



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:50 am BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	<b>NOT EXECUTED</b>
EDS	:	<b>NOT EXECUTED</b>
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

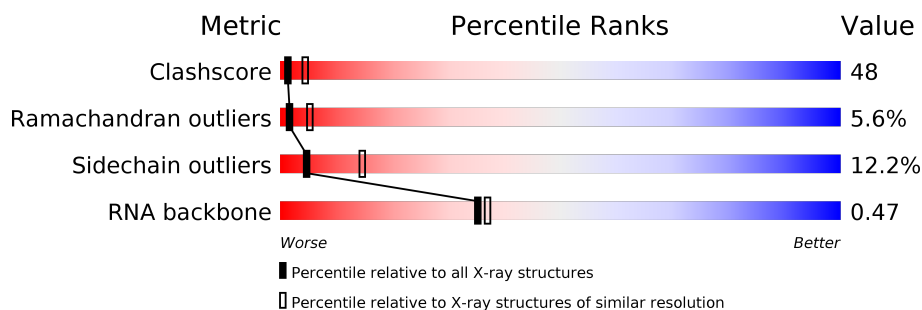
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	75	 27% 39% 35%
1	D	75	 25% 43% 31% .
2	A	862	 37% 52% 9% .
2	B	862	 36% 51% 12% .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17368 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			

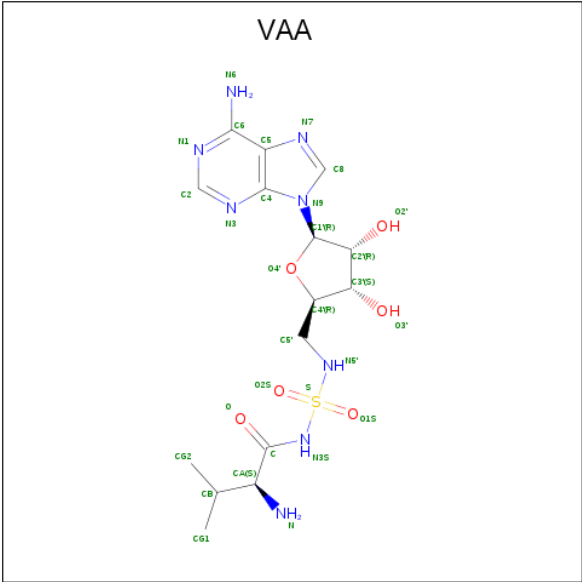
- Molecule 2 is a protein called VALYL-TRNA SYNTHETASE.

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 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: C<sub>15</sub>H<sub>24</sub>N<sub>8</sub>O<sub>6</sub>S).



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.

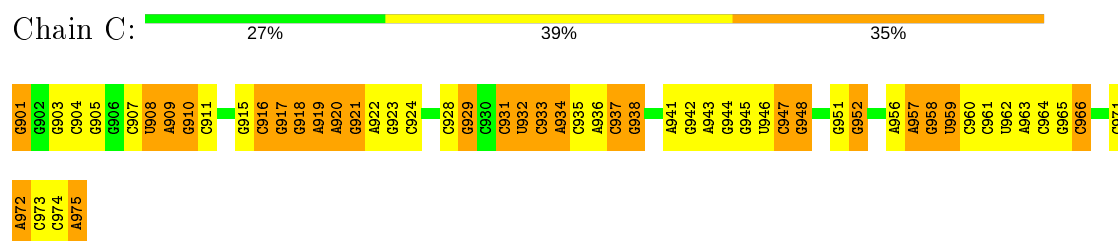
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	19	Total	O	0	0
			19	19		
5	D	11	Total	O	0	0
			11	11		
5	A	67	Total	O	0	0
			67	67		
5	B	61	Total	O	0	0
			61	61		

### 3 Residue-property plots

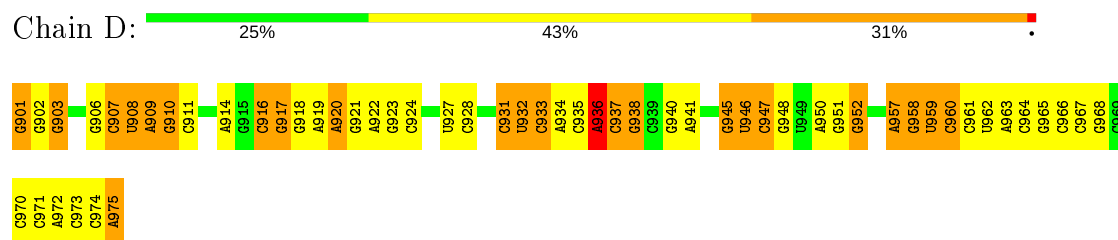
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

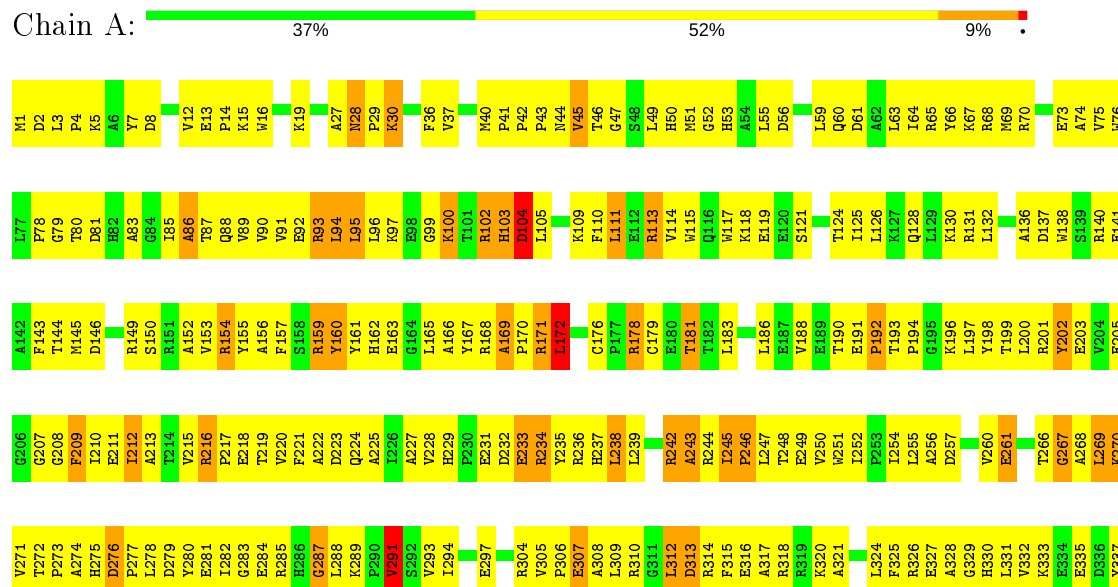
#### • Molecule 1: TRNA(VAL)

