Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:08 PM GMT

PDB ID	:	1IVS
Title	:	CRYSTAL STRUCTURE OF THERMUS THERMOPHILUS VALYL-TRNA SYNTHETASE COMPLEXED WITH TRNA(VAL) AND VALYL-ADENYLATE ANALOGUE
Authors	:	Fukai, S.; Nureki, O.; Sekine, S.-I.; Shimada, A.; Vassylyev, D.G.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2002-03-29
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:

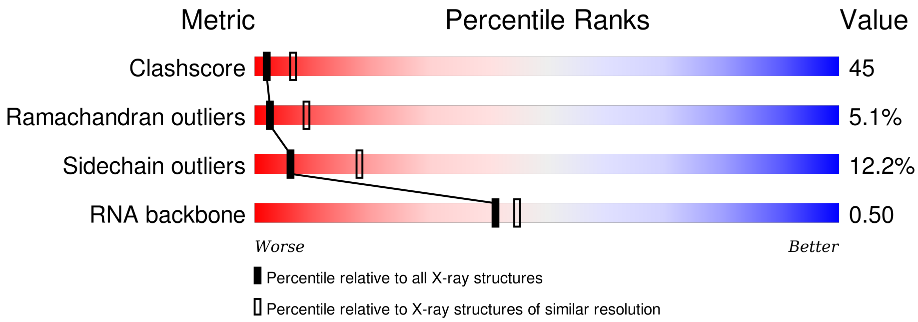
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

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 <=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	C	75	29% 43% 23% 5%
1	D	75	20% 53% 25% •
2	A	862	39% 51% 9% •
2	B	862	37% 51% 11% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17424 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.

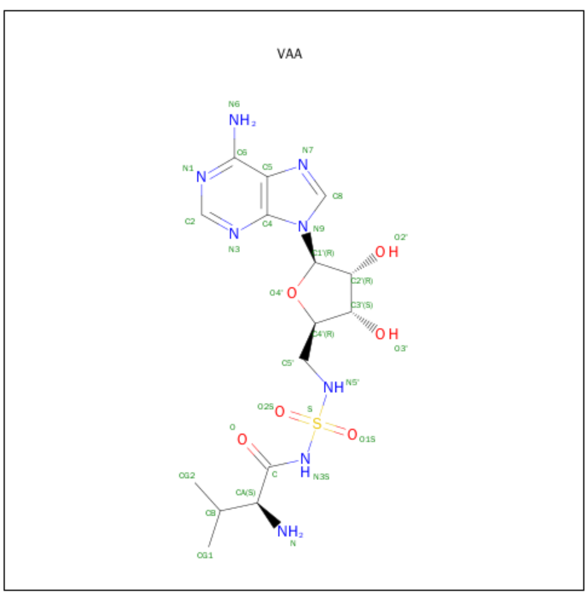
- Molecule 1 is a RNA chain called tRNA (Val).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	75	Total	C	N	O	P	0	0	0
			1603	714	293	521	75			
1	D	75	Total	C	N	O	P	0	0	0
			1603	714	293	521	75			

- Molecule 2 is a protein called Valyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	862	Total	C	N	O	S	0	0	0
			6970	4449	1228	1266	27			
2	B	862	Total	C	N	O	S	0	0	0
			6970	4449	1228	1266	27			

- Molecule 3 is N-[VALINYL]-N'-[ADENOSYL]-DIAMINOSUFONE (three-letter code: VAA) (formula: $C_{15}H_{24}N_8O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 30	C 15	N 8	O 6	S 1	0	0
3	B	1	Total 30	C 15	N 8	O 6	S 1	0	0

- Molecule 4 is water.

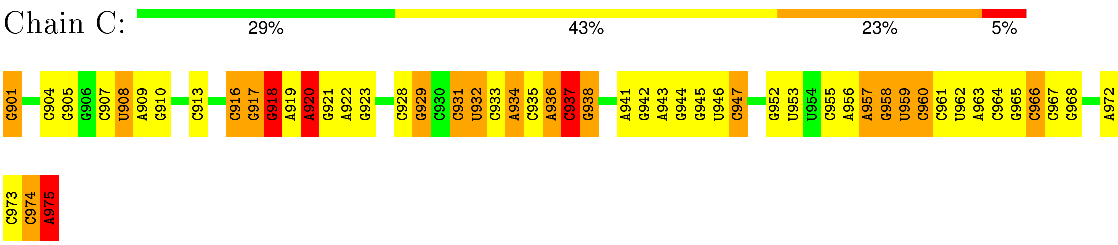
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	101	Total 101	O 101	0	0
4	B	75	Total 75	O 75	0	0
4	C	29	Total 29	O 29	0	0
4	D	13	Total 13	O 13	0	0

3 Residue-property plots (i)

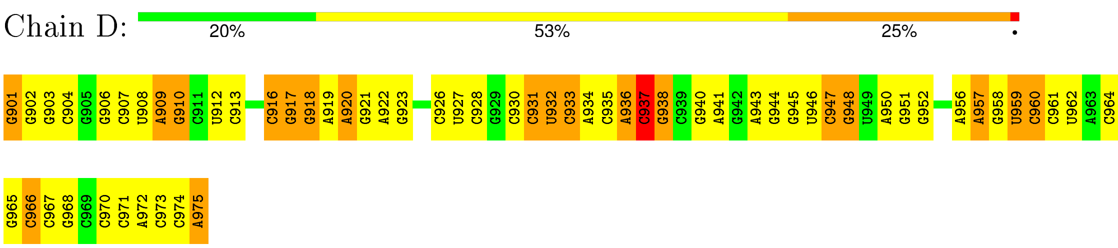
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

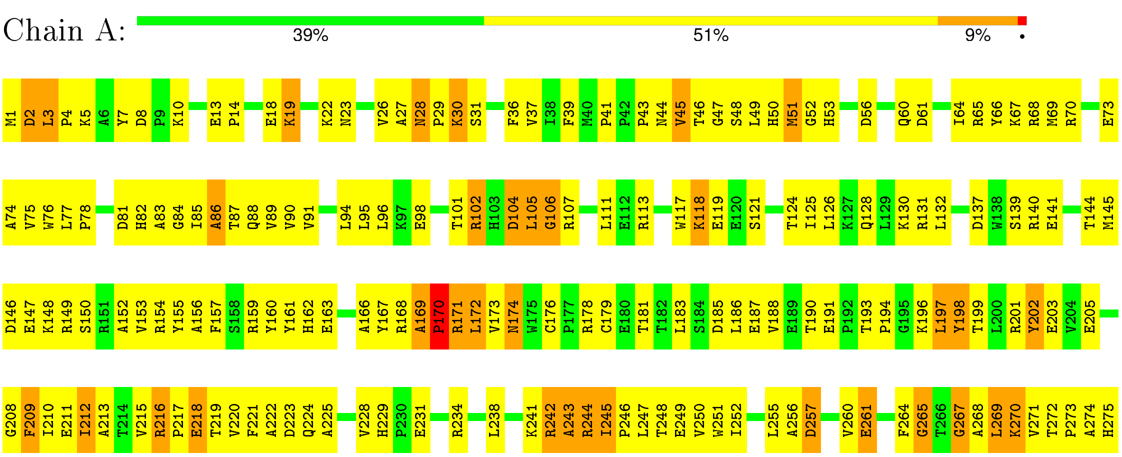
- Molecule 1: tRNA (Val)

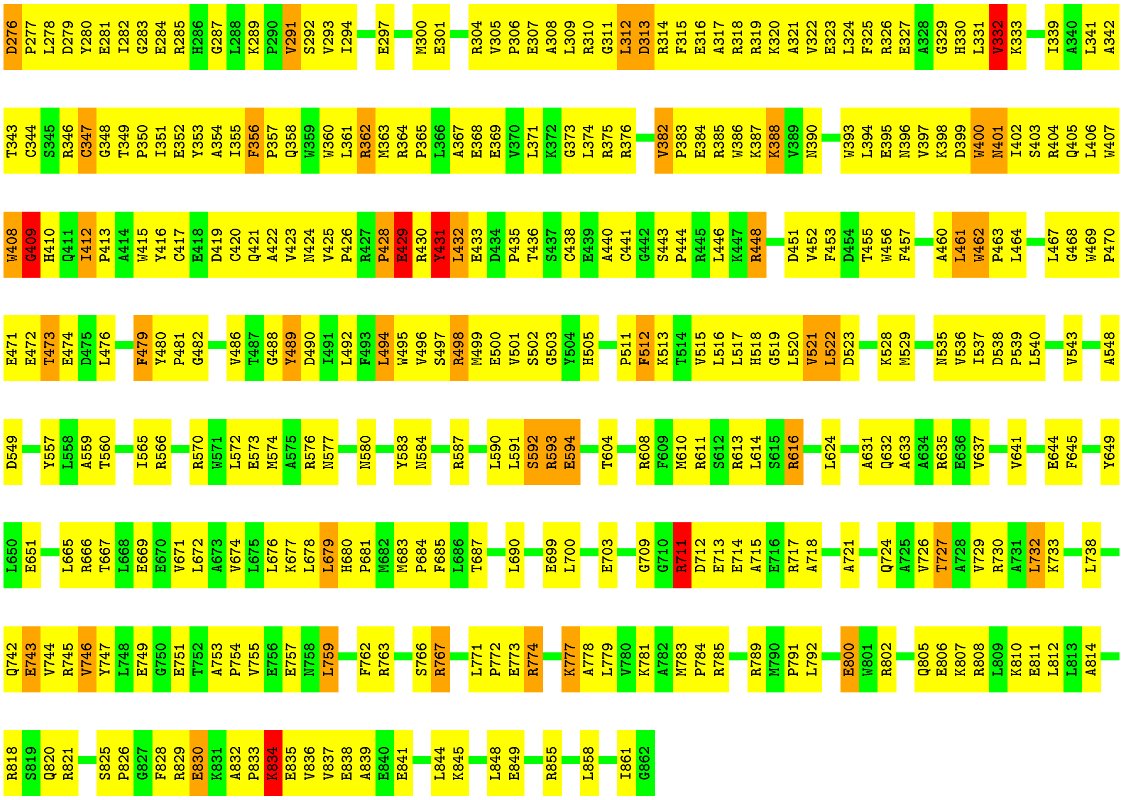


- Molecule 1: tRNA (Val)



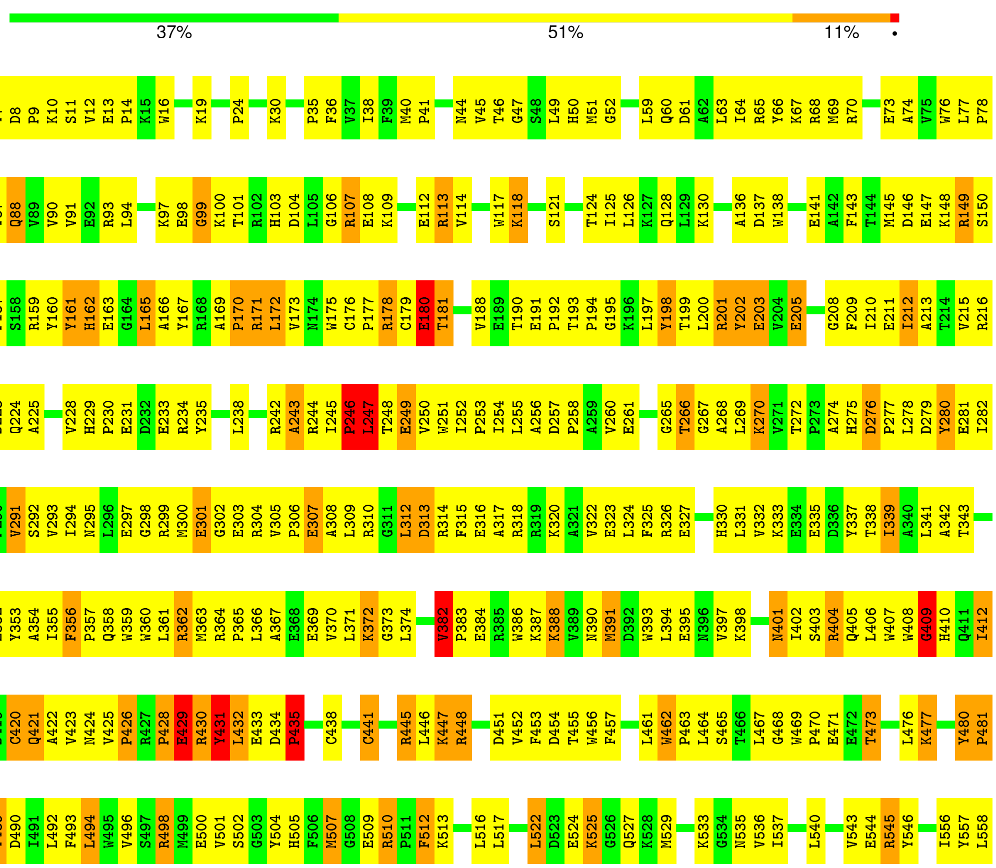
- Molecule 2: Valyl-tRNA synthetase

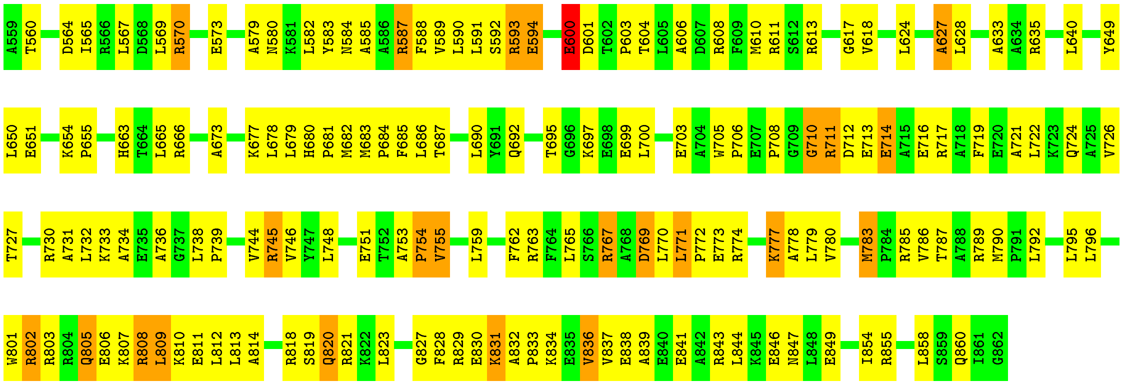




- Molecule 2: Valyl-tRNA synthetase

Chain B:




A559 T560 D564 I565 R566 L567 D568 L569 R570 E573 A579 N580 K581 L582 Y583 N584 A585 A586 R587 F588 V589 L590 L591 S592 R593 E594 E600 D601 T602 P603 T604 L605 A606 D607 R608 F609 M610 R611 S612 R613 G617 V618 L624 A627 L628 A633 A634 R635 L640 Y649
L650 E651 K654 P655 H663 T664 L665 R666 A673 K677 L678 L679 H680 P681 M682 M683 P684 F685 L686 T687 L690 Y691 Q692 T695 G696 K697 E698 E699 L700 E703 A704 W705 P706 E707 P708 G709 G710 R711 D712 E713 E714 A715 E716 R717 A718 F719 E720 A721 L722 K723 Q724 A725 V726
T727 R730 A731 L732 K733 A734 E735 A736 G737 L738 P739 V744 R745 V746 Y747 L748 E751 T752 A753 P754 V755 L759 F762 R763 F764 L765 S766 R767 A768 D769 L770 L771 P772 E773 R774 K777 A778 L779 V780 M783 P784 R785 V786 T787 A788 R789 M790 P791 L792 L795 L796
W801 R802 R803 R804 Q805 E806 K807 R808 L809 K810 E811 L812 L813 A814 R818 S819 Q820 R821 K822 L823 G827 F828 R829 E830 K831 A832 P833 K834 E835 V836 V837 E838 A839 E840 E841 A842 R843 L844 K845 E846 N847 L848 E849 I854 R855 L858 S859 Q860 I861 G862

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	411.81Å 411.81Å 81.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.90	Depositor
% Data completeness (in resolution range)	96.5 (40.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17424	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

5 Model quality (i)

5.1 Standard geometry (i)

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

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	C	0.49	1/1791 (0.1%)	0.82	4/2789 (0.1%)
1	D	0.49	1/1791 (0.1%)	0.79	1/2789 (0.0%)
2	A	0.45	0/7143	0.68	2/9678 (0.0%)
2	B	0.46	0/7143	0.70	3/9678 (0.0%)
All	All	0.46	2/17868 (0.0%)	0.72	10/24934 (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
1	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	901	G	OP3-P	-7.20	1.52	1.61
1	C	901	G	OP3-P	-7.03	1.52	1.61

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	975	A	C4'-C3'-O3'	7.18	127.36	113.00
1	C	947	C	N1-C1'-C2'	6.45	122.38	114.00
2	B	382	VAL	C-N-CD	6.04	141.09	128.40
1	D	937	C	C2'-C3'-O3'	5.90	123.14	113.70
2	B	409	GLY	N-CA-C	5.43	126.67	113.10
2	A	244	ARG	N-CA-C	-5.26	96.79	111.00
2	B	3	LEU	N-CA-C	5.21	125.08	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	920	A	N9-C1'-C2'	5.20	120.76	114.00
1	C	937	C	C2'-C3'-O3'	5.08	121.83	113.70
2	A	409	GLY	N-CA-C	5.05	125.73	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	918	G	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1603	0	816	63	0
1	D	1603	0	816	56	0
2	A	6970	0	6949	682	1
2	B	6970	0	6949	725	0
3	A	30	0	24	5	0
3	B	30	0	24	1	0
4	A	101	0	0	16	0
4	B	75	0	0	12	0
4	C	29	0	0	0	0
4	D	13	0	0	1	0
All	All	17424	0	15578	1490	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 45.

