:HH11	1:C:307:ARG:HG3	1.24	0.98
1:D:298:ARG:HH21	1:D:427:TYR:HB2	1.26	0.98
1:A:711:LYS:NZ	1:A:711:LYS:HB2	1.75	0.98
1:A:720:ARG:HG2	1:A:720:ARG:HH11	1.29	0.98
1:A:196:LEU:HA	5:A:2085:HOH:O	1.64	0.98
1:D:829:ARG:O	1:D:833:VAL:HG23	1.62	0.97
1:A:632:ARG:NH1	1:A:632:ARG:HB2	1.79	0.97
1:B:423:ARG:HE	2:H:12:DT:H4'	1.29	0.97
1:D:663:LYS:HG2	1:D:664:GLY:H	1.27	0.97
1:D:348:PRO:HG3	5:D:2092:HOH:O	1.62	0.97
1:D:681:ILE:O	1:D:685:VAL:HG22	1.64	0.97
1:C:457:TYR:CE1	1:C:521:VAL:HG11	1.98	0.97
1:C:806:SER:O	1:C:816:THR:HG23	1.65	0.97
1:A:668:THR:CG2	1:A:669:GLN:HE22	1.79	0.96
1:B:573:ILE:HD12	1:B:573:ILE:C	1.85	0.96
1:B:290:GLY:HA2	5:B:2134:HOH:O	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:TYR:HA	1:B:666:MET:HE2	1.47	0.96
1:A:92:VAL:HG12	1:A:99:ARG:HG3	1.44	0.96
1:A:99:ARG:HG2	1:A:99:ARG:HH11	1.27	0.95
1:D:275:PRO:HD2	5:D:2086:HOH:O	1.66	0.95
1:B:748:ASN:HD21	1:B:751:PHE:H	1.09	0.95
1:C:45:GLU:HG2	5:C:2038:HOH:O	1.65	0.95
1:A:113:ALA:O	1:A:117:ILE:HG13	1.64	0.95
1:A:93:LYS:HA	1:A:99:ARG:NH2	1.80	0.95
1:A:704:LYS:HE2	4:G:5:DA:OP1	1.66	0.95
1:A:342:THR:HG22	1:A:348:PRO:HG2	1.47	0.95
1:C:532:LEU:HD23	1:C:534:LEU:HD23	1.49	0.95
1:A:711:LYS:HB2	1:A:711:LYS:HZ3	1.25	0.94
1:C:422:TRP:HB3	5:C:2101:HOH:O	1.66	0.94
1:A:202:SER:HB2	5:A:2088:HOH:O	1.64	0.94
1:B:58:GLN:HG3	1:B:67:ASN:HD22	1.30	0.93
1:A:428:ALA:H	1:A:435:GLN:HE21	1.15	0.93
1:B:532:LEU:HD12	1:B:533:PRO:HD2	1.50	0.93
1:A:746:ARG:NH1	1:A:746:ARG:HB3	1.83	0.92
1:D:272:VAL:HA	5:D:2115:HOH:O	1.67	0.92
1:B:158:GLU:HG2	1:B:195:LEU:HD22	1.50	0.92
1:C:423:ARG:NH2	1:C:784:HIS:ND1	2.18	0.92
1:A:428:ALA:H	1:A:435:GLN:NE2	1.68	0.92
1:C:80:LYS:HD3	1:C:224:THR:HG22	1.52	0.92
1:C:428:ALA:H	1:C:435:GLN:HE22	1.10	0.91
1:B:59:LEU:HA	1:B:64:VAL:HG22	1.52	0.91
1:B:744:GLN:HA	1:B:756:ARG:HE	1.31	0.91
1:B:854:HIS:CD2	1:B:856:SER:H	1.88	0.91
1:B:423:ARG:NE	2:H:12:DT:H4'	1.84	0.91
1:A:751:PHE:HB3	1:A:752:LEU:HD12	1.52	0.91
1:D:560:ASN:O	1:D:881:ALA:HB2	1.70	0.91
1:C:485:ASN:HD22	1:C:488:ASN:HD22	1.09	0.91
1:A:562:LEU:CD2	1:A:870:LEU:HD11	2.00	0.91
1:D:806:SER:O	1:D:816:THR:HG23	1.72	0.90
2:K:2:DG:H2''	2:K:3:DG:H8	1.35	0.90
1:D:153:ARG:HH22	1:D:201:TRP:HE1	1.20	0.90
1:B:236:VAL:HG21	1:B:239:GLN:HE21	1.34	0.90
1:C:340:VAL:O	1:C:343:LYS:HG2	1.69	0.90
1:B:647:ARG:HH22	1:B:671:ASN:HD22	1.01	0.89
1:A:641:SER:HA	2:E:10:DC:H5'	1.53	0.89
1:D:155:ARG:HA	1:D:163:LYS:HD3	1.54	0.89
1:D:794:THR:OG1	1:D:831:THR:HG21	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:633:SER:HA	1:D:649:GLN:HE22	1.37	0.89
2:E:2:DG:H2"	2:E:3:DG:N7	1.87	0.89
1:B:133:THR:HA	1:B:243:THR:HG22	1.54	0.89
1:A:109:ILE:HD11	1:A:149:ALA:HB2	1.54	0.89
1:B:748:ASN:ND2	1:B:751:PHE:H	1.71	0.89
1:A:155:ARG:HB3	1:A:155:ARG:HH11	1.35	0.89
1:C:141:ILE:O	1:C:145:ILE:HG12	1.71	0.89
1:A:208:ASP:O	1:A:212:VAL:HG23	1.71	0.89
1:A:269:GLN:HE22	1:A:407:LYS:HZ3	1.15	0.89
1:C:16:LEU:H	1:C:16:LEU:HD23	1.38	0.88
1:C:147:ASP:HB3	1:C:750:MET:HE1	1.52	0.88
1:A:169:GLN:O	1:A:173:ARG:HG2	1.72	0.88
1:B:244:ILE:HB	5:B:2084:HOH:O	1.74	0.88
1:C:14:ILE:HG23	1:C:288:ALA:HB1	1.54	0.88
1:B:438:ASP:OD2	1:B:508:PRO:HD2	1.73	0.88
1:A:140:ALA:HA	5:A:2071:HOH:O	1.72	0.88
1:A:398:LEU:HD23	1:A:398:LEU:C	1.95	0.88
1:C:560:ASN:O	1:C:881:ALA:HB2	1.72	0.87
1:C:374:LEU:HD12	1:C:374:LEU:H	1.39	0.87
1:C:551:ARG:CG	1:C:551:ARG:HH11	1.88	0.87
1:D:751:PHE:HB3	1:D:752:LEU:HD12	1.54	0.87
1:A:155:ARG:HB3	1:A:155:ARG:NH1	1.88	0.87
1:B:560:ASN:O	1:B:881:ALA:HB2	1.73	0.87
1:C:720:ARG:HH11	1:C:720:ARG:HG2	1.40	0.87
1:B:18:ALA:HA	5:B:2040:HOH:O	1.74	0.87
2:K:3:DG:H2"	2:K:4:DA:C8	2.08	0.87
1:C:281:ILE:HG22	1:C:282:THR:HG23	1.54	0.87
1:C:549:MET:HB3	1:C:836:TYR:HE1	1.40	0.86
1:C:154:ILE:HG23	1:C:190:MET:HE1	1.54	0.86
1:B:607:GLU:HG2	5:B:2274:HOH:O	1.73	0.86
1:D:352:ILE:HA	5:D:2098:HOH:O	1.76	0.86
1:D:231:ARG:HD2	1:D:240:ASP:OD1	1.76	0.86
1:D:315:GLU:HA	1:D:315:GLU:OE2	1.72	0.86
1:A:100:PRO:HG2	1:A:103:PHE:HB2	1.56	0.86
1:C:870:LEU:HD23	1:C:872:LEU:HD23	1.58	0.86
1:C:481:PHE:HB2	5:C:2113:HOH:O	1.74	0.85
1:B:347:CYS:HB3	1:B:350:GLU:HG3	1.56	0.85
1:C:169:GLN:HB3	5:C:2062:HOH:O	1.74	0.85
1:B:546:PHE:HD1	1:B:549:MET:HE3	1.39	0.85
1:D:43:SER:HA	1:D:46:MET:HE2	1.56	0.85
1:B:790:HIS:CD2	1:B:831:THR:CG2	2.59	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HA	1:A:64:VAL:HG22	1.59	0.85
1:A:730:PRO:HD3	1:A:786:GLN:HE22	1.41	0.85
1:C:164:LYS:N	1:C:164:LYS:HE2	1.90	0.85
1:A:84:ARG:HG3	1:A:223:SER:HB3	1.55	0.85
1:B:146:GLU:OE2	1:B:201:TRP:HB3	1.77	0.85
1:B:59:LEU:HD23	1:B:64:VAL:HG21	1.59	0.84
2:K:3:DG:H3'	5:K:2007:HOH:O	1.76	0.84
1:A:195:LEU:HD11	5:A:2076:HOH:O	1.76	0.84
1:B:715:THR:HB	5:B:2302:HOH:O	1.75	0.84
1:B:208:ASP:O	1:B:212:VAL:HG23	1.77	0.84
1:B:152:GLY:HA2	5:B:2088:HOH:O	1.75	0.84
1:C:849:PHE:HD2	1:C:853:LEU:HD21	1.41	0.84
1:B:43:SER:OG	1:B:269:GLN:HG3	1.76	0.84
1:C:826:LYS:O	1:C:830:GLU:HG3	1.77	0.84
1:A:854:HIS:CD2	1:A:856:SER:H	1.96	0.84
1:B:249:GLU:HB2	5:B:2120:HOH:O	1.76	0.84
1:D:146:GLU:OE2	1:D:201:TRP:HB3	1.78	0.84
1:B:790:HIS:CD2	1:B:831:THR:HG23	2.13	0.84
1:B:579:ASN:HA	1:B:582:LEU:HD12	1.57	0.84
1:A:126:LEU:HB3	5:A:2070:HOH:O	1.76	0.84
1:D:632:ARG:HG2	5:N:2010:HOH:O	1.77	0.84
1:C:428:ALA:N	1:C:435:GLN:NE2	2.26	0.84
1:A:560:ASN:O	1:A:881:ALA:HB2	1.78	0.84
1:D:438:ASP:OD2	1:D:508:PRO:HG2	1.78	0.84
1:B:332:LYS:HG2	5:B:2152:HOH:O	1.77	0.83
1:D:729:THR:HG23	1:D:733:PHE:O	1.78	0.83
1:B:123:LEU:HD11	5:B:2082:HOH:O	1.78	0.83
1:A:92:VAL:CG1	1:A:99:ARG:HG3	2.08	0.83
1:B:120:LYS:HD2	1:B:752:LEU:HD21	1.58	0.83
1:A:143:ARG:HB3	5:A:2071:HOH:O	1.77	0.83
1:B:113:ALA:O	1:B:117:ILE:HG13	1.77	0.83
1:D:153:ARG:NH2	1:D:201:TRP:HE1	1.76	0.83
1:A:24:LEU:HD21	1:A:287:TRP:CD2	2.14	0.83
1:D:582:LEU:HB3	1:D:621:LEU:HD21	1.61	0.83
1:B:281:ILE:HG22	1:B:282:THR:HG23	1.58	0.83
1:A:724:ALA:HB2	1:A:738:GLU:HG3	1.61	0.83
1:B:50:ARG:HG2	1:B:50:ARG:NH1	1.74	0.83
1:C:485:ASN:ND2	1:C:488:ASN:HD22	1.76	0.83
1:D:347:CYS:SG	1:D:350:GLU:HG2	2.19	0.83
1:D:11:PHE:CZ	1:D:44:TYR:HB3	2.13	0.82
1:A:560:ASN:HD21	1:A:567:VAL:HG13	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:SER:CA	2:E:10:DC:H5'	2.09	0.82
1:A:347:CYS:HB3	1:A:350:GLU:HG3	1.60	0.82
1:A:398:LEU:HD23	1:A:398:LEU:O	1.80	0.82
4:M:1:DG:H1'	4:M:2:DT:H71	1.60	0.82
1:A:632:ARG:HD3	5:A:2249:HOH:O	1.78	0.82
1:C:423:ARG:HE	1:C:781:ASN:ND2	1.78	0.82
1:A:744:GLN:O	1:A:745:THR:HG23	1.79	0.82
1:D:585:ASP:OD2	1:D:613:THR:HB	1.79	0.82
1:B:169:GLN:O	1:B:173:ARG:HG2	1.80	0.82
1:D:587:ILE:HG13	5:D:2136:HOH:O	1.80	0.82
3:L:1:G:H5''	5:L:2001:HOH:O	1.78	0.82
1:A:705:LEU:HD22	1:A:857:GLN:HB2	1.62	0.82
1:B:769:ILE:HG12	5:B:2306:HOH:O	1.80	0.82
1:D:292:ARG:HG3	1:D:292:ARG:O	1.77	0.82
1:B:329:LYS:HD3	1:B:447:ALA:HA	1.60	0.82
1:A:425:ARG:HD3	1:A:811:HIS:CD2	2.14	0.82
1:A:100:PRO:HB3	5:A:2064:HOH:O	1.78	0.81
1:D:573:ILE:HA	1:D:576:LYS:HD3	1.62	0.81
1:D:486:HIS:O	1:D:490:MET:HG2	1.80	0.81
1:D:711:LYS:HG2	1:D:718:ILE:HA	1.62	0.81
1:A:217:ILE:O	1:A:221:ILE:HG13	1.80	0.81
1:A:89:PHE:HA	1:A:103:PHE:HE1	1.45	0.81
1:C:769:ILE:HG21	5:C:2154:HOH:O	1.78	0.81
1:D:155:ARG:HB2	1:D:163:LYS:HE2	1.63	0.81
1:D:116:TYR:OH	1:D:752:LEU:HD22	1.79	0.81
1:A:226:MET:HG3	1:A:250:TYR:HD1	1.45	0.81
1:B:751:PHE:HB3	1:B:752:LEU:HD12	1.61	0.81
1:B:401:MET:HE3	1:B:401:MET:HA	1.61	0.81
1:A:18:ALA:O	1:A:19:ILE:HG12	1.80	0.81
1:D:339:ASN:O	1:D:343:LYS:HD2	1.81	0.81
1:B:236:VAL:HG21	1:B:239:GLN:NE2	1.94	0.81
1:A:379:ARG:HA	5:A:2149:HOH:O	1.80	0.81
1:B:16:LEU:H	1:B:16:LEU:HD23	1.46	0.81
1:B:206:LYS:O	1:B:210:ILE:HG12	1.81	0.81
1:B:647:ARG:NH2	1:B:671:ASN:ND2	2.29	0.80
1:C:751:PHE:HB3	1:C:752:LEU:HD12	1.62	0.80
1:D:206:LYS:O	1:D:210:ILE:HG12	1.81	0.80
1:C:530:CYS:SG	1:C:818:PRO:HG2	2.20	0.80
1:D:744:GLN:HA	1:D:756:ARG:HH11	1.45	0.80
1:A:120:LYS:HE3	1:A:752:LEU:CD2	2.10	0.80
1:B:546:PHE:CD1	1:B:549:MET:HE3	2.16	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:HG2	1:A:34:ARG:CZ	2.09	0.80
1:D:332:LYS:HE2	5:D:2011:HOH:O	1.80	0.80
1:D:648:GLN:O	1:D:652:GLU:HG2	1.82	0.80
1:D:91:GLU:O	1:D:95:LYS:HD2	1.82	0.80
1:C:11:PHE:HB2	5:C:2018:HOH:O	1.80	0.80
1:C:711:LYS:NZ	1:C:711:LYS:HB2	1.96	0.80
1:A:315:GLU:OE2	1:A:318:LYS:HD3	1.82	0.80
1:D:154:ILE:HG23	1:D:190:MET:HE1	1.63	0.80
1:B:59:LEU:HD23	1:B:64:VAL:CG2	2.12	0.80
1:C:229:LEU:HD12	1:C:243:THR:O	1.82	0.80
1:A:421:ASP:OD2	1:A:427:TYR:HE1	1.65	0.80
1:B:730:PRO:CD	1:B:786:GLN:HE22	1.95	0.80
1:C:551:ARG:HG3	1:C:551:ARG:HH11	1.45	0.80
1:B:7:ALA:HB3	5:B:2024:HOH:O	1.81	0.79
2:H:6:DT:H1'	5:H:2008:HOH:O	1.81	0.79
2:E:8:DG:H5'	5:E:2005:HOH:O	1.82	0.79
1:A:134:VAL:HB	1:A:244:ILE:HD11	1.64	0.79
1:C:452:ILE:HD11	1:C:457:TYR:HA	1.64	0.79
1:A:746:ARG:HH11	1:A:746:ARG:HB3	1.47	0.79
1:C:50:ARG:HH11	1:C:50:ARG:HG2	1.45	0.79
1:B:711:LYS:HA	1:B:719:LEU:HD13	1.64	0.79
1:C:181:ALA:O	1:C:185:VAL:HG22	1.82	0.79
1:C:428:ALA:N	1:C:435:GLN:HE22	1.79	0.79
1:D:450:LYS:HD3	5:D:2119:HOH:O	1.82	0.79
1:A:155:ARG:O	1:A:155:ARG:HD2	1.83	0.79
1:B:714:LYS:NZ	1:B:714:LYS:HA	1.98	0.79
1:C:468:ALA:HB2	1:C:511:PHE:CE1	2.18	0.79
1:A:804:ILE:HG23	1:A:816:THR:HG21	1.63	0.79
1:D:570:ILE:O	1:D:574:VAL:HG23	1.82	0.79
1:D:84:ARG:HD3	1:D:84:ARG:C	2.03	0.79
1:A:608:LYS:HG2	5:A:2240:HOH:O	1.81	0.79
1:C:147:ASP:HB3	1:C:750:MET:CE	2.13	0.78
1:A:495:SER:HB3	1:A:498:GLU:HG3	1.65	0.78
1:B:829:ARG:HH11	1:B:829:ARG:HG3	1.47	0.78
1:C:455:GLU:HA	5:C:2110:HOH:O	1.81	0.78
1:C:19:ILE:HG21	5:C:2027:HOH:O	1.83	0.78
1:B:790:HIS:HD2	1:B:831:THR:HG23	1.48	0.78
1:C:663:LYS:HG2	1:C:664:GLY:H	1.47	0.78
1:B:489:ILE:HG21	1:B:518:TYR:CD1	2.19	0.78
1:A:648:GLN:NE2	1:A:652:GLU:OE1	2.16	0.78
1:B:84:ARG:HD2	1:B:219:MET:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:PHE:CZ	1:A:261:LEU:HD23	2.19	0.78
1:D:109:ILE:HD12	1:D:109:ILE:H	1.49	0.78
1:C:84:ARG:NE	1:C:222:GLU:OE1	2.16	0.77
1:B:663:LYS:HG2	1:B:664:GLY:N	1.97	0.77
1:A:423:ARG:HE	1:A:781:ASN:HD22	1.31	0.77
1:C:236:VAL:HB	1:C:239:GLN:HB2	1.66	0.77
2:K:2:DG:H2''	2:K:3:DG:C8	2.19	0.77
1:D:497:LEU:HD12	5:D:2125:HOH:O	1.84	0.77
1:A:281:ILE:HG22	1:A:282:THR:HG23	1.66	0.77
1:A:372:GLU:HG3	5:A:2014:HOH:O	1.83	0.77
1:B:537:ASP:O	1:B:882:PHE:HB2	1.84	0.77
1:D:355:ILE:HA	5:D:2102:HOH:O	1.82	0.77
1:D:82:ILE:HD13	1:D:112:GLU:OE2	1.84	0.77
1:C:871:ASN:HA	5:C:2183:HOH:O	1.82	0.77
1:B:257:ARG:HG2	5:B:2125:HOH:O	1.85	0.77
1:D:219:MET:HE2	5:D:2030:HOH:O	1.85	0.77
1:D:572:GLY:O	1:D:576:LYS:HG3	1.85	0.77
1:D:103:PHE:HB2	5:D:2029:HOH:O	1.83	0.77
2:N:5:DA:H1'	2:N:6:DT:H5'	1.67	0.77
1:A:88:TRP:CH2	1:A:100:PRO:HG3	2.20	0.77
1:C:210:ILE:O	1:C:214:VAL:HG23	1.85	0.76
1:B:96:ARG:HG3	5:B:2031:HOH:O	1.85	0.76
1:A:14:ILE:HG23	1:A:288:ALA:HB1	1.67	0.76
4:M:4:DG:H4'	4:M:5:DA:OP1	1.84	0.76
1:D:744:GLN:HG2	1:D:756:ARG:HD3	1.67	0.76
1:A:122:THR:HG22	1:A:126:LEU:HD12	1.66	0.76
1:A:88:TRP:HH2	1:A:100:PRO:HG3	1.50	0.76
1:B:150:ARG:HD3	1:B:151:PHE:CE2	2.20	0.76
1:B:151:PHE:CD1	1:B:183:MET:HB3	2.20	0.76
1:B:137:VAL:HG12	1:B:141:ILE:HD11	1.68	0.76
1:D:16:LEU:HD13	1:D:38:ALA:HB2	1.68	0.76
1:B:50:ARG:HH11	1:B:50:ARG:CG	1.89	0.76
1:A:632:ARG:CZ	1:A:632:ARG:HB2	2.15	0.76
1:B:159:ALA:HB1	1:B:163:LYS:N	1.99	0.76
1:D:16:LEU:HA	1:D:37:LEU:HD12	1.67	0.76
1:D:853:LEU:HD22	1:D:857:GLN:HG3	1.66	0.76
1:A:197:GLY:HA2	5:A:2087:HOH:O	1.84	0.76
1:B:853:LEU:HD22	1:B:857:GLN:HG3	1.66	0.76
1:A:217:ILE:HG22	1:A:221:ILE:HD11	1.68	0.76
1:A:281:ILE:HD11	1:A:308:TYR:HB3	1.67	0.76
1:D:34:ARG:HB3	5:D:2022:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:MET:SD	5:A:2060:HOH:O	2.43	0.76
1:B:692:ALA:O	1:B:696:MET:HG3	1.85	0.76
1:D:829:ARG:HG3	1:D:829:ARG:HH11	1.50	0.76
1:C:231:ARG:HG2	1:C:234:ALA:HB2	1.65	0.75
1:C:794:THR:OG1	1:C:831:THR:HG21	1.86	0.75
1:B:748:ASN:HD21	1:B:751:PHE:N	1.83	0.75
1:A:143:ARG:HA	5:A:2073:HOH:O	1.86	0.75
1:A:724:ALA:CB	1:A:738:GLU:HG3	2.16	0.75
1:A:720:ARG:HG2	1:A:720:ARG:NH1	2.02	0.75
1:A:150:ARG:NH1	5:A:2075:HOH:O	2.20	0.75
5:C:2147:HOH:O	4:M:1:DG:H4'	1.85	0.75
1:C:738:GLU:OE2	5:C:2158:HOH:O	2.03	0.75
1:D:314:PRO:HA	5:D:2084:HOH:O	1.86	0.75
1:B:79:PRO:HB3	5:B:2071:HOH:O	1.85	0.75
1:B:309:GLU:HG2	5:B:2142:HOH:O	1.86	0.75
1:C:437:ASN:H	1:C:437:ASN:HD22	1.34	0.75
1:B:50:ARG:NH2	1:B:267:MET:HG2	2.00	0.75
1:D:307:ARG:HD2	5:D:2081:HOH:O	1.85	0.75
1:D:298:ARG:NH2	1:D:427:TYR:HB2	2.01	0.75
1:B:236:VAL:HB	1:B:239:GLN:HB2	1.67	0.75
2:E:4:DA:H2''	2:E:5:DA:C8	2.21	0.75
1:A:84:ARG:HE	1:A:222:GLU:HB2	1.52	0.75
1:A:882:PHE:CD1	1:A:882:PHE:N	2.52	0.75
1:A:325:ASN:HB3	5:A:2134:HOH:O	1.86	0.75
1:D:126:LEU:HD21	1:D:244:ILE:HG22	1.69	0.75
1:A:60:LYS:HG2	1:A:60:LYS:O	1.84	0.75
1:A:669:GLN:HE21	1:A:669:GLN:N	1.85	0.75
1:D:479:ILE:O	1:D:483:GLU:HG3	1.87	0.75
1:A:452:ILE:HD12	1:A:818:PRO:HB2	1.68	0.75
1:C:78:LEU:O	1:C:82:ILE:HG13	1.87	0.74
1:B:679:LYS:HG2	5:B:2299:HOH:O	1.86	0.74
1:D:402:LEU:HG	1:D:439:MET:HE1	1.69	0.74
1:A:592:ASN:OD1	1:A:611:LEU:HA	1.87	0.74
1:B:473:VAL:HG11	1:B:477:GLU:HB3	1.69	0.74
1:A:631:LYS:O	1:A:635:MET:HG2	1.87	0.74
1:C:422:TRP:HE3	5:C:2101:HOH:O	1.69	0.74
1:C:549:MET:HB3	1:C:836:TYR:CE1	2.23	0.74
1:B:106:LEU:HD21	1:B:212:VAL:CG1	2.17	0.74
1:A:269:GLN:HA	5:A:2113:HOH:O	1.85	0.74
1:B:882:PHE:O	1:B:883:ALA:HB3	1.87	0.74
1:B:712:ASP:HB3	5:B:2302:HOH:O	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:CYS:SG	1:A:350:GLU:HG2	2.28	0.74
1:D:355:ILE:HG13	5:D:2104:HOH:O	1.87	0.74
1:A:591:ASP:OD2	1:A:591:ASP:N	2.20	0.74
1:C:59:LEU:HA	1:C:64:VAL:HG22	1.69	0.74
4:G:3:DC:H2"	4:G:4:DG:OP2	1.85	0.74
1:A:109:ILE:CD1	1:A:149:ALA:HB2	2.17	0.74
1:B:15:GLU:OE2	1:B:19:ILE:HG12	1.87	0.74
1:C:171:ASN:HB3	3:L:2:C:H4'	1.69	0.74
1:B:43:SER:HG	1:B:269:GLN:HG3	1.49	0.74
1:C:557:ARG:HD2	5:C:2129:HOH:O	1.87	0.74
1:C:423:ARG:HE	1:C:781:ASN:HD22	1.35	0.74
4:P:1:DG:N2	5:P:2001:HOH:O	2.20	0.74
1:B:234:ALA:HB1	5:B:2112:HOH:O	1.85	0.74
1:A:269:GLN:NE2	1:A:407:LYS:HZ3	1.86	0.74
1:B:119:ILE:HG13	5:B:2069:HOH:O	1.88	0.74
1:A:206:LYS:HD3	1:A:206:LYS:H	1.53	0.74
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.53	0.74
1:D:11:PHE:CE1	1:D:44:TYR:HB3	2.23	0.74
1:A:665:LEU:HG	5:A:2262:HOH:O	1.86	0.74
1:B:551:ARG:HG2	5:B:2240:HOH:O	1.87	0.74
1:B:15:GLU:HA	5:B:2034:HOH:O	1.88	0.73
1:A:663:LYS:CG	1:A:664:GLY:H	2.01	0.73
1:C:218:GLU:HG2	5:C:2070:HOH:O	1.88	0.73
1:D:810:ILE:HB	1:D:813:SER:HB3	1.69	0.73
1:B:744:GLN:CA	1:B:756:ARG:HE	2.01	0.73
1:A:206:LYS:O	1:A:210:ILE:HG12	1.88	0.73
1:C:711:LYS:CG	1:C:718:ILE:HA	2.17	0.73
1:C:303:LYS:CE	1:C:740:LYS:HZ1	2.01	0.73
1:C:88:TRP:O	1:C:92:VAL:HG23	1.89	0.73
1:A:269:GLN:NE2	1:A:407:LYS:NZ	2.33	0.73
1:D:272:VAL:HB	5:D:2021:HOH:O	1.87	0.73
1:B:407:LYS:NZ	5:B:2175:HOH:O	2.18	0.73
1:D:164:LYS:HE2	1:D:164:LYS:HA	1.69	0.73
1:C:134:VAL:HG12	1:C:242:GLU:O	1.89	0.73
1:B:215:ARG:C	1:B:219:MET:HE2	2.09	0.73
1:A:84:ARG:HE	1:A:222:GLU:CB	2.02	0.73
1:B:796:VAL:O	1:B:800:GLU:HG3	1.87	0.73
1:B:726:HIS:HB2	1:B:736:TRP:CD1	2.23	0.73
1:B:158:GLU:HA	1:B:195:LEU:HD22	1.68	0.73
1:A:126:LEU:HD22	1:A:246:LEU:HB2	1.71	0.73
1:C:199:GLU:HG2	1:C:201:TRP:HD1	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:18:DC:OP2	5:K:2015:HOH:O	2.07	0.73
1:B:748:ASN:ND2	1:B:752:LEU:H	1.86	0.73
1:A:698:TRP:HE3	1:A:699:LEU:HD23	1.53	0.73
1:B:422:TRP:HB3	5:B:2182:HOH:O	1.88	0.73
1:B:423:ARG:NH2	1:B:784:HIS:ND1	2.35	0.73
1:D:573:ILE:HA	1:D:576:LYS:CD	2.19	0.73
1:C:374:LEU:H	1:C:374:LEU:CD1	2.02	0.73
1:C:109:ILE:HD11	1:C:149:ALA:HB2	1.68	0.73
1:B:681:ILE:O	1:B:685:VAL:HG13	1.89	0.73
1:D:176:HIS:HA	5:D:2052:HOH:O	1.89	0.73
1:B:480:LYS:O	1:B:484:GLU:HG3	1.89	0.73
1:C:882:PHE:HD1	1:C:882:PHE:H	1.34	0.73
1:A:51:PHE:HZ	1:A:261:LEU:HD23	1.53	0.73
1:D:882:PHE:HD1	1:D:882:PHE:H	1.36	0.72
1:B:744:GLN:HA	1:B:756:ARG:NE	2.03	0.72
1:C:668:THR:HG22	1:C:669:GLN:OE1	1.88	0.72
1:C:597:VAL:HB	5:C:2141:HOH:O	1.87	0.72
1:B:829:ARG:HH11	1:B:829:ARG:CG	2.01	0.72
1:C:727:TRP:HA	1:C:848:GLN:HE21	1.53	0.72
1:B:250:TYR:HD2	5:B:2121:HOH:O	1.71	0.72
1:B:347:CYS:CB	1:B:350:GLU:HG3	2.18	0.72
1:C:711:LYS:HG2	1:C:718:ILE:HA	1.69	0.72
1:B:596:THR:O	5:B:2264:HOH:O	2.07	0.72
4:J:4:DG:H2''	4:J:5:DA:C8	2.23	0.72
4:J:5:DA:H3'	5:J:2003:HOH:O	1.89	0.72
1:B:73:LEU:HD11	1:B:254:ILE:HG13	1.70	0.72
1:C:120:LYS:HZ3	1:C:752:LEU:HD11	1.54	0.72
1:D:109:ILE:HG21	5:D:2041:HOH:O	1.89	0.72
1:C:437:ASN:ND2	1:C:440:THR:H	1.86	0.72
1:D:378:LYS:HD2	5:D:2007:HOH:O	1.88	0.72
1:D:45:GLU:HG2	5:D:2024:HOH:O	1.88	0.72
1:B:354:ALA:HB2	5:B:2221:HOH:O	1.88	0.72
1:A:349:VAL:O	1:A:349:VAL:HG12	1.87	0.72
1:B:546:PHE:HD1	1:B:549:MET:CE	2.02	0.72
1:B:730:PRO:HD3	5:B:2308:HOH:O	1.89	0.72
1:A:134:VAL:CB	1:A:244:ILE:HD11	2.19	0.72
1:C:574:VAL:O	1:C:578:VAL:HG23	1.90	0.72
1:D:300:HIS:HB2	5:D:2078:HOH:O	1.90	0.72
1:B:14:ILE:HG23	1:B:288:ALA:HB1	1.72	0.72
4:G:5:DA:H2''	4:G:6:DT:C7	2.17	0.72