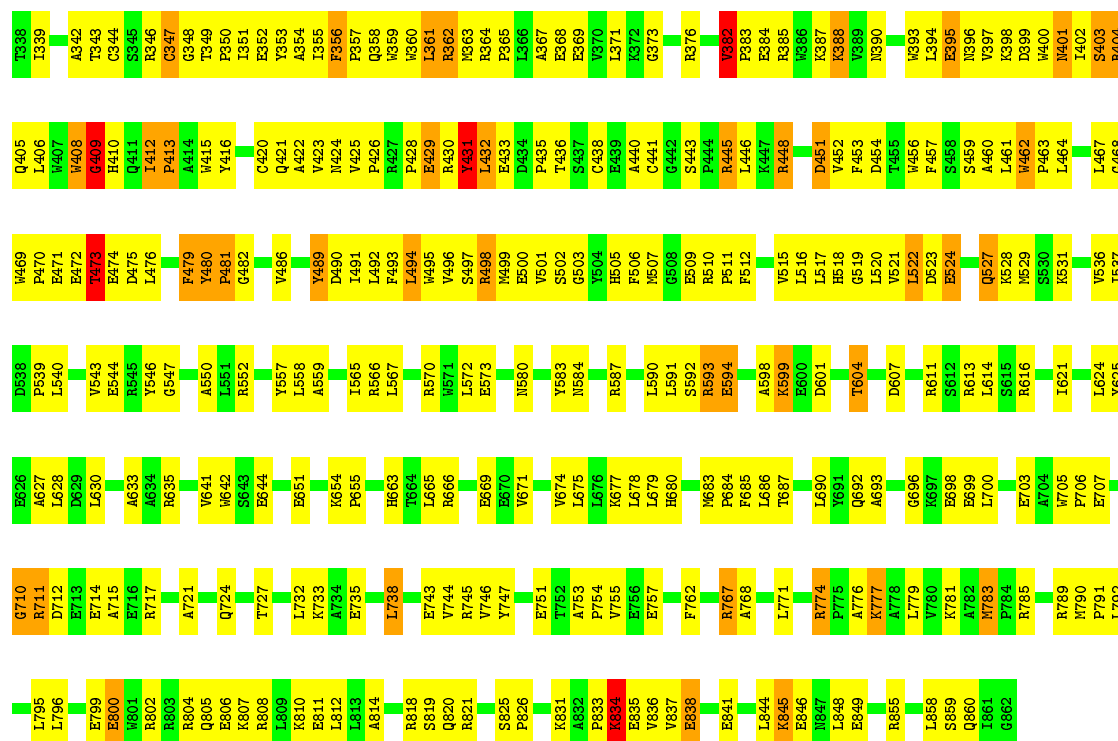


#### • Molecule 1: TRNA(VAL)

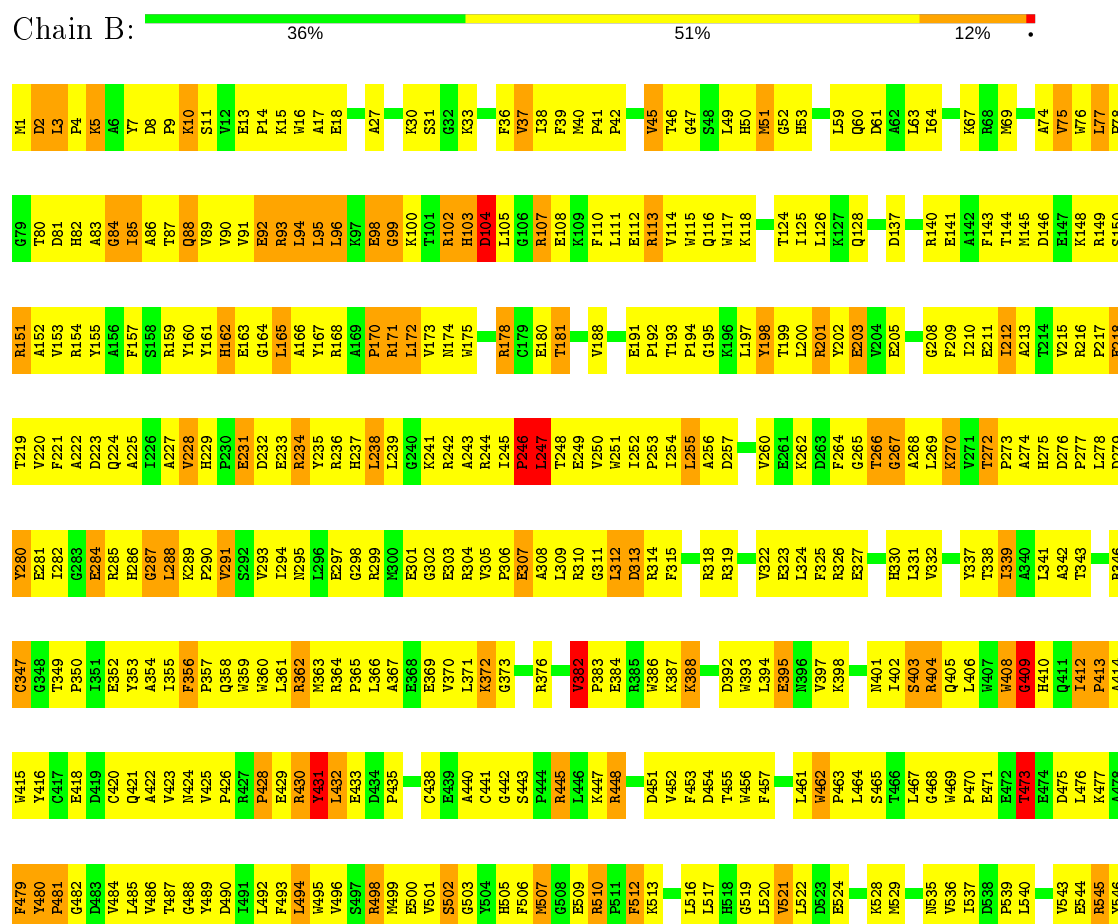


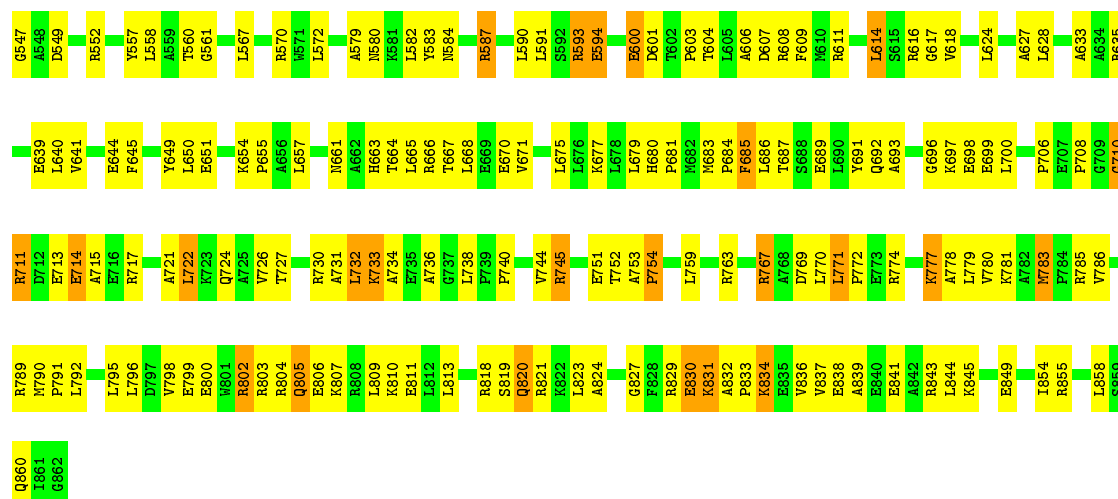
#### • Molecule 2: VALYL-TRNA SYNTHETASE





- Molecule 2: VALYL-TRNA SYNTHETASE





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	52.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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 48.

