



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 09:07 PM GMT

PDB ID : 1GAX
Title : CRYSTAL STRUCTURE OF THERMUS THERMOPHILUS VALYL-
TRNA SYNTHETASE COMPLEXED WITH TRNA(VAL) AND VALYL-
ADENYLATE ANALOGUE
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Deposited on : 2000-06-23
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

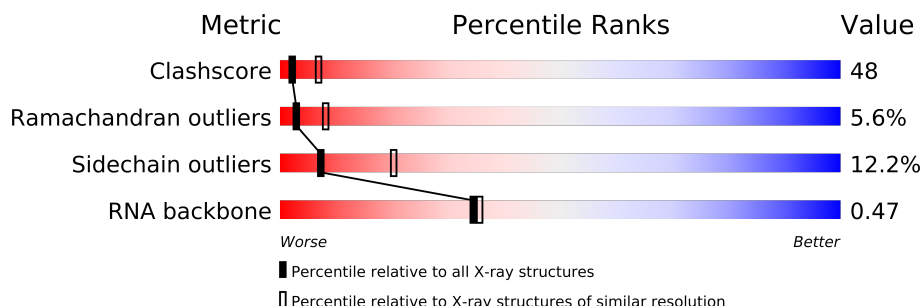
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	75	
1	D	75	
2	A	862	
2	B	862	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17368 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

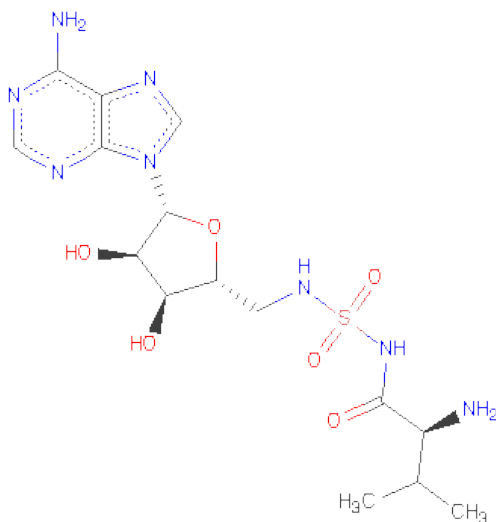
- Molecule 2 is a protein called VALYL-TRNA SYNTHETASE.

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Zn	0	0
			2	2		
3	A	2	Total	Zn	0	0
			2	2		

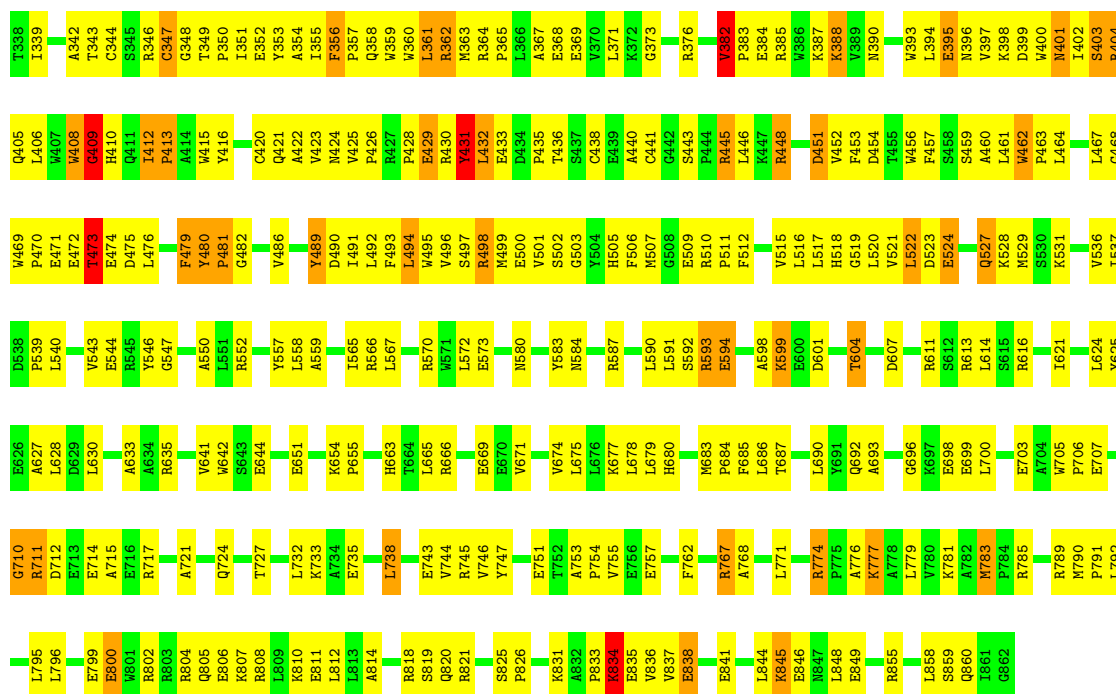
- Molecule 4 is N-[VALINYLYL]-N'-[ADENOSYL]-DIAMINOSUFONE (three-letter code: VAA) (formula: C₁₅H₂₄N₈O₆S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	67	Total	O	0	0
			67	67		
5	B	61	Total	O	0	0
			61	61		
5	C	19	Total	O	0	0
			19	19		
5	D	11	Total	O	0	0
			11	11		



• Molecule 2: VALYL-TRNA SYNTHETASE

Chain B:

Q860	W790	E639	R789	E644	E649	E654	E661	E669	E670	E671	E675	E676	E677	E678	E679	E680	E681	E682	E683	E684	E685	E686	E687	E688	E689	E690	E691	E692	E693	E696	E697	E698	E699	E700	P706	E707	E708	E709	G710																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
T861	P791	E713	R791	E716	E721	E724	E726	E736	E737	E738	E744	E745	E751	E752	E753	E754	E759	E763	E767	E768	E769	E770	E771	E772	E773	E774	E777	E778	E779	E780	E781	E782	E783	E784	E785	E786																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G862	L792	E714	L792	A715	R717	Q724	W726	T727	R730	A731	L732	K733	A734	E735	A736	G737	L738	P739	P740	V744	R745	E751	T752	P754	L759	R763	R767	A768	D769	L770	L771	P772	E773	R774	K777	A778	L779	V780	K781	A782	W783	P784	R785	V786																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
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4 Data and refinement statistics

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)	30.00 – 2.90	Depositor
% Data completeness (in resolution range)	96.5 (30.00-2.90)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.272	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17368	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.47	1/1791 (0.1%)	0.78	0/2789
1	D	0.46	1/1791 (0.1%)	0.78	1/2789 (0.0%)
2	A	0.44	0/7143	0.69	3/9678 (0.0%)
2	B	0.43	0/7143	0.68	2/9678 (0.0%)
All	All	0.44	2/17868 (0.0%)	0.71	6/24934 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	901	G	OP3-P	-7.02	1.52	1.61
1	D	901	G	OP3-P	-6.91	1.52	1.61

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	172	LEU	CA-CB-CG	7.55	132.66	115.30
1	D	936	A	N9-C1'-C2'	6.97	123.06	114.00
2	B	382	VAL	C-N-CD	5.74	140.45	128.40
2	B	409	GLY	N-CA-C	5.50	126.84	113.10
2	A	409	GLY	N-CA-C	5.13	125.93	113.10
2	A	382	VAL	C-N-CD	5.06	139.03	128.40

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1603	0	816	67	0
1	D	1603	0	816	66	0
2	A	6970	0	6943	728	0
2	B	6970	0	6942	751	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	30	0	24	3	0
4	B	30	0	24	4	0
5	A	67	0	0	13	0
5	B	61	0	0	17	0
5	C	19	0	0	0	0
5	D	11	0	0	1	0
All	All	17368	0	15565	1571	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 48.

All (1571) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:777:LYS:H	2:B:777:LYS:HE3	1.06	1.18
2:B:201:ARG:HE	2:B:211:GLU:HB3	1.02	1.17
2:A:102:ARG:HH21	2:A:104:ASP:HA	1.04	1.16
2:A:382:VAL:HG11	2:A:516:LEU:HD12	1.19	1.16
2:A:28:ASN:HD21	2:A:30:LYS:HG2	1.05	1.13
2:B:382:VAL:HG23	2:B:383:PRO:CD	1.78	1.12
2:A:382:VAL:HG23	2:A:383:PRO:HD3	1.27	1.12
2:A:382:VAL:HG23	2:A:383:PRO:CD	1.81	1.11
2:B:382:VAL:HG23	2:B:383:PRO:HD3	1.28	1.10
2:B:388:LYS:H	2:B:388:LYS:HE2	1.12	1.08
2:A:777:LYS:H	2:A:777:LYS:HD3	1.18	1.07
2:A:494:LEU:H	2:A:494:LEU:HD23	1.16	1.05
2:A:171:ARG:HH22	2:A:364:ARG:NH2	1.56	1.02
2:A:448:ARG:HD3	2:A:448:ARG:H	1.24	1.01
2:A:102:ARG:NH2	2:A:104:ASP:HA	1.76	1.01
1:D:975:A:H3'	2:B:215:VAL:HG23	1.41	1.01
2:B:225:ALA:HA	2:B:252:ILE:HG23	1.41	1.00
1:C:928:C:H2'	1:C:929:G:H5''	1.42	0.99
2:A:220:VAL:HG12	2:A:270:LYS:HZ3	1.24	0.99

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:855:ARG:HH22	2:B:810:LYS:HE3	1.27	0.99
2:A:50:HIS:HD2	2:A:52:GLY:H	1.05	0.99
2:B:448:ARG:HD3	2:B:448:ARG:H	1.27	0.97
2:A:282:ILE:HA	2:A:285:ARG:HD3	1.45	0.97
2:A:225:ALA:HA	2:A:252:ILE:HG23	1.44	0.97
1:C:971:C:H2'	1:C:972:A:H5''	1.45	0.97
2:B:201:ARG:HD3	2:B:332:VAL:HG21	1.47	0.96
2:A:172:LEU:HB3	2:A:355:ILE:HD13	1.44	0.96
2:B:248:THR:HG23	2:B:250:VAL:H	1.27	0.95
2:B:5:LYS:HD2	2:B:5:LYS:H	1.28	0.94
2:B:785:ARG:HA	2:B:785:ARG:HH11	1.32	0.94
2:A:5:LYS:H	2:A:5:LYS:HD2	1.31	0.94
2:B:201:ARG:NE	2:B:211:GLU:HB3	1.83	0.94
2:B:201:ARG:HH11	2:B:332:VAL:HG11	1.31	0.94
2:A:37:VAL:HG21	2:A:479:PHE:HB2	1.50	0.93
2:B:494:LEU:HD23	2:B:494:LEU:H	1.30	0.93
2:A:178:ARG:HG2	2:A:347:CYS:SG	2.08	0.93
2:A:95:LEU:HD22	2:A:95:LEU:H	1.34	0.92
1:C:932:U:HO2'	1:C:933:C:H5	0.97	0.92
2:B:102:ARG:NH2	2:B:104:ASP:HA	1.83	0.92
2:B:777:LYS:N	2:B:777:LYS:HE3	1.85	0.91
2:A:28:ASN:ND2	2:A:30:LYS:HG2	1.83	0.91
2:B:245:ILE:HB	2:B:248:THR:CG2	2.01	0.91
2:A:388:LYS:NZ	2:A:388:LYS:H	1.67	0.91
2:B:382:VAL:HG11	2:B:516:LEU:HD12	1.51	0.91
2:A:281:GLU:O	2:A:285:ARG:HG3	1.69	0.91
2:B:361:LEU:HD12	2:B:402:ILE:HD11	1.51	0.91
2:B:789:ARG:HB2	2:B:789:ARG:NH1	1.86	0.90
2:B:412:ILE:HD12	2:B:413:PRO:HD2	1.54	0.90
2:B:282:ILE:HA	2:B:285:ARG:HD3	1.52	0.90
2:B:745:ARG:HH11	2:B:745:ARG:HB3	1.36	0.89
2:B:275:HIS:HE1	2:B:294:ILE:HB	1.34	0.89
2:A:382:VAL:CG2	2:A:383:PRO:HD3	2.01	0.89
1:C:928:C:C2'	1:C:929:G:H5''	2.02	0.89
2:B:295:ASN:HD21	2:B:299:ARG:HB2	1.38	0.89
2:A:178:ARG:HB2	2:A:178:ARG:HH11	1.38	0.88
2:B:248:THR:HG23	2:B:249:GLU:N	1.89	0.88
2:B:382:VAL:CG2	2:B:383:PRO:HD3	2.04	0.88
2:A:494:LEU:H	2:A:494:LEU:CD2	1.86	0.88
2:B:382:VAL:HG22	2:B:516:LEU:HA	1.53	0.88
2:A:388:LYS:N	2:A:388:LYS:HZ2	1.71	0.88
2:B:777:LYS:CE	2:B:777:LYS:H	1.85	0.87