4:P:4:DG:H2''	4:P:5:DA:C8	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:778:ILE:HG23	1:D:779:ALA:N	2.04	0.72
1:D:80:LYS:HD3	1:D:224:THR:HG22	1.72	0.72
1:B:882:PHE:O	1:B:883:ALA:CB	2.37	0.72
1:D:582:LEU:HD11	1:D:625:VAL:HG21	1.70	0.72
1:D:347:CYS:HB3	1:D:350:GLU:HG2	1.70	0.72
1:A:58:GLN:OE1	1:A:67:ASN:HB2	1.89	0.72
1:C:486:HIS:CE1	1:C:490:MET:HG3	2.25	0.72
1:C:630:THR:O	1:C:634:VAL:HG12	1.89	0.72
1:B:165:ASN:HA	5:B:2093:HOH:O	1.89	0.72
1:C:96:ARG:HH11	1:C:96:ARG:HG2	1.55	0.72
1:C:333:LYS:HB3	1:C:516:PHE:CD2	2.24	0.71
1:B:720:ARG:NH1	1:B:720:ARG:HG2	2.01	0.71
1:A:745:THR:H	1:A:756:ARG:HD3	1.55	0.71
1:A:84:ARG:HB3	5:A:2060:HOH:O	1.88	0.71
1:A:882:PHE:O	1:A:883:ALA:HB3	1.90	0.71
1:C:485:ASN:HD22	1:C:488:ASN:ND2	1.86	0.71
1:A:324:GLN:HE21	1:A:417:PRO:HA	1.55	0.71
1:C:737:GLN:HE22	1:C:778:ILE:HA	1.54	0.71
1:A:568:GLN:OE1	1:B:565:GLU:HB2	1.89	0.71
1:B:50:ARG:NH1	1:B:50:ARG:CG	2.51	0.71
1:D:347:CYS:CB	1:D:350:GLU:HG2	2.20	0.71
1:A:872:LEU:O	1:A:875:ILE:HG13	1.89	0.71
1:A:72:PRO:HB3	5:A:2110:HOH:O	1.90	0.71
1:A:247:ALA:HB1	5:A:2098:HOH:O	1.89	0.71
1:B:826:LYS:O	1:B:830:GLU:HG3	1.89	0.71
1:A:425:ARG:HD3	1:A:811:HIS:HD2	1.56	0.71
1:D:854:HIS:CD2	1:D:856:SER:H	2.08	0.71
1:A:57:ARG:O	1:A:60:LYS:HE2	1.90	0.71
1:D:810:ILE:HG22	3:O:8:U:H5'	1.73	0.71
1:C:154:ILE:CG2	1:C:190:MET:HE1	2.21	0.71
1:B:546:PHE:CD1	1:B:549:MET:CE	2.73	0.71
1:A:77:LEU:HD21	1:A:226:MET:SD	2.30	0.71
1:B:118:THR:HG23	1:B:141:ILE:HG21	1.71	0.71
1:C:59:LEU:HD23	1:C:64:VAL:HG22	1.73	0.71
1:A:342:THR:HG22	1:A:348:PRO:CG	2.18	0.71
1:C:720:ARG:NH1	1:C:720:ARG:HG2	2.05	0.71
1:D:315:GLU:OE2	1:D:318:LYS:HD3	1.90	0.71
1:B:72:PRO:HG3	1:B:257:ARG:HG3	1.72	0.70
1:A:220:LEU:HG	5:A:2101:HOH:O	1.91	0.70
1:B:452:ILE:HG23	1:B:453:GLY:N	2.06	0.70
1:C:713:LYS:HA	1:C:713:LYS:HZ3	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:421:ASP:OD2	1:D:423:ARG:NH1	2.25	0.70
2:E:12:DT:H2''	2:E:13:DC:H5'	1.74	0.70
1:D:14:ILE:HG23	1:D:288:ALA:HB1	1.72	0.70
1:C:529:ASN:HB2	5:C:2124:HOH:O	1.92	0.70
1:A:479:ILE:O	1:A:483:GLU:HG3	1.90	0.70
1:A:746:ARG:HH11	1:A:746:ARG:CB	2.04	0.70
1:B:236:VAL:CB	1:B:239:GLN:HB2	2.20	0.70
1:C:869:ASN:N	1:C:869:ASN:HD22	1.88	0.70
1:C:437:ASN:H	1:C:437:ASN:ND2	1.88	0.70
1:C:109:ILE:CG1	1:C:149:ALA:HB2	2.21	0.70
1:D:553:GLU:HA	1:D:870:LEU:HD12	1.72	0.70
1:D:182:PHE:O	1:D:185:VAL:HG22	1.91	0.70
1:A:51:PHE:CE2	1:A:261:LEU:HB3	2.26	0.70
1:A:17:ALA:HA	5:A:2048:HOH:O	1.91	0.70
1:D:289:ASN:HB3	5:D:2074:HOH:O	1.90	0.70
2:K:12:DT:H2''	2:K:13:DC:H5'	1.73	0.70
1:D:402:LEU:HG	1:D:439:MET:CE	2.22	0.70
1:A:191:LEU:HA	5:A:2085:HOH:O	1.92	0.70
1:C:208:ASP:N	1:C:208:ASP:OD2	2.24	0.70
1:D:441:LYS:HD3	5:D:2117:HOH:O	1.90	0.70
1:C:355:ILE:HA	5:C:2094:HOH:O	1.91	0.70
1:A:105:PHE:HB3	1:A:204:TRP:CZ2	2.26	0.70
1:A:308:TYR:HE2	1:A:734:PRO:HG2	1.56	0.70
1:B:355:ILE:HA	5:B:2165:HOH:O	1.91	0.70
1:A:347:CYS:HB3	1:A:350:GLU:CG	2.20	0.70
1:A:871:ASN:HD21	1:A:873:ARG:HB2	1.56	0.70
1:A:51:PHE:HE2	1:A:261:LEU:HB3	1.56	0.70
1:C:201:TRP:O	1:C:204:TRP:HB2	1.92	0.70
1:C:307:ARG:NH1	1:C:307:ARG:HG3	2.03	0.69
1:B:236:VAL:CG1	1:B:239:GLN:HB2	2.22	0.69
1:A:308:TYR:HA	1:A:311:VAL:HG23	1.74	0.69
1:A:698:TRP:CE3	1:A:699:LEU:HD23	2.26	0.69
1:A:120:LYS:CE	1:A:752:LEU:HD21	2.15	0.69
1:B:423:ARG:HE	2:H:12:DT:C4'	2.03	0.69
1:A:236:VAL:HB	1:A:239:GLN:HB2	1.74	0.69
1:D:113:ALA:O	1:D:117:ILE:HG13	1.92	0.69
1:C:402:LEU:HG	1:C:439:MET:CE	2.23	0.69
1:A:32:LEU:HD12	1:A:272:VAL:CG1	2.22	0.69
1:D:710:VAL:HG13	1:D:720:ARG:HB3	1.74	0.69
1:A:619:GLN:O	1:A:622:ALA:HB3	1.92	0.69
3:I:6:G:H3'	5:I:2011:HOH:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HD11	1:C:259:GLY:C	2.13	0.69
1:C:108:GLU:HA	1:C:108:GLU:OE1	1.91	0.69
1:D:40:GLU:OE1	1:D:286:TYR:HB3	1.91	0.69
1:B:21:PHE:HD1	1:B:21:PHE:O	1.76	0.69
1:D:248:PRO:O	1:D:252:GLU:HG3	1.93	0.69
1:A:663:LYS:HG2	1:A:664:GLY:H	1.57	0.69
1:A:860:LYS:O	1:A:860:LYS:HD3	1.93	0.69
1:B:85:ILE:HG12	1:B:219:MET:SD	2.33	0.69
1:A:402:LEU:O	1:A:406:ASN:ND2	2.24	0.69
1:A:427:TYR:HA	1:A:435:GLN:HE22	1.57	0.69
4:G:1:DG:H2"	4:G:2:DT:OP2	1.93	0.69
1:C:706:LEU:HD21	1:C:849:PHE:HB2	1.74	0.69
1:C:860:LYS:O	1:C:860:LYS:HD2	1.93	0.69
1:A:571:TYR:HD1	1:A:634:VAL:HG11	1.57	0.69
1:A:88:TRP:O	1:A:92:VAL:HG23	1.93	0.69
1:A:121:THR:HG22	5:A:2069:HOH:O	1.93	0.69
1:B:58:GLN:HG3	1:B:67:ASN:ND2	2.05	0.69
1:A:308:TYR:CE2	1:A:734:PRO:HG2	2.28	0.69
1:D:170:LEU:O	1:D:179:LYS:HE2	1.93	0.69
1:C:308:TYR:CE2	1:C:734:PRO:HG2	2.28	0.69
1:A:159:ALA:HB1	1:A:163:LYS:N	2.08	0.69
1:D:109:ILE:HG13	1:D:149:ALA:HB2	1.74	0.69
4:M:7:DT:H2"	4:M:8:DC:C6	2.28	0.69
1:C:713:LYS:NZ	1:C:713:LYS:HA	2.07	0.69
2:N:12:DT:H2"	2:N:13:DC:H5'	1.75	0.69
1:A:172:LYS:HA	5:A:2080:HOH:O	1.92	0.69
1:B:553:GLU:OE1	1:B:869:ASN:N	2.18	0.69
1:B:386:ARG:NH2	3:I:5:C:OP2	2.26	0.69
1:B:120:LYS:HD2	1:B:752:LEU:CD2	2.23	0.69
1:D:64:VAL:HA	5:D:2026:HOH:O	1.92	0.69
1:A:517:GLU:OE1	1:A:517:GLU:HA	1.93	0.69
1:A:375:THR:HG22	1:A:375:THR:O	1.93	0.69
1:C:505:GLN:O	1:C:508:PRO:HD3	1.92	0.68
1:C:437:ASN:HD22	1:C:437:ASN:N	1.91	0.68
1:A:118:THR:CG2	1:A:141:ILE:HD13	2.23	0.68
1:C:656:GLN:HB3	1:C:657:PRO:CD	2.22	0.68
1:D:281:ILE:HD11	1:D:308:TYR:HB3	1.75	0.68
1:C:752:LEU:HB3	5:C:2160:HOH:O	1.91	0.68
1:B:870:LEU:HD23	1:B:871:ASN:N	2.07	0.68
1:D:704:LYS:HE3	1:D:860:LYS:NZ	2.08	0.68
1:C:92:VAL:HG12	1:C:99:ARG:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:HD23	5:B:2083:HOH:O	1.92	0.68
1:C:373:ALA:HB1	1:C:377:TRP:HE1	1.59	0.68
1:A:308:TYR:HA	1:A:311:VAL:CG2	2.23	0.68
2:N:5:DA:H2"	2:N:6:DT:OP2	1.92	0.68
1:C:669:GLN:HG2	1:C:672:GLN:HE21	1.58	0.68
3:I:4:G:N7	5:I:2006:HOH:O	2.24	0.68
1:B:335:LEU:HD22	1:B:339:ASN:ND2	2.09	0.68
1:D:19:ILE:HG23	1:D:20:PRO:HD2	1.75	0.68
1:A:425:ARG:NH2	1:A:784:HIS:HD2	1.91	0.68
1:B:680:LEU:N	1:B:680:LEU:HD12	2.09	0.68
1:A:592:ASN:OD1	1:A:611:LEU:HD23	1.92	0.68
1:D:236:VAL:HG11	1:D:239:GLN:HB2	1.75	0.68
1:B:215:ARG:O	1:B:219:MET:HG3	1.93	0.68
1:A:730:PRO:CD	1:A:786:GLN:HE22	2.06	0.68
1:C:616:LEU:HD23	1:C:619:GLN:OE1	1.93	0.68
1:A:448:LYS:HE2	5:A:2287:HOH:O	1.94	0.68
1:A:546:PHE:CZ	1:A:783:VAL:CG2	2.75	0.68
1:D:804:ILE:HG23	1:D:816:THR:HG21	1.76	0.68
1:B:553:GLU:H	1:B:553:GLU:CD	1.96	0.68
1:D:608:LYS:HG3	5:D:2142:HOH:O	1.93	0.68
1:A:116:TYR:CE2	1:A:752:LEU:HD22	2.29	0.68
1:C:159:ALA:HB1	1:C:163:LYS:N	2.08	0.68
1:B:325:ASN:HB3	5:B:2147:HOH:O	1.93	0.68
1:B:143:ARG:NH1	1:B:209:SER:OG	2.27	0.68
1:B:92:VAL:HG22	5:B:2075:HOH:O	1.94	0.68
1:C:801:LYS:HE3	1:C:801:LYS:O	1.93	0.68
1:B:51:PHE:HD2	1:B:51:PHE:O	1.77	0.68
1:B:790:HIS:NE2	1:B:831:THR:HG22	2.09	0.68
1:A:423:ARG:HE	1:A:781:ASN:ND2	1.91	0.68
1:A:226:MET:HB3	5:A:2101:HOH:O	1.93	0.68
1:D:84:ARG:HD2	1:D:219:MET:HG2	1.74	0.68
1:C:849:PHE:CD2	1:C:853:LEU:HD21	2.27	0.67
1:D:84:ARG:HG2	1:D:84:ARG:HH11	1.57	0.67
1:D:596:THR:HG23	5:D:2143:HOH:O	1.92	0.67
1:B:165:ASN:OD1	1:B:165:ASN:N	2.27	0.67
1:D:181:ALA:O	1:D:185:VAL:HG13	1.94	0.67
1:A:112:GLU:H	1:A:112:GLU:CD	1.98	0.67
1:C:232:GLN:HB2	1:C:241:SER:O	1.94	0.67
1:A:882:PHE:O	1:A:883:ALA:CB	2.42	0.67
1:A:713:LYS:O	1:A:714:LYS:HE2	1.94	0.67
1:B:650:VAL:HA	5:B:2281:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:GLN:HB3	1:B:657:PRO:CD	2.24	0.67
1:D:816:THR:OG1	1:D:824:LEU:HD23	1.94	0.67
2:H:12:DT:H2"	2:H:13:DC:H5'	1.76	0.67
1:A:89:PHE:HE2	1:A:107:GLN:HG3	1.60	0.67
4:P:8:DC:H2"	4:P:9:DC:OP2	1.94	0.67
1:A:485:ASN:HD22	1:A:488:ASN:HD22	1.41	0.67
1:C:126:LEU:HD23	1:C:132:THR:CG2	2.24	0.67
1:C:109:ILE:CD1	1:C:149:ALA:HB2	2.24	0.67
1:C:72:PRO:HG2	5:C:2043:HOH:O	1.93	0.67
1:B:505:GLN:HG3	1:B:511:PHE:CD2	2.30	0.67
1:A:22:ASN:ND2	5:A:2043:HOH:O	2.27	0.67
1:B:138:ALA:O	1:B:213:GLY:HA3	1.94	0.67
1:D:351:ASP:N	5:D:2097:HOH:O	2.19	0.67
1:A:421:ASP:OD2	1:A:427:TYR:CE1	2.47	0.67
1:A:150:ARG:HD2	1:A:201:TRP:CG	2.30	0.67
1:A:225:GLY:HA3	5:A:2099:HOH:O	1.95	0.67
1:B:324:GLN:NE2	1:B:418:TYR:H	1.91	0.67
1:C:324:GLN:HE21	1:C:418:TYR:H	1.40	0.67
1:C:151:PHE:CD1	1:C:183:MET:HB3	2.30	0.67
1:D:326:THR:HG23	1:D:806:SER:HA	1.74	0.67
1:A:794:THR:OG1	1:A:831:THR:HG21	1.93	0.67
1:D:488:ASN:HB3	1:D:501:TRP:CE3	2.30	0.67
1:D:630:THR:O	1:D:634:VAL:HG12	1.95	0.67
1:C:711:LYS:HG2	1:C:717:GLU:C	2.15	0.67
1:C:15:GLU:HG2	1:C:18:ALA:O	1.94	0.67
1:C:374:LEU:HD12	1:C:374:LEU:N	2.10	0.67
1:D:726:HIS:CD2	1:D:727:TRP:N	2.63	0.67
1:B:215:ARG:O	1:B:219:MET:HE2	1.95	0.66
1:A:109:ILE:N	1:A:109:ILE:HD12	2.10	0.66
1:C:191:LEU:HB2	5:C:2066:HOH:O	1.94	0.66
1:C:324:GLN:NE2	1:C:418:TYR:H	1.93	0.66
1:A:879:ASP:HB2	5:A:2307:HOH:O	1.95	0.66
1:B:346:HIS:HA	1:B:395:ARG:HH11	1.60	0.66
1:B:55:PHE:HE1	1:B:69:ALA:CB	2.08	0.66
1:A:55:PHE:CE2	1:A:59:LEU:HD11	2.30	0.66
1:D:298:ARG:HH21	1:D:427:TYR:CB	2.05	0.66
1:A:105:PHE:HB3	1:A:204:TRP:CH2	2.30	0.66
1:B:737:GLN:NE2	1:B:739:TYR:HE2	1.93	0.66
1:B:881:ALA:HA	5:B:2352:HOH:O	1.94	0.66
1:D:183:MET:HE3	5:D:2048:HOH:O	1.95	0.66
1:B:422:TRP:HE3	5:B:2182:HOH:O	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:THR:HG21	1:A:216:CYS:HB3	1.77	0.66
1:A:220:LEU:HA	5:A:2097:HOH:O	1.95	0.66
1:B:416:PHE:HD1	1:B:430:SER:HG	1.43	0.66
1:A:15:GLU:HB2	1:A:19:ILE:HG12	1.76	0.66
1:C:21:PHE:HE1	5:C:2031:HOH:O	1.77	0.66
4:P:4:DG:H1'	5:P:2005:HOH:O	1.95	0.66
1:A:623:TYR:CD1	1:A:663:LYS:HE3	2.31	0.66
1:D:766:ASP:HA	5:D:2161:HOH:O	1.95	0.66
1:B:432:PHE:CE2	1:B:444:LEU:HD21	2.31	0.66
1:C:292:ARG:N	1:C:293:PRO:HD3	2.11	0.66
1:D:669:GLN:HG2	1:D:672:GLN:NE2	2.10	0.66
3:L:4:G:N7	5:L:2004:HOH:O	2.29	0.66
1:A:882:PHE:H	1:A:882:PHE:HD1	1.37	0.66
1:B:215:ARG:HG3	1:B:219:MET:CE	2.26	0.66
1:A:205:HIS:O	1:A:207:GLU:N	2.29	0.66
1:C:303:LYS:HE2	1:C:740:LYS:NZ	2.10	0.66
1:C:417:PRO:HG2	1:C:429:VAL:HB	1.77	0.66
1:C:552:ASP:HB2	1:C:691:ALA:HB2	1.77	0.66
1:A:118:THR:HG22	1:A:141:ILE:HD13	1.78	0.66
1:B:324:GLN:HE21	1:B:418:TYR:H	1.44	0.66
1:B:536:PHE:HB3	1:B:882:PHE:HB3	1.76	0.66
1:B:231:ARG:HH11	1:B:242:GLU:HB2	1.61	0.66
1:B:24:LEU:HD13	1:B:33:ALA:HA	1.79	0.66
1:B:423:ARG:HH11	1:B:423:ARG:HB2	1.61	0.65
1:C:606:SER:HB2	5:C:2141:HOH:O	1.96	0.65
1:B:573:ILE:HD11	1:B:688:THR:HG21	1.78	0.65
1:B:574:VAL:O	1:B:578:VAL:HG23	1.96	0.65
1:D:155:ARG:HB2	5:D:2044:HOH:O	1.95	0.65
1:A:398:LEU:CD2	1:A:398:LEU:C	2.64	0.65
1:C:116:TYR:OH	1:C:752:LEU:HD22	1.96	0.65
1:A:227:VAL:HB	1:A:244:ILE:HG22	1.77	0.65
1:A:452:ILE:HG22	1:A:528:TYR:O	1.95	0.65
1:C:656:GLN:HG2	5:C:2148:HOH:O	1.96	0.65
1:C:312:TYR:CZ	1:C:314:PRO:HG2	2.30	0.65
1:B:110:LYS:HG2	1:B:112:GLU:OE1	1.96	0.65
1:B:331:ASN:HB2	1:B:445:THR:HG22	1.79	0.65
1:A:711:LYS:NZ	1:A:711:LYS:CB	2.52	0.65
1:B:21:PHE:C	1:B:21:PHE:CD1	2.69	0.65
1:B:730:PRO:HD3	1:B:786:GLN:HE22	1.61	0.65
1:B:96:ARG:HD3	5:B:2078:HOH:O	1.95	0.65
1:D:337:VAL:O	1:D:341:ILE:HG12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:VAL:O	1:A:470:VAL:HG12	1.97	0.65
1:C:551:ARG:HE	1:C:872:LEU:HD11	1.60	0.65
1:A:219:MET:HB3	5:A:2060:HOH:O	1.96	0.65
1:B:182:PHE:O	1:B:185:VAL:HG22	1.96	0.65
1:B:867:LYS:HE2	5:B:2240:HOH:O	1.95	0.65
1:C:15:GLU:CG	1:C:18:ALA:H	2.08	0.65
1:C:103:PHE:CE2	1:C:107:GLN:NE2	2.64	0.65
1:C:577:LYS:HE3	5:C:2135:HOH:O	1.96	0.65
1:A:36:GLN:HG3	1:A:273:VAL:HG22	1.79	0.65
1:C:307:ARG:CG	1:C:307:ARG:HH11	2.04	0.65
1:B:54:MET:O	1:B:58:GLN:HG2	1.96	0.65
1:C:32:LEU:HG	1:C:272:VAL:HG12	1.77	0.65
1:D:692:ALA:O	1:D:696:MET:HG3	1.96	0.65
1:A:720:ARG:NH1	1:A:721:LYS:O	2.29	0.65
1:D:663:LYS:HG2	1:D:664:GLY:N	2.07	0.65
1:A:457:TYR:CD1	1:A:521:VAL:HG11	2.32	0.65
3:F:1:G:H2'	3:F:2:C:C6	2.32	0.65
4:G:5:DA:C2'	4:G:6:DT:H71	2.19	0.65
1:C:333:LYS:HB3	1:C:516:PHE:HE2	1.56	0.65
2:K:7:DC:H2"	2:K:8:DG:O5'	1.94	0.65
1:D:155:ARG:CB	1:D:163:LYS:HE2	2.27	0.65
1:B:111:PRO:HG2	1:B:112:GLU:OE2	1.97	0.65
1:B:391:ARG:HB3	1:B:391:ARG:HH11	1.61	0.65
1:B:278:TRP:HE1	1:B:324:GLN:HE22	1.45	0.65
1:B:690:VAL:O	1:B:694:GLU:HG3	1.97	0.65
1:D:319:ALA:CB	1:D:792:ARG:HG2	2.27	0.65
1:A:571:TYR:CD1	1:A:634:VAL:HG11	2.32	0.65
1:D:36:GLN:HG3	1:D:273:VAL:HG22	1.79	0.65
1:B:256:THR:HG22	5:B:2124:HOH:O	1.96	0.65
1:B:374:LEU:HD12	1:B:374:LEU:H	1.60	0.65
1:C:333:LYS:CB	1:C:516:PHE:CE2	2.76	0.65
1:D:281:ILE:HG12	1:D:309:GLU:HA	1.78	0.65
1:B:599:ASP:HA	5:B:2267:HOH:O	1.97	0.65
1:A:99:ARG:NH1	1:A:99:ARG:HG2	1.98	0.64
1:D:719:LEU:CD1	1:D:719:LEU:N	2.59	0.64
1:D:220:LEU:HG	5:D:2059:HOH:O	1.97	0.64
1:A:540:CYS:HB3	5:A:2024:HOH:O	1.97	0.64
1:A:276:LYS:HD2	1:A:283:GLY:O	1.96	0.64
1:C:704:LYS:HE3	5:M:2006:HOH:O	1.97	0.64
1:D:159:ALA:HB1	1:D:163:LYS:N	2.11	0.64
1:B:717:GLU:HA	5:B:2305:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ILE:HD11	1:A:308:TYR:CB	2.27	0.64
1:D:59:LEU:HD23	1:D:64:VAL:HG22	1.79	0.64
1:D:786:GLN:HG3	1:D:836:TYR:OH	1.96	0.64
1:B:791:LEU:HD21	1:B:809:LEU:HD13	1.79	0.64
1:D:824:LEU:HD12	1:D:824:LEU:O	1.97	0.64
1:C:751:PHE:C	1:C:752:LEU:HD12	2.18	0.64
1:A:714:LYS:NZ	1:A:714:LYS:HA	2.13	0.64
1:A:485:ASN:HD22	1:A:488:ASN:ND2	1.96	0.64
1:A:170:LEU:HD12	1:A:183:MET:HE1	1.80	0.64
1:A:119:ILE:HD12	5:A:2059:HOH:O	1.96	0.64
1:D:663:LYS:HE3	1:D:666:MET:CE	2.28	0.64
1:A:292:ARG:O	1:A:292:ARG:HG3	1.97	0.64
2:K:9:DA:N6	4:M:1:DG:N2	2.45	0.64
1:C:73:LEU:HG	5:C:2043:HOH:O	1.96	0.64
1:D:141:ILE:O	1:D:145:ILE:HG12	1.98	0.64
1:A:40:GLU:OE1	1:A:286:TYR:HB3	1.98	0.64
1:A:595:VAL:HG22	5:A:2237:HOH:O	1.97	0.64
1:C:291:ARG:HB2	5:C:2079:HOH:O	1.96	0.64
1:C:341:ILE:HD12	1:C:348:PRO:HB3	1.78	0.64
1:A:668:THR:CG2	1:A:669:GLN:NE2	2.43	0.64
1:B:77:LEU:HD12	1:B:224:THR:HG21	1.79	0.64
3:L:1:G:H2'	3:L:2:C:C6	2.32	0.64
1:A:425:ARG:NH2	1:A:784:HIS:CD2	2.66	0.64
1:B:663:LYS:CG	1:B:664:GLY:H	1.94	0.64
1:D:790:HIS:NE2	1:D:832:MET:HB2	2.13	0.64
1:C:816:THR:OG1	1:C:824:LEU:HD22	1.98	0.64
1:C:422:TRP:CH2	2:K:12:DT:H5"	2.33	0.64
1:A:80:LYS:HE2	1:A:224:THR:HG22	1.79	0.64
1:B:148:GLU:OE2	1:B:148:GLU:HA	1.97	0.64
1:C:455:GLU:HA	1:C:455:GLU:OE1	1.98	0.64
1:A:32:LEU:HD12	1:A:272:VAL:HG12	1.79	0.64
1:C:68:ALA:HB3	1:C:261:LEU:HD21	1.79	0.64
1:C:115:ALA:O	1:C:119:ILE:HG12	1.97	0.64
1:C:828:VAL:HB	1:C:883:ALA:HA	1.78	0.64
1:B:132:THR:HB	5:B:2083:HOH:O	1.98	0.64
1:B:55:PHE:HE1	1:B:69:ALA:HB3	1.62	0.64
1:A:391:ARG:HG2	1:A:391:ARG:HH11	1.63	0.64
1:D:423:ARG:NH2	1:D:784:HIS:ND1	2.45	0.64
1:A:150:ARG:HD2	1:A:201:TRP:CD1	2.33	0.64
5:A:2025:HOH:O	1:B:553:GLU:HG3	1.97	0.64
1:A:565:GLU:HG3	5:A:2225:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:TYR:CD1	1:C:521:VAL:HG11	2.32	0.63
3:I:1:G:H2'	3:I:2:C:C6	2.34	0.63
1:B:401:MET:HE1	1:B:432:PHE:HA	1.80	0.63
1:D:335:LEU:HD22	1:D:339:ASN:ND2	2.13	0.63
2:K:18:DC:H2"	5:K:2016:HOH:O	1.99	0.63
1:C:162:PHE:CG	5:C:2059:HOH:O	2.51	0.63
1:C:804:ILE:HG23	1:C:816:THR:HG21	1.80	0.63
1:B:71:LYS:N	1:B:72:PRO:HD2	2.14	0.63
1:C:162:PHE:HB3	5:C:2059:HOH:O	1.99	0.63
1:B:639:TYR:O	2:H:10:DC:H4'	1.97	0.63
1:B:28:TYR:O	1:B:32:LEU:HD23	1.98	0.63
1:C:549:MET:HE2	1:C:841:VAL:HG21	1.81	0.63
1:D:133:THR:HA	1:D:243:THR:HG22	1.79	0.63
1:A:648:GLN:O	1:A:652:GLU:HG2	1.97	0.63
1:B:473:VAL:CG1	1:B:477:GLU:CB	2.76	0.63
1:A:58:GLN:HG3	1:A:67:ASN:HD22	1.64	0.63
1:C:15:GLU:HG2	1:C:18:ALA:H	1.62	0.63
1:B:475:PHE:HE1	1:B:478:ARG:NH1	1.97	0.63
1:C:522:GLN:OE1	1:C:522:GLN:HA	1.97	0.63
1:D:537:ASP:H	1:D:882:PHE:HD2	1.46	0.63
1:B:225:GLY:O	1:B:247:ALA:HB2	1.98	0.63
1:C:532:LEU:HD23	1:C:534:LEU:CD2	2.24	0.63
1:A:428:ALA:HB3	1:A:433:ASN:ND2	2.13	0.63
1:D:84:ARG:NH1	1:D:84:ARG:HG2	2.13	0.63
1:C:652:GLU:HA	1:C:656:GLN:HB2	1.81	0.63
1:C:183:MET:HA	1:C:183:MET:CE	2.29	0.63
1:D:291:ARG:HB2	5:D:2076:HOH:O	1.97	0.63
1:B:34:ARG:HD3	5:B:2049:HOH:O	1.97	0.63
1:A:881:ALA:O	1:A:882:PHE:C	2.34	0.63
1:A:181:ALA:O	1:A:185:VAL:HG13	1.99	0.63
1:C:303:LYS:NZ	1:C:740:LYS:NZ	2.46	0.63
1:C:726:HIS:HB3	5:C:2155:HOH:O	1.97	0.63
1:D:552:ASP:HB2	1:D:691:ALA:HB2	1.81	0.63
1:C:113:ALA:O	1:C:117:ILE:HG13	1.97	0.63
1:C:532:LEU:CD2	1:C:534:LEU:HD23	2.27	0.63
1:D:796:VAL:HA	5:D:2167:HOH:O	1.98	0.63
1:B:138:ALA:HA	1:B:141:ILE:HD12	1.80	0.63
1:D:34:ARG:HG2	5:D:2023:HOH:O	1.98	0.63
1:A:568:GLN:CD	1:B:565:GLU:HB2	2.19	0.63
1:A:710:VAL:HG13	1:A:720:ARG:HB3	1.81	0.63
1:C:123:LEU:O	1:C:127:THR:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:MET:HE2	1:C:183:MET:HA	1.81	0.63
1:B:375:THR:HG22	1:B:375:THR:O	1.99	0.63
1:B:714:LYS:HA	1:B:714:LYS:HZ3	1.63	0.63
1:C:755:PHE:N	1:C:755:PHE:HD1	1.95	0.63
1:D:161:HIS:O	1:D:164:LYS:HG2	1.98	0.63
1:C:146:GLU:OE2	1:C:201:TRP:HB3	1.99	0.63
1:A:437:ASN:ND2	1:A:440:THR:H	1.97	0.63
1:A:529:ASN:HD22	1:A:529:ASN:C	2.02	0.63
1:A:499:ASN:HA	5:A:2188:HOH:O	1.97	0.63
1:D:824:LEU:HD12	1:D:828:VAL:HG13	1.81	0.62
1:B:573:ILE:O	1:B:573:ILE:HD12	1.98	0.62
1:A:205:HIS:NE2	1:A:206:LYS:HE2	2.13	0.62
1:C:779:ALA:O	1:C:783:VAL:HG22	1.99	0.62
1:C:587:ILE:HG22	1:C:588:ASN:ND2	2.13	0.62
1:B:322:ILE:HD13	1:B:799:HIS:CG	2.34	0.62