All (1571) 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: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
1:D:975:A:H3'	2:B:215:VAL:HG23	1.41	1.01
2:A:102:ARG:NH2	2:A:104:ASP:HA	1.76	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	Interatomic distance (Å)	Clash overlap (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
2:B:102:ARG:NH2	2:B:104:ASP:HA	1.83	0.92
1:C:932:U:HO2'	1:C:933:C:H5	0.97	0.92
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:B:777:LYS:N	2:B:777:LYS:HE3	1.85	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:282:ILE:HA	2:B:285:ARG:HD3	1.52	0.90
2:B:412:ILE:HD12	2:B:413:PRO:HD2	1.54	0.90
2:B:745:ARG:HB3	2:B:745:ARG:HH11	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:A:494:LEU:H	2:A:494:LEU:CD2	1.86	0.88
2:B:382:VAL:CG2	2:B:383:PRO:HD3	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:178:ARG:HB2	2:A:178:ARG:NH1	1.89	0.87
2:B:777:LYS:CE	2:B:777:LYS:H	1.85	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:A:680:HIS:HA	2:A:687:THR:HG21	1.58	0.85
2:B:499:MET:CE	2:B:512:PHE:HE2	1.89	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:680:HIS:HA	2:B:687:THR:HG21	1.60	0.84
1:D:918:G:O6	2:B:833:PRO:HD3	1.77	0.84
2:B:93:ARG:HD2	2:B:94:LEU:HG	1.59	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:307:GLU:C	2:B:309:LEU:H	1.79	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:A:460:ALA:HB2	2:A:498:ARG:HB3	1.60	0.83
2:A:371:LEU:HD21	2:A:394:LEU:HB2	1.58	0.83
2:A:777:LYS:HD3	2:A:777:LYS:N	1.93	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:A:289:LYS:HD3	2:A:289:LYS:H	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:418:GLU:OE1	2:B:445:ARG:HD2	1.80	0.81
2:B:778:ALA:HB1	2:B:790:MET:O	1.80	0.81
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:A:326:ARG:HB3	2:A:331:LEU:HD23	1.61	0.80
2:B:529:MET:HE2	2:B:537:ILE:H	1.47	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:412:ILE:HA	2:A:453:PHE:HE1	1.47	0.79
2:A:459:SER:O	2:A:495:TRP:HZ3	1.64	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:A:834:LYS:HD2	2:A:834:LYS:H	1.48	0.78
2:B:745:ARG:HB2	2:B:771:LEU:HD23	1.64	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:A:732:LEU:HD13	2:A:781:LYS:HB2	1.63	0.78
2:B:364:ARG:NH2	2:B:398:LYS:HG3	1.99	0.78
2:A:47:GLY:H	2:A:117:TRP:HZ2	1.30	0.78
1:C:971:C:C2'	1:C:972:A:H5''	2.13	0.78
2:A:521:VAL:HG23	2:A:529:MET:HE3	1.64	0.78
2:A:751:GLU:HB2	2:A:785:ARG:HH21	1.49	0.78
2:B:202:TYR:O	2:B:210:ILE:HG22	1.84	0.78
2:B:819:SER:O	2:B:823:LEU:HD23	1.84	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:359:TRP:HB2	2:B:403:SER:OG	1.85	0.77
2:B:738:LEU:HD23	2:B:744:VAL:HG11	1.67	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:412:ILE:HA	2:A:453:PHE:CE1	2.21	0.75
2:A:50:HIS:CD2	2:A:52:GLY:H	1.97	0.75
2:A:820:GLN:HG2	2:B:844:LEU:HD23	1.68	0.75
2:B:69:MET:HE1	2:B:680:HIS:HB3	1.65	0.75
1:D:975:A:H3'	2:B:215:VAL:CG2	2.15	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:A:593:ARG:HH11	2:A:593:ARG:HG3	1.51	0.75
2:B:91:VAL:O	2:B:96:LEU:HD23	1.86	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:473:THR:HG23	2:A:476:LEU:H	1.49	0.74
2:A:93:ARG:HD2	2:A:94:LEU:HG	1.68	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:A:235:TYR:O	2:A:236:ARG:HD3	1.87	0.74
2:B:448:ARG:N	2:B:448:ARG:HD3	2.01	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:A:845:LYS:O	2:A:849:GLU:HG3	1.89	0.72
2:A:85:ILE:O	2:A:89:VAL:HG23	1.89	0.72
2:B:201:ARG:HB3	2:B:211:GLU:HA	1.70	0.72
2:B:361:LEU:HB2	2:B:402:ILE:CD1	2.19	0.72
2:A:202:TYR:O	2:A:210:ILE:HG22	1.88	0.72
2:A:28:ASN:HD21	2:A:30:LYS:CG	1.94	0.72
2:A:666:ARG:HH11	2:A:666:ARG:HG3	1.54	0.72
2:B:228:VAL:O	2:B:256:ALA:HA	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:557:TYR:CE1	2:A:635:ARG:HB3	2.24	0.71
2:B:352:GLU:HG2	2:B:353:TYR:N	2.05	0.71
2:A:178:ARG:HH11	2:A:178:ARG:CB	2.04	0.71
2:B:494:LEU:CD2	2:B:494:LEU:H	2.02	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:A:428:PRO:HB2	2:A:429:GLU:OE1	1.91	0.71
2:B:13:GLU:HA	2:B:685:PHE:HD2	1.55	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
2:A:431:TYR:CE1	2:A:432:LEU:HD12	2.26	0.71
2:B:480:TYR:O	2:B:482:GLY:N	2.23	0.71
1:D:975:A:H8	2:B:213:ALA:O	1.72	0.71
1:D:902:G:C3'	1:D:903:G:H5''	2.20	0.70
2:A:201:ARG:HG2	2:A:211:GLU:HB3	1.71	0.70
2:B:245:ILE:HG13	2:B:252:ILE:HD13	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:A:501:VAL:HG12	2:A:502:SER:N	2.06	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: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
2:A:45:VAL:HG23	2:A:81:ASP:O	1.92	0.70
2:B:150:SER:O	2:B:153:VAL:HG22	1.92	0.70
2:B:173:VAL:C	2:B:174:ASN:HD22	1.95	0.70
2:B:540:LEU:O	2:B:543:VAL:HG22	1.92	0.70
2:B:651:GLU:HA	2:B:651:GLU:OE1	1.91	0.70
1:C:957:A:H4'	1:C:958:G:OP1	1.91	0.70
2:A:5:LYS:N	2:A:5:LYS:HD2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:92:GLU:HA	2:A:96:LEU:HD12	1.75	0.69
2:B:77:LEU:H	2:B:77:LEU:HD12	1.57	0.69
2:A:242:ARG:NH1	2:A:251:TRP:HB3	2.06	0.69
2:A:331:LEU:HD12	2:A:332:VAL:H	1.58	0.69
2:A:105:LEU:H	2:A:105:LEU:HD23	1.57	0.69
2:B:324:LEU:H	2:B:324:LEU:HD22	1.56	0.69
2:B:361:LEU:HB2	2:B:402:ILE:HD11	1.74	0.69
2:B:473:THR:CG2	2:B:476:LEU:H	2.06	0.69
2:B:486:VAL:HG22	2:B:516:LEU:HD22	1.75	0.69
2:A:171:ARG:NH2	2:A:364:ARG:NH2	2.38	0.69
2:B:220:VAL:HG21	2:B:325:PHE:HZ	1.56	0.69
2:B:382:VAL:HG11	2:B:516:LEU:CD1	2.20	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:153:VAL:HG23	2:A:154:ARG:N	2.08	0.68
2:A:224:GLN:HE22	2:A:304:ARG:NH2	1.92	0.68
2:A:441:CYS:SG	2:A:443:SER:HB3	2.32	0.68
2:B:248:THR:HG23	2:B:250:VAL:N	2.06	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:99:GLY:O	2:A:100:LYS:HG2	1.93	0.68
2:A:248:THR:HG23	2:A:250:VAL:N	2.08	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:260:VAL:HG22	2:B:269:LEU:CD2	2.23	0.67
2:B:680:HIS:HD2	2:B:687:THR:CG2	2.07	0.67
2:A:304:ARG:HG3	2:A:304:ARG:NH1	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:VAL:HG23	2:B:383:PRO:HD2	1.75	0.67
1:D:922:A:H2'	1:D:923:G:H8	1.60	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:B:82:HIS:O	2:B:87:THR:OG1	2.11	0.67
2:A:126:LEU:O	2:A:130:LYS:HG2	1.94	0.67
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:A:233:GLU:HB2	2:A:237:HIS:HE1	1.60	0.67
2:B:171:ARG:HH12	2:B:364:ARG:HH21	1.41	0.67
2:B:545:ARG:HB3	2:B:546:TYR:CD1	2.30	0.67
2:A:233:GLU:O	2:A:234:ARG:O	2.12	0.67
2:A:332:VAL:HG22	2:A:333:LYS:N	2.09	0.67
2:A:497:SER:HA	2:A:500:GLU:OE1	1.94	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:B:384:GLU:N	5:B:2040:HOH:O	2.28	0.67
2:B:464:LEU:HB3	2:B:469:TRP:HB3	1.77	0.67
2:A:234:ARG:HH22	2:A:267:GLY:H	1.42	0.67
2:A:218:GLU:CD	2:A:318:ARG:HB3	2.15	0.67
2:A:382:VAL:CG2	2:A:517:LEU:H	2.07	0.67
2:B:480:TYR:HB3	2:B:481:PRO:HD3	1.77	0.67
2:B:802:ARG:HG3	2:B:803:ARG:N	2.08	0.67
2:A:167:TYR:CE2	2:A:360:TRP:HB2	2.30	0.67
2:B:270:LYS:CB	2:B:270:LYS:HZ2	2.08	0.67
2:B:404:ARG:HG2	2:B:406:LEU:HD12	1.75	0.67
2:A:416:TYR:CD2	2:A:423:VAL:HG12	2.31	0.66
2:B:245:ILE:HB	2:B:248:THR:HG22	1.74	0.66
2:B:830:GLU:HG2	2:B:831:LYS:NZ	2.10	0.66
2:A:289:LYS:H	2:A:289:LYS:CD	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:VAL:HG13	2:B:310:ARG:HD3	1.78	0.66
2:B:468:GLY:C	2:B:470:PRO:HD2	2.16	0.66
2:B:496:VAL:O	2:B:500:GLU:HG3	1.96	0.66
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:B:277:PRO:HD3	2:B:353:TYR:CD2	2.30	0.65
2:A:224:GLN:NE2	2:A:304:ARG:NH2	2.43	0.65
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:A:469:TRP:O	2:A:470:PRO:C	2.34	0.65
2:B:307:GLU:C	2:B:309:LEU:N	2.50	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:832:ALA:HB1	2:B:833:PRO:HD2	1.79	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:B:415:TRP:CE3	2:B:448:ARG:HB3	2.32	0.65
2:A:94:LEU:HB2	2:A:95:LEU:HD22	1.78	0.65
2:A:845:LYS:NZ	2:B:820:GLN:HE22	1.94	0.65