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:178:ARG:HB2	2:A:178:ARG:NH1	1.89	0.87
2:B:529:MET:HE2	2:B:537:ILE:N	1.88	0.87
2:B:558:LEU:HA	5:B:2020:HOH:O	1.74	0.87
2:A:388:LYS:HZ2	2:A:388:LYS:H	0.90	0.87
2:B:245:ILE:HB	2:B:248:THR:HG21	1.56	0.87
2:A:248:THR:HG23	2:A:250:VAL:H	1.39	0.87
2:A:186:LEU:H	2:A:186:LEU:HD12	1.40	0.86
2:A:382:VAL:CG2	2:A:516:LEU:HA	2.05	0.85
2:B:499:MET:CE	2:B:512:PHE:HE2	1.89	0.85
2:A:680:HIS:HA	2:A:687:THR:HG21	1.58	0.85
1:D:902:G:H3'	1:D:903:G:H5''	1.57	0.84
2:A:83:ALA:HB1	2:A:86:ALA:HB3	1.58	0.84
1:D:901:G:N2	1:D:972:A:H1'	1.91	0.84
2:B:93:ARG:HD2	2:B:94:LEU:HG	1.59	0.84
1:D:918:G:O6	2:B:833:PRO:HD3	1.77	0.84
2:B:680:HIS:HA	2:B:687:THR:HG21	1.60	0.84
2:B:277:PRO:HD3	2:B:353:TYR:CE2	2.13	0.84
2:B:159:ARG:O	2:B:163:GLU:HG3	1.78	0.84
2:A:326:ARG:HG3	2:A:327:GLU:N	1.90	0.83
2:B:352:GLU:HG2	2:B:353:TYR:H	1.43	0.83
2:B:382:VAL:CG2	2:B:516:LEU:HA	2.08	0.83
2:B:388:LYS:HE2	2:B:388:LYS:N	1.93	0.83
2:B:307:GLU:C	2:B:309:LEU:H	1.79	0.83
2:A:460:ALA:HB2	2:A:498:ARG:HB3	1.60	0.83
2:A:777:LYS:HD3	2:A:777:LYS:N	1.93	0.83
2:A:371:LEU:HD21	2:A:394:LEU:HB2	1.58	0.83
2:B:246:PRO:O	2:B:247:LEU:HB2	1.76	0.83
2:B:361:LEU:HD21	2:B:366:LEU:HD11	1.58	0.83
2:A:382:VAL:HG22	2:A:516:LEU:HA	1.61	0.82
2:A:282:ILE:HA	2:A:285:ARG:CD	2.09	0.82
2:A:169:ALA:HB1	2:A:170:PRO:HD2	1.61	0.82
2:A:51:MET:HE3	2:A:537:ILE:HB	1.60	0.82
2:A:448:ARG:HD3	2:A:448:ARG:N	1.93	0.82
2:A:358:GLN:HE22	2:A:405:GLN:HE22	1.27	0.82
2:B:47:GLY:H	2:B:117:TRP:HZ2	1.24	0.82
2:A:224:GLN:NE2	2:A:304:ARG:HH22	1.78	0.81
2:B:281:GLU:O	2:B:285:ARG:HG3	1.78	0.81
2:A:277:PRO:HD3	2:A:353:TYR:CE2	2.14	0.81
2:B:753:ALA:HB3	2:B:754:PRO:HD3	1.63	0.81
2:B:778:ALA:HB1	2:B:790:MET:O	1.80	0.81
2:B:418:GLU:OE1	2:B:445:ARG:HD2	1.80	0.81
2:A:289:LYS:HD3	2:A:289:LYS:H	1.43	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:438:CYS:SG	2:A:440:ALA:HB3	2.21	0.80
2:B:789:ARG:HB2	2:B:789:ARG:HH11	1.44	0.80
2:A:810:LYS:HE3	2:B:855:ARG:HH22	1.44	0.80
2:B:529:MET:HE2	2:B:537:ILE:H	1.47	0.80
2:A:326:ARG:HB3	2:A:331:LEU:HD23	1.61	0.80
2:B:248:THR:CG2	2:B:250:VAL:H	1.94	0.80
2:A:326:ARG:HG3	2:A:327:GLU:H	1.43	0.80
2:A:426:PRO:HG3	2:A:435:PRO:HD3	1.63	0.79
2:A:459:SER:O	2:A:495:TRP:HZ3	1.64	0.79
2:A:412:ILE:HA	2:A:453:PHE:HE1	1.47	0.79
2:B:88:GLN:HG3	2:B:406:LEU:HD22	1.64	0.79
2:B:522:LEU:HD23	2:B:528:LYS:HA	1.65	0.79
2:A:855:ARG:NH2	2:B:810:LYS:HE3	1.96	0.79
2:B:745:ARG:HB2	2:B:771:LEU:HD23	1.64	0.78
2:A:834:LYS:HD2	2:A:834:LYS:H	1.48	0.78
2:A:473:THR:CG2	2:A:476:LEU:H	1.95	0.78
2:A:352:GLU:HG2	2:A:353:TYR:H	1.47	0.78
1:C:908:U:H5'	1:C:948:G:OP2	1.84	0.78
2:B:364:ARG:NH2	2:B:398:LYS:HG3	1.99	0.78
2:A:732:LEU:HD13	2:A:781:LYS:HB2	1.63	0.78
1:C:971:C:C2'	1:C:972:A:H5''	2.13	0.78
2:A:47:GLY:H	2:A:117:TRP:HZ2	1.30	0.78
2:B:202:TYR:O	2:B:210:ILE:HG22	1.84	0.78
2:A:521:VAL:HG23	2:A:529:MET:HE3	1.64	0.78
2:B:819:SER:O	2:B:823:LEU:HD23	1.84	0.78
2:A:751:GLU:HB2	2:A:785:ARG:HH21	1.49	0.78
2:A:516:LEU:HD13	2:A:628:LEU:HD13	1.65	0.77
2:B:82:HIS:HB2	2:B:408:TRP:NE1	1.99	0.77
2:A:245:ILE:O	2:A:248:THR:HG22	1.84	0.77
2:A:50:HIS:HD2	2:A:52:GLY:N	1.82	0.77
2:B:805:GLN:H	2:B:805:GLN:HE21	1.31	0.77
2:A:220:VAL:HG12	2:A:270:LYS:NZ	1.99	0.77
2:A:222:ALA:HB2	2:A:293:VAL:HG13	1.67	0.77
2:A:304:ARG:HG3	2:A:304:ARG:HH11	1.48	0.77
2:B:738:LEU:HD23	2:B:744:VAL:HG11	1.67	0.77
2:B:359:TRP:HB2	2:B:403:SER:OG	1.85	0.77
2:A:614:LEU:HD22	2:A:671:VAL:HG13	1.67	0.76
2:A:468:GLY:C	2:A:470:PRO:HD2	2.06	0.76
2:A:245:ILE:CG2	2:A:252:ILE:HD13	2.15	0.76
2:B:358:GLN:HE22	2:B:405:GLN:HE22	1.33	0.76
2:A:680:HIS:HD2	2:A:687:THR:CG2	1.96	0.76
2:A:245:ILE:HG12	2:A:248:THR:CG2	2.15	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:975:A:HG3'	2:B:215:VAL:CG2	2.15	0.75
2:A:50:HIS:CD2	2:A:52:GLY:H	1.97	0.75
2:B:69:MET:HE1	2:B:680:HIS:HB3	1.65	0.75
2:A:412:ILE:HA	2:A:453:PHE:CE1	2.21	0.75
2:A:820:GLN:HG2	2:B:844:LEU:HD23	1.68	0.75
2:B:225:ALA:HA	2:B:252:ILE:CG2	2.16	0.75
2:B:145:MET:HG3	2:B:410:HIS:CD2	2.22	0.75
2:B:7:TYR:CZ	2:B:686:LEU:HD13	2.20	0.75
2:B:91:VAL:O	2:B:96:LEU:HD23	1.86	0.75
2:A:593:ARG:HH11	2:A:593:ARG:HG3	1.51	0.75
2:B:153:VAL:HG23	2:B:154:ARG:N	2.02	0.74
2:B:275:HIS:CE1	2:B:294:ILE:HB	2.20	0.74
2:B:167:TYR:CE2	2:B:360:TRP:HB2	2.21	0.74
2:A:93:ARG:HD2	2:A:94:LEU:HG	1.68	0.74
2:A:473:THR:HG23	2:A:476:LEU:H	1.49	0.74
2:A:202:TYR:HE1	2:A:330:HIS:CG	2.06	0.74
2:A:424:ASN:ND2	2:A:446:LEU:HD21	2.02	0.74
2:B:448:ARG:N	2:B:448:ARG:HD3	2.01	0.74
2:A:235:TYR:O	2:A:236:ARG:HD3	1.87	0.74
2:A:169:ALA:O	2:A:357:PRO:HA	1.88	0.73
2:B:220:VAL:HG12	2:B:270:LYS:HZ3	1.53	0.73
2:B:37:VAL:HG21	2:B:479:PHE:HB2	1.70	0.73
2:B:584:ASN:HA	2:B:587:ARG:HB3	1.68	0.73
2:B:304:ARG:HG3	2:B:304:ARG:HH11	1.52	0.73
2:A:159:ARG:O	2:A:163:GLU:HB2	1.88	0.73
2:B:245:ILE:O	2:B:247:LEU:N	2.21	0.73
2:A:201:ARG:HG2	2:A:211:GLU:HA	1.71	0.73
2:A:436:THR:HA	5:A:1013:HOH:O	1.89	0.73
2:B:143:PHE:HB3	2:B:146:ASP:HB3	1.71	0.73
2:A:66:TYR:O	2:A:70:ARG:HB2	1.88	0.73
2:B:201:ARG:HB3	2:B:211:GLU:HA	1.70	0.72
2:A:85:ILE:O	2:A:89:VAL:HG23	1.89	0.72
2:B:361:LEU:HB2	2:B:402:ILE:CD1	2.19	0.72
2:A:845:LYS:O	2:A:849:GLU:HG3	1.89	0.72
2:A:28:ASN:HD21	2:A:30:LYS:CG	1.94	0.72
2:A:202:TYR:O	2:A:210:ILE:HG22	1.88	0.72
2:A:666:ARG:HG3	2:A:666:ARG:HH11	1.54	0.72
2:B:228:VAL:O	2:B:256:ALA:HA	1.90	0.72
2:A:221:PHE:CE2	2:A:306:PRO:HD3	2.25	0.72
2:A:724:GLN:HE22	2:A:785:ARG:H	1.38	0.72
2:A:494:LEU:N	2:A:494:LEU:HD23	1.98	0.72
1:D:959:U:H5''	1:D:960:C:OP2	1.90	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:178:ARG:HG3	2:A:179:CYS:SG	2.30	0.71
2:A:476:LEU:O	2:A:476:LEU:HD23	1.90	0.71
2:B:280:TYR:O	2:B:284:GLU:HG2	1.90	0.71
2:A:415:TRP:CZ3	2:A:448:ARG:HD2	2.25	0.71
2:B:352:GLU:HG2	2:B:353:TYR:N	2.05	0.71
2:A:557:TYR:CE1	2:A:635:ARG:HB3	2.24	0.71
2:B:494:LEU:CD2	2:B:494:LEU:H	2.02	0.71
2:A:178:ARG:HH11	2:A:178:ARG:CB	2.04	0.71
2:B:501:VAL:HG13	2:B:502:SER:N	2.05	0.71
2:B:745:ARG:HB3	2:B:745:ARG:NH1	2.06	0.71
2:B:13:GLU:HA	2:B:685:PHE:HD2	1.55	0.71
2:A:428:PRO:HB2	2:A:429:GLU:OE1	1.91	0.71
2:A:225:ALA:HA	2:A:252:ILE:CG2	2.19	0.71
2:A:416:TYR:CE2	2:A:423:VAL:HG12	2.25	0.71
2:A:428:PRO:O	2:A:431:TYR:HB3	1.90	0.71
2:B:462:TRP:H	2:B:463:PRO:CD	2.04	0.71
1:D:975:A:H8	2:B:213:ALA:O	1.72	0.71
2:B:480:TYR:O	2:B:482:GLY:N	2.23	0.71
2:A:431:TYR:CE1	2:A:432:LEU:HD12	2.26	0.71
1:D:902:G:C3'	1:D:903:G:H5''	2.20	0.70
2:B:245:ILE:HG13	2:B:252:ILE:HD13	1.71	0.70
2:A:201:ARG:HG2	2:A:211:GLU:HB3	1.71	0.70
2:B:118:LYS:HD3	2:B:143:PHE:CZ	2.27	0.70
2:A:460:ALA:CB	2:A:498:ARG:HB3	2.20	0.70
2:B:248:THR:OG1	2:B:250:VAL:HG23	1.91	0.70
2:B:469:TRP:N	2:B:470:PRO:HD2	2.07	0.70
2:A:501:VAL:HG12	2:A:502:SER:N	2.06	0.70
2:A:245:ILE:HG21	2:A:252:ILE:HD13	1.74	0.70
2:B:201:ARG:HD3	2:B:332:VAL:CG2	2.21	0.70
2:A:171:ARG:HH22	2:A:364:ARG:HH22	1.37	0.70
1:C:957:A:H4'	1:C:958:G:OP1	1.91	0.70
2:B:150:SER:O	2:B:153:VAL:HG22	1.92	0.70
2:B:540:LEU:O	2:B:543:VAL:HG22	1.92	0.70
2:B:173:VAL:C	2:B:174:ASN:HD22	1.95	0.70
2:B:651:GLU:HA	2:B:651:GLU:OE1	1.91	0.70
2:A:45:VAL:HG23	2:A:81:ASP:O	1.92	0.70
2:A:5:LYS:N	2:A:5:LYS:HD2	2.07	0.69
2:B:326:ARG:HG2	2:B:327:GLU:N	2.07	0.69
2:A:518:HIS:HD2	2:A:519:GLY:O	1.73	0.69
2:B:732:LEU:HD13	2:B:781:LYS:HB2	1.73	0.69
2:A:1:MET:HE1	2:A:690:LEU:HD23	1.74	0.69
2:B:41:PRO:HD2	2:B:60:GLN:HE22	1.55	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:77:LEU:H	2:B:77:LEU:HD12	1.57	0.69
2:A:92:GLU:HA	2:A:96:LEU:HD12	1.75	0.69
2:A:331:LEU:HD12	2:A:332:VAL:H	1.58	0.69
2:A:242:ARG:NH1	2:A:251:TRP:HB3	2.06	0.69
2:B:486:VAL:HG22	2:B:516:LEU:HD22	1.75	0.69
2:B:382:VAL:HG11	2:B:516:LEU:CD1	2.20	0.69
2:A:171:ARG:NH2	2:A:364:ARG:NH2	2.38	0.69
2:A:105:LEU:H	2:A:105:LEU:HD23	1.57	0.69
2:B:361:LEU:HB2	2:B:402:ILE:HD11	1.74	0.69
2:B:220:VAL:HG21	2:B:325:PHE:HZ	1.56	0.69
2:B:473:THR:CG2	2:B:476:LEU:H	2.06	0.69
2:B:324:LEU:HD22	2:B:324:LEU:H	1.56	0.69
2:B:473:THR:HG22	2:B:476:LEU:HB3	1.73	0.69
2:A:448:ARG:CD	2:A:448:ARG:H	1.99	0.69
2:A:462:TRP:H	2:A:463:PRO:HD2	1.57	0.68
2:A:93:ARG:CG	2:A:94:LEU:H	2.06	0.68
2:A:777:LYS:H	2:A:777:LYS:CD	2.00	0.68
2:B:371:LEU:HD21	2:B:394:LEU:HB2	1.74	0.68
2:A:224:GLN:HE22	2:A:304:ARG:NH2	1.92	0.68
2:B:248:THR:HG23	2:B:250:VAL:N	2.06	0.68
2:A:441:CYS:SG	2:A:443:SER:HB3	2.32	0.68
2:A:153:VAL:HG23	2:A:154:ARG:N	2.08	0.68
1:C:917:G:O2'	1:C:918:G:OP1	2.11	0.68
2:A:171:ARG:HH22	2:A:364:ARG:HH21	1.40	0.68
1:C:933:C:O5'	1:C:933:C:H6	1.76	0.68
1:D:922:A:H2'	1:D:923:G:C8	2.29	0.68
2:B:680:HIS:CD2	2:B:684:PRO:HA	2.29	0.68
2:A:537:ILE:HD11	2:A:567:LEU:HD22	1.76	0.68
2:A:248:THR:HG23	2:A:250:VAL:N	2.08	0.68
2:A:99:GLY:O	2:A:100:LYS:HG2	1.93	0.68
2:A:343:THR:HB	2:A:348:GLY:O	1.94	0.68
2:A:522:LEU:HD12	2:A:566:ARG:HA	1.75	0.68
2:B:248:THR:HG23	2:B:249:GLU:H	1.57	0.67
2:B:680:HIS:HD2	2:B:687:THR:CG2	2.07	0.67
2:B:260:VAL:HG22	2:B:269:LEU:CD2	2.23	0.67
2:B:382:VAL:HG23	2:B:383:PRO:HD2	1.75	0.67
2:A:304:ARG:HG3	2:A:304:ARG:NH1	2.07	0.67
1:D:922:A:H2'	1:D:923:G:H8	1.60	0.67
2:B:82:HIS:O	2:B:87:THR:OG1	2.11	0.67
2:B:153:VAL:HG21	2:B:410:HIS:ND1	2.08	0.67
2:B:3:LEU:HD21	2:B:590:LEU:HD12	1.75	0.67
2:A:126:LEU:O	2:A:130:LYS:HG2	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:162:HIS:NE2	2:A:425:VAL:O	2.22	0.67
2:A:169:ALA:HB1	2:A:170:PRO:CD	2.24	0.67
2:B:171:ARG:HH12	2:B:364:ARG:HH21	1.41	0.67
2:A:233:GLU:HB2	2:A:237:HIS:HE1	1.60	0.67
2:B:545:ARG:HB3	2:B:546:TYR:CD1	2.30	0.67
2:B:384:GLU:N	5:B:2040:HOH:O	2.28	0.67
2:A:332:VAL:HG22	2:A:333:LYS:N	2.09	0.67
2:A:233:GLU:O	2:A:234:ARG:O	2.12	0.67
2:A:613:ARG:HH21	2:A:644:GLU:HG3	1.59	0.67
2:A:806:GLU:HA	2:A:858:LEU:HD21	1.76	0.67
2:A:497:SER:HA	2:A:500:GLU:OE1	1.94	0.67
2:B:464:LEU:HB3	2:B:469:TRP:HB3	1.77	0.67
2:A:382:VAL:CG2	2:A:517:LEU:H	2.07	0.67
2:A:218:GLU:CD	2:A:318:ARG:HB3	2.15	0.67
2:B:480:TYR:HB3	2:B:481:PRO:HD3	1.77	0.67
2:A:234:ARG:HH22	2:A:267:GLY:H	1.42	0.67
2:B:802:ARG:HG3	2:B:803:ARG:N	2.08	0.67
2:B:404:ARG:HG2	2:B:406:LEU:HD12	1.75	0.67
2:A:167:TYR:CE2	2:A:360:TRP:HB2	2.30	0.67
2:B:270:LYS:HZ2	2:B:270:LYS:CB	2.08	0.67
2:B:245:ILE:HB	2:B:248:THR:HG22	1.74	0.66
2:A:416:TYR:CD2	2:A:423:VAL:HG12	2.31	0.66
2:B:830:GLU:HG2	2:B:831:LYS:NZ	2.10	0.66
2:A:289:LYS:CD	2:A:289:LYS:H	2.08	0.66
2:A:810:LYS:HE3	2:B:855:ARG:NH2	2.10	0.66
2:A:277:PRO:HD3	2:A:353:TYR:CD2	2.29	0.66
2:A:172:LEU:CB	2:A:355:ILE:HD13	2.24	0.66
2:A:93:ARG:HG2	2:A:94:LEU:H	1.61	0.66
2:A:320:LYS:O	2:A:324:LEU:HD23	1.96	0.66
2:B:524:GLU:OE1	2:B:567:LEU:HD23	1.96	0.66
2:A:201:ARG:HG2	2:A:211:GLU:CB	2.25	0.66
2:A:711:ARG:O	2:A:711:ARG:HG3	1.96	0.66
2:B:307:GLU:O	2:B:309:LEU:N	2.29	0.66
2:B:462:TRP:C	2:B:464:LEU:H	1.99	0.66
2:A:248:THR:CG2	2:A:250:VAL:H	2.07	0.66
2:B:468:GLY:C	2:B:470:PRO:HD2	2.16	0.66
2:B:305:VAL:HG13	2:B:310:ARG:HD3	1.78	0.66
2:B:496:VAL:O	2:B:500:GLU:HG3	1.96	0.66
2:B:277:PRO:HD3	2:B:353:TYR:CD2	2.30	0.65
2:A:234:ARG:HG2	2:A:235:TYR:N	2.11	0.65
2:A:153:VAL:HG21	2:A:410:HIS:ND1	2.10	0.65
2:A:224:GLN:NE2	2:A:304:ARG:NH2	2.43	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:45:VAL:HG11	2:A:118:LYS:HA	1.79	0.65
2:A:172:LEU:CD2	2:A:353:TYR:HB3	2.26	0.65
2:B:307:GLU:C	2:B:309:LEU:N	2.50	0.65
2:A:469:TRP:O	2:A:470:PRO:C	2.34	0.65
2:B:832:ALA:HB1	2:B:833:PRO:HD2	1.79	0.65
2:A:358:GLN:HB2	2:A:360:TRP:HE1	1.61	0.65
2:B:237:HIS:H	2:B:238:LEU:HD23	1.62	0.65
2:B:415:TRP:CE3	2:B:448:ARG:HB3	2.32	0.65
2:B:221:PHE:O	2:B:304:ARG:NH1	2.30	0.65
2:B:438:CYS:SG	2:B:440:ALA:HB3	2.36	0.65
2:A:94:LEU:HB2	2:A:95:LEU:HD22	1.78	0.65
1:C:947:C:H2'	1:C:958:G:O2'	1.97	0.65
2:A:845:LYS:NZ	2:B:820:GLN:HE22	1.94	0.65
2:B:501:VAL:HG13	2:B:502:SER:H	1.62	0.65
2:B:349:THR:HG23	2:B:350:PRO:HD2	1.79	0.65
1:D:931:C:H5''	1:D:932:U:OP2	1.97	0.64
1:C:975:A:H3'	2:A:215:VAL:HG22	1.79	0.64
2:B:545:ARG:HD2	2:B:546:TYR:CE1	2.31	0.64
2:A:480:TYR:HB3	2:A:481:PRO:HD3	1.79	0.64
2:A:250:VAL:HG21	2:A:304:ARG:HD2	1.78	0.64
2:A:201:ARG:CD	2:A:211:GLU:HB3	2.27	0.64
2:B:326:ARG:HG2	2:B:327:GLU:H	1.63	0.64
1:C:918:G:O6	2:A:833:PRO:CD	2.45	0.64
1:D:964:C:H2'	1:D:965:G:H8	1.62	0.64
2:A:245:ILE:HG12	2:A:248:THR:HG22	1.79	0.64
2:A:216:ARG:NH1	2:A:314:ARG:HH21	1.96	0.64
2:B:92:GLU:HG3	2:B:102:ARG:HD2	1.78	0.64
2:A:343:THR:HA	2:A:350:PRO:HA	1.78	0.64
2:B:448:ARG:HB2	5:B:2029:HOH:O	1.96	0.64
2:A:242:ARG:HB3	2:A:242:ARG:HH11	1.62	0.64
2:B:260:VAL:HG22	2:B:269:LEU:HD21	1.79	0.64
2:A:314:ARG:NH2	2:A:352:GLU:HG3	2.12	0.64
2:B:412:ILE:HD12	2:B:413:PRO:CD	2.28	0.64
2:B:47:GLY:N	2:B:117:TRP:HZ2	1.96	0.64
2:A:159:ARG:HG3	2:A:159:ARG:HH11	1.63	0.64
2:B:392:ASP:HA	2:B:395:GLU:HB2	1.80	0.64
2:B:126:LEU:HD11	2:B:141:GLU:OE1	1.98	0.64
2:A:93:ARG:O	2:A:94:LEU:C	2.37	0.63
2:B:295:ASN:ND2	2:B:299:ARG:HB2	2.12	0.63
1:D:957:A:H4'	1:D:959:U:H5	1.64	0.63
2:A:216:ARG:HH12	2:A:314:ARG:HH21	1.46	0.63
1:D:901:G:H22	1:D:972:A:H1'	1.63	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:352:GLU:HG2	2:A:353:TYR:N	2.14	0.63
2:B:306:PRO:O	2:B:309:LEU:HB3	1.99	0.63
1:C:920:A:H2'	1:C:945:G:O6	1.97	0.63
2:B:388:LYS:H	2:B:388:LYS:CE	2.00	0.63
2:B:91:VAL:HA	2:B:95:LEU:HD12	1.80	0.63
2:A:289:LYS:HD3	2:A:289:LYS:N	2.13	0.63
2:A:19:LYS:HE2	2:A:699:GLU:OE2	1.98	0.63
2:B:372:LYS:NZ	2:B:372:LYS:HA	2.12	0.63
2:A:202:TYR:HE1	2:A:330:HIS:ND1	1.97	0.63
2:B:651:GLU:OE1	2:B:654:LYS:HE3	1.98	0.63
2:B:591:LEU:O	2:B:594:GLU:HB2	1.99	0.63
2:A:382:VAL:HG21	2:A:516:LEU:HA	1.80	0.63
2:B:654:LYS:HB2	2:B:655:PRO:HD3	1.80	0.63
2:A:522:LEU:HB3	2:A:528:LYS:HA	1.80	0.63
1:C:937:C:O2'	1:C:938:G:OP1	2.15	0.63
2:B:366:LEU:HB3	2:B:501:VAL:CG2	2.28	0.63
2:B:823:LEU:HD12	2:B:829:ARG:NH1	2.14	0.63
2:A:90:VAL:O	2:A:95:LEU:HD23	1.98	0.63
2:B:86:ALA:O	2:B:90:VAL:HG23	1.98	0.63
2:B:372:LYS:HZ3	2:B:372:LYS:HA	1.64	0.63
2:B:293:VAL:HA	2:B:301:GLU:O	1.99	0.63
2:B:593:ARG:HH11	2:B:593:ARG:HG3	1.63	0.63
2:A:95:LEU:CD2	2:A:95:LEU:H	2.10	0.62
2:B:789:ARG:CB	2:B:789:ARG:HH11	2.10	0.62
2:A:420:CYS:HB2	2:A:441:CYS:HB3	1.80	0.62
2:A:178:ARG:HG3	2:A:179:CYS:N	2.14	0.62
2:B:171:ARG:HH12	2:B:364:ARG:NH2	1.97	0.62
2:B:201:ARG:HE	2:B:211:GLU:CB	1.96	0.62
2:A:503:GLY:HA3	2:A:511:PRO:HG3	1.82	0.62
2:A:37:VAL:CG2	2:A:479:PHE:HB2	2.27	0.62
2:B:304:ARG:NH1	2:B:304:ARG:HG3	2.12	0.62
2:B:82:HIS:HB2	2:B:408:TRP:HE1	1.61	0.62
2:A:385:ARG:HB3	5:A:1025:HOH:O	2.00	0.62
2:A:733:LYS:HZ1	2:A:767:ARG:HB3	1.64	0.62
2:A:315:PHE:O	2:A:318:ARG:HG2	2.00	0.62
2:B:785:ARG:HA	2:B:785:ARG:NH1	2.09	0.62
2:A:593:ARG:HG3	2:A:593:ARG:NH1	2.14	0.62
2:B:202:TYR:CE2	2:B:203:GLU:HB2	2.35	0.62
2:B:431:TYR:CE1	2:B:432:LEU:HD22	2.34	0.62
2:B:412:ILE:HA	2:B:453:PHE:CE1	2.34	0.62
2:A:387:LYS:HB3	2:A:388:LYS:NZ	2.15	0.62
2:B:153:VAL:CG2	2:B:154:ARG:H	2.12	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:451:ASP:O	2:A:452:VAL:HG23	2.00	0.62
2:A:95:LEU:O	2:A:99:GLY:HA3	2.00	0.62
2:B:234:ARG:HG3	2:B:234:ARG:HH11	1.64	0.62
2:A:462:TRP:C	2:A:464:LEU:H	2.04	0.62
1:C:973:C:O2	2:A:278:LEU:HD13	2.00	0.62
2:B:153:VAL:CG2	2:B:154:ARG:N	2.62	0.62
2:A:733:LYS:NZ	2:A:767:ARG:HB3	2.14	0.62
2:B:7:TYR:HB2	2:B:583:TYR:CD2	2.36	0.61
2:B:61:ASP:CG	2:B:552:ARG:HH22	2.04	0.61
2:A:221:PHE:CD2	2:A:306:PRO:HD3	2.35	0.61
2:A:85:ILE:O	2:A:88:GLN:HB3	2.00	0.61
2:A:83:ALA:HB3	2:A:87:THR:OG1	2.00	0.61
2:A:51:MET:CE	2:A:537:ILE:HB	2.29	0.61
2:A:807:LYS:O	2:A:811:GLU:HG3	2.00	0.61
2:A:224:GLN:HE22	2:A:304:ARG:HH22	1.46	0.61
2:B:306:PRO:HD2	2:B:309:LEU:HD23	1.82	0.61
2:A:234:ARG:HG2	2:A:235:TYR:H	1.63	0.61
2:B:216:ARG:HA	2:B:318:ARG:NH2	2.15	0.61
1:D:974:C:O2'	1:D:975:A:H5''	2.00	0.61
2:B:492:LEU:HD12	2:B:496:VAL:HB	1.82	0.61
2:A:332:VAL:CG2	2:A:333:LYS:N	2.62	0.61
1:D:937:C:O2'	1:D:938:G:OP1	2.12	0.61
1:D:973:C:H1'	2:B:278:LEU:HB2	1.81	0.61
2:B:102:ARG:HH21	2:B:104:ASP:HA	1.62	0.61
2:B:469:TRP:C	2:B:471:GLU:N	2.49	0.61
2:A:41:PRO:O	2:A:43:PRO:HD3	2.00	0.61
2:B:49:LEU:HD21	2:B:125:ILE:HG23	1.81	0.61
2:A:105:LEU:O	2:A:109:LYS:HB2	2.00	0.61
2:A:808:ARG:NH2	2:A:812:LEU:HD21	2.15	0.61
2:B:441:CYS:SG	2:B:443:SER:HB3	2.40	0.61
2:A:692:GLN:NE2	2:A:698:GLU:HA	2.14	0.61
2:A:837:VAL:HG13	2:A:838:GLU:N	2.16	0.61
1:C:929:G:H5'	1:C:929:G:H8	1.65	0.61
2:A:102:ARG:NE	2:A:102:ARG:O	2.33	0.61
1:C:928:C:C3'	1:C:929:G:H5''	2.31	0.61
2:A:331:LEU:HD12	2:A:332:VAL:N	2.16	0.61
2:A:382:VAL:HG23	2:A:383:PRO:HD2	1.78	0.60
2:A:44:ASN:HB3	2:A:83:ALA:HB2	1.82	0.60
2:B:363:MET:HE3	2:B:363:MET:HA	1.83	0.60