1:B:335:LEU:HB2	5:B:2150:HOH:O	1.97	0.62
1:D:36:GLN:CG	1:D:273:VAL:HG22	2.29	0.62
1:A:138:ALA:O	1:A:213:GLY:HA3	1.99	0.62
1:D:744:GLN:HA	1:D:756:ARG:NH1	2.14	0.62
1:C:711:LYS:HG2	1:C:717:GLU:O	1.99	0.62
1:A:159:ALA:O	1:A:163:LYS:HB2	1.99	0.62
1:D:748:ASN:HB2	1:D:753:GLY:CA	2.29	0.62
1:C:133:THR:CA	1:C:243:THR:HG22	2.16	0.62
1:B:350:GLU:OE2	1:B:394:ARG:NH2	2.27	0.62
1:B:790:HIS:NE2	1:B:831:THR:CG2	2.62	0.62
1:A:77:LEU:CD2	1:A:226:MET:SD	2.87	0.62
1:C:491:ALA:HB1	1:C:499:ASN:HD22	1.62	0.62
1:D:698:TRP:CZ3	1:D:842:LEU:HG	2.34	0.62
1:C:128:SER:HA	5:C:2055:HOH:O	1.98	0.62
1:C:42:GLU:OE1	1:C:407:LYS:NZ	2.27	0.62
1:D:138:ALA:O	1:D:213:GLY:HA3	1.98	0.62
1:B:812:ASP:OD2	3:I:8:U:O2'	2.09	0.62
1:B:162:PHE:HE1	1:B:190:MET:HG2	1.64	0.62
1:B:236:VAL:HG11	1:B:239:GLN:HB2	1.81	0.62
1:B:281:ILE:HG23	1:B:305:LEU:HD21	1.81	0.62
1:C:303:LYS:HE2	1:C:740:LYS:HZ1	1.63	0.62
1:D:882:PHE:O	1:D:883:ALA:HB3	1.98	0.62
1:B:881:ALA:CA	5:B:2352:HOH:O	2.47	0.62
1:C:169:GLN:O	1:C:173:ARG:HG2	2.00	0.62
1:D:164:LYS:HE2	1:D:164:LYS:CA	2.30	0.62
1:D:553:GLU:HA	1:D:870:LEU:CD1	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ALA:O	1:A:37:LEU:HG	1.99	0.62
1:A:881:ALA:C	5:A:2310:HOH:O	2.38	0.62
1:D:632:ARG:NH1	1:D:632:ARG:H	1.97	0.62
1:C:50:ARG:HH11	1:C:50:ARG:CG	2.12	0.62
1:D:109:ILE:CG2	5:D:2041:HOH:O	2.47	0.62
3:O:1:G:H2'	3:O:2:C:C6	2.34	0.62
1:C:428:ALA:H	1:C:435:GLN:HE21	1.41	0.62
1:D:677:MET:O	1:D:681:ILE:HG13	2.00	0.62
1:D:746:ARG:NH1	1:D:746:ARG:HB3	2.15	0.62
1:B:183:MET:HE1	1:B:186:VAL:HG21	1.82	0.62
1:D:700:LYS:NZ	1:D:700:LYS:HB2	2.14	0.62
1:D:713:LYS:HZ3	1:D:713:LYS:HA	1.63	0.62
1:B:748:ASN:ND2	1:B:751:PHE:N	2.43	0.62
1:D:236:VAL:CG1	1:D:239:GLN:HB2	2.29	0.62
1:C:4:ILE:HG21	5:C:2019:HOH:O	1.99	0.62
1:B:268:PHE:HB3	1:B:286:TYR:OH	1.99	0.62
1:A:113:ALA:O	1:A:117:ILE:CG1	2.44	0.62
1:D:335:LEU:HD22	1:D:335:LEU:O	1.99	0.62
1:D:88:TRP:HA	1:D:91:GLU:CD	2.21	0.62
1:C:50:ARG:NH1	1:C:50:ARG:HG2	2.09	0.62
1:B:195:LEU:HB3	5:B:2100:HOH:O	2.00	0.62
1:D:814:PHE:HE1	1:D:883:ALA:CB	2.12	0.62
5:C:2147:HOH:O	4:M:2:DT:H5'	2.00	0.62
2:H:5:DA:H2''	2:H:6:DT:OP2	1.98	0.62
1:C:636:THR:O	1:C:641:SER:OG	2.18	0.62
1:C:560:ASN:OD1	1:C:568:GLN:HB2	1.99	0.61
1:B:744:GLN:HA	1:B:756:ARG:HH21	1.65	0.61
1:C:846:TYR:CD1	1:C:850:ALA:HB2	2.35	0.61
1:A:21:PHE:HD1	1:A:21:PHE:O	1.83	0.61
1:C:755:PHE:N	1:C:755:PHE:CD1	2.67	0.61
1:D:56:GLU:CD	1:D:57:ARG:N	2.54	0.61
2:N:9:DA:OP2	5:N:2009:HOH:O	2.16	0.61
1:A:116:TYR:OH	1:A:752:LEU:HD22	2.00	0.61
1:D:350:GLU:OE1	1:D:350:GLU:HA	2.00	0.61
1:C:418:TYR:HD2	1:C:426:VAL:CG1	2.13	0.61
1:C:570:ILE:HA	1:C:573:ILE:HG22	1.82	0.61
1:A:332:LYS:HE2	1:A:410:ASN:ND2	2.15	0.61
1:D:826:LYS:O	1:D:830:GLU:HG3	1.99	0.61
1:B:158:GLU:HG2	1:B:195:LEU:CD2	2.26	0.61
1:D:881:ALA:O	1:D:882:PHE:C	2.38	0.61
1:B:80:LYS:CD	1:B:224:THR:HG22	2.28	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:746:ARG:HH12	1:D:754:GLN:H	1.48	0.61
1:D:347:CYS:HB3	1:D:350:GLU:CG	2.31	0.61
1:D:730:PRO:HD2	1:D:786:GLN:HE22	1.65	0.61
1:B:109:ILE:HD12	1:B:109:ILE:H	1.65	0.61
1:B:6:ILE:HB	1:B:48:GLU:OE2	2.01	0.61
1:C:514:PHE:CD1	1:C:515:CYS:N	2.68	0.61
1:D:828:VAL:O	1:D:831:THR:HG22	2.00	0.61
1:C:303:LYS:CE	1:C:740:LYS:NZ	2.63	0.61
1:D:869:ASN:ND2	1:D:869:ASN:N	2.47	0.61
1:D:391:ARG:HB3	1:D:391:ARG:HH11	1.66	0.61
1:A:11:PHE:HZ	1:A:263:GLY:HA2	1.66	0.61
1:B:14:ILE:HG13	5:B:2134:HOH:O	2.00	0.61
1:A:742:PRO:HB3	1:A:744:GLN:OE1	2.00	0.61
1:B:881:ALA:O	1:B:882:PHE:C	2.37	0.61
1:B:51:PHE:O	1:B:51:PHE:CD2	2.53	0.61
1:A:249:GLU:HA	1:A:252:GLU:OE1	2.01	0.61
1:C:226:MET:HA	1:C:250:TYR:CD1	2.36	0.61
2:H:3:DG:H2"	2:H:4:DA:OP2	2.00	0.61
1:C:882:PHE:O	1:C:883:ALA:HB3	1.99	0.61
1:C:869:ASN:N	1:C:869:ASN:ND2	2.46	0.61
1:D:66:ASP:OD2	1:D:752:LEU:HD23	1.99	0.61
1:B:155:ARG:NH2	1:B:749:LEU:HD23	2.15	0.61
1:A:71:LYS:N	1:A:72:PRO:HD2	2.15	0.61
1:C:410:ASN:HA	5:C:2098:HOH:O	1.98	0.61
1:B:571:TYR:CD1	1:B:631:LYS:HA	2.35	0.61
1:B:472:LYS:HB2	5:B:2206:HOH:O	2.00	0.61
1:D:120:LYS:HG3	1:D:752:LEU:HD21	1.82	0.61
1:A:229:LEU:HD13	1:A:244:ILE:CD1	2.31	0.61
1:C:768:GLU:OE2	5:C:2165:HOH:O	2.16	0.61
1:B:743:ILE:O	1:B:743:ILE:HG22	1.99	0.61
1:D:326:THR:HA	5:D:2087:HOH:O	2.01	0.61
1:D:43:SER:HA	1:D:46:MET:CE	2.28	0.61
1:A:30:GLU:HG2	1:A:34:ARG:NH1	2.15	0.61
1:C:109:ILE:HG13	1:C:149:ALA:HB2	1.83	0.61
1:A:246:LEU:HB3	5:A:2108:HOH:O	1.99	0.61
1:D:332:LYS:HG2	5:D:2011:HOH:O	2.00	0.61
1:C:105:PHE:CE1	1:C:208:ASP:HB3	2.36	0.61
1:B:552:ASP:HB2	1:B:691:ALA:HB2	1.82	0.61
1:D:534:LEU:HD11	1:D:818:PRO:HG3	1.81	0.61
5:A:2258:HOH:O	2:E:10:DC:H5	1.82	0.61
1:C:38:ALA:HA	5:C:2034:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:ASP:H	1:B:882:PHE:HD2	1.47	0.61
1:B:401:MET:CE	1:B:432:PHE:HD1	2.14	0.61
1:C:19:ILE:CD1	1:C:20:PRO:HD2	2.31	0.61
4:J:3:DC:H2'	5:J:2002:HOH:O	2.01	0.61
1:D:132:THR:HA	5:D:2037:HOH:O	2.00	0.61
1:A:553:GLU:HB2	5:A:2222:HOH:O	2.01	0.61
1:A:380:ALA:O	1:A:384:VAL:HG23	2.01	0.61
1:C:536:PHE:HB3	1:C:882:PHE:CB	2.24	0.60
2:E:4:DA:H5''	5:E:2003:HOH:O	2.00	0.60
1:D:16:LEU:HB2	5:D:2022:HOH:O	2.00	0.60
1:A:871:ASN:ND2	1:A:873:ARG:HB2	2.15	0.60
2:N:12:DT:H2''	2:N:13:DC:C5'	2.31	0.60
1:B:632:ARG:CD	1:B:632:ARG:H	2.14	0.60
1:C:809:LEU:C	1:C:810:ILE:HG13	2.22	0.60
1:A:182:PHE:O	1:A:185:VAL:HG22	2.00	0.60
1:B:16:LEU:HD13	1:B:38:ALA:HA	1.83	0.60
1:D:226:MET:HB3	5:D:2059:HOH:O	2.01	0.60
1:B:355:ILE:HB	5:B:2167:HOH:O	2.01	0.60
1:D:56:GLU:CD	1:D:56:GLU:C	2.59	0.60
1:D:9:ASN:HA	1:D:12:SER:HB3	1.83	0.60
1:B:216:CYS:HA	1:B:219:MET:CE	2.31	0.60
1:A:84:ARG:HH21	1:A:222:GLU:HB3	1.67	0.60
1:D:34:ARG:HD3	5:D:2016:HOH:O	2.00	0.60
1:A:546:PHE:CE2	1:A:783:VAL:HG21	2.36	0.60
1:C:227:VAL:HG12	1:C:245:GLU:O	2.02	0.60
2:K:12:DT:H2''	2:K:13:DC:C5'	2.31	0.60
1:C:173:ARG:NH2	5:C:2062:HOH:O	2.34	0.60
1:D:16:LEU:HA	1:D:37:LEU:CD1	2.31	0.60
1:B:437:ASN:HD22	1:B:437:ASN:C	2.05	0.60
1:C:554:VAL:HG23	5:C:2128:HOH:O	2.00	0.60
1:A:825:PHE:CZ	1:A:829:ARG:NH2	2.68	0.60
1:C:229:LEU:HD13	1:C:244:ILE:CD1	2.31	0.60
1:A:632:ARG:HB2	1:A:632:ARG:HH11	1.63	0.60
1:A:117:ILE:O	1:A:121:THR:OG1	2.16	0.60
1:B:221:ILE:HG12	1:B:227:VAL:O	2.01	0.60
1:D:120:LYS:HD3	1:D:120:LYS:C	2.22	0.60
1:B:881:ALA:C	5:B:2352:HOH:O	2.37	0.60
1:D:64:VAL:HG21	1:D:127:THR:HG21	1.82	0.60
1:C:4:ILE:CG2	5:C:2019:HOH:O	2.48	0.60
1:A:388:ASP:OD1	1:A:392:LYS:HE2	2.01	0.60
1:D:298:ARG:NH2	1:D:427:TYR:CB	2.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:ARG:HD3	1:D:103:PHE:HE2	1.67	0.60
1:A:882:PHE:N	1:A:882:PHE:HD1	1.96	0.60
2:E:9:DA:H2"	2:E:10:DC:OP1	2.00	0.60
1:D:87:ASP:O	1:D:91:GLU:HG3	2.02	0.60
1:A:663:LYS:HA	5:A:2262:HOH:O	2.01	0.60
1:B:499:ASN:HB3	5:B:2219:HOH:O	2.02	0.60
1:B:37:LEU:HD22	1:B:288:ALA:HB2	1.84	0.60
1:A:730:PRO:CD	1:A:786:GLN:NE2	2.64	0.60
1:C:727:TRP:NE1	1:C:735:VAL:HG11	2.17	0.60
1:D:473:VAL:O	1:D:478:ARG:NE	2.20	0.60
1:A:583:GLN:O	1:A:587:ILE:HG12	2.02	0.60
1:A:861:MET:CE	1:A:862:PRO:HD2	2.32	0.60
1:C:421:ASP:OD2	1:C:423:ARG:NH1	2.34	0.60
1:B:401:MET:CE	1:B:432:PHE:HB2	2.32	0.60
1:A:110:LYS:HG2	1:A:112:GLU:OE1	2.02	0.60
1:C:226:MET:HA	1:C:250:TYR:HD1	1.66	0.60
1:B:162:PHE:CD1	1:B:190:MET:SD	2.95	0.60
1:C:347:CYS:HG	1:C:350:GLU:HG2	1.67	0.60
1:A:536:PHE:HB3	1:A:882:PHE:CB	2.25	0.60
1:B:752:LEU:HD12	1:B:752:LEU:N	2.16	0.60
1:B:178:TYR:HE2	5:B:2095:HOH:O	1.84	0.60
1:B:116:TYR:CE2	1:B:752:LEU:HD22	2.36	0.59
1:B:262:ALA:HB2	5:B:2059:HOH:O	2.02	0.59
1:A:6:ILE:HG23	1:A:10:ASP:OD2	2.02	0.59
1:C:719:LEU:N	1:C:719:LEU:HD12	2.16	0.59
1:C:333:LYS:CB	1:C:516:PHE:CD2	2.85	0.59
1:B:307:ARG:HB3	1:B:736:TRP:CZ3	2.38	0.59
1:A:110:LYS:O	1:A:114:VAL:HG23	2.01	0.59
1:A:115:ALA:O	1:A:119:ILE:HG12	2.02	0.59
1:C:54:MET:O	1:C:58:GLN:HG2	2.02	0.59
1:A:78:LEU:N	1:A:79:PRO:HD2	2.16	0.59
2:K:6:DT:C6	2:K:6:DT:H5'	2.37	0.59
1:A:30:GLU:CD	1:A:34:ARG:NH2	2.56	0.59
1:D:778:ILE:HG23	1:D:779:ALA:H	1.66	0.59
1:B:565:GLU:N	5:B:2252:HOH:O	2.25	0.59
1:C:551:ARG:NH1	1:C:551:ARG:CG	2.52	0.59
1:B:739:TYR:HB2	1:B:774:GLN:OE1	2.02	0.59
2:H:9:DA:H2"	2:H:10:DC:OP1	2.02	0.59
1:C:482:ILE:HD12	1:C:514:PHE:CZ	2.37	0.59
1:B:539:SER:HB2	1:B:544:GLN:OE1	2.02	0.59
1:B:19:ILE:HD12	1:B:20:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HH21	1:A:222:GLU:CD	2.04	0.59
1:A:21:PHE:CD1	1:A:21:PHE:C	2.76	0.59
1:A:275:PRO:HD3	1:A:415:TRP:CB	2.32	0.59
1:A:236:VAL:HG11	1:A:239:GLN:CG	2.31	0.59
1:B:99:ARG:H	1:B:99:ARG:HD2	1.68	0.59
1:C:573:ILE:O	1:C:577:LYS:HG3	2.03	0.59
1:C:854:HIS:CD2	1:C:856:SER:H	2.21	0.59
1:A:120:LYS:HG3	1:A:752:LEU:HD21	1.83	0.59
1:A:89:PHE:HA	1:A:103:PHE:CE1	2.33	0.59
1:B:751:PHE:HB3	1:B:752:LEU:CD1	2.33	0.59
1:D:292:ARG:HA	5:D:2075:HOH:O	2.02	0.59
1:A:30:GLU:OE1	1:A:34:ARG:NH2	2.34	0.59
1:D:88:TRP:HA	1:D:91:GLU:OE2	2.02	0.59
1:D:81:MET:HE2	1:D:220:LEU:HD13	1.84	0.59
1:A:438:ASP:OD2	1:A:509:PHE:N	2.35	0.59
1:B:517:GLU:O	1:B:521:VAL:HG23	2.02	0.59
1:D:32:LEU:N	1:D:32:LEU:HD12	2.18	0.59
1:A:55:PHE:CD2	1:A:59:LEU:HD11	2.37	0.59
1:B:116:TYR:HE1	5:B:2315:HOH:O	1.85	0.59
1:C:14:ILE:HG23	1:C:288:ALA:CB	2.32	0.59
1:D:573:ILE:HD12	1:D:573:ILE:O	2.01	0.59
1:D:227:VAL:HG13	5:D:2059:HOH:O	2.03	0.59
1:C:689:VAL:O	1:C:689:VAL:HG23	2.02	0.59
1:A:814:PHE:CE1	1:A:883:ALA:HB2	2.38	0.59
1:C:492:CYS:SG	1:C:501:TRP:HE3	2.26	0.59
1:D:810:ILE:CG2	3:O:8:U:H5'	2.33	0.59
1:A:269:GLN:HE22	1:A:407:LYS:HZ2	1.46	0.59
1:B:473:VAL:CG1	1:B:477:GLU:HB2	2.33	0.59
1:B:669:GLN:HB3	1:B:672:GLN:HB2	1.85	0.59
1:A:468:ALA:HA	1:A:505:GLN:HB3	1.85	0.59
1:A:649:GLN:O	1:A:653:ASP:HB2	2.03	0.59
1:C:881:ALA:O	1:C:883:ALA:N	2.35	0.59
1:D:663:LYS:HE3	1:D:666:MET:HE1	1.85	0.59
1:C:236:VAL:CB	1:C:239:GLN:HB2	2.33	0.59
1:B:256:THR:HB	5:B:2122:HOH:O	2.03	0.59
1:A:6:ILE:O	1:A:10:ASP:HB3	2.03	0.59
1:D:380:ALA:O	1:D:384:VAL:HG23	2.03	0.59
1:C:743:ILE:HG12	5:C:2164:HOH:O	2.03	0.59
1:B:410:ASN:HA	5:B:2177:HOH:O	2.03	0.59
1:A:47:GLY:O	1:A:50:ARG:HB3	2.02	0.59
1:A:264:ILE:O	1:A:264:ILE:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:PHE:HA	1:C:882:PHE:HD2	1.67	0.58
1:A:170:LEU:HD12	1:A:183:MET:CE	2.33	0.58
1:C:5:ASN:OD1	1:C:7:ALA:HB3	2.02	0.58
1:D:462:ILE:HG22	1:D:466:ASN:ND2	2.18	0.58
1:C:110:LYS:HE2	1:C:112:GLU:OE1	2.02	0.58
1:B:749:LEU:HD21	5:B:2088:HOH:O	2.03	0.58
1:D:582:LEU:CB	1:D:621:LEU:HD21	2.31	0.58
1:C:711:LYS:NZ	1:C:711:LYS:CB	2.64	0.58
1:D:437:ASN:ND2	1:D:440:THR:H	2.01	0.58
1:A:236:VAL:CB	1:A:239:GLN:HB2	2.33	0.58
1:A:142:GLY:HA2	5:A:2072:HOH:O	2.01	0.58
1:D:432:PHE:CE2	1:D:444:LEU:HD21	2.39	0.58
1:A:209:SER:HB2	5:A:2092:HOH:O	2.02	0.58
1:A:668:THR:HG22	1:A:669:GLN:HE21	1.59	0.58
1:B:623:TYR:CA	1:B:666:MET:HE2	2.29	0.58
2:H:12:DT:H2''	2:H:13:DC:C5'	2.33	0.58
1:A:806:SER:O	1:A:816:THR:CG2	2.51	0.58
1:B:787:ASP:C	1:B:787:ASP:OD1	2.41	0.58
1:D:686:SER:HA	1:D:693:VAL:HG21	1.85	0.58
1:A:377:TRP:HB3	5:A:2148:HOH:O	2.03	0.58
1:D:475:PHE:H	1:D:475:PHE:HD1	1.51	0.58
1:D:116:TYR:CD2	1:D:746:ARG:NH2	2.72	0.58
1:C:188:ALA:HA	5:C:2066:HOH:O	2.03	0.58
1:C:437:ASN:HD21	1:C:440:THR:H	1.50	0.58
1:B:109:ILE:HG13	1:B:149:ALA:HB2	1.84	0.58
1:C:791:LEU:O	1:C:795:VAL:HG23	2.03	0.58
1:D:158:GLU:HG2	1:D:195:LEU:HD13	1.86	0.58
1:B:82:ILE:HG22	5:B:2073:HOH:O	2.03	0.58
1:A:854:HIS:HD2	1:A:856:SER:OG	1.86	0.58
2:K:3:DG:H2''	2:K:4:DA:N7	2.18	0.58
1:A:84:ARG:CG	1:A:223:SER:HB3	2.31	0.58
4:M:2:DT:H2''	4:M:3:DC:O5'	2.02	0.58
1:B:561:LEU:C	1:B:562:LEU:HD23	2.24	0.58
1:D:534:LEU:HD23	1:D:534:LEU:N	2.19	0.58
1:C:138:ALA:O	1:C:213:GLY:HA3	2.02	0.58
1:C:881:ALA:O	1:C:882:PHE:C	2.42	0.58
1:B:43:SER:HA	1:B:46:MET:CE	2.34	0.58
1:D:226:MET:HA	1:D:250:TYR:CD1	2.39	0.58
1:A:689:VAL:O	1:A:689:VAL:HG23	2.04	0.58
1:B:77:LEU:HD21	1:B:226:MET:SD	2.44	0.58
1:D:286:TYR:CE1	1:D:417:PRO:HG3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HA	1:B:64:VAL:CG2	2.32	0.58
1:A:105:PHE:CD2	1:A:105:PHE:N	2.69	0.58
1:C:551:ARG:HB2	1:C:868:GLY:H	1.68	0.58
1:D:226:MET:HA	1:D:250:TYR:HD1	1.68	0.58
1:C:301:SER:HB2	1:C:303:LYS:HG3	1.86	0.58
1:A:70:ALA:C	1:A:72:PRO:HD2	2.24	0.58
1:D:551:ARG:NH2	1:D:836:TYR:O	2.22	0.58
1:D:609:VAL:HG12	5:D:2148:HOH:O	2.03	0.58
1:C:229:LEU:HD13	1:C:244:ILE:HD13	1.85	0.58
1:A:881:ALA:O	1:A:883:ALA:N	2.37	0.58
1:D:348:PRO:CG	5:D:2092:HOH:O	2.32	0.58
2:H:17:DG:H2''	2:H:18:DC:C6	2.38	0.58
1:A:116:TYR:HE2	1:A:752:LEU:HD22	1.68	0.58
1:A:632:ARG:NH1	1:A:632:ARG:CB	2.62	0.58
1:A:571:TYR:CD1	1:A:634:VAL:CG1	2.87	0.58
1:D:617:ALA:O	1:D:621:LEU:HG	2.03	0.58
1:C:56:GLU:OE1	1:C:57:ARG:N	2.36	0.58
1:A:163:LYS:HB3	1:A:164:LYS:NZ	2.18	0.58
1:C:825:PHE:O	1:C:829:ARG:NH1	2.37	0.58
1:D:677:MET:HG3	1:D:681:ILE:HD11	1.85	0.58
1:B:748:ASN:ND2	1:B:752:LEU:N	2.52	0.58
1:B:155:ARG:CZ	1:B:749:LEU:HD23	2.34	0.58
1:A:423:ARG:NH2	1:A:784:HIS:ND1	2.50	0.58
2:K:17:DG:H2''	2:K:18:DC:C6	2.39	0.58
1:D:182:PHE:O	1:D:186:VAL:HG23	2.02	0.58
1:D:6:ILE:O	1:D:10:ASP:HB3	2.04	0.58
1:D:475:PHE:HE1	1:D:880:PHE:CD1	2.20	0.58
1:B:313:MET:HE3	5:B:2143:HOH:O	2.04	0.58
1:B:479:ILE:O	1:B:483:GLU:HG3	2.03	0.58
1:C:829:ARG:HH11	1:C:829:ARG:HG3	1.69	0.57
4:G:2:DT:H2'	5:G:2001:HOH:O	2.04	0.57
1:D:352:ILE:HG22	5:D:2101:HOH:O	2.04	0.57
1:C:120:LYS:NZ	1:C:752:LEU:HD11	2.19	0.57
1:A:806:SER:O	1:A:816:THR:HG23	2.03	0.57
2:N:5:DA:H1'	2:N:6:DT:C5'	2.34	0.57
1:A:552:ASP:HB2	1:A:691:ALA:HB2	1.86	0.57
1:B:746:ARG:HB3	1:B:746:ARG:CZ	2.33	0.57
1:C:105:PHE:HE1	1:C:208:ASP:HB3	1.69	0.57
1:B:6:ILE:HG23	1:B:10:ASP:CG	2.24	0.57
1:A:229:LEU:HD13	1:A:244:ILE:HD13	1.85	0.57
1:B:475:PHE:CE1	1:B:478:ARG:NH1	2.72	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PRO:HD2	5:B:2144:HOH:O	2.04	0.57
2:N:17:DG:H2"	2:N:18:DC:C6	2.39	0.57
1:B:433:ASN:HB2	1:B:434:PRO:CD	2.34	0.57
1:B:671:ASN:HB2	5:B:2297:HOH:O	2.03	0.57
1:A:828:VAL:CG1	1:A:883:ALA:HA	2.34	0.57
1:C:777:GLY:O	1:C:781:ASN:HB2	2.05	0.57
1:C:425:ARG:HH21	1:C:784:HIS:CD2	2.23	0.57
1:C:551:ARG:NH1	1:C:551:ARG:HG2	2.19	0.57
1:C:281:ILE:CG2	1:C:282:THR:HG23	2.32	0.57
1:D:583:GLN:O	1:D:587:ILE:HG12	2.02	0.57
1:C:711:LYS:HB2	1:C:711:LYS:HZ3	1.67	0.57
2:H:7:DC:H5'	5:H:2008:HOH:O	2.05	0.57
1:B:419:ASN:N	1:B:419:ASN:HD22	2.01	0.57
1:D:555:GLY:O	1:D:559:VAL:HG22	2.05	0.57
1:A:829:ARG:HG3	1:A:829:ARG:HH11	1.69	0.57
1:D:105:PHE:HB3	5:D:2033:HOH:O	2.03	0.57
1:D:873:ARG:HH11	1:D:876:LEU:HD11	1.69	0.57
1:B:187:GLU:CD	1:B:199:GLU:OE2	2.43	0.57
1:D:832:MET:HG2	1:D:875:ILE:HD13	1.85	0.57
1:D:881:ALA:O	1:D:883:ALA:N	2.37	0.57
1:B:532:LEU:HD12	1:B:533:PRO:CD	2.30	0.57
1:D:551:ARG:HB2	1:D:868:GLY:H	1.69	0.57
1:C:491:ALA:HB1	1:C:499:ASN:ND2	2.19	0.57
1:D:74:ILE:HD12	5:D:2027:HOH:O	2.04	0.57
1:B:326:THR:HG23	1:B:806:SER:HA	1.86	0.57
1:B:15:GLU:OE2	1:B:18:ALA:O	2.22	0.57
1:C:158:GLU:OE2	1:C:195:LEU:HB3	2.04	0.57
1:D:134:VAL:HG12	1:D:242:GLU:O	2.04	0.57
1:D:322:ILE:HG13	5:D:2167:HOH:O	2.04	0.57
1:A:452:ILE:HD12	1:A:818:PRO:CB	2.34	0.57
1:C:681:ILE:O	1:C:685:VAL:HG13	2.05	0.57
1:D:437:ASN:C	1:D:437:ASN:HD22	2.08	0.57
1:C:810:ILE:O	1:C:810:ILE:HG22	2.03	0.57
1:D:154:ILE:HG23	1:D:190:MET:CE	2.33	0.57
1:C:96:ARG:HG2	1:C:96:ARG:NH1	2.18	0.57
1:A:164:LYS:HZ3	1:A:164:LYS:N	2.03	0.57
1:A:111:PRO:HG2	1:A:112:GLU:OE2	2.04	0.57
1:B:51:PHE:C	1:B:51:PHE:CD2	2.78	0.57
1:C:719:LEU:N	1:C:719:LEU:CD1	2.68	0.57
1:A:338:ALA:O	1:A:342:THR:HG23	2.04	0.57
1:C:463:HIS:HA	1:C:466:ASN:HD22	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:604:GLU:HG3	5:D:2141:HOH:O	2.04	0.57
1:C:172:LYS:HD2	3:L:3:G:H5"	1.85	0.57
1:A:204:TRP:HA	1:A:208:ASP:OD2	2.04	0.57
1:A:347:CYS:CB	1:A:350:GLU:HG3	2.34	0.57
1:C:30:GLU:HA	5:C:2031:HOH:O	2.05	0.57
1:C:96:ARG:H	1:C:96:ARG:HD2	1.69	0.57
1:C:860:LYS:HB2	5:C:2182:HOH:O	2.05	0.57
1:A:332:LYS:CE	1:A:410:ASN:HD22	2.18	0.57
1:A:78:LEU:O	1:A:82:ILE:HG13	2.05	0.57
1:D:281:ILE:HD11	1:D:308:TYR:CB	2.34	0.57
1:B:573:ILE:HD12	1:B:574:VAL:N	2.19	0.57
1:C:312:TYR:HA	5:C:2087:HOH:O	2.05	0.57
1:B:389:LYS:HA	1:B:392:LYS:HE2	1.86	0.57
1:D:52:ARG:HH21	1:D:52:ARG:HG3	1.70	0.57
1:C:882:PHE:N	1:C:882:PHE:HD1	2.03	0.56
2:E:12:DT:H2"	2:E:13:DC:C5'	2.35	0.56
1:C:154:ILE:HG23	1:C:190:MET:CE	2.32	0.56
1:A:213:GLY:O	1:A:217:ILE:HG13	2.05	0.56
1:C:810:ILE:CG2	3:L:8:U:H5'	2.35	0.56
1:C:555:GLY:HA3	5:C:2126:HOH:O	2.05	0.56
1:C:563:PRO:HB3	1:C:877:GLU:O	2.04	0.56
1:C:199:GLU:HG2	1:C:201:TRP:CD1	2.37	0.56
4:J:4:DG:H2"	4:J:5:DA:H8	1.68	0.56
1:D:475:PHE:N	1:D:476:PRO:HD2	2.20	0.56
1:C:502:TRP:CG	1:C:512:LEU:HD13	2.40	0.56
1:B:336:ALA:O	1:B:340:VAL:HG23	2.04	0.56
1:B:158:GLU:HA	1:B:195:LEU:CD2	2.36	0.56
1:B:710:VAL:CG1	1:B:720:ARG:HB3	2.36	0.56
1:B:84:ARG:HA	1:B:84:ARG:HH11	1.68	0.56
1:B:84:ARG:HD2	1:B:219:MET:CB	2.33	0.56
2:E:6:DT:H2"	2:E:7:DC:C5	2.40	0.56
1:A:155:ARG:CB	1:A:749:LEU:HD21	2.34	0.56
1:A:211:HIS:HB2	5:A:2093:HOH:O	2.05	0.56
1:A:214:VAL:O	1:A:218:GLU:HG3	2.05	0.56
1:D:632:ARG:HA	1:D:635:MET:HG2	1.86	0.56