All (1490) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:VAL:HG23	2:B:383:PRO:CD	1.71	1.20
2:B:448:ARG:HD3	2:B:448:ARG:H	1.05	1.18
2:A:282:ILE:HA	2:A:285:ARG:HD3	1.31	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:VAL:HG23	2:B:383:PRO:HD3	1.29	1.12
2:A:777:LYS:H	2:A:777:LYS:HD3	0.98	1.12
2:A:382:VAL:HG23	2:A:383:PRO:CD	1.78	1.12
2:A:28:ASN:HD21	2:A:30:LYS:HG2	1.15	1.11
2:B:777:LYS:H	2:B:777:LYS:HE3	1.09	1.08
2:A:855:ARG:HH22	2:B:810:LYS:HE2	1.18	1.08
2:A:448:ARG:HD3	2:A:448:ARG:H	0.92	1.07
2:B:412:ILE:HD12	2:B:413:PRO:HD2	1.35	1.06
2:A:494:LEU:H	2:A:494:LEU:HD23	1.13	1.05
2:A:382:VAL:HG23	2:A:383:PRO:HD3	1.06	1.05
2:A:171:ARG:HH22	2:A:364:ARG:NH2	1.55	1.04
2:B:225:ALA:HA	2:B:252:ILE:HG23	1.42	1.01
2:A:540:LEU:HA	2:A:543:VAL:HG12	1.40	1.00
2:B:382:VAL:CG2	2:B:516:LEU:HA	1.91	1.00
2:A:224:GLN:HE22	2:A:304:ARG:NH2	1.58	1.00
2:A:810:LYS:HE3	2:B:855:ARG:HH22	1.26	0.99
1:C:928:C:H2'	1:C:929:G:H5"	1.41	0.99
2:A:448:ARG:HD3	2:A:448:ARG:N	1.76	0.98
2:A:37:VAL:HG21	2:A:479:PHE:HB2	1.45	0.97
2:A:382:VAL:CG2	2:A:383:PRO:HD3	1.95	0.97
2:B:282:ILE:HA	2:B:285:ARG:HD3	1.48	0.96
2:B:745:ARG:HB3	2:B:745:ARG:HH11	1.31	0.96
2:A:777:LYS:HD3	2:A:777:LYS:N	1.81	0.95
2:A:186:LEU:H	2:A:186:LEU:HD12	1.30	0.95
2:B:448:ARG:N	2:B:448:ARG:HD3	1.80	0.95
2:A:225:ALA:HA	2:A:252:ILE:HG23	1.48	0.94
2:A:358:GLN:HE22	2:A:405:GLN:HE22	1.10	0.94
2:B:382:VAL:HG22	2:B:516:LEU:HA	1.48	0.94
2:B:494:LEU:HD23	2:B:494:LEU:H	1.31	0.94
2:A:448:ARG:CD	2:A:448:ARG:H	1.82	0.93
2:A:159:ARG:O	2:A:163:GLU:HB2	1.69	0.93
2:A:382:VAL:HG21	2:A:516:LEU:HD12	1.46	0.92
2:A:224:GLN:HE22	2:A:304:ARG:HH22	1.01	0.92
2:B:805:GLN:H	2:B:805:GLN:HE21	1.17	0.92
2:B:248:THR:HG23	2:B:249:GLU:N	1.84	0.92
2:A:50:HIS:HD2	2:A:52:GLY:H	1.16	0.91
1:D:918:G:O6	2:B:833:PRO:HD2	1.70	0.91
2:B:201:ARG:HE	2:B:211:GLU:HB3	1.36	0.91
2:B:248:THR:HG23	2:B:250:VAL:H	1.33	0.91
1:D:932:U:HO2'	1:D:933:C:H5	1.13	0.91
2:B:210:ILE:HD13	2:B:238:LEU:HD13	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:220:VAL:HG12	2:A:270:LYS:HZ1	1.34	0.90
2:B:245:ILE:HB	2:B:248:THR:CG2	2.00	0.90
2:A:777:LYS:H	2:A:777:LYS:CD	1.84	0.90
2:B:245:ILE:HB	2:B:248:THR:HG21	1.53	0.90
2:B:246:PRO:O	2:B:247:LEU:HB2	1.71	0.90
2:B:522:LEU:HD11	2:B:564:ASP:HB3	1.54	0.90
2:A:171:ARG:HH22	2:A:364:ARG:HH22	1.19	0.89
2:A:855:ARG:NH2	2:B:810:LYS:HE2	1.86	0.89
1:C:928:C:C2’	1:C:929:G:H5”	2.03	0.88
2:B:295:ASN:HD21	2:B:299:ARG:HB2	1.39	0.88
2:A:388:LYS:HZ2	2:A:388:LYS:H	0.90	0.88
2:A:224:GLN:NE2	2:A:304:ARG:HH22	1.72	0.88
2:B:5:LYS:HD2	2:B:5:LYS:H	1.36	0.88
2:B:421:GLN:N	2:B:421:GLN:HE21	1.71	0.88
2:B:382:VAL:CG2	2:B:383:PRO:HD3	2.04	0.87
2:B:388:LYS:HD2	2:B:388:LYS:H	1.37	0.87
2:B:248:THR:HG23	2:B:249:GLU:H	1.38	0.87
2:A:201:ARG:HG2	2:A:211:GLU:HB3	1.55	0.86
2:B:789:ARG:HB2	2:B:789:ARG:HH11	1.37	0.86
2:B:248:THR:OG1	2:B:250:VAL:HG23	1.76	0.86
2:B:101:THR:HG22	2:B:104:ASP:OD2	1.75	0.86
2:A:245:ILE:O	2:A:248:THR:HG22	1.76	0.86
2:B:777:LYS:CE	2:B:777:LYS:H	1.88	0.86
2:A:83:ALA:HB1	2:A:86:ALA:HB3	1.58	0.86
2:A:352:GLU:HG2	2:A:353:TYR:H	1.41	0.85
2:A:5:LYS:H	2:A:5:LYS:HD2	1.40	0.85
2:B:358:GLN:HE22	2:B:405:GLN:HE22	1.19	0.85
2:B:98:GLU:HG3	2:B:99:GLY:H	1.42	0.85
2:B:220:VAL:HG12	2:B:270:LYS:HZ3	1.42	0.84
2:A:382:VAL:CG2	2:A:516:LEU:HA	2.06	0.84
2:B:201:ARG:NE	2:B:211:GLU:HB3	1.91	0.84
2:A:178:ARG:HG2	2:A:347:CYS:SG	2.18	0.84
2:A:494:LEU:H	2:A:494:LEU:CD2	1.90	0.84
2:B:361:LEU:HD12	2:B:402:ILE:HD11	1.58	0.83
2:A:751:GLU:HB2	2:A:785:ARG:HH21	1.41	0.83
2:B:823:LEU:HD12	2:B:829:ARG:NH1	1.93	0.83
2:A:171:ARG:HD2	4:A:1088:HOH:O	1.79	0.83
2:A:277:PRO:HD3	2:A:353:TYR:CE2	2.12	0.83
2:A:486:VAL:HG22	2:A:516:LEU:HD23	1.60	0.83
2:A:388:LYS:NZ	2:A:388:LYS:H	1.75	0.83
1:D:936:A:H4’	1:D:937:C:O5’	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:LEU:HG	2:B:313:ASP:H	1.41	0.83
2:B:307:GLU:C	2:B:309:LEU:H	1.82	0.83
2:B:201:ARG:HH11	2:B:332:VAL:HG11	1.44	0.82
2:B:789:ARG:HB2	2:B:789:ARG:NH1	1.94	0.82
2:A:593:ARG:HH11	2:A:593:ARG:HG3	1.45	0.82
2:B:777:LYS:N	2:B:777:LYS:HE3	1.92	0.82
2:B:324:LEU:H	2:B:324:LEU:HD22	1.44	0.82
2:B:516:LEU:HD12	2:B:628:LEU:HD13	1.62	0.82
2:A:499:MET:CE	2:A:512:PHE:HE2	1.93	0.81
2:B:277:PRO:HD3	2:B:353:TYR:CE2	2.16	0.81
2:A:176:CYS:SG	2:A:178:ARG:HB3	2.20	0.81
2:A:28:ASN:ND2	2:A:30:LYS:HG2	1.95	0.81
1:C:936:A:H4'	1:C:937:C:O5'	1.81	0.81
2:B:100:LYS:HB3	2:B:104:ASP:OD2	1.82	0.80
2:B:201:ARG:HD3	2:B:332:VAL:HG21	1.62	0.80
2:A:171:ARG:HH12	2:A:364:ARG:HH21	1.28	0.80
2:B:202:TYR:HE1	2:B:330:HIS:ND1	1.80	0.80
2:B:304:ARG:HG3	2:B:304:ARG:HH11	1.46	0.80
2:B:374:LEU:HD12	2:B:374:LEU:H	1.47	0.80
2:A:382:VAL:HG22	2:A:516:LEU:HA	1.64	0.79
2:B:202:TYR:HE1	2:B:330:HIS:CG	1.99	0.79
1:C:964:C:H2'	1:C:965:G:H8	1.48	0.79
2:A:540:LEU:HA	2:A:543:VAL:CG1	2.12	0.79
2:A:281:GLU:O	2:A:285:ARG:HG3	1.83	0.79
2:A:436:THR:HA	4:A:1040:HOH:O	1.82	0.79
2:A:45:VAL:HG23	2:A:81:ASP:O	1.83	0.79
2:B:361:LEU:HD21	2:B:366:LEU:HD11	1.65	0.79
2:B:388:LYS:HD2	2:B:388:LYS:N	1.98	0.78
2:B:352:GLU:HG2	2:B:353:TYR:H	1.48	0.78
2:A:248:THR:HG23	2:A:250:VAL:H	1.49	0.78
2:B:248:THR:CG2	2:B:250:VAL:H	1.95	0.78
2:B:118:LYS:HD3	2:B:143:PHE:CZ	2.18	0.78
2:A:426:PRO:HG3	2:A:435:PRO:HD3	1.66	0.78
2:A:503:GLY:HA3	2:A:511:PRO:HG3	1.65	0.78
2:B:438:CYS:SG	2:B:441:CYS:HB3	2.24	0.77
2:A:326:ARG:HG3	2:A:327:GLU:N	1.99	0.77
2:B:522:LEU:N	2:B:522:LEU:HD12	1.99	0.77
2:B:680:HIS:HD2	2:B:687:THR:CG2	1.98	0.77
2:B:677:LYS:HD2	2:B:706:PRO:HG3	1.66	0.77
2:A:438:CYS:SG	2:A:440:ALA:HB3	2.25	0.77
2:A:210:ILE:HD13	2:A:238:LEU:HD13	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:VAL:HG21	2:B:516:LEU:HA	1.65	0.76
2:A:245:ILE:HG12	2:A:248:THR:CG2	2.15	0.76
2:B:805:GLN:N	2:B:805:GLN:HE21	1.81	0.76
2:A:416:TYR:CE2	2:A:423:VAL:HG12	2.20	0.76
2:A:343:THR:HB	2:A:348:GLY:O	1.86	0.76
2:B:68:ARG:HB2	2:B:74:ALA:HB2	1.67	0.76
2:B:819:SER:O	2:B:823:LEU:HD23	1.85	0.76
2:A:169:ALA:O	2:A:357:PRO:HA	1.85	0.76
2:B:225:ALA:HA	2:B:252:ILE:CG2	2.14	0.75
2:B:201:ARG:HG3	2:B:332:VAL:HG11	1.67	0.75
2:B:358:GLN:NE2	2:B:405:GLN:HE22	1.85	0.75
2:A:557:TYR:CE1	2:A:635:ARG:HB3	2.21	0.75
2:B:496:VAL:O	2:B:500:GLU:HG3	1.86	0.75
2:A:275:HIS:CE1	2:A:294:ILE:HG12	2.22	0.75
2:A:304:ARG:HG3	2:A:304:ARG:HH11	1.51	0.75
2:A:733:LYS:NZ	2:A:767:ARG:HB3	2.01	0.75
2:A:1:MET:HE1	2:A:690:LEU:HD23	1.67	0.75
2:B:529:MET:HE2	2:B:536:VAL:HA	1.69	0.75
2:A:320:LYS:O	2:A:324:LEU:HD23	1.86	0.75
2:B:257:ASP:OD1	2:B:282:ILE:HG12	1.87	0.75
2:A:171:ARG:NH2	2:A:364:ARG:NH2	2.33	0.75
2:B:361:LEU:HB2	2:B:402:ILE:HD11	1.68	0.74
2:A:614:LEU:HD22	2:A:671:VAL:HG13	1.69	0.74
2:B:680:HIS:HA	2:B:687:THR:HG21	1.68	0.74
2:A:476:LEU:O	2:A:476:LEU:HD23	1.88	0.74
2:A:245:ILE:CG2	2:A:252:ILE:HD13	2.16	0.74
2:A:473:THR:HG23	2:A:476:LEU:H	1.52	0.74
2:A:201:ARG:HG2	2:A:211:GLU:CB	2.15	0.74
2:A:371:LEU:HD21	2:A:394:LEU:HB2	1.68	0.74
2:B:242:ARG:HE	2:B:251:TRP:HB3	1.52	0.74
2:A:362:ARG:NH2	4:A:1068:HOH:O	2.21	0.74
2:B:113:ARG:HH11	2:B:113:ARG:HB2	1.52	0.74
2:A:188:VAL:HG23	2:A:343:THR:O	1.88	0.74
2:B:382:VAL:HG23	2:B:383:PRO:HD2	1.65	0.73
2:A:388:LYS:N	2:A:388:LYS:HZ2	1.76	0.73
2:A:202:TYR:O	2:A:210:ILE:HG22	1.87	0.73
2:A:202:TYR:HE1	2:A:330:HIS:CE1	2.07	0.73
2:B:51:MET:HE2	2:B:537:ILE:HB	1.70	0.73
2:A:412:ILE:HA	2:A:453:PHE:HE1	1.53	0.73
1:D:932:U:O2'	1:D:933:C:H5	1.70	0.73
2:B:818:ARG:HA	2:B:821:ARG:HH12	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:680:HIS:HA	2:A:687:THR:HG21	1.70	0.73
2:B:480:TYR:O	2:B:482:GLY:N	2.21	0.73
2:A:806:GLU:HA	2:A:858:LEU:HD21	1.70	0.73
2:B:161:TYR:CD1	2:B:425:VAL:HB	2.23	0.73
2:B:201:ARG:CD	2:B:211:GLU:HB3	2.18	0.72
2:A:126:LEU:O	2:A:130:LYS:HG2	1.89	0.72
2:B:613:ARG:HH21	2:B:640:LEU:HD13	1.54	0.72
2:A:724:GLN:HE22	2:A:785:ARG:H	1.35	0.72
2:A:496:VAL:O	2:A:500:GLU:HG3	1.89	0.72
2:A:808:ARG:NH2	2:A:812:LEU:HD21	2.04	0.72
1:C:975:A:H3'	2:A:215:VAL:HG23	1.70	0.72
2:A:220:VAL:HG12	2:A:270:LYS:NZ	2.05	0.72
2:A:222:ALA:HB2	2:A:293:VAL:HG13	1.69	0.72
2:A:462:TRP:H	2:A:463:PRO:HD2	1.53	0.72
2:B:245:ILE:O	2:B:247:LEU:N	2.23	0.72
2:A:332:VAL:HG22	2:A:333:LYS:N	2.02	0.72
2:A:785:ARG:HG3	4:A:1060:HOH:O	1.89	0.72
2:B:753:ALA:HB3	2:B:754:PRO:HD3	1.70	0.72
2:B:90:VAL:O	2:B:94:LEU:HG	1.90	0.72
2:A:818:ARG:HA	2:A:821:ARG:HH12	1.55	0.72
2:A:448:ARG:HD2	4:A:1082:HOH:O	1.89	0.72
2:B:202:TYR:O	2:B:210:ILE:HG22	1.90	0.71
1:D:937:C:O2'	1:D:938:G:OP1	2.05	0.71
2:B:584:ASN:HA	2:B:587:ARG:HB3	1.72	0.71
2:A:289:LYS:HD3	2:A:289:LYS:H	1.54	0.71
2:B:83:ALA:HB1	2:B:86:ALA:HB3	1.71	0.71
2:A:50:HIS:CD2	2:A:52:GLY:H	2.05	0.71
2:B:153:VAL:HG23	2:B:154:ARG:N	2.05	0.71
2:B:448:ARG:H	2:B:448:ARG:CD	1.94	0.71
2:A:543:VAL:HG23	2:A:548:ALA:N	2.06	0.71
2:A:714:GLU:HG3	2:A:715:ALA:H	1.54	0.71
2:B:293:VAL:HA	2:B:301:GLU:O	1.91	0.70
2:A:118:LYS:O	2:A:118:LYS:HD2	1.90	0.70
2:A:733:LYS:HZ1	2:A:767:ARG:HB3	1.56	0.70
2:A:680:HIS:HD2	2:A:684:PRO:HA	1.55	0.70
2:B:382:VAL:HG11	2:B:516:LEU:HD12	1.72	0.70
2:A:244:ARG:NH2	4:A:1055:HOH:O	2.14	0.70
2:B:305:VAL:HG13	2:B:310:ARG:HD3	1.71	0.70
2:A:242:ARG:O	2:A:243:ALA:HB2	1.92	0.70
2:B:818:ARG:HA	2:B:821:ARG:NH1	2.06	0.70
2:A:50:HIS:HD2	2:A:52:GLY:N	1.88	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:529:MET:HE2	2:A:536:VAL:HA	1.72	0.70
2:B:751:GLU:HB2	2:B:785:ARG:HH21	1.55	0.70
2:A:51:MET:HE3	2:A:537:ILE:HB	1.72	0.70
2:A:313:ASP:O	2:A:317:ALA:HB2	1.92	0.70
2:B:383:PRO:HB2	2:B:386:TRP:CD1	2.27	0.70
2:B:416:TYR:HA	2:B:422:ALA:O	1.91	0.70
2:A:431:TYR:CE1	2:A:432:LEU:HD12	2.27	0.70
2:A:460:ALA:HB2	2:A:498:ARG:HB3	1.74	0.69
2:B:242:ARG:O	2:B:243:ALA:HB2	1.91	0.69
2:B:149:ARG:HG3	2:B:465:SER:OG	1.91	0.69
2:B:7:TYR:CZ	2:B:686:LEU:HD13	2.26	0.69
2:A:45:VAL:HG11	2:A:118:LYS:HA	1.75	0.69
2:A:522:LEU:HB3	2:A:528:LYS:HA	1.73	0.69
2:A:834:LYS:HD2	2:A:834:LYS:H	1.57	0.69
2:A:358:GLN:NE2	2:A:405:GLN:HE22	1.88	0.69
2:A:201:ARG:CG	2:A:211:GLU:HB3	2.22	0.69
1:D:973:C:H1'	2:B:278:LEU:HB2	1.73	0.69
2:A:224:GLN:NE2	2:A:291:VAL:HG11	2.08	0.69
2:B:170:PRO:O	2:B:355:ILE:HG23	1.93	0.69
2:B:322:VAL:O	2:B:325:PHE:HB2	1.92	0.69
2:A:306:PRO:HG2	2:A:309:LEU:HB3	1.73	0.69
2:B:361:LEU:HB2	2:B:402:ILE:CD1	2.22	0.69
1:C:957:A:H4'	1:C:958:G:OP1	1.92	0.69
2:B:802:ARG:HH11	2:B:802:ARG:HB2	1.58	0.69
2:B:372:LYS:NZ	2:B:372:LYS:HA	2.07	0.69
2:A:304:ARG:HG3	2:A:304:ARG:NH1	2.07	0.69
2:A:610:MET:HG2	2:A:649:TYR:CD2	2.27	0.69
2:A:7:TYR:HB2	2:A:583:TYR:CD2	2.27	0.69
2:A:205:GLU:HB2	2:A:242:ARG:HB2	1.72	0.69
2:B:680:HIS:CD2	2:B:684:PRO:HA	2.28	0.68
2:A:43:PRO:HB2	2:A:125:ILE:HD13	1.75	0.68
2:B:248:THR:CG2	2:B:249:GLU:H	1.97	0.68
2:B:464:LEU:HB3	2:B:469:TRP:CB	2.24	0.68
2:A:312:LEU:HD21	2:A:316:GLU:HG2	1.75	0.68
2:B:201:ARG:HD2	2:B:211:GLU:HB3	1.75	0.68
2:B:145:MET:HG3	2:B:410:HIS:CD2	2.27	0.68
2:A:807:LYS:O	2:A:811:GLU:HG3	1.92	0.68
2:B:352:GLU:HG2	2:B:353:TYR:N	2.06	0.68
2:B:745:ARG:HB3	2:B:745:ARG:NH1	2.06	0.68
2:A:394:LEU:O	2:A:397:VAL:HG23	1.92	0.68
2:A:680:HIS:CD2	2:A:684:PRO:HA	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:GLN:HE21	2:B:421:GLN:H	1.40	0.68
2:A:593:ARG:HG3	2:A:593:ARG:NH1	2.07	0.68
2:A:412:ILE:HA	2:A:453:PHE:CE1	2.27	0.68
2:B:420:CYS:SG	2:B:422:ALA:HB2	2.32	0.68
2:B:295:ASN:ND2	2:B:299:ARG:HB2	2.09	0.68
2:B:462:TRP:H	2:B:463:PRO:CD	2.07	0.68
2:A:712:ASP:HB3	2:A:715:ALA:HB3	1.75	0.68
2:B:270:LYS:CB	2:B:270:LYS:HZ2	2.06	0.68
2:A:540:LEU:CA	2:A:543:VAL:HG12	2.21	0.68
2:A:300:MET:HB2	2:A:311:GLY:H	1.57	0.68
2:B:13:GLU:HA	2:B:685:PHE:HD2	1.59	0.68
2:B:245:ILE:HB	2:B:248:THR:HG22	1.76	0.68
2:B:421:GLN:HE21	2:B:421:GLN:CA	2.06	0.68
2:A:468:GLY:C	2:A:470:PRO:HD2	2.14	0.68
2:A:492:LEU:O	2:A:492:LEU:HG	1.92	0.68
2:A:171:ARG:NH1	2:A:364:ARG:HH21	1.90	0.68
2:B:47:GLY:H	2:B:117:TRP:HZ2	1.39	0.68
2:B:464:LEU:HB3	2:B:469:TRP:HB3	1.75	0.68
2:B:409:GLY:HA3	2:B:452:VAL:CG1	2.24	0.67
2:A:845:LYS:O	2:A:849:GLU:HG3	1.93	0.67
2:A:216:ARG:HB3	2:A:219:THR:HG23	1.76	0.67
2:A:401:ASN:HD22	2:A:402:ILE:N	1.92	0.67
2:B:387:LYS:HG2	2:B:388:LYS:HE2	1.75	0.67
2:B:7:TYR:HB2	2:B:583:TYR:CD2	2.28	0.67
2:A:170:PRO:HA	2:A:356:PHE:O	1.94	0.67
2:B:802:ARG:O	2:B:806:GLU:HB2	1.95	0.67
2:A:183:LEU:HD21	2:A:344:CYS:SG	2.35	0.67
2:B:415:TRP:HA	2:B:447:LYS:O	1.95	0.67
2:A:382:VAL:HG21	2:A:516:LEU:HA	1.75	0.67
2:A:297:GLU:N	2:A:297:GLU:OE1	2.28	0.67
2:B:415:TRP:O	2:B:424:ASN:N	2.24	0.66
2:A:591:LEU:O	2:A:594:GLU:HB2	1.94	0.66
2:B:593:ARG:HB2	2:B:665:LEU:HD21	1.76	0.66
2:B:304:ARG:NH1	2:B:304:ARG:HG3	2.08	0.66
2:A:225:ALA:HA	2:A:252:ILE:CG2	2.25	0.66
2:B:372:LYS:HZ3	2:B:372:LYS:HA	1.58	0.66
2:B:501:VAL:HG13	2:B:502:SER:N	2.10	0.66
2:A:162:HIS:NE2	2:A:425:VAL:O	2.20	0.66
2:B:221:PHE:O	2:B:304:ARG:NH1	2.28	0.66
2:A:167:TYR:CE2	2:A:360:TRP:HB2	2.30	0.66
2:B:382:VAL:CG2	2:B:383:PRO:CD	2.62	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:383:PRO:HB2	2:A:386:TRP:CD1	2.30	0.66
2:B:312:LEU:HG	2:B:313:ASP:N	2.10	0.66
2:B:778:ALA:HB1	2:B:790:MET:O	1.95	0.66