2:B:270:LYS:HZ2	2:B:270:LYS:HB3	1.64	0.60
2:A:201:ARG:HG2	2:A:211:GLU:CA	2.31	0.60
2:A:183:LEU:HD21	2:A:344:CYS:SG	2.41	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:275:HIS:CE1	2:A:294:ILE:HG23	2.36	0.60
2:B:641:VAL:HG22	2:B:675:LEU:HD13	1.82	0.60
2:B:415:TRP:CZ3	2:B:448:ARG:HB3	2.36	0.60
1:C:931:C:H4'	1:C:932:U:OP2	2.00	0.60
2:A:665:LEU:O	2:A:669:GLU:HG3	2.01	0.60
2:B:650:LEU:HD23	2:B:650:LEU:O	2.00	0.60
2:A:312:LEU:HG	2:A:313:ASP:H	1.66	0.60
2:B:724:GLN:HB3	2:B:783:MET:HG2	1.82	0.60
2:A:242:ARG:HH11	2:A:242:ARG:CB	2.12	0.60
2:B:494:LEU:N	2:B:494:LEU:HD23	2.10	0.60
2:B:382:VAL:CG1	2:B:516:LEU:HD12	2.27	0.60
2:A:170:PRO:HA	2:A:356:PHE:O	2.01	0.60
2:A:248:THR:HG21	2:A:250:VAL:HB	1.84	0.60
2:A:424:ASN:HD22	2:A:446:LEU:HD21	1.63	0.60
2:B:361:LEU:CD1	2:B:402:ILE:HD11	2.30	0.60
1:D:920:A:H2'	1:D:945:G:O6	2.02	0.60
2:A:186:LEU:N	2:A:186:LEU:HD12	2.14	0.60
2:B:367:ALA:O	2:B:371:LEU:HG	2.02	0.60
2:B:272:THR:H	2:B:279:ASP:HB3	1.66	0.60
2:A:841:GLU:OE1	2:B:824:ALA:HA	2.00	0.60
2:B:161:TYR:CD1	2:B:425:VAL:HB	2.37	0.60
2:B:40:MET:HA	2:B:60:GLN:HE22	1.67	0.60
2:A:92:GLU:O	2:A:96:LEU:HB2	2.02	0.60
1:C:918:G:N2	1:C:956:A:H1'	2.17	0.60
4:B:1990:VAA:H5'1	4:B:1990:VAA:O	2.01	0.60
2:A:5:LYS:H	2:A:5:LYS:CD	2.09	0.60
2:B:343:THR:HG22	2:B:350:PRO:HA	1.84	0.60
2:A:87:THR:O	2:A:91:VAL:HG23	2.02	0.60
2:B:161:TYR:CE1	2:B:425:VAL:HB	2.37	0.59
2:A:459:SER:O	2:A:495:TRP:CZ3	2.52	0.59
2:A:593:ARG:HG2	2:A:593:ARG:O	2.02	0.59
1:C:964:C:H2'	1:C:965:G:H8	1.66	0.59
2:A:171:ARG:HH12	2:A:364:ARG:HH21	1.49	0.59
2:B:312:LEU:HG	2:B:313:ASP:H	1.65	0.59
2:B:714:GLU:O	2:B:717:ARG:HG2	2.02	0.59
2:A:680:HIS:CD2	2:A:687:THR:CG2	2.81	0.59
2:A:429:GLU:H	2:A:429:GLU:CD	2.04	0.59
2:A:744:VAL:O	2:A:768:ALA:HA	2.02	0.59
2:B:480:TYR:HE2	2:B:509:GLU:HG3	1.67	0.59
2:B:341:LEU:CD1	2:B:343:THR:HG23	2.32	0.59
2:A:221:PHE:HA	2:A:245:ILE:HD11	1.82	0.59
2:B:624:LEU:HD12	2:B:633:ALA:HA	1.85	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:201:ARG:CG	2:A:211:GLU:HB3	2.33	0.59
2:B:220:VAL:HG21	2:B:325:PHE:CZ	2.37	0.59
2:A:155:TYR:HD1	2:A:431:TYR:CD2	2.21	0.59
2:A:118:LYS:O	2:A:118:LYS:HD3	2.01	0.59
1:C:961:C:O2'	1:C:962:U:H5'	2.03	0.59
2:B:834:LYS:O	2:B:838:GLU:HG2	2.03	0.59
2:A:69:MET:HB2	2:A:703:GLU:O	2.03	0.59
2:A:529:MET:HG2	2:A:536:VAL:HG12	1.85	0.59
2:A:361:LEU:HB2	2:A:402:ILE:HD13	1.85	0.59
2:A:592:SER:C	2:A:594:GLU:H	2.04	0.59
2:A:515:VAL:HG12	2:A:517:LEU:HD22	1.84	0.59
2:A:225:ALA:CA	2:A:252:ILE:HG23	2.27	0.59
2:B:13:GLU:HA	2:B:685:PHE:CD2	2.37	0.59
2:B:362:ARG:O	2:B:365:PRO:HD2	2.02	0.59
2:B:153:VAL:HG23	2:B:154:ARG:H	1.65	0.59
2:A:771:LEU:HD11	2:A:791:PRO:HG2	1.83	0.59
2:A:28:ASN:ND2	2:A:30:LYS:H	2.00	0.59
2:A:66:TYR:OH	2:A:70:ARG:NH1	2.35	0.59
2:B:85:ILE:HG23	2:B:86:ALA:N	2.18	0.59
2:A:810:LYS:CE	2:B:855:ARG:HH22	2.16	0.59
2:B:152:ALA:HA	2:B:470:PRO:HB3	1.85	0.59
2:B:387:LYS:HB3	2:B:388:LYS:HZ1	1.68	0.58
2:B:297:GLU:N	2:B:297:GLU:OE2	2.36	0.58
2:B:394:LEU:O	2:B:397:VAL:HG23	2.03	0.58
2:B:805:GLN:H	2:B:805:GLN:NE2	2.00	0.58
2:A:145:MET:HG2	2:A:410:HIS:CD2	2.37	0.58
1:D:964:C:H2'	1:D:965:G:C8	2.37	0.58
2:B:593:ARG:HG3	2:B:593:ARG:NH1	2.15	0.58
2:B:312:LEU:CG	2:B:313:ASP:H	2.16	0.58
2:B:146:ASP:OD1	2:B:149:ARG:HB2	2.02	0.58
2:B:464:LEU:HB3	2:B:469:TRP:CB	2.33	0.58
2:A:624:LEU:HD12	2:A:633:ALA:HA	1.85	0.58
2:A:753:ALA:HB3	2:A:754:PRO:HD3	1.83	0.58
2:B:202:TYR:CG	2:B:203:GLU:N	2.70	0.58
2:B:516:LEU:HD12	2:B:628:LEU:HD13	1.86	0.58
2:B:172:LEU:HD23	2:B:354:ALA:O	2.03	0.58
2:B:270:LYS:CB	2:B:270:LYS:NZ	2.66	0.58
2:B:473:THR:HG22	2:B:476:LEU:CB	2.32	0.58
2:B:178:ARG:HG2	2:B:347:CYS:SG	2.42	0.58
2:A:245:ILE:HG22	2:A:252:ILE:HD13	1.85	0.58
2:A:469:TRP:N	2:A:470:PRO:HD2	2.19	0.58
2:B:312:LEU:HG	2:B:313:ASP:N	2.18	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:385:ARG:HH11	2:A:385:ARG:HG3	1.68	0.58
2:A:346:ARG:HB2	2:A:346:ARG:NH1	2.19	0.58
2:B:217:PRO:O	2:B:220:VAL:HG22	2.04	0.58
2:B:467:LEU:O	2:B:473:THR:HG21	2.03	0.58
2:B:234:ARG:NH1	2:B:235:TYR:HB2	2.18	0.58
2:A:274:ALA:HB2	2:A:291:VAL:H	1.67	0.58
2:B:151:ARG:HG2	2:B:151:ARG:HH11	1.67	0.58
2:B:198:TYR:CD2	2:B:198:TYR:N	2.71	0.58
2:B:225:ALA:CA	2:B:252:ILE:HG23	2.27	0.58
2:B:684:PRO:O	2:B:687:THR:HG22	2.03	0.58
2:B:50:HIS:HD2	2:B:52:GLY:N	2.00	0.58
2:A:248:THR:OG1	2:A:250:VAL:HG23	2.03	0.58
2:A:855:ARG:HD3	2:B:813:LEU:HD12	1.84	0.58
2:B:160:TYR:HE2	2:B:505:HIS:CD2	2.22	0.58
2:A:244:ARG:HB2	2:A:251:TRP:CZ2	2.39	0.58
2:A:224:GLN:O	2:A:225:ALA:HB2	2.04	0.58
2:B:393:TRP:CE3	2:B:394:LEU:HD23	2.39	0.58
2:B:202:TYR:CE2	2:B:244:ARG:NE	2.72	0.58
2:B:480:TYR:O	2:B:481:PRO:C	2.42	0.58
2:B:1:MET:HE3	2:B:693:ALA:HB3	1.86	0.58
2:A:242:ARG:O	2:A:243:ALA:HB2	2.04	0.58
2:B:322:VAL:O	2:B:325:PHE:HB2	2.03	0.58
2:A:367:ALA:O	2:A:371:LEU:HG	2.04	0.58
2:A:358:GLN:NE2	2:A:405:GLN:HE22	1.99	0.58
2:A:153:VAL:CG2	2:A:154:ARG:N	2.66	0.58
2:A:833:PRO:C	2:A:835:GLU:H	2.06	0.58
2:B:83:ALA:HA	2:B:455:THR:HG21	1.85	0.57
1:C:959:U:H5''	1:C:960:C:OP2	2.02	0.57
2:B:151:ARG:HG2	2:B:151:ARG:NH1	2.19	0.57
2:A:64:ILE:HG23	2:A:74:ALA:HB1	1.84	0.57
2:A:280:TYR:O	2:A:284:GLU:HG2	2.03	0.57
2:B:105:LEU:H	2:B:105:LEU:HD23	1.68	0.57
2:B:84:GLY:HA2	2:B:408:TRP:HD1	1.69	0.57
2:A:188:VAL:HG23	2:A:343:THR:O	2.04	0.57
2:B:198:TYR:N	2:B:198:TYR:HD2	2.02	0.57
1:D:973:C:O2	1:D:973:C:H2'	2.04	0.57
2:B:172:LEU:HD21	2:B:353:TYR:HB3	1.85	0.57
2:A:598:ALA:O	2:A:599:LYS:HE2	2.03	0.57
2:A:515:VAL:HG12	2:A:517:LEU:CD2	2.35	0.57
2:B:805:GLN:N	2:B:805:GLN:HE21	2.02	0.57
2:B:286:HIS:HB2	2:B:288:LEU:HD21	1.86	0.57
2:A:486:VAL:HG22	2:A:516:LEU:CD2	2.34	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:488:GLY:O	2:B:490:ASP:N	2.36	0.57
2:A:170:PRO:O	2:A:171:ARG:C	2.42	0.57
2:A:312:LEU:HG	2:A:313:ASP:N	2.20	0.57
2:B:245:ILE:CB	2:B:248:THR:HG22	2.35	0.57
2:A:202:TYR:OH	2:A:244:ARG:CZ	2.52	0.57
2:B:146:ASP:OD2	2:B:149:ARG:NH2	2.33	0.57
2:A:45:VAL:HG12	2:A:121:SER:HB3	1.87	0.57
1:C:918:G:O6	2:A:833:PRO:HD2	2.03	0.57
2:B:830:GLU:C	2:B:831:LYS:HE3	2.24	0.57
4:A:990:VAA:O	4:A:990:VAA:H5'1	2.04	0.57
2:B:666:ARG:NH2	5:B:1993:HOH:O	2.33	0.57
2:B:59:LEU:O	2:B:63:LEU:HD23	2.04	0.57
2:B:409:GLY:HA3	2:B:452:VAL:CG1	2.34	0.57
2:A:382:VAL:O	2:A:383:PRO:C	2.41	0.57
2:A:172:LEU:HB2	2:A:354:ALA:O	2.05	0.57
2:B:248:THR:CG2	2:B:249:GLU:H	2.13	0.57
2:B:87:THR:O	2:B:91:VAL:HG23	2.05	0.57
2:A:453:PHE:CD2	2:A:457:PHE:CD2	2.93	0.57
2:B:469:TRP:O	2:B:470:PRO:C	2.41	0.57
2:A:118:LYS:C	2:A:118:LYS:HD3	2.25	0.57
2:A:3:LEU:HD21	2:A:590:LEU:HD12	1.85	0.57
2:B:677:LYS:HD2	2:B:706:PRO:HG3	1.86	0.57
2:A:383:PRO:O	2:A:384:GLU:HB3	2.04	0.56
2:A:855:ARG:CD	2:B:809:LEU:HD12	2.35	0.56
1:C:932:U:O2	1:C:932:U:H2'	2.05	0.56
2:B:93:ARG:HH11	2:B:93:ARG:HG3	1.70	0.56
2:B:680:HIS:CD2	2:B:687:THR:CG2	2.88	0.56
2:B:287:GLY:C	2:B:288:LEU:HD23	2.25	0.56
2:A:313:ASP:O	2:A:317:ALA:HB2	2.04	0.56
1:D:973:C:C2	2:B:278:LEU:HD13	2.40	0.56
2:A:844:LEU:HD23	2:B:820:GLN:HG2	1.87	0.56
2:B:324:LEU:HD22	2:B:324:LEU:N	2.20	0.56
2:B:603:PRO:HA	2:B:663:HIS:CD2	2.39	0.56
2:B:303:GLU:OE2	2:B:303:GLU:HA	2.04	0.56
2:A:217:PRO:O	2:A:220:VAL:HG13	2.05	0.56
2:B:415:TRP:HB2	2:B:424:ASN:HB2	1.87	0.56
1:C:971:C:C3'	1:C:972:A:H5''	2.35	0.56
2:B:529:MET:HE2	2:B:536:VAL:HA	1.87	0.56
2:A:394:LEU:O	2:A:397:VAL:HG23	2.06	0.56
2:A:238:LEU:HD23	2:A:238:LEU:H	1.71	0.56
2:B:149:ARG:NH1	2:B:465:SER:O	2.36	0.56
2:A:819:SER:HB2	2:A:844:LEU:HD13	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:233:GLU:CD	2:B:234:ARG:N	2.58	0.56
2:A:61:ASP:OD1	2:A:65:ARG:HG3	2.06	0.56
2:A:236:ARG:HA	2:A:238:LEU:CD2	2.35	0.56
1:D:933:C:H3'	1:D:933:C:H6	1.70	0.56
2:B:462:TRP:C	2:B:464:LEU:N	2.57	0.56
2:B:238:LEU:O	2:B:254:ILE:HG21	2.05	0.56
2:A:245:ILE:HG23	2:A:248:THR:HG21	1.88	0.56
2:B:501:VAL:CG1	2:B:502:SER:H	2.19	0.56
2:A:234:ARG:C	2:A:236:ARG:H	2.08	0.56
2:B:188:VAL:HG23	2:B:343:THR:O	2.05	0.56
2:B:726:VAL:HG12	2:B:730:ARG:NH1	2.20	0.56
2:A:393:TRP:CE3	2:A:394:LEU:HD23	2.40	0.56
2:A:229:HIS:CD2	2:A:231:GLU:H	2.24	0.56
2:B:495:TRP:CE3	4:B:1990:VAA:HG21	2.40	0.56
2:B:216:ARG:HA	2:B:318:ARG:HH21	1.70	0.56
2:A:833:PRO:HB2	2:A:836:VAL:HG12	1.88	0.56
2:B:102:ARG:HE	2:B:102:ARG:C	2.06	0.56
2:B:1:MET:HE1	2:B:689:GLU:HG3	1.88	0.56
1:C:973:C:O2'	1:C:974:C:H5''	2.06	0.56
2:B:152:ALA:HB2	2:B:470:PRO:HD3	1.88	0.56
2:A:124:THR:O	2:A:128:GLN:HG3	2.06	0.56
2:A:196:LYS:HB3	2:A:198:TYR:CE1	2.41	0.56
2:B:557:TYR:CE1	2:B:635:ARG:HB3	2.41	0.56
2:B:456:TRP:CE3	2:B:494:LEU:O	2.59	0.55
2:B:103:HIS:O	2:B:104:ASP:C	2.44	0.55
2:B:239:LEU:HA	2:B:254:ILE:HG22	1.87	0.55
1:D:916:C:H5''	1:D:917:G:OP1	2.06	0.55
2:B:266:THR:O	2:B:268:ALA:N	2.40	0.55
2:B:149:ARG:HD3	2:B:465:SER:HB2	1.88	0.55
2:A:234:ARG:CG	2:A:235:TYR:H	2.15	0.55
2:B:361:LEU:HD21	2:B:366:LEU:CD1	2.33	0.55
2:B:322:VAL:HG13	2:B:323:GLU:OE1	2.06	0.55
2:B:85:ILE:HG23	2:B:86:ALA:H	1.71	0.55
2:B:501:VAL:CG1	2:B:502:SER:N	2.69	0.55
2:A:785:ARG:HG3	5:A:1031:HOH:O	2.07	0.55
2:B:193:THR:CG2	2:B:194:PRO:HD2	2.36	0.55
1:C:975:A:C3'	2:A:215:VAL:HG22	2.36	0.55
1:C:973:C:C2	2:A:278:LEU:HD13	2.42	0.55
2:B:257:ASP:OD2	2:B:282:ILE:HG12	2.06	0.55
2:B:792:LEU:HD12	2:B:796:LEU:HD12	1.89	0.55
1:C:974:C:O2'	1:C:975:A:H5''	2.06	0.55
2:A:271:VAL:HG12	2:A:273:PRO:HD3	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:795:LEU:O	2:B:796:LEU:HD23	2.06	0.55
2:A:159:ARG:CG	2:A:159:ARG:HH11	2.18	0.55
2:B:524:GLU:CD	2:B:524:GLU:H	2.10	0.55
1:D:932:U:O2'	1:D:933:C:C5	2.57	0.55
2:B:246:PRO:O	2:B:247:LEU:CB	2.50	0.55
2:B:50:HIS:CD2	2:B:52:GLY:H	2.24	0.55
2:A:205:GLU:HB2	2:A:242:ARG:HB2	1.89	0.54
2:B:232:ASP:OD1	2:B:234:ARG:NE	2.40	0.54
2:B:178:ARG:HE	2:B:178:ARG:HA	1.72	0.54
2:B:587:ARG:HH11	2:B:587:ARG:CG	2.20	0.54
2:B:722:LEU:O	2:B:726:VAL:HG23	2.07	0.54
2:A:310:ARG:HG3	2:A:310:ARG:O	2.07	0.54
2:B:516:LEU:HD13	2:B:628:LEU:HD22	1.89	0.54
2:A:404:ARG:HG2	2:A:406:LEU:HD12	1.89	0.54
2:A:408:TRP:O	2:A:409:GLY:O	2.25	0.54
2:A:415:TRP:O	2:A:424:ASN:N	2.38	0.54
2:B:409:GLY:HA3	2:B:452:VAL:HG13	1.88	0.54
2:A:215:VAL:O	2:A:318:ARG:NH2	2.41	0.54
2:B:298:GLY:O	2:B:314:ARG:HB3	2.08	0.54
1:C:916:C:H5''	1:C:917:G:OP1	2.08	0.54
2:A:724:GLN:HE22	2:A:785:ARG:N	2.05	0.54
2:A:266:THR:O	2:A:268:ALA:N	2.40	0.54
2:B:200:LEU:HD21	2:B:325:PHE:CD1	2.43	0.54
2:A:64:ILE:HG13	2:A:76:TRP:HB2	1.89	0.54
2:A:799:GLU:O	2:A:802:ARG:HB3	2.07	0.54
1:D:927:U:O2'	1:D:928:C:H5'	2.07	0.54
2:B:627:ALA:O	2:B:628:LEU:HB2	2.06	0.54
2:A:246:PRO:O	2:A:247:LEU:HB2	2.06	0.54
2:B:107:ARG:HH11	2:B:107:ARG:HB3	1.71	0.54
2:A:498:ARG:HG2	2:A:498:ARG:HH11	1.72	0.54
1:D:918:G:O6	2:B:833:PRO:CD	2.54	0.54
2:A:326:ARG:HA	2:A:331:LEU:HB3	1.90	0.54
2:B:233:GLU:O	2:B:235:TYR:N	2.41	0.54
2:A:260:VAL:HG22	2:A:269:LEU:HD21	1.89	0.54
2:A:393:TRP:HB2	2:A:493:PHE:CE2	2.43	0.54
1:C:947:C:O2'	1:C:948:G:P	2.65	0.54
2:A:233:GLU:HB2	2:A:237:HIS:CE1	2.41	0.54
2:A:845:LYS:HA	2:A:845:LYS:HE3	1.90	0.54
2:B:830:GLU:HG2	2:B:831:LYS:HZ2	1.72	0.54
1:D:933:C:C6	1:D:933:C:H3'	2.43	0.54
2:A:712:ASP:HB3	2:A:715:ALA:HB3	1.89	0.54
2:B:487:THR:O	2:B:517:LEU:HA	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:366:LEU:HB3	2:B:501:VAL:HG21	1.90	0.53
2:B:680:HIS:HD2	2:B:684:PRO:HA	1.71	0.53
2:B:397:VAL:HG12	2:B:398:LYS:H	1.72	0.53
2:B:358:GLN:NE2	2:B:405:GLN:HE22	2.02	0.53
2:B:341:LEU:C	2:B:341:LEU:HD13	2.27	0.53
2:A:4:PRO:O	2:A:587:ARG:NE	2.41	0.53
2:B:211:GLU:C	2:B:266:THR:HG21	2.28	0.53
1:C:973:C:H1'	2:A:278:LEU:HB2	1.88	0.53
2:A:680:HIS:CD2	2:A:684:PRO:HA	2.44	0.53
2:A:326:ARG:C	2:A:328:ALA:H	2.12	0.53
2:B:543:VAL:HG23	2:B:544:GLU:N	2.23	0.53
2:A:145:MET:HG2	2:A:410:HIS:NE2	2.23	0.53
1:C:922:A:H2'	1:C:923:G:C8	2.43	0.53
2:A:171:ARG:NH2	2:A:364:ARG:HH21	2.04	0.53
2:A:855:ARG:HH22	2:B:810:LYS:CE	2.11	0.53
2:A:476:LEU:C	2:A:476:LEU:HD23	2.28	0.53
2:A:242:ARG:NH1	2:A:251:TRP:CB	2.70	0.53
2:B:202:TYR:HE2	2:B:244:ARG:CD	2.22	0.53
2:A:221:PHE:O	2:A:304:ARG:NH1	2.42	0.53
2:B:245:ILE:O	2:B:248:THR:HG22	2.08	0.53
2:B:785:ARG:CA	2:B:785:ARG:HH11	2.14	0.53
2:A:683:MET:O	2:A:687:THR:CG2	2.57	0.53
2:B:1:MET:HG2	2:B:2:ASP:H	1.72	0.53
2:B:692:GLN:O	2:B:696:GLY:N	2.40	0.53
2:A:307:GLU:C	2:A:309:LEU:H	2.11	0.53
2:A:46:THR:HG22	2:A:90:VAL:HG21	1.89	0.53
2:B:499:MET:HE3	2:B:512:PHE:HE2	1.72	0.53
2:B:383:PRO:HG2	5:B:2016:HOH:O	2.09	0.53
2:A:462:TRP:C	2:A:464:LEU:N	2.62	0.53
2:A:393:TRP:HE3	2:A:394:LEU:HD23	1.74	0.53
2:A:666:ARG:CG	2:A:666:ARG:HH11	2.20	0.53
2:B:428:PRO:O	2:B:431:TYR:HB3	2.07	0.53
2:B:777:LYS:O	2:B:777:LYS:HD2	2.09	0.53
2:B:387:LYS:HB3	2:B:388:LYS:NZ	2.24	0.53
2:A:318:ARG:HA	2:A:321:ALA:HB3	1.91	0.53
2:B:738:LEU:HD23	2:B:744:VAL:CG1	2.38	0.53
2:B:305:VAL:HG22	2:B:310:ARG:HB2	1.90	0.53
2:A:467:LEU:O	2:A:473:THR:HG21	2.09	0.53
2:B:382:VAL:C	2:B:384:GLU:N	2.59	0.53
2:A:186:LEU:H	2:A:186:LEU:CD1	2.16	0.53
2:B:778:ALA:HB1	2:B:790:MET:C	2.29	0.53
2:A:724:GLN:NE2	2:A:785:ARG:HB2	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:462:TRP:H	2:B:463:PRO:HD2	1.73	0.53
2:A:522:LEU:CD1	2:A:566:ARG:HA	2.39	0.53
2:A:131:ARG:O	2:A:131:ARG:HD2	2.09	0.53
2:B:382:VAL:O	2:B:383:PRO:C	2.43	0.52
1:D:973:C:O2'	1:D:974:C:H5''	2.08	0.52
2:A:110:PHE:O	2:A:114:VAL:HG23	2.09	0.52
2:A:239:LEU:HA	2:A:254:ILE:CG2	2.40	0.52
2:B:820:GLN:NE2	2:B:821:ARG:N	2.57	0.52
2:A:376:ARG:HB2	2:A:376:ARG:HH11	1.75	0.52
2:A:59:LEU:HD23	2:A:630:LEU:HD12	1.91	0.52
2:B:5:LYS:CD	2:B:5:LYS:H	2.02	0.52
2:B:352:GLU:HA	5:B:2001:HOH:O	2.09	0.52
2:B:326:ARG:CG	2:B:327:GLU:N	2.72	0.52
2:B:710:GLY:O	2:B:711:ARG:HB3	2.10	0.52
2:B:487:THR:HG23	2:B:517:LEU:CD2	2.39	0.52
2:A:306:PRO:HD2	2:A:309:LEU:HD23	1.90	0.52
2:B:680:HIS:CA	2:B:687:THR:HG21	2.37	0.52
2:B:171:ARG:HH22	2:B:398:LYS:CG	2.21	0.52
2:B:124:THR:O	2:B:128:GLN:HG3	2.09	0.52
2:A:424:ASN:HD22	2:A:446:LEU:CD2	2.23	0.52
2:A:202:TYR:OH	2:A:244:ARG:NH2	2.42	0.52
2:A:332:VAL:HG22	2:A:333:LYS:H	1.74	0.52
2:A:469:TRP:C	2:A:471:GLU:N	2.58	0.52
2:A:239:LEU:HA	2:A:254:ILE:HG22	1.90	0.52
2:A:202:TYR:CE1	2:A:330:HIS:CG	2.94	0.52
2:B:229:HIS:CD2	2:B:231:GLU:H	2.27	0.52
1:D:932:U:HO2'	1:D:933:C:H5	1.50	0.52
2:A:540:LEU:HA	2:A:543:VAL:HG13	1.92	0.52
2:A:97:LYS:HG2	2:A:102:ARG:HB3	1.92	0.52
2:A:387:LYS:HB3	2:A:388:LYS:HZ2	1.73	0.52
2:A:168:ARG:HA	2:A:358:GLN:O	2.10	0.52
2:A:154:ARG:HH11	2:A:154:ARG:HG3	1.75	0.52
2:A:1:MET:CE	2:A:690:LEU:HD23	2.38	0.52
2:B:692:GLN:HE21	2:B:698:GLU:HA	1.75	0.52
2:B:740:PRO:O	2:B:767:ARG:HG2	2.10	0.52
2:A:220:VAL:HG23	2:A:221:PHE:N	2.25	0.52
2:B:687:THR:HG23	2:B:700:LEU:HD23	1.92	0.52
2:B:414:ALA:HA	2:B:425:VAL:HG22	1.92	0.52
2:A:359:TRP:H	2:A:403:SER:HG	1.55	0.52
2:B:501:VAL:C	2:B:503:GLY:H	2.12	0.52
2:A:684:PRO:O	2:A:687:THR:HG22	2.10	0.52
2:B:358:GLN:NE2	2:B:403:SER:HB2	2.25	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:469:TRP:O	2:B:471:GLU:N	2.43	0.52
2:B:155:TYR:HD1	2:B:431:TYR:CD2	2.27	0.52
1:D:940:G:O2'	1:D:941:A:H5'	2.10	0.52
2:B:210:ILE:HG23	2:B:210:ILE:O	2.10	0.52
2:B:382:VAL:O	2:B:384:GLU:N	2.43	0.52
2:A:157:PHE:HD2	2:A:413:PRO:HG2	1.75	0.52
2:B:371:LEU:HD21	2:B:394:LEU:CB	2.39	0.52
2:B:506:PHE:C	2:B:507:MET:HG2	2.29	0.52
2:B:3:LEU:HD11	2:B:590:LEU:CD1	2.40	0.52
2:A:126:LEU:HD11	2:A:141:GLU:OE1	2.10	0.52
2:B:616:ARG:HG2	5:B:2024:HOH:O	2.09	0.52
2:B:114:VAL:HG11	2:B:408:TRP:CE3	2.45	0.52
2:B:162:HIS:NE2	2:B:425:VAL:O	2.40	0.52
2:B:148:LYS:HE2	5:B:2027:HOH:O	2.10	0.52
2:A:181:THR:OG1	2:A:404:ARG:HG3	2.10	0.52
2:A:88:GLN:NE2	2:A:110:PHE:CE2	2.78	0.51
2:B:805:GLN:HB3	2:B:858:LEU:HD21	1.91	0.51
2:A:714:GLU:HG3	2:A:715:ALA:N	2.24	0.51
2:B:614:LEU:CD1	2:B:671:VAL:HG13	2.41	0.51
2:A:306:PRO:HG2	2:A:309:LEU:CB	2.40	0.51
2:A:199:THR:O	2:A:332:VAL:HG13	2.10	0.51
2:A:593:ARG:HB2	2:A:665:LEU:HD21	1.92	0.51
2:A:591:LEU:O	2:A:594:GLU:HB2	2.10	0.51
2:A:486:VAL:HG22	2:A:516:LEU:HD23	1.90	0.51
2:B:529:MET:HG3	2:B:535:ASN:O	2.09	0.51
2:B:819:SER:HB2	2:B:844:LEU:HD13	1.91	0.51
2:A:157:PHE:CD2	2:A:413:PRO:HG2	2.45	0.51
2:A:469:TRP:HB2	2:A:476:LEU:HD12	1.92	0.51
2:A:473:THR:HG23	2:A:475:ASP:N	2.26	0.51
2:B:170:PRO:HA	2:B:356:PHE:O	2.10	0.51
2:A:306:PRO:HG2	2:A:309:LEU:HB3	1.93	0.51
2:B:499:MET:HE2	2:B:512:PHE:HE2	1.75	0.51
2:B:266:THR:C	2:B:268:ALA:H	2.12	0.51
2:A:250:VAL:HG12	2:A:252:ILE:HD12	1.93	0.51
2:B:224:GLN:O	2:B:225:ALA:HB2	2.09	0.51
2:B:408:TRP:O	2:B:409:GLY:O	2.29	0.51
2:B:412:ILE:HG23	2:B:451:ASP:O	2.11	0.51
2:A:160:TYR:HB3	2:A:166:ALA:HB2	1.92	0.51
2:B:731:ALA:O	2:B:734:ALA:HB3	2.10	0.51