1:D:719:LEU:N	1:D:719:LEU:HD12	2.21	0.56
1:D:406:ASN:HB2	5:D:2112:HOH:O	2.04	0.56
4:M:5:DA:H2"	4:M:6:DT:H72	1.87	0.56
1:A:56:GLU:C	1:A:56:GLU:OE1	2.43	0.56
1:D:737:GLN:HE22	1:D:778:ILE:HA	1.68	0.56
1:B:873:ARG:HD2	5:B:2345:HOH:O	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:PRO:HG2	1:B:429:VAL:HB	1.87	0.56
1:C:633:SER:HB3	1:C:646:PHE:CE1	2.41	0.56
1:B:6:ILE:O	1:B:10:ASP:HB3	2.05	0.56
1:D:422:TRP:C	1:D:422:TRP:CD1	2.79	0.56
1:B:342:THR:HG22	1:B:348:PRO:HG3	1.87	0.56
1:A:84:ARG:NH2	1:A:222:GLU:HB3	2.20	0.56
1:C:778:ILE:HG23	1:C:779:ALA:N	2.19	0.56
1:A:118:THR:CG2	1:A:216:CYS:HB3	2.35	0.56
1:A:391:ARG:NH1	1:A:391:ARG:HG2	2.19	0.56
1:A:721:LYS:HE2	5:A:2268:HOH:O	2.06	0.56
1:B:14:ILE:CG1	5:B:2134:HOH:O	2.54	0.56
1:D:43:SER:CA	1:D:46:MET:HE2	2.31	0.56
1:A:663:LYS:CG	1:A:664:GLY:N	2.68	0.56
1:C:6:ILE:O	1:C:10:ASP:HB3	2.06	0.56
1:D:52:ARG:HG3	1:D:52:ARG:NH2	2.20	0.56
1:B:89:PHE:O	1:B:93:LYS:HG3	2.05	0.56
1:A:487:GLU:HA	1:A:487:GLU:OE1	2.05	0.56
1:A:669:GLN:NE2	1:A:669:GLN:N	2.53	0.56
1:A:176:HIS:HA	5:A:2081:HOH:O	2.05	0.56
1:A:92:VAL:HG11	1:A:100:PRO:HD2	1.87	0.56
2:K:2:DG:H5'	5:K:2004:HOH:O	2.06	0.56
1:A:109:ILE:CG1	1:A:149:ALA:HB2	2.36	0.56
1:D:335:LEU:CD2	1:D:339:ASN:ND2	2.69	0.56
1:C:871:ASN:ND2	1:C:873:ARG:HB2	2.21	0.56
1:B:450:LYS:HE2	1:B:817:ILE:HD11	1.88	0.56
4:G:4:DG:H2''	4:G:5:DA:C8	2.41	0.56
1:B:854:HIS:HD2	1:B:856:SER:OG	1.89	0.56
1:D:339:ASN:O	1:D:343:LYS:CD	2.53	0.56
1:A:227:VAL:HB	1:A:244:ILE:CG2	2.35	0.56
1:A:312:TYR:CZ	1:A:314:PRO:HG3	2.41	0.56
1:D:811:HIS:HD2	5:D:2168:HOH:O	1.89	0.56
1:D:268:PHE:HB3	1:D:286:TYR:OH	2.05	0.56
1:B:67:ASN:O	1:B:71:LYS:HG3	2.06	0.56
1:C:711:LYS:HG3	1:C:718:ILE:HA	1.86	0.56
1:C:726:HIS:HD2	1:C:735:VAL:O	1.89	0.56
1:A:6:ILE:HG23	1:A:10:ASP:CG	2.25	0.56
1:A:215:ARG:HG2	5:A:2065:HOH:O	2.05	0.56
1:B:21:PHE:C	1:B:23:THR:H	2.09	0.56
1:A:592:ASN:OD1	1:A:611:LEU:CD2	2.53	0.56
1:B:473:VAL:CG1	1:B:477:GLU:HB3	2.34	0.56
1:C:631:LYS:O	1:C:634:VAL:HG13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:ILE:HG23	1:A:779:ALA:N	2.21	0.56
1:C:346:HIS:CE1	1:C:391:ARG:NH2	2.74	0.56
1:A:473:VAL:O	1:A:478:ARG:NE	2.36	0.56
1:B:349:VAL:HG12	1:B:349:VAL:O	2.06	0.56
1:C:829:ARG:HD3	1:C:875:ILE:O	2.05	0.56
1:B:423:ARG:NE	1:B:781:ASN:ND2	2.53	0.56
1:D:318:LYS:NZ	1:D:800:GLU:OE2	2.34	0.56
1:A:218:GLU:O	1:A:222:GLU:HG3	2.06	0.56
1:B:281:ILE:CG2	1:B:282:THR:HG23	2.33	0.56
1:C:631:LYS:HE2	1:C:635:MET:SD	2.46	0.56
1:C:313:MET:HA	5:C:2156:HOH:O	2.06	0.56
1:B:698:TRP:CZ2	1:B:864:LEU:HD21	2.41	0.56
1:A:580:GLU:OE2	5:A:2231:HOH:O	2.17	0.56
1:A:182:PHE:HB2	5:A:2082:HOH:O	2.05	0.55
1:D:335:LEU:HD11	1:D:406:ASN:OD1	2.06	0.55
1:B:657:PRO:HA	5:B:2292:HOH:O	2.06	0.55
1:B:324:GLN:CG	1:B:417:PRO:HA	2.36	0.55
1:C:155:ARG:HB3	1:C:155:ARG:NH1	2.21	0.55
1:C:78:LEU:N	1:C:79:PRO:HD2	2.22	0.55
1:D:213:GLY:O	1:D:217:ILE:HG13	2.06	0.55
1:C:2:ASN:N	5:C:2003:HOH:O	2.40	0.55
1:D:428:ALA:H	1:D:435:GLN:HE22	1.54	0.55
1:B:332:LYS:N	5:B:2151:HOH:O	2.35	0.55
1:D:201:TRP:O	1:D:204:TRP:HB2	2.05	0.55
1:D:711:LYS:HA	1:D:719:LEU:HD13	1.87	0.55
4:M:6:DT:H2"	4:M:7:DT:OP2	2.07	0.55
1:D:220:LEU:O	1:D:220:LEU:HD12	2.05	0.55
1:A:595:VAL:HG13	5:A:2237:HOH:O	2.06	0.55
1:C:791:LEU:HD21	1:C:809:LEU:HD22	1.87	0.55
1:B:308:TYR:HA	1:B:311:VAL:HG23	1.87	0.55
1:D:231:ARG:HG2	1:D:234:ALA:HB2	1.88	0.55
1:A:210:ILE:O	1:A:214:VAL:HG23	2.07	0.55
1:B:170:LEU:CD2	1:B:179:LYS:HD3	2.37	0.55
1:B:422:TRP:CD1	1:B:422:TRP:O	2.59	0.55
1:C:553:GLU:HG2	1:C:554:VAL:N	2.22	0.55
1:D:462:ILE:HG22	1:D:466:ASN:HD21	1.71	0.55
1:C:614:LYS:HE2	5:C:2137:HOH:O	2.06	0.55
1:D:342:THR:HA	5:D:2092:HOH:O	2.07	0.55
1:C:373:ALA:O	1:C:377:TRP:CD1	2.60	0.55
1:B:148:GLU:OE2	1:B:749:LEU:HB2	2.05	0.55
1:A:230:HIS:HE2	1:A:245:GLU:CG	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:LYS:N	1:C:72:PRO:HD2	2.22	0.55
1:C:272:VAL:O	1:C:415:TRP:HZ3	1.89	0.55
1:B:391:ARG:NH1	1:B:391:ARG:HB3	2.21	0.55
1:B:374:LEU:N	1:B:374:LEU:HD12	2.21	0.55
1:B:158:GLU:HB3	1:B:190:MET:CE	2.36	0.55
1:D:150:ARG:HG3	1:D:201:TRP:NE1	2.20	0.55
1:A:105:PHE:HE1	5:A:2093:HOH:O	1.89	0.55
1:B:401:MET:HE1	1:B:432:PHE:CA	2.36	0.55
1:C:432:PHE:CE1	1:C:440:THR:HG23	2.42	0.55
1:D:59:LEU:HA	1:D:64:VAL:HG22	1.87	0.55
1:B:99:ARG:HG2	1:B:103:PHE:CE2	2.42	0.55
1:B:669:GLN:HG2	1:B:672:GLN:HE21	1.71	0.55
1:C:230:HIS:CD2	1:C:230:HIS:H	2.24	0.55
1:A:179:LYS:HD3	5:A:2081:HOH:O	2.06	0.55
1:B:158:GLU:HA	1:B:195:LEU:HD13	1.89	0.55
1:D:448:LYS:HE3	5:D:2087:HOH:O	2.07	0.55
2:K:2:DG:C2'	2:K:3:DG:C8	2.89	0.55
1:C:291:ARG:C	1:C:293:PRO:HD3	2.26	0.55
1:B:676:TYR:O	1:B:679:LYS:HB3	2.06	0.55
1:A:551:ARG:NH2	1:A:836:TYR:O	2.39	0.55
1:D:428:ALA:H	1:D:435:GLN:NE2	2.04	0.55
1:D:278:TRP:CD2	1:D:284:GLY:HA3	2.42	0.55
1:A:633:SER:HB3	1:A:646:PHE:CD1	2.42	0.55
1:B:157:LEU:HG	1:B:158:GLU:N	2.21	0.55
1:D:420:MET:HA	1:D:425:ARG:O	2.07	0.55
1:A:169:GLN:HB2	1:A:182:PHE:CZ	2.42	0.55
1:B:711:LYS:HB3	1:B:717:GLU:O	2.07	0.55
1:B:126:LEU:HA	5:B:2083:HOH:O	2.05	0.55
1:A:448:LYS:HG2	5:A:2287:HOH:O	2.07	0.55
1:A:714:LYS:HZ3	1:A:714:LYS:HA	1.71	0.55
1:C:324:GLN:HE21	1:C:418:TYR:N	2.05	0.55
1:B:159:ALA:O	1:B:163:LYS:HB2	2.06	0.55
1:C:882:PHE:O	1:C:883:ALA:CB	2.54	0.55
1:D:327:ALA:HB3	1:D:448:LYS:HE2	1.88	0.55
1:C:422:TRP:CE2	1:C:423:ARG:HD2	2.41	0.55
2:K:4:DA:H2''	2:K:5:DA:OP2	2.07	0.55
1:C:16:LEU:HD13	1:C:38:ALA:HB2	1.88	0.55
1:A:154:ILE:HA	1:A:158:GLU:HB2	1.88	0.55
1:C:21:PHE:C	1:C:23:THR:H	2.10	0.55
1:B:99:ARG:HB3	1:B:103:PHE:CD2	2.42	0.55
1:D:552:ASP:OD1	1:D:555:GLY:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:553:GLU:HG2	1:C:554:VAL:H	1.72	0.55
1:D:158:GLU:OE1	1:D:195:LEU:HD22	2.07	0.55
1:A:313:MET:HB2	1:A:316:VAL:CG2	2.37	0.55
1:B:315:GLU:OE2	1:B:318:LYS:HD3	2.07	0.55
2:K:6:DT:H2"	2:K:7:DC:C5	2.42	0.55
1:C:120:LYS:HG3	1:C:752:LEU:HD21	1.89	0.55
1:D:84:ARG:CG	1:D:84:ARG:HH11	2.19	0.55
1:D:14:ILE:HG22	5:D:2014:HOH:O	2.06	0.55
1:A:110:LYS:HE2	1:A:112:GLU:OE1	2.07	0.55
1:B:632:ARG:HD3	1:B:632:ARG:H	1.71	0.55
1:D:69:ALA:HA	1:D:257:ARG:HD2	1.89	0.55
1:C:754:GLN:HG2	5:C:2160:HOH:O	2.05	0.54
1:C:711:LYS:HG2	1:C:718:ILE:CA	2.36	0.54
1:B:489:ILE:CG2	1:B:518:TYR:CD1	2.88	0.54
1:D:227:VAL:HB	1:D:244:ILE:HG23	1.89	0.54
1:A:142:GLY:CA	5:A:2072:HOH:O	2.55	0.54
1:C:434:PRO:HG3	1:C:444:LEU:HD13	1.89	0.54
1:C:36:GLN:HA	1:C:36:GLN:OE1	2.05	0.54
1:B:567:VAL:HG22	1:B:880:PHE:CG	2.43	0.54
1:D:150:ARG:HA	1:D:201:TRP:CZ2	2.42	0.54
1:D:551:ARG:NH1	1:D:872:LEU:CD1	2.71	0.54
1:B:804:ILE:HG12	1:B:820:ASP:HB3	1.89	0.54
1:D:794:THR:HG21	1:D:828:VAL:HG12	1.89	0.54
1:B:80:LYS:HD3	1:B:223:SER:O	2.08	0.54
1:A:804:ILE:HG12	1:A:820:ASP:HB3	1.89	0.54
1:C:656:GLN:HB3	1:C:657:PRO:HD3	1.89	0.54
1:D:713:LYS:NZ	1:D:713:LYS:HA	2.22	0.54
1:D:873:ARG:NH1	1:D:876:LEU:HD11	2.23	0.54
1:C:676:TYR:O	1:C:679:LYS:HB3	2.08	0.54
1:B:12:SER:HA	5:B:2033:HOH:O	2.06	0.54
1:A:571:TYR:CD1	1:A:631:LYS:HA	2.42	0.54
1:A:204:TRP:HZ2	5:A:2067:HOH:O	1.89	0.54
1:C:846:TYR:HA	1:C:849:PHE:CE1	2.43	0.54
1:A:230:HIS:CD2	1:A:230:HIS:H	2.25	0.54
1:D:217:ILE:O	1:D:221:ILE:HG13	2.07	0.54
1:C:395:ARG:O	1:C:399:GLU:HG3	2.07	0.54
1:A:826:LYS:HG2	1:A:830:GLU:OE2	2.08	0.54
1:B:272:VAL:CG1	1:B:411:HIS:HD2	2.20	0.54
1:C:475:PHE:N	1:C:476:PRO:HD2	2.22	0.54
1:B:710:VAL:HG12	1:B:720:ARG:HB3	1.89	0.54
1:B:216:CYS:HA	1:B:219:MET:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ALA:HB3	1:A:433:ASN:HD22	1.72	0.54
1:C:702:ALA:O	1:C:706:LEU:HD12	2.07	0.54
1:B:401:MET:HE2	1:B:432:PHE:HD1	1.73	0.54
1:D:169:GLN:O	1:D:173:ARG:HG2	2.07	0.54
1:B:73:LEU:CD1	1:B:254:ILE:HG13	2.38	0.54
1:A:726:HIS:HB2	1:A:736:TRP:CD1	2.43	0.54
1:C:790:HIS:NE2	1:C:832:MET:HB2	2.22	0.54
1:D:134:VAL:HA	5:D:2038:HOH:O	2.06	0.54
1:B:155:ARG:HB3	5:B:2088:HOH:O	2.07	0.54
1:C:47:GLY:O	1:C:50:ARG:HB3	2.08	0.54
1:D:84:ARG:HD3	1:D:84:ARG:O	2.06	0.54
1:C:57:ARG:HD2	5:C:2041:HOH:O	2.07	0.54
1:D:56:GLU:OE2	1:D:57:ARG:N	2.41	0.54
1:D:56:GLU:OE1	1:D:60:LYS:HB2	2.06	0.54
1:C:514:PHE:C	1:C:514:PHE:CD1	2.80	0.54
1:A:881:ALA:CA	5:A:2310:HOH:O	2.55	0.54
1:B:221:ILE:HG12	1:B:227:VAL:HG23	1.89	0.54
1:B:21:PHE:C	1:B:23:THR:N	2.61	0.54
1:A:14:ILE:HG23	1:A:288:ALA:CB	2.37	0.54
2:E:17:DG:H2"	2:E:18:DC:C6	2.41	0.54
1:A:71:LYS:N	1:A:72:PRO:CD	2.71	0.54
1:B:130:ASP:O	1:B:132:THR:HG23	2.07	0.54
1:D:869:ASN:HD22	1:D:869:ASN:N	2.06	0.54
1:A:468:ALA:HB3	5:A:2175:HOH:O	2.08	0.54
1:D:108:GLU:HG3	5:D:2034:HOH:O	2.07	0.54
1:B:264:ILE:O	1:B:264:ILE:HG22	2.08	0.54
1:C:229:LEU:HD11	1:C:242:GLU:HG2	1.89	0.54
1:B:720:ARG:HH11	1:B:720:ARG:CG	2.06	0.54
1:A:814:PHE:N	1:A:814:PHE:CD1	2.75	0.54
1:B:18:ALA:O	1:B:19:ILE:HG12	2.08	0.54
1:B:432:PHE:CZ	1:B:444:LEU:HD21	2.43	0.54
1:C:19:ILE:O	1:C:21:PHE:N	2.39	0.54
1:D:80:LYS:CD	1:D:224:THR:HG22	2.37	0.54
1:A:6:ILE:HB	1:A:48:GLU:OE2	2.08	0.54
1:D:824:LEU:O	1:D:828:VAL:HG13	2.08	0.54
1:D:814:PHE:CE1	1:D:883:ALA:HB2	2.43	0.54
1:B:21:PHE:O	1:B:21:PHE:CD1	2.59	0.54
1:B:404:GLN:HG2	1:B:432:PHE:HB3	1.90	0.54
1:D:446:LEU:HD12	1:D:817:ILE:HG22	1.90	0.54
1:A:308:TYR:O	1:A:311:VAL:HG23	2.08	0.54
3:I:4:G:H5'	5:I:2003:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:PHE:C	1:B:51:PHE:HD2	2.10	0.54
1:C:324:GLN:HE21	1:C:417:PRO:HA	1.73	0.54
1:B:391:ARG:CB	1:B:391:ARG:HH11	2.20	0.54
1:B:644:PHE:CE2	2:H:9:DA:C4	2.95	0.54
1:B:631:LYS:HD3	1:B:632:ARG:HH11	1.72	0.54
1:A:486:HIS:HD2	1:A:518:TYR:OH	1.90	0.54
1:C:825:PHE:CZ	1:C:829:ARG:NH2	2.76	0.54
1:A:341:ILE:HD12	1:A:348:PRO:HB3	1.90	0.54
1:A:713:LYS:C	1:A:713:LYS:HE3	2.28	0.54
3:F:6:G:N7	5:F:2013:HOH:O	2.34	0.54
1:D:230:HIS:H	1:D:230:HIS:CD2	2.26	0.54
1:A:669:GLN:CA	1:A:669:GLN:HE21	2.21	0.53
1:B:115:ALA:O	1:B:119:ILE:HG12	2.09	0.53
1:D:16:LEU:HD22	1:D:38:ALA:HA	1.90	0.53
1:A:623:TYR:HD1	1:A:663:LYS:HE3	1.72	0.53
1:C:646:PHE:HD1	1:C:649:GLN:OE1	1.90	0.53
1:A:422:TRP:O	1:A:422:TRP:CD1	2.62	0.53
1:B:116:TYR:CD1	1:B:746:ARG:NH2	2.76	0.53
1:B:754:GLN:HG3	5:B:2065:HOH:O	2.07	0.53
1:C:92:VAL:CG1	1:C:99:ARG:HG3	2.38	0.53
1:D:58:GLN:HB3	5:D:2026:HOH:O	2.09	0.53
1:B:99:ARG:HD2	1:B:99:ARG:N	2.23	0.53
1:C:582:LEU:HB3	1:C:621:LEU:HD21	1.90	0.53
1:C:473:VAL:HG13	1:C:477:GLU:HB2	1.89	0.53
1:A:63:GLU:HA	5:A:2057:HOH:O	2.08	0.53
1:A:109:ILE:H	1:A:109:ILE:HD12	1.71	0.53
1:A:80:LYS:HE2	1:A:223:SER:O	2.08	0.53
1:C:120:LYS:HZ3	1:C:752:LEU:CD1	2.20	0.53
1:B:651:LEU:O	1:B:656:GLN:HB2	2.09	0.53
1:C:570:ILE:HA	1:C:573:ILE:CG2	2.37	0.53
1:A:842:LEU:O	1:A:845:PHE:HB3	2.08	0.53
1:D:162:PHE:HB2	5:D:2045:HOH:O	2.07	0.53
1:B:50:ARG:HH21	1:B:267:MET:HG2	1.72	0.53
1:B:7:ALA:HB1	5:B:2057:HOH:O	2.09	0.53
1:B:748:ASN:HD22	1:B:752:LEU:N	2.05	0.53
1:C:551:ARG:HE	1:C:872:LEU:HD21	1.72	0.53
1:D:349:VAL:C	5:D:2096:HOH:O	2.46	0.53
1:B:416:PHE:HD1	1:B:430:SER:OG	1.90	0.53
1:A:161:HIS:O	1:A:164:LYS:HG2	2.08	0.53
1:B:552:ASP:O	1:B:870:LEU:HD12	2.08	0.53
1:D:32:LEU:CD1	1:D:32:LEU:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ILE:HB	5:B:2174:HOH:O	2.08	0.53
1:A:100:PRO:HG2	1:A:103:PHE:CB	2.35	0.53
1:C:182:PHE:O	1:C:185:VAL:HG23	2.09	0.53
1:C:205:HIS:O	1:C:207:GLU:N	2.41	0.53
1:B:278:TRP:CD2	1:B:284:GLY:HA3	2.44	0.53
1:B:324:GLN:HE21	1:B:418:TYR:N	2.06	0.53
1:B:162:PHE:CE1	1:B:190:MET:SD	3.02	0.53
1:D:414:ILE:HA	5:D:2115:HOH:O	2.08	0.53
1:D:151:PHE:CD1	1:D:183:MET:HB3	2.44	0.53
2:E:7:DC:C4	2:E:8:DG:N7	2.77	0.53
1:B:155:ARG:O	1:B:155:ARG:HG2	2.07	0.53
1:A:652:GLU:HA	1:A:656:GLN:HB2	1.91	0.53
1:D:37:LEU:HD13	5:D:2014:HOH:O	2.09	0.53
1:C:64:VAL:HG21	1:C:127:THR:HG21	1.90	0.53
1:B:726:HIS:CD2	1:B:736:TRP:NE1	2.76	0.53
1:A:141:ILE:O	1:A:145:ILE:HG12	2.08	0.53
1:D:743:ILE:HG13	1:D:766:ASP:O	2.08	0.53
1:D:730:PRO:CD	1:D:786:GLN:HE22	2.21	0.53
1:D:379:ARG:HA	5:D:2109:HOH:O	2.09	0.53
1:B:840:ASP:O	1:B:842:LEU:N	2.42	0.53
1:B:797:TRP:CH2	1:B:801:LYS:HG3	2.42	0.53
1:C:227:VAL:CG1	1:C:244:ILE:HG22	2.38	0.53
1:B:158:GLU:HB3	1:B:190:MET:HE1	1.90	0.53
1:C:164:LYS:CA	1:C:164:LYS:HE2	2.39	0.53
1:B:712:ASP:OD2	1:B:714:LYS:HB2	2.09	0.53
1:D:486:HIS:C	1:D:486:HIS:HD1	2.12	0.53
1:A:21:PHE:C	1:A:23:THR:H	2.12	0.53
1:C:205:HIS:C	1:C:207:GLU:N	2.62	0.53
1:B:346:HIS:HA	1:B:395:ARG:NH1	2.23	0.53
1:D:32:LEU:CD1	1:D:32:LEU:H	2.22	0.53
1:A:846:TYR:HD2	1:A:849:PHE:CZ	2.27	0.53
1:C:544:GLN:HG2	1:C:561:LEU:HD13	1.90	0.53
1:C:180:LYS:HG2	1:C:184:GLN:OE1	2.08	0.53
1:C:146:GLU:HB2	1:C:204:TRP:CZ3	2.43	0.53
4:P:4:DG:H2"	4:P:5:DA:H8	1.71	0.53
1:D:319:ALA:HB1	1:D:792:ARG:HG2	1.91	0.53
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.09	0.53
1:D:36:GLN:HG3	1:D:273:VAL:CG2	2.38	0.53
1:D:201:TRP:HA	1:D:204:TRP:CD1	2.44	0.53
1:B:537:ASP:N	1:B:882:PHE:HD2	2.07	0.53
1:B:719:LEU:HD12	1:B:719:LEU:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:TYR:CA	1:A:311:VAL:HG23	2.39	0.53
2:K:15:DC:H2"	2:K:16:DC:O5'	2.08	0.53
1:A:114:VAL:HG13	1:A:145:ILE:HD12	1.91	0.53
1:B:44:TYR:OH	1:B:292:ARG:HB3	2.08	0.53
1:A:19:ILE:O	1:A:21:PHE:N	2.39	0.53
1:C:416:PHE:CE2	1:C:434:PRO:HD3	2.44	0.53
1:C:35:GLU:OE2	1:C:272:VAL:HG11	2.09	0.53
1:C:854:HIS:HD2	1:C:856:SER:OG	1.92	0.53
1:C:5:ASN:HD21	1:C:7:ALA:C	2.12	0.53
1:D:412:LYS:N	5:D:2114:HOH:O	2.36	0.53
1:A:217:ILE:HG22	1:A:221:ILE:CD1	2.38	0.52
1:A:134:VAL:CG2	1:A:244:ILE:HD11	2.39	0.52
1:A:656:GLN:HB3	1:A:657:PRO:CD	2.39	0.52
1:B:551:ARG:HB2	1:B:868:GLY:H	1.72	0.52
1:C:68:ALA:CB	1:C:261:LEU:HD21	2.39	0.52
1:A:82:ILE:HG21	5:A:2068:HOH:O	2.10	0.52
1:D:71:LYS:N	1:D:72:PRO:HD2	2.25	0.52
1:B:490:MET:HE2	1:B:522:GLN:HG3	1.91	0.52
1:B:614:LYS:HB3	5:B:2261:HOH:O	2.08	0.52
1:B:393:SER:HB3	5:H:2017:HOH:O	2.09	0.52
1:D:623:TYR:CD1	1:D:663:LYS:HE2	2.43	0.52
1:B:573:ILE:CD1	1:B:573:ILE:C	2.60	0.52
1:B:257:ARG:HB2	5:B:2123:HOH:O	2.09	0.52
2:E:4:DA:H2"	2:E:5:DA:N7	2.24	0.52
1:A:105:PHE:CE1	1:A:208:ASP:HB3	2.44	0.52
1:C:16:LEU:HD13	1:C:38:ALA:CB	2.39	0.52
1:B:105:PHE:HB3	1:B:204:TRP:CZ2	2.45	0.52
1:A:423:ARG:NE	1:A:781:ASN:ND2	2.56	0.52
1:C:120:LYS:HG3	1:C:752:LEU:CD2	2.39	0.52
1:D:109:ILE:HG12	5:D:2041:HOH:O	2.09	0.52
1:D:85:ILE:HG22	1:D:89:PHE:CE1	2.45	0.52
1:B:231:ARG:HD2	1:B:240:ASP:OD1	2.09	0.52
1:B:39:LEU:HD13	1:B:272:VAL:CG2	2.39	0.52
1:D:411:HIS:HB3	5:D:2114:HOH:O	2.08	0.52
1:A:395:ARG:HG3	1:A:395:ARG:O	2.09	0.52
1:A:632:ARG:HH11	1:A:632:ARG:CB	2.20	0.52
1:B:116:TYR:HE2	1:B:752:LEU:HD22	1.74	0.52
1:A:428:ALA:N	1:A:435:GLN:NE2	2.48	0.52
1:D:353:PRO:HD3	5:D:2098:HOH:O	2.10	0.52
1:B:168:GLU:OE1	1:B:169:GLN:N	2.33	0.52
1:D:574:VAL:O	1:D:578:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:VAL:HG21	5:D:2029:HOH:O	2.09	0.52
1:D:16:LEU:HD13	1:D:38:ALA:CB	2.38	0.52
1:B:551:ARG:N	5:B:2240:HOH:O	2.41	0.52
1:D:710:VAL:HG21	1:D:854:HIS:CD2	2.44	0.52
1:C:424:GLY:HA3	5:C:2102:HOH:O	2.09	0.52
1:D:588:ASN:N	1:D:588:ASN:HD22	2.06	0.52
1:A:106:LEU:HD21	5:A:2094:HOH:O	2.09	0.52
1:B:74:ILE:HG22	1:B:755:PHE:HE2	1.74	0.52
1:A:372:GLU:N	5:A:2145:HOH:O	2.41	0.52
1:B:63:GLU:OE1	2:H:18:DC:H2"	2.09	0.52
1:A:312:TYR:HB3	5:A:2131:HOH:O	2.10	0.52
1:C:556:GLY:O	1:C:561:LEU:HB2	2.09	0.52
1:D:21:PHE:C	1:D:23:THR:H	2.12	0.52
1:B:881:ALA:O	1:B:883:ALA:N	2.42	0.52
1:A:205:HIS:C	1:A:207:GLU:H	2.13	0.52
1:A:122:THR:HG22	1:A:126:LEU:CD1	2.35	0.52
1:A:347:CYS:CB	1:A:350:GLU:CG	2.87	0.52
1:D:278:TRP:CE3	1:D:284:GLY:HA3	2.45	0.52
1:B:9:ASN:HA	1:B:12:SER:HB3	1.91	0.52
1:C:756:ARG:HG2	5:C:2161:HOH:O	2.09	0.52
1:D:806:SER:O	1:D:816:THR:CG2	2.51	0.52
1:B:595:VAL:HG12	1:B:596:THR:N	2.25	0.52
1:C:792:ARG:O	1:C:796:VAL:HG23	2.10	0.52
1:A:555:GLY:O	1:A:559:VAL:HG22	2.08	0.52
1:A:668:THR:C	1:A:669:GLN:HE21	2.12	0.52
1:D:15:GLU:HB2	1:D:18:ALA:O	2.09	0.52
1:D:36:GLN:HG2	5:D:2021:HOH:O	2.10	0.52
1:A:146:GLU:HG3	1:A:204:TRP:CE3	2.44	0.52
1:A:21:PHE:C	1:A:23:THR:N	2.63	0.52
1:C:752:LEU:N	1:C:752:LEU:HD12	2.25	0.52
1:C:402:LEU:HG	1:C:439:MET:HE2	1.91	0.52
1:D:59:LEU:CD2	1:D:64:VAL:HG22	2.39	0.52
1:D:264:ILE:HB	5:D:2068:HOH:O	2.10	0.52
1:D:177:VAL:HG12	1:D:178:TYR:HD2	1.75	0.52
1:A:629:VAL:HG11	1:A:677:MET:HE3	1.92	0.52
1:A:677:MET:O	1:A:681:ILE:HG13	2.10	0.52
1:B:557:ARG:NH1	5:B:2244:HOH:O	2.43	0.52
1:A:743:ILE:HG22	1:A:743:ILE:O	2.10	0.52
1:D:545:HIS:O	1:D:549:MET:HG2	2.10	0.52
2:E:2:DG:H2"	2:E:3:DG:C8	2.42	0.52
1:B:401:MET:HE1	1:B:432:PHE:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:HD13	1:D:651:LEU:O	2.10	0.52
1:A:243:THR:O	1:A:244:ILE:HD13	2.09	0.52
1:D:81:MET:HE1	1:D:220:LEU:HB2	1.91	0.52
1:A:163:LYS:HB3	1:A:164:LYS:HZ3	1.73	0.52
2:N:11:DA:H2''	2:N:12:DT:O5'	2.10	0.52
1:C:814:PHE:N	1:C:814:PHE:CD1	2.78	0.52
1:B:203:SER:O	1:B:205:HIS:N	2.43	0.52
1:B:146:GLU:HG3	1:B:204:TRP:CE3	2.45	0.52
1:D:347:CYS:O	1:D:349:VAL:N	2.43	0.52
1:B:232:GLN:HG2	1:B:241:SER:O	2.10	0.52
1:B:812:ASP:OD1	3:I:8:U:O3'	2.26	0.52
1:A:692:ALA:O	1:A:696:MET:HG3	2.09	0.52