2:B:303:GLU:OE2	2:B:303:GLU:HA	1.94	0.66
2:A:315:PHE:C	2:A:317:ALA:H	1.97	0.66
2:A:494:LEU:N	2:A:494:LEU:HD23	1.97	0.66
2:A:224:GLN:HE21	2:A:291:VAL:HG11	1.61	0.66
2:A:157:PHE:HD2	2:A:413:PRO:HG2	1.60	0.66
1:C:918:G:O6	2:A:833:PRO:HD3	1.96	0.66
2:B:41:PRO:HD2	2:B:60:GLN:HE22	1.60	0.66
2:A:316:GLU:OE1	2:A:319:ARG:HD2	1.96	0.66
2:B:193:THR:CG2	2:B:194:PRO:HD2	2.26	0.66
2:B:771:LEU:HD13	2:B:772:PRO:HD2	1.77	0.65
2:B:388:LYS:HB3	4:B:1032:HOH:O	1.96	0.65
2:B:473:THR:HG23	2:B:476:LEU:H	1.61	0.65
2:B:169:ALA:O	2:B:357:PRO:HA	1.96	0.65
2:A:855:ARG:HD3	2:B:813:LEU:HD12	1.79	0.65
2:B:494:LEU:CD2	2:B:494:LEU:H	2.05	0.65
2:B:167:TYR:CE2	2:B:360:TRP:HB2	2.31	0.65
2:A:86:ALA:HA	2:A:346:ARG:HD3	1.77	0.65
2:A:23:ASN:HB3	4:A:1005:HOH:O	1.97	0.65
2:A:289:LYS:HD3	2:A:289:LYS:N	2.12	0.65
2:B:260:VAL:HG22	2:B:269:LEU:CD2	2.25	0.65
2:B:349:THR:HG23	2:B:350:PRO:HD2	1.79	0.65
2:B:651:GLU:OE1	2:B:654:LYS:HE3	1.97	0.65
2:A:522:LEU:HD12	2:A:566:ARG:HA	1.79	0.65
2:B:371:LEU:HD21	2:B:394:LEU:HB2	1.76	0.65
2:B:270:LYS:HZ2	2:B:270:LYS:HB3	1.60	0.65
2:A:358:GLN:HE22	2:A:405:GLN:NE2	1.90	0.65
2:A:153:VAL:HG23	2:A:154:ARG:N	2.10	0.65
2:B:188:VAL:HG23	2:B:343:THR:O	1.97	0.65
2:B:414:ALA:HA	2:B:425:VAL:HG22	1.79	0.64
2:B:190:THR:HG22	2:B:342:ALA:HB2	1.78	0.64
2:B:415:TRP:CE3	2:B:448:ARG:HB3	2.32	0.64
2:A:242:ARG:NH1	2:A:251:TRP:HB3	2.12	0.64
2:B:480:TYR:HB3	2:B:481:PRO:HD3	1.80	0.64
2:A:47:GLY:H	2:A:117:TRP:HZ2	1.45	0.64
2:B:272:THR:H	2:B:279:ASP:HB3	1.62	0.64
2:A:186:LEU:H	2:A:186:LEU:CD1	2.09	0.64
2:B:306:PRO:HD2	2:B:309:LEU:HD23	1.78	0.64
2:B:588:PHE:CD2	2:B:650:LEU:HD11	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:HIS:HD2	2:B:52:GLY:H	1.45	0.64
2:A:294:ILE:HG22	2:A:300:MET:SD	2.37	0.64
2:B:201:ARG:NH1	2:B:332:VAL:HG11	2.13	0.64
2:A:154:ARG:HD2	4:A:1058:HOH:O	1.98	0.64
2:B:275:HIS:HE1	2:B:294:ILE:HB	1.63	0.64
2:B:220:VAL:HA	2:B:223:ASP:OD2	1.97	0.64
2:B:415:TRP:CZ3	2:B:448:ARG:HB3	2.33	0.64
2:B:179:CYS:O	2:B:181:THR:HG22	1.95	0.64
2:A:245:ILE:HG22	2:A:252:ILE:HD13	1.79	0.64
2:B:307:GLU:C	2:B:309:LEU:N	2.51	0.64
1:D:918:G:H21	1:D:956:A:H1'	1.64	0.63
2:A:66:TYR:O	2:A:70:ARG:HB2	1.97	0.63
2:A:326:ARG:HB3	2:A:331:LEU:HD23	1.80	0.63
2:B:488:GLY:O	2:B:490:ASP:N	2.31	0.63
2:B:278:LEU:O	2:B:281:GLU:HB3	1.98	0.63
2:B:307:GLU:O	2:B:309:LEU:N	2.31	0.63
2:A:248:THR:CG2	2:A:250:VAL:H	2.11	0.63
2:B:398:LYS:HD2	2:B:398:LYS:N	2.14	0.63
2:B:83:ALA:HB3	2:B:87:THR:OG1	1.99	0.63
2:A:810:LYS:HG3	2:B:855:ARG:NH2	2.14	0.63
1:D:959:U:H5"	1:D:960:C:OP2	1.99	0.63
2:A:416:TYR:HE2	2:A:423:VAL:HG12	1.62	0.63
2:B:651:GLU:HA	2:B:651:GLU:OE1	1.99	0.63
2:B:50:HIS:HD2	2:B:52:GLY:N	1.96	0.63
2:A:160:TYR:HB3	2:A:166:ALA:HB2	1.80	0.63
2:A:256:ALA:O	2:A:257:ASP:HB2	1.99	0.63
3:A:990:VAA:O	3:A:990:VAA:H5'1	1.98	0.63
2:A:726:VAL:O	2:A:730:ARG:HG2	1.98	0.63
2:A:499:MET:HE3	2:A:512:PHE:HE2	1.63	0.63
1:C:937:C:O2'	1:C:938:G:OP1	2.09	0.63
2:B:272:THR:N	2:B:279:ASP:HB3	2.14	0.63
2:B:50:HIS:CD2	2:B:52:GLY:H	2.16	0.63
2:B:198:TYR:CD2	2:B:198:TYR:N	2.66	0.63
2:B:49:LEU:HD21	2:B:125:ILE:HG23	1.80	0.63
2:B:220:VAL:O	2:B:223:ASP:HB2	1.99	0.62
1:C:928:C:C3'	1:C:929:G:H5"	2.28	0.62
2:B:277:PRO:HD3	2:B:353:TYR:CD2	2.34	0.62
2:A:155:TYR:HD1	2:A:431:TYR:CD2	2.17	0.62
2:B:834:LYS:O	2:B:838:GLU:HG2	2.00	0.62
2:B:545:ARG:HB3	2:B:546:TYR:CD1	2.34	0.62
2:B:374:LEU:N	2:B:374:LEU:HD12	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:TRP:N	2:B:470:PRO:HD2	2.14	0.62
2:A:497:SER:HA	2:A:500:GLU:OE1	2.00	0.62
2:B:178:ARG:HG3	2:B:179:CYS:SG	2.39	0.62
2:A:87:THR:O	2:A:91:VAL:HG23	1.99	0.62
2:B:654:LYS:HB2	2:B:655:PRO:HD3	1.81	0.62
2:A:810:LYS:HE3	2:B:855:ARG:NH2	2.08	0.62
2:B:201:ARG:HH11	2:B:201:ARG:HG3	1.63	0.62
2:B:312:LEU:CG	2:B:313:ASP:H	2.09	0.62
2:A:346:ARG:HB2	2:A:346:ARG:NH1	2.14	0.62
2:B:501:VAL:HG13	2:B:502:SER:H	1.65	0.62
2:B:374:LEU:CD1	2:B:374:LEU:H	2.13	0.62
2:B:358:GLN:NE2	2:B:403:SER:HB2	2.15	0.62
2:B:198:TYR:N	2:B:198:TYR:HD2	1.98	0.62
2:A:169:ALA:HB1	2:A:170:PRO:CD	2.29	0.62
2:B:159:ARG:O	2:B:163:GLU:HB2	2.00	0.62
2:B:802:ARG:HG3	2:B:803:ARG:N	2.13	0.62
2:B:220:VAL:HG21	2:B:325:PHE:HZ	1.64	0.62
2:A:714:GLU:HG3	2:A:715:ALA:N	2.14	0.62
1:C:918:G:N2	1:C:956:A:H1'	2.15	0.62
2:B:830:GLU:C	2:B:831:LYS:HE3	2.20	0.62
2:B:733:LYS:HB3	2:B:733:LYS:NZ	2.15	0.62
2:B:789:ARG:CB	2:B:789:ARG:HH11	2.12	0.62
2:B:65:ARG:O	2:B:69:MET:HG2	2.00	0.62
2:B:229:HIS:CD2	2:B:231:GLU:H	2.18	0.62
2:B:82:HIS:HB2	2:B:408:TRP:NE1	2.15	0.61
2:B:44:ASN:HB3	2:B:83:ALA:HB2	1.80	0.61
2:B:370:VAL:HG12	2:B:374:LEU:HD11	1.81	0.61
2:A:845:LYS:NZ	2:B:820:GLN:HE22	1.97	0.61
2:B:611:ARG:HH22	2:B:666:ARG:HH21	1.48	0.61
2:B:591:LEU:O	2:B:594:GLU:HB2	1.99	0.61
2:A:352:GLU:HG2	2:A:353:TYR:N	2.12	0.61
2:A:473:THR:CG2	2:A:476:LEU:H	2.12	0.61
2:B:3:LEU:HD21	2:B:590:LEU:HD12	1.81	0.61
2:A:732:LEU:HD13	2:A:781:LYS:HB2	1.80	0.61
1:C:973:C:O2	2:A:278:LEU:HD13	2.00	0.61
1:D:931:C:H5"	1:D:932:U:OP2	1.99	0.61
2:B:171:ARG:HH12	2:B:364:ARG:NH2	1.98	0.61
2:B:680:HIS:CD2	2:B:687:THR:CG2	2.81	0.61
1:D:964:C:H2'	1:D:965:G:H8	1.65	0.61
2:A:198:TYR:CD2	2:A:198:TYR:N	2.68	0.61
1:D:933:C:H3'	1:D:933:C:H6	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:MET:HE2	2:B:537:ILE:N	2.16	0.61
2:B:153:VAL:CG2	2:B:154:ARG:N	2.64	0.61
2:B:805:GLN:N	2:B:805:GLN:NE2	2.47	0.61
2:A:66:TYR:OH	2:A:70:ARG:NH1	2.34	0.61
2:B:556:ILE:HD12	2:B:682:MET:HG2	1.83	0.61
2:A:244:ARG:HB2	2:A:251:TRP:CZ2	2.36	0.61
1:D:940:G:O2'	1:D:941:A:H5'	2.01	0.61
1:C:929:G:H5'	1:C:929:G:H8	1.66	0.60
2:A:666:ARG:HH11	2:A:666:ARG:HG3	1.65	0.60
2:A:94:LEU:O	2:A:98:GLU:HG3	2.01	0.60
2:B:222:ALA:HB2	2:B:293:VAL:HG22	1.82	0.60
2:A:221:PHE:CD2	2:A:306:PRO:HD3	2.36	0.60
2:A:326:ARG:HG3	2:A:327:GLU:H	1.64	0.60
2:A:153:VAL:HG21	2:A:410:HIS:ND1	2.15	0.60
2:B:162:HIS:NE2	2:B:425:VAL:O	2.31	0.60
2:A:171:ARG:HH12	2:A:364:ARG:NH2	1.96	0.60
2:A:95:LEU:O	2:A:98:GLU:HB2	2.01	0.60
2:B:540:LEU:O	2:B:543:VAL:HG22	2.01	0.60
2:B:324:LEU:N	2:B:324:LEU:HD22	2.16	0.60
2:B:150:SER:O	2:B:153:VAL:HG22	2.00	0.60
2:A:316:GLU:HA	2:A:319:ARG:HH11	1.65	0.60
2:B:124:THR:O	2:B:128:GLN:HG3	2.02	0.60
2:A:248:THR:HG23	2:A:250:VAL:N	2.16	0.60
2:A:401:ASN:HD22	2:A:401:ASN:C	2.03	0.60
2:A:201:ARG:CD	2:A:211:GLU:HB3	2.32	0.60
2:A:85:ILE:O	2:A:89:VAL:HG23	2.02	0.60
2:B:468:GLY:C	2:B:470:PRO:HD2	2.21	0.60
2:A:412:ILE:HB	2:A:453:PHE:CE1	2.36	0.60
1:C:961:C:O2'	1:C:962:U:H5'	2.02	0.60
1:D:975:A:H3'	2:B:215:VAL:HG23	1.82	0.60
2:B:242:ARG:NE	2:B:251:TRP:HB3	2.16	0.60
2:A:245:ILE:HG23	2:A:248:THR:HG21	1.82	0.60
2:B:613:ARG:NH2	2:B:640:LEU:HD13	2.16	0.60
2:A:429:GLU:H	2:A:429:GLU:CD	2.04	0.60
2:B:248:THR:HG23	2:B:250:VAL:N	2.13	0.60
2:B:270:LYS:CB	2:B:270:LYS:NZ	2.64	0.60
2:A:844:LEU:O	2:A:848:LEU:HD23	2.01	0.60
1:D:922:A:H2'	1:D:923:G:C8	2.37	0.60
2:B:326:ARG:HG3	2:B:327:GLU:N	2.17	0.60
2:A:28:ASN:ND2	2:A:30:LYS:H	1.99	0.59
2:A:498:ARG:HG2	2:A:498:ARG:HH11	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:387:LYS:HB3	2:A:388:LYS:NZ	2.16	0.59
2:A:680:HIS:HD2	2:A:687:THR:CG2	2.15	0.59
2:B:480:TYR:O	2:B:481:PRO:C	2.39	0.59
2:A:833:PRO:C	2:A:835:GLU:H	2.04	0.59
2:A:198:TYR:N	2:A:198:TYR:HD2	1.99	0.59
2:B:161:TYR:CE1	2:B:425:VAL:HB	2.37	0.59
2:B:289:LYS:HD2	2:B:289:LYS:H	1.66	0.59
2:B:126:LEU:O	2:B:130:LYS:HG2	2.01	0.59
2:B:172:LEU:HD23	2:B:354:ALA:O	2.02	0.59
2:A:4:PRO:HD2	2:A:583:TYR:OH	2.02	0.59
2:B:220:VAL:HG12	2:B:270:LYS:NZ	2.17	0.59
2:B:40:MET:HA	2:B:60:GLN:HE22	1.68	0.59
2:A:124:THR:O	2:A:128:GLN:HG3	2.02	0.59
2:A:46:THR:HG22	2:A:90:VAL:HG21	1.85	0.59
2:B:383:PRO:HB2	2:B:386:TRP:HD1	1.67	0.59
2:B:238:LEU:O	2:B:254:ILE:HG21	2.02	0.59
2:B:161:TYR:C	2:B:163:GLU:H	2.06	0.59
2:A:153:VAL:CG2	2:A:154:ARG:N	2.66	0.59
1:D:927:U:O2'	1:D:928:C:H5'	2.02	0.59
2:B:228:VAL:O	2:B:256:ALA:HA	2.03	0.59
2:B:382:VAL:O	2:B:383:PRO:C	2.39	0.59
2:B:346:ARG:CZ	2:B:346:ARG:HB2	2.33	0.59
1:C:935:C:H1'	2:A:584:ASN:ND2	2.17	0.59
2:B:88:GLN:HG3	2:B:406:LEU:HD22	1.85	0.59
2:B:383:PRO:HG2	4:B:1003:HOH:O	2.02	0.59
2:A:495:TRP:NE1	3:A:990:VAA:HG21	2.17	0.59
2:A:855:ARG:HG3	2:B:809:LEU:CD1	2.33	0.58
2:B:409:GLY:HA3	2:B:452:VAL:HG13	1.84	0.58
2:A:245:ILE:H	2:A:248:THR:CG2	2.16	0.58
2:B:617:GLY:HA3	2:B:640:LEU:HD22	1.84	0.58
2:A:529:MET:HE2	2:A:537:ILE:N	2.18	0.58
2:A:364:ARG:HD2	4:A:1056:HOH:O	2.02	0.58
2:A:314:ARG:NH2	2:A:352:GLU:HG3	2.18	0.58
2:A:264:PHE:CD2	2:A:265:GLY:N	2.71	0.58
2:B:738:LEU:HD23	2:B:744:VAL:HG11	1.84	0.58
2:B:13:GLU:HA	2:B:685:PHE:CD2	2.37	0.58
1:D:918:G:O6	2:B:833:PRO:CD	2.46	0.58
2:B:201:ARG:HG3	2:B:201:ARG:NH1	2.18	0.58
2:B:366:LEU:HB3	2:B:501:VAL:CG2	2.33	0.58
2:A:145:MET:HG2	2:A:410:HIS:CD2	2.38	0.58
2:B:246:PRO:O	2:B:247:LEU:CB	2.48	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:220:VAL:HA	2:A:270:LYS:HE3	1.85	0.58
2:B:202:TYR:CE1	2:B:330:HIS:CG	2.87	0.58
2:B:837:VAL:O	2:B:841:GLU:HG3	2.02	0.58
2:B:391:MET:O	2:B:395:GLU:HB2	2.04	0.58
2:B:324:LEU:CD2	2:B:324:LEU:H	2.15	0.58
2:A:202:TYR:HE1	2:A:330:HIS:ND1	2.00	0.58
2:A:293:VAL:HG23	2:A:294:ILE:HG23	1.85	0.58
2:B:666:ARG:NH2	4:B:1047:HOH:O	2.33	0.58
2:B:151:ARG:HG2	2:B:151:ARG:HH11	1.68	0.58
2:B:109:LYS:O	2:B:112:GLU:HB2	2.03	0.58
2:B:170:PRO:HA	2:B:356:PHE:O	2.04	0.58
2:B:281:GLU:O	2:B:285:ARG:HG3	2.03	0.58
2:B:522:LEU:H	2:B:522:LEU:HD12	1.68	0.58
2:B:197:LEU:HB2	2:B:337:TYR:HB2	1.85	0.58
2:A:684:PRO:O	2:A:687:THR:HG22	2.03	0.57
2:B:397:VAL:C	2:B:398:LYS:HD2	2.25	0.57
2:A:170:PRO:O	2:A:355:ILE:HG23	2.04	0.57
2:B:456:TRP:CE3	2:B:494:LEU:O	2.57	0.57
2:A:680:HIS:CD2	2:A:687:THR:HG21	2.38	0.57
2:B:600:GLU:HG2	2:B:601:ASP:N	2.20	0.57
2:A:3:LEU:HD21	2:A:590:LEU:HD12	1.85	0.57
2:B:412:ILE:HA	2:B:453:PHE:CE1	2.40	0.57
2:B:454:ASP:O	2:B:457:PHE:N	2.31	0.57
2:A:248:THR:OG1	2:A:250:VAL:HG23	2.05	0.57
2:B:312:LEU:O	2:B:313:ASP:O	2.23	0.57
2:A:131:ARG:O	2:A:131:ARG:HD2	2.05	0.57
2:A:280:TYR:O	2:A:284:GLU:HG2	2.04	0.57
2:B:469:TRP:O	2:B:470:PRO:C	2.39	0.57
2:B:245:ILE:O	2:B:248:THR:HG22	2.04	0.57
2:B:492:LEU:HD12	2:B:496:VAL:HB	1.87	0.57
2:A:714:GLU:CG	2:A:715:ALA:H	2.17	0.57
2:B:371:LEU:HD21	2:B:394:LEU:CB	2.34	0.57
2:A:282:ILE:HA	2:A:285:ARG:CD	2.21	0.57
2:B:245:ILE:HG13	2:B:252:ILE:HD13	1.85	0.57
2:B:266:THR:O	2:B:268:ALA:N	2.38	0.57
2:A:202:TYR:OH	2:A:244:ARG:NH2	2.38	0.57
2:A:395:GLU:HA	2:A:395:GLU:OE2	2.04	0.57
2:A:169:ALA:HB1	2:A:170:PRO:HD2	1.87	0.57
2:A:5:LYS:N	2:A:5:LYS:HD2	2.16	0.57
2:A:592:SER:C	2:A:594:GLU:H	2.08	0.57
2:B:148:LYS:HD2	2:B:468:GLY:HA2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:473:THR:HG22	2:B:476:LEU:HB3	1.86	0.57
2:A:188:VAL:HG21	2:A:351:ILE:HD13	1.86	0.57
2:B:36:PHE:CD1	2:B:67:LYS:HG3	2.39	0.57
2:B:151:ARG:NH1	2:B:151:ARG:HG2	2.20	0.56
2:B:759:LEU:CD1	2:B:763:ARG:HE	2.18	0.56
2:A:415:TRP:CE3	2:A:448:ARG:HB3	2.40	0.56
2:A:456:TRP:HB3	2:A:498:ARG:HH12	1.70	0.56
2:B:172:LEU:HB2	2:B:280:TYR:CD1	2.41	0.56
2:B:823:LEU:HD11	2:B:841:GLU:HG2	1.87	0.56
2:A:289:LYS:H	2:A:289:LYS:CD	2.18	0.56
2:B:230:PRO:HG2	2:B:258:PRO:HG3	1.86	0.56
2:A:415:TRP:O	2:A:424:ASN:N	2.36	0.56
2:B:473:THR:CG2	2:B:476:LEU:H	2.17	0.56
2:A:4:PRO:O	2:A:587:ARG:NE	2.38	0.56
2:B:382:VAL:HG21	2:B:516:LEU:CA	2.36	0.56
2:A:13:GLU:OE2	2:A:548:ALA:HB3	2.06	0.56
2:A:468:GLY:C	2:A:470:PRO:CD	2.74	0.56
2:B:260:VAL:HG22	2:B:269:LEU:HD21	1.87	0.56
2:A:157:PHE:HD2	2:A:413:PRO:CG	2.18	0.56
2:B:7:TYR:CE2	2:B:686:LEU:HD13	2.39	0.56
2:A:777:LYS:O	2:A:778:ALA:HB2	2.06	0.56
2:B:777:LYS:O	2:B:777:LYS:HD2	2.05	0.56
2:B:680:HIS:HB3	2:B:681:PRO:HD3	1.88	0.56
2:A:467:LEU:O	2:A:473:THR:CG2	2.54	0.56
2:A:84:GLY:HA3	2:A:455:THR:OG1	2.04	0.56
2:A:107:ARG:HA	2:A:407:TRP:CZ3	2.40	0.56
2:A:65:ARG:O	2:A:69:MET:HG2	2.05	0.56
2:B:724:GLN:HB3	2:B:783:MET:HG2	1.87	0.56
2:A:317:ALA:O	2:A:321:ALA:HB2	2.06	0.56
2:A:199:THR:HA	2:A:212:ILE:O	2.07	0.56
2:A:157:PHE:CD2	2:A:413:PRO:HG2	2.41	0.56
2:A:855:ARG:HG3	2:B:809:LEU:HD12	1.88	0.55
2:B:217:PRO:HD2	2:B:318:ARG:HE	1.71	0.55
2:A:245:ILE:HG12	2:A:248:THR:HB	1.88	0.55
2:B:341:LEU:C	2:B:341:LEU:HD13	2.27	0.55
1:D:975:A:H8	2:B:213:ALA:O	1.89	0.55
2:A:105:LEU:O	2:A:106:GLY:O	2.24	0.55
2:A:408:TRP:O	2:A:409:GLY:O	2.24	0.55
2:A:260:VAL:HG22	2:A:269:LEU:HD21	1.88	0.55
1:D:917:G:H4'	1:D:918:G:OP1	2.06	0.55
2:B:201:ARG:CD	2:B:332:VAL:HG21	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:922:A:H2'	1:D:923:G:H8	1.72	0.55
2:B:714:GLU:O	2:B:717:ARG:HB3	2.05	0.55
2:A:424:ASN:ND2	2:A:446:LEU:HD21	2.21	0.55
2:A:170:PRO:O	2:A:171:ARG:O	2.24	0.55
2:A:202:TYR:OH	2:A:244:ARG:CZ	2.53	0.55
2:A:343:THR:HA	2:A:350:PRO:HA	1.88	0.55
2:A:412:ILE:HG13	2:A:413:PRO:HD2	1.88	0.55
2:A:480:TYR:HB3	2:A:481:PRO:HD3	1.89	0.55
2:B:306:PRO:O	2:B:309:LEU:HB3	2.05	0.55
2:A:557:TYR:O	2:A:635:ARG:NH2	2.36	0.55
2:B:114:VAL:HG11	2:B:408:TRP:CE3	2.42	0.55
2:A:747:TYR:CE2	2:A:749:GLU:HG2	2.42	0.55
2:B:202:TYR:CE1	2:B:330:HIS:ND1	2.69	0.55
2:B:469:TRP:C	2:B:471:GLU:N	2.58	0.55
2:B:445:ARG:HB2	4:B:1037:HOH:O	2.06	0.55