2:A:316:GLU:OE1	2:A:316:GLU:HA	2.11	0.51
2:A:103:HIS:O	2:A:104:ASP:C	2.49	0.51
2:B:160:TYR:CE2	2:B:505:HIS:CD2	2.98	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:4:PRO:HD2	2:B:583:TYR:OH	2.11	0.51
2:A:213:ALA:HB3	5:A:1044:HOH:O	2.10	0.51
2:A:312:LEU:CG	2:A:313:ASP:H	2.23	0.51
2:B:467:LEU:O	2:B:473:THR:CG2	2.59	0.51
2:A:56:ASP:O	2:A:60:GLN:HG3	2.11	0.51
2:A:349:THR:HG23	2:A:350:PRO:HD2	1.93	0.51
2:A:480:TYR:O	2:A:482:GLY:N	2.44	0.51
2:B:600:GLU:HG2	2:B:601:ASP:N	2.25	0.51
2:A:738:LEU:HD11	2:A:796:LEU:HD23	1.93	0.51
2:B:90:VAL:O	2:B:95:LEU:HD12	2.10	0.51
2:B:170:PRO:O	2:B:355:ILE:HG23	2.11	0.51
2:B:733:LYS:HG3	2:B:738:LEU:HB2	1.93	0.51
2:B:312:LEU:CG	2:B:313:ASP:N	2.74	0.51
2:B:234:ARG:NH1	2:B:234:ARG:HG3	2.26	0.51
2:A:779:LEU:HD13	2:A:792:LEU:HD21	1.91	0.51
2:A:255:LEU:HD12	2:A:255:LEU:C	2.31	0.51
2:A:383:PRO:O	2:A:384:GLU:CB	2.59	0.51
2:A:172:LEU:HB3	2:A:355:ILE:CD1	2.27	0.51
2:A:222:ALA:HB2	2:A:293:VAL:CG1	2.39	0.51
2:B:593:ARG:HB2	2:B:665:LEU:HD21	1.92	0.51
2:A:13:GLU:HA	2:A:685:PHE:CD2	2.46	0.51
2:A:825:SER:OG	2:A:826:PRO:HD2	2.11	0.51
1:C:931:C:H2'	1:C:931:C:O2	2.10	0.50
2:B:165:LEU:HD13	2:B:366:LEU:HD21	1.93	0.50
2:A:228:VAL:HG12	2:A:229:HIS:O	2.11	0.50
2:B:220:VAL:HG12	2:B:270:LYS:NZ	2.24	0.50
2:A:441:CYS:SG	2:A:443:SER:CB	2.99	0.50
2:B:233:GLU:O	2:B:234:ARG:C	2.49	0.50
2:B:593:ARG:HG2	2:B:593:ARG:O	2.11	0.50
2:A:539:PRO:O	2:A:543:VAL:HG13	2.11	0.50
2:A:382:VAL:CG2	2:A:383:PRO:CD	2.68	0.50
2:B:382:VAL:HG11	2:B:516:LEU:CG	2.41	0.50
2:B:779:LEU:CD1	2:B:792:LEU:HD13	2.41	0.50
2:B:805:GLN:N	2:B:805:GLN:NE2	2.59	0.50
2:B:7:TYR:HB2	2:B:583:TYR:CG	2.46	0.50
2:A:202:TYR:HE2	2:A:244:ARG:HD3	1.74	0.50
2:A:611:ARG:NH1	5:A:1006:HOH:O	2.45	0.50
2:A:176:CYS:SG	2:A:178:ARG:HB3	2.51	0.50
2:A:680:HIS:CA	2:A:687:THR:HG21	2.36	0.50
2:A:469:TRP:O	2:A:469:TRP:CG	2.64	0.50
2:B:807:LYS:O	2:B:811:GLU:HG3	2.12	0.50
2:B:63:LEU:HD11	2:B:628:LEU:HD23	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:84:GLY:HA2	2:B:408:TRP:CD1	2.46	0.50
2:B:85:ILE:O	2:B:88:GLN:HB2	2.12	0.50
2:B:161:TYR:HA	2:B:166:ALA:HB3	1.92	0.50
2:B:37:VAL:HG13	2:B:75:VAL:HB	1.92	0.50
2:A:193:THR:HG23	2:A:194:PRO:HD2	1.94	0.50
2:B:338:THR:O	2:B:338:THR:HG23	2.11	0.50
2:A:297:GLU:N	2:A:297:GLU:OE1	2.43	0.50
2:B:382:VAL:CG2	2:B:383:PRO:CD	2.68	0.50
2:A:680:HIS:CD2	2:A:687:THR:HG21	2.47	0.50
2:A:412:ILE:HB	2:A:453:PHE:CE1	2.46	0.50
2:A:233:GLU:O	2:A:234:ARG:C	2.49	0.50
2:B:220:VAL:O	2:B:223:ASP:HB2	2.12	0.50
2:B:148:LYS:HD2	2:B:468:GLY:HA2	1.94	0.50
1:D:936:A:H1'	1:D:938:G:N7	2.27	0.50
1:C:964:C:H2'	1:C:965:G:C8	2.45	0.50
2:A:859:SER:HB2	2:B:806:GLU:OE1	2.11	0.50
2:A:172:LEU:HD23	2:A:353:TYR:HB3	1.93	0.50
2:A:304:ARG:O	2:A:305:VAL:C	2.50	0.50
2:A:371:LEU:HD21	2:A:394:LEU:CB	2.37	0.50
2:B:7:TYR:CE2	2:B:686:LEU:HD13	2.46	0.50
2:A:474:GLU:HB3	5:A:1056:HOH:O	2.11	0.50
1:D:909:A:H4'	1:D:910:G:OP1	2.10	0.50
2:B:854:ILE:O	2:B:858:LEU:HD23	2.12	0.50
2:B:469:TRP:C	2:B:471:GLU:H	2.13	0.50
2:B:593:ARG:HH11	2:B:593:ARG:CG	2.25	0.50
2:B:498:ARG:HG2	2:B:498:ARG:HH11	1.77	0.50
2:A:157:PHE:HD2	2:A:413:PRO:CG	2.25	0.50
2:B:239:LEU:HA	2:B:254:ILE:CG2	2.42	0.50
2:A:412:ILE:HG13	2:A:413:PRO:HD2	1.93	0.50
2:B:356:PHE:CD2	2:B:357:PRO:HD2	2.47	0.50
2:A:845:LYS:NZ	2:B:820:GLN:NE2	2.59	0.50
2:B:469:TRP:HD1	2:B:507:MET:HE1	1.77	0.50
2:A:747:TYR:CZ	2:A:774:ARG:HB2	2.46	0.50
2:A:456:TRP:CE3	2:A:494:LEU:O	2.65	0.49
2:A:307:GLU:H	2:A:307:GLU:CD	2.14	0.49
2:B:217:PRO:HD2	2:B:318:ARG:NE	2.27	0.49
2:A:153:VAL:CG2	2:A:154:ARG:H	2.25	0.49
2:B:420:CYS:HB2	2:B:441:CYS:HB3	1.94	0.49
2:A:789:ARG:HG2	2:A:789:ARG:HH11	1.77	0.49
2:B:85:ILE:O	2:B:89:VAL:HG23	2.11	0.49
2:B:145:MET:HG3	2:B:410:HIS:NE2	2.27	0.49
2:A:234:ARG:HH22	2:A:267:GLY:N	2.07	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:232:ASP:O	2:B:236:ARG:HG2	2.12	0.49
2:A:433:GLU:HA	5:A:1022:HOH:O	2.12	0.49
1:C:904:C:H2'	1:C:905:G:H8	1.77	0.49
2:A:463:PRO:HD3	2:A:499:MET:SD	2.52	0.49
2:A:257:ASP:OD2	2:A:282:ILE:HB	2.11	0.49
2:B:783:MET:HB2	2:B:786:VAL:O	2.13	0.49
1:C:932:U:C2'	1:C:932:U:O2	2.59	0.49
2:A:247:LEU:HD23	2:A:325:PHE:CE1	2.47	0.49
2:A:228:VAL:HG22	2:A:268:ALA:HB2	1.93	0.49
2:B:469:TRP:N	2:B:470:PRO:CD	2.75	0.49
2:B:41:PRO:HD2	2:B:60:GLN:NE2	2.24	0.49
2:A:105:LEU:HD21	2:A:110:PHE:HD1	1.78	0.49
2:A:845:LYS:HZ2	2:B:820:GLN:HE22	1.60	0.49
1:D:960:C:O2'	1:D:961:C:H5'	2.13	0.49
2:B:113:ARG:HA	2:B:116:GLN:NE2	2.28	0.49
2:B:102:ARG:HH21	2:B:105:LEU:H	1.60	0.49
2:A:491:ILE:O	2:A:495:TRP:HB3	2.12	0.49
2:B:524:GLU:N	2:B:524:GLU:OE2	2.36	0.49
2:A:462:TRP:O	2:A:464:LEU:N	2.46	0.49
2:B:833:PRO:HG2	2:B:836:VAL:HB	1.93	0.49
2:B:549:ASP:OD2	2:B:685:PHE:HB2	2.13	0.49
2:A:753:ALA:O	2:A:757:GLU:HG3	2.13	0.49
2:B:51:MET:HB3	2:B:521:VAL:HG21	1.94	0.49
2:A:494:LEU:N	2:A:494:LEU:CD2	2.62	0.49
2:A:700:LEU:HA	2:A:703:GLU:HG2	1.95	0.49
2:B:45:VAL:O	2:B:117:TRP:NE1	2.42	0.49
2:A:68:ARG:C	2:A:70:ARG:H	2.16	0.49
2:B:473:THR:HG23	2:B:476:LEU:H	1.77	0.49
2:B:827:GLY:O	2:B:831:LYS:HB2	2.13	0.49
2:B:341:LEU:HD11	2:B:343:THR:HG23	1.94	0.49
2:B:799:GLU:HG3	2:B:800:GLU:N	2.28	0.49
2:A:279:ASP:HA	2:A:282:ILE:HG12	1.95	0.49
2:B:370:VAL:HG22	2:B:501:VAL:HA	1.95	0.49
2:B:501:VAL:O	2:B:503:GLY:N	2.46	0.49
2:B:312:LEU:O	2:B:313:ASP:O	2.30	0.49
2:A:844:LEU:O	2:A:848:LEU:HD23	2.13	0.49
2:B:484:VAL:HG12	2:B:486:VAL:HG23	1.94	0.49
2:B:802:ARG:HH11	2:B:802:ARG:HB2	1.78	0.49
2:A:598:ALA:C	2:A:599:LYS:HE2	2.33	0.49
1:C:922:A:H2'	1:C:923:G:H8	1.78	0.49
2:A:543:VAL:CG2	2:A:544:GLU:N	2.76	0.49
2:A:190:THR:HG22	2:A:342:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:935:C:H1'	2:A:584:ASN:ND2	2.28	0.49
2:B:845:LYS:O	2:B:849:GLU:HG3	2.12	0.49
2:B:294:ILE:HD13	2:B:299:ARG:O	2.13	0.49
2:B:314:ARG:HG3	2:B:315:PHE:CD2	2.48	0.49
2:A:150:SER:O	2:A:153:VAL:HG22	2.13	0.49
2:B:3:LEU:HD11	2:B:590:LEU:HD12	1.94	0.49
2:B:771:LEU:HD13	2:B:772:PRO:HD2	1.96	0.48
2:A:680:HIS:HD2	2:A:687:THR:HG23	1.77	0.48
2:A:242:ARG:HH11	2:A:242:ARG:CG	2.26	0.48
2:A:212:ILE:HD11	2:A:268:ALA:C	2.34	0.48
2:B:315:PHE:O	2:B:318:ARG:HB3	2.13	0.48
2:B:802:ARG:NH1	2:B:802:ARG:HB2	2.28	0.48
2:A:227:ALA:HB3	2:A:269:LEU:HG	1.94	0.48
2:B:202:TYR:CD2	2:B:244:ARG:HB3	2.48	0.48
2:B:272:THR:N	2:B:279:ASP:HB3	2.27	0.48
2:A:36:PHE:CD1	2:A:67:LYS:HG3	2.48	0.48
2:B:241:LYS:N	2:B:241:LYS:HD2	2.28	0.48
2:B:102:ARG:O	2:B:103:HIS:C	2.52	0.48
2:B:2:ASP:O	2:B:4:PRO:HD3	2.13	0.48
2:A:200:LEU:HD21	2:A:325:PHE:CD2	2.48	0.48
2:A:429:GLU:OE1	2:A:429:GLU:N	2.46	0.48
2:B:38:ILE:O	2:B:77:LEU:HD12	2.13	0.48
1:D:933:C:C6	1:D:933:C:C3'	2.97	0.48
1:C:965:G:H2'	1:C:966:C:C6	2.49	0.48
2:A:63:LEU:O	2:A:67:LYS:HG2	2.13	0.48
1:C:911:C:H6	1:C:911:C:O5'	1.97	0.48
2:B:448:ARG:H	2:B:448:ARG:CD	2.08	0.48
2:B:397:VAL:HG12	2:B:398:LYS:N	2.28	0.48
2:B:217:PRO:HD2	2:B:318:ARG:HE	1.78	0.48
2:B:270:LYS:HB2	2:B:270:LYS:NZ	2.29	0.48
2:B:193:THR:HG23	2:B:194:PRO:HD2	1.96	0.48
2:A:193:THR:O	2:A:339:ILE:HG12	2.14	0.48
2:B:415:TRP:HA	2:B:447:LYS:O	2.14	0.48
2:B:89:VAL:O	2:B:93:ARG:N	2.47	0.48
2:B:462:TRP:N	2:B:463:PRO:CD	2.74	0.48
2:B:543:VAL:O	2:B:547:GLY:N	2.46	0.48
2:B:830:GLU:O	2:B:831:LYS:HE3	2.14	0.48
2:A:489:TYR:N	2:A:517:LEU:HD12	2.28	0.48
2:A:315:PHE:C	2:A:317:ALA:H	2.17	0.48
2:B:415:TRP:CZ3	2:B:448:ARG:HD2	2.48	0.48
2:A:89:VAL:HG21	2:A:346:ARG:HG2	1.94	0.48
2:B:238:LEU:HD23	2:B:238:LEU:N	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:7:TYR:CD1	2:A:8:ASP:N	2.81	0.48
2:B:759:LEU:O	2:B:763:ARG:HG2	2.14	0.48
2:B:498:ARG:O	2:B:501:VAL:HG12	2.13	0.48
1:D:967:C:O2'	1:D:968:G:H5'	2.12	0.48
1:D:971:C:O2'	1:D:972:A:H5'	2.14	0.48
2:A:724:GLN:HB3	2:A:783:MET:HG2	1.95	0.48
2:B:441:CYS:SG	2:B:443:SER:CB	3.02	0.48
2:A:520:LEU:HA	4:A:990:VAA:N1	2.29	0.48
2:A:28:ASN:HD22	2:A:28:ASN:C	2.16	0.48
1:D:971:C:C2'	1:D:972:A:H5'	2.43	0.48
2:A:834:LYS:NZ	2:A:834:LYS:HB3	2.29	0.48
2:B:738:LEU:CD1	2:B:738:LEU:N	2.76	0.48
2:B:1:MET:HE3	2:B:693:ALA:CB	2.42	0.48
2:B:462:TRP:O	2:B:464:LEU:N	2.47	0.48
2:A:118:LYS:HE3	2:A:143:PHE:CE2	2.49	0.48
2:A:145:MET:HG2	2:A:410:HIS:HE2	1.77	0.48
2:B:50:HIS:CD2	2:B:52:GLY:N	2.81	0.48
2:B:175:TRP:CZ2	2:B:180:GLU:HA	2.49	0.48
2:B:195:GLY:HA3	2:B:339:ILE:HD11	1.95	0.48
2:A:272:THR:H	2:A:279:ASP:HB3	1.78	0.48
2:A:80:THR:O	2:A:143:PHE:HD1	1.97	0.48
2:B:222:ALA:HB2	2:B:293:VAL:HG13	1.94	0.48
2:A:49:LEU:HG	2:A:128:GLN:OE1	2.13	0.48
1:C:934:A:N3	2:A:584:ASN:HB3	2.29	0.48
2:A:28:ASN:ND2	2:A:28:ASN:C	2.67	0.47
2:B:386:TRP:HB2	5:B:2040:HOH:O	2.13	0.47
2:A:270:LYS:CB	2:A:270:LYS:HZ2	2.27	0.47
2:B:164:GLY:O	2:B:166:ALA:N	2.47	0.47
2:A:459:SER:C	2:A:495:TRP:HZ3	2.17	0.47
2:A:202:TYR:CD1	2:A:246:PRO:HG3	2.49	0.47
1:C:951:G:H5'	1:C:952:G:OP2	2.13	0.47
2:A:171:ARG:NH1	2:A:364:ARG:HH21	2.10	0.47
2:A:307:GLU:O	2:A:309:LEU:N	2.47	0.47
1:D:901:G:H22	1:D:972:A:C1'	2.27	0.47
2:A:440:ALA:HA	5:A:1051:HOH:O	2.14	0.47
2:B:587:ARG:HG3	2:B:587:ARG:HH11	1.78	0.47
2:B:492:LEU:HD12	2:B:492:LEU:O	2.13	0.47
2:B:9:PRO:C	2:B:11:SER:H	2.18	0.47
2:A:326:ARG:CG	2:A:327:GLU:H	2.20	0.47
2:B:393:TRP:HB2	2:B:493:PHE:CE2	2.49	0.47
2:A:266:THR:C	2:A:268:ALA:H	2.17	0.47
2:A:518:HIS:CD2	2:A:519:GLY:O	2.62	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:78:PRO:HG2	2:B:141:GLU:HA	1.96	0.47
2:A:625:TYR:C	2:A:627:ALA:H	2.17	0.47
2:B:382:VAL:C	2:B:384:GLU:H	2.17	0.47
2:B:382:VAL:CG2	2:B:517:LEU:H	2.27	0.47
2:B:724:GLN:HE22	2:B:785:ARG:HB2	1.79	0.47
2:B:485:LEU:HD22	2:B:512:PHE:CE2	2.49	0.47
2:A:201:ARG:HG3	2:A:332:VAL:HG11	1.95	0.47
2:B:115:TRP:HA	2:B:118:LYS:HB3	1.96	0.47
2:B:236:ARG:HA	2:B:238:LEU:HD23	1.96	0.47
2:A:93:ARG:CG	2:A:94:LEU:N	2.77	0.47
2:B:234:ARG:HG3	2:B:235:TYR:N	2.29	0.47
2:A:404:ARG:HG2	2:A:406:LEU:CD1	2.45	0.47
2:A:273:PRO:HB3	2:A:280:TYR:HA	1.95	0.47
2:A:160:TYR:CE2	2:A:505:HIS:CD2	3.03	0.47
2:A:604:THR:HG23	2:A:607:ASP:OD1	2.15	0.47
2:B:202:TYR:CE2	2:B:244:ARG:HB3	2.49	0.47
2:A:170:PRO:HB2	2:A:355:ILE:HG22	1.96	0.47
2:B:249:GLU:OE1	2:B:249:GLU:HA	2.14	0.47
2:B:724:GLN:NE2	2:B:785:ARG:HB2	2.29	0.47
2:B:277:PRO:O	2:B:281:GLU:HB2	2.15	0.47
2:A:467:LEU:O	2:A:473:THR:CG2	2.62	0.47
2:B:363:MET:CA	2:B:363:MET:HE3	2.44	0.47
2:A:429:GLU:N	2:A:429:GLU:CD	2.68	0.47
2:B:780:VAL:HG12	2:B:781:LYS:N	2.30	0.47
2:A:1:MET:HE2	2:A:693:ALA:CB	2.45	0.47
2:B:324:LEU:CD2	2:B:324:LEU:H	2.23	0.47
2:A:509:GLU:HG2	2:A:510:ARG:H	1.79	0.47
2:B:818:ARG:NH2	5:B:2004:HOH:O	2.47	0.47
2:B:202:TYR:CD1	2:B:330:HIS:CE1	3.03	0.47
2:B:197:LEU:HB2	2:B:337:TYR:HB2	1.97	0.47
2:A:601:ASP:OD1	2:A:663:HIS:HB2	2.15	0.47
2:A:157:PHE:O	2:A:160:TYR:HB2	2.15	0.47
1:C:908:U:C2	1:C:915:G:O6	2.68	0.47
1:C:947:C:HO2'	1:C:948:G:P	2.37	0.47
2:A:159:ARG:NH1	2:A:163:GLU:OE1	2.43	0.47
2:B:149:ARG:CD	2:B:465:SER:HB2	2.44	0.47
2:B:473:THR:HG23	2:B:475:ASP:N	2.29	0.47
1:C:962:U:H2'	1:C:963:A:C8	2.49	0.47
2:B:50:HIS:HD2	2:B:52:GLY:H	1.60	0.47
2:A:128:GLN:O	2:A:132:LEU:HG	2.15	0.47
2:A:13:GLU:N	2:A:14:PRO:HD2	2.30	0.47
1:D:911:C:H6	1:D:911:C:O5'	1.98	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:202:TYR:HE2	2:B:244:ARG:HD3	1.80	0.47
1:D:973:C:H2'	1:D:974:C:H5'	1.97	0.47
2:A:88:GLN:HE22	2:A:110:PHE:HE2	1.63	0.47
2:B:91:VAL:HG12	2:B:96:LEU:CD2	2.44	0.47
1:D:935:C:H1'	2:B:584:ASN:ND2	2.30	0.47
1:C:962:U:H2'	1:C:963:A:H8	1.79	0.47
2:A:831:LYS:HD3	2:A:831:LYS:N	2.29	0.47
2:A:395:GLU:HA	2:A:395:GLU:OE2	2.14	0.47
2:A:105:LEU:HD21	2:A:110:PHE:HB2	1.97	0.46
2:B:280:TYR:C	2:B:280:TYR:CD2	2.87	0.46
1:C:921:G:O2'	1:C:922:A:H5'	2.14	0.46
2:A:217:PRO:HD2	2:A:218:GLU:OE1	2.15	0.46
2:B:724:GLN:HE22	2:B:785:ARG:H	1.62	0.46
2:B:236:ARG:O	2:B:237:HIS:ND1	2.48	0.46
2:A:136:ALA:O	2:A:138:TRP:N	2.47	0.46
2:B:416:TYR:HA	2:B:422:ALA:O	2.15	0.46
2:A:88:GLN:NE2	2:A:110:PHE:HE2	2.13	0.46
2:A:232:ASP:C	2:A:234:ARG:N	2.67	0.46
2:B:543:VAL:CG2	2:B:544:GLU:N	2.79	0.46
2:A:520:LEU:HA	4:A:990:VAA:C2	2.45	0.46
2:B:319:ARG:O	2:B:319:ARG:HG3	2.15	0.46
2:B:225:ALA:CA	2:B:252:ILE:CG2	2.91	0.46
2:A:273:PRO:HA	2:A:280:TYR:CA	2.46	0.46
2:A:65:ARG:HH11	2:A:680:HIS:CE1	2.32	0.46
2:A:521:VAL:HA	2:A:565:ILE:O	2.16	0.46
2:A:522:LEU:HD12	2:A:522:LEU:O	2.15	0.46
2:A:276:ASP:OD1	2:A:278:LEU:N	2.49	0.46
2:B:416:TYR:CD2	2:B:423:VAL:HG22	2.50	0.46
2:A:105:LEU:HD21	2:A:110:PHE:CD1	2.51	0.46
2:A:496:VAL:O	2:A:500:GLU:HG3	2.15	0.46
2:A:361:LEU:O	2:A:363:MET:N	2.48	0.46
2:B:607:ASP:OD2	2:B:664:THR:HA	2.16	0.46
2:A:855:ARG:CZ	2:B:810:LYS:HG3	2.46	0.46
2:B:745:ARG:CB	2:B:771:LEU:HD23	2.42	0.46
2:A:153:VAL:HG12	2:A:461:LEU:HD23	1.97	0.46
2:B:798:VAL:HG13	2:B:799:GLU:N	2.31	0.46
2:B:561:GLY:HA2	5:B:2025:HOH:O	2.15	0.46
2:A:111:LEU:O	2:A:115:TRP:HD1	1.98	0.46
2:B:274:ALA:HB2	2:B:290:PRO:HB2	1.96	0.46
1:C:928:C:H2'	1:C:929:G:C5'	2.29	0.46
2:A:282:ILE:HA	2:A:285:ARG:CG	2.46	0.46
2:B:273:PRO:HA	2:B:280:TYR:HA	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:932:U:O2'	1:D:933:C:H5	1.94	0.46
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.15	0.46
2:A:382:VAL:HG21	2:A:517:LEU:N	2.30	0.46
2:B:393:TRP:CZ3	2:B:394:LEU:HD23	2.51	0.46
2:A:592:SER:C	2:A:594:GLU:N	2.68	0.46
2:B:331:LEU:HD12	2:B:332:VAL:N	2.31	0.46
2:A:61:ASP:CG	2:A:552:ARG:HH22	2.19	0.46
2:A:326:ARG:CG	2:A:327:GLU:N	2.69	0.46
2:B:236:ARG:HA	2:B:238:LEU:CD2	2.46	0.46
2:B:606:ALA:O	2:B:609:PHE:HB3	2.16	0.46
2:A:102:ARG:O	2:A:103:HIS:C	2.53	0.46
2:A:705:TRP:CD2	2:A:706:PRO:HD2	2.51	0.46
2:A:369:GLU:OE2	2:A:505:HIS:HA	2.16	0.46
2:B:364:ARG:N	2:B:365:PRO:HD2	2.31	0.46
2:A:275:HIS:CE1	2:A:294:ILE:CG2	2.99	0.46
2:A:745:ARG:HB3	2:A:771:LEU:HD21	1.98	0.46
2:B:36:PHE:CD1	2:B:67:LYS:HG3	2.51	0.45
2:A:776:ALA:HB3	2:A:777:LYS:HD3	1.98	0.45
2:B:39:PHE:HE1	2:B:482:GLY:HA3	1.80	0.45
2:A:47:GLY:N	2:A:117:TRP:HZ2	2.07	0.45
2:A:385:ARG:NH1	2:A:385:ARG:HG3	2.30	0.45
2:A:651:GLU:HA	2:A:651:GLU:OE2	2.15	0.45
2:B:452:VAL:CG1	2:B:453:PHE:N	2.80	0.45
2:B:454:ASP:O	2:B:457:PHE:N	2.33	0.45
2:A:412:ILE:HG13	2:A:413:PRO:N	2.30	0.45
2:A:416:TYR:HE2	2:A:423:VAL:HG12	1.77	0.45
2:A:558:LEU:HA	5:A:1028:HOH:O	2.16	0.45
2:A:261:GLU:HA	2:A:261:GLU:OE1	2.15	0.45
2:A:248:THR:HG23	2:A:249:GLU:N	2.29	0.45
2:A:415:TRP:CE3	2:A:448:ARG:HB3	2.51	0.45
2:B:579:ALA:HB2	2:B:683:MET:HE1	1.98	0.45
2:A:326:ARG:HB3	2:A:331:LEU:CD2	2.41	0.45
1:D:945:G:C2'	1:D:946:U:O5'	2.65	0.45
2:A:363:MET:HE3	2:A:363:MET:HA	1.98	0.45
2:A:314:ARG:HG3	2:A:315:PHE:CD2	2.52	0.45
2:B:160:TYR:HD2	2:B:165:LEU:HD12	1.82	0.45
2:A:239:LEU:HD12	2:A:254:ILE:O	2.17	0.45
2:B:469:TRP:CD1	2:B:507:MET:HE1	2.51	0.45
2:A:524:GLU:CD	2:A:524:GLU:H	2.19	0.45
2:A:27:ALA:O	2:A:140:ARG:NH2	2.49	0.45
2:A:245:ILE:HG21	2:A:252:ILE:CD1	2.45	0.45
2:A:855:ARG:HD2	2:B:809:LEU:HD12	1.97	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:370:VAL:CG2	2:B:501:VAL:HA	2.47	0.45
2:B:778:ALA:HB2	2:B:791:PRO:HA	1.97	0.45
2:B:738:LEU:HD12	2:B:738:LEU:N	2.31	0.45
2:A:242:ARG:O	2:A:254:ILE:HD13	2.16	0.45
2:B:469:TRP:CD1	2:B:507:MET:CE	2.99	0.45
2:B:341:LEU:HD13	2:B:342:ALA:N	2.32	0.45
2:A:451:ASP:HB3	2:A:452:VAL:H	1.55	0.45
2:B:49:LEU:HG	2:B:128:GLN:OE1	2.15	0.45
2:B:618:VAL:HG12	2:B:708:PRO:HG3	1.98	0.45
2:A:170:PRO:O	2:A:355:ILE:HG23	2.16	0.45
2:B:250:VAL:HG12	2:B:252:ILE:HD12	1.99	0.45
2:A:732:LEU:HD12	2:A:732:LEU:HA	1.71	0.45
2:A:238:LEU:HA	5:A:1005:HOH:O	2.16	0.45
1:D:962:U:H2'	1:D:963:A:H8	1.81	0.45
2:B:273:PRO:HA	2:B:280:TYR:CA	2.47	0.45
2:A:480:TYR:HE2	2:A:509:GLU:HB3	1.82	0.45
2:A:547:GLY:O	2:A:550:ALA:HB3	2.17	0.45
2:A:774:ARG:C	2:A:774:ARG:HD3	2.37	0.45
2:A:546:TYR:CD2	2:A:572:LEU:HB3	2.51	0.45
2:B:683:MET:O	2:B:687:THR:CG2	2.65	0.45
2:A:160:TYR:HE2	2:A:505:HIS:CD2	2.35	0.45
2:A:774:ARG:HH11	2:A:774:ARG:HG3	1.82	0.45
2:A:216:ARG:HH12	2:A:314:ARG:NH2	2.15	0.45
1:C:929:G:H5'	1:C:929:G:C8	2.49	0.45
2:A:210:ILE:O	2:A:210:ILE:HG23	2.17	0.45
2:A:543:VAL:O	2:A:547:GLY:N	2.50	0.45
2:B:759:LEU:HD13	2:B:759:LEU:C	2.37	0.45
2:A:651:GLU:HA	2:A:654:LYS:HD3	1.99	0.45
2:A:642:TRP:O	2:A:642:TRP:HD1	2.00	0.45
2:B:201:ARG:HB3	2:B:210:ILE:O	2.15	0.45
2:A:855:ARG:HG3	2:B:809:LEU:HD12	1.99	0.45
2:A:271:VAL:HG22	2:A:282:ILE:HD11	1.99	0.45
1:C:908:U:H1'	1:C:947:C:O2	2.17	0.45
2:B:823:LEU:HD11	2:B:841:GLU:HG2	1.97	0.45
2:A:234:ARG:C	2:A:236:ARG:N	2.70	0.45
2:B:219:THR:O	2:B:272:THR:HG21	2.17	0.45
2:A:814:ALA:O	2:A:818:ARG:HG3	2.17	0.45
2:A:306:PRO:CD	2:A:309:LEU:HD23	2.47	0.45
2:B:7:TYR:CD1	2:B:8:ASP:N	2.85	0.45
2:A:161:TYR:CD1	2:A:161:TYR:C	2.90	0.45