1:C:947:C:H2'	1:C:958:G:O2'	1.97	0.65
2:B:349:THR:HG23	2:B:350:PRO:HD2	1.79	0.65
2:B:501:VAL:HG13	2:B:502:SER:H	1.62	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:A:480:TYR:HB3	2:A:481:PRO:HD3	1.79	0.64
2:B:545:ARG:HD2	2:B:546:TYR:CE1	2.31	0.64
2:A:201:ARG:CD	2:A:211:GLU:HB3	2.27	0.64
2:A:250:VAL:HG21	2:A:304:ARG:HD2	1.78	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:A:343:THR:HA	2:A:350:PRO:HA	1.78	0.64
2:B:92:GLU:HG3	2:B:102:ARG:HD2	1.78	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:B:448:ARG:HB2	5:B:2029:HOH:O	1.96	0.64
2:A:314:ARG:NH2	2:A:352:GLU:HG3	2.12	0.64
2:B:47:GLY:N	2:B:117:TRP:HZ2	1.96	0.64
2:B:412:ILE:HD12	2:B:413:PRO:CD	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:ARG:HG3	2:A:159:ARG:HH11	1.63	0.64
2:B:126:LEU:HD11	2:B:141:GLU:OE1	1.98	0.64
2:B:392:ASP:HA	2:B:395:GLU:HB2	1.80	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
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:A:19:LYS:HE2	2:A:699:GLU:OE2	1.98	0.63
2:A:289:LYS:HD3	2:A:289:LYS:N	2.13	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:202:TYR:HE1	2:A:330:HIS:ND1	1.97	0.63
2:B:372:LYS:NZ	2:B:372:LYS:HA	2.12	0.63
2:B:591:LEU:O	2:B:594:GLU:HB2	1.99	0.63
2:B:651:GLU:OE1	2:B:654:LYS:HE3	1.98	0.63
2:A:382:VAL:HG21	2:A:516:LEU:HA	1.80	0.63
2:A:522:LEU:HB3	2:A:528:LYS:HA	1.80	0.63
2:B:654:LYS:HB2	2:B:655:PRO:HD3	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:372:LYS:HZ3	2:B:372:LYS:HA	1.64	0.63
2:B:86:ALA:O	2:B:90:VAL:HG23	1.98	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:420:CYS:HB2	2:A:441:CYS:HB3	1.80	0.62
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: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:A:37:VAL:CG2	2:A:479:PHE:HB2	2.27	0.62
2:A:503:GLY:HA3	2:A:511:PRO:HG3	1.82	0.62
2:B:201:ARG:HE	2:B:211:GLU:CB	1.96	0.62
2:B:304:ARG:NH1	2:B:304:ARG:HG3	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:HIS:HB2	2:B:408:TRP:HE1	1.61	0.62
2:A:315:PHE:O	2:A:318:ARG:HG2	2.00	0.62
2:A:593:ARG:HG3	2:A:593:ARG:NH1	2.14	0.62
2:B:785:ARG:HA	2:B:785:ARG:NH1	2.09	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:A:387:LYS:HB3	2:A:388:LYS:NZ	2.15	0.62
2:A:451:ASP:O	2:A:452:VAL:HG23	2.00	0.62
2:B:153:VAL:CG2	2:B:154:ARG:H	2.12	0.62
2:B:412:ILE:HA	2:B:453:PHE:CE1	2.34	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
2:A:733:LYS:NZ	2:A:767:ARG:HB3	2.14	0.62
2:B:153:VAL:CG2	2:B:154:ARG:N	2.62	0.62
1:C:973:C:O2	2:A:278:LEU:HD13	2.00	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: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:83:ALA:HB3	2:A:87:THR:OG1	2.00	0.61
2:A:85:ILE:O	2:A:88:GLN:HB3	2.00	0.61
2:A:224:GLN:HE22	2:A:304:ARG:HH22	1.46	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
2:B:306:PRO:HD2	2:B:309:LEU:HD23	1.82	0.61
2:B:492:LEU:HD12	2:B:496:VAL:HB	1.82	0.61
1:D:974:C:O2'	1:D:975:A:H5''	2.00	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
2:A:41:PRO:O	2:A:43:PRO:HD3	2.00	0.61
2:B:102:ARG:HH21	2:B:104:ASP:HA	1.62	0.61
2:B:49:LEU:HD21	2:B:125:ILE:HG23	1.81	0.61
1:D:973:C:H1'	2:B:278:LEU:HB2	1.81	0.61
2:B:469:TRP:C	2:B:471:GLU:N	2.49	0.61
2:A:105:LEU:O	2:A:109:LYS:HB2	2.00	0.61
2:A:692:GLN:NE2	2:A:698:GLU:HA	2.14	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:837:VAL:HG13	2:A:838:GLU:N	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:331:LEU:HD12	2:A:332:VAL:N	2.16	0.61
1:C:928:C:C3'	1:C:929:G:H5''	2.31	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:270:LYS:HZ2	2:B:270:LYS:HB3	1.64	0.60
2:B:363:MET:HE3	2:B:363:MET:HA	1.83	0.60
2:A:183:LEU:HD21	2:A:344:CYS:SG	2.41	0.60
2:A:201:ARG:HG2	2:A:211:GLU:CA	2.31	0.60
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:A:665:LEU:O	2:A:669:GLU:HG3	2.01	0.60
2:B:415:TRP:CZ3	2:B:448:ARG:HB3	2.36	0.60
2:B:650:LEU:HD23	2:B:650:LEU:O	2.00	0.60
1:C:931:C:H4'	1:C:932:U:OP2	2.00	0.60
2:A:242:ARG:HH11	2:A:242:ARG:CB	2.12	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:B:494:LEU:N	2:B:494:LEU:HD23	2.10	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
2:B:382:VAL:CG1	2:B:516:LEU:HD12	2.27	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:A:841:GLU:OE1	2:B:824:ALA:HA	2.00	0.60
2:B:272:THR:H	2:B:279:ASP:HB3	1.66	0.60
2:B:367:ALA:O	2:B:371:LEU:HG	2.02	0.60
2:A:92:GLU:O	2:A:96:LEU:HB2	2.02	0.60
2:B:40:MET:HA	2:B:60:GLN:HE22	1.67	0.60
2:B:161:TYR:CD1	2:B:425:VAL:HB	2.37	0.60
1:C:918:G:N2	1:C:956:A:H1'	2.17	0.60
2:A:5:LYS:H	2:A:5:LYS:CD	2.09	0.60
4:B:1990:VAA:H5'1	4:B:1990:VAA:O	2.01	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: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
2:B:161:TYR:CE1	2:B:425:VAL:HB	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:429:GLU:H	2:A:429:GLU:CD	2.04	0.59
2:A:680:HIS:CD2	2:A:687:THR:CG2	2.81	0.59
2:A:744:VAL:O	2:A:768:ALA:HA	2.02	0.59
2:B:341:LEU:CD1	2:B:343:THR:HG23	2.32	0.59
2:B:480:TYR:HE2	2:B:509:GLU:HG3	1.67	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
2:A:118:LYS:O	2:A:118:LYS:HD3	2.01	0.59
2:A:201:ARG:CG	2:A:211:GLU:HB3	2.33	0.59
2:A:155:TYR:HD1	2:A:431:TYR:CD2	2.21	0.59
2:B:220:VAL:HG21	2:B:325:PHE:CZ	2.37	0.59
2:B:834:LYS:O	2:B:838:GLU:HG2	2.03	0.59
1:C:961:C:O2'	1:C:962:U:H5'	2.03	0.59
2:A:361:LEU:HB2	2:A:402:ILE:HD13	1.85	0.59
2:A:529:MET:HG2	2:A:536:VAL:HG12	1.85	0.59
2:A:592:SER:C	2:A:594:GLU:H	2.04	0.59
2:A:69:MET:HB2	2:A:703:GLU:O	2.03	0.59
2:A:225:ALA:CA	2:A:252:ILE:HG23	2.27	0.59
2:A:515:VAL:HG12	2:A:517:LEU:HD22	1.84	0.59
2:A:771:LEU:HD11	2:A:791:PRO:HG2	1.83	0.59
2:B:153:VAL:HG23	2:B:154:ARG:H	1.65	0.59
2:B:362:ARG:O	2:B:365:PRO:HD2	2.02	0.59
2:B:13:GLU:HA	2:B:685:PHE:CD2	2.37	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:152:ALA:HA	2:B:470:PRO:HB3	1.85	0.59
2:A:810:LYS:CE	2:B:855:ARG:HH22	2.16	0.59
2:B:85:ILE:HG23	2:B:86:ALA:N	2.18	0.59
2:A:145:MET:HG2	2:A:410:HIS:CD2	2.37	0.58
2:B:297:GLU:N	2:B:297:GLU:OE2	2.36	0.58
2:B:387:LYS:HB3	2:B:388:LYS:HZ1	1.68	0.58
2:B:394:LEU:O	2:B:397:VAL:HG23	2.03	0.58
2:B:593:ARG:HG3	2:B:593:ARG:NH1	2.15	0.58
2:B:805:GLN:H	2:B:805:GLN:NE2	2.00	0.58
1:D:964:C:H2'	1:D:965:G:C8	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:146:ASP:OD1	2:B:149:ARG:HB2	2.02	0.58
2:B:312:LEU:CG	2:B:313:ASP:H	2.16	0.58
2:B:464:LEU:HB3	2:B:469:TRP:CB	2.33	0.58
2:B:172:LEU:HD23	2:B:354:ALA:O	2.03	0.58
2:B:178:ARG:HG2	2:B:347:CYS:SG	2.42	0.58
2:B:202:TYR:CG	2:B:203:GLU:N	2.70	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:516:LEU:HD12	2:B:628:LEU:HD13	1.86	0.58
2:A:245:ILE:HG22	2:A:252:ILE:HD13	1.85	0.58
2:A:385:ARG:HH11	2:A:385:ARG:HG3	1.68	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
2:A:274:ALA:HB2	2:A:291:VAL:H	1.67	0.58
2:A:346:ARG:HB2	2:A:346:ARG:NH1	2.19	0.58
2:B:151:ARG:HG2	2:B:151:ARG:HH11	1.67	0.58
2:B:198:TYR:N	2:B:198:TYR:CD2	2.71	0.58
2:B:217:PRO:O	2:B:220:VAL:HG22	2.04	0.58
2:B:234:ARG:NH1	2:B:235:TYR:HB2	2.18	0.58
2:B:467:LEU:O	2:B:473:THR:HG21	2.03	0.58
2:B:225:ALA:CA	2:B:252:ILE:HG23	2.27	0.58
2:B:50:His:HD2	2:B:52:GLY:N	2.00	0.58
2:B:684:PRO:O	2:B:687:THR:HG22	2.03	0.58
2:A:244:ARG:HB2	2:A:251:TRP:CZ2	2.39	0.58
2:A:248:THR:OG1	2:A:250:VAL:HG23	2.03	0.58
2:B:160:TYR:HE2	2:B:505:His:CD2	2.22	0.58
2:A:855:ARG:HD3	2:B:813:LEU:HD12	1.84	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:A:242:ARG:O	2:A:243:ALA:HB2	2.04	0.58
2:B:1:MET:HE3	2:B:693:ALA:HB3	1.86	0.58
2:B:202:TYR:CE2	2:B:244:ARG:NE	2.72	0.58
2:B:322:VAL:O	2:B:325:PHE:HB2	2.03	0.58
2:B:480:TYR:O	2:B:481:PRO:C	2.42	0.58
2:A:153:VAL:CG2	2:A:154:ARG:N	2.66	0.58
2:A:358:GLN:NE2	2:A:405:GLN:HE22	1.99	0.58
2:A:367:ALA:O	2:A:371:LEU:HG	2.04	0.58
2:A:833:PRO:C	2:A:835:GLU:H	2.06	0.58
2:B:151:ARG:NH1	2:B:151:ARG:HG2	2.19	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:188:VAL:HG23	2:A:343:THR:O	2.04	0.57