2:A:146:ASP:OD1	2:A:149:ARG:HB2	2.06	0.55
2:B:805:GLN:H	2:B:805:GLN:NE2	1.96	0.55
1:C:965:G:H2'	1:C:966:C:C6	2.42	0.55
2:B:830:GLU:HG2	2:B:831:LYS:NZ	2.22	0.55
2:A:711:ARG:HG2	2:A:711:ARG:HH11	1.72	0.55
2:A:172:LEU:HD23	2:A:354:ALA:O	2.07	0.55
2:B:146:ASP:OD1	2:B:149:ARG:HB2	2.07	0.55
2:A:467:LEU:O	2:A:473:THR:HG21	2.07	0.55
2:B:153:VAL:CG2	2:B:154:ARG:H	2.20	0.55
2:B:2:ASP:O	2:B:4:PRO:HD3	2.06	0.55
2:A:837:VAL:HG13	2:A:838:GLU:N	2.21	0.55
2:A:28:ASN:HD22	2:A:28:ASN:C	2.11	0.54
2:B:416:TYR:CD2	2:B:423:VAL:HG22	2.42	0.54
2:A:221:PHE:CE2	2:A:306:PRO:HD3	2.42	0.54
2:A:401:ASN:C	2:A:401:ASN:ND2	2.60	0.54
2:A:680:HIS:CD2	2:A:687:THR:CG2	2.90	0.54
2:A:282:ILE:CA	2:A:285:ARG:HD3	2.22	0.54
2:B:242:ARG:HH21	2:B:251:TRP:HB2	1.72	0.54
1:C:931:C:H2'	1:C:931:C:O2	2.08	0.54
2:A:49:LEU:HG	2:A:128:GLN:OE1	2.07	0.54
2:B:35:PRO:HA	2:B:73:GLU:HB2	1.88	0.54
2:A:759:LEU:HD12	2:A:763:ARG:HD2	1.89	0.54
2:B:462:TRP:H	2:B:463:PRO:HD2	1.71	0.54
1:C:964:C:H2'	1:C:965:G:C8	2.36	0.54
2:A:460:ALA:HA	2:A:499:MET:HG3	1.89	0.54
2:B:245:ILE:CB	2:B:248:THR:HG22	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:27:ALA:O	2:A:140:ARG:NH2	2.41	0.54
2:A:358:GLN:HB2	2:A:360:TRP:HE1	1.73	0.54
2:A:228:VAL:HG22	2:A:268:ALA:HB2	1.89	0.54
2:B:498:ARG:O	2:B:501:VAL:HG12	2.07	0.54
2:B:143:PHE:HB3	2:B:146:ASP:HB3	1.90	0.54
2:A:242:ARG:HH11	2:A:251:TRP:HB3	1.72	0.54
2:A:242:ARG:O	2:A:243:ALA:CB	2.56	0.54
2:B:161:TYR:O	2:B:163:GLU:N	2.40	0.54
2:B:341:LEU:CD1	2:B:343:THR:HG23	2.38	0.54
2:A:196:LYS:HB3	2:A:198:TYR:CE2	2.42	0.54
2:B:452:VAL:HG12	2:B:453:PHE:O	2.07	0.54
2:A:248:THR:HG23	2:A:249:GLU:N	2.22	0.54
2:A:250:VAL:HG21	2:A:304:ARG:HD2	1.89	0.54
1:C:916:C:C6	1:C:916:C:OP2	2.60	0.54
2:B:714:GLU:O	2:B:717:ARG:N	2.41	0.54
1:D:947:C:HO2'	1:D:948:G:P	2.30	0.54
2:A:501:VAL:HG12	2:A:502:SER:N	2.22	0.54
2:B:201:ARG:HD2	2:B:211:GLU:CB	2.37	0.54
2:B:680:HIS:CD2	2:B:687:THR:HG21	2.43	0.54
2:A:473:THR:OG1	2:A:474:GLU:N	2.41	0.54
2:B:814:ALA:O	2:B:818:ARG:HG3	2.07	0.54
2:A:448:ARG:NH1	2:A:448:ARG:O	2.40	0.54
2:B:118:LYS:HD3	2:B:143:PHE:CE1	2.43	0.54
2:B:467:LEU:O	2:B:473:THR:HG21	2.07	0.54
2:A:61:ASP:OD1	2:A:65:ARG:HG3	2.08	0.54
2:A:376:ARG:HB2	2:A:376:ARG:HH11	1.73	0.54
2:B:107:ARG:HA	2:B:407:TRP:CE3	2.43	0.54
2:A:364:ARG:N	2:A:365:PRO:HD2	2.23	0.54
2:A:221:PHE:HA	2:A:245:ILE:HD11	1.88	0.54
2:A:593:ARG:HH11	2:A:593:ARG:CG	2.19	0.54
2:A:349:THR:HG23	2:A:350:PRO:HD2	1.90	0.54
2:B:153:VAL:HG11	2:B:410:HIS:ND1	2.23	0.54
2:B:315:PHE:C	2:B:317:ALA:H	2.10	0.54
2:A:593:ARG:HB2	2:A:665:LEU:HD21	1.90	0.53
2:A:242:ARG:NH1	2:A:251:TRP:CB	2.71	0.53
2:A:462:TRP:C	2:A:464:LEU:H	2.11	0.53
2:A:416:TYR:CD2	2:A:423:VAL:HG12	2.43	0.53
2:B:529:MET:HE1	2:B:537:ILE:HB	1.89	0.53
2:A:845:LYS:HE3	2:B:820:GLN:OE1	2.09	0.53
2:A:613:ARG:NH2	2:A:644:GLU:HG3	2.24	0.53
2:B:155:TYR:HD1	2:B:431:TYR:CD2	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:525:LYS:HD2	2:B:525:LYS:N	2.23	0.53
2:A:271:VAL:HG12	2:A:273:PRO:HD3	1.89	0.53
2:B:255:LEU:HD12	2:B:255:LEU:O	2.08	0.53
2:B:277:PRO:O	2:B:281:GLU:HB2	2.08	0.53
2:A:277:PRO:HD3	2:A:353:TYR:CD2	2.44	0.53
2:A:469:TRP:O	2:A:470:PRO:C	2.40	0.53
2:B:178:ARG:HG2	2:B:347:CYS:SG	2.48	0.53
2:B:795:LEU:O	2:B:796:LEU:HD23	2.08	0.53
2:B:87:THR:O	2:B:91:VAL:HG23	2.08	0.53
2:A:456:TRP:HB3	2:A:498:ARG:NH1	2.23	0.53
2:B:527:GLN:HE21	2:B:533:LYS:HE2	1.72	0.53
1:C:904:C:H2'	1:C:905:G:H8	1.73	0.53
2:A:37:VAL:CG2	2:A:479:PHE:HB2	2.28	0.53
2:B:172:LEU:HB2	2:B:280:TYR:CE1	2.42	0.53
2:A:431:TYR:HE1	2:A:432:LEU:HD12	1.74	0.53
2:A:404:ARG:HG2	2:A:406:LEU:HD12	1.90	0.53
2:B:69:MET:CE	2:B:680:HIS:ND1	2.71	0.53
2:A:747:TYR:CZ	2:A:774:ARG:HB2	2.44	0.53
2:B:217:PRO:O	2:B:220:VAL:HG22	2.09	0.53
2:A:217:PRO:O	2:A:220:VAL:HG13	2.09	0.53
2:A:593:ARG:HG2	2:A:593:ARG:O	2.08	0.53
2:A:398:LYS:O	2:A:399:ASP:C	2.47	0.53
2:A:85:ILE:O	2:A:88:GLN:HB3	2.09	0.53
2:A:234:ARG:HH21	2:A:267:GLY:HA3	1.73	0.53
2:B:242:ARG:HE	2:B:251:TRP:CB	2.22	0.53
2:A:346:ARG:HH11	2:A:346:ARG:HB2	1.72	0.53
2:B:359:TRP:HB2	2:B:403:SER:OG	2.09	0.53
2:B:152:ALA:HB2	2:B:470:PRO:HD3	1.89	0.53
2:A:82:HIS:CB	2:A:145:MET:HE2	2.38	0.53
2:A:315:PHE:C	2:A:317:ALA:N	2.63	0.53
2:B:430:ARG:O	2:B:432:LEU:N	2.42	0.53
1:C:922:A:H2'	1:C:923:G:H8	1.74	0.53
2:B:98:GLU:HG3	2:B:99:GLY:N	2.18	0.53
2:A:171:ARG:HB2	4:A:1088:HOH:O	2.09	0.53
2:A:522:LEU:CD1	2:A:566:ARG:HA	2.39	0.53
2:B:86:ALA:O	2:B:90:VAL:HG23	2.08	0.53
2:B:388:LYS:CD	2:B:388:LYS:N	2.72	0.53
2:B:160:TYR:HE2	2:B:505:HIS:CD2	2.27	0.53
2:A:771:LEU:HD11	2:A:791:PRO:HG2	1.91	0.53
2:A:774:ARG:HG3	2:A:774:ARG:HH11	1.74	0.52
2:B:361:LEU:CD1	2:B:402:ILE:HD11	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:GLY:O	2:B:310:ARG:NH1	2.38	0.52
2:B:193:THR:HG23	2:B:194:PRO:HD2	1.89	0.52
1:C:922:A:H2'	1:C:923:G:C8	2.45	0.52
2:A:229:HIS:CD2	2:A:231:GLU:H	2.28	0.52
1:D:909:A:H4'	1:D:910:G:OP1	2.08	0.52
2:A:499:MET:CE	2:A:512:PHE:CE2	2.83	0.52
2:A:245:ILE:HG12	2:A:248:THR:CB	2.39	0.52
2:B:834:LYS:HD2	2:B:834:LYS:H	1.73	0.52
2:A:665:LEU:O	2:A:669:GLU:HG3	2.09	0.52
2:A:469:TRP:O	2:A:469:TRP:CG	2.62	0.52
2:B:807:LYS:O	2:B:811:GLU:HG3	2.08	0.52
2:A:753:ALA:HB3	2:A:754:PRO:HD3	1.90	0.52
2:A:64:ILE:HG23	2:A:74:ALA:HB1	1.91	0.52
2:B:416:TYR:N	2:B:447:LYS:O	2.38	0.52
2:B:244:ARG:NH2	4:B:992:HOH:O	2.17	0.52
2:B:326:ARG:HB3	2:B:331:LEU:HD23	1.91	0.52
2:B:93:ARG:O	2:B:97:LYS:HG3	2.10	0.52
2:A:430:ARG:HB3	2:A:433:GLU:OE2	2.10	0.52
2:B:516:LEU:CD1	2:B:628:LEU:HD13	2.38	0.52
2:A:382:VAL:HG11	2:A:516:LEU:CD1	2.40	0.52
2:B:217:PRO:HD2	2:B:318:ARG:NE	2.24	0.52
2:B:297:GLU:N	2:B:297:GLU:OE2	2.43	0.52
2:B:299:ARG:NH2	2:B:312:LEU:HD12	2.25	0.52
2:A:341:LEU:HD21	2:A:350:PRO:HB3	1.92	0.52
2:A:469:TRP:N	2:A:470:PRO:CD	2.71	0.52
2:A:78:PRO:HG2	2:A:141:GLU:HA	1.91	0.52
1:C:967:C:O2'	1:C:968:G:H5'	2.10	0.52
1:C:920:A:H2'	1:C:945:G:O6	2.10	0.52
2:B:724:GLN:HE22	2:B:785:ARG:H	1.57	0.52
2:B:736:ALA:CB	2:B:738:LEU:HD13	2.40	0.52
1:D:901:G:N2	1:D:972:A:H1'	2.25	0.52
2:B:382:VAL:HG11	2:B:516:LEU:CD1	2.40	0.52
2:A:529:MET:HG3	2:A:535:ASN:O	2.10	0.52
2:B:429:GLU:O	2:B:430:ARG:HG2	2.10	0.52
2:A:101:THR:O	2:A:104:ASP:HB2	2.10	0.52
2:A:520:LEU:HA	3:A:990:VAA:N1	2.25	0.52
2:B:593:ARG:HG3	2:B:593:ARG:NH1	2.24	0.52
2:B:382:VAL:C	2:B:384:GLU:N	2.63	0.52
2:B:82:HIS:O	2:B:87:THR:OG1	2.17	0.52
2:A:306:PRO:HG2	2:A:309:LEU:CB	2.39	0.52
2:A:453:PHE:CD2	2:A:457:PHE:CD2	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:724:GLN:HE22	2:B:785:ARG:HB2	1.74	0.52
2:A:216:ARG:HG2	2:A:218:GLU:OE1	2.09	0.52
2:B:618:VAL:HG12	2:B:708:PRO:HG3	1.92	0.52
2:A:278:LEU:O	2:A:282:ILE:HG12	2.10	0.52
2:A:221:PHE:HB2	2:A:293:VAL:HG11	1.91	0.52
1:D:932:U:O2'	1:D:933:C:C5	2.45	0.52
2:B:820:GLN:NE2	2:B:821:ARG:N	2.57	0.52
2:A:529:MET:HE2	2:A:536:VAL:CA	2.40	0.52
2:A:651:GLU:HA	2:A:651:GLU:OE2	2.10	0.52
2:B:101:THR:HG23	2:B:104:ASP:H	1.74	0.51
2:A:201:ARG:NH2	2:A:332:VAL:HG21	2.25	0.51
2:A:83:ALA:HB3	2:A:87:THR:OG1	2.10	0.51
2:A:202:TYR:CD2	2:A:203:GLU:N	2.78	0.51
2:A:462:TRP:C	2:A:464:LEU:N	2.64	0.51
2:A:361:LEU:O	2:A:363:MET:N	2.42	0.51
2:B:778:ALA:HB3	2:B:789:ARG:HG2	1.93	0.51
2:B:467:LEU:O	2:B:473:THR:CG2	2.58	0.51
2:B:489:TYR:HA	2:B:517:LEU:HD22	1.90	0.51
2:B:202:TYR:OH	2:B:244:ARG:CZ	2.59	0.51
2:B:200:LEU:HD21	2:B:325:PHE:CE1	2.45	0.51
2:B:751:GLU:HB2	2:B:785:ARG:NH2	2.25	0.51
2:B:362:ARG:O	2:B:365:PRO:HD2	2.10	0.51
2:A:369:GLU:OE2	2:A:505:HIS:HA	2.09	0.51
2:A:759:LEU:HD12	2:A:763:ARG:CD	2.40	0.51
2:A:279:ASP:HA	2:A:282:ILE:CG1	2.40	0.51
1:D:973:C:C2	2:B:278:LEU:HD13	2.46	0.51
2:B:181:THR:OG1	2:B:404:ARG:HG3	2.10	0.51
2:A:96:LEU:C	2:A:98:GLU:H	2.14	0.51
1:C:934:A:N3	2:A:584:ASN:HB3	2.25	0.51
2:A:197:LEU:HD21	2:A:213:ALA:HB1	1.93	0.51
2:A:818:ARG:HA	2:A:821:ARG:NH1	2.22	0.51
2:A:388:LYS:N	2:A:388:LYS:HD3	2.26	0.51
2:B:69:MET:HB2	2:B:703:GLU:O	2.11	0.51
2:B:161:TYR:HD1	2:B:425:VAL:HB	1.70	0.51
2:B:593:ARG:HH11	2:B:593:ARG:HG3	1.75	0.51
1:C:918:G:O6	2:A:833:PRO:CD	2.57	0.51
2:A:64:ILE:HG13	2:A:76:TRP:HB2	1.93	0.51
2:A:802:ARG:NH2	2:A:861:ILE:HG22	2.25	0.51
1:D:902:G:O6	1:D:970:C:N3	2.44	0.51
2:A:279:ASP:HA	2:A:282:ILE:HG12	1.93	0.51
2:A:260:VAL:HG13	2:A:269:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ILE:HD12	2:B:413:PRO:CD	2.24	0.51
2:B:462:TRP:C	2:B:464:LEU:H	2.15	0.51
2:B:724:GLN:NE2	2:B:785:ARG:HB2	2.25	0.51
1:D:964:C:H2'	1:D:965:G:C8	2.44	0.51
2:B:9:PRO:C	2:B:11:SER:H	2.14	0.51
2:A:5:LYS:H	2:A:5:LYS:CD	2.18	0.51
2:B:370:VAL:HG12	2:B:374:LEU:CD1	2.41	0.51
2:A:522:LEU:HD12	2:A:522:LEU:O	2.11	0.51
2:B:745:ARG:HH11	2:B:745:ARG:CB	2.14	0.50
2:B:494:LEU:N	2:B:494:LEU:HD23	2.13	0.50
1:C:933:C:O5'	1:C:933:C:H6	1.94	0.50
2:B:149:ARG:CD	2:B:465:SER:OG	2.59	0.50
1:D:967:C:O2'	1:D:968:G:H5'	2.11	0.50
2:B:748:LEU:CD1	2:B:755:VAL:HG21	2.41	0.50
2:A:19:LYS:HE3	2:A:699:GLU:OE2	2.11	0.50
2:A:498:ARG:NH1	2:A:498:ARG:HG2	2.26	0.50
2:B:529:MET:HE2	2:B:537:ILE:H	1.75	0.50
2:B:349:THR:CG2	2:B:350:PRO:HD2	2.41	0.50
2:A:201:ARG:CZ	2:A:211:GLU:OE1	2.60	0.50
1:C:932:U:O2	1:C:932:U:H2'	2.09	0.50
2:B:529:MET:HA	2:B:535:ASN:OD1	2.10	0.50
2:B:565:ILE:HG22	2:B:565:ILE:O	2.11	0.50
2:A:518:HIS:CD2	2:A:519:GLY:O	2.65	0.50
2:A:224:GLN:O	2:A:225:ALA:HB2	2.10	0.50
2:A:307:GLU:C	2:A:309:LEU:H	2.14	0.50
2:A:203:GLU:O	2:A:243:ALA:HA	2.10	0.50
2:B:613:ARG:HH21	2:B:640:LEU:CD1	2.24	0.50
2:A:460:ALA:CB	2:A:498:ARG:HB3	2.42	0.50
2:B:322:VAL:HG13	2:B:323:GLU:N	2.27	0.50
2:A:150:SER:O	2:A:153:VAL:HG22	2.11	0.50
2:A:153:VAL:HG11	2:A:410:HIS:CE1	2.46	0.50
2:B:85:ILE:HG23	2:B:86:ALA:N	2.27	0.50
2:B:224:GLN:O	2:B:225:ALA:HB2	2.11	0.50
2:A:152:ALA:HB2	2:A:470:PRO:HG3	1.93	0.50
2:A:46:THR:CG2	2:A:90:VAL:HG21	2.40	0.50
2:B:487:THR:O	2:B:517:LEU:HA	2.11	0.50
2:A:26:VAL:HG22	2:A:139:SER:HB3	1.94	0.50
2:B:424:ASN:ND2	2:B:446:LEU:HD21	2.26	0.50
2:A:155:TYR:OH	2:A:159:ARG:HD2	2.12	0.50
2:B:501:VAL:CG1	2:B:502:SER:H	2.25	0.50
2:B:683:MET:O	2:B:687:THR:CG2	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:846:GLU:HA	2:B:849:GLU:HB2	1.92	0.50
2:A:307:GLU:H	2:A:307:GLU:CD	2.15	0.50
2:A:387:LYS:HB3	2:A:388:LYS:CE	2.42	0.50
2:A:196:LYS:CB	2:A:198:TYR:HE2	2.25	0.50
2:A:518:HIS:HD2	2:A:519:GLY:O	1.95	0.50
2:B:415:TRP:HB2	2:B:424:ASN:HB2	1.94	0.49
1:D:933:C:C6	1:D:933:C:H3'	2.46	0.49
2:B:165:LEU:HD13	2:B:366:LEU:HD21	1.94	0.49
1:C:932:U:OP1	1:C:933:C:OP2	2.30	0.49
2:A:260:VAL:HG22	2:A:269:LEU:CD2	2.42	0.49
2:A:276:ASP:OD1	2:A:278:LEU:N	2.45	0.49
2:A:382:VAL:HG11	2:A:516:LEU:HD13	1.93	0.49
2:B:205:GLU:HB2	2:B:242:ARG:HB2	1.92	0.49
2:A:666:ARG:HH11	2:A:666:ARG:CG	2.25	0.49
2:A:69:MET:HB2	2:A:703:GLU:O	2.11	0.49
2:A:250:VAL:HG12	2:A:252:ILE:HD12	1.93	0.49
2:A:744:VAL:CG1	2:A:745:ARG:N	2.75	0.49
2:A:488:GLY:O	2:A:490:ASP:N	2.45	0.49
2:B:409:GLY:HA3	2:B:452:VAL:HG11	1.92	0.49
2:A:171:ARG:NH2	2:A:364:ARG:HH21	2.11	0.49
2:B:469:TRP:CG	2:B:469:TRP:O	2.66	0.49
2:A:385:ARG:HB3	4:A:1038:HOH:O	2.11	0.49
2:A:246:PRO:O	2:A:247:LEU:HB2	2.11	0.49
2:A:500:GLU:HA	2:A:511:PRO:HG2	1.93	0.49
2:B:64:ILE:HG23	2:B:74:ALA:HB1	1.94	0.49
2:A:218:GLU:N	2:A:218:GLU:OE1	2.38	0.49
2:B:179:CYS:C	2:B:180:GLU:HG2	2.31	0.49
2:A:373:GLY:O	2:A:376:ARG:N	2.45	0.49
2:B:415:TRP:HZ3	4:B:1022:HOH:O	1.95	0.49
2:B:501:VAL:CG1	2:B:502:SER:N	2.75	0.49
2:A:82:HIS:HB2	2:A:145:MET:HE2	1.95	0.49
2:B:587:ARG:HH11	2:B:587:ARG:CG	2.25	0.49
2:B:272:THR:H	2:B:279:ASP:CB	2.26	0.49
2:B:294:ILE:CD1	2:B:300:MET:SD	3.00	0.49
2:A:198:TYR:CE1	2:A:322:VAL:HG21	2.48	0.49
2:B:454:ASP:O	2:B:455:THR:C	2.50	0.49
2:B:242:ARG:O	2:B:243:ALA:CB	2.57	0.49
2:B:248:THR:CG2	2:B:249:GLU:N	2.52	0.49
2:B:149:ARG:CG	2:B:465:SER:OG	2.60	0.49
2:B:326:ARG:HE	2:B:331:LEU:HD23	1.76	0.49
2:A:611:ARG:NH1	4:A:1004:HOH:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:LEU:CD2	2:B:354:ALA:H	2.26	0.49
2:B:352:GLU:HA	4:B:1010:HOH:O	2.12	0.49
2:B:498:ARG:HG2	2:B:498:ARG:HH11	1.78	0.49
2:A:412:ILE:HG13	2:A:413:PRO:CD	2.42	0.49
2:A:680:HIS:HD2	2:A:687:THR:HG21	1.74	0.49
2:A:51:MET:CE	2:A:537:ILE:HB	2.41	0.49
2:B:540:LEU:HA	2:B:543:VAL:HG22	1.95	0.49
1:C:959:U:H5"	1:C:960:C:OP2	2.12	0.49
2:A:753:ALA:O	2:A:757:GLU:HG3	2.13	0.49
2:B:487:THR:HG23	2:B:517:LEU:HD23	1.94	0.49
2:A:382:VAL:O	2:A:383:PRO:C	2.49	0.49
2:A:358:GLN:NE2	2:A:403:SER:HB2	2.28	0.49
2:B:680:HIS:HD2	2:B:687:THR:HG21	1.74	0.49
2:B:363:MET:HE3	2:B:363:MET:HA	1.95	0.49
2:A:711:ARG:HG2	2:A:711:ARG:NH1	2.27	0.49
2:B:85:ILE:HG23	2:B:86:ALA:H	1.78	0.48
2:A:245:ILE:H	2:A:248:THR:HG22	1.77	0.48
2:B:745:ARG:HB2	2:B:771:LEU:CD2	2.43	0.48
2:A:412:ILE:HG13	2:A:413:PRO:N	2.27	0.48
2:B:755:VAL:HG12	2:B:762:PHE:CG	2.47	0.48
2:A:36:PHE:CD1	2:A:67:LYS:HD3	2.48	0.48
2:B:322:VAL:HG13	2:B:323:GLU:OE1	2.13	0.48
2:A:401:ASN:ND2	2:A:403:SER:H	2.10	0.48
2:A:155:TYR:CD1	2:A:431:TYR:CD2	3.00	0.48
2:B:153:VAL:HG21	2:B:410:HIS:ND1	2.27	0.48
2:A:529:MET:CE	2:A:536:VAL:HA	2.43	0.48
2:B:280:TYR:C	2:B:280:TYR:CD2	2.86	0.48