1:B:158:GLU:CA	1:B:195:LEU:HD22	2.37	0.52
1:B:754:GLN:HE22	3:I:1:G:H4'	1.75	0.52
1:D:215:ARG:CG	5:D:2030:HOH:O	2.58	0.52
1:B:422:TRP:CD1	1:B:422:TRP:C	2.83	0.52
1:A:551:ARG:CZ	1:A:872:LEU:HD11	2.40	0.52
1:B:99:ARG:HB3	1:B:103:PHE:HD2	1.74	0.52
1:D:743:ILE:HD12	1:D:766:ASP:HB2	1.92	0.52
1:A:50:ARG:HG2	1:A:50:ARG:NH1	2.24	0.52
1:D:422:TRP:O	1:D:422:TRP:CD1	2.63	0.51
1:B:14:ILE:HG22	1:B:14:ILE:O	2.11	0.51
1:A:777:GLY:O	1:A:781:ASN:HB2	2.11	0.51
1:C:19:ILE:HG23	1:C:20:PRO:HD2	1.91	0.51
1:B:185:VAL:HG23	1:B:186:VAL:N	2.24	0.51
1:B:374:LEU:H	1:B:374:LEU:CD1	2.23	0.51
1:D:882:PHE:O	1:D:883:ALA:CB	2.58	0.51
1:D:154:ILE:CG2	1:D:190:MET:HE1	2.38	0.51
1:B:341:ILE:HG13	1:B:348:PRO:HB3	1.91	0.51
2:H:6:DT:H2''	2:H:7:DC:C5	2.44	0.51
1:C:21:PHE:C	1:C:23:THR:N	2.61	0.51
1:D:560:ASN:OD1	1:D:568:GLN:HB2	2.09	0.51
1:D:623:TYR:HD1	1:D:666:MET:HE1	1.75	0.51
1:C:425:ARG:HH21	1:C:784:HIS:CG	2.28	0.51
1:A:105:PHE:HA	5:A:2067:HOH:O	2.11	0.51
1:D:318:LYS:O	1:D:322:ILE:HG12	2.11	0.51
1:A:706:LEU:HD21	1:A:849:PHE:HB2	1.91	0.51
1:C:572:GLY:O	1:C:576:LYS:HG3	2.11	0.51
1:C:329:LYS:HG3	1:C:445:THR:HG23	1.92	0.51
1:D:721:LYS:HG2	1:D:722:ARG:N	2.24	0.51
1:B:398:LEU:C	1:B:398:LEU:CD2	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ALA:CB	1:A:120:LYS:HG2	2.39	0.51
1:A:824:LEU:O	1:A:828:VAL:HG23	2.09	0.51
1:D:199:GLU:HG3	1:D:201:TRP:HD1	1.75	0.51
1:A:143:ARG:NH1	5:A:2073:HOH:O	2.42	0.51
1:D:89:PHE:CD2	1:D:103:PHE:HE1	2.28	0.51
1:C:546:PHE:CE1	1:C:783:VAL:HG13	2.46	0.51
1:A:228:SER:HA	5:A:2100:HOH:O	2.09	0.51
1:A:517:GLU:HG3	1:A:532:LEU:HB2	1.92	0.51
1:A:183:MET:HB2	5:A:2084:HOH:O	2.10	0.51
1:D:556:GLY:O	1:D:561:LEU:HB2	2.10	0.51
1:D:655:ILE:HD12	1:D:674:ALA:HB2	1.92	0.51
1:B:253:ALA:HB1	5:B:2001:HOH:O	2.10	0.51
1:A:386:ARG:HG3	3:F:4:G:H5"	1.93	0.51
1:B:747:LEU:HD13	5:B:2316:HOH:O	2.10	0.51
1:D:19:ILE:HG23	1:D:20:PRO:CD	2.39	0.51
1:D:829:ARG:HD3	1:D:875:ILE:CG2	2.40	0.51
1:B:227:VAL:HB	1:B:244:ILE:CG2	2.41	0.51
1:C:373:ALA:C	1:C:377:TRP:NE1	2.64	0.51
1:C:308:TYR:HA	1:C:311:VAL:HG23	1.93	0.51
1:A:142:GLY:N	5:A:2072:HOH:O	2.43	0.51
1:C:743:ILE:HD12	1:C:766:ASP:HB3	1.92	0.51
1:A:47:GLY:HA3	1:A:265:SER:O	2.10	0.51
1:B:308:TYR:HA	1:B:311:VAL:CG2	2.41	0.51
1:C:480:LYS:O	1:C:484:GLU:HG3	2.11	0.51
1:C:398:LEU:C	1:C:398:LEU:HD23	2.31	0.51
1:A:704:LYS:HZ2	1:A:860:LYS:HD2	1.75	0.51
1:C:828:VAL:O	1:C:831:THR:HG22	2.11	0.51
1:D:814:PHE:CE1	1:D:883:ALA:CB	2.92	0.51
2:K:6:DT:H2"	2:K:7:DC:OP2	2.10	0.51
1:D:153:ARG:NH2	1:D:201:TRP:NE1	2.52	0.51
1:B:92:VAL:HG12	1:B:99:ARG:HG3	1.93	0.51
1:C:275:PRO:HB2	1:C:324:GLN:HG2	1.93	0.51
1:D:871:ASN:HD21	1:D:873:ARG:HB2	1.75	0.51
1:D:2:ASN:HB2	5:D:2002:HOH:O	2.10	0.51
1:C:25:ALA:HA	1:C:29:GLY:O	2.11	0.51
1:B:53:LYS:O	1:B:56:GLU:HB3	2.11	0.51
1:A:860:LYS:O	1:A:862:PRO:HD3	2.10	0.51
1:D:275:PRO:HG2	1:D:324:GLN:HG2	1.92	0.51
1:C:120:LYS:CD	1:C:752:LEU:HD11	2.41	0.51
1:D:78:LEU:N	1:D:79:PRO:HD2	2.25	0.51
1:B:178:TYR:CD1	1:B:178:TYR:N	2.77	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:VAL:CG1	1:C:477:GLU:HB2	2.41	0.51
1:D:25:ALA:HA	1:D:29:GLY:O	2.11	0.51
1:C:730:PRO:HD2	1:C:786:GLN:NE2	2.25	0.51
1:D:454:LYS:HG3	1:D:455:GLU:N	2.25	0.51
1:D:882:PHE:N	1:D:882:PHE:CD1	2.71	0.51
1:D:272:VAL:O	1:D:272:VAL:HG12	2.11	0.51
1:D:633:SER:CA	1:D:649:GLN:HE22	2.14	0.51
1:A:208:ASP:HA	5:A:2093:HOH:O	2.10	0.51
1:C:154:ILE:HD13	1:C:190:MET:HE1	1.92	0.51
1:C:191:LEU:HD23	1:C:195:LEU:O	2.11	0.51
4:M:4:DG:H2"	4:M:5:DA:C8	2.46	0.51
1:B:726:HIS:HD2	1:B:736:TRP:CE2	2.28	0.51
1:C:744:GLN:HB3	1:C:756:ARG:HB3	1.92	0.51
1:D:47:GLY:HA3	1:D:265:SER:O	2.11	0.51
1:A:861:MET:HE3	1:A:862:PRO:HD2	1.93	0.51
1:D:281:ILE:CG2	1:D:282:THR:HG23	2.30	0.51
1:A:720:ARG:HD2	1:A:852:GLN:O	2.10	0.51
1:B:423:ARG:NH2	2:H:12:DT:O4'	2.44	0.51
1:D:242:GLU:HG3	5:D:2060:HOH:O	2.11	0.51
1:C:751:PHE:HB3	1:C:752:LEU:CD1	2.39	0.51
1:C:205:HIS:C	1:C:207:GLU:H	2.14	0.51
1:C:59:LEU:HA	1:C:64:VAL:CG2	2.41	0.51
1:C:199:GLU:O	1:C:199:GLU:HG2	2.11	0.51
1:B:648:GLN:O	1:B:652:GLU:HG2	2.11	0.51
1:D:335:LEU:HD12	5:D:2090:HOH:O	2.11	0.50
1:A:230:HIS:CD2	1:A:232:GLN:HE22	2.29	0.50
1:C:608:LYS:HG3	5:C:2141:HOH:O	2.12	0.50
1:C:317:TYR:O	1:C:321:ASN:ND2	2.42	0.50
1:A:457:TYR:CE2	1:A:461:LYS:HD3	2.45	0.50
1:B:600:GLU:HG3	5:B:2268:HOH:O	2.11	0.50
1:D:791:LEU:HG	1:D:809:LEU:HD22	1.93	0.50
1:B:540:CYS:HB3	5:B:2238:HOH:O	2.11	0.50
1:C:422:TRP:CE3	5:C:2101:HOH:O	2.53	0.50
1:C:373:ALA:HB3	1:C:374:LEU:HD12	1.93	0.50
1:D:210:ILE:O	1:D:214:VAL:HG23	2.11	0.50
1:D:84:ARG:HB2	1:D:223:SER:HB3	1.94	0.50
1:D:165:ASN:O	1:D:169:GLN:NE2	2.45	0.50
1:B:597:VAL:HG22	5:B:2264:HOH:O	2.12	0.50
1:D:553:GLU:HG2	1:D:554:VAL:N	2.26	0.50
1:B:562:LEU:HD23	1:B:562:LEU:N	2.26	0.50
1:B:737:GLN:HE21	1:B:739:TYR:HE2	1.57	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ALA:O	1:A:119:ILE:CD1	2.59	0.50
1:B:797:TRP:CZ2	1:B:801:LYS:HG3	2.46	0.50
1:B:729:THR:HB	1:B:789:SER:HB2	1.93	0.50
1:D:546:PHE:CE1	1:D:783:VAL:HG13	2.46	0.50
1:B:25:ALA:HA	1:B:29:GLY:O	2.11	0.50
2:E:10:DC:H2"	2:E:11:DA:OP2	2.12	0.50
1:C:663:LYS:HG2	1:C:664:GLY:N	2.24	0.50
1:D:85:ILE:HG22	1:D:89:PHE:CD1	2.46	0.50
1:C:57:ARG:HD3	5:K:2015:HOH:O	2.11	0.50
1:D:778:ILE:CG2	1:D:779:ALA:N	2.74	0.50
1:D:720:ARG:HG2	1:D:720:ARG:NH1	2.26	0.50
1:A:272:VAL:O	1:A:272:VAL:HG12	2.11	0.50
1:A:160:LYS:NZ	1:A:161:HIS:NE2	2.58	0.50
1:C:386:ARG:HD3	3:L:4:G:H5"	1.94	0.50
1:D:871:ASN:ND2	1:D:873:ARG:HB2	2.26	0.50
1:B:93:LYS:HB2	5:B:2076:HOH:O	2.11	0.50
1:B:47:GLY:HA3	1:B:265:SER:O	2.12	0.50
1:D:394:ARG:HD3	3:O:5:C:O3'	2.11	0.50
1:D:659:ILE:HG12	1:D:664:GLY:HA3	1.94	0.50
1:C:11:PHE:CE1	1:C:44:TYR:HB3	2.47	0.50
1:A:236:VAL:HG11	1:A:239:GLN:HG3	1.92	0.50
1:A:713:LYS:C	1:A:714:LYS:HG2	2.32	0.50
2:H:9:DA:H5"	5:H:2011:HOH:O	2.10	0.50
1:D:511:PHE:CE2	1:D:515:CYS:SG	3.04	0.50
1:D:814:PHE:HE1	1:D:883:ALA:HB1	1.77	0.50
1:B:744:GLN:HA	1:B:756:ARG:NH2	2.25	0.50
1:C:269:GLN:HE22	1:C:407:LYS:NZ	2.09	0.50
1:C:133:THR:HA	1:C:243:THR:CG2	2.20	0.50
1:B:714:LYS:HZ2	1:B:714:LYS:HA	1.76	0.50
1:C:846:TYR:CE1	1:C:850:ALA:HB2	2.47	0.50
1:A:21:PHE:CD1	1:A:21:PHE:O	2.64	0.50
1:A:281:ILE:CG2	1:A:282:THR:HG23	2.39	0.50
1:D:551:ARG:NH1	1:D:872:LEU:HD12	2.27	0.50
1:C:162:PHE:O	1:C:162:PHE:CD2	2.65	0.50
1:A:48:GLU:HB2	5:A:2112:HOH:O	2.11	0.50
1:A:50:ARG:HH11	1:A:50:ARG:CG	2.24	0.50
1:C:495:SER:HB3	5:C:2118:HOH:O	2.12	0.50
1:B:854:HIS:CG	1:B:855:GLU:N	2.80	0.50
1:B:748:ASN:HD22	1:B:752:LEU:H	1.59	0.50
1:B:19:ILE:CD1	1:B:20:PRO:HD2	2.42	0.50
1:D:704:LYS:HE3	5:D:2175:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:TYR:C	1:B:419:ASN:HD22	2.15	0.50
1:B:322:ILE:CD1	1:B:799:HIS:CG	2.95	0.50
1:C:809:LEU:O	1:C:810:ILE:HG13	2.12	0.50
1:B:60:LYS:HG2	1:B:60:LYS:O	2.12	0.50
1:C:568:GLN:HB3	5:C:2130:HOH:O	2.11	0.50
1:D:21:PHE:C	1:D:23:THR:N	2.63	0.50
1:D:414:ILE:HG22	5:D:2115:HOH:O	2.12	0.50
1:B:828:VAL:HB	1:B:883:ALA:HA	1.94	0.50
1:D:639:TYR:O	2:N:10:DC:H4'	2.12	0.50
1:A:313:MET:HB2	1:A:316:VAL:HG23	1.94	0.50
1:C:729:THR:HB	1:C:789:SER:HB2	1.92	0.50
1:D:422:TRP:CD1	1:D:423:ARG:HG3	2.47	0.50
1:C:164:LYS:CE	1:C:164:LYS:N	2.69	0.50
1:B:452:ILE:CG2	1:B:453:GLY:N	2.75	0.50
1:B:791:LEU:C	1:B:791:LEU:HD23	2.32	0.50
1:B:427:TYR:HA	1:B:435:GLN:HE22	1.76	0.50
1:A:176:HIS:C	1:A:176:HIS:ND1	2.66	0.49
1:D:229:LEU:HD12	1:D:243:THR:O	2.13	0.49
1:D:585:ASP:OD2	1:D:613:THR:CB	2.57	0.49
1:A:19:ILE:HG23	1:A:20:PRO:HD2	1.94	0.49
1:C:47:GLY:HA3	1:C:265:SER:O	2.12	0.49
1:B:407:LYS:HG2	1:B:408:PHE:CE2	2.47	0.49
1:C:328:TRP:O	1:C:413:ALA:HA	2.12	0.49
1:D:311:VAL:HG11	1:D:734:PRO:HG3	1.93	0.49
1:A:59:LEU:HD23	1:A:64:VAL:CG1	2.43	0.49
1:A:404:GLN:HG2	1:A:432:PHE:HB2	1.92	0.49
1:A:861:MET:HE2	1:A:862:PRO:HD2	1.93	0.49
1:C:304:ALA:HB1	5:C:2085:HOH:O	2.12	0.49
1:A:56:GLU:OE1	1:A:57:ARG:N	2.45	0.49
1:D:261:LEU:HD12	5:D:2068:HOH:O	2.13	0.49
1:D:180:LYS:HG3	1:D:750:MET:CE	2.43	0.49
1:A:65:ALA:HB3	5:A:2057:HOH:O	2.12	0.49
1:B:215:ARG:HG3	1:B:219:MET:HE2	1.95	0.49
1:D:322:ILE:HD12	1:D:799:HIS:CD2	2.46	0.49
1:D:576:LYS:O	1:D:580:GLU:HG3	2.11	0.49
1:C:774:GLN:HG2	5:C:2154:HOH:O	2.12	0.49
1:C:120:LYS:HD2	1:C:752:LEU:HD11	1.94	0.49
1:D:656:GLN:N	1:D:657:PRO:HD2	2.27	0.49
1:C:292:ARG:O	1:C:292:ARG:HG3	2.12	0.49
5:A:2233:HOH:O	1:B:683:GLU:HB3	2.12	0.49
1:C:742:PRO:HD2	5:C:2159:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:TYR:CZ	1:A:752:LEU:HD22	2.48	0.49
1:B:164:LYS:HD3	5:B:2092:HOH:O	2.12	0.49
1:B:74:ILE:HG13	1:B:119:ILE:HG21	1.95	0.49
1:C:78:LEU:N	1:C:79:PRO:CD	2.75	0.49
1:B:19:ILE:HD12	5:B:2046:HOH:O	2.12	0.49
1:B:350:GLU:HG3	5:B:2161:HOH:O	2.12	0.49
1:A:158:GLU:HA	1:A:195:LEU:HD22	1.94	0.49
1:B:718:ILE:HG13	5:B:2305:HOH:O	2.12	0.49
1:C:203:SER:O	1:C:205:HIS:N	2.46	0.49
1:B:181:ALA:O	1:B:185:VAL:HG13	2.12	0.49
1:B:452:ILE:HG23	1:B:453:GLY:H	1.76	0.49
1:B:788:GLY:HA2	5:B:2323:HOH:O	2.11	0.49
1:A:473:VAL:HG22	1:A:474:PRO:HD2	1.93	0.49
1:A:681:ILE:O	1:A:685:VAL:HG22	2.12	0.49
1:C:329:LYS:HG3	1:C:445:THR:CG2	2.43	0.49
1:B:495:SER:CB	5:B:2218:HOH:O	2.59	0.49
1:C:101:THR:O	1:C:104:GLN:HG2	2.12	0.49
1:C:392:LYS:O	1:C:396:ILE:HG12	2.12	0.49
1:D:203:SER:O	1:D:205:HIS:N	2.46	0.49
1:C:420:MET:HA	1:C:425:ARG:O	2.13	0.49
1:C:339:ASN:O	1:C:343:LYS:HD2	2.12	0.49
1:A:246:LEU:CD2	1:A:251:ALA:HB2	2.42	0.49
1:A:425:ARG:HH21	1:A:784:HIS:HD2	1.57	0.49
1:A:275:PRO:HD3	1:A:415:TRP:HB2	1.94	0.49
1:A:332:LYS:CE	1:A:410:ASN:ND2	2.76	0.49
1:C:537:ASP:OD1	1:C:813:SER:HB2	2.13	0.49
1:B:56:GLU:OE1	1:B:56:GLU:C	2.51	0.49
1:C:602:THR:CG2	1:C:604:GLU:HB2	2.43	0.49
1:D:616:LEU:HD13	1:D:676:TYR:HB2	1.95	0.49
1:D:706:LEU:HD21	1:D:849:PHE:HB2	1.93	0.49
1:A:828:VAL:O	1:A:831:THR:HG22	2.12	0.49
1:B:84:ARG:CA	1:B:84:ARG:HH11	2.26	0.49
1:B:401:MET:CE	1:B:432:PHE:HA	2.42	0.49
1:A:309:GLU:HG2	1:A:310:ASP:OD1	2.13	0.49
1:C:437:ASN:ND2	1:C:440:THR:HB	2.27	0.49
1:A:44:TYR:OH	1:A:292:ARG:HB3	2.12	0.49
4:P:5:DA:H2"	4:P:6:DT:C7	2.43	0.49
1:A:391:ARG:CG	1:A:391:ARG:HH11	2.25	0.49
1:A:270:PRO:HD2	1:A:408:PHE:HE2	1.76	0.49
1:B:532:LEU:CD1	1:B:533:PRO:HD2	2.32	0.49
1:C:16:LEU:HD13	1:C:38:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:LEU:CD2	1:C:872:LEU:HD23	2.37	0.49
4:M:1:DG:H1'	4:M:2:DT:C7	2.38	0.49
2:E:15:DC:H2''	2:E:16:DC:O5'	2.12	0.49
1:B:231:ARG:NH1	1:B:242:GLU:HB2	2.28	0.49
1:C:402:LEU:HG	1:C:439:MET:HE1	1.93	0.49
1:D:9:ASN:HA	1:D:12:SER:CB	2.42	0.49
1:B:312:TYR:CE1	1:B:314:PRO:HG3	2.48	0.49
4:J:8:DC:H2''	4:J:9:DC:OP2	2.13	0.49
1:A:31:ARG:NH2	5:A:2047:HOH:O	2.45	0.49
1:B:705:LEU:HD23	1:B:705:LEU:N	2.24	0.49
1:C:452:ILE:HG23	1:C:453:GLY:N	2.28	0.49
1:B:233:ASN:CB	1:B:239:GLN:HB3	2.42	0.49
1:C:727:TRP:HA	1:C:848:GLN:NE2	2.23	0.49
4:P:5:DA:H2''	4:P:6:DT:H72	1.95	0.49
1:C:546:PHE:CZ	1:C:783:VAL:HG13	2.48	0.49
1:B:322:ILE:HD13	1:B:799:HIS:CD2	2.48	0.49
1:A:602:THR:CG2	1:A:604:GLU:HB2	2.42	0.49
1:C:352:ILE:C	5:C:2093:HOH:O	2.50	0.49
1:B:331:ASN:C	5:B:2150:HOH:O	2.52	0.49
1:B:159:ALA:HA	1:B:162:PHE:HB3	1.93	0.49
1:D:155:ARG:CG	1:D:163:LYS:HE2	2.43	0.49
1:B:141:ILE:O	1:B:145:ILE:HG12	2.13	0.49
1:B:278:TRP:HE1	1:B:324:GLN:NE2	2.09	0.49
1:D:422:TRP:O	1:D:422:TRP:HD1	1.95	0.49
1:C:463:HIS:CD2	5:C:2111:HOH:O	2.66	0.49
1:B:15:GLU:HB2	1:B:19:ILE:HG12	1.95	0.49
1:B:347:CYS:SG	1:B:350:GLU:HG2	2.53	0.49
1:D:99:ARG:HD3	1:D:103:PHE:CE2	2.46	0.49
1:B:230:HIS:HB2	5:B:2109:HOH:O	2.11	0.49
1:A:112:GLU:N	1:A:112:GLU:CD	2.64	0.49
1:B:51:PHE:HE1	1:B:261:LEU:HB3	1.78	0.49
1:A:553:GLU:CD	1:A:553:GLU:H	2.16	0.49
2:N:16:DC:H2''	2:N:17:DG:O5'	2.12	0.49
1:C:446:LEU:HB2	1:C:531:SER:O	2.12	0.49
1:B:159:ALA:O	1:B:160:LYS:C	2.52	0.48
1:B:423:ARG:HE	1:B:781:ASN:ND2	2.11	0.48
1:A:205:HIS:C	1:A:207:GLU:N	2.64	0.48
1:A:85:ILE:HG13	5:A:2060:HOH:O	2.13	0.48
1:A:230:HIS:HE2	1:A:245:GLU:CD	2.16	0.48
1:D:82:ILE:HG21	1:D:112:GLU:OE2	2.13	0.48
1:C:778:ILE:CG2	1:C:779:ALA:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:854:HIS:CG	1:D:855:GLU:N	2.81	0.48
1:D:337:VAL:HG12	1:D:341:ILE:HD11	1.94	0.48
1:D:418:TYR:C	1:D:419:ASN:HD22	2.16	0.48
1:B:78:LEU:N	1:B:79:PRO:HD2	2.27	0.48
1:A:243:THR:C	1:A:244:ILE:HD13	2.34	0.48
1:A:229:LEU:HD12	1:A:243:THR:O	2.13	0.48
1:A:275:PRO:HB2	1:A:324:GLN:HG2	1.95	0.48
1:A:118:THR:HG23	1:A:141:ILE:HD13	1.92	0.48
1:C:42:GLU:O	1:C:46:MET:HG3	2.13	0.48
1:D:475:PHE:CD1	1:D:475:PHE:N	2.81	0.48
2:H:17:DG:H2"	2:H:18:DC:C5	2.49	0.48
1:C:582:LEU:HD11	1:C:625:VAL:HG21	1.95	0.48
1:A:571:TYR:CE1	1:A:634:VAL:CG1	2.97	0.48
1:B:347:CYS:SG	1:B:350:GLU:CG	3.02	0.48
1:B:401:MET:CE	1:B:432:PHE:CD1	2.94	0.48
1:B:206:LYS:HE2	1:B:207:GLU:OE2	2.13	0.48
1:C:19:ILE:HD12	1:C:20:PRO:HD2	1.94	0.48
1:C:205:HIS:CG	1:C:207:GLU:HG2	2.48	0.48
1:C:59:LEU:HD23	1:C:64:VAL:CG2	2.43	0.48
1:C:633:SER:HB3	1:C:646:PHE:CD1	2.47	0.48
1:B:437:ASN:ND2	1:B:440:THR:H	2.11	0.48
1:D:475:PHE:HE1	1:D:880:PHE:HD1	1.60	0.48
1:A:842:LEU:HD23	1:A:864:LEU:HD23	1.94	0.48
1:B:60:LYS:HD3	5:B:2062:HOH:O	2.13	0.48
1:D:828:VAL:HB	1:D:883:ALA:HA	1.95	0.48
1:B:78:LEU:HD21	1:B:116:TYR:CD1	2.48	0.48
1:C:711:LYS:HZ2	1:C:711:LYS:HB2	1.77	0.48
1:A:242:GLU:N	5:A:2106:HOH:O	2.46	0.48
1:C:609:VAL:O	1:C:672:GLN:NE2	2.46	0.48
1:D:595:VAL:HG12	1:D:596:THR:N	2.27	0.48
1:B:437:ASN:C	1:B:437:ASN:ND2	2.67	0.48
1:A:6:ILE:HG22	1:A:10:ASP:HB3	1.95	0.48
1:A:710:VAL:CG1	1:A:720:ARG:HB3	2.42	0.48
1:D:269:GLN:NE2	1:D:404:GLN:OE1	2.40	0.48
1:B:41:HIS:NE2	1:B:45:GLU:OE2	2.46	0.48
1:B:170:LEU:HD22	1:B:179:LYS:HD3	1.96	0.48
1:C:84:ARG:HH21	1:C:222:GLU:CD	2.16	0.48
2:N:4:DA:N3	5:N:2006:HOH:O	2.35	0.48
1:D:727:TRP:HB3	1:D:845:PHE:CD1	2.48	0.48
1:D:868:GLY:C	1:D:869:ASN:HD22	2.16	0.48
1:A:170:LEU:HD23	1:A:170:LEU:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:MET:HE1	1:B:522:GLN:HB2	1.94	0.48
1:C:789:SER:O	1:C:793:LYS:HG3	2.14	0.48
1:C:229:LEU:CD1	1:C:244:ILE:HD13	2.44	0.48
1:D:423:ARG:HE	1:D:781:ASN:ND2	2.11	0.48
1:B:463:HIS:HD2	1:B:535:ALA:H	1.62	0.48
1:D:150:ARG:HG3	1:D:201:TRP:CD1	2.49	0.48
1:B:401:MET:HE2	1:B:432:PHE:CD1	2.48	0.48
1:A:315:GLU:OE2	1:A:318:LYS:CD	2.58	0.48
1:B:230:HIS:CE1	1:B:232:GLN:HE22	2.32	0.48
1:A:292:ARG:NH1	1:A:292:ARG:HG2	2.26	0.48
1:C:28:TYR:CE2	1:C:274:PRO:HD2	2.47	0.48
1:C:9:ASN:HA	1:C:12:SER:HB3	1.95	0.48
1:D:27:HIS:HB3	1:D:28:TYR:CD1	2.48	0.48
1:D:537:ASP:N	1:D:882:PHE:HD2	2.11	0.48
1:A:854:HIS:CG	1:A:855:GLU:N	2.82	0.48
1:C:551:ARG:NE	1:C:872:LEU:HD21	2.28	0.48
1:B:404:GLN:HG2	1:B:432:PHE:CB	2.43	0.48
1:A:164:LYS:NZ	1:A:164:LYS:N	2.62	0.48
1:A:457:TYR:CZ	1:A:461:LYS:HD3	2.48	0.48
1:B:698:TRP:CZ2	1:B:864:LEU:CD2	2.97	0.48
1:A:374:LEU:C	1:A:376:ALA:H	2.15	0.48
1:B:84:ARG:HG3	1:B:223:SER:HB3	1.95	0.48
1:C:816:THR:HG22	1:C:817:ILE:H	1.79	0.48
1:C:84:ARG:HD3	1:C:84:ARG:C	2.33	0.48
4:M:5:DA:H2"	4:M:6:DT:C7	2.43	0.48
1:A:695:ALA:O	1:A:699:LEU:HG	2.14	0.48
1:C:5:ASN:C	1:C:5:ASN:ND2	2.67	0.48
2:N:15:DC:H2"	2:N:16:DC:O5'	2.14	0.48
1:A:563:PRO:HB3	1:A:877:GLU:O	2.14	0.48
1:B:226:MET:HA	1:B:250:TYR:CD1	2.49	0.48
1:C:316:VAL:CG1	1:C:420:MET:HE1	2.44	0.48
2:K:6:DT:H5"	5:K:2009:HOH:O	2.14	0.48
1:D:42:GLU:HG2	1:D:46:MET:CE	2.44	0.48
1:B:401:MET:CE	1:B:432:PHE:CB	2.91	0.48
1:A:315:GLU:HB3	5:A:2132:HOH:O	2.13	0.48
1:B:829:ARG:NH1	1:B:829:ARG:CG	2.68	0.48
1:C:619:GLN:O	1:C:622:ALA:HB3	2.14	0.48
1:A:281:ILE:HD11	1:A:308:TYR:C	2.34	0.48
4:M:6:DT:C2'	4:M:7:DT:H72	2.44	0.48
2:K:16:DC:H2"	2:K:17:DG:O5'	2.14	0.48
2:K:17:DG:H2"	2:K:18:DC:C5	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:GLN:NE2	1:A:418:TYR:H	2.12	0.48
1:C:162:PHE:CB	5:C:2059:HOH:O	2.59	0.48
1:C:789:SER:HA	1:C:792:ARG:NH2	2.29	0.48
1:C:329:LYS:HD2	1:C:447:ALA:HA	1.94	0.48
1:D:829:ARG:HH11	1:D:829:ARG:CG	2.21	0.48
1:D:315:GLU:CA	1:D:315:GLU:OE2	2.50	0.48
1:C:706:LEU:HD11	1:C:849:PHE:CD2	2.49	0.48
2:N:4:DA:H2''	2:N:5:DA:OP2	2.14	0.48
1:A:82:ILE:O	1:A:86:ASN:ND2	2.47	0.48
1:C:194:GLY:O	1:C:196:LEU:HD23	2.14	0.48
2:N:2:DG:H2''	2:N:3:DG:C8	2.49	0.48
1:B:291:ARG:C	1:B:293:PRO:HD3	2.34	0.47
1:D:19:ILE:O	1:D:21:PHE:N	2.39	0.47
2:K:8:DG:OP2	5:K:2011:HOH:O	2.20	0.47
1:B:305:LEU:HD23	1:B:305:LEU:O	2.13	0.47
1:C:468:ALA:HB2	1:C:511:PHE:HE1	1.74	0.47
1:D:111:PRO:HG2	1:D:112:GLU:OE1	2.14	0.47
1:C:56:GLU:OE1	1:C:57:ARG:CA	2.62	0.47
1:C:278:TRP:N	1:C:321:ASN:OD1	2.45	0.47
1:D:53:LYS:O	1:D:56:GLU:HB3	2.13	0.47
1:A:78:LEU:N	1:A:79:PRO:CD	2.77	0.47
1:C:475:PHE:N	5:C:2112:HOH:O	2.28	0.47
1:D:19:ILE:CD1	1:D:20:PRO:HD2	2.43	0.47
1:C:463:HIS:ND1	1:C:532:LEU:HD21	2.29	0.47
1:A:155:ARG:HH11	1:A:155:ARG:CB	2.18	0.47
1:A:425:ARG:CZ	1:A:784:HIS:CD2	2.97	0.47
1:B:151:PHE:HD1	1:B:183:MET:HB3	1.78	0.47
1:C:303:LYS:NZ	1:C:740:LYS:HZ1	2.11	0.47
1:C:797:TRP:CZ2	1:C:801:LYS:HG3	2.49	0.47
1:C:36:GLN:HG2	1:C:273:VAL:HG22	1.95	0.47
1:A:11:PHE:N	5:A:2034:HOH:O	2.30	0.47
1:D:158:GLU:CD	1:D:195:LEU:HB3	2.35	0.47