2:B:302:GLY:O	2:B:310:ARG:NH1	2.35	0.45
1:D:945:G:H2'	1:D:946:U:O5'	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:102:ARG:NH1	5:A:1008:HOH:O	2.49	0.44
2:B:487:THR:HG23	2:B:517:LEU:HD23	1.99	0.44
2:B:45:VAL:HG13	2:B:81:ASP:O	2.17	0.44
2:A:212:ILE:CD1	2:A:268:ALA:O	2.65	0.44
2:B:148:LYS:HD2	2:B:468:GLY:CA	2.47	0.44
2:B:469:TRP:HA	2:B:476:LEU:HD22	1.99	0.44
2:A:45:VAL:CG1	2:A:118:LYS:HA	2.46	0.44
2:B:254:ILE:HG22	2:B:254:ILE:O	2.17	0.44
2:B:242:ARG:HB2	2:B:251:TRP:HE3	1.81	0.44
2:B:31:SER:C	2:B:33:LYS:N	2.71	0.44
2:A:422:ALA:HB1	5:A:1009:HOH:O	2.17	0.44
2:A:217:PRO:O	2:A:220:VAL:HG22	2.18	0.44
2:B:501:VAL:C	2:B:503:GLY:N	2.70	0.44
2:A:518:HIS:C	2:A:518:HIS:CD2	2.91	0.44
2:B:233:GLU:OE2	2:B:234:ARG:N	2.50	0.44
2:A:401:ASN:O	2:A:404:ARG:NH2	2.51	0.44
2:B:774:ARG:HH11	2:B:774:ARG:HG2	1.82	0.44
2:A:382:VAL:CG2	2:A:517:LEU:N	2.77	0.44
1:C:975:A:H8	2:A:213:ALA:O	2.01	0.44
2:B:93:ARG:C	2:B:94:LEU:O	2.52	0.44
2:B:680:HIS:HB3	2:B:681:PRO:HD3	1.98	0.44
2:B:691:TYR:HB2	2:B:700:LEU:HD22	1.99	0.44
2:B:69:MET:HE3	2:B:681:PRO:HG3	1.98	0.44
2:A:473:THR:HG22	2:A:476:LEU:CB	2.47	0.44
2:B:218:GLU:CG	2:B:318:ARG:HB2	2.47	0.44
2:A:837:VAL:HG13	2:A:838:GLU:H	1.80	0.44
2:A:755:VAL:HG13	2:A:762:PHE:CG	2.52	0.44
2:A:30:LYS:HG2	2:A:30:LYS:H	1.65	0.44
2:B:277:PRO:CD	2:B:353:TYR:CE2	2.93	0.44
2:A:333:LYS:HG2	2:A:335:GLU:OE1	2.17	0.44
2:A:397:VAL:HG12	2:A:398:LYS:H	1.81	0.44
2:A:454:ASP:O	2:A:457:PHE:N	2.39	0.44
2:A:232:ASP:O	2:A:233:GLU:C	2.56	0.44
2:A:364:ARG:N	2:A:365:PRO:HD2	2.33	0.44
2:A:94:LEU:O	2:A:95:LEU:C	2.56	0.44
2:A:557:TYR:HE1	2:A:635:ARG:HB3	1.77	0.44
2:B:546:TYR:CD1	2:B:546:TYR:N	2.86	0.44
1:C:909:A:O2'	1:C:910:G:N7	2.46	0.44
2:B:488:GLY:N	4:B:1990:VAA:O2'	2.45	0.44
2:A:86:ALA:HA	2:A:346:ARG:HD3	2.00	0.44
2:B:408:TRP:CE3	2:B:408:TRP:HA	2.52	0.44
2:B:361:LEU:CD2	2:B:366:LEU:CD1	2.96	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:412:ILE:HG13	2:A:413:PRO:CD	2.48	0.44
2:A:473:THR:HG22	2:A:476:LEU:HB2	1.99	0.44
2:A:724:GLN:NE2	2:A:785:ARG:H	2.10	0.44
2:B:546:TYR:CD2	2:B:572:LEU:HB3	2.53	0.44
2:A:613:ARG:NH2	2:A:644:GLU:HG3	2.31	0.44
2:A:808:ARG:HD2	2:A:808:ARG:HA	1.84	0.44
1:D:914:A:H4'	2:B:560:THR:HG21	1.99	0.44
2:B:361:LEU:HB2	2:B:402:ILE:HD12	1.98	0.44
2:A:152:ALA:HA	2:A:470:PRO:HB3	1.99	0.44
2:B:50:HIS:C	2:B:50:HIS:CD2	2.91	0.44
1:D:952:G:N3	1:D:952:G:H2'	2.32	0.44
2:A:472:GLU:HG2	2:A:472:GLU:O	2.17	0.44
2:A:492:LEU:O	2:A:492:LEU:HG	2.16	0.44
2:B:212:ILE:HD12	2:B:268:ALA:O	2.18	0.44
2:B:499:MET:CE	2:B:512:PHE:CE2	2.82	0.44
2:B:140:ARG:NH1	2:B:475:ASP:OD1	2.50	0.44
2:B:349:THR:CG2	2:B:350:PRO:HD2	2.45	0.44
2:B:382:VAL:HG21	2:B:516:LEU:HA	1.93	0.44
2:B:415:TRP:HZ3	2:B:448:ARG:HD2	1.81	0.44
2:B:312:LEU:CD1	2:B:313:ASP:H	2.31	0.44
2:B:322:VAL:HG13	2:B:323:GLU:N	2.32	0.44
2:B:539:PRO:O	2:B:543:VAL:HG13	2.18	0.44
2:A:621:ILE:HD12	2:A:678:LEU:HD13	2.00	0.44
2:B:373:GLY:O	2:B:376:ARG:N	2.50	0.44
2:B:110:PHE:C	2:B:112:GLU:N	2.70	0.44
2:B:387:LYS:HB3	2:B:388:LYS:CE	2.48	0.43
2:A:463:PRO:HG3	2:A:511:PRO:HB3	2.00	0.43
2:A:362:ARG:O	2:A:365:PRO:HG2	2.18	0.43
2:B:181:THR:OG1	2:B:404:ARG:HG3	2.18	0.43
2:B:408:TRP:HE3	2:B:408:TRP:HA	1.83	0.43
2:B:94:LEU:O	2:B:96:LEU:N	2.51	0.43
2:B:745:ARG:NH1	2:B:745:ARG:CB	2.79	0.43
2:B:362:ARG:C	2:B:365:PRO:HD2	2.38	0.43
2:A:751:GLU:OE2	2:A:785:ARG:NE	2.50	0.43
2:B:200:LEU:HD21	2:B:325:PHE:CE1	2.53	0.43
1:D:958:G:H2'	1:D:959:U:H5'	2.00	0.43
2:B:831:LYS:HE3	2:B:831:LYS:CA	2.48	0.43
2:B:227:ALA:HA	2:B:255:LEU:HD12	1.99	0.43
2:B:102:ARG:O	2:B:104:ASP:N	2.51	0.43
2:A:388:LYS:N	2:A:388:LYS:HD3	2.34	0.43
2:B:17:ALA:HB2	2:B:685:PHE:HE2	1.82	0.43
2:A:821:ARG:O	2:A:825:SER:HB2	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:906:G:N2	1:D:967:C:C2	2.86	0.43
2:A:486:VAL:HG22	2:A:516:LEU:HD22	2.00	0.43
2:A:456:TRP:HB3	2:A:498:ARG:NH1	2.33	0.43
2:B:91:VAL:HG12	2:B:96:LEU:HD21	2.00	0.43
2:B:272:THR:H	2:B:279:ASP:CB	2.30	0.43
2:A:710:GLY:O	2:A:711:ARG:HB3	2.18	0.43
2:B:714:GLU:O	2:B:717:ARG:N	2.52	0.43
2:B:274:ALA:HB3	2:B:291:VAL:O	2.18	0.43
2:A:40:MET:CE	2:A:79:GLY:H	2.31	0.43
2:A:800:GLU:OE1	2:A:800:GLU:HA	2.18	0.43
2:B:157:PHE:CD2	2:B:413:PRO:HG2	2.54	0.43
2:B:404:ARG:HG2	2:B:406:LEU:CD1	2.44	0.43
2:B:425:VAL:HA	2:B:426:PRO:HD2	1.82	0.43
2:A:326:ARG:CA	2:A:331:LEU:HB3	2.47	0.43
2:A:833:PRO:C	2:A:835:GLU:N	2.71	0.43
2:B:269:LEU:HB2	5:B:2007:HOH:O	2.19	0.43
2:A:692:GLN:HE21	2:A:698:GLU:HA	1.82	0.43
2:A:489:TYR:HD1	2:A:490:ASP:N	2.17	0.43
2:A:221:PHE:HA	2:A:245:ILE:CD1	2.48	0.43
2:A:415:TRP:HB2	2:A:424:ASN:HB2	2.00	0.43
2:A:46:THR:CG2	2:A:90:VAL:HG21	2.48	0.43
2:A:56:ASP:OD1	2:A:518:HIS:HE1	2.01	0.43
2:A:49:LEU:HD21	2:A:125:ILE:HG23	2.01	0.43
2:B:107:ARG:O	2:B:111:LEU:HB3	2.19	0.43
2:B:262:LYS:HG2	5:B:2014:HOH:O	2.19	0.43
2:B:785:ARG:CA	2:B:785:ARG:NH1	2.80	0.43
2:A:93:ARG:HG2	2:A:94:LEU:N	2.30	0.43
2:B:454:ASP:O	2:B:455:THR:C	2.56	0.43
2:B:160:TYR:CE2	2:B:505:HIS:HD2	2.37	0.43
1:D:971:C:O5'	1:D:971:C:H6	2.01	0.43
2:B:685:PHE:HD1	2:B:685:PHE:H	1.67	0.43
2:A:412:ILE:CA	2:A:453:PHE:CE1	2.99	0.43
2:A:161:TYR:C	2:A:163:GLU:H	2.22	0.43
2:B:144:THR:O	2:B:149:ARG:HB3	2.18	0.43
2:B:242:ARG:O	2:B:243:ALA:HB2	2.19	0.43
2:B:519:GLY:C	2:B:520:LEU:HD23	2.38	0.43
2:A:170:PRO:HB2	2:A:355:ILE:CG2	2.49	0.43
2:B:88:GLN:CG	2:B:406:LEU:HD22	2.43	0.43
2:A:69:MET:CE	2:A:680:HIS:ND1	2.81	0.43
1:D:923:G:H2'	1:D:924:C:C6	2.53	0.43
2:A:480:TYR:O	2:A:481:PRO:C	2.57	0.43
2:A:507:MET:C	2:A:509:GLU:H	2.21	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:938:G:P	5:D:71:HOH:O	2.76	0.43
2:B:699:GLU:OE1	2:B:699:GLU:HA	2.19	0.43
2:A:218:GLU:CD	2:A:218:GLU:H	2.19	0.43
2:A:49:LEU:HD22	2:A:53:HIS:ND1	2.33	0.43
1:C:904:C:H2'	1:C:905:G:C8	2.54	0.43
2:A:314:ARG:HH22	2:A:352:GLU:HG3	1.79	0.43
2:A:362:ARG:HB3	2:A:365:PRO:HG3	2.01	0.43
2:B:84:GLY:O	2:B:85:ILE:C	2.57	0.43
2:A:810:LYS:HG3	2:B:855:ARG:NH2	2.34	0.43
1:D:962:U:H2'	1:D:963:A:C8	2.54	0.43
2:B:692:GLN:HA	2:B:697:LYS:O	2.18	0.43
2:B:262:LYS:HA	2:B:267:GLY:HA2	2.01	0.43
2:B:248:THR:CG2	2:B:249:GLU:N	2.56	0.43
2:A:855:ARG:NH2	2:B:810:LYS:HG3	2.33	0.43
2:A:44:ASN:C	2:A:46:THR:H	2.23	0.43
2:B:102:ARG:NE	2:B:102:ARG:O	2.28	0.43
2:A:398:LYS:O	2:A:399:ASP:C	2.56	0.43
2:A:209:PHE:O	2:A:238:LEU:HD12	2.19	0.43
2:A:833:PRO:O	2:A:837:VAL:HG12	2.18	0.43
2:A:744:VAL:CG1	2:A:745:ARG:N	2.82	0.43
2:A:64:ILE:HD13	2:A:64:ILE:HA	1.83	0.43
2:B:210:ILE:O	2:B:210:ILE:CG2	2.67	0.42
2:A:498:ARG:NH1	2:A:498:ARG:HG2	2.33	0.42
2:A:460:ALA:O	2:A:499:MET:HA	2.19	0.42
2:A:313:ASP:CG	2:A:314:ARG:N	2.73	0.42
2:A:216:ARG:HA	2:A:318:ARG:NH2	2.34	0.42
2:A:69:MET:O	2:A:705:TRP:N	2.51	0.42
2:A:155:TYR:CD1	2:A:431:TYR:CD2	3.04	0.42
2:B:692:GLN:HG3	2:B:697:LYS:O	2.18	0.42
2:B:614:LEU:HD11	2:B:671:VAL:HG13	2.01	0.42
2:A:7:TYR:CE2	2:A:686:LEU:HD13	2.53	0.42
1:D:918:G:C6	2:B:833:PRO:CD	3.02	0.42
2:A:420:CYS:O	2:A:420:CYS:SG	2.77	0.42
2:A:721:ALA:HB3	2:A:754:PRO:HG2	1.99	0.42
2:A:531:LYS:NZ	5:A:1041:HOH:O	2.49	0.42
2:B:244:ARG:NH2	5:B:1991:HOH:O	2.26	0.42
2:A:312:LEU:CG	2:A:313:ASP:N	2.81	0.42
2:A:405:GLN:N	2:A:405:GLN:CD	2.73	0.42
2:A:70:ARG:HH11	2:A:70:ARG:HG2	1.85	0.42
2:B:238:LEU:HD23	2:B:238:LEU:H	1.83	0.42
2:A:255:LEU:HD12	2:A:255:LEU:O	2.19	0.42
2:A:304:ARG:HH11	2:A:304:ARG:CG	2.23	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:469:TRP:N	2:A:470:PRO:CD	2.82	0.42
2:A:812:LEU:HD23	2:A:812:LEU:HA	1.87	0.42
2:B:714:GLU:O	2:B:715:ALA:C	2.58	0.42
1:C:960:C:O2'	1:C:961:C:H5'	2.18	0.42
2:B:639:GLU:O	2:B:640:LEU:C	2.56	0.42
2:A:546:TYR:HE2	2:A:573:GLU:HG2	1.84	0.42
2:B:91:VAL:HA	2:B:95:LEU:CD1	2.48	0.42
2:A:247:LEU:HD23	2:A:325:PHE:HE1	1.84	0.42
2:A:143:PHE:O	2:A:145:MET:N	2.53	0.42
2:A:196:LYS:HB3	2:A:198:TYR:HE1	1.80	0.42
2:A:260:VAL:HG22	2:A:269:LEU:CD2	2.49	0.42
2:B:98:GLU:O	2:B:99:GLY:O	2.37	0.42
2:B:171:ARG:NH2	2:B:398:LYS:HG2	2.34	0.42
2:A:45:VAL:CG1	2:A:121:SER:HB3	2.48	0.42
2:A:42:PRO:HB2	2:A:81:ASP:N	2.35	0.42
2:B:430:ARG:O	2:B:432:LEU:N	2.53	0.42
2:B:666:ARG:O	2:B:670:GLU:HG3	2.19	0.42
2:A:283:GLY:O	2:A:288:LEU:HG	2.20	0.42
2:B:721:ALA:HB2	2:B:751:GLU:OE1	2.19	0.42
2:A:103:HIS:O	2:A:104:ASP:O	2.37	0.42
2:B:752:THR:O	2:B:753:ALA:C	2.57	0.42
2:B:544:GLU:CD	2:B:544:GLU:C	2.79	0.42
1:C:918:G:O2'	1:C:919:A:O5'	2.35	0.42
2:B:233:GLU:O	2:B:236:ARG:N	2.52	0.42
2:B:617:GLY:HA3	2:B:640:LEU:HD22	2.01	0.42
2:A:170:PRO:O	2:A:171:ARG:O	2.37	0.42
2:A:221:PHE:O	2:A:304:ARG:HG3	2.20	0.42
2:B:93:ARG:NH1	2:B:93:ARG:HG3	2.35	0.42
2:B:482:GLY:O	2:B:512:PHE:HA	2.20	0.42
2:B:171:ARG:HH22	2:B:398:LYS:HD2	1.84	0.42
2:B:405:GLN:N	2:B:405:GLN:CD	2.73	0.42
2:A:232:ASP:O	2:A:234:ARG:N	2.53	0.42
2:A:228:VAL:O	2:A:256:ALA:HA	2.19	0.42
2:B:223:ASP:HA	2:B:272:THR:HG23	2.01	0.42
2:B:10:LYS:NZ	2:B:544:GLU:HG2	2.34	0.42
2:A:506:PHE:C	2:A:507:MET:HG2	2.40	0.42
2:A:3:LEU:N	2:A:4:PRO:HD3	2.35	0.42
1:D:951:G:H5'	1:D:952:G:OP2	2.20	0.42
2:B:202:TYR:O	2:B:203:GLU:O	2.38	0.42
2:B:252:ILE:HG23	2:B:253:PRO:HD2	2.02	0.42
1:C:971:C:H2'	1:C:972:A:C5'	2.32	0.42
2:B:103:HIS:O	2:B:104:ASP:O	2.38	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:558:LEU:HD23	5:B:2020:HOH:O	2.20	0.42
2:B:837:VAL:O	2:B:841:GLU:HG3	2.20	0.42
2:B:313:ASP:CG	2:B:314:ARG:H	2.23	0.42
2:A:159:ARG:NH1	2:A:159:ARG:CG	2.78	0.42
2:B:148:LYS:O	2:B:148:LYS:HG3	2.20	0.42
2:B:38:ILE:HG22	2:B:76:TRP:CD1	2.55	0.42
2:B:649:TYR:CE2	2:B:668:LEU:HD23	2.55	0.42
2:A:201:ARG:CZ	2:A:332:VAL:HG21	2.50	0.42
2:B:778:ALA:HA	2:B:792:LEU:HB2	2.01	0.42
2:B:736:ALA:CB	2:B:738:LEU:HD13	2.49	0.42
2:A:155:TYR:OH	2:A:159:ARG:HD3	2.20	0.42
2:B:644:GLU:O	2:B:645:PHE:C	2.58	0.42
2:B:516:LEU:CD1	2:B:628:LEU:HD13	2.48	0.41
2:B:416:TYR:N	2:B:447:LYS:O	2.36	0.41
2:B:168:ARG:HA	2:B:358:GLN:O	2.20	0.41
2:B:469:TRP:CG	2:B:469:TRP:O	2.72	0.41
2:A:692:GLN:O	2:A:696:GLY:N	2.41	0.41
2:B:640:LEU:O	2:B:644:GLU:HB2	2.20	0.41
2:A:73:GLU:O	2:A:75:VAL:HG23	2.19	0.41
1:C:941:A:H2'	1:C:942:G:O5'	2.20	0.41
2:B:202:TYR:CD2	2:B:203:GLU:HB2	2.56	0.41
2:A:489:TYR:CD1	2:A:490:ASP:N	2.88	0.41
2:B:809:LEU:HD13	2:B:813:LEU:HG	2.02	0.41
2:B:83:ALA:HA	2:B:455:THR:CG2	2.49	0.41
2:A:438:CYS:C	2:A:440:ALA:H	2.23	0.41
1:D:957:A:H4'	1:D:959:U:C5	2.50	0.41
1:D:961:C:O2'	1:D:962:U:H5'	2.20	0.41
2:A:540:LEU:O	2:A:543:VAL:HG22	2.20	0.41
2:A:859:SER:OG	2:A:860:GLN:N	2.53	0.41
2:B:42:PRO:HB2	2:B:80:THR:C	2.40	0.41
2:A:717:ARG:NH1	2:A:717:ARG:HB2	2.33	0.41
2:B:210:ILE:HD12	2:B:210:ILE:HA	1.90	0.41
2:B:165:LEU:O	2:B:361:LEU:HA	2.19	0.41
2:B:161:TYR:O	2:B:163:GLU:N	2.53	0.41
2:A:732:LEU:CD1	2:A:781:LYS:HB2	2.40	0.41
2:A:724:GLN:HE22	2:A:785:ARG:HB2	1.85	0.41
2:B:221:PHE:O	2:B:304:ARG:HG3	2.21	0.41
2:A:666:ARG:CG	2:A:666:ARG:NH1	2.80	0.41
2:A:193:THR:CG2	2:A:194:PRO:HD2	2.49	0.41
2:B:64:ILE:HG23	2:B:74:ALA:HB1	2.01	0.41
2:A:146:ASP:OD1	2:A:149:ARG:HB2	2.20	0.41
2:B:199:THR:O	2:B:332:VAL:HG22	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:975:A:OP2	2:A:337:TYR:OH	2.28	0.41
1:C:901:G:N2	1:C:972:A:H1'	2.36	0.41
2:B:453:PHE:CD2	2:B:457:PHE:CD2	3.09	0.41
2:B:46:THR:CG2	2:B:90:VAL:HG21	2.51	0.41
2:B:93:ARG:O	2:B:94:LEU:O	2.38	0.41
2:B:745:ARG:H	2:B:745:ARG:HG2	1.74	0.41
2:B:297:GLU:HB2	2:B:299:ARG:HG2	2.02	0.41
2:B:680:HIS:CD2	2:B:687:THR:HG21	2.56	0.41
2:B:170:PRO:C	2:B:171:ARG:O	2.56	0.41
2:A:210:ILE:HA	2:A:210:ILE:HD12	1.86	0.41
2:B:323:GLU:C	2:B:325:PHE:N	2.74	0.41
2:B:433:GLU:O	2:B:435:PRO:HD3	2.20	0.41
2:A:401:ASN:C	2:A:401:ASN:ND2	2.73	0.41
2:A:7:TYR:HB2	2:A:583:TYR:CD2	2.55	0.41
2:B:611:ARG:HE	2:B:667:THR:HG23	1.86	0.41
2:B:212:ILE:CA	2:B:266:THR:HG21	2.51	0.41
2:B:388:LYS:CE	2:B:388:LYS:N	2.71	0.41
2:A:326:ARG:C	2:A:328:ALA:N	2.74	0.41
2:A:844:LEU:HD23	2:B:820:GLN:CG	2.50	0.41
2:B:108:GLU:O	2:B:112:GLU:HB2	2.20	0.41
2:A:242:ARG:NH1	2:A:242:ARG:CG	2.82	0.41
1:C:918:G:H21	1:C:956:A:H1'	1.84	0.41
2:A:599:LYS:HE2	2:A:599:LYS:HA	2.01	0.41
2:A:55:LEU:HD11	2:A:559:ALA:HB2	2.03	0.41
2:B:520:LEU:HA	4:B:1990:VAA:C2	2.51	0.41
2:B:487:THR:OG1	2:B:488:GLY:N	2.53	0.41
2:A:415:TRP:HZ3	2:A:448:ARG:HD2	1.81	0.41
2:B:83:ALA:HB1	2:B:86:ALA:HB3	2.02	0.41
2:B:587:ARG:NH1	2:B:587:ARG:CG	2.79	0.41
2:B:233:GLU:C	2:B:235:TYR:N	2.73	0.41
2:B:49:LEU:HD22	2:B:53:HIS:ND1	2.35	0.41
2:B:600:GLU:O	2:B:661:ASN:HA	2.20	0.41
1:D:973:C:O2	1:D:973:C:C2'	2.69	0.41
2:B:161:TYR:C	2:B:163:GLU:H	2.24	0.41
2:A:157:PHE:CD2	2:A:413:PRO:CG	3.04	0.41
2:B:611:ARG:NE	2:B:667:THR:HG23	2.36	0.41
2:A:15:LYS:HG3	2:A:16:TRP:N	2.36	0.41
2:B:15:LYS:HG3	2:B:16:TRP:N	2.36	0.41
2:A:225:ALA:CA	2:A:252:ILE:CG2	2.94	0.41
2:B:5:LYS:N	2:B:5:LYS:HD2	2.13	0.41
2:B:46:THR:HG22	2:B:87:THR:HA	2.03	0.41
2:B:745:ARG:HB2	2:B:771:LEU:CD2	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:903:G:N2	1:D:970:C:H1'	2.36	0.41
2:A:397:VAL:HG12	2:A:398:LYS:N	2.36	0.41
2:A:358:GLN:HB2	2:A:360:TRP:NE1	2.32	0.41
2:B:736:ALA:HB3	2:B:738:LEU:HD13	2.02	0.41
2:B:27:ALA:CB	2:B:75:VAL:HG13	2.51	0.41
2:A:154:ARG:NH1	2:A:154:ARG:HG3	2.36	0.41
2:B:231:GLU:C	2:B:233:GLU:H	2.24	0.41
2:A:408:TRP:HE3	2:A:408:TRP:HA	1.86	0.41
2:A:779:LEU:HD13	2:A:792:LEU:CD2	2.51	0.41
1:D:909:A:O2'	1:D:910:G:N7	2.39	0.41
1:D:907:C:H5''	1:D:908:U:OP2	2.20	0.41
1:C:943:A:H2'	1:C:944:G:O4'	2.20	0.41
2:B:510:ARG:CZ	2:B:513:LYS:HG2	2.51	0.41
2:B:713:GLU:HB3	5:B:2034:HOH:O	2.21	0.41
2:B:839:ALA:O	2:B:843:ARG:HG3	2.21	0.41
1:C:946:U:H3'	1:C:946:U:H6	1.85	0.41
2:B:63:LEU:O	2:B:67:LYS:HB2	2.21	0.41
2:A:448:ARG:NH1	2:A:448:ARG:HG2	2.36	0.41
2:A:273:PRO:HA	2:A:280:TYR:HA	2.02	0.41
2:B:13:GLU:N	2:B:14:PRO:CD	2.83	0.41
2:B:369:GLU:O	2:B:372:LYS:HB3	2.21	0.41
2:A:373:GLY:O	2:A:376:ARG:N	2.54	0.41
2:B:804:ARG:O	2:B:807:LYS:N	2.54	0.41
2:A:7:TYR:HB2	2:A:583:TYR:CG	2.56	0.41
2:B:228:VAL:CG2	2:B:268:ALA:HB2	2.51	0.40
1:D:973:C:C2'	1:D:974:C:H5''	2.51	0.40
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.86	0.40
2:B:312:LEU:HD12	2:B:313:ASP:H	1.86	0.40
1:D:934:A:N3	2:B:584:ASN:HB3	2.36	0.40
2:A:76:TRP:O	2:A:78:PRO:HD3	2.21	0.40
2:A:401:ASN:HD22	2:A:401:ASN:C	2.24	0.40
1:C:909:A:H61	1:C:921:G:H3'	1.85	0.40
2:A:523:ASP:OD2	2:A:527:GLN:HG3	2.22	0.40
2:B:201:ARG:CG	2:B:332:VAL:HG11	2.51	0.40
2:B:416:TYR:CE2	2:B:423:VAL:HG22	2.56	0.40
2:A:223:ASP:HA	2:A:271:VAL:O	2.22	0.40
2:B:281:GLU:O	2:B:285:ARG:CG	2.62	0.40
2:B:684:PRO:HG2	2:B:685:PHE:CD1	2.56	0.40
2:B:364:ARG:H	2:B:364:ARG:HG2	1.57	0.40
2:B:371:LEU:O	2:B:372:LYS:C	2.59	0.40
2:A:431:TYR:C	2:A:431:TYR:CD1	2.94	0.40
1:D:931:C:O5'	1:D:931:C:H6	2.03	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:859:SER:O	2:A:860:GLN:C	2.60	0.40
2:B:607:ASP:O	2:B:609:PHE:N	2.54	0.40
2:A:735:GLU:HG2	2:A:804:ARG:NH1	2.36	0.40
2:A:641:VAL:HG22	2:A:675:LEU:HD13	2.02	0.40
2:B:211:GLU:H	2:B:211:GLU:HG2	1.61	0.40
2:A:220:VAL:HA	2:A:270:LYS:HE3	2.03	0.40
2:A:846:GLU:HA	2:A:849:GLU:HG3	2.02	0.40
2:A:156:ALA:CB	2:A:461:LEU:HD21	2.51	0.40
2:B:38:ILE:HA	5:B:2041:HOH:O	2.20	0.40
2:B:438:CYS:O	2:B:442:GLY:HA2	2.22	0.40
1:C:961:C:C2'	1:C:962:U:H5'	2.51	0.40
2:A:624:LEU:HD12	2:A:633:ALA:CA	2.51	0.40
1:C:923:G:H2'	1:C:924:C:O4'	2.21	0.40
2:B:657:LEU:HD21	2:B:664:THR:HG22	2.03	0.40
1:D:950:A:H2'	1:D:951:G:O4'	2.22	0.40
2:A:102:ARG:O	2:A:104:ASP:N	2.55	0.40
2:B:92:GLU:O	2:B:96:LEU:HB2	2.22	0.40
2:B:363:MET:C	2:B:365:PRO:HD2	2.42	0.40
2:A:231:GLU:C	2:A:233:GLU:H	2.24	0.40
2:B:3:LEU:HD11	2:B:590:LEU:CB	2.52	0.40
2:A:790:MET:HA	2:A:791:PRO:HD3	1.97	0.40
2:A:12:VAL:O	2:A:15:LYS:HG2	2.22	0.40
2:B:264:PHE:O	2:B:265:GLY:C	2.60	0.40
2:A:28:ASN:HD22	2:A:29:PRO:CD	2.34	0.40
2:B:448:ARG:HH11	2:B:448:ARG:HG2	1.87	0.40
2:B:89:VAL:HG21	2:B:346:ARG:HG3	2.04	0.40
2:A:326:ARG:O	2:A:329:GLY:N	2.45	0.40
2:B:358:GLN:HB3	2:B:359:TRP:H	1.76	0.40
2:B:582:LEU:O	2:B:583:TYR:C	2.59	0.40
2:A:242:ARG:O	2:A:243:ALA:CB	2.69	0.40
1:D:947:C:C5	1:D:958:G:H5''	2.56	0.40
2:A:837:VAL:CG1	2:A:838:GLU:N	2.82	0.40
1:C:918:G:N2	1:C:956:A:C1'	2.84	0.40
2:B:301:GLU:HA	2:B:310:ARG:HG3	2.04	0.40
2:A:767:ARG:HG2	2:A:767:ARG:HH11	1.87	0.40
2:B:430:ARG:HB3	2:B:433:GLU:OE2	2.20	0.40
2:A:789:ARG:HG2	2:A:789:ARG:NH1	2.37	0.40
2:A:430:ARG:HB3	2:A:433:GLU:OE2	2.22	0.40
2:A:287:GLY:O	2:A:288:LEU:HD23	2.21	0.40
2:A:674:VAL:O	2:A:677:LYS:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	860/862 (100%)	676 (79%)	139 (16%)	45 (5%)	3	10
2	B	860/862 (100%)	652 (76%)	156 (18%)	52 (6%)	2	7
All	All	1720/1724 (100%)	1328 (77%)	295 (17%)	97 (6%)	3	8