2:A:829:ARG:HH21	2:B:829:ARG:NH1	2.11	0.48
2:B:78:PRO:HG2	2:B:141:GLU:HA	1.95	0.48
2:B:175:TRP:O	2:B:177:PRO:HD3	2.13	0.48
2:A:31:SER:HB3	2:A:73:GLU:HG3	1.96	0.48
2:B:82:HIS:HB2	2:B:408:TRP:HE1	1.78	0.48
2:A:216:ARG:HG3	2:A:318:ARG:NH2	2.28	0.48
2:B:4:PRO:HD2	2:B:583:TYR:OH	2.13	0.48
2:B:831:LYS:HE3	2:B:831:LYS:CA	2.44	0.48
2:B:63:LEU:O	2:B:67:LYS:HB2	2.14	0.48
2:A:31:SER:CB	2:A:73:GLU:HG3	2.43	0.48
2:B:808:ARG:HG2	2:B:854:ILE:CD1	2.44	0.48
2:B:338:THR:O	2:B:338:THR:HG23	2.13	0.48
2:B:46:THR:HG22	2:B:90:VAL:HG21	1.94	0.48
2:A:218:GLU:CD	2:A:318:ARG:HB3	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:387:LYS:HB3	2:A:388:LYS:HZ1	1.76	0.48
2:A:181:THR:OG1	2:A:404:ARG:HG3	2.13	0.48
2:A:845:LYS:HZ1	2:B:820:GLN:HE22	1.59	0.48
2:B:736:ALA:HB3	2:B:738:LEU:HD13	1.95	0.48
2:A:193:THR:HG23	2:A:194:PRO:HD2	1.96	0.48
1:C:973:C:C2	2:A:278:LEU:HD13	2.48	0.48
1:D:965:G:H2'	1:D:966:C:C6	2.48	0.48
2:B:333:LYS:HE2	2:B:335:GLU:OE1	2.13	0.48
1:C:946:U:H3'	1:C:946:U:C6	2.48	0.48
2:A:400:TRP:O	2:A:402:ILE:HD12	2.13	0.48
2:B:684:PRO:HG2	2:B:685:PHE:CD1	2.49	0.48
2:B:7:TYR:CD1	2:B:8:ASP:N	2.81	0.48
2:B:806:GLU:HA	2:B:858:LEU:HD11	1.96	0.48
2:A:18:GLU:HG3	2:A:22:LYS:HD3	1.96	0.48
2:B:710:GLY:O	2:B:711:ARG:HB3	2.13	0.48
2:B:298:GLY:O	2:B:314:ARG:HB3	2.14	0.48
2:B:274:ALA:HB3	2:B:291:VAL:O	2.13	0.48
2:A:810:LYS:HG3	2:B:855:ARG:CZ	2.44	0.48
2:B:358:GLN:HE22	2:B:405:GLN:NE2	2.00	0.48
2:B:405:GLN:N	2:B:405:GLN:CD	2.67	0.48
2:A:476:LEU:C	2:A:476:LEU:HD23	2.34	0.48
2:A:714:GLU:O	2:A:717:ARG:N	2.46	0.48
2:B:488:GLY:O	2:B:490:ASP:OD1	2.31	0.48
2:A:362:ARG:O	2:A:365:PRO:HG2	2.14	0.48
2:B:579:ALA:HB2	2:B:683:MET:HE1	1.95	0.48
2:A:397:VAL:HG12	2:A:398:LYS:N	2.29	0.48
2:A:833:PRO:HD2	2:A:836:VAL:CG1	2.44	0.48
2:B:712:ASP:O	2:B:716:GLU:HG3	2.13	0.48
2:A:383:PRO:HB2	2:A:386:TRP:HD1	1.76	0.47
1:C:917:G:H5'	1:C:959:U:O2	2.13	0.47
1:C:973:C:H1'	2:A:278:LEU:HB2	1.95	0.47
2:B:46:THR:CG2	2:B:90:VAL:HG21	2.45	0.47
2:A:197:LEU:CD2	2:A:213:ALA:HB1	2.44	0.47
1:C:961:C:C2'	1:C:962:U:H5'	2.43	0.47
2:B:839:ALA:O	2:B:843:ARG:HG3	2.14	0.47
2:B:730:ARG:HH12	2:B:765:LEU:HB3	1.79	0.47
2:A:456:TRP:CE3	2:A:494:LEU:O	2.67	0.47
1:D:957:A:H4'	1:D:959:U:H5	1.80	0.47
2:B:199:THR:HA	2:B:212:ILE:O	2.15	0.47
2:B:361:LEU:HD21	2:B:366:LEU:CD1	2.40	0.47
2:A:729:VAL:HG11	2:A:766:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:408:TRP:HA	2:A:408:TRP:CE3	2.49	0.47
2:B:783:MET:HB2	2:B:786:VAL:O	2.13	0.47
2:A:538:ASP:OD1	2:A:539:PRO:HD2	2.14	0.47
1:C:941:A:H2'	1:C:942:G:O5'	2.14	0.47
2:A:225:ALA:CA	2:A:252:ILE:HG23	2.31	0.47
2:A:416:TYR:HA	2:A:422:ALA:O	2.14	0.47
2:A:289:LYS:N	2:A:289:LYS:CD	2.77	0.47
2:B:305:VAL:CG1	2:B:310:ARG:HD3	2.41	0.47
2:B:193:THR:HG22	2:B:194:PRO:HD2	1.94	0.47
2:A:76:TRP:O	2:A:78:PRO:HD3	2.15	0.47
2:B:433:GLU:HA	4:B:1046:HOH:O	2.13	0.47
2:A:28:ASN:ND2	2:A:28:ASN:C	2.68	0.47
2:A:431:TYR:C	2:A:431:TYR:CD1	2.87	0.47
2:A:667:THR:O	2:A:671:VAL:HG23	2.14	0.47
2:B:393:TRP:CE3	2:B:394:LEU:HD23	2.49	0.47
2:B:831:LYS:N	2:B:831:LYS:HE3	2.30	0.47
2:B:510:ARG:HH11	2:B:510:ARG:HG3	1.78	0.47
2:B:524:GLU:N	2:B:524:GLU:OE2	2.39	0.47
2:A:382:VAL:CG2	2:A:383:PRO:CD	2.70	0.47
2:B:282:ILE:CA	2:B:285:ARG:HD3	2.34	0.47
2:A:185:ASP:O	2:A:188:VAL:HG12	2.14	0.47
2:B:537:ILE:HD12	2:B:567:LEU:HD22	1.97	0.47
2:A:371:LEU:HD21	2:A:394:LEU:CB	2.41	0.47
2:A:480:TYR:O	2:A:482:GLY:N	2.47	0.47
2:A:613:ARG:HH21	2:A:644:GLU:HG3	1.78	0.47
2:B:160:TYR:CE2	2:B:505:HIS:CD2	3.02	0.47
2:A:772:PRO:HG2	2:A:773:GLU:H	1.79	0.47
2:A:13:GLU:N	2:A:14:PRO:HD2	2.29	0.47
2:A:245:ILE:N	2:A:248:THR:HG22	2.29	0.47
2:B:280:TYR:HD2	2:B:280:TYR:C	2.17	0.47
2:B:833:PRO:HG2	2:B:836:VAL:HB	1.97	0.47
2:B:421:GLN:NE2	2:B:421:GLN:CA	2.76	0.47
2:A:408:TRP:HE3	2:A:408:TRP:HA	1.80	0.47
2:A:215:VAL:HG11	2:A:339:ILE:HG21	1.97	0.47
2:A:160:TYR:CE2	2:A:505:HIS:CD2	3.03	0.47
2:B:233:GLU:C	2:B:235:TYR:H	2.17	0.47
2:B:477:LYS:HD2	2:B:477:LYS:O	2.15	0.47
1:D:916:C:H5"	1:D:917:G:OP1	2.14	0.47
1:C:932:U:C2'	1:C:932:U:O2	2.62	0.47
2:A:210:ILE:CD1	2:A:238:LEU:HD13	2.42	0.47
2:A:2:ASP:O	2:A:4:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:733:LYS:HZ2	2:B:733:LYS:HB3	1.80	0.47
2:A:430:ARG:NE	2:A:433:GLU:OE2	2.48	0.47
2:B:401:ASN:C	2:B:401:ASN:ND2	2.68	0.47
2:B:695:THR:OG1	2:B:697:LYS:HG2	2.14	0.47
2:B:383:PRO:O	2:B:384:GLU:HB3	2.14	0.47
2:A:212:ILE:HD11	2:A:268:ALA:C	2.36	0.47
2:B:462:TRP:C	2:B:464:LEU:N	2.67	0.47
2:B:3:LEU:HB3	2:B:587:ARG:HD3	1.97	0.47
2:B:422:ALA:HA	4:B:1017:HOH:O	2.13	0.47
2:A:364:ARG:CD	4:A:1056:HOH:O	2.63	0.47
2:B:244:ARG:HB2	2:B:251:TRP:CZ2	2.50	0.47
2:B:270:LYS:HB2	2:B:270:LYS:NZ	2.30	0.47
2:B:224:GLN:OE1	2:B:291:VAL:HG11	2.15	0.47
1:D:917:G:O2'	1:D:918:G:O4'	2.32	0.47
2:A:393:TRP:CE3	2:A:394:LEU:HD23	2.48	0.47
1:D:971:C:O5'	1:D:971:C:H6	1.98	0.47
2:B:200:LEU:HD21	2:B:325:PHE:CD1	2.50	0.46
2:A:220:VAL:HG23	2:A:221:PHE:N	2.30	0.46
2:A:304:ARG:O	2:A:305:VAL:C	2.51	0.46
2:B:13:GLU:HB2	2:B:14:PRO:HD3	1.97	0.46
1:C:901:G:N2	1:C:972:A:H1'	2.30	0.46
2:B:221:PHE:O	2:B:304:ARG:HG3	2.15	0.46
2:A:186:LEU:N	2:A:186:LEU:HD12	2.14	0.46
2:A:367:ALA:O	2:A:371:LEU:HG	2.15	0.46
2:A:312:LEU:O	2:A:313:ASP:O	2.33	0.46
2:B:275:HIS:CE1	2:B:294:ILE:HB	2.49	0.46
2:B:121:SER:O	2:B:125:ILE:HG13	2.16	0.46
2:B:434:ASP:O	2:B:435:PRO:C	2.53	0.46
2:B:447:LYS:NZ	2:B:447:LYS:HA	2.30	0.46
2:A:28:ASN:HD22	2:A:29:PRO:N	2.13	0.46
1:D:956:A:H5'	1:D:957:A:OP1	2.15	0.46
2:A:469:TRP:C	2:A:471:GLU:N	2.66	0.46
2:A:397:VAL:HG12	2:A:398:LYS:H	1.80	0.46
2:A:153:VAL:CG2	2:A:154:ARG:H	2.28	0.46
2:A:683:MET:O	2:A:687:THR:CG2	2.63	0.46
2:B:482:GLY:O	2:B:513:LYS:HG3	2.15	0.46
2:B:801:TRP:CH2	2:B:858:LEU:HD23	2.50	0.46
2:B:731:ALA:O	2:B:734:ALA:HB3	2.16	0.46
2:A:275:HIS:HE1	2:A:294:ILE:HG12	1.76	0.46
1:D:916:C:H4'	1:D:917:G:O5'	2.15	0.46
2:B:66:TYR:CE2	2:B:70:ARG:HD3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:699:GLU:HA	2:A:699:GLU:OE1	2.14	0.46
2:A:855:ARG:CZ	2:B:810:LYS:HE2	2.43	0.46
2:B:408:TRP:O	2:B:409:GLY:O	2.33	0.46
2:A:45:VAL:HG12	2:A:121:SER:HB3	1.97	0.46
2:A:452:VAL:CG1	2:A:453:PHE:N	2.78	0.46
2:B:786:VAL:HG22	2:B:787:THR:N	2.31	0.46
2:B:362:ARG:C	2:B:365:PRO:HD2	2.36	0.46
2:B:364:ARG:N	2:B:365:PRO:HD2	2.30	0.46
2:A:521:VAL:HA	2:A:565:ILE:O	2.16	0.46
2:B:603:PRO:HG3	2:B:663:HIS:ND1	2.31	0.46
2:A:279:ASP:HA	2:A:282:ILE:HD11	1.98	0.46
2:B:471:GLU:O	4:B:1041:HOH:O	2.21	0.46
2:A:409:GLY:HA3	2:A:452:VAL:HG13	1.98	0.46
2:B:343:THR:HG22	2:B:350:PRO:HA	1.97	0.46
2:B:487:THR:HG23	2:B:517:LEU:CD2	2.46	0.46
2:A:637:VAL:HG21	2:A:679:LEU:CD2	2.46	0.46
2:A:255:LEU:H	2:A:255:LEU:HG	1.61	0.46
2:A:307:GLU:O	2:A:309:LEU:N	2.49	0.46
2:B:745:ARG:NH1	2:B:745:ARG:CB	2.76	0.46
2:B:370:VAL:O	2:B:373:GLY:N	2.46	0.46
2:B:153:VAL:HG11	2:B:410:HIS:CE1	2.50	0.46
2:A:196:LYS:CB	2:A:198:TYR:CE2	2.99	0.46
2:A:382:VAL:CG2	2:A:517:LEU:H	2.28	0.46
2:B:159:ARG:HG3	2:B:159:ARG:HH11	1.80	0.46
2:B:393:TRP:HB2	2:B:493:PHE:CE2	2.51	0.46
2:A:746:VAL:CG1	2:A:747:TYR:N	2.79	0.46
2:A:156:ALA:CB	2:A:461:LEU:HD21	2.45	0.46
1:C:908:U:H6	1:C:908:U:O5'	1.99	0.46
2:A:245:ILE:HG12	2:A:248:THR:HG21	1.97	0.46
2:B:266:THR:C	2:B:268:ALA:H	2.18	0.46
2:A:272:THR:H	2:A:279:ASP:HB3	1.81	0.46
2:B:366:LEU:O	2:B:369:GLU:HB2	2.16	0.46
2:A:39:PHE:CE2	2:A:463:PRO:HA	2.51	0.46
2:B:428:PRO:C	2:B:430:ARG:H	2.19	0.46
2:A:441:CYS:SG	2:A:443:SER:CB	3.04	0.46
1:C:929:G:H5'	1:C:929:G:C8	2.48	0.45
1:D:933:C:C6	1:D:933:C:C3'	2.99	0.45
2:A:201:ARG:HG2	2:A:211:GLU:CA	2.46	0.45
2:B:469:TRP:N	2:B:470:PRO:CD	2.77	0.45
2:A:145:MET:HG2	2:A:410:HIS:NE2	2.31	0.45
2:A:727:THR:HA	2:A:730:ARG:CG	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:947:C:O2'	1:D:948:G:OP2	2.33	0.45
2:A:417:CYS:C	2:A:419:ASP:H	2.20	0.45
2:B:5:LYS:CD	2:B:5:LYS:H	2.08	0.45
2:A:212:ILE:CD1	2:A:268:ALA:O	2.65	0.45
2:B:469:TRP:HD1	2:B:507:MET:HE1	1.82	0.45
2:B:473:THR:HG22	2:B:476:LEU:CB	2.44	0.45
2:A:845:LYS:HA	2:A:845:LYS:HE3	1.98	0.45
2:A:318:ARG:HA	2:A:321:ALA:HB3	1.98	0.45
2:B:624:LEU:HD12	2:B:633:ALA:HA	1.98	0.45
2:A:77:LEU:N	2:A:77:LEU:HD22	2.32	0.45
2:B:148:LYS:HD2	2:B:468:GLY:CA	2.45	0.45
2:B:190:THR:HG22	2:B:342:ALA:CB	2.46	0.45
2:A:231:GLU:HA	2:A:231:GLU:OE1	2.16	0.45
2:B:710:GLY:O	2:B:711:ARG:CB	2.64	0.45
2:B:101:THR:HG23	2:B:103:HIS:N	2.32	0.45
2:A:362:ARG:C	2:A:365:PRO:HD2	2.37	0.45
2:B:250:VAL:HG12	2:B:252:ILE:HD12	1.98	0.45
2:A:274:ALA:HB2	2:A:291:VAL:H	1.80	0.45
2:B:229:HIS:HD2	2:B:231:GLU:H	1.61	0.45
2:A:247:LEU:N	2:A:247:LEU:HD22	2.31	0.45
2:A:820:GLN:HG2	2:B:844:LEU:HD23	1.99	0.45
2:A:495:TRP:CD1	3:A:990:VAA:HG21	2.52	0.45
2:B:361:LEU:CD2	2:B:366:LEU:HD11	2.43	0.45
2:B:529:MET:HE2	2:B:536:VAL:CA	2.42	0.45
1:D:934:A:C6	1:D:935:C:N4	2.85	0.45
2:A:714:GLU:O	2:A:715:ALA:C	2.55	0.45
2:B:759:LEU:HD13	2:B:763:ARG:HE	1.82	0.45
2:B:221:PHE:C	2:B:223:ASP:H	2.20	0.45
2:A:224:GLN:NE2	2:A:304:ARG:NH2	2.41	0.45
2:B:49:LEU:HB2	2:B:128:GLN:OE1	2.16	0.45
2:A:401:ASN:ND2	2:A:403:SER:N	2.64	0.45
1:D:957:A:H4'	1:D:959:U:C5	2.52	0.45
2:A:202:TYR:CE1	2:A:330:HIS:CE1	2.96	0.45
2:A:70:ARG:HA	2:A:70:ARG:HD2	1.68	0.45
2:A:128:GLN:O	2:A:132:LEU:HG	2.16	0.45
2:A:49:LEU:HA	2:A:53:HIS:ND1	2.32	0.45
2:B:195:GLY:HA3	2:B:339:ILE:HD11	1.99	0.45
2:A:800:GLU:OE1	2:A:800:GLU:HA	2.17	0.45
2:A:261:GLU:HA	2:A:261:GLU:OE1	2.17	0.45
2:A:111:LEU:O	2:A:111:LEU:HD13	2.16	0.45
2:B:585:ALA:O	2:B:589:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:332:VAL:HG13	2:A:333:LYS:H	1.82	0.45
2:A:326:ARG:O	2:A:329:GLY:N	2.49	0.45
2:A:469:TRP:HB2	2:A:476:LEU:HD12	1.98	0.45
2:A:680:HIS:CA	2:A:687:THR:HG21	2.43	0.45
2:A:714:GLU:CG	2:A:715:ALA:N	2.75	0.45
1:C:955:C:H1'	2:A:828:PHE:HA	1.99	0.45
2:B:808:ARG:HG2	2:B:854:ILE:HD13	1.99	0.45
2:A:56:ASP:O	2:A:60:GLN:HG3	2.17	0.45
2:B:44:ASN:ND2	3:B:991:VAA:N3S	2.65	0.45
1:D:961:C:O2'	1:D:962:U:H5'	2.17	0.45
2:B:69:MET:HE1	2:B:680:HIS:ND1	2.32	0.45
2:B:171:ARG:HH12	2:B:364:ARG:HH21	1.64	0.45
2:B:50:HIS:CD2	2:B:52:GLY:N	2.79	0.45
2:A:429:GLU:N	2:A:429:GLU:CD	2.70	0.45
2:B:759:LEU:HD11	2:B:763:ARG:HE	1.82	0.45
2:A:13:GLU:HA	2:A:685:PHE:CD2	2.52	0.45
2:A:839:ALA:C	2:A:841:GLU:H	2.19	0.45
2:B:593:ARG:HG2	2:B:593:ARG:O	2.17	0.45
2:B:173:VAL:HG12	2:B:360:TRP:HZ2	1.82	0.45
2:A:674:VAL:O	2:A:677:LYS:HB2	2.16	0.45
2:B:225:ALA:HB1	2:B:255:LEU:HD21	1.99	0.44
2:A:245:ILE:HG21	2:A:252:ILE:HD13	1.96	0.44
2:B:148:LYS:HE2	4:B:1061:HOH:O	2.17	0.44
2:A:312:LEU:HG	2:A:313:ASP:N	2.32	0.44
2:B:831:LYS:HA	2:B:831:LYS:HE3	1.98	0.44
2:A:482:GLY:O	2:A:513:LYS:HG3	2.17	0.44
2:B:401:ASN:HD22	2:B:401:ASN:C	2.19	0.44
2:B:812:LEU:HD22	2:B:847:ASN:O	2.17	0.44
2:B:257:ASP:OD1	2:B:282:ILE:HG23	2.17	0.44
2:B:280:TYR:O	2:B:284:GLU:HG2	2.17	0.44
2:B:341:LEU:HD13	2:B:342:ALA:N	2.32	0.44
2:B:294:ILE:HD13	2:B:300:MET:SD	2.57	0.44
2:B:59:LEU:O	2:B:63:LEU:HD23	2.18	0.44
2:A:759:LEU:HD12	2:A:763:ARG:HG3	1.99	0.44
2:A:494:LEU:N	2:A:494:LEU:CD2	2.63	0.44
2:A:549:ASP:OD1	2:A:683:MET:HA	2.17	0.44
2:A:806:GLU:CA	2:A:858:LEU:HD21	2.42	0.44
2:A:808:ARG:HD2	2:A:808:ARG:HA	1.84	0.44
2:A:68:ARG:C	2:A:70:ARG:H	2.20	0.44
2:A:746:VAL:HG13	2:A:747:TYR:N	2.33	0.44
1:D:947:C:O2'	1:D:948:G:P	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:443:SER:OG	2:A:444:PRO:HD2	2.17	0.44
2:B:283:GLY:HA2	2:B:288:LEU:HG	1.99	0.44
2:A:678:LEU:O	2:A:681:PRO:HD2	2.18	0.44
2:B:221:PHE:HB2	2:B:293:VAL:HG11	1.98	0.44
2:A:221:PHE:HA	2:A:245:ILE:CD1	2.47	0.44
2:B:277:PRO:CD	2:B:353:TYR:CE2	2.94	0.44
2:B:172:LEU:HD21	2:B:353:TYR:HB3	1.97	0.44
2:A:592:SER:C	2:A:594:GLU:N	2.70	0.44
2:A:41:PRO:O	2:A:43:PRO:HD3	2.17	0.44
2:B:393:TRP:CZ3	2:B:394:LEU:HD23	2.52	0.44
1:C:962:U:H2'	1:C:963:A:C8	2.52	0.44
2:A:789:ARG:HG2	2:A:789:ARG:HH11	1.82	0.44
2:A:201:ARG:NE	2:A:332:VAL:HG11	2.32	0.44
2:A:814:ALA:O	2:A:818:ARG:HG3	2.17	0.44
2:A:833:PRO:C	2:A:835:GLU:N	2.71	0.44
2:B:398:LYS:CD	2:B:398:LYS:N	2.81	0.44
2:B:543:VAL:HG23	2:B:544:GLU:N	2.32	0.44
2:B:201:ARG:HH11	2:B:332:VAL:CG1	2.22	0.44
2:B:684:PRO:O	2:B:687:THR:HG22	2.17	0.44
2:B:418:GLU:HG3	2:B:445:ARG:O	2.17	0.44
2:B:722:LEU:O	2:B:726:VAL:HG23	2.17	0.44
2:B:202:TYR:HE1	2:B:330:HIS:CE1	2.34	0.44
2:B:202:TYR:HE2	2:B:244:ARG:HD3	1.83	0.44
2:B:529:MET:CE	2:B:537:ILE:N	2.80	0.44
2:B:582:LEU:O	2:B:583:TYR:C	2.55	0.44
2:B:179:CYS:O	2:B:180:GLU:C	2.56	0.44
2:B:606:ALA:HB1	2:B:649:TYR:CD1	2.53	0.44
2:B:106:GLY:C	2:B:108:GLU:N	2.69	0.44
2:B:223:ASP:HB2	2:B:245:ILE:HD13	2.00	0.44
2:A:201:ARG:HG2	2:A:211:GLU:HA	2.00	0.44
1:C:932:U:HO2'	1:C:933:C:H5	1.61	0.44
1:D:935:C:H1'	2:B:584:ASN:ND2	2.32	0.44
2:B:305:VAL:HG22	2:B:310:ARG:HB2	1.99	0.44
2:B:7:TYR:HB2	2:B:583:TYR:CG	2.53	0.44
1:C:955:C:O2	2:A:832:ALA:HB2	2.17	0.44
2:A:837:VAL:CG1	2:A:838:GLU:N	2.81	0.44
2:B:233:GLU:C	2:B:235:TYR:N	2.71	0.44
2:A:573:GLU:O	2:A:574:MET:C	2.56	0.44
2:B:416:TYR:CE2	2:B:423:VAL:HG22	2.53	0.44
2:B:448:ARG:HG2	2:B:448:ARG:NH1	2.33	0.44