2:B:105:LEU:H	2:B:105:LEU:HD23	1.68	0.57
2:B:198:TYR:N	2:B:198:TYR:HD2	2.02	0.57
2:B:84:GLY:HA2	2:B:408:TRP:HD1	1.69	0.57
2:A:598:ALA:O	2:A:599:LYS:HE2	2.03	0.57
2:B:172:LEU:HD21	2:B:353:TYR:HB3	1.85	0.57
1:D:973:C:O2	1:D:973:C:H2'	2.04	0.57
2:A:515:VAL:HG12	2:A:517:LEU:CD2	2.35	0.57
2:B:286:HIS:HB2	2:B:288:LEU:HD21	1.86	0.57
2:B:805:GLN:N	2:B:805:GLN:HE21	2.02	0.57
2:A:170:PRO:O	2:A:171:ARG:C	2.42	0.57
2:A:202:TYR:OH	2:A:244:ARG:CZ	2.52	0.57
2:A:312:LEU:HG	2:A:313:ASP:N	2.20	0.57
2:A:45:VAL:HG12	2:A:121:SER:HB3	1.87	0.57
2:A:486:VAL:HG22	2:A:516:LEU:CD2	2.34	0.57
2:B:146:ASP:OD2	2:B:149:ARG:NH2	2.33	0.57
2:B:245:ILE:CB	2:B:248:THR:HG22	2.35	0.57
2:B:488:GLY:O	2:B:490:ASP:N	2.36	0.57
1:C:918:G:O6	2:A:833:PRO:HD2	2.03	0.57
4:A:990:VAA:O	4:A:990:VAA:H5'1	2.04	0.57
2:B:830:GLU:C	2:B:831:LYS:HE3	2.24	0.57
2:B:666:ARG:NH2	5:B:1993:HOH:O	2.33	0.57
2:B:409:GLY:HA3	2:B:452:VAL:CG1	2.34	0.57
2:B:59:LEU:O	2:B:63:LEU:HD23	2.04	0.57
2:A:118:LYS:C	2:A:118:LYS:HD3	2.25	0.57
2:A:172:LEU:HB2	2:A:354:ALA:O	2.05	0.57
2:A:382:VAL:O	2:A:383:PRO:C	2.41	0.57
2:A:453:PHE:CD2	2:A:457:PHE:CD2	2.93	0.57
2:A:3:LEU:HD21	2:A:590:LEU:HD12	1.85	0.57
2:B:248:THR:CG2	2:B:249:GLU:H	2.13	0.57
2:B:469:TRP:O	2:B:470:PRO:C	2.41	0.57
2:B:677:LYS:HD2	2:B:706:PRO:HG3	1.86	0.57
2:B:87:THR:O	2:B:91:VAL:HG23	2.05	0.57
2:A:383:PRO:O	2:A:384:GLU:HB3	2.04	0.56
2:B:287:GLY:C	2:B:288:LEU:HD23	2.25	0.56
2:B:680:HIS:CD2	2:B:687:THR:CG2	2.88	0.56
2:A:855:ARG:CD	2:B:809:LEU:HD12	2.35	0.56
2:B:93:ARG:HH11	2:B:93:ARG:HG3	1.70	0.56
1:C:932:U:O2	1:C:932:U:H2'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:313:ASP:O	2:A:317:ALA:HB2	2.04	0.56
2:A:844:LEU:HD23	2:B:820:GLN:HG2	1.87	0.56
1:D:973:C:C2	2:B:278:LEU:HD13	2.40	0.56
2:B:303:GLU:OE2	2:B:303:GLU:HA	2.04	0.56
2:B:324:LEU:N	2:B:324:LEU:HD22	2.20	0.56
2:B:603:PRO:HA	2:B:663:HIS:CD2	2.39	0.56
2:A:238:LEU:HD23	2:A:238:LEU:H	1.71	0.56
2:B:233:GLU:CD	2:B:234:ARG:N	2.58	0.56
2:B:415:TRP:HB2	2:B:424:ASN:HB2	1.87	0.56
2:B:149:ARG:NH1	2:B:465:SER:O	2.36	0.56
2:A:217:PRO:O	2:A:220:VAL:HG13	2.05	0.56
2:A:394:LEU:O	2:A:397:VAL:HG23	2.06	0.56
2:A:819:SER:HB2	2:A:844:LEU:HD13	1.87	0.56
2:B:529:MET:HE2	2:B:536:VAL:HA	1.87	0.56
1:C:971:C:C3'	1:C:972:A:H5''	2.35	0.56
2:A:236:ARG:HA	2:A:238:LEU:CD2	2.35	0.56
2:A:61:ASP:OD1	2:A:65:ARG:HG3	2.06	0.56
1:D:933:C:H3'	1:D:933:C:H6	1.70	0.56
2:B:238:LEU:O	2:B:254:ILE:HG21	2.05	0.56
2:B:462:TRP:C	2:B:464:LEU:N	2.57	0.56
2:A:234:ARG:C	2:A:236:ARG:H	2.08	0.56
2:A:245:ILE:HG23	2:A:248:THR:HG21	1.88	0.56
2:B:188:VAL:HG23	2:B:343:THR:O	2.05	0.56
2:B:501:VAL:CG1	2:B:502:SER:H	2.19	0.56
2:B:726:VAL:HG12	2:B:730:ARG:NH1	2.20	0.56
2:A:229:HIS:CD2	2:A:231:GLU:H	2.24	0.56
2:A:393:TRP:CE3	2:A:394:LEU:HD23	2.40	0.56
2:A:833:PRO:HB2	2:A:836:VAL:HG12	1.88	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: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
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:152:ALA:HB2	2:B:470:PRO:HD3	1.88	0.56
2:B:557:TYR:CE1	2:B:635:ARG:HB3	2.41	0.56
1:C:973:C:O2'	1:C:974:C:H5''	2.06	0.56
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
2:B:456:TRP:CE3	2:B:494:LEU:O	2.59	0.55
1:D:916:C:H5''	1:D:917:G:OP1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:322:VAL:HG13	2:B:323:GLU:OE1	2.06	0.55
2:B:361:LEU:HD21	2:B:366:LEU:CD1	2.33	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
2:B:501:VAL:CG1	2:B:502:SER:N	2.69	0.55
2:B:85:ILE:HG23	2:B:86:ALA:H	1.71	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
2:A:159:ARG:CG	2:A:159:ARG:HH11	2.18	0.55
2:A:271:VAL:HG12	2:A:273:PRO:HD3	1.88	0.55
2:B:795:LEU:O	2:B:796:LEU:HD23	2.06	0.55
1:C:974:C:O2'	1:C:975:A:H5''	2.06	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:178:ARG:HA	2:B:178:ARG:HE	1.72	0.54
2:B:232:ASP:OD1	2:B:234:ARG:NE	2.40	0.54
2:A:310:ARG:HG3	2:A:310:ARG:O	2.07	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: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:B:516:LEU:HD13	2:B:628:LEU:HD22	1.89	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:266:THR:O	2:A:268:ALA:N	2.40	0.54
2:A:64:ILE:HG13	2:A:76:TRP:HB2	1.89	0.54
2:A:724:GLN:HE22	2:A:785:ARG:N	2.05	0.54
2:A:799:GLU:O	2:A:802:ARG:HB3	2.07	0.54
2:B:200:LEU:HD21	2:B:325:PHE:CD1	2.43	0.54
1:D:927:U:O2'	1:D:928:C:H5'	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:246:PRO:O	2:A:247:LEU:HB2	2.06	0.54
2:B:107:ARG:HB3	2:B:107:ARG:HH11	1.71	0.54
2:B:627:ALA:O	2:B:628:LEU:HB2	2.06	0.54
2:A:260:VAL:HG22	2:A:269:LEU:HD21	1.89	0.54
2:A:326:ARG:HA	2:A:331:LEU:HB3	1.90	0.54
2:A:498:ARG:HH11	2:A:498:ARG:HG2	1.72	0.54
2:B:233:GLU:O	2:B:235:TYR:N	2.41	0.54
1:D:918:G:O6	2:B:833:PRO:CD	2.54	0.54
2:A:233:GLU:HB2	2:A:237:HIS:CE1	2.41	0.54
2:A:393:TRP:HB2	2:A:493:PHE:CE2	2.43	0.54
2:A:712:ASP:HB3	2:A:715:ALA:HB3	1.89	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:C:947:C:O2'	1:C:948:G:P	2.65	0.54
1:D:933:C:C6	1:D:933:C:H3'	2.43	0.54
2:B:341:LEU:C	2:B:341:LEU:HD13	2.27	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:366:LEU:HB3	2:B:501:VAL:HG21	1.90	0.53
2:B:487:THR:O	2:B:517:LEU:HA	2.08	0.53
2:B:680:HIS:HD2	2:B:684:PRO:HA	1.71	0.53
2:A:4:PRO:O	2:A:587:ARG:NE	2.41	0.53
2:A:326:ARG:C	2:A:328:ALA:H	2.12	0.53
2:A:145:MET:HG2	2:A:410:HIS:NE2	2.23	0.53
2:A:680:HIS:CD2	2:A:684:PRO:HA	2.44	0.53
2:B:211:GLU:C	2:B:266:THR:HG21	2.28	0.53
2:B:543:VAL:HG23	2:B:544:GLU:N	2.23	0.53
1:C:922:A:H2'	1:C:923:G:C8	2.43	0.53
1:C:973:C:H1'	2:A:278:LEU:HB2	1.88	0.53
2:A:171:ARG:NH2	2:A:364:ARG:HH21	2.04	0.53
2:A:242:ARG:NH1	2:A:251:TRP:CB	2.70	0.53
2:A:476:LEU:C	2:A:476:LEU:HD23	2.28	0.53
2:A:855:ARG:HH22	2:B:810:LYS:CE	2.11	0.53
2:A:221:PHE:O	2:A:304:ARG:NH1	2.42	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:202:TYR:HE2	2:B:244:ARG:CD	2.22	0.53
2:B:245:ILE:O	2:B:248:THR:HG22	2.08	0.53
2:B:692:GLN:O	2:B:696:GLY:N	2.40	0.53
2:B:785:ARG:CA	2:B:785:ARG:HH11	2.14	0.53
2:A:307:GLU:C	2:A:309:LEU:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:393:TRP:HE3	2:A:394:LEU:HD23	1.74	0.53
2:A:462:TRP:C	2:A:464:LEU:N	2.62	0.53
2:A:666:ARG:HH11	2:A:666:ARG:CG	2.20	0.53
2:B:383:PRO:HG2	5:B:2016:HOH:O	2.09	0.53
2:B:428:PRO:O	2:B:431:TYR:HB3	2.07	0.53
2:A:318:ARG:HA	2:A:321:ALA:HB3	1.91	0.53
2:B:305:VAL:HG22	2:B:310:ARG:HB2	1.90	0.53
2:B:387:LYS:HB3	2:B:388:LYS:NZ	2.24	0.53
2:B:738:LEU:HD23	2:B:744:VAL:CG1	2.38	0.53
2:B:777:LYS:O	2:B:777:LYS:HD2	2.09	0.53
2:A:467:LEU:O	2:A:473:THR:HG21	2.09	0.53
2:A:131:ARG:O	2:A:131:ARG:HD2	2.09	0.53
2:A:186:LEU:H	2:A:186:LEU:CD1	2.16	0.53
2:A:522:LEU:CD1	2:A:566:ARG:HA	2.39	0.53
2:A:724:GLN:NE2	2:A:785:ARG:HB2	2.24	0.53
2:B:382:VAL:C	2:B:384:GLU:N	2.59	0.53
2:B:462:TRP:H	2:B:463:PRO:HD2	1.73	0.53
2:B:778:ALA:HB1	2:B:790:MET:C	2.29	0.53
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: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:382:VAL:O	2:B:383:PRO:C	2.43	0.52
2:B:820:GLN:NE2	2:B:821:ARG:N	2.57	0.52
1:D:973:C:O2'	1:D:974:C:H5''	2.08	0.52
2:B:326:ARG:CG	2:B:327:GLU:N	2.72	0.52
2:B:352:GLU:HA	5:B:2001:HOH:O	2.09	0.52
2:B:5:LYS:CD	2:B:5:LYS:H	2.02	0.52
2:B:710:GLY:O	2:B:711:ARG:HB3	2.10	0.52
2:A:306:PRO:HD2	2:A:309:LEU:HD23	1.90	0.52
2:B:124:THR:O	2:B:128:GLN:HG3	2.09	0.52
2:B:171:ARG:HH22	2:B:398:LYS:CG	2.21	0.52
2:B:487:THR:HG23	2:B:517:LEU:CD2	2.39	0.52
2:B:680:HIS:CA	2:B:687:THR:HG21	2.37	0.52
2:A:202:TYR:OH	2:A:244:ARG:NH2	2.42	0.52
2:A:424:ASN:HD22	2:A:446:LEU:CD2	2.23	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:A:332:VAL:HG22	2:A:333:LYS:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:469:TRP:C	2:A:471:GLU:N	2.58	0.52
2:A:540:LEU:HA	2:A:543:VAL:HG13	1.92	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:97:LYS:HG2	2:A:102:ARG:HB3	1.92	0.52