2:H:16:DC:H2''	2:H:17:DG:O5'	2.14	0.47
1:B:218:GLU:O	1:B:222:GLU:HB2	2.14	0.47
1:D:28:TYR:CE2	1:D:274:PRO:HD2	2.49	0.47
1:B:577:LYS:HD2	5:B:2301:HOH:O	2.13	0.47
2:K:6:DT:C2'	2:K:7:DC:C5	2.96	0.47
1:D:352:ILE:HG12	5:D:2098:HOH:O	2.14	0.47
1:B:711:LYS:CA	1:B:719:LEU:HD13	2.39	0.47
1:A:318:LYS:O	1:A:322:ILE:HG13	2.14	0.47
1:C:19:ILE:HG23	1:C:20:PRO:CD	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:693:VAL:O	1:D:697:ASN:ND2	2.34	0.47
1:A:120:LYS:HD2	1:A:752:LEU:HD11	1.96	0.47
1:C:488:ASN:HB3	1:C:501:TRP:CE3	2.50	0.47
1:B:236:VAL:CG2	1:B:239:GLN:HE21	2.16	0.47
1:C:163:LYS:C	1:C:164:LYS:HE2	2.34	0.47
1:A:221:ILE:O	5:A:2096:HOH:O	2.20	0.47
2:H:5:DA:H1'	2:H:6:DT:H5'	1.96	0.47
1:D:179:LYS:HB2	5:D:2052:HOH:O	2.15	0.47
1:C:105:PHE:HE2	5:C:2015:HOH:O	1.98	0.47
1:B:324:GLN:HE21	1:B:417:PRO:CA	2.27	0.47
1:D:2:ASN:N	5:D:2001:HOH:O	2.47	0.47
1:C:134:VAL:O	1:C:134:VAL:HG22	2.15	0.47
1:B:215:ARG:HG3	1:B:219:MET:HE1	1.97	0.47
1:A:707:ALA:HB2	1:A:774:GLN:HG2	1.97	0.47
1:A:51:PHE:HD2	1:A:262:ALA:HB2	1.79	0.47
1:A:6:ILE:HD11	1:A:259:GLY:O	2.14	0.47
1:D:550:LEU:HD23	1:D:550:LEU:HA	1.62	0.47
1:A:120:LYS:HE2	5:A:2057:HOH:O	2.14	0.47
1:B:804:ILE:HG22	1:B:807:PHE:CZ	2.49	0.47
1:B:720:ARG:NH2	1:B:857:GLN:OE1	2.43	0.47
1:A:720:ARG:CG	1:A:720:ARG:NH1	2.69	0.47
1:D:229:LEU:HD11	1:D:242:GLU:HG2	1.96	0.47
1:D:651:LEU:HD13	1:D:651:LEU:C	2.35	0.47
1:C:146:GLU:HG3	1:C:204:TRP:CD2	2.49	0.47
1:C:57:ARG:HH12	2:K:17:DG:H3'	1.80	0.47
1:A:532:LEU:HD12	1:A:533:PRO:HD2	1.97	0.47
1:B:122:THR:HG22	1:B:126:LEU:HD11	1.97	0.47
1:B:51:PHE:CE1	1:B:261:LEU:HB3	2.50	0.47
2:N:17:DG:H2'	2:N:18:DC:C5	2.50	0.47
1:C:796:VAL:O	1:C:800:GLU:HG3	2.13	0.47
1:A:556:GLY:O	1:A:561:LEU:HB2	2.14	0.47
1:D:354:ALA:HB2	5:D:2100:HOH:O	2.14	0.47
1:C:427:TYR:HA	1:C:435:GLN:HE22	1.79	0.47
1:D:829:ARG:HD3	1:D:875:ILE:HG22	1.96	0.47
1:D:666:MET:SD	1:D:666:MET:N	2.86	0.47
1:D:324:GLN:HG3	1:D:417:PRO:HA	1.96	0.47
1:A:745:THR:N	1:A:756:ARG:HD3	2.27	0.47
2:K:6:DT:H2'	2:K:6:DT:H6	1.57	0.47
1:A:705:LEU:CD2	1:A:857:GLN:HB2	2.39	0.47
1:D:84:ARG:HH11	1:D:84:ARG:HA	1.80	0.47
1:C:686:SER:HA	1:C:693:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD12	1:A:272:VAL:HG11	1.94	0.47
1:C:72:PRO:HG3	1:C:257:ARG:HG3	1.97	0.47
1:C:278:TRP:CD2	1:C:284:GLY:HA3	2.49	0.47
1:A:180:LYS:HA	5:A:2084:HOH:O	2.15	0.47
1:B:39:LEU:HA	5:B:2052:HOH:O	2.15	0.47
1:D:861:MET:CE	1:D:862:PRO:HD2	2.45	0.47
1:C:349:VAL:O	1:C:349:VAL:HG12	2.15	0.47
1:B:810:ILE:O	1:B:811:HIS:HB2	2.14	0.47
1:D:333:LYS:HD2	1:D:516:PHE:CD1	2.50	0.47
1:D:134:VAL:HG22	1:D:134:VAL:O	2.14	0.47
1:C:748:ASN:HD22	1:C:751:PHE:H	1.61	0.47
1:A:324:GLN:HE21	1:A:417:PRO:CA	2.25	0.47
1:D:726:HIS:HD2	1:D:727:TRP:H	1.63	0.47
1:B:698:TRP:CH2	1:B:864:LEU:HD21	2.50	0.47
1:B:811:HIS:HD2	5:B:2185:HOH:O	1.97	0.47
1:A:231:ARG:HG2	1:A:234:ALA:HB2	1.95	0.47
1:B:327:ALA:HB2	5:B:2195:HOH:O	2.13	0.47
4:M:2:DT:H1'	4:M:3:DC:H5'	1.96	0.47
1:A:292:ARG:CG	1:A:292:ARG:HH11	2.26	0.47
1:D:224:THR:HA	5:D:2028:HOH:O	2.15	0.47
1:B:458:TYR:CD1	1:B:479:ILE:HD11	2.50	0.47
1:B:125:CYS:O	1:B:128:SER:CB	2.63	0.47
1:B:713:LYS:HG2	5:H:2003:HOH:O	2.15	0.47
1:B:642:LYS:O	1:B:643:GLU:C	2.53	0.47
1:B:854:HIS:HD2	1:B:856:SER:H	1.55	0.47
1:C:463:HIS:HD2	5:C:2111:HOH:O	1.98	0.47
1:A:745:THR:HA	5:A:2271:HOH:O	2.15	0.47
1:D:154:ILE:HD12	1:D:183:MET:SD	2.54	0.47
1:B:828:VAL:CG1	1:B:883:ALA:HA	2.45	0.47
1:D:335:LEU:CD1	1:D:339:ASN:HD21	2.28	0.47
1:A:30:GLU:HG2	1:A:34:ARG:NH2	2.28	0.47
1:A:134:VAL:HG23	1:A:244:ILE:HD11	1.96	0.47
1:B:474:PRO:HG2	1:B:477:GLU:OE2	2.15	0.47
1:A:332:LYS:HE3	1:A:409:ALA:O	2.14	0.47
1:D:517:GLU:HG3	1:D:532:LEU:HB2	1.97	0.47
1:A:576:LYS:O	1:A:580:GLU:HG3	2.14	0.47
1:B:164:LYS:CD	5:B:2092:HOH:O	2.62	0.46
1:D:268:PHE:CD1	1:D:286:TYR:HE2	2.32	0.46
2:E:4:DA:H2''	2:E:5:DA:H8	1.76	0.46
1:C:16:LEU:CD1	1:C:38:ALA:HB2	2.44	0.46
1:D:353:PRO:HB2	5:D:2101:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:ALA:O	1:C:160:LYS:C	2.52	0.46
1:D:720:ARG:HH11	1:D:720:ARG:HG2	1.79	0.46
1:A:829:ARG:NH1	1:A:878:SER:O	2.48	0.46
1:B:490:MET:CE	1:B:522:GLN:HG3	2.45	0.46
1:D:140:ALA:HA	5:D:2040:HOH:O	2.15	0.46
1:A:562:LEU:HD23	1:A:562:LEU:N	2.28	0.46
1:A:404:GLN:HG2	1:A:432:PHE:CB	2.45	0.46
1:A:859:ASP:OD1	1:A:860:LYS:N	2.48	0.46
1:D:829:ARG:CD	1:D:875:ILE:O	2.63	0.46
1:D:268:PHE:CD1	1:D:286:TYR:CE2	3.04	0.46
1:A:201:TRP:O	1:A:204:TRP:HB2	2.15	0.46
1:B:42:GLU:HA	1:B:45:GLU:HG3	1.96	0.46
1:C:619:GLN:NE2	1:C:666:MET:O	2.46	0.46
1:D:89:PHE:HE2	1:D:107:GLN:HA	1.80	0.46
1:D:644:PHE:CE1	4:P:1:DG:N2	2.83	0.46
1:C:53:LYS:HE2	1:C:53:LYS:HB3	1.66	0.46
1:A:160:LYS:NZ	5:A:2077:HOH:O	2.47	0.46
1:A:553:GLU:HG2	1:A:554:VAL:N	2.29	0.46
1:C:502:TRP:CE2	1:C:512:LEU:HD22	2.50	0.46
1:D:793:LYS:NZ	1:D:834:ASP:OD2	2.42	0.46
1:C:412:LYS:N	1:C:412:LYS:HD2	2.29	0.46
1:C:229:LEU:HD21	1:C:242:GLU:OE2	2.16	0.46
1:A:854:HIS:CD2	1:A:856:SER:OG	2.68	0.46
1:C:804:ILE:HG12	1:C:820:ASP:HB3	1.97	0.46
1:B:269:GLN:HB3	1:B:270:PRO:CD	2.46	0.46
1:C:711:LYS:HG2	1:C:718:ILE:N	2.30	0.46
1:D:78:LEU:O	1:D:82:ILE:HG13	2.14	0.46
1:D:700:LYS:HZ2	1:D:700:LYS:HB2	1.80	0.46
5:A:2080:HOH:O	3:F:3:G:H5'	2.16	0.46
1:C:651:LEU:C	1:C:651:LEU:HD13	2.35	0.46
1:C:15:GLU:HG3	1:C:18:ALA:H	1.77	0.46
1:B:402:LEU:HG	1:B:439:MET:HE1	1.96	0.46
1:B:840:ASP:O	1:B:841:VAL:C	2.54	0.46
1:D:412:LYS:O	1:D:413:ALA:HB2	2.15	0.46
1:D:390:ALA:O	1:D:394:ARG:HG3	2.16	0.46
1:C:595:VAL:HG12	1:C:596:THR:N	2.30	0.46
1:B:619:GLN:O	1:B:622:ALA:HB3	2.16	0.46
1:D:18:ALA:O	1:D:19:ILE:HG12	2.15	0.46
1:B:720:ARG:NH1	1:B:720:ARG:CG	2.68	0.46
1:A:745:THR:O	1:A:746:ARG:HG3	2.16	0.46
1:C:833:VAL:HG22	1:C:872:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ARG:O	1:B:179:LYS:HE2	2.15	0.46
2:H:6:DT:C1'	5:H:2008:HOH:O	2.52	0.46
1:D:571:TYR:HD2	1:D:627:ARG:NH2	2.14	0.46
1:D:337:VAL:HG21	1:D:512:LEU:HD21	1.96	0.46
1:B:433:ASN:HB2	1:B:434:PRO:HD2	1.97	0.46
1:C:642:LYS:O	1:C:643:GLU:C	2.51	0.46
1:D:801:LYS:HD3	1:D:801:LYS:C	2.36	0.46
1:B:445:THR:OG1	1:B:446:LEU:N	2.48	0.46
1:C:452:ILE:HD11	1:C:457:TYR:CA	2.41	0.46
4:G:7:DT:H72	5:G:2002:HOH:O	2.15	0.46
1:C:698:TRP:HZ2	1:C:846:TYR:HD2	1.63	0.46
1:A:137:VAL:HG12	1:A:217:ILE:HD11	1.96	0.46
1:C:56:GLU:OE1	1:C:57:ARG:HA	2.15	0.46
1:C:57:ARG:NH1	2:K:17:DG:H3'	2.31	0.46
1:B:565:GLU:O	1:B:565:GLU:OE2	2.33	0.46
1:D:437:ASN:ND2	1:D:437:ASN:H	2.13	0.46
1:A:546:PHE:CZ	1:A:783:VAL:HG21	2.47	0.46
4:P:2:DT:H4'	5:P:2003:HOH:O	2.15	0.46
4:J:1:DG:H1'	5:J:2001:HOH:O	2.14	0.46
1:B:174:VAL:HG22	5:I:2002:HOH:O	2.15	0.46
1:B:276:LYS:HD2	1:B:283:GLY:O	2.15	0.46
1:B:216:CYS:HA	1:B:219:MET:HE2	1.97	0.46
1:A:342:THR:HA	1:A:348:PRO:HG3	1.97	0.46
1:B:257:ARG:HG2	1:B:257:ARG:HH11	1.81	0.46
1:B:463:HIS:CD2	1:B:535:ALA:H	2.34	0.46
1:B:102:ALA:HB1	1:B:106:LEU:HD12	1.98	0.46
1:C:718:ILE:HB	5:C:2153:HOH:O	2.14	0.46
2:E:17:DG:H2''	2:E:18:DC:C5	2.51	0.46
4:P:3:DC:H2''	4:P:4:DG:OP2	2.16	0.46
1:C:270:PRO:HG3	1:C:416:PHE:HE1	1.79	0.46
1:D:118:THR:HG23	1:D:141:ILE:HD13	1.98	0.46
1:B:510:CYS:HB3	5:B:2225:HOH:O	2.14	0.46
1:B:706:LEU:HD11	1:B:849:PHE:CG	2.50	0.46
1:B:781:ASN:HD21	2:H:12:DT:H5'	1.81	0.46
1:D:623:TYR:CD1	1:D:666:MET:HE1	2.51	0.46
1:C:817:ILE:HD11	1:C:820:ASP:OD2	2.16	0.46
1:A:433:ASN:C	1:A:433:ASN:OD1	2.54	0.46
2:E:13:DC:H2''	2:E:14:DG:C5'	2.46	0.46
1:C:710:VAL:CG1	1:C:720:ARG:HB3	2.45	0.46
1:B:166:VAL:C	1:B:168:GLU:OE1	2.54	0.46
1:B:16:LEU:H	1:B:16:LEU:CD2	2.20	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:HIS:CD2	1:A:232:GLN:NE2	2.84	0.46
1:A:281:ILE:HD13	1:A:309:GLU:HA	1.96	0.46
1:C:199:GLU:O	1:C:199:GLU:CG	2.63	0.46
1:C:727:TRP:NE1	1:C:735:VAL:CG1	2.78	0.46
1:C:577:LYS:HB3	1:C:577:LYS:HE2	1.59	0.46
1:A:778:ILE:HG23	1:A:779:ALA:H	1.81	0.46
1:C:155:ARG:HB3	1:C:155:ARG:CZ	2.46	0.46
1:C:487:GLU:HB2	5:C:2116:HOH:O	2.15	0.46
1:D:679:LYS:HE2	1:D:679:LYS:HB2	1.66	0.46
1:B:223:SER:HA	5:B:2106:HOH:O	2.16	0.46
1:D:656:GLN:HB3	1:D:657:PRO:CD	2.45	0.46
1:C:711:LYS:HZ3	1:C:711:LYS:CB	2.27	0.46
1:A:57:ARG:CZ	2:E:18:DC:OP2	2.64	0.46
1:A:57:ARG:HG2	1:A:60:LYS:HZ3	1.80	0.46
1:B:676:TYR:O	1:B:680:LEU:HD13	2.16	0.46
1:B:324:GLN:HE21	1:B:417:PRO:HA	1.80	0.46
1:C:645:GLY:O	1:C:649:GLN:HG3	2.16	0.46
1:C:502:TRP:CD1	1:C:512:LEU:HD13	2.51	0.46
1:B:842:LEU:HA	1:B:842:LEU:HD12	1.72	0.46
1:A:561:LEU:HD12	1:A:561:LEU:HA	1.69	0.46
1:A:65:ALA:N	5:A:2057:HOH:O	2.42	0.46
1:D:274:PRO:HD3	1:D:415:TRP:CZ3	2.51	0.46
1:B:21:PHE:HD1	1:B:21:PHE:C	2.15	0.46
1:C:644:PHE:CD1	2:K:9:DA:C2	3.04	0.46
1:B:416:PHE:HE1	1:B:432:PHE:O	1.98	0.46
1:C:109:ILE:N	1:C:109:ILE:HD12	2.31	0.46
1:A:375:THR:CG2	1:A:375:THR:O	2.63	0.46
3:F:1:G:H5"	5:F:2002:HOH:O	2.16	0.46
1:A:595:VAL:HG12	1:A:596:THR:N	2.31	0.46
1:B:706:LEU:HD21	1:B:849:PHE:HB2	1.98	0.46
1:B:512:LEU:HD11	1:B:516:PHE:CZ	2.51	0.46
1:B:71:LYS:N	1:B:72:PRO:CD	2.78	0.46
1:D:39:LEU:CD2	1:D:272:VAL:HG23	2.46	0.46
1:A:185:VAL:HG23	1:A:186:VAL:N	2.31	0.46
1:C:868:GLY:C	1:C:869:ASN:HD22	2.19	0.46
1:D:746:ARG:NH1	1:D:754:GLN:O	2.49	0.46
1:C:19:ILE:HD13	1:C:20:PRO:HD2	1.97	0.46
1:B:232:GLN:O	1:B:240:ASP:HA	2.16	0.46
1:B:17:ALA:HA	5:B:2049:HOH:O	2.16	0.46
1:A:6:ILE:CG2	1:A:10:ASP:CG	2.84	0.46
1:B:787:ASP:OD1	1:B:788:GLY:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:744:GLN:O	1:C:745:THR:OG1	2.27	0.46
1:B:619:GLN:NE2	1:B:666:MET:O	2.49	0.45
1:B:663:LYS:HE3	1:B:666:MET:HE2	1.98	0.45
1:C:453:GLY:O	1:C:526:LEU:HD22	2.17	0.45
1:A:89:PHE:CE2	1:A:107:GLN:HG3	2.46	0.45
1:B:123:LEU:O	1:B:127:THR:HG23	2.16	0.45
1:A:24:LEU:HD21	1:A:287:TRP:CE2	2.51	0.45
1:C:610:LYS:O	1:C:611:LEU:C	2.52	0.45
1:C:208:ASP:O	1:C:212:VAL:HG23	2.16	0.45
1:B:418:TYR:HD2	1:B:426:VAL:HG12	1.80	0.45
1:C:89:PHE:HE2	1:C:107:GLN:HA	1.80	0.45
1:A:577:LYS:HE2	1:A:580:GLU:OE1	2.16	0.45
1:B:727:TRP:HB2	5:B:2307:HOH:O	2.15	0.45
1:C:126:LEU:HD23	1:C:132:THR:HG22	1.96	0.45
1:B:746:ARG:NH1	5:B:2315:HOH:O	2.49	0.45
1:B:64:VAL:HG21	1:B:127:THR:HG21	1.96	0.45
1:B:233:ASN:OD1	1:B:239:GLN:HB3	2.16	0.45
1:C:16:LEU:HD13	5:C:2034:HOH:O	2.16	0.45
1:A:84:ARG:NH2	1:A:222:GLU:CD	2.70	0.45
1:A:80:LYS:CE	1:A:224:THR:HG22	2.44	0.45
1:B:677:MET:HG3	1:B:681:ILE:HD12	1.97	0.45
1:D:567:VAL:HG22	1:D:880:PHE:CG	2.51	0.45
1:A:481:PHE:HD2	1:A:482:ILE:HD13	1.81	0.45
1:B:804:ILE:HG23	1:B:816:THR:HG21	1.99	0.45
1:D:828:VAL:HG23	1:D:829:ARG:N	2.31	0.45
1:B:688:THR:HG23	5:B:2301:HOH:O	2.15	0.45
1:C:422:TRP:CZ2	1:C:423:ARG:HD2	2.51	0.45
1:D:749:LEU:HD11	5:D:2044:HOH:O	2.15	0.45
1:D:582:LEU:CD1	1:D:625:VAL:HG21	2.43	0.45
1:D:449:GLY:HA3	1:D:531:SER:HB3	1.97	0.45
1:C:437:ASN:HD22	1:C:440:THR:HB	1.82	0.45
1:D:173:ARG:O	1:D:179:LYS:HE3	2.17	0.45
1:D:379:ARG:HG2	5:D:2146:HOH:O	2.16	0.45
1:C:730:PRO:CD	1:C:786:GLN:NE2	2.80	0.45
1:B:859:ASP:OD1	1:B:859:ASP:C	2.54	0.45
1:A:709:GLU:O	1:A:711:LYS:HG3	2.16	0.45
1:C:422:TRP:HH2	2:K:12:DT:H5"	1.78	0.45
1:C:77:LEU:C	1:C:79:PRO:HD2	2.37	0.45
1:B:744:GLN:C	1:B:745:THR:HG1	2.19	0.45
1:D:717:GLU:O	1:D:719:LEU:CD1	2.64	0.45
1:B:16:LEU:HD13	1:B:38:ALA:CA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:810:ILE:O	1:D:812:ASP:N	2.50	0.45
1:A:551:ARG:HB2	1:A:868:GLY:H	1.80	0.45
1:A:486:HIS:O	1:A:490:MET:HG2	2.17	0.45
1:A:706:LEU:HB2	5:A:2265:HOH:O	2.15	0.45
1:A:269:GLN:NE2	1:A:407:LYS:HZ2	2.09	0.45
1:A:185:VAL:CG2	1:A:186:VAL:N	2.79	0.45
1:C:173:ARG:CZ	5:C:2062:HOH:O	2.63	0.45
1:C:706:LEU:HD21	1:C:849:PHE:CB	2.43	0.45
1:D:700:LYS:HA	1:D:778:ILE:HG21	1.98	0.45
1:B:561:LEU:HB3	1:B:562:LEU:HD23	1.97	0.45
1:B:561:LEU:HD23	1:B:870:LEU:HD11	1.98	0.45
1:B:6:ILE:HG23	1:B:10:ASP:OD2	2.16	0.45
1:B:62:GLY:CA	1:B:124:ALA:HA	2.45	0.45
1:C:550:LEU:HD21	1:C:865:PRO:HG2	1.97	0.45
1:B:420:MET:HA	1:B:425:ARG:O	2.17	0.45
4:G:5:DA:P	5:G:2004:HOH:O	2.75	0.45
1:C:532:LEU:CD2	1:C:534:LEU:CD2	2.92	0.45
1:D:159:ALA:HB2	1:D:190:MET:HE1	1.99	0.45
1:B:244:ILE:O	1:B:245:GLU:OE2	2.34	0.45
1:B:19:ILE:O	1:B:21:PHE:N	2.42	0.45
1:B:680:LEU:N	1:B:680:LEU:CD1	2.79	0.45
1:A:529:ASN:HD22	1:A:530:CYS:N	2.14	0.45
1:B:632:ARG:HA	1:B:635:MET:HG2	1.97	0.45
1:C:854:HIS:CG	1:C:855:GLU:N	2.84	0.45
1:A:50:ARG:CG	1:A:50:ARG:NH1	2.77	0.45
1:D:72:PRO:HG3	1:D:257:ARG:HG3	1.99	0.45
1:A:481:PHE:CD2	1:A:482:ILE:HD13	2.52	0.45
1:A:352:ILE:HA	1:A:353:PRO:HD3	1.88	0.45
1:D:433:ASN:HB2	1:D:434:PRO:CD	2.47	0.45
1:D:457:TYR:CE1	1:D:521:VAL:HG11	2.52	0.45
1:B:247:ALA:HB3	1:B:250:TYR:HD1	1.82	0.45
1:B:577:LYS:HE2	1:B:687:VAL:CG2	2.47	0.45
1:C:549:MET:SD	1:C:842:LEU:HD13	2.56	0.45
1:A:84:ARG:NE	1:A:222:GLU:CB	2.76	0.45
1:C:850:ALA:O	1:C:853:LEU:HG	2.16	0.45
1:D:644:PHE:CD2	1:D:644:PHE:C	2.89	0.45
1:C:6:ILE:HD11	1:C:259:GLY:O	2.16	0.45
1:D:474:PRO:O	1:D:478:ARG:HG3	2.16	0.45
1:A:25:ALA:HA	1:A:29:GLY:O	2.17	0.45
1:A:59:LEU:HA	1:A:64:VAL:CG2	2.39	0.45
1:B:84:ARG:HB2	1:B:223:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:MET:HA	1:A:425:ARG:O	2.16	0.45
1:C:727:TRP:CE2	1:C:735:VAL:HG11	2.52	0.45
1:C:571:TYR:HD1	1:C:634:VAL:HG11	1.82	0.45
1:C:685:VAL:HG23	1:C:686:SER:N	2.32	0.45
1:A:629:VAL:HG11	1:A:677:MET:CE	2.46	0.45
1:C:819:ALA:C	5:C:2175:HOH:O	2.55	0.45
1:B:331:ASN:HB2	1:B:445:THR:CG2	2.45	0.45
1:B:161:HIS:O	1:B:164:LYS:HG2	2.16	0.45
1:B:463:HIS:CD2	1:B:534:LEU:HA	2.52	0.45
1:B:744:GLN:HA	1:B:756:ARG:CZ	2.47	0.45
2:E:13:DC:H2''	2:E:14:DG:H5'	1.99	0.45
1:B:595:VAL:HG12	5:B:2264:HOH:O	2.16	0.45
1:A:417:PRO:HG2	1:A:429:VAL:HB	1.99	0.45
1:B:112:GLU:CD	1:B:112:GLU:H	2.20	0.45
1:A:392:LYS:O	1:A:396:ILE:HG12	2.17	0.45
1:A:82:ILE:O	1:A:86:ASN:CG	2.56	0.45
1:B:458:TYR:CE1	1:B:479:ILE:HD11	2.52	0.45
1:C:629:VAL:O	1:C:629:VAL:HG12	2.16	0.45
1:C:882:PHE:N	1:C:882:PHE:CD1	2.67	0.45
1:A:560:ASN:ND2	1:A:880:PHE:CB	2.80	0.45
1:B:247:ALA:HB3	1:B:250:TYR:CD1	2.52	0.45
1:A:632:ARG:HA	1:A:635:MET:HG3	1.99	0.45
1:A:89:PHE:HZ	1:A:106:LEU:O	2.00	0.45
1:B:171:ASN:HB3	3:I:2:C:H4'	1.99	0.45
2:E:3:DG:H2''	2:E:4:DA:OP2	2.16	0.45
1:A:109:ILE:N	1:A:109:ILE:CD1	2.80	0.45
1:B:102:ALA:HB1	1:B:106:LEU:CD1	2.47	0.45
1:D:632:ARG:HH11	1:D:632:ARG:HB2	1.81	0.45
1:B:206:LYS:HG2	1:B:207:GLU:OE2	2.17	0.45
1:A:133:THR:HG22	1:A:243:THR:HG22	1.99	0.45
1:A:58:GLN:OE1	1:A:66:ASP:O	2.34	0.45
1:C:780:PRO:O	1:C:783:VAL:HG23	2.17	0.45
1:C:162:PHE:CE2	1:C:165:ASN:HB2	2.52	0.45
1:A:553:GLU:HG2	1:A:554:VAL:H	1.82	0.45
1:A:840:ASP:O	1:A:842:LEU:N	2.50	0.45
1:B:125:CYS:O	1:B:128:SER:HB3	2.17	0.45
1:A:463:HIS:CD2	1:A:534:LEU:HA	2.51	0.45
1:A:54:MET:HG3	5:A:2055:HOH:O	2.16	0.45
1:A:573:ILE:HD12	1:A:573:ILE:C	2.38	0.45
1:C:419:ASN:HD22	1:C:419:ASN:HA	1.48	0.45
1:B:647:ARG:HG2	1:B:675:GLY:HA2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:LYS:HA	5:B:2150:HOH:O	2.17	0.44
1:D:27:HIS:HB3	1:D:28:TYR:CE1	2.51	0.44
1:A:560:ASN:ND2	1:A:880:PHE:HB2	2.31	0.44
1:B:423:ARG:NE	2:H:12:DT:C4'	2.68	0.44
1:B:752:LEU:HB2	1:B:753:GLY:H	1.48	0.44
1:B:532:LEU:O	1:B:818:PRO:HD3	2.18	0.44
1:C:147:ASP:CB	1:C:750:MET:HE1	2.36	0.44
1:B:221:ILE:CD1	1:B:229:LEU:HB2	2.47	0.44
1:C:611:LEU:HD22	1:C:615:ALA:CB	2.47	0.44
1:C:206:LYS:O	1:C:210:ILE:HG12	2.18	0.44
1:D:737:GLN:HG2	1:D:774:GLN:HE22	1.83	0.44
1:C:860:LYS:O	1:C:860:LYS:CD	2.63	0.44
1:A:76:THR:C	1:A:79:PRO:HD2	2.38	0.44
1:A:514:PHE:CD1	1:A:515:CYS:N	2.85	0.44
1:C:541:SER:O	1:C:545:HIS:HD2	1.99	0.44
1:B:857:GLN:HA	5:B:2340:HOH:O	2.18	0.44
1:A:560:ASN:ND2	1:A:567:VAL:HG13	2.21	0.44
1:A:854:HIS:HD2	1:A:856:SER:H	1.53	0.44
1:C:526:LEU:HA	1:C:526:LEU:HD23	1.72	0.44
1:B:573:ILE:CD1	1:B:688:THR:HG21	2.45	0.44
1:C:80:LYS:HD3	1:C:224:THR:CG2	2.35	0.44
1:A:811:HIS:HA	5:A:2283:HOH:O	2.16	0.44
1:B:185:VAL:CG2	1:B:186:VAL:N	2.79	0.44
1:D:170:LEU:O	1:D:173:ARG:HB2	2.17	0.44
1:C:257:ARG:HD3	1:C:261:LEU:HD13	1.97	0.44
1:C:275:PRO:HB2	1:C:324:GLN:CG	2.47	0.44
1:A:726:HIS:CD2	1:A:736:TRP:NE1	2.86	0.44
1:B:847:ASP:OD1	1:B:847:ASP:N	2.50	0.44
1:B:748:ASN:HB3	1:B:752:LEU:C	2.38	0.44
1:B:401:MET:HE1	1:B:432:PHE:CB	2.46	0.44
1:B:183:MET:HA	1:B:183:MET:CE	2.47	0.44
1:C:726:HIS:CD2	1:C:727:TRP:N	2.86	0.44
1:D:54:MET:O	1:D:58:GLN:HG2	2.17	0.44
1:D:789:SER:HA	1:D:792:ARG:NH2	2.32	0.44
1:A:332:LYS:HE2	1:A:410:ASN:HD22	1.78	0.44
1:D:276:LYS:HD2	1:D:283:GLY:O	2.16	0.44
1:C:81:MET:O	1:C:85:ILE:HG13	2.18	0.44
1:A:666:MET:HB3	1:A:666:MET:HE3	1.83	0.44
1:A:711:LYS:HG2	1:A:718:ILE:HA	1.99	0.44
1:A:746:ARG:CZ	1:A:746:ARG:HB3	2.43	0.44
2:K:5:DA:H2''	2:K:6:DT:OP2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLU:CA	1:C:108:GLU:OE1	2.64	0.44
1:D:859:ASP:OD2	1:D:860:LYS:N	2.51	0.44
1:C:801:LYS:CE	1:C:801:LYS:O	2.64	0.44
1:C:89:PHE:HE2	1:C:107:GLN:HG3	1.83	0.44
1:D:543:ILE:HG21	1:D:689:VAL:HG11	1.99	0.44
1:C:482:ILE:HD12	1:C:514:PHE:HZ	1.81	0.44
1:C:448:LYS:O	1:C:448:LYS:HG3	2.17	0.44
1:A:744:GLN:H	1:A:744:GLN:HG3	1.51	0.44
1:C:860:LYS:O	1:C:862:PRO:HD3	2.18	0.44