2:B:101:THR:HG22	2:B:104:ASP:CG	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ASP:HB2	2:B:245:ILE:CD1	2.48	0.44
2:B:202:TYR:OH	2:B:244:ARG:NH2	2.51	0.44
2:B:323:GLU:C	2:B:325:PHE:N	2.71	0.44
2:A:173:VAL:HG12	2:A:360:TRP:HZ2	1.83	0.44
2:A:85:ILE:HG23	2:A:86:ALA:N	2.32	0.44
2:A:774:ARG:HG3	2:A:774:ARG:NH1	2.33	0.44
2:A:19:LYS:HE3	2:A:699:GLU:CD	2.39	0.44
1:C:941:A:C2'	1:C:942:G:O5'	2.66	0.44
2:A:572:LEU:HA	2:A:572:LEU:HD23	1.81	0.44
1:D:912:U:H2'	1:D:913:C:O5'	2.18	0.44
2:A:171:ARG:CZ	2:A:364:ARG:HH21	2.31	0.43
2:B:202:TYR:O	2:B:203:GLU:O	2.36	0.43
2:B:274:ALA:HB1	2:B:292:SER:OG	2.17	0.43
2:B:201:ARG:HH11	2:B:201:ARG:CG	2.31	0.43
1:D:923:G:N2	2:B:570:ARG:NH2	2.66	0.43
2:B:429:GLU:C	2:B:430:ARG:HG2	2.37	0.43
2:A:190:THR:HG22	2:A:342:ALA:HB2	1.99	0.43
2:A:641:VAL:O	2:A:645:PHE:HB3	2.18	0.43
2:A:576:ARG:NH1	2:A:577:ASN:OD1	2.51	0.43
2:A:279:ASP:O	2:A:283:GLY:N	2.43	0.43
1:C:931:C:O4'	1:C:936:A:N6	2.52	0.43
2:B:469:TRP:HA	2:B:476:LEU:HD22	1.99	0.43
2:B:364:ARG:H	2:B:364:ARG:HG2	1.53	0.43
2:B:510:ARG:NH1	2:B:510:ARG:HG3	2.32	0.43
2:B:12:VAL:O	2:B:16:TRP:HD1	2.01	0.43
2:B:627:ALA:O	2:B:628:LEU:HB2	2.18	0.43
2:B:225:ALA:CA	2:B:252:ILE:CG2	2.92	0.43
2:A:766:SER:O	2:A:767:ARG:CB	2.66	0.43
2:A:7:TYR:HB2	2:A:583:TYR:CG	2.53	0.43
2:B:176:CYS:SG	2:B:347:CYS:SG	3.16	0.43
2:B:738:LEU:HD23	2:B:744:VAL:CG1	2.47	0.43
2:B:261:GLU:OE2	2:B:261:GLU:HA	2.18	0.43
2:A:382:VAL:CG2	2:A:516:LEU:HD12	2.33	0.43
2:A:199:THR:HB	2:A:332:VAL:HG13	1.99	0.43
2:B:778:ALA:HA	2:B:792:LEU:HB2	2.01	0.43
2:A:839:ALA:C	2:A:841:GLU:N	2.71	0.43
2:A:312:LEU:CD2	2:A:316:GLU:HG2	2.44	0.43
2:B:592:SER:C	2:B:594:GLU:H	2.20	0.43
2:B:157:PHE:O	2:B:160:TYR:N	2.52	0.43
2:A:8:ASP:OD1	2:A:10:LYS:HB2	2.18	0.43
2:B:486:VAL:HG22	2:B:516:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ILE:HG23	2:B:451:ASP:O	2.18	0.43
2:A:211:GLU:O	2:A:212:ILE:HD12	2.19	0.43
2:A:202:TYR:HE1	2:A:330:HIS:CG	2.36	0.43
2:A:255:LEU:HD12	2:A:255:LEU:O	2.19	0.43
2:A:441:CYS:SG	2:A:443:SER:HB2	2.59	0.43
2:A:326:ARG:CG	2:A:327:GLU:N	2.74	0.43
2:A:529:MET:HE2	2:A:537:ILE:H	1.82	0.43
1:C:918:G:N2	1:C:956:A:C1'	2.81	0.43
2:B:428:PRO:O	2:B:430:ARG:N	2.50	0.43
2:A:255:LEU:HD12	2:A:255:LEU:C	2.38	0.43
2:A:148:LYS:NZ	4:A:1063:HOH:O	2.45	0.43
2:A:28:ASN:HD22	2:A:29:PRO:CD	2.32	0.43
2:B:99:GLY:C	2:B:100:LYS:HD2	2.39	0.43
2:B:245:ILE:CA	2:B:248:THR:HG22	2.48	0.43
1:D:936:A:O4'	1:D:938:G:C8	2.72	0.43
2:A:241:LYS:HB3	2:A:242:ARG:H	1.61	0.43
2:A:844:LEU:HD23	2:B:820:GLN:HG2	2.01	0.43
2:A:683:MET:O	2:A:687:THR:HB	2.18	0.43
2:A:196:LYS:HB2	2:A:198:TYR:HE2	1.84	0.43
2:A:718:ALA:O	2:A:721:ALA:HB3	2.18	0.43
1:D:943:A:H2'	1:D:944:G:O4'	2.18	0.43
2:A:632:GLN:O	2:A:633:ALA:C	2.56	0.43
2:A:452:VAL:HG12	2:A:453:PHE:N	2.33	0.43
2:B:587:ARG:HG3	2:B:587:ARG:HH11	1.83	0.43
2:B:126:LEU:HD23	2:B:126:LEU:HA	1.84	0.43
2:A:759:LEU:HD12	2:A:763:ARG:CG	2.49	0.43
2:A:373:GLY:O	2:A:374:LEU:C	2.55	0.43
2:B:160:TYR:HB3	2:B:166:ALA:HB2	2.01	0.43
2:A:743:GLU:O	2:A:744:VAL:HG23	2.19	0.43
2:B:610:MET:HG2	2:B:649:TYR:CD2	2.53	0.43
2:A:304:ARG:HH11	2:A:304:ARG:CG	2.25	0.43
2:B:771:LEU:HD12	2:B:773:GLU:H	1.84	0.43
2:A:145:MET:HE3	2:A:408:TRP:CZ2	2.54	0.43
2:B:161:TYR:C	2:B:163:GLU:N	2.71	0.43
2:B:145:MET:HG3	2:B:410:HIS:NE2	2.34	0.43
2:B:448:ARG:HH11	2:B:448:ARG:HG2	1.82	0.43
2:B:225:ALA:CA	2:B:252:ILE:HG23	2.31	0.43
2:B:216:ARG:HA	2:B:318:ARG:NH2	2.33	0.43
2:A:405:GLN:CD	2:A:405:GLN:N	2.72	0.43
2:A:469:TRP:HB2	2:A:476:LEU:CD1	2.49	0.43
2:A:216:ARG:HB3	2:A:219:THR:CG2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:828:PHE:CE2	2:A:837:VAL:HG23	2.54	0.43
2:A:73:GLU:O	2:A:75:VAL:HG23	2.19	0.43
2:B:774:ARG:HH11	2:B:774:ARG:HG2	1.84	0.43
2:A:608:ARG:NH2	4:A:1057:HOH:O	2.52	0.43
2:B:210:ILE:CD1	2:B:238:LEU:HD13	2.36	0.42
1:D:932:U:H3'	1:D:932:U:OP1	2.19	0.42
1:C:913:C:OP1	2:A:566:ARG:HB3	2.19	0.42
2:B:830:GLU:O	2:B:831:LYS:HE3	2.19	0.42
2:B:130:LYS:HE3	2:B:138:TRP:CD1	2.54	0.42
1:D:906:G:N2	1:D:967:C:C2	2.87	0.42
2:A:637:VAL:CG2	2:A:679:LEU:CD2	2.97	0.42
2:B:827:GLY:O	2:B:828:PHE:C	2.58	0.42
2:B:412:ILE:CG2	2:B:451:ASP:O	2.66	0.42
2:B:220:VAL:HG21	2:B:325:PHE:CZ	2.50	0.42
2:A:178:ARG:HG3	2:A:179:CYS:N	2.33	0.42
2:A:45:VAL:CG1	2:A:118:LYS:HA	2.47	0.42
2:A:242:ARG:HB3	2:A:251:TRP:HE3	1.83	0.42
2:B:480:TYR:HE2	2:B:509:GLU:HG3	1.83	0.42
2:B:3:LEU:HD21	2:B:590:LEU:CD1	2.47	0.42
2:B:41:PRO:HD2	2:B:60:GLN:NE2	2.30	0.42
2:A:247:LEU:HD23	2:A:325:PHE:CE1	2.54	0.42
2:A:515:VAL:HG12	2:A:517:LEU:HD13	2.00	0.42
2:A:170:PRO:HB2	2:A:355:ILE:HG22	2.01	0.42
2:A:152:ALA:CA	2:A:470:PRO:HG3	2.49	0.42
2:A:160:TYR:HE2	2:A:505:HIS:CD2	2.37	0.42
2:B:136:ALA:O	2:B:138:TRP:N	2.52	0.42
2:B:557:TYR:CE1	2:B:635:ARG:HB3	2.53	0.42
2:A:672:LEU:O	2:A:676:LEU:HG	2.19	0.42
2:B:221:PHE:HB3	2:B:304:ARG:HB2	2.01	0.42
2:A:310:ARG:HG3	2:A:310:ARG:O	2.18	0.42
2:B:212:ILE:HD12	2:B:268:ALA:O	2.19	0.42
2:B:297:GLU:HB2	2:B:299:ARG:HG2	2.01	0.42
2:A:371:LEU:O	2:A:375:ARG:HB2	2.19	0.42
1:C:918:G:C2	1:C:956:A:N3	2.87	0.42
2:A:247:LEU:HD23	2:A:325:PHE:HE1	1.85	0.42
2:A:272:THR:N	2:A:279:ASP:HB3	2.34	0.42
2:A:245:ILE:HG12	2:A:248:THR:HG22	1.98	0.42
2:A:209:PHE:O	2:A:238:LEU:HD21	2.20	0.42
2:A:766:SER:O	2:A:767:ARG:HB2	2.19	0.42
2:B:372:LYS:CA	2:B:372:LYS:NZ	2.80	0.42
2:A:2:ASP:O	2:A:4:PRO:CD	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:50:HIS:C	2:B:50:HIS:CD2	2.93	0.42
2:B:738:LEU:HA	2:B:739:PRO:HD3	1.89	0.42
1:D:920:A:H2'	1:D:945:G:O6	2.20	0.42
1:D:960:C:O2'	1:D:961:C:H5'	2.19	0.42
2:B:361:LEU:CD2	2:B:366:LEU:CD1	2.97	0.42
2:B:462:TRP:N	2:B:463:PRO:CD	2.77	0.42
2:A:833:PRO:HD2	2:A:836:VAL:HG11	2.02	0.42
1:C:918:G:H21	1:C:956:A:H1'	1.83	0.42
2:A:825:SER:OG	2:A:826:PRO:HD2	2.18	0.42
2:A:755:VAL:HG13	2:A:762:PHE:CG	2.54	0.42
2:A:88:GLN:OE1	2:A:406:LEU:HD22	2.19	0.42
2:B:683:MET:O	2:B:687:THR:HG22	2.19	0.42
2:B:482:GLY:O	2:B:512:PHE:HA	2.20	0.42
2:B:721:ALA:HB3	2:B:754:PRO:HG2	2.01	0.42
1:C:946:U:H3'	1:C:946:U:H6	1.84	0.42
2:A:417:CYS:SG	2:A:441:CYS:SG	3.17	0.42
1:C:943:A:H2'	1:C:944:G:O4'	2.19	0.42
2:A:456:TRP:CB	2:A:498:ARG:HH12	2.33	0.42
2:B:802:ARG:NH1	2:B:802:ARG:HB2	2.32	0.42
2:B:339:ILE:H	2:B:339:ILE:HG13	1.67	0.42
2:A:674:VAL:HA	2:A:677:LYS:HG3	2.02	0.42
2:B:217:PRO:CG	2:B:318:ARG:HG3	2.49	0.42
2:A:140:ARG:HH12	2:A:479:PHE:HZ	1.67	0.42
1:C:931:C:O2'	1:C:932:U:P	2.78	0.42
2:A:412:ILE:HB	2:A:453:PHE:CZ	2.55	0.42
2:B:190:THR:HA	2:B:342:ALA:HA	2.01	0.42
2:B:544:GLU:C	2:B:544:GLU:CD	2.78	0.42
2:B:19:LYS:HE2	2:B:699:GLU:OE2	2.20	0.42
2:B:382:VAL:O	2:B:384:GLU:N	2.53	0.42
2:B:453:PHE:CD2	2:B:457:PHE:CD2	3.08	0.42
2:A:220:VAL:HA	2:A:223:ASP:OD2	2.20	0.42
2:A:249:GLU:HA	2:A:249:GLU:OE1	2.20	0.42
2:B:469:TRP:CD1	2:B:507:MET:HE3	2.54	0.42
2:B:529:MET:HG3	2:B:535:ASN:O	2.20	0.42
2:B:294:ILE:HD11	2:B:300:MET:SD	2.60	0.42
2:B:233:GLU:O	2:B:235:TYR:N	2.53	0.42
2:B:1:MET:HE1	2:B:690:LEU:HA	2.02	0.42
2:B:420:CYS:HG	2:B:441:CYS:HB3	1.85	0.41
2:A:273:PRO:HG3	2:A:283:GLY:HA3	2.02	0.41
2:B:94:LEU:O	2:B:98:GLU:HG2	2.20	0.41
2:B:833:PRO:O	2:B:834:LYS:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:202:TYR:CE1	2:A:330:HIS:ND1	2.85	0.41
2:A:216:ARG:HD2	2:A:219:THR:CG2	2.50	0.41
2:B:178:ARG:CG	2:B:347:CYS:SG	3.08	0.41
2:B:326:ARG:CG	2:B:327:GLU:N	2.82	0.41
1:D:904:C:H1'	4:D:171:HOH:O	2.20	0.41
2:A:178:ARG:HG3	2:A:179:CYS:SG	2.60	0.41
2:B:397:VAL:HG12	2:B:398:LYS:H	1.84	0.41
2:B:431:TYR:CZ	2:B:432:LEU:HD23	2.55	0.41
1:C:952:G:O2'	1:C:953:U:H5'	2.20	0.41
2:B:420:CYS:HG	2:B:438:CYS:HG	1.68	0.41
2:B:210:ILE:HD12	2:B:210:ILE:HA	1.89	0.41
2:B:323:GLU:C	2:B:325:PHE:H	2.23	0.41
2:A:221:PHE:O	2:A:304:ARG:HG3	2.19	0.41
2:B:201:ARG:HD2	2:B:211:GLU:HA	2.02	0.41
2:B:469:TRP:CD1	2:B:507:MET:CE	3.03	0.41
2:B:821:ARG:HH11	2:B:821:ARG:CB	2.33	0.41
2:A:216:ARG:HG2	2:A:218:GLU:CD	2.41	0.41
2:B:830:GLU:CG	2:B:831:LYS:NZ	2.83	0.41
2:A:428:PRO:HB2	2:A:429:GLU:OE1	2.20	0.41
2:A:747:TYR:CE2	2:A:774:ARG:HB2	2.56	0.41
2:B:692:GLN:HA	2:B:697:LYS:O	2.20	0.41
2:B:293:VAL:CA	2:B:301:GLU:O	2.66	0.41
2:A:422:ALA:HB1	4:A:1000:HOH:O	2.20	0.41
1:C:975:A:H8	2:A:213:ALA:O	2.03	0.41
2:B:738:LEU:HD12	2:B:738:LEU:N	2.35	0.41
1:C:946:U:C3'	1:C:946:U:C6	3.03	0.41
2:A:624:LEU:HD13	2:A:633:ALA:N	2.35	0.41
1:C:974:C:H6	1:C:974:C:H3'	1.85	0.41
2:A:779:LEU:HD13	2:A:792:LEU:CD2	2.49	0.41
2:B:318:ARG:C	2:B:320:LYS:H	2.23	0.41
2:B:370:VAL:HG22	2:B:501:VAL:HA	2.02	0.41
2:A:417:CYS:SG	2:A:419:ASP:HB2	2.61	0.41
2:B:84:GLY:HA2	2:B:408:TRP:HD1	1.84	0.41
2:A:170:PRO:C	2:A:171:ARG:O	2.57	0.41
2:B:276:ASP:HA	2:B:277:PRO:HD2	1.86	0.41
2:B:779:LEU:CD1	2:B:792:LEU:HD13	2.51	0.41
2:B:117:TRP:O	2:B:118:LYS:C	2.59	0.41
1:C:955:C:C2'	1:C:956:A:H5'	2.51	0.41
2:A:101:THR:O	2:A:102:ARG:C	2.59	0.41
2:A:362:ARG:O	2:A:365:PRO:HD2	2.20	0.41
2:B:252:ILE:HG23	2:B:253:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:220:VAL:HG12	2:A:270:LYS:CE	2.51	0.41
1:C:929:G:C5'	1:C:929:G:H8	2.33	0.41
2:B:280:TYR:CD2	2:B:284:GLU:HG2	2.55	0.41
2:A:161:TYR:C	2:A:163:GLU:H	2.24	0.41
2:B:211:GLU:C	2:B:266:THR:HG21	2.41	0.41
2:B:473:THR:CG2	2:B:476:LEU:HB3	2.51	0.41
2:A:101:THR:O	2:A:104:ASP:N	2.54	0.41
2:A:228:VAL:O	2:A:256:ALA:HA	2.21	0.41
2:B:462:TRP:HB3	2:B:463:PRO:HD3	2.02	0.41
2:B:537:ILE:HD12	2:B:567:LEU:CD2	2.51	0.41
2:B:783:MET:HA	2:B:783:MET:HE2	2.01	0.41
1:C:952:G:H2'	1:C:953:U:C6	2.56	0.41
2:B:678:LEU:HD23	2:B:705:TRP:CZ2	2.56	0.41
2:A:382:VAL:C	2:A:384:GLU:N	2.72	0.41
2:A:280:TYR:CE1	2:A:355:ILE:HD11	2.55	0.41
2:B:248:THR:OG1	2:B:249:GLU:N	2.50	0.41
2:B:225:ALA:CB	2:B:255:LEU:HD21	2.51	0.41
2:B:746:VAL:C	2:B:771:LEU:HB2	2.40	0.41
1:D:931:C:C6	1:D:931:C:O5'	2.74	0.41
2:B:780:VAL:HG22	2:B:789:ARG:HG3	2.03	0.41
2:A:829:ARG:NH2	2:A:841:GLU:OE2	2.53	0.41
2:B:680:HIS:HD2	2:B:684:PRO:HA	1.79	0.41
2:B:61:ASP:OD1	2:B:65:ARG:NE	2.53	0.41
2:A:153:VAL:HG11	2:A:410:HIS:ND1	2.35	0.41
2:A:684:PRO:C	2:A:687:THR:HG22	2.41	0.41
2:B:425:VAL:HA	2:B:426:PRO:HD2	1.86	0.41
2:A:462:TRP:O	2:A:464:LEU:N	2.53	0.41
2:B:363:MET:C	2:B:365:PRO:HD2	2.41	0.41
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.85	0.41
2:B:188:VAL:HG21	2:B:351:ILE:HD13	2.03	0.41
2:B:763:ARG:HH12	2:B:769:ASP:CG	2.23	0.41
2:B:107:ARG:HB3	2:B:107:ARG:HH11	1.85	0.41
2:B:489:TYR:C	2:B:489:TYR:CD1	2.93	0.41
2:B:9:PRO:O	2:B:11:SER:N	2.54	0.41
2:A:193:THR:CG2	2:A:194:PRO:HD2	2.51	0.41
2:A:779:LEU:HD13	2:A:792:LEU:HD21	2.02	0.41
2:A:472:GLU:HG2	2:A:472:GLU:O	2.20	0.41
1:D:950:A:H2'	1:D:951:G:O4'	2.21	0.41
2:A:830:GLU:N	2:A:830:GLU:CD	2.74	0.41
2:B:242:ARG:HA	2:B:252:ILE:O	2.21	0.41
2:B:745:ARG:H	2:B:745:ARG:HG2	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:45:VAL:HG12	2:A:45:VAL:O	2.20	0.41
2:A:341:LEU:HD23	2:A:343:THR:HG23	2.03	0.41
2:A:51:MET:HE1	2:A:537:ILE:CG2	2.51	0.41
2:A:501:VAL:O	2:A:502:SER:C	2.59	0.41
2:A:424:ASN:HD22	2:A:446:LEU:CD2	2.32	0.40
2:A:362:ARG:O	2:A:365:PRO:CG	2.69	0.40
2:A:305:VAL:CG1	2:A:310:ARG:HB3	2.52	0.40
2:B:353:TYR:O	2:B:354:ALA:HB2	2.21	0.40
2:B:366:LEU:HB3	2:B:501:VAL:HG21	2.02	0.40
2:B:149:ARG:O	2:B:152:ALA:N	2.52	0.40
2:A:467:LEU:O	2:A:473:THR:HG22	2.19	0.40
2:B:485:LEU:HD22	2:B:512:PHE:CE2	2.57	0.40
2:B:367:ALA:O	2:B:371:LEU:HG	2.21	0.40
2:B:546:TYR:HE2	2:B:573:GLU:HG2	1.87	0.40
2:A:616:ARG:HH12	2:A:711:ARG:HB2	1.86	0.40
1:C:921:G:O2'	1:C:922:A:H5'	2.21	0.40
1:D:909:A:O2'	1:D:910:G:N7	2.37	0.40
2:B:558:LEU:HB2	2:B:565:ILE:HD13	2.03	0.40
2:B:700:LEU:N	4:B:1006:HOH:O	2.53	0.40
2:A:174:ASN:OD1	2:A:174:ASN:N	2.53	0.40
2:B:382:VAL:HG11	2:B:516:LEU:CG	2.51	0.40
2:B:313:ASP:HB3	2:B:316:GLU:HB2	2.03	0.40
2:A:44:ASN:HB3	2:A:83:ALA:HB2	2.03	0.40
2:A:593:ARG:O	2:A:594:GLU:O	2.40	0.40
1:C:904:C:H2'	1:C:905:G:C8	2.54	0.40
2:B:748:LEU:HD12	2:B:755:VAL:HG21	2.02	0.40
2:B:494:LEU:N	2:B:494:LEU:CD2	2.79	0.40
2:B:832:ALA:HB1	2:B:833:PRO:HD2	2.04	0.40
2:A:349:THR:CG2	2:A:350:PRO:HD2	2.52	0.40
2:B:173:VAL:HG12	2:B:360:TRP:CZ2	2.55	0.40
2:A:727:THR:HA	2:A:730:ARG:HG2	2.02	0.40
2:B:738:LEU:CD1	2:B:738:LEU:N	2.84	0.40
2:B:67:LYS:O	2:B:70:ARG:HB3	2.20	0.40
2:A:721:ALA:HB3	2:A:754:PRO:HG2	2.03	0.40
2:B:38:ILE:HG22	2:B:76:TRP:CD1	2.56	0.40
2:A:415:TRP:HB2	2:A:424:ASN:HB2	2.03	0.40
2:A:393:TRP:HE3	2:A:394:LEU:HD23	1.87	0.40
2:A:313:ASP:HB3	2:A:316:GLU:HB3	2.03	0.40
1:C:916:C:H4'	1:C:959:U:O2	2.22	0.40
2:A:429:GLU:OE1	2:A:429:GLU:N	2.54	0.40
2:B:326:ARG:HG3	2:B:327:GLU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LYS:HD3	2:B:138:TRP:CZ2	2.56	0.40
2:A:559:ALA:O	2:A:631:ALA:HB2	2.21	0.40
2:A:270:LYS:HZ3	2:A:270:LYS:CB	2.35	0.40
2:A:44:ASN:ND2	3:A:990:VAA:N3S	2.69	0.40
1:D:934:A:C6	2:B:650:LEU:HD23	2.55	0.40
2:A:717:ARG:HB2	2:A:717:ARG:NH1	2.37	0.40
2:B:170:PRO:O	2:B:171:ARG:O	2.40	0.40
1:C:960:C:O2'	1:C:961:C:H5'	2.21	0.40
1:D:926:C:O2'	1:D:927:U:H5'	2.21	0.40
2:A:700:LEU:HA	2:A:703:GLU:HG2	2.04	0.40
2:B:713:GLU:H	2:B:713:GLU:CD	2.25	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:742:GLN:OE1	2:A:742:GLN:OE1[7_555]	2.19	0.01