2:A:154:ARG:HG3	2:A:154:ARG:HH11	1.75	0.52
2:A:1:MET:CE	2:A:690:LEU:HD23	2.38	0.52
2:A:168:ARG:HA	2:A:358:GLN:O	2.10	0.52
2:A:387:LYS:HB3	2:A:388:LYS:HZ2	1.73	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:A:359:TRP:H	2:A:403:SER:HG	1.55	0.52
2:B:414:ALA:HA	2:B:425:VAL:HG22	1.92	0.52
2:B:687:THR:HG23	2:B:700:LEU:HD23	1.92	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
2:B:155:TYR:HD1	2:B:431:TYR:CD2	2.27	0.52
2:B:469:TRP:O	2:B:471:GLU:N	2.43	0.52
2:B:501:VAL:C	2:B:503:GLY:H	2.12	0.52
1:D:940:G:O2'	1:D:941:A:H5'	2.10	0.52
2:A:126:LEU:HD11	2:A:141:GLU:OE1	2.10	0.52
2:A:157:PHE:HD2	2:A:413:PRO:HG2	1.75	0.52
2:B:210:ILE:HG23	2:B:210:ILE:O	2.10	0.52
2:B:371:LEU:HD21	2:B:394:LEU:CB	2.39	0.52
2:B:382:VAL:O	2:B:384:GLU:N	2.43	0.52
2:B:3:LEU:HD11	2:B:590:LEU:CD1	2.40	0.52
2:B:506:PHE:C	2:B:507:MET:HG2	2.29	0.52
2:B:616:ARG:HG2	5:B:2024:HOH:O	2.09	0.52
2:A:181:THR:OG1	2:A:404:ARG:HG3	2.10	0.52
2:B:148:LYS:HE2	5:B:2027:HOH:O	2.10	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:A:88:GLN:NE2	2:A:110:PHE:CE2	2.78	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:B:805:GLN:HB3	2:B:858:LEU:HD21	1.91	0.51
2:A:199:THR:O	2:A:332:VAL:HG13	2.10	0.51
2:A:306:PRO:HG2	2:A:309:LEU:CB	2.40	0.51
2:A:591:LEU:O	2:A:594:GLU:HB2	2.10	0.51
2:A:593:ARG:HB2	2:A:665:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:160:TYR:HB3	2:A:166:ALA:HB2	1.92	0.51
2:A:250:VAL:HG12	2:A:252:ILE:HD12	1.93	0.51
2:A:316:GLU:OE1	2:A:316:GLU:HA	2.11	0.51
2:B:224:GLN:O	2:B:225:ALA:HB2	2.09	0.51
2:B:266:THR:C	2:B:268:ALA:H	2.12	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:B:731:ALA:O	2:B:734:ALA:HB3	2.10	0.51
2:A:103:HIS:O	2:A:104:ASP:C	2.49	0.51
2:B:4:PRO:HD2	2:B:583:TYR:OH	2.11	0.51
2:B:160:TYR:CE2	2:B:505:HIS:CD2	2.98	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: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:A:56:ASP:O	2:A:60:GLN:HG3	2.11	0.51
2:A:738:LEU:HD11	2:A:796:LEU:HD23	1.93	0.51
2:B:467:LEU:O	2:B:473:THR:CG2	2.59	0.51
2:B:600:GLU:HG2	2:B:601:ASP:N	2.25	0.51
2:A:255:LEU:HD12	2:A:255:LEU:C	2.31	0.51
2:A:779:LEU:HD13	2:A:792:LEU:HD21	1.91	0.51
2:B:170:PRO:O	2:B:355:ILE:HG23	2.11	0.51
2:B:234:ARG:NH1	2:B:234:ARG:HG3	2.26	0.51
2:B:312:LEU:CG	2:B:313:ASP:N	2.74	0.51
2:B:733:LYS:HG3	2:B:738:LEU:HB2	1.93	0.51
2:B:90:VAL:O	2:B:95:LEU:HD12	2.10	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:A:383:PRO:O	2:A:384:GLU:CB	2.59	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
2:B:593:ARG:HB2	2:B:665:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:228:VAL:HG12	2:A:229:HIS:O	2.11	0.50
2:A:441:CYS:SG	2:A:443:SER:CB	2.99	0.50
2:A:539:PRO:O	2:A:543:VAL:HG13	2.11	0.50
2:B:165:LEU:HD13	2:B:366:LEU:HD21	1.93	0.50
2:B:220:VAL:HG12	2:B:270:LYS:NZ	2.24	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
1:C:931:C:H2'	1:C:931:C:O2	2.10	0.50
2:A:202:TYR:HE2	2:A:244:ARG:HD3	1.74	0.50
2:A:382:VAL:CG2	2:A:383:PRO:CD	2.68	0.50
2:A:611:ARG:NH1	5:A:1006:HOH:O	2.45	0.50
2:B:382:VAL:HG11	2:B:516:LEU:CG	2.41	0.50
2:B:7:TYR:HB2	2:B:583:TYR:CG	2.46	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:A:176:CYS:SG	2:A:178:ARG:HB3	2.51	0.50
2:A:469:TRP:O	2:A:469:TRP:CG	2.64	0.50
2:A:680:HIS:CA	2:A:687:THR:HG21	2.36	0.50
2:B:807:LYS:O	2:B:811:GLU:HG3	2.12	0.50
2:A:193:THR:HG23	2:A:194:PRO:HD2	1.94	0.50
2:A:297:GLU:N	2:A:297:GLU:OE1	2.43	0.50
2:B:161:TYR:HA	2:B:166:ALA:HB3	1.92	0.50
2:B:338:THR:O	2:B:338:THR:HG23	2.11	0.50
2:B:84:GLY:HA2	2:B:408:TRP:CD1	2.46	0.50
2:B:63:LEU:HD11	2:B:628:LEU:HD23	1.93	0.50
2:B:37:VAL:HG13	2:B:75:VAL:HB	1.92	0.50
2:B:85:ILE:O	2:B:88:GLN:HB2	2.12	0.50
2:A:233:GLU:O	2:A:234:ARG:C	2.49	0.50
2:A:412:ILE:HB	2:A:453:PHE:CE1	2.46	0.50
2:A:680:HIS:CD2	2:A:687:THR:HG21	2.47	0.50
2:B:220:VAL:O	2:B:223:ASP:HB2	2.12	0.50
2:B:382:VAL:CG2	2:B:383:PRO:CD	2.68	0.50
2:B:148:LYS:HD2	2:B:468:GLY:HA2	1.94	0.50
2:A:859:SER:HB2	2:B:806:GLU:OE1	2.11	0.50
1:C:964:C:H2'	1:C:965:G:C8	2.45	0.50
1:D:936:A:H1'	1:D:938:G:N7	2.27	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:A:474:GLU:HB3	5:A:1056:HOH:O	2.11	0.50
2:B:7:TYR:CE2	2:B:686:LEU:HD13	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:909:A:H4'	1:D:910:G:OP1	2.10	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:854:ILE:O	2:B:858:LEU:HD23	2.12	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:B:498:ARG:HG2	2:B:498:ARG:HH11	1.77	0.50
2:A:412:ILE:HG13	2:A:413:PRO:HD2	1.93	0.50
2:A:747:TYR:CZ	2:A:774:ARG:HB2	2.46	0.50
2:A:845:LYS:NZ	2:B:820:GLN:NE2	2.59	0.50
2:B:356:PHE:CD2	2:B:357:PRO:HD2	2.47	0.50
2:B:469:TRP:HD1	2:B:507:MET:HE1	1.77	0.50
2:A:153:VAL:CG2	2:A:154:ARG:H	2.25	0.49
2:A:307:GLU:H	2:A:307:GLU:CD	2.14	0.49
2:A:456:TRP:CE3	2:A:494:LEU:O	2.65	0.49
2:A:789:ARG:HG2	2:A:789:ARG:HH11	1.77	0.49
2:B:217:PRO:HD2	2:B:318:ARG:NE	2.27	0.49
2:B:420:CYS:HB2	2:B:441:CYS:HB3	1.94	0.49
2:A:234:ARG:HH22	2:A:267:GLY:N	2.07	0.49
2:A:433:GLU:HA	5:A:1022:HOH:O	2.12	0.49
2:B:232:ASP:O	2:B:236:ARG:HG2	2.12	0.49
2:B:145:MET:HG3	2:B:410:HIS:NE2	2.27	0.49
2:B:85:ILE:O	2:B:89:VAL:HG23	2.11	0.49
1:C:904:C:H2'	1:C:905:G:H8	1.77	0.49
2:A:228:VAL:HG22	2:A:268:ALA:HB2	1.93	0.49
2:A:247:LEU:HD23	2:A:325:PHE:CE1	2.47	0.49
2:A:257:ASP:OD2	2:A:282:ILE:HB	2.11	0.49
2:A:463:PRO:HD3	2:A:499:MET:SD	2.52	0.49
2:B:41:PRO:HD2	2:B:60:GLN:NE2	2.24	0.49
2:B:469:TRP:N	2:B:470:PRO:CD	2.75	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:105:LEU:HD21	2:A:110:PHE:HD1	1.78	0.49
2:B:113:ARG:HA	2:B:116:GLN:NE2	2.28	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:A:491:ILE:O	2:A:495:TRP:HB3	2.12	0.49
2:B:102:ARG:HH21	2:B:105:LEU:H	1.60	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:A:753:ALA:O	2:A:757:GLU:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:51:MET:HB3	2:B:521:VAL:HG21	1.94	0.49
2:B:549:ASP:OD2	2:B:685:PHE:HB2	2.13	0.49
2:B:833:PRO:HG2	2:B:836:VAL:HB	1.93	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:A:68:ARG:C	2:A:70:ARG:H	2.16	0.49
2:B:341:LEU:HD11	2:B:343:THR:HG23	1.94	0.49
2:B:45:VAL:O	2:B:117:TRP:NE1	2.42	0.49
2:B:473:THR:HG23	2:B:476:LEU:H	1.77	0.49
2:B:799:GLU:HG3	2:B:800:GLU:N	2.28	0.49
2:B:827:GLY:O	2:B:831:LYS:HB2	2.13	0.49
2:A:279:ASP:HA	2:A:282:ILE:HG12	1.95	0.49
2:A:844:LEU:O	2:A:848:LEU:HD23	2.13	0.49
2:B:312:LEU:O	2:B:313:ASP:O	2.30	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:A:190:THR:HG22	2:A:342:ALA:HA	1.95	0.49
2:A:543:VAL:CG2	2:A:544:GLU:N	2.76	0.49
2:A:598:ALA:C	2:A:599:LYS:HE2	2.33	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:B:845:LYS:O	2:B:849:GLU:HG3	2.12	0.49
1:C:922:A:H2'	1:C:923:G:H8	1.78	0.49
1:C:935:C:H1'	2:A:584:ASN:ND2	2.28	0.49
2:A:150:SER:O	2:A:153:VAL:HG22	2.13	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:B:3:LEU:HD11	2:B:590:LEU:HD12	1.94	0.49
2:A:212:ILE:HD11	2:A:268:ALA:C	2.34	0.48
2:A:242:ARG:HH11	2:A:242:ARG:CG	2.26	0.48
2:A:227:ALA:HB3	2:A:269:LEU:HG	1.94	0.48
2:A:680:HIS:HD2	2:A:687:THR:HG23	1.77	0.48
2:B:315:PHE:O	2:B:318:ARG:HB3	2.13	0.48
2:B:771:LEU:HD13	2:B:772:PRO:HD2	1.96	0.48
2:B:802:ARG:NH1	2:B:802:ARG:HB2	2.28	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:63:LEU:O	2:A:67:LYS:HG2	2.13	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:B:38:ILE:O	2:B:77:LEU:HD12	2.13	0.48
1:C:911:C:H6	1:C:911:C:O5'	1.97	0.48
1:C:965:G:H2'	1:C:966:C:C6	2.49	0.48
1:D:933:C:C6	1:D:933:C:C3'	2.97	0.48
2:A:193:THR:O	2:A:339:ILE:HG12	2.14	0.48
2:B:193:THR:HG23	2:B:194:PRO:HD2	1.96	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:397:VAL:HG12	2:B:398:LYS:N	2.28	0.48
2:B:448:ARG:H	2:B:448:ARG:CD	2.08	0.48
2:B:415:TRP:HA	2:B:447:LYS:O	2.14	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:B:89:VAL:O	2:B:93:ARG:N	2.47	0.48
2:A:315:PHE:C	2:A:317:ALA:H	2.17	0.48
2:A:489:TYR:N	2:A:517:LEU:HD12	2.28	0.48