All (97) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	94	LEU
2	A	103	HIS
2	A	104	ASP
2	A	234	ARG
2	A	312	LEU
2	A	313	ASP
2	A	351	ILE
2	A	362	ARG
2	A	409	GLY
2	A	473	THR
2	A	594	GLU
2	A	711	ARG
2	B	103	HIS
2	B	104	ASP
2	B	162	HIS
2	B	165	LEU
2	B	203	GLU
2	B	246	PRO
2	B	247	LEU
2	B	312	LEU
2	B	313	ASP
2	B	409	GLY
2	B	489	TYR
2	B	594	GLU
2	B	711	ARG
2	A	45	VAL
2	A	100	LYS

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Mol	Chain	Res	Type
2	A	144	THR
2	A	165	LEU
2	A	203	GLU
2	A	243	ALA
2	A	267	GLY
2	A	287	GLY
2	A	395	GLU
2	A	451	ASP
2	B	10	LYS
2	B	99	GLY
2	B	267	GLY
2	B	287	GLY
2	B	307	GLU
2	B	362	ARG
2	B	429	GLU
2	B	431	TYR
2	B	473	THR
2	B	710	GLY
2	A	93	ARG
2	A	95	LEU
2	A	113	ARG
2	A	137	ASP
2	A	219	THR
2	A	445	ARG
2	B	45	VAL
2	B	92	GLU
2	B	98	GLU
2	B	234	ARG
2	B	308	ALA
2	B	481	PRO
2	B	502	SER
2	B	834	LYS
2	A	171	ARG
2	A	192	PRO
2	A	208	GLY
2	B	95	LEU
2	B	100	LYS
2	B	137	ASP
2	B	170	PRO
2	B	205	GLU
2	B	462	TRP
2	B	685	PHE