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	
2	A	860/862 (100%)	683 (79%)	141 (16%)	36 (4%)	3	13
2	B	860/862 (100%)	670 (78%)	139 (16%)	51 (6%)	2	6
All	All	1720/1724 (100%)	1353 (79%)	280 (16%)	87 (5%)	2	9

All (87) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	106	GLY
2	A	171	ARG

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Mol	Chain	Res	Type
2	A	243	ALA
2	A	257	ASP
2	A	312	LEU
2	A	313	ASP
2	A	362	ARG
2	A	409	GLY
2	A	473	THR
2	A	594	GLU
2	B	162	HIS
2	B	165	LEU
2	B	203	GLU
2	B	243	ALA
2	B	246	PRO
2	B	247	LEU
2	B	249	GLU
2	B	312	LEU
2	B	313	ASP
2	B	409	GLY
2	B	431	TYR
2	B	489	TYR
2	B	594	GLU
2	B	711	ARG
2	A	45	VAL
2	A	102	ARG
2	A	332	VAL
2	A	451	ASP
2	A	489	TYR
2	B	2	ASP
2	B	10	LYS
2	B	45	VAL
2	B	267	GLY
2	B	307	GLU
2	B	429	GLU
2	B	435	PRO
2	B	462	TRP
2	B	473	THR
2	B	627	ALA
2	B	710	GLY
2	A	86	ALA
2	A	170	PRO
2	A	287	GLY
2	A	429	GLU