1:D:319:ALA:HB3	1:D:792:ARG:HG2	1.97	0.44
1:D:463:HIS:CD2	1:D:534:LEU:HA	2.52	0.44
1:D:532:LEU:O	1:D:818:PRO:HD3	2.17	0.44
1:A:625:VAL:C	1:A:626:THR:HG23	2.37	0.44
1:A:320:ILE:HG12	1:A:320:ILE:H	1.62	0.44
1:C:709:GLU:HG2	1:C:709:GLU:O	2.16	0.44
1:A:711:LYS:HB3	1:A:717:GLU:O	2.17	0.44
1:D:619:GLN:O	1:D:622:ALA:HB3	2.17	0.44
1:D:159:ALA:O	1:D:160:LYS:C	2.56	0.44
1:C:164:LYS:NZ	5:C:2060:HOH:O	2.50	0.44
1:A:203:SER:O	1:A:205:HIS:N	2.49	0.44
1:A:229:LEU:HD11	1:A:242:GLU:HG2	2.00	0.44
1:A:133:THR:HA	1:A:243:THR:HA	2.00	0.44
1:A:804:ILE:CG2	1:A:816:THR:HG21	2.38	0.44
1:D:81:MET:HE2	1:D:220:LEU:HA	2.00	0.44
1:B:230:HIS:O	1:B:232:GLN:NE2	2.48	0.44
2:K:15:DC:H2"	2:K:16:DC:C5'	2.47	0.44
1:C:5:ASN:HA	1:C:52:ARG:HH11	1.82	0.44
1:B:272:VAL:HG13	1:B:411:HIS:CD2	2.53	0.44
1:B:427:TYR:N	1:B:427:TYR:CD1	2.85	0.44
1:A:569:ASP:CG	1:A:627:ARG:HH21	2.21	0.44
1:C:227:VAL:HG12	1:C:244:ILE:HG22	2.00	0.44
1:A:65:ALA:HB3	1:A:120:LYS:HE2	2.00	0.44
1:B:195:LEU:N	5:B:2099:HOH:O	2.49	0.44
1:D:327:ALA:CB	1:D:448:LYS:HE2	2.47	0.44
2:H:13:DC:H2"	2:H:14:DG:C5'	2.48	0.44
1:D:663:LYS:CG	1:D:664:GLY:N	2.76	0.44
1:B:534:LEU:HD11	1:B:818:PRO:HG3	2.00	0.44
1:A:744:GLN:HB3	1:A:756:ARG:HB2	2.00	0.44
1:A:155:ARG:HB3	1:A:749:LEU:HD21	2.00	0.44
1:C:16:LEU:HD13	1:C:38:ALA:CA	2.47	0.44
1:D:120:LYS:HD3	1:D:120:LYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:717:GLU:O	1:D:719:LEU:HD13	2.18	0.44
1:C:630:THR:HG22	1:C:681:ILE:HD13	2.00	0.44
1:D:185:VAL:HG23	1:D:186:VAL:N	2.32	0.44
1:A:159:ALA:O	1:A:160:LYS:C	2.56	0.44
1:C:416:PHE:O	1:C:418:TYR:CD1	2.70	0.44
1:D:463:HIS:CE1	5:D:2121:HOH:O	2.70	0.44
1:D:328:TRP:O	1:D:413:ALA:HA	2.18	0.44
1:D:389:LYS:NZ	3:O:3:G:O2'	2.51	0.44
1:B:335:LEU:HD22	1:B:339:ASN:CG	2.37	0.44
1:B:720:ARG:HE	1:B:854:HIS:H	1.65	0.44
1:D:232:GLN:NE2	1:D:243:THR:OG1	2.51	0.44
1:D:349:VAL:HG12	5:D:2096:HOH:O	2.18	0.44
1:C:313:MET:N	1:C:314:PRO:HD3	2.32	0.44
1:C:273:VAL:HA	1:C:415:TRP:CZ3	2.52	0.44
1:B:880:PHE:N	1:B:880:PHE:CD1	2.81	0.44
1:C:349:VAL:HG13	1:C:503:ALA:O	2.17	0.44
1:B:630:THR:O	1:B:634:VAL:CG1	2.66	0.44
1:A:176:HIS:HD2	1:A:751:PHE:CE1	2.36	0.44
1:A:631:LYS:O	1:A:634:VAL:HG12	2.18	0.44
1:B:257:ARG:CG	5:B:2125:HOH:O	2.57	0.44
1:C:718:ILE:HD12	5:C:2153:HOH:O	2.17	0.44
1:C:454:LYS:HG3	1:C:455:GLU:N	2.32	0.44
1:D:30:GLU:O	1:D:34:ARG:HG3	2.18	0.44
2:E:15:DC:H2''	2:E:16:DC:C5'	2.47	0.44
1:A:247:ALA:HA	1:A:248:PRO:HD3	1.88	0.44
1:D:236:VAL:CB	1:D:239:GLN:HB2	2.48	0.44
1:C:326:THR:O	1:C:415:TRP:CD1	2.71	0.44
1:C:479:ILE:HA	1:C:479:ILE:HD13	1.88	0.44
1:A:378:LYS:HD2	1:A:378:LYS:HA	1.90	0.44
1:A:645:GLY:HA3	2:E:10:DC:OP2	2.18	0.43
1:D:751:PHE:HD2	1:D:752:LEU:HD11	1.82	0.43
1:D:42:GLU:HG2	1:D:46:MET:HE1	1.99	0.43
1:B:281:ILE:HG23	1:B:305:LEU:CD2	2.46	0.43
1:D:641:SER:HA	2:N:10:DC:H5'	1.99	0.43
1:D:337:VAL:HG11	1:D:502:TRP:CZ2	2.52	0.43
1:A:115:ALA:O	1:A:119:ILE:CG1	2.66	0.43
1:D:873:ARG:HH11	1:D:876:LEU:CD1	2.30	0.43
1:B:412:LYS:O	1:B:413:ALA:HB2	2.17	0.43
1:D:487:GLU:OE1	1:D:487:GLU:HA	2.17	0.43
1:A:178:TYR:N	1:A:178:TYR:CD2	2.86	0.43
1:D:348:PRO:CD	5:D:2092:HOH:O	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:NE	1:A:222:GLU:HB3	2.33	0.43
1:C:455:GLU:O	1:C:458:TYR:HB3	2.18	0.43
1:A:449:GLY:C	1:A:529:ASN:HD21	2.22	0.43
1:C:790:HIS:HD1	1:C:790:HIS:C	2.21	0.43
1:C:143:ARG:NH1	1:C:209:SER:HB2	2.33	0.43
1:B:193:LYS:HB2	1:B:194:GLY:H	1.55	0.43
1:A:269:GLN:HB3	1:A:270:PRO:CD	2.49	0.43
1:C:536:PHE:CE1	1:C:825:PHE:HD2	2.36	0.43
1:A:641:SER:CB	2:E:10:DC:H5'	2.48	0.43
1:A:104:GLN:HB2	1:A:105:PHE:CD2	2.54	0.43
1:C:720:ARG:NH2	1:C:857:GLN:OE1	2.34	0.43
1:D:651:LEU:O	1:D:656:GLN:HB2	2.18	0.43
1:A:232:GLN:HB2	1:A:241:SER:O	2.19	0.43
1:A:308:TYR:C	1:A:311:VAL:HG23	2.38	0.43
1:C:404:GLN:HG2	1:C:432:PHE:HB2	2.00	0.43
1:B:231:ARG:HG2	1:B:234:ALA:HB2	2.00	0.43
1:C:779:ALA:HB3	1:C:780:PRO:CD	2.48	0.43
1:B:88:TRP:O	1:B:92:VAL:HG23	2.18	0.43
1:A:825:PHE:CE2	1:A:829:ARG:NH2	2.87	0.43
1:A:700:LYS:HA	1:A:778:ILE:HG21	2.00	0.43
1:A:422:TRP:C	1:A:422:TRP:CD1	2.90	0.43
1:D:750:MET:HG2	1:D:750:MET:H	1.64	0.43
1:D:663:LYS:HE3	1:D:666:MET:HE3	2.01	0.43
1:D:231:ARG:NH1	1:D:242:GLU:HB2	2.33	0.43
1:D:450:LYS:HD2	1:D:817:ILE:HD11	2.01	0.43
1:D:446:LEU:HD12	1:D:817:ILE:CG2	2.48	0.43
1:D:148:GLU:CG	5:D:2041:HOH:O	2.65	0.43
1:D:726:HIS:CD2	1:D:727:TRP:H	2.33	0.43
1:A:115:ALA:O	1:A:119:ILE:HD11	2.17	0.43
1:B:6:ILE:O	1:B:8:LYS:N	2.40	0.43
1:A:249:GLU:CG	5:A:2109:HOH:O	2.66	0.43
1:A:779:ALA:O	1:A:780:PRO:C	2.56	0.43
1:D:177:VAL:HG12	1:D:178:TYR:CD2	2.53	0.43
1:C:741:LYS:HG2	5:C:2159:HOH:O	2.16	0.43
1:B:663:LYS:CG	1:B:664:GLY:N	2.64	0.43
1:B:221:ILE:CG1	1:B:227:VAL:HG23	2.49	0.43
1:D:446:LEU:HB2	1:D:531:SER:O	2.19	0.43
1:B:825:PHE:CE2	1:B:829:ARG:NH2	2.87	0.43
1:A:14:ILE:O	1:A:16:LEU:HD23	2.18	0.43
1:A:57:ARG:HB3	1:A:60:LYS:HZ1	1.83	0.43
1:C:514:PHE:HD1	1:C:515:CYS:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ARG:HG3	1:A:829:ARG:NH1	2.32	0.43
1:A:842:LEU:HD23	1:A:864:LEU:CD2	2.47	0.43
1:D:372:GLU:HB2	5:D:2105:HOH:O	2.17	0.43
1:B:157:LEU:HG	1:B:195:LEU:CD2	2.48	0.43
1:D:281:ILE:HA	1:D:281:ILE:HD12	1.67	0.43
1:B:781:ASN:HD21	2:H:12:DT:C5'	2.31	0.43
1:B:754:GLN:HB3	1:B:755:PHE:H	1.54	0.43
1:D:163:LYS:O	1:D:166:VAL:HB	2.19	0.43
1:B:719:LEU:CD1	1:B:719:LEU:N	2.81	0.43
1:A:230:HIS:HE2	1:A:245:GLU:HG2	1.84	0.43
1:C:871:ASN:O	1:C:873:ARG:N	2.52	0.43
1:D:571:TYR:HD1	1:D:634:VAL:HG11	1.82	0.43
1:A:481:PHE:C	1:A:481:PHE:CD2	2.91	0.43
1:C:217:ILE:O	1:C:221:ILE:HG13	2.19	0.43
1:D:828:VAL:CG2	1:D:883:ALA:HA	2.48	0.43
1:C:459:TRP:HB3	1:C:534:LEU:CD1	2.49	0.43
1:C:147:ASP:OD1	1:C:180:LYS:HE3	2.18	0.43
1:D:46:MET:HE1	1:D:269:GLN:OE1	2.19	0.43
1:B:730:PRO:CG	1:B:786:GLN:HE22	2.31	0.43
1:C:623:TYR:HA	1:C:666:MET:HE1	1.99	0.43
1:D:148:GLU:HG3	5:D:2041:HOH:O	2.18	0.43
2:N:6:DT:H2'	5:N:2008:HOH:O	2.19	0.43
2:N:5:DA:C2	4:P:7:DT:O2	2.72	0.43
1:C:700:LYS:HA	1:C:778:ILE:HG21	2.01	0.43
1:B:656:GLN:HB3	1:B:657:PRO:HD2	2.00	0.43
1:B:272:VAL:HG13	1:B:411:HIS:HD2	1.82	0.43
1:D:374:LEU:C	1:D:376:ALA:H	2.21	0.43
1:C:523:HIS:N	1:C:523:HIS:CD2	2.84	0.43
1:B:668:THR:O	1:B:670:PRO:HD3	2.19	0.43
2:H:13:DC:H2''	2:H:14:DG:H5'	2.01	0.43
1:B:236:VAL:HG11	1:B:239:GLN:NE2	2.34	0.43
1:C:154:ILE:HD13	1:C:190:MET:CE	2.48	0.43
1:D:353:PRO:CD	5:D:2098:HOH:O	2.65	0.43
1:D:343:LYS:HB3	1:D:343:LYS:HE3	1.90	0.43
1:C:664:GLY:HA2	1:C:667:PHE:CD2	2.54	0.43
1:B:275:PRO:HD3	1:B:415:TRP:CB	2.48	0.43
1:A:651:LEU:C	1:A:651:LEU:HD13	2.39	0.43
1:A:61:ALA:HB3	1:A:63:GLU:HG3	2.01	0.43
1:C:828:VAL:C	1:C:831:THR:HG22	2.38	0.43
1:A:881:ALA:HA	5:A:2310:HOH:O	2.16	0.43
1:A:814:PHE:HE1	1:A:883:ALA:HB2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:THR:HB	5:B:2107:HOH:O	2.18	0.43
1:B:201:TRP:O	1:B:204:TRP:HB2	2.19	0.43
1:B:106:LEU:HD21	1:B:212:VAL:HG13	1.97	0.43
1:A:24:LEU:HD21	1:A:287:TRP:CG	2.51	0.43
1:D:406:ASN:CB	5:D:2112:HOH:O	2.64	0.43
1:D:215:ARG:HA	1:D:215:ARG:HD2	1.81	0.43
5:B:2341:HOH:O	4:J:5:DA:H5''	2.18	0.43
1:C:632:ARG:HG2	5:C:2145:HOH:O	2.19	0.43
1:D:567:VAL:HA	1:D:880:PHE:CD2	2.54	0.43
1:B:833:VAL:HG12	1:B:834:ASP:N	2.32	0.43
1:A:621:LEU:HA	1:A:621:LEU:HD23	1.82	0.43
1:A:294:LEU:HA	1:A:294:LEU:HD23	1.79	0.43
1:B:162:PHE:CD2	1:B:162:PHE:O	2.71	0.43
1:B:164:LYS:N	1:B:164:LYS:HE3	2.33	0.43
1:A:772:HIS:CE1	4:G:6:DT:H5'	2.53	0.43
1:B:7:ALA:CB	5:B:2057:HOH:O	2.67	0.43
1:D:829:ARG:HD3	1:D:875:ILE:O	2.19	0.43
1:B:216:CYS:N	1:B:219:MET:HE2	2.33	0.43
1:C:158:GLU:HG2	1:C:195:LEU:CD2	2.49	0.43
1:C:195:LEU:HA	1:C:195:LEU:HD12	1.81	0.43
1:B:42:GLU:HG2	1:B:46:MET:CE	2.49	0.43
1:D:490:MET:CE	1:D:522:GLN:HG3	2.49	0.43
1:B:16:LEU:HD13	1:B:38:ALA:CB	2.49	0.43
1:D:126:LEU:HD21	1:D:244:ILE:CG2	2.42	0.43
1:D:101:THR:HG21	5:D:2055:HOH:O	2.18	0.43
1:D:668:THR:O	1:D:670:PRO:HD3	2.19	0.43
1:B:610:LYS:O	1:B:611:LEU:C	2.57	0.43
1:B:296:LEU:O	1:B:296:LEU:HG	2.18	0.43
1:C:231:ARG:CZ	1:C:242:GLU:HB2	2.49	0.42
1:C:828:VAL:O	1:C:831:THR:CG2	2.67	0.42
1:D:274:PRO:HD3	1:D:415:TRP:CH2	2.54	0.42
1:B:401:MET:HE3	1:B:432:PHE:HD1	1.83	0.42
1:D:93:LYS:HA	1:D:99:ARG:HH12	1.83	0.42
1:B:726:HIS:CD2	1:B:736:TRP:CE2	3.07	0.42
1:C:810:ILE:HB	1:C:813:SER:HB3	1.99	0.42
1:D:722:ARG:HD2	1:D:768:GLU:OE2	2.19	0.42
1:A:234:ALA:HA	1:A:240:ASP:OD2	2.19	0.42
1:C:509:PHE:N	1:C:509:PHE:CD2	2.87	0.42
1:B:343:LYS:HB3	1:B:343:LYS:HE3	1.76	0.42
1:B:629:VAL:HG12	1:B:629:VAL:O	2.18	0.42
1:C:807:PHE:N	1:C:807:PHE:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ARG:HG3	1:D:420:MET:O	2.19	0.42
1:B:709:GLU:O	1:B:711:LYS:HG3	2.20	0.42
1:A:724:ALA:HA	1:A:774:GLN:NE2	2.34	0.42
1:A:298:ARG:HG3	1:A:420:MET:O	2.18	0.42
1:C:746:ARG:HB2	1:C:754:GLN:O	2.19	0.42
1:D:578:VAL:HG13	1:D:680:LEU:HB3	2.00	0.42
1:B:141:ILE:HG13	1:B:141:ILE:H	1.58	0.42
2:N:12:DT:H2''	2:N:13:DC:O5'	2.20	0.42
1:C:641:SER:HA	2:K:10:DC:H5'	2.01	0.42
1:D:6:ILE:HG23	1:D:10:ASP:CG	2.40	0.42
1:A:8:LYS:O	1:A:12:SER:HB2	2.18	0.42
1:B:699:LEU:O	1:B:778:ILE:HG21	2.19	0.42
1:B:83:ALA:O	1:B:87:ASP:OD2	2.37	0.42
1:C:231:ARG:NH2	1:C:242:GLU:HB2	2.34	0.42
1:A:63:GLU:C	5:A:2057:HOH:O	2.57	0.42
1:A:828:VAL:HB	1:A:883:ALA:HA	2.01	0.42
1:C:485:ASN:ND2	1:C:488:ASN:ND2	2.53	0.42
1:C:833:VAL:O	1:C:837:GLU:HG3	2.19	0.42
1:B:146:GLU:HG3	1:B:204:TRP:CD2	2.54	0.42
1:B:717:GLU:HB3	5:B:2302:HOH:O	2.19	0.42
1:D:505:GLN:O	1:D:508:PRO:HD3	2.18	0.42
1:A:20:PRO:HA	5:A:2043:HOH:O	2.19	0.42
1:C:291:ARG:HD3	1:C:291:ARG:HA	1.74	0.42
1:C:615:ALA:O	1:C:619:GLN:HG3	2.19	0.42
1:C:677:MET:O	1:C:681:ILE:HG13	2.18	0.42
1:A:163:LYS:HD2	1:A:166:VAL:HB	1.99	0.42
1:D:337:VAL:HG11	1:D:502:TRP:CH2	2.54	0.42
1:B:322:ILE:CD1	1:B:799:HIS:CD2	3.02	0.42
1:D:846:TYR:CD1	1:D:846:TYR:C	2.93	0.42
1:A:512:LEU:HG	1:A:516:PHE:CE2	2.53	0.42
1:B:98:LYS:NZ	5:B:2080:HOH:O	2.52	0.42
1:B:605:ILE:N	5:B:2273:HOH:O	2.52	0.42
1:D:316:VAL:HG12	1:D:317:TYR:N	2.34	0.42
1:A:131:ASN:C	1:A:131:ASN:OD1	2.57	0.42
1:B:331:ASN:HA	5:B:2151:HOH:O	2.18	0.42
1:C:457:TYR:HD1	1:C:521:VAL:HG21	1.84	0.42
1:A:226:MET:HG3	1:A:250:TYR:CD1	2.37	0.42
1:C:274:PRO:HA	1:C:275:PRO:HD3	1.90	0.42
1:B:6:ILE:CB	1:B:48:GLU:OE2	2.66	0.42
1:C:502:TRP:CZ2	1:C:512:LEU:HD22	2.55	0.42
1:B:253:ALA:CB	5:B:2001:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:VAL:CG1	1:C:503:ALA:O	2.68	0.42
1:A:625:VAL:C	1:A:626:THR:CG2	2.85	0.42
1:B:700:LYS:HA	1:B:778:ILE:HG21	2.01	0.42
1:D:643:GLU:HG3	1:D:682:TRP:CB	2.50	0.42
1:D:326:THR:HG23	1:D:806:SER:CA	2.46	0.42
1:D:659:ILE:HA	1:D:663:LYS:O	2.19	0.42
1:D:275:PRO:HG2	1:D:324:GLN:CG	2.50	0.42
2:E:11:DA:H2''	2:E:12:DT:O5'	2.19	0.42
1:C:551:ARG:HD3	1:C:872:LEU:HD21	2.01	0.42
1:D:137:VAL:HG21	5:D:2038:HOH:O	2.20	0.42
1:A:372:GLU:HB2	5:A:2014:HOH:O	2.19	0.42
1:B:182:PHE:O	1:B:186:VAL:HG23	2.20	0.42
1:C:418:TYR:HD2	1:C:426:VAL:HG12	1.82	0.42
1:D:9:ASN:CA	1:D:12:SER:HB3	2.49	0.42
1:D:6:ILE:O	1:D:8:LYS:N	2.44	0.42
1:A:685:VAL:HG23	1:A:686:SER:N	2.35	0.42
1:B:852:GLN:HB2	1:B:852:GLN:HE21	1.47	0.42
1:A:59:LEU:HD23	1:A:64:VAL:HG13	2.00	0.42
1:C:453:GLY:C	1:C:526:LEU:HD22	2.40	0.42
1:B:59:LEU:HD23	1:B:64:VAL:HG22	1.99	0.42
1:A:205:HIS:CD2	1:A:206:LYS:HE2	2.53	0.42
1:B:582:LEU:CD2	1:B:620:TRP:HB2	2.50	0.42
1:C:748:ASN:ND2	1:C:751:PHE:H	2.17	0.42
1:A:322:ILE:HD13	1:A:799:HIS:CD2	2.54	0.42
1:A:14:ILE:HG22	1:A:14:ILE:O	2.20	0.42
1:C:632:ARG:HA	1:C:635:MET:HG2	2.02	0.42
1:B:475:PHE:HE1	1:B:478:ARG:HH12	1.65	0.42
4:J:3:DC:C2'	5:J:2002:HOH:O	2.62	0.42
1:B:313:MET:N	1:B:314:PRO:HD3	2.33	0.42
1:B:455:GLU:O	1:B:458:TYR:HB3	2.19	0.42
1:B:490:MET:HE1	1:B:522:GLN:CB	2.50	0.42
1:C:448:LYS:CG	1:C:448:LYS:O	2.67	0.42
1:B:412:LYS:HA	1:B:412:LYS:HD2	1.83	0.42
1:C:98:LYS:HB3	1:C:98:LYS:HE2	1.91	0.42
1:A:722:ARG:HB3	1:A:722:ARG:HE	1.27	0.42
1:A:270:PRO:HD2	1:A:408:PHE:CE2	2.53	0.42
1:D:666:MET:HG2	1:D:667:PHE:CD1	2.54	0.42
1:C:79:PRO:HG2	1:C:80:LYS:H	1.84	0.42
1:D:109:ILE:HG23	1:D:148:GLU:HG3	2.01	0.42
4:M:7:DT:H2''	4:M:8:DC:C5	2.55	0.42
4:M:8:DC:H2''	4:M:9:DC:OP2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLU:HB3	5:B:2117:HOH:O	2.19	0.42
1:A:274:PRO:HA	1:A:275:PRO:HD3	1.94	0.42
1:D:488:ASN:HB3	1:D:501:TRP:CZ3	2.54	0.42
1:C:89:PHE:CE2	1:C:107:GLN:HA	2.55	0.42
1:D:748:ASN:HB2	1:D:753:GLY:HA2	1.99	0.42
1:C:810:ILE:HG22	3:L:8:U:H5'	2.01	0.42
1:C:346:HIS:ND1	1:C:391:ARG:NH2	2.67	0.42
1:D:846:TYR:CD1	1:D:850:ALA:HB2	2.55	0.42
1:D:152:GLY:O	1:D:156:ASP:OD2	2.38	0.42
1:D:852:GLN:HB2	1:D:852:GLN:HE21	1.52	0.42
1:A:814:PHE:CE1	1:A:883:ALA:CB	3.02	0.42
1:B:14:ILE:HG23	1:B:288:ALA:CB	2.46	0.42
1:A:340:VAL:HG12	1:A:341:ILE:N	2.34	0.42
2:K:11:DA:H2''	2:K:12:DT:O5'	2.19	0.42
1:D:754:GLN:O	1:D:755:PHE:O	2.37	0.42
1:D:229:LEU:O	1:D:229:LEU:HG	2.18	0.42
1:A:77:LEU:HD22	1:A:226:MET:SD	2.60	0.42
1:A:292:ARG:NH1	1:A:292:ARG:CG	2.83	0.42
1:C:57:ARG:CD	5:C:2041:HOH:O	2.67	0.42
1:C:845:PHE:O	1:C:848:GLN:HB2	2.20	0.42
1:C:68:ALA:HB3	1:C:261:LEU:CD2	2.45	0.42
1:C:15:GLU:HG2	1:C:18:ALA:N	2.32	0.42
1:D:836:TYR:HB2	1:D:872:LEU:HD13	2.02	0.42
1:A:249:GLU:N	1:A:249:GLU:OE1	2.50	0.42
1:C:474:PRO:HB2	1:C:476:PRO:HD2	2.02	0.42
1:B:713:LYS:HA	1:B:713:LYS:HD2	1.79	0.42
1:A:573:ILE:HD11	1:A:688:THR:CG2	2.49	0.42
1:C:586:ALA:HB3	5:C:2136:HOH:O	2.20	0.42
1:C:665:LEU:HA	1:C:665:LEU:HD23	1.88	0.42
1:B:860:LYS:HG2	1:B:860:LYS:O	2.20	0.42
1:A:790:HIS:CD2	1:A:790:HIS:O	2.73	0.42
1:C:231:ARG:HD2	1:C:240:ASP:OD1	2.20	0.42
1:B:160:LYS:NZ	1:B:161:HIS:CE1	2.88	0.42
1:C:827:ALA:O	1:C:831:THR:HG22	2.19	0.42
1:D:829:ARG:HG3	1:D:829:ARG:NH1	2.26	0.42
1:B:754:GLN:NE2	3:I:1:G:H4'	2.34	0.42
1:D:220:LEU:CG	5:D:2059:HOH:O	2.63	0.42
1:D:247:ALA:HA	1:D:248:PRO:HD3	1.87	0.42
1:A:57:ARG:HA	1:A:60:LYS:HB3	2.02	0.42
1:B:231:ARG:CD	1:B:240:ASP:OD1	2.67	0.42
1:C:71:LYS:N	1:C:72:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:MET:HE3	1:C:317:TYR:CE2	2.55	0.42
1:A:810:ILE:O	1:A:812:ASP:N	2.53	0.42
1:B:11:PHE:N	5:B:2030:HOH:O	2.47	0.42
4:G:8:DC:N4	5:G:2010:HOH:O	2.52	0.42
1:B:550:LEU:HA	1:B:550:LEU:HD23	1.68	0.42
1:C:333:LYS:C	1:C:516:PHE:HE2	2.24	0.42
1:D:326:THR:O	1:D:415:TRP:CD1	2.73	0.42
1:A:571:TYR:HE1	1:A:634:VAL:HG13	1.85	0.42
1:D:416:PHE:HA	1:D:417:PRO:HD2	1.95	0.42
1:B:746:ARG:NH1	1:B:754:GLN:O	2.53	0.42
1:C:16:LEU:H	1:C:16:LEU:CD2	2.14	0.42
1:B:43:SER:HA	1:B:46:MET:HE3	2.01	0.42
1:C:171:ASN:O	3:L:2:C:O2'	2.37	0.42
1:D:573:ILE:HD12	1:D:573:ILE:C	2.40	0.42
1:C:611:LEU:HD22	1:C:615:ALA:HB1	2.02	0.42
1:A:542:GLY:HA2	1:A:783:VAL:HG11	2.01	0.42
1:A:713:LYS:CA	1:A:713:LYS:HE3	2.50	0.42
1:D:689:VAL:HA	5:D:2133:HOH:O	2.19	0.42
1:D:698:TRP:CE3	1:D:842:LEU:HG	2.55	0.42
1:D:346:HIS:CD2	1:D:391:ARG:NH2	2.88	0.42
1:A:522:GLN:HG2	1:A:522:GLN:H	1.50	0.42
1:C:473:VAL:O	1:C:478:ARG:NE	2.33	0.42
1:D:47:GLY:O	1:D:50:ARG:HB3	2.20	0.42
1:B:706:LEU:HD11	1:B:849:PHE:CB	2.50	0.42
1:A:823:ASN:N	5:A:2294:HOH:O	2.45	0.42
1:C:350:GLU:OE1	1:C:350:GLU:HA	2.20	0.41
1:B:84:ARG:CG	1:B:223:SER:HB3	2.50	0.41
1:C:457:TYR:CE1	1:C:521:VAL:CG1	2.88	0.41
2:K:13:DC:H2''	2:K:14:DG:C5'	2.50	0.41
1:B:54:MET:HA	5:B:2061:HOH:O	2.19	0.41
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.92	0.41
1:D:349:VAL:HG11	1:D:503:ALA:O	2.20	0.41
1:D:402:LEU:HG	1:D:439:MET:HE2	1.99	0.41
1:D:710:VAL:CG1	1:D:720:ARG:HB3	2.46	0.41
1:D:639:TYR:CE2	2:N:11:DA:C6	3.07	0.41
1:A:583:GLN:HB3	1:A:583:GLN:HE21	1.44	0.41
1:C:329:LYS:HB2	1:C:329:LYS:HE3	1.84	0.41
1:B:655:ILE:O	1:B:659:ILE:HG13	2.20	0.41
1:D:207:GLU:OE1	1:D:207:GLU:HA	2.20	0.41
1:B:431:MET:HB3	1:B:431:MET:HE2	1.86	0.41
1:A:179:LYS:HE2	1:A:750:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:ILE:HD12	1:D:20:PRO:HD2	2.01	0.41
1:B:15:GLU:HB2	1:B:18:ALA:O	2.19	0.41
1:D:322:ILE:HD12	1:D:799:HIS:NE2	2.35	0.41
1:B:166:VAL:O	1:B:168:GLU:OE1	2.38	0.41
1:C:292:ARG:N	1:C:293:PRO:CD	2.83	0.41
1:C:205:HIS:HD2	1:C:206:LYS:HD3	1.86	0.41
1:B:551:ARG:NH2	1:B:836:TYR:O	2.53	0.41
1:D:588:ASN:N	1:D:588:ASN:ND2	2.69	0.41
5:A:2164:HOH:O	3:F:7:A:H1'	2.20	0.41
1:D:21:PHE:C	1:D:21:PHE:CD1	2.94	0.41
1:C:304:ALA:HA	1:C:307:ARG:NH1	2.36	0.41
1:C:137:VAL:O	1:C:141:ILE:HG13	2.20	0.41
1:C:454:LYS:HG3	1:C:455:GLU:H	1.85	0.41
1:C:402:LEU:HD23	1:C:402:LEU:HA	1.78	0.41
1:C:801:LYS:NZ	5:C:2174:HOH:O	2.51	0.41
1:D:488:ASN:O	1:D:491:ALA:HB3	2.20	0.41
1:B:475:PHE:HA	1:B:478:ARG:HD2	2.01	0.41
1:D:801:LYS:O	1:D:801:LYS:CE	2.69	0.41
1:D:647:ARG:HG2	1:D:675:GLY:HA2	2.00	0.41
1:A:727:TRP:CZ2	1:A:735:VAL:HG21	2.55	0.41
1:D:23:THR:O	1:D:27:HIS:HB2	2.20	0.41
1:A:828:VAL:HG11	1:A:883:ALA:HA	2.02	0.41
1:D:422:TRP:HZ2	1:D:781:ASN:OD1	2.02	0.41
2:H:11:DA:H2''	2:H:12:DT:O5'	2.19	0.41
1:D:285:GLY:HA2	1:D:324:GLN:NE2	2.34	0.41
1:A:109:ILE:HG13	1:A:149:ALA:HB2	2.01	0.41
1:B:882:PHE:CD1	1:B:882:PHE:N	2.84	0.41
1:D:335:LEU:CD2	1:D:339:ASN:HD21	2.33	0.41