2:A:7:TYR:CD1	2:A:8:ASP:N	2.81	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
2:B:415:TRP:CZ3	2:B:448:ARG:HD2	2.48	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
2:A:724:GLN:HB3	2:A:783:MET:HG2	1.95	0.48
2:A:520:LEU:HA	4:A:990:VAA:N1	2.29	0.48
2:B:441:CYS:SG	2:B:443:SER:CB	3.02	0.48
1:D:971:C:O2'	1:D:972:A:H5'	2.14	0.48
2:A:118:LYS:HE3	2:A:143:PHE:CE2	2.49	0.48
2:A:28:ASN:HD22	2:A:28:ASN:C	2.16	0.48
2:A:145:MET:HG2	2:A:410:HIS:HE2	1.77	0.48
2:A:834:LYS:HB3	2:A:834:LYS:NZ	2.29	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:B:462:TRP:O	2:B:464:LEU:N	2.47	0.48
2:B:50:HIS:CD2	2:B:52:GLY:N	2.81	0.48
2:B:1:MET:HE3	2:B:693:ALA:CB	2.42	0.48
2:B:738:LEU:CD1	2:B:738:LEU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:971:C:C2'	1:D:972:A:H5'	2.43	0.48
2:A:80:THR:O	2:A:143:PHE:HD1	1.97	0.48
2:A:272:THR:H	2:A:279:ASP:HB3	1.78	0.48
2:A:49:LEU:HG	2:A:128:GLN:OE1	2.13	0.48
2:B:222:ALA:HB2	2:B:293:VAL:HG13	1.94	0.48
1:C:934:A:N3	2:A:584:ASN:HB3	2.29	0.48
2:A:202:TYR:CD1	2:A:246:PRO:HG3	2.49	0.47
2:A:270:LYS:CB	2:A:270:LYS:HZ2	2.27	0.47
2:A:28:ASN:ND2	2:A:28:ASN:C	2.67	0.47
2:A:459:SER:C	2:A:495:TRP:HZ3	2.17	0.47
2:B:164:GLY:O	2:B:166:ALA:N	2.47	0.47
2:B:386:TRP:HB2	5:B:2040:HOH:O	2.13	0.47
1:C:951:G:H5'	1:C:952:G:OP2	2.13	0.47
2:A:307:GLU:O	2:A:309:LEU:N	2.47	0.47
2:A:171:ARG:NH1	2:A:364:ARG:HH21	2.10	0.47
2:A:440:ALA:HA	5:A:1051:HOH:O	2.14	0.47
2:B:9:PRO:C	2:B:11:SER:H	2.18	0.47
2:B:492:LEU:HD12	2:B:492:LEU:O	2.13	0.47
2:B:587:ARG:HG3	2:B:587:ARG:HH11	1.78	0.47
1:D:901:G:H22	1:D:972:A:C1'	2.27	0.47
2:A:266:THR:C	2:A:268:ALA:H	2.17	0.47
2:A:326:ARG:CG	2:A:327:GLU:H	2.20	0.47
2:A:518:HIS:CD2	2:A:519:GLY:O	2.62	0.47
2:A:625:TYR:C	2:A:627:ALA:H	2.17	0.47
2:B:393:TRP:HB2	2:B:493:PHE:CE2	2.49	0.47
2:B:78:PRO:HG2	2:B:141:GLU:HA	1.96	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: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:485:LEU:HD22	2:B:512:PHE:CE2	2.49	0.47
2:B:724:GLN:HE22	2:B:785:ARG:HB2	1.79	0.47
2:A:404:ARG:HG2	2:A:406:LEU:CD1	2.45	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: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:A:429:GLU:N	2:A:429:GLU:CD	2.68	0.47
2:A:467:LEU:O	2:A:473:THR:CG2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:509:GLU:HG2	2:A:510:ARG:H	1.79	0.47
2:B:202:TYR:CE2	2:B:244:ARG:HB3	2.49	0.47
2:B:249:GLU:OE1	2:B:249:GLU:HA	2.14	0.47
2:B:277:PRO:O	2:B:281:GLU:HB2	2.15	0.47
2:B:324:LEU:CD2	2:B:324:LEU:H	2.23	0.47
2:B:724:GLN:NE2	2:B:785:ARG:HB2	2.29	0.47
2:A:1:MET:HE2	2:A:693:ALA:CB	2.45	0.47
2:A:170:PRO:HB2	2:A:355:ILE:HG22	1.96	0.47
2:B:363:MET:CA	2:B:363:MET:HE3	2.44	0.47
2:B:780:VAL:HG12	2:B:781:LYS:N	2.30	0.47
2:B:818:ARG:NH2	5:B:2004:HOH:O	2.47	0.47
2:A:601:ASP:OD1	2:A:663:HIS:HB2	2.15	0.47
2:B:197:LEU:HB2	2:B:337:TYR:HB2	1.97	0.47
2:B:202:TYR:CD1	2:B:330:HIS:CE1	3.03	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
2:A:157:PHE:O	2:A:160:TYR:HB2	2.15	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
2:B:50:HIS:HD2	2:B:52:GLY:H	1.60	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
1:C:962:U:H2'	1:C:963:A:C8	2.49	0.47
1:D:911:C:H6	1:D:911:C:O5'	1.98	0.47
2:A:88:GLN:HE22	2:A:110:PHE:HE2	1.63	0.47
2:A:395:GLU:HA	2:A:395:GLU:OE2	2.14	0.47
2:A:831:LYS:N	2:A:831:LYS:HD3	2.29	0.47
2:B:202:TYR:HE2	2:B:244:ARG:HD3	1.80	0.47
1:D:935:C:H1'	2:B:584:ASN:ND2	2.30	0.47
2:B:91:VAL:HG12	2:B:96:LEU:CD2	2.44	0.47
1:C:962:U:H2'	1:C:963:A:H8	1.79	0.47
1:D:973:C:H2'	1:D:974:C:H5'	1.97	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:136:ALA:O	2:A:138:TRP:N	2.47	0.46
2:A:217:PRO:HD2	2:A:218:GLU:OE1	2.15	0.46
2:B:236:ARG:O	2:B:237:HIS:ND1	2.48	0.46
2:B:724:GLN:HE22	2:B:785:ARG:H	1.62	0.46
2:A:232:ASP:C	2:A:234:ARG:N	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:520:LEU:HA	4:A:990:VAA:C2	2.45	0.46
2:A:88:GLN:NE2	2:A:110:PHE:HE2	2.13	0.46
2:B:319:ARG:O	2:B:319:ARG:HG3	2.15	0.46
2:B:416:TYR:HA	2:B:422:ALA:O	2.15	0.46
2:B:543:VAL:CG2	2:B:544:GLU:N	2.79	0.46
2:A:273:PRO:HA	2:A:280:TYR:CA	2.46	0.46
2:A:522:LEU:HD12	2:A:522:LEU:O	2.15	0.46
2:A:521:VAL:HA	2:A:565:ILE:O	2.16	0.46
2:A:65:ARG:HH11	2:A:680:HIS:CE1	2.32	0.46
2:B:225:ALA:CA	2:B:252:ILE:CG2	2.91	0.46
2:A:105:LEU:HD21	2:A:110:PHE:CD1	2.51	0.46
2:A:276:ASP:OD1	2:A:278:LEU:N	2.49	0.46
2:A:361:LEU:O	2:A:363:MET:N	2.48	0.46
2:A:496:VAL:O	2:A:500:GLU:HG3	2.15	0.46
2:B:416:TYR:CD2	2:B:423:VAL:HG22	2.50	0.46
2:B:607:ASP:OD2	2:B:664:THR:HA	2.16	0.46
2:A:111:LEU:O	2:A:115:TRP:HD1	1.98	0.46
2:A:153:VAL:HG12	2:A:461:LEU:HD23	1.97	0.46
2:B:274:ALA:HB2	2:B:290:PRO:HB2	1.96	0.46
2:B:561:GLY:HA2	5:B:2025:HOH:O	2.15	0.46
2:B:745:ARG:CB	2:B:771:LEU:HD23	2.42	0.46
2:B:798:VAL:HG13	2:B:799:GLU:N	2.31	0.46
2:A:855:ARG:CZ	2:B:810:LYS:HG3	2.46	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
2:B:644:GLU:HA	2:B:644:GLU:OE1	2.15	0.46
1:C:928:C:H2'	1:C:929:G:C5'	2.29	0.46
1:D:932:U:O2'	1:D:933:C:H5	1.94	0.46
2:A:382:VAL:HG21	2:A:517:LEU:N	2.30	0.46
2:A:592:SER:C	2:A:594:GLU:N	2.68	0.46
2:B:393:TRP:CZ3	2:B:394:LEU:HD23	2.51	0.46
2:A:326:ARG:CG	2:A:327:GLU:N	2.69	0.46
2:A:61:ASP:CG	2:A:552:ARG:HH22	2.19	0.46
2:B:236:ARG:HA	2:B:238:LEU:CD2	2.46	0.46
2:B:331:LEU:HD12	2:B:332:VAL:N	2.31	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:275:HIS:CE1	2:A:294:ILE:CG2	2.99	0.46
2:A:369:GLU:OE2	2:A:505:HIS:HA	2.16	0.46
2:A:705:TRP:CD2	2:A:706:PRO:HD2	2.51	0.46
2:A:745:ARG:HB3	2:A:771:LEU:HD21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ARG:N	2:B:365:PRO:HD2	2.31	0.46
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: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:B:36:PHE:CD1	2:B:67:LYS:HG3	2.51	0.45
2:A:261:GLU:HA	2:A:261:GLU:OE1	2.15	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: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:248:THR:HG23	2:A:249:GLU:N	2.29	0.45
2:A:326:ARG:HB3	2:A:331:LEU:CD2	2.41	0.45
2:A:363:MET:HE3	2:A:363:MET:HA	1.98	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
1:D:945:G:C2'	1:D:946:U:O5'	2.65	0.45
2:A:239:LEU:HD12	2:A:254:ILE:O	2.17	0.45
2:A:27:ALA:O	2:A:140:ARG:NH2	2.49	0.45
2:A:314:ARG:HG3	2:A:315:PHE:CD2	2.52	0.45
2:A:524:GLU:CD	2:A:524:GLU:H	2.19	0.45
2:B:160:TYR:HD2	2:B:165:LEU:HD12	1.82	0.45
2:B:469:TRP:CD1	2:B:507:MET:HE1	2.51	0.45
2:A:242:ARG:O	2:A:254:ILE:HD13	2.16	0.45
2:A:245:ILE:HG21	2:A:252:ILE:CD1	2.45	0.45
2:A:451:ASP:HB3	2:A:452:VAL:H	1.55	0.45
2:A:855:ARG:HD2	2:B:809:LEU:HD12	1.97	0.45
2:B:49:LEU:HG	2:B:128:GLN:OE1	2.15	0.45
2:B:341:LEU:HD13	2:B:342:ALA:N	2.32	0.45
2:B:370:VAL:CG2	2:B:501:VAL:HA	2.47	0.45
2:B:469:TRP:CD1	2:B:507:MET:CE	2.99	0.45
2:B:618:VAL:HG12	2:B:708:PRO:HG3	1.98	0.45
2:B:738:LEU:HD12	2:B:738:LEU:N	2.31	0.45
2:B:778:ALA:HB2	2:B:791:PRO:HA	1.97	0.45
2:A:170:PRO:O	2:A:355:ILE:HG23	2.16	0.45
2:A:238:LEU:HA	5:A:1005:HOH:O	2.16	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:546:TYR:CD2	2:A:572:LEU:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:732:LEU:HD12	2:A:732:LEU:HA	1.71	0.45
2:A:774:ARG:C	2:A:774:ARG:HD3	2.37	0.45
2:B:250:VAL:HG12	2:B:252:ILE:HD12	1.99	0.45
2:B:273:PRO:HA	2:B:280:TYR:CA	2.47	0.45
1:D:962:U:H2'	1:D:963:A:H8	1.81	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:B:683:MET:O	2:B:687:THR:CG2	2.65	0.45
2:A:210:ILE:O	2:A:210:ILE:HG23	2.17	0.45
2:A:216:ARG:HH12	2:A:314:ARG:NH2	2.15	0.45
2:A:543:VAL:O	2:A:547:GLY:N	2.50	0.45
2:A:642:TRP:O	2:A:642:TRP:HD1	2.00	0.45
2:A:651:GLU:HA	2:A:654:LYS:HD3	1.99	0.45
2:B:759:LEU:HD13	2:B:759:LEU:C	2.37	0.45
1:C:929:G:H5'	1:C:929:G:C8	2.49	0.45
2:A:234:ARG:C	2:A:236:ARG:N	2.70	0.45
2:A:271:VAL:HG22	2:A:282:ILE:HD11	1.99	0.45
2:A:814:ALA:O	2:A:818:ARG:HG3	2.17	0.45
2:B:201:ARG:HB3	2:B:210:ILE:O	2.15	0.45
2:B:219:THR:O	2:B:272:THR:HG21	2.17	0.45