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Mol	Chain	Res	Type
2	A	711	ARG
2	B	3	LEU
2	B	99	GLY
2	B	137	ASP
2	B	161	TYR
2	B	180	GLU
2	B	208	GLY
2	B	308	ALA
2	B	362	ARG
2	B	569	LEU
2	A	3	LEU
2	A	169	ALA
2	A	308	ALA
2	A	523	ASP
2	B	171	ARG
2	B	714	GLU
2	B	754	PRO
2	A	137	ASP
2	A	431	TYR
2	A	462	TRP
2	A	713	GLU
2	B	170	PRO
2	B	391	MET
2	B	480	TYR
2	B	481	PRO
2	B	600	GLU
2	B	673	ALA
2	B	719	PHE
2	A	144	THR
2	A	267	GLY
2	A	834	LYS
2	B	234	ARG
2	B	767	ARG
2	A	428	PRO
2	A	709	GLY
2	B	428	PRO
2	B	24	PRO
2	B	382	VAL
2	B	426	PRO
2	A	208	GLY
2	A	265	GLY
2	A	784	PRO

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Mol	Chain	Res	Type
2	B	265	GLY

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	
2	A	724/724 (100%)	640 (88%)	84 (12%)	7	20
2	B	724/724 (100%)	632 (87%)	92 (13%)	5	16
All	All	1448/1448 (100%)	1272 (88%)	176 (12%)	6	18

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	ASP
2	A	19	LYS
2	A	28	ASN
2	A	30	LYS
2	A	48	SER
2	A	51	MET
2	A	104	ASP
2	A	105	LEU
2	A	113	ARG
2	A	118	LYS
2	A	119	GLU
2	A	147	GLU
2	A	168	ARG
2	A	170	PRO
2	A	172	LEU
2	A	174	ASN
2	A	187	GLU
2	A	191	GLU
2	A	197	LEU
2	A	198	TYR
2	A	202	TYR
2	A	209	PHE

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Mol	Chain	Res	Type
2	A	212	ILE
2	A	216	ARG
2	A	218	GLU
2	A	242	ARG
2	A	245	ILE
2	A	261	GLU
2	A	269	LEU
2	A	270	LYS
2	A	276	ASP
2	A	291	VAL
2	A	292	SER
2	A	301	GLU
2	A	323	GLU
2	A	332	VAL
2	A	347	CYS
2	A	356	PHE
2	A	368	GLU
2	A	382	VAL
2	A	388	LYS
2	A	390	ASN
2	A	396	ASN
2	A	400	TRP
2	A	401	ASN
2	A	408	TRP
2	A	412	ILE
2	A	420	CYS
2	A	421	GLN
2	A	429	GLU
2	A	431	TYR
2	A	432	LEU
2	A	448	ARG
2	A	461	LEU
2	A	479	PHE
2	A	489	TYR
2	A	494	LEU
2	A	498	ARG
2	A	512	PHE
2	A	521	VAL
2	A	522	LEU
2	A	560	THR
2	A	570	ARG
2	A	580	ASN

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Mol	Chain	Res	Type
2	A	592	SER
2	A	593	ARG
2	A	604	THR
2	A	616	ARG
2	A	679	LEU
2	A	711	ARG
2	A	727	THR
2	A	732	LEU
2	A	738	LEU
2	A	743	GLU
2	A	746	VAL
2	A	759	LEU
2	A	767	ARG
2	A	774	ARG
2	A	777	LYS
2	A	783	MET
2	A	800	GLU
2	A	805	GLN
2	A	830	GLU
2	A	834	LYS
2	B	2	ASP
2	B	5	LYS
2	B	30	LYS
2	B	77	LEU
2	B	88	GLN
2	B	107	ARG
2	B	113	ARG
2	B	118	LYS
2	B	147	GLU
2	B	149	ARG
2	B	151	ARG
2	B	172	LEU
2	B	178	ARG
2	B	180	GLU
2	B	181	THR
2	B	191	GLU
2	B	192	PRO
2	B	198	TYR
2	B	201	ARG
2	B	202	TYR
2	B	205	GLU
2	B	209	PHE

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Mol	Chain	Res	Type
2	B	212	ILE
2	B	218	GLU
2	B	246	PRO
2	B	247	LEU
2	B	266	THR
2	B	270	LYS
2	B	276	ASP
2	B	280	TYR
2	B	284	GLU
2	B	291	VAL
2	B	301	GLU
2	B	339	ILE
2	B	346	ARG
2	B	356	PHE
2	B	372	LYS
2	B	388	LYS
2	B	390	ASN
2	B	401	ASN
2	B	404	ARG
2	B	412	ILE
2	B	413	PRO
2	B	420	CYS
2	B	421	GLN
2	B	429	GLU
2	B	430	ARG
2	B	431	TYR
2	B	432	LEU
2	B	435	PRO
2	B	441	CYS
2	B	445	ARG
2	B	447	LYS
2	B	448	ARG
2	B	461	LEU
2	B	477	LYS
2	B	494	LEU
2	B	498	ARG
2	B	504	TYR
2	B	507	MET
2	B	510	ARG
2	B	512	PHE
2	B	522	LEU
2	B	525	LYS

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Mol	Chain	Res	Type
2	B	545	ARG
2	B	560	THR
2	B	570	ARG
2	B	580	ASN
2	B	587	ARG
2	B	593	ARG
2	B	600	GLU
2	B	604	THR
2	B	608	ARG
2	B	679	LEU
2	B	727	THR
2	B	732	LEU
2	B	745	ARG
2	B	755	VAL
2	B	767	ARG
2	B	769	ASP
2	B	770	LEU
2	B	771	LEU
2	B	777	LYS
2	B	783	MET
2	B	802	ARG
2	B	805	GLN
2	B	808	ARG
2	B	809	LEU
2	B	820	GLN
2	B	831	LYS
2	B	836	VAL
2	B	860	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	28	ASN
2	A	50	HIS
2	A	60	GLN
2	A	224	GLN
2	A	229	HIS
2	A	358	GLN
2	A	390	ASN
2	A	401	ASN
2	A	424	ASN
2	A	505	HIS

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Mol	Chain	Res	Type
2	A	518	HIS
2	A	580	ASN
2	A	584	ASN
2	A	680	HIS
2	A	692	GLN
2	A	724	GLN
2	A	860	GLN
2	B	50	HIS
2	B	60	GLN
2	B	229	HIS
2	B	358	GLN
2	B	390	ASN
2	B	421	GLN
2	B	424	ASN
2	B	518	HIS
2	B	527	GLN
2	B	580	ASN
2	B	584	ASN
2	B	663	HIS
2	B	692	GLN
2	B	724	GLN
2	B	805	GLN
2	B	820	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	22 (29%)	9 (12%)
1	D	74/75 (98%)	28 (37%)	9 (12%)
All	All	148/150 (98%)	50 (33%)	18 (12%)

All (50) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	907	C
1	C	908	U
1	C	910	G
1	C	916	C
1	C	917	G
1	C	918	G
1	C	919	A

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Mol	Chain	Res	Type
1	C	920	A
1	C	929	G
1	C	931	C
1	C	932	U
1	C	934	A
1	C	936	A
1	C	937	C
1	C	938	G
1	C	947	C
1	C	958	G
1	C	959	U
1	C	960	C
1	C	966	C
1	C	974	C
1	C	975	A
1	D	903	G
1	D	908	U
1	D	909	A
1	D	910	G
1	D	916	C
1	D	917	G
1	D	918	G
1	D	919	A
1	D	920	A
1	D	921	G
1	D	930	C
1	D	931	C
1	D	932	U
1	D	933	C
1	D	936	A
1	D	937	C
1	D	938	G
1	D	946	U
1	D	947	C
1	D	948	G
1	D	952	G
1	D	957	A
1	D	958	G
1	D	959	U
1	D	960	C
1	D	966	C
1	D	974	C

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Mol	Chain	Res	Type
1	D	975	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	907	C
1	C	909	A
1	C	917	G
1	C	931	C
1	C	936	A
1	C	937	C
1	C	947	C
1	C	957	A
1	C	959	U
1	D	907	C
1	D	909	A
1	D	916	C
1	D	917	G
1	D	936	A
1	D	937	C
1	D	947	C
1	D	957	A
1	D	959	U

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	VAA	A	990	-	25,32,32	3.59	11 (44%)	27,48,48	1.88	6 (22%)
3	VAA	B	991	-	25,32,32	3.71	9 (36%)	27,48,48	2.10	5 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VAA	A	990	-	-	0/17/39/39	0/3/3/3
3	VAA	B	991	-	-	0/17/39/39	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	990	VAA	C5'-N5'	-7.61	1.32	1.47
3	B	991	VAA	C5'-N5'	-7.39	1.33	1.47
3	A	990	VAA	C5'-C4'	-4.36	1.41	1.51
3	A	990	VAA	C8-N7	-3.15	1.28	1.34
3	B	991	VAA	C8-N7	-2.62	1.29	1.34
3	A	990	VAA	C3'-C2'	-2.16	1.47	1.53
3	B	991	VAA	C3'-C2'	-2.10	1.47	1.53
3	A	990	VAA	C2-N3	2.29	1.36	1.32
3	B	991	VAA	C2-N3	2.41	1.36	1.32
3	A	990	VAA	O2S-S	3.43	1.47	1.43
3	B	991	VAA	C4-N3	3.44	1.40	1.35
3	A	990	VAA	C4-N3	3.54	1.40	1.35
3	B	991	VAA	S-N3S	4.95	1.74	1.63
3	A	990	VAA	O4'-C1'	5.03	1.47	1.41
3	A	990	VAA	S-N3S	5.22	1.74	1.63
3	B	991	VAA	O4'-C1'	5.41	1.48	1.41
3	A	990	VAA	S-N5'	7.72	1.69	1.61
3	A	990	VAA	O1S-S	8.43	1.53	1.43
3	B	991	VAA	O1S-S	8.64	1.53	1.43
3	B	991	VAA	S-N5'	10.63	1.72	1.61

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	991	VAA	O2S-S-O1S	-6.31	109.75	120.04
3	A	990	VAA	O2S-S-O1S	-5.33	111.34	120.04
3	B	991	VAA	C1'-N9-C4	-4.37	120.36	126.94
3	A	990	VAA	C-N3S-S	-3.45	119.22	124.05
3	B	991	VAA	C-N3S-S	-3.28	119.45	124.05
3	A	990	VAA	C1'-N9-C4	-3.01	122.39	126.94
3	A	990	VAA	N3-C2-N1	-2.42	127.04	128.89
3	A	990	VAA	C4'-C5'-N5'	-2.40	107.48	112.56
3	B	991	VAA	N3-C2-N1	-2.08	127.30	128.89
3	A	990	VAA	O-C-N3S	2.02	125.15	121.62
3	B	991	VAA	O4'-C1'-N9	4.10	116.67	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	990	VAA	5	0
3	B	991	VAA	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

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

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

6.3 Carbohydrates (i)

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

6.4 Ligands (i)

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

6.5 Other polymers (i)

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