1:D:335:LEU:HD21	1:D:406:ASN:OD1	2.19	0.41
1:D:109:ILE:HD12	1:D:109:ILE:N	2.26	0.41
1:B:473:VAL:HG13	1:B:474:PRO:HD2	2.03	0.41
1:B:596:THR:HB	5:B:2263:HOH:O	2.20	0.41
1:D:553:GLU:HB2	5:D:2135:HOH:O	2.19	0.41
1:C:860:LYS:O	1:C:862:PRO:CD	2.69	0.41
1:C:416:PHE:O	1:C:418:TYR:CE1	2.74	0.41
1:B:110:LYS:HE2	1:B:112:GLU:OE1	2.20	0.41
1:C:272:VAL:HG12	1:C:272:VAL:O	2.20	0.41
1:C:32:LEU:HD12	1:C:32:LEU:HA	1.74	0.41
1:A:151:PHE:CD1	1:A:183:MET:HB3	2.56	0.41
1:D:543:ILE:CG2	1:D:559:VAL:HG11	2.50	0.41
1:D:602:THR:CG2	1:D:604:GLU:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:ILE:HB	1:A:813:SER:HB3	2.02	0.41
1:B:476:PRO:HG2	5:B:2209:HOH:O	2.19	0.41
1:D:712:ASP:OD2	1:D:714:LYS:HB2	2.20	0.41
1:A:269:GLN:HG2	1:A:404:GLN:OE1	2.21	0.41
1:D:829:ARG:NH1	1:D:829:ARG:CG	2.79	0.41
2:E:5:DA:H2"	2:E:6:DT:O5'	2.19	0.41
1:B:723:CYS:C	5:B:2306:HOH:O	2.58	0.41
1:C:50:ARG:HG2	5:C:2039:HOH:O	2.19	0.41
1:D:737:GLN:OE1	1:D:774:GLN:NE2	2.53	0.41
1:C:15:GLU:HB3	1:C:18:ALA:O	2.20	0.41
1:C:277:PRO:HA	1:C:321:ASN:OD1	2.21	0.41
1:B:4:ILE:HD12	1:B:256:THR:HA	2.02	0.41
1:D:594:VAL:HA	1:D:609:VAL:HA	2.02	0.41
1:B:264:ILE:C	1:B:266:PRO:HD3	2.41	0.41
1:A:748:ASN:HB2	1:A:753:GLY:CA	2.51	0.41
1:C:229:LEU:HD11	1:C:242:GLU:CG	2.50	0.41
4:G:1:DG:C2	4:G:2:DT:O4	2.73	0.41
1:C:549:MET:CE	1:C:841:VAL:HG21	2.50	0.41
1:B:347:CYS:HA	1:B:348:PRO:HD3	1.93	0.41
1:D:656:GLN:HB3	1:D:657:PRO:HD3	2.03	0.41
1:C:206:LYS:H	1:C:206:LYS:HD3	1.85	0.41
1:A:665:LEU:HB2	5:A:2027:HOH:O	2.20	0.41
1:C:778:ILE:HD12	1:C:778:ILE:HA	1.87	0.41
1:A:529:ASN:ND2	1:A:529:ASN:C	2.72	0.41
1:B:516:PHE:HB2	5:B:2226:HOH:O	2.21	0.41
1:A:642:LYS:O	1:A:643:GLU:C	2.57	0.41
1:D:772:HIS:CD2	2:N:8:DG:H5"	2.55	0.41
1:A:669:GLN:CG	1:A:672:GLN:NE2	2.64	0.41
1:B:663:LYS:HE3	1:B:666:MET:CE	2.51	0.41
1:D:777:GLY:O	1:D:781:ASN:HB2	2.20	0.41
1:B:577:LYS:HE2	1:B:687:VAL:HG23	2.01	0.41
1:A:93:LYS:HA	1:A:99:ARG:HH22	1.76	0.41
1:B:257:ARG:HA	5:B:2125:HOH:O	2.20	0.41
1:D:150:ARG:O	1:D:153:ARG:HB3	2.21	0.41
4:G:7:DT:C7	5:G:2002:HOH:O	2.68	0.41
1:C:754:GLN:HB3	1:C:755:PHE:H	1.53	0.41
1:C:507:SER:HA	1:C:508:PRO:HD2	1.85	0.41
1:B:489:ILE:CG2	1:B:518:TYR:HD1	2.32	0.41
1:A:656:GLN:HB3	1:A:657:PRO:HD3	2.03	0.41
1:C:437:ASN:C	1:C:437:ASN:ND2	2.74	0.41
1:B:551:ARG:NE	5:B:2240:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:632:ARG:HD2	1:C:653:ASP:OD2	2.20	0.41
1:C:6:ILE:HG22	1:C:10:ASP:CG	2.41	0.41
1:C:308:TYR:HA	1:C:311:VAL:CG2	2.50	0.41
1:B:871:ASN:O	1:B:873:ARG:N	2.53	0.41
1:C:269:GLN:HE22	1:C:407:LYS:HZ3	1.68	0.41
1:A:332:LYS:NZ	1:A:410:ASN:ND2	2.68	0.41
1:D:846:TYR:CE1	1:D:850:ALA:HB2	2.55	0.41
1:A:810:ILE:HG22	3:F:8:U:H5'	2.01	0.41
1:C:286:TYR:CD2	1:C:294:LEU:HD11	2.56	0.41
1:C:176:HIS:C	1:C:176:HIS:ND1	2.73	0.41
1:D:423:ARG:HE	1:D:781:ASN:HD22	1.67	0.41
1:D:204:TRP:HB3	5:D:2057:HOH:O	2.20	0.41
1:C:164:LYS:O	1:C:168:GLU:OE1	2.39	0.41
1:B:582:LEU:HB3	1:B:621:LEU:HD21	2.03	0.41
1:D:654:THR:C	1:D:657:PRO:HD2	2.41	0.41
1:B:231:ARG:NH2	5:B:2110:HOH:O	2.54	0.41
1:C:630:THR:O	1:C:634:VAL:CG1	2.63	0.41
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.82	0.41
1:A:163:LYS:C	1:A:164:LYS:HZ3	2.23	0.41
1:D:860:LYS:O	1:D:860:LYS:HD3	2.21	0.41
1:B:791:LEU:HA	1:B:814:PHE:HE2	1.85	0.41
1:C:645:GLY:HA3	2:K:10:DC:OP2	2.21	0.41
1:A:249:GLU:N	1:A:249:GLU:CD	2.74	0.41
2:H:15:DC:H2''	2:H:16:DC:O5'	2.21	0.41
1:D:611:LEU:HB2	1:D:616:LEU:HD21	2.02	0.41
1:A:2:ASN:N	5:A:2002:HOH:O	2.53	0.41
1:A:526:LEU:HA	1:A:526:LEU:HD23	1.86	0.41
1:A:62:GLY:C	1:A:64:VAL:H	2.23	0.41
1:A:120:LYS:CG	1:A:752:LEU:HD21	2.49	0.41
1:B:13:ASP:OD1	1:B:291:ARG:NH1	2.51	0.41
1:D:326:THR:HG23	5:D:2087:HOH:O	2.20	0.41
1:D:425:ARG:NH1	1:D:784:HIS:CE1	2.89	0.41
1:A:711:LYS:HA	1:A:719:LEU:HD13	2.03	0.41
1:D:468:ALA:HA	1:D:505:GLN:HB3	2.03	0.41
1:C:44:TYR:OH	1:C:292:ARG:HB3	2.21	0.41
1:A:229:LEU:HD11	1:A:242:GLU:CG	2.51	0.41
1:A:806:SER:O	1:A:816:THR:HG22	2.19	0.41
1:B:137:VAL:HG12	1:B:217:ILE:HD11	2.01	0.41
1:D:312:TYR:CZ	1:D:314:PRO:HG3	2.55	0.41
1:A:267:MET:HE3	2:E:16:DC:OP1	2.21	0.41
1:D:700:LYS:NZ	1:D:700:LYS:CB	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:ASN:O	1:D:441:LYS:HG3	2.21	0.41
1:C:6:ILE:O	1:C:8:LYS:N	2.43	0.41
1:B:386:ARG:HE	3:I:5:C:P	2.44	0.41
1:B:395:ARG:O	1:B:395:ARG:HG3	2.20	0.41
1:D:341:ILE:HG12	1:D:341:ILE:H	1.73	0.41
1:D:291:ARG:C	1:D:293:PRO:HD3	2.41	0.41
1:D:60:LYS:HE2	1:D:60:LYS:HB3	1.68	0.41
1:D:8:LYS:HB3	1:D:9:ASN:H	1.49	0.41
1:A:6:ILE:O	1:A:8:LYS:N	2.42	0.41
1:B:198:GLY:O	1:B:199:GLU:HB2	2.21	0.41
1:A:518:TYR:O	1:A:522:GLN:HG2	2.21	0.41
1:B:495:SER:HB2	1:B:498:GLU:HB2	2.03	0.41
1:B:276:LYS:NZ	1:B:283:GLY:O	2.40	0.41
1:D:452:ILE:HD11	1:D:457:TYR:HA	2.02	0.41
1:B:98:LYS:HB3	1:B:98:LYS:HE2	1.78	0.41
1:A:753:GLY:O	1:A:754:GLN:HG2	2.20	0.41
1:D:192:SER:C	1:D:193:LYS:HG3	2.42	0.41
1:A:775:GLU:HG2	1:A:775:GLU:O	2.20	0.41
1:C:787:ASP:C	1:C:787:ASP:OD1	2.58	0.41
1:A:582:LEU:HD23	1:A:582:LEU:HA	1.89	0.41
1:A:497:LEU:HA	1:A:497:LEU:HD23	1.77	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.60	0.41
1:D:472:LYS:HD2	1:D:472:LYS:HA	1.96	0.41
1:B:247:ALA:HA	1:B:248:PRO:HD3	1.92	0.41
1:D:619:GLN:NE2	1:D:666:MET:O	2.54	0.41
1:D:652:GLU:HA	1:D:656:GLN:HB2	2.02	0.41
1:C:664:GLY:HA2	1:C:667:PHE:HD2	1.86	0.41
1:A:416:PHE:HA	1:A:417:PRO:HD2	1.99	0.41
1:A:437:ASN:C	1:A:437:ASN:HD22	2.24	0.41
1:D:70:ALA:O	1:D:74:ILE:HG13	2.21	0.41
1:B:476:PRO:HG2	5:B:2249:HOH:O	2.21	0.41
1:D:563:PRO:HB3	1:D:877:GLU:O	2.21	0.41
1:A:720:ARG:HD3	1:A:854:HIS:HB2	2.02	0.40
1:C:154:ILE:HA	1:C:158:GLU:HB2	2.02	0.40
1:D:352:ILE:CG2	5:D:2101:HOH:O	2.65	0.40
1:B:347:CYS:SG	1:B:350:GLU:HG3	2.62	0.40
1:B:416:PHE:CE1	1:B:432:PHE:O	2.75	0.40
1:C:120:LYS:HZ2	1:C:752:LEU:HG	1.85	0.40
1:A:244:ILE:O	1:A:245:GLU:CD	2.59	0.40
4:M:4:DG:H1'	4:M:5:DA:C8	2.56	0.40
1:B:324:GLN:HG3	1:B:417:PRO:HA	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:MET:CE	1:C:317:TYR:CE2	3.04	0.40
1:D:840:ASP:O	1:D:842:LEU:N	2.54	0.40
1:B:353:PRO:HB2	5:B:2164:HOH:O	2.21	0.40
1:C:430:SER:O	1:C:433:ASN:ND2	2.46	0.40
1:D:540:CYS:O	1:D:541:SER:C	2.59	0.40
1:C:126:LEU:HD11	1:C:227:VAL:HG11	2.04	0.40
1:B:292:ARG:N	1:B:293:PRO:HD3	2.37	0.40
1:B:710:VAL:O	1:B:710:VAL:HG13	2.20	0.40
1:D:134:VAL:CG1	5:D:2067:HOH:O	2.69	0.40
1:B:749:LEU:CD2	5:B:2088:HOH:O	2.64	0.40
1:A:419:ASN:HB3	1:A:420:MET:H	1.77	0.40
1:C:468:ALA:HA	1:C:505:GLN:HB3	2.02	0.40
1:A:51:PHE:CE2	1:A:261:LEU:HD23	2.56	0.40
1:D:93:LYS:NZ	5:D:2032:HOH:O	2.52	0.40
1:D:247:ALA:HB3	1:D:250:TYR:HB2	2.03	0.40
1:A:292:ARG:CG	1:A:292:ARG:O	2.66	0.40
1:C:53:LYS:O	1:C:56:GLU:HB3	2.21	0.40
1:C:651:LEU:O	1:C:656:GLN:HB2	2.21	0.40
1:D:551:ARG:HH12	1:D:872:LEU:HD12	1.85	0.40
1:D:291:ARG:HA	1:D:291:ARG:HD3	1.81	0.40
1:A:389:LYS:HA	1:A:392:LYS:HE3	2.03	0.40
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.85	0.40
1:A:632:ARG:NH1	5:A:2251:HOH:O	2.55	0.40
1:D:729:THR:H	1:D:729:THR:HG23	1.60	0.40
1:D:236:VAL:HB	1:D:239:GLN:HB2	2.04	0.40
1:D:475:PHE:HD1	1:D:475:PHE:N	2.17	0.40
1:D:849:PHE:O	1:D:850:ALA:C	2.59	0.40
1:D:642:LYS:O	1:D:643:GLU:C	2.56	0.40
1:A:74:ILE:CG2	1:A:755:PHE:HZ	2.34	0.40
1:A:789:SER:HA	1:A:792:ARG:NH2	2.36	0.40
1:B:158:GLU:CG	1:B:195:LEU:HD22	2.36	0.40
1:C:463:HIS:HA	1:C:466:ASN:ND2	2.34	0.40
1:C:373:ALA:CB	1:C:377:TRP:HE1	2.31	0.40
1:A:308:TYR:HA	1:A:311:VAL:HG21	2.03	0.40
1:D:85:ILE:H	1:D:85:ILE:HG13	1.62	0.40
2:E:16:DC:H2''	2:E:17:DG:O5'	2.22	0.40
1:C:57:ARG:NH1	2:K:18:DC:OP2	2.55	0.40
1:C:632:ARG:CG	5:C:2145:HOH:O	2.69	0.40
1:A:141:ILE:HG22	5:A:2072:HOH:O	2.21	0.40
1:B:439:MET:O	1:B:440:THR:C	2.58	0.40
1:A:59:LEU:O	1:A:61:ALA:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:882:PHE:N	1:D:882:PHE:HD1	2.09	0.40
1:B:171:ASN:ND2	1:B:171:ASN:N	2.69	0.40
1:B:155:ARG:CB	5:B:2088:HOH:O	2.65	0.40
2:K:9:DA:N6	4:M:1:DG:H21	2.18	0.40
1:D:486:HIS:C	1:D:486:HIS:ND1	2.72	0.40
1:A:30:GLU:CG	1:A:34:ARG:NH2	2.84	0.40
1:C:663:LYS:HE3	1:C:666:MET:HE1	2.02	0.40
1:D:109:ILE:H	1:D:109:ILE:CD1	2.27	0.40
1:C:594:VAL:HA	1:C:609:VAL:HA	2.03	0.40
1:A:58:GLN:CG	1:A:67:ASN:HD22	2.34	0.40
1:B:737:GLN:O	1:B:774:GLN:NE2	2.55	0.40
1:D:130:ASP:O	1:D:132:THR:HG23	2.22	0.40
1:C:791:LEU:HA	1:C:814:PHE:HE2	1.86	0.40
1:A:505:GLN:O	1:A:508:PRO:HD3	2.22	0.40
1:C:172:LYS:HE3	1:C:172:LYS:HB3	1.78	0.40
1:C:170:LEU:HD22	1:C:179:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	851/883 (96%)	740 (87%)	94 (11%)	17 (2%)	9	33
1	B	851/883 (96%)	736 (86%)	98 (12%)	17 (2%)	9	33
1	C	851/883 (96%)	737 (87%)	93 (11%)	21 (2%)	7	27
1	D	851/883 (96%)	735 (86%)	96 (11%)	20 (2%)	7	29
All	All	3404/3532 (96%)	2948 (87%)	381 (11%)	75 (2%)	8	31

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLY
1	A	199	GLU
1	A	539	SER
1	A	663	LYS
1	A	755	PHE
1	B	194	GLY
1	B	199	GLU
1	B	539	SER
1	B	755	PHE
1	C	194	GLY
1	C	199	GLU
1	C	539	SER
1	C	755	PHE
1	D	194	GLY
1	D	199	GLU
1	D	539	SER
1	D	755	PHE
1	A	7	ALA
1	A	206	LYS
1	B	7	ALA
1	B	15	GLU
1	B	200	ALA
1	B	663	LYS
1	B	882	PHE
1	C	7	ALA
1	C	15	GLU
1	C	200	ALA
1	C	240	ASP
1	C	663	LYS
1	D	7	ALA
1	D	15	GLU
1	D	200	ALA
1	D	663	LYS
1	D	882	PHE
1	A	15	GLU
1	A	60	LYS
1	A	200	ALA
1	A	841	VAL
1	B	14	ILE
1	B	204	TRP
1	B	872	LEU
1	C	60	LYS
1	C	204	TRP

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Mol	Chain	Res	Type
1	C	206	LYS
1	C	872	LEU
1	C	882	PHE
1	D	14	ILE
1	D	204	TRP
1	D	240	ASP
1	D	841	VAL
1	A	14	ILE
1	A	240	ASP
1	B	745	THR
1	C	631	LYS
1	C	745	THR
1	C	841	VAL
1	D	872	LEU
1	A	745	THR
1	A	882	PHE
1	C	14	ILE
1	C	508	PRO
1	D	348	PRO
1	D	353	PRO
1	D	745	THR
1	A	353	PRO
1	B	240	ASP
1	B	631	LYS
1	B	841	VAL
1	D	60	LYS
1	D	508	PRO
1	B	4	ILE
1	C	4	ILE
1	C	348	PRO
1	D	4	ILE
1	A	810	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	703/729 (96%)	615 (88%)	88 (12%)	6	17
1	B	703/729 (96%)	619 (88%)	84 (12%)	6	19
1	C	703/729 (96%)	623 (89%)	80 (11%)	7	21
1	D	703/729 (96%)	628 (89%)	75 (11%)	8	24
All	All	2812/2916 (96%)	2485 (88%)	327 (12%)	7	20

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	16	LEU
1	A	21	PHE
1	A	32	LEU
1	A	36	GLN
1	A	50	ARG
1	A	54	MET
1	A	56	GLU
1	A	77	LEU
1	A	84	ARG
1	A	96	ARG
1	A	99	ARG
1	A	101	THR
1	A	105	PHE
1	A	118	THR
1	A	119	ILE
1	A	121	THR
1	A	155	ARG
1	A	162	PHE
1	A	176	HIS
1	A	184	GLN
1	A	202	SER
1	A	206	LYS
1	A	228	SER
1	A	230	HIS
1	A	245	GLU
1	A	257	ARG
1	A	274	PRO
1	A	279	THR
1	A	302	LYS
1	A	305	LEU
1	A	335	LEU
1	A	343	LYS

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Mol	Chain	Res	Type
1	A	377	TRP
1	A	379	ARG
1	A	391	ARG
1	A	399	GLU
1	A	402	LEU
1	A	422	TRP
1	A	423	ARG
1	A	437	ASN
1	A	452	ILE
1	A	454	LYS
1	A	472	LYS
1	A	514	PHE
1	A	517	GLU
1	A	527	SER
1	A	529	ASN
1	A	553	GLU
1	A	559	VAL
1	A	561	LEU
1	A	573	ILE
1	A	577	LYS
1	A	583	GLN
1	A	591	ASP
1	A	601	ASN
1	A	632	ARG
1	A	633	SER
1	A	635	MET
1	A	654	THR
1	A	656	GLN
1	A	666	MET
1	A	669	GLN
1	A	670	PRO
1	A	700	LYS
1	A	701	SER
1	A	704	LYS
1	A	710	VAL
1	A	713	LYS
1	A	714	LYS
1	A	722	ARG
1	A	731	ASP
1	A	735	VAL
1	A	738	GLU
1	A	741	LYS

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Mol	Chain	Res	Type
1	A	744	GLN
1	A	746	ARG
1	A	766	ASP
1	A	786	GLN
1	A	791	LEU
1	A	814	PHE
1	A	816	THR
1	A	828	VAL
1	A	842	LEU
1	A	852	GLN
1	A	859	ASP
1	A	867	LYS
1	A	882	PHE
1	B	16	LEU
1	B	19	ILE
1	B	21	PHE
1	B	27	HIS
1	B	39	LEU
1	B	46	MET
1	B	50	ARG
1	B	51	PHE
1	B	54	MET
1	B	56	GLU
1	B	84	ARG
1	B	96	ARG
1	B	116	TYR
1	B	143	ARG
1	B	164	LYS
1	B	165	ASN
1	B	168	GLU
1	B	170	LEU
1	B	192	SER
1	B	196	LEU
1	B	206	LYS
1	B	222	GLU
1	B	245	GLU
1	B	257	ARG
1	B	261	LEU
1	B	265	SER
1	B	272	VAL
1	B	274	PRO
1	B	289	ASN

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Mol	Chain	Res	Type
1	B	292	ARG
1	B	305	LEU
1	B	307	ARG
1	B	333	LYS
1	B	335	LEU
1	B	386	ARG
1	B	388	ASP
1	B	391	ARG
1	B	393	SER
1	B	398	LEU
1	B	412	LYS
1	B	422	TRP
1	B	423	ARG
1	B	437	ASN
1	B	445	THR
1	B	477	GLU
1	B	480	LYS
1	B	495	SER
1	B	514	PHE
1	B	529	ASN
1	B	553	GLU
1	B	561	LEU
1	B	565	GLU
1	B	573	ILE
1	B	601	ASN
1	B	632	ARG
1	B	634	VAL
1	B	651	LEU
1	B	654	THR
1	B	666	MET
1	B	668	THR
1	B	669	GLN
1	B	685	VAL
1	B	714	LYS
1	B	722	ARG
1	B	725	VAL
1	B	734	PRO
1	B	735	VAL
1	B	745	THR
1	B	749	LEU
1	B	751	PHE
1	B	752	LEU

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Mol	Chain	Res	Type
1	B	769	ILE
1	B	783	VAL
1	B	785	SER
1	B	786	GLN
1	B	787	ASP
1	B	818	PRO
1	B	828	VAL
1	B	829	ARG
1	B	831	THR
1	B	842	LEU
1	B	852	GLN
1	B	859	ASP
1	B	867	LYS
1	C	5	ASN
1	C	15	GLU
1	C	16	LEU
1	C	19	ILE
1	C	32	LEU
1	C	36	GLN
1	C	50	ARG
1	C	56	GLU
1	C	81	MET
1	C	84	ARG
1	C	96	ARG
1	C	120	LYS
1	C	132	THR
1	C	143	ARG
1	C	155	ARG
1	C	162	PHE
1	C	170	LEU
1	C	185	VAL
1	C	206	LYS
1	C	208	ASP
1	C	227	VAL
1	C	230	HIS
1	C	241	SER
1	C	257	ARG
1	C	266	PRO
1	C	279	THR
1	C	291	ARG
1	C	293	PRO
1	C	303	LYS

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Mol	Chain	Res	Type
1	C	305	LEU
1	C	307	ARG
1	C	313	MET
1	C	350	GLU
1	C	378	LYS
1	C	379	ARG
1	C	397	SER
1	C	412	LYS
1	C	419	ASN
1	C	422	TRP
1	C	423	ARG
1	C	437	ASN
1	C	472	LYS
1	C	473	VAL
1	C	514	PHE
1	C	532	LEU
1	C	551	ARG
1	C	561	LEU
1	C	601	ASN
1	C	632	ARG
1	C	634	VAL
1	C	641	SER
1	C	643	GLU
1	C	652	GLU
1	C	654	THR
1	C	666	MET
1	C	669	GLN
1	C	670	PRO
1	C	694	GLU
1	C	730	PRO
1	C	731	ASP
1	C	734	PRO
1	C	735	VAL
1	C	744	GLN
1	C	749	LEU
1	C	754	GLN
1	C	755	PHE
1	C	768	GLU
1	C	783	VAL
1	C	787	ASP
1	C	801	LYS
1	C	814	PHE

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Mol	Chain	Res	Type
1	C	816	THR
1	C	823	ASN
1	C	838	SER
1	C	855	GLU
1	C	859	ASP
1	C	860	LYS
1	C	869	ASN
1	C	870	LEU
1	C	882	PHE
1	D	5	ASN
1	D	16	LEU
1	D	19	ILE
1	D	27	HIS
1	D	48	GLU
1	D	50	ARG
1	D	52	ARG
1	D	54	MET
1	D	56	GLU
1	D	77	LEU
1	D	84	ARG
1	D	120	LYS
1	D	135	GLN
1	D	143	ARG
1	D	171	ASN
1	D	206	LYS
1	D	230	HIS
1	D	257	ARG
1	D	274	PRO
1	D	279	THR
1	D	281	ILE
1	D	294	LEU
1	D	305	LEU
1	D	315	GLU
1	D	335	LEU
1	D	343	LYS
1	D	346	HIS
1	D	351	ASP
1	D	388	ASP
1	D	391	ARG
1	D	393	SER
1	D	402	LEU
1	D	404	GLN

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Mol	Chain	Res	Type
1	D	422	TRP
1	D	423	ARG
1	D	437	ASN
1	D	472	LYS
1	D	475	PHE
1	D	495	SER
1	D	497	LEU
1	D	539	SER
1	D	553	GLU
1	D	561	LEU
1	D	573	ILE
1	D	577	LYS
1	D	585	ASP
1	D	601	ASN
1	D	632	ARG
1	D	666	MET
1	D	685	VAL
1	D	689	VAL
1	D	701	SER
1	D	710	VAL
1	D	714	LYS
1	D	719	LEU
1	D	722	ARG
1	D	730	PRO
1	D	735	VAL
1	D	746	ARG
1	D	750	MET
1	D	751	PHE
1	D	752	LEU
1	D	783	VAL
1	D	787	ASP
1	D	801	LYS
1	D	816	THR
1	D	824	LEU
1	D	829	ARG
1	D	831	THR
1	D	834	ASP
1	D	842	LEU
1	D	855	GLU
1	D	869	ASN
1	D	870	LEU
1	D	882	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (130) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	107	GLN
1	A	131	ASN
1	A	171	ASN
1	A	184	GLN
1	A	232	GLN
1	A	239	GLN
1	A	269	GLN
1	A	289	ASN
1	A	324	GLN
1	A	410	ASN
1	A	419	ASN
1	A	435	GLN
1	A	437	ASN
1	A	463	HIS
1	A	485	ASN
1	A	486	HIS
1	A	529	ASN
1	A	544	GLN
1	A	568	GLN
1	A	583	GLN
1	A	588	ASN
1	A	669	GLN
1	A	672	GLN
1	A	726	HIS
1	A	737	GLN
1	A	781	ASN
1	A	786	GLN
1	A	811	HIS
1	A	823	ASN
1	A	852	GLN
1	A	854	HIS
1	A	869	ASN
1	A	871	ASN
1	B	161	HIS
1	B	171	ASN
1	B	211	HIS
1	B	239	GLN
1	B	324	GLN
1	B	404	GLN
1	B	411	HIS

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Mol	Chain	Res	Type
1	B	419	ASN
1	B	435	GLN
1	B	437	ASN
1	B	463	HIS
1	B	485	ASN
1	B	499	ASN
1	B	529	ASN
1	B	619	GLN
1	B	656	GLN
1	B	671	ASN
1	B	672	GLN
1	B	726	HIS
1	B	737	GLN
1	B	744	GLN
1	B	748	ASN
1	B	754	GLN
1	B	781	ASN
1	B	786	GLN
1	B	811	HIS
1	B	823	ASN
1	B	852	GLN
1	B	854	HIS
1	C	5	ASN
1	C	86	ASN
1	C	107	GLN
1	C	171	ASN
1	C	211	HIS
1	C	230	HIS
1	C	233	ASN
1	C	239	GLN
1	C	269	GLN
1	C	289	ASN
1	C	324	GLN
1	C	404	GLN
1	C	410	ASN
1	C	419	ASN
1	C	435	GLN
1	C	437	ASN
1	C	466	ASN
1	C	485	ASN
1	C	486	HIS
1	C	499	ASN

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Mol	Chain	Res	Type
1	C	545	HIS
1	C	588	ASN
1	C	726	HIS
1	C	737	GLN
1	C	744	GLN
1	C	748	ASN
1	C	754	GLN
1	C	781	ASN
1	C	786	GLN
1	C	823	ASN
1	C	848	GLN
1	C	854	HIS
1	C	869	ASN
1	C	871	ASN
1	D	86	ASN
1	D	171	ASN
1	D	184	GLN
1	D	232	GLN
1	D	239	GLN
1	D	289	ASN
1	D	324	GLN
1	D	339	ASN
1	D	346	HIS
1	D	406	ASN
1	D	410	ASN
1	D	419	ASN
1	D	435	GLN
1	D	437	ASN
1	D	463	HIS
1	D	485	ASN
1	D	522	GLN
1	D	544	GLN
1	D	588	ASN
1	D	649	GLN
1	D	671	ASN
1	D	726	HIS
1	D	737	GLN
1	D	744	GLN
1	D	772	HIS
1	D	774	GLN
1	D	781	ASN
1	D	786	GLN

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Mol	Chain	Res	Type
1	D	823	ASN
1	D	852	GLN
1	D	854	HIS
1	D	869	ASN
1	D	871	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	F	7/12 (58%)	0	0
3	I	7/12 (58%)	0	0
3	L	7/12 (58%)	0	0
3	O	7/12 (58%)	0	0
All	All	28/48 (58%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.