2:A:855:ARG:HG3	2:B:809:LEU:HD12	1.99	0.45
2:B:823:LEU:HD11	2:B:841:GLU:HG2	1.97	0.45
1:C:908:U:H1'	1:C:947:C:O2	2.17	0.45
2:A:161:TYR:CD1	2:A:161:TYR:C	2.90	0.45
2:A:306:PRO:CD	2:A:309:LEU:HD23	2.47	0.45
2:B:302:GLY:O	2:B:310:ARG:NH1	2.35	0.45
2:B:7:TYR:CD1	2:B:8:ASP:N	2.85	0.45
1:D:945:G:H2'	1:D:946:U:O5'	2.17	0.45
2:A:102:ARG:NH1	5:A:1008:HOH:O	2.49	0.44
2:A:45:VAL:CG1	2:A:118:LYS:HA	2.46	0.44
2:A:212:ILE:CD1	2:A:268:ALA:O	2.65	0.44
2:A:422:ALA:HB1	5:A:1009:HOH:O	2.17	0.44
2:B:148:LYS:HD2	2:B:468:GLY:CA	2.47	0.44
2:B:242:ARG:HB2	2:B:251:TRP:HE3	1.81	0.44
2:B:254:ILE:HG22	2:B:254:ILE:O	2.17	0.44
2:B:31:SER:C	2:B:33:LYS:N	2.71	0.44
2:B:45:VAL:HG13	2:B:81:ASP:O	2.17	0.44
2:B:469:TRP:HA	2:B:476:LEU:HD22	1.99	0.44
2:B:487:THR:HG23	2:B:517:LEU:HD23	1.99	0.44
2:A:217:PRO:O	2:A:220:VAL:HG22	2.18	0.44
2:A:401:ASN:O	2:A:404:ARG:NH2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:501:VAL:C	2:B:503:GLY:N	2.70	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
2:A:473:THR:HG22	2:A:476:LEU:CB	2.47	0.44
2:A:755:VAL:HG13	2:A:762:PHE:CG	2.52	0.44
2:A:837:VAL:HG13	2:A:838:GLU:H	1.80	0.44
2:B:218:GLU:CG	2:B:318:ARG:HB2	2.47	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:B:93:ARG:C	2:B:94:LEU:O	2.52	0.44
1:C:975:A:H8	2:A:213:ALA:O	2.01	0.44
2:A:232:ASP:O	2:A:233:GLU:C	2.56	0.44
2:A:30:LYS:HG2	2:A:30:LYS:H	1.65	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:B:277:PRO:CD	2:B:353:TYR:CE2	2.93	0.44
2:A:364:ARG:N	2:A:365:PRO:HD2	2.33	0.44
2:A:557:TYR:HE1	2:A:635:ARG:HB3	1.77	0.44
2:A:94:LEU:O	2:A:95:LEU:C	2.56	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:A:86:ALA:HA	2:A:346:ARG:HD3	2.00	0.44
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:613:ARG:NH2	2:A:644:GLU:HG3	2.31	0.44
2:A:724:GLN:NE2	2:A:785:ARG:H	2.10	0.44
2:A:808:ARG:HD2	2:A:808:ARG:HA	1.84	0.44
2:B:488:GLY:N	4:B:1990:VAA:O2'	2.45	0.44
2:B:361:LEU:CD2	2:B:366:LEU:CD1	2.96	0.44
2:B:408:TRP:CE3	2:B:408:TRP:HA	2.52	0.44
2:B:546:TYR:CD2	2:B:572:LEU:HB3	2.53	0.44
1:D:914:A:H4'	2:B:560:THR:HG21	1.99	0.44
2:A:152:ALA:HA	2:A:470:PRO:HB3	1.99	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:361:LEU:HB2	2:B:402:ILE:HD12	1.98	0.44
2:B:50:HIS:C	2:B:50:HIS:CD2	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:952:G:N3	1:D:952:G:H2'	2.32	0.44
2:B:212:ILE:HD12	2:B:268:ALA:O	2.18	0.44
2:B:349:THR:CG2	2:B:350:PRO:HD2	2.45	0.44
2:B:140:ARG:NH1	2:B:475:ASP:OD1	2.50	0.44
2:B:499:MET:CE	2:B:512:PHE:CE2	2.82	0.44
2:A:621:ILE:HD12	2:A:678:LEU:HD13	2.00	0.44
2:B:110:PHE:C	2:B:112:GLU:N	2.70	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:373:GLY:O	2:B:376:ARG:N	2.50	0.44
2:B:415:TRP:HZ3	2:B:448:ARG:HD2	1.81	0.44
2:B:382:VAL:HG21	2:B:516:LEU:HA	1.93	0.44
2:B:539:PRO:O	2:B:543:VAL:HG13	2.18	0.44
2:A:362:ARG:O	2:A:365:PRO:HG2	2.18	0.43
2:A:463:PRO:HG3	2:A:511:PRO:HB3	2.00	0.43
2:A:751:GLU:OE2	2:A:785:ARG:NE	2.50	0.43
2:B:181:THR:OG1	2:B:404:ARG:HG3	2.18	0.43
2:B:227:ALA:HA	2:B:255:LEU:HD12	1.99	0.43
2:B:200:LEU:HD21	2:B:325:PHE:CE1	2.53	0.43
2:B:362:ARG:C	2:B:365:PRO:HD2	2.38	0.43
2:B:387:LYS:HB3	2:B:388:LYS:CE	2.48	0.43
2:B:408:TRP:HE3	2:B:408:TRP:HA	1.83	0.43
2:B:745:ARG:NH1	2:B:745:ARG:CB	2.79	0.43
2:B:831:LYS:HE3	2:B:831:LYS:CA	2.48	0.43
2:B:94:LEU:O	2:B:96:LEU:N	2.51	0.43
1:D:958:G:H2'	1:D:959:U:H5'	2.00	0.43
2:A:388:LYS:HD3	2:A:388:LYS:N	2.34	0.43
2:A:821:ARG:O	2:A:825:SER:HB2	2.17	0.43
2:B:102:ARG:O	2:B:104:ASP:N	2.51	0.43
2:B:17:ALA:HB2	2:B:685:PHE:HE2	1.82	0.43
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:A:710:GLY:O	2:A:711:ARG:HB3	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:272:THR:H	2:B:279:ASP:CB	2.30	0.43
2:B:274:ALA:HB3	2:B:291:VAL:O	2.18	0.43
2:B:714:GLU:O	2:B:717:ARG:N	2.52	0.43
2:B:91:VAL:HG12	2:B:96:LEU:HD21	2.00	0.43
2:A:326:ARG:CA	2:A:331:LEU:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:692:GLN:HE21	2:A:698:GLU:HA	1.82	0.43
2:A:833:PRO:C	2:A:835:GLU:N	2.71	0.43
2:B:157:PHE:CD2	2:B:413:PRO:HG2	2.54	0.43
2:B:269:LEU:HB2	5:B:2007:HOH:O	2.19	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: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:489:TYR:HD1	2:A:490:ASP:N	2.17	0.43
2:A:49:LEU:HD21	2:A:125:ILE:HG23	2.01	0.43
2:A:56:ASP:OD1	2:A:518:HIS:HE1	2.01	0.43
2:A:46:THR:CG2	2:A:90:VAL:HG21	2.48	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:A:161:TYR:C	2:A:163:GLU:H	2.22	0.43
2:A:412:ILE:CA	2:A:453:PHE:CE1	2.99	0.43
2:A:93:ARG:HG2	2:A:94:LEU:N	2.30	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: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
2:B:685:PHE:HD1	2:B:685:PHE:H	1.67	0.43
2:B:785:ARG:CA	2:B:785:ARG:NH1	2.80	0.43
1:D:971:C:O5'	1:D:971:C:H6	2.01	0.43
2:A:170:PRO:HB2	2:A:355:ILE:CG2	2.49	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
2:A:69:MET:CE	2:A:680:HIS:ND1	2.81	0.43
2:B:88:GLN:CG	2:B:406:LEU:HD22	2.43	0.43
2:B:519:GLY:C	2:B:520:LEU:HD23	2.38	0.43
2:B:699:GLU:OE1	2:B:699:GLU:HA	2.19	0.43
1:D:923:G:H2'	1:D:924:C:C6	2.53	0.43
1:D:938:G:P	5:D:71:HOH:O	2.76	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:262:LYS:HA	2:B:267:GLY:HA2	2.01	0.43
2:B:692:GLN:HA	2:B:697:LYS:O	2.18	0.43
2:A:810:LYS:HG3	2:B:855:ARG:NH2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:GLY:O	2:B:85:ILE:C	2.57	0.43
1:D:962:U:H2'	1:D:963:A:C8	2.54	0.43
2:A:209:PHE:O	2:A:238:LEU:HD12	2.19	0.43
2:A:398:LYS:O	2:A:399:ASP:C	2.56	0.43
2:A:44:ASN:C	2:A:46:THR:H	2.23	0.43
2:A:64:ILE:HD13	2:A:64:ILE:HA	1.83	0.43
2:A:744:VAL:CG1	2:A:745:ARG:N	2.82	0.43
2:A:833:PRO:O	2:A:837:VAL:HG12	2.18	0.43
2:A:855:ARG:NH2	2:B:810:LYS:HG3	2.33	0.43
2:B:102:ARG:NE	2:B:102:ARG:O	2.28	0.43
2:B:248:THR:CG2	2:B:249:GLU:N	2.56	0.43
2:A:216:ARG:HA	2:A:318:ARG:NH2	2.34	0.42
2:A:313:ASP:CG	2:A:314:ARG:N	2.73	0.42
2:A:155:TYR:CD1	2:A:431:TYR:CD2	3.04	0.42
2:A:460:ALA:O	2:A:499:MET:HA	2.19	0.42
2:A:498:ARG:NH1	2:A:498:ARG:HG2	2.33	0.42
2:A:69:MET:O	2:A:705:TRP:N	2.51	0.42
2:A:7:TYR:CE2	2:A:686:LEU:HD13	2.53	0.42
2:B:210:ILE:O	2:B:210:ILE:CG2	2.67	0.42
2:B:614:LEU:HD11	2:B:671:VAL:HG13	2.01	0.42
2:B:692:GLN:HG3	2:B:697:LYS:O	2.18	0.42
2:A:420:CYS:O	2:A:420:CYS:SG	2.77	0.42
2:A:531:LYS:NZ	5:A:1041:HOH:O	2.49	0.42
2:A:721:ALA:HB3	2:A:754:PRO:HG2	1.99	0.42
1:D:918:G:C6	2:B:833:PRO:CD	3.02	0.42
2:A:255:LEU:HD12	2:A:255:LEU:O	2.19	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:B:244:ARG:NH2	5:B:1991:HOH:O	2.26	0.42
2:A:304:ARG:HH11	2:A:304:ARG:CG	2.23	0.42
2:A:469:TRP:N	2:A:470:PRO:CD	2.82	0.42
2:A:546:TYR:HE2	2:A:573:GLU:HG2	1.84	0.42
2:A:812:LEU:HD23	2:A:812:LEU:HA	1.87	0.42
2:B:639:GLU:O	2:B:640:LEU:C	2.56	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:247:LEU:HD23	2:A:325:PHE:HE1	1.84	0.42
2:B:91:VAL:HA	2:B:95:LEU:CD1	2.48	0.42
2:B:98:GLU:O	2:B:99:GLY:O	2.37	0.42
2:A:45:VAL:CG1	2:A:121:SER:HB3	2.48	0.42
2:A:283:GLY:O	2:A:288:LEU:HG	2.20	0.42
2:A:42:PRO:HB2	2:A:81:ASP:N	2.35	0.42
2:B:171:ARG:NH2	2:B:398:LYS:HG2	2.34	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: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:233:GLU:O	2:B:236:ARG:N	2.52	0.42
2:B:544:GLU:CD	2:B:544:GLU:C	2.79	0.42
2:B:617:GLY:HA3	2:B:640:LEU:HD22	2.01	0.42
2:B:752:THR:O	2:B:753:ALA:C	2.57	0.42
1:C:918:G:O2'	1:C:919:A:O5'	2.35	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:A:228:VAL:O	2:A:256:ALA:HA	2.19	0.42
2:A:232:ASP:O	2:A:234:ARG:N	2.53	0.42
2:A:3:LEU:N	2:A:4:PRO:HD3	2.35	0.42
2:A:506:PHE:C	2:A:507:MET:HG2	2.40	0.42
2:B:10:LYS:NZ	2:B:544:GLU:HG2	2.34	0.42
2:B:171:ARG:HH22	2:B:398:LYS:HD2	1.84	0.42
2:B:223:ASP:HA	2:B:272:THR:HG23	2.01	0.42
2:B:405:GLN:N	2:B:405:GLN:CD	2.73	0.42
2:B:482:GLY:O	2:B:512:PHE:HA	2.20	0.42
2:B:93:ARG:NH1	2:B:93:ARG:HG3	2.35	0.42
1:D:951:G:H5'	1:D:952:G:OP2	2.20	0.42
2:A:159:ARG:NH1	2:A:159:ARG:CG	