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Mol	Chain	Res	Type
2	B	714	GLU
2	A	86	ALA
2	A	308	ALA
2	A	431	TYR
2	A	462	TRP
2	B	3	LEU
2	B	84	GLY
2	B	94	LEU
2	B	96	LEU
2	B	171	ARG
2	B	395	GLU
2	A	710	GLY
2	A	834	LYS
2	B	480	TYR
2	A	169	ALA
2	A	382	VAL
2	B	85	ILE
2	B	208	GLY
2	B	311	GLY
2	A	291	VAL
2	A	481	PRO
2	A	207	GLY
2	B	754	PRO
2	A	246	PRO
2	A	655	PRO
2	B	382	VAL
2	B	428	PRO
2	A	480	TYR

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	724/724 (100%)	641 (88%)	83 (12%)	8	23
2	B	724/724 (100%)	630 (87%)	94 (13%)	6	17
All	All	1448/1448 (100%)	1271 (88%)	177 (12%)	7	20

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	ASP
2	A	28	ASN
2	A	30	LYS
2	A	102	ARG
2	A	104	ASP
2	A	111	LEU
2	A	113	ARG
2	A	119	GLU
2	A	154	ARG
2	A	159	ARG
2	A	160	TYR
2	A	172	LEU
2	A	178	ARG
2	A	181	THR
2	A	191	GLU
2	A	192	PRO
2	A	197	LEU
2	A	202	TYR
2	A	209	PHE
2	A	212	ILE
2	A	216	ARG
2	A	233	GLU
2	A	238	LEU
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	307	GLU
2	A	347	CYS
2	A	356	PHE
2	A	361	LEU
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	403	SER

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Mol	Chain	Res	Type
2	A	404	ARG
2	A	408	TRP
2	A	412	ILE
2	A	413	PRO
2	A	421	GLN
2	A	429	GLU
2	A	431	TYR
2	A	432	LEU
2	A	445	ARG
2	A	448	ARG
2	A	473	THR
2	A	479	PHE
2	A	489	TYR
2	A	494	LEU
2	A	498	ARG
2	A	512	PHE
2	A	522	LEU
2	A	524	GLU
2	A	527	GLN
2	A	570	ARG
2	A	580	ASN
2	A	593	ARG
2	A	599	LYS
2	A	604	THR
2	A	616	ARG
2	A	679	LEU
2	A	707	GLU
2	A	727	THR
2	A	738	LEU
2	A	743	GLU
2	A	746	VAL
2	A	767	ARG
2	A	774	ARG
2	A	777	LYS
2	A	783	MET
2	A	795	LEU
2	A	800	GLU
2	A	805	GLN
2	A	834	LYS
2	A	838	GLU
2	A	845	LYS
2	B	2	ASP

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Mol	Chain	Res	Type
2	B	5	LYS
2	B	18	GLU
2	B	30	LYS
2	B	37	VAL
2	B	51	MET
2	B	75	VAL
2	B	77	LEU
2	B	88	GLN
2	B	93	ARG
2	B	102	ARG
2	B	104	ASP
2	B	107	ARG
2	B	113	ARG
2	B	151	ARG
2	B	172	LEU
2	B	178	ARG
2	B	181	THR
2	B	191	GLU
2	B	192	PRO
2	B	198	TYR
2	B	201	ARG
2	B	209	PHE
2	B	212	ILE
2	B	218	GLU
2	B	228	VAL
2	B	231	GLU
2	B	238	LEU
2	B	246	PRO
2	B	247	LEU
2	B	255	LEU
2	B	266	THR
2	B	270	LYS
2	B	272	THR
2	B	276	ASP
2	B	280	TYR
2	B	284	GLU
2	B	288	LEU
2	B	289	LYS
2	B	291	VAL
2	B	339	ILE
2	B	347	CYS
2	B	356	PHE

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Mol	Chain	Res	Type
2	B	372	LYS
2	B	388	LYS
2	B	401	ASN
2	B	403	SER
2	B	404	ARG
2	B	408	TRP
2	B	412	ILE
2	B	413	PRO
2	B	421	GLN
2	B	430	ARG
2	B	431	TYR
2	B	432	LEU
2	B	445	ARG
2	B	448	ARG
2	B	461	LEU
2	B	473	THR
2	B	477	LYS
2	B	479	PHE
2	B	494	LEU
2	B	498	ARG
2	B	507	MET
2	B	510	ARG
2	B	512	PHE
2	B	521	VAL
2	B	545	ARG
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	614	LEU
2	B	679	LEU
2	B	722	LEU
2	B	727	THR
2	B	732	LEU
2	B	733	LYS
2	B	745	ARG
2	B	767	ARG
2	B	769	ASP
2	B	770	LEU

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Mol	Chain	Res	Type
2	B	771	LEU
2	B	777	LYS
2	B	783	MET
2	B	802	ARG
2	B	805	GLN
2	B	820	GLN
2	B	830	GLU
2	B	831	LYS
2	B	860	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	28	ASN
2	A	50	HIS
2	A	224	GLN
2	A	229	HIS
2	A	237	HIS
2	A	330	HIS
2	A	358	GLN
2	A	390	ASN
2	A	401	ASN
2	A	411	GLN
2	A	424	ASN
2	A	505	HIS
2	A	518	HIS
2	A	527	GLN
2	A	580	ASN
2	A	584	ASN
2	A	692	GLN
2	A	724	GLN
2	A	758	ASN
2	A	860	GLN
2	B	50	HIS
2	B	60	GLN
2	B	116	GLN
2	B	174	ASN
2	B	229	HIS
2	B	275	HIS
2	B	330	HIS
2	B	358	GLN
2	B	396	ASN

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Mol	Chain	Res	Type
2	B	401	ASN
2	B	411	GLN
2	B	505	HIS
2	B	518	HIS
2	B	563	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 ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	74/75 (98%)	26 (35%)	10 (13%)
1	D	74/75 (98%)	27 (36%)	7 (9%)
All	All	148/150 (98%)	53 (35%)	17 (11%)

All (53) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	903	G
1	C	907	C
1	C	908	U
1	C	909	A
1	C	910	G
1	C	917	G
1	C	918	G
1	C	919	A
1	C	920	A
1	C	921	G
1	C	929	G
1	C	931	C
1	C	932	U
1	C	933	C
1	C	934	A
1	C	936	A
1	C	937	C
1	C	938	G

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Mol	Chain	Res	Type
1	C	947	C
1	C	948	G
1	C	952	G
1	C	958	G
1	C	959	U
1	C	966	C
1	C	972	A
1	C	975	A
1	D	903	G
1	D	907	C
1	D	908	U
1	D	909	A
1	D	910	G
1	D	916	C
1	D	917	G
1	D	919	A
1	D	920	A
1	D	921	G
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	945	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	975	A

All (17) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	907	C
1	C	909	A
1	C	916	C

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Mol	Chain	Res	Type
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	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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
4	VAA	A	990	-	32,32,32	3.34	12 (37%)	48,48,48	2.19	9 (18%)
4	VAA	B	1990	-	32,32,32	3.21	11 (34%)	48,48,48	2.07	11 (22%)

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
4	VAA	A	990	-	-	0/23/39/39	0/1/3/3
4	VAA	B	1990	-	-	0/23/39/39	0/1/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1990	VAA	S-N5'	8.99	1.69	1.61
4	A	990	VAA	S-N3S	8.83	1.74	1.63
4	B	1990	VAA	S-N3S	8.13	1.73	1.63
4	A	990	VAA	S-N5'	8.08	1.69	1.61
4	A	990	VAA	O1S-S	7.61	1.52	1.43
4	B	1990	VAA	O1S-S	6.58	1.51	1.43
4	A	990	VAA	C5'-N5'	-6.53	1.31	1.47
4	B	1990	VAA	C5'-N5'	-5.89	1.33	1.47
4	A	990	VAA	C4-N9	4.43	1.44	1.37
4	A	990	VAA	O4'-C1'	4.42	1.48	1.41
4	B	1990	VAA	O4'-C1'	4.32	1.48	1.41
4	A	990	VAA	C5'-C4'	-4.17	1.41	1.51
4	B	1990	VAA	C4-N9	4.04	1.43	1.37
4	B	1990	VAA	C5'-C4'	-3.56	1.42	1.51
4	A	990	VAA	C8-N7	-3.41	1.27	1.34
4	B	1990	VAA	C4-N3	3.05	1.40	1.35
4	A	990	VAA	C4-N3	2.99	1.40	1.35
4	B	1990	VAA	C8-N7	-2.94	1.28	1.34
4	A	990	VAA	O2S-S	2.37	1.46	1.43
4	B	1990	VAA	C8-N9	2.28	1.40	1.36
4	A	990	VAA	C8-N9	2.19	1.39	1.36
4	B	1990	VAA	C2-N3	2.13	1.36	1.32
4	A	990	VAA	C2-N3	2.03	1.36	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	990	VAA	C5'-N5'-S	-6.80	106.46	119.14
4	B	1990	VAA	C5'-N5'-S	-6.09	107.80	119.14
4	A	990	VAA	O2S-S-O1S	-6.01	111.01	120.12
4	B	1990	VAA	O2S-S-O1S	-5.20	112.23	120.12
4	A	990	VAA	C-N3S-S	-5.17	117.87	124.35
4	A	990	VAA	C8-N9-C4	-5.03	103.06	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1990	VAA	C8-N9-C4	-4.61	103.38	106.90
4	B	1990	VAA	C-N3S-S	-4.13	119.18	124.35
4	B	1990	VAA	C8-N9-C1'	4.08	134.41	126.38
4	B	1990	VAA	CB-CA-C	-4.06	106.16	111.79
4	A	990	VAA	C8-N9-C1'	3.73	133.74	126.38
4	A	990	VAA	CB-CA-C	-3.63	106.76	111.79
4	B	1990	VAA	O4'-C1'-N9	2.86	111.10	108.44
4	B	1990	VAA	O1S-S-N5'	-2.80	101.73	106.35
4	B	1990	VAA	C1'-N9-C4	-2.56	122.21	126.64
4	A	990	VAA	O1S-S-N5'	-2.50	102.22	106.35
4	B	1990	VAA	O2S-S-N3S	2.40	112.98	106.89
4	A	990	VAA	O2S-S-N3S	2.29	112.70	106.89
4	A	990	VAA	C5'-C4'-C3'	-2.06	112.96	116.76
4	B	1990	VAA	C5'-C4'-C3'	-2.04	113.00	116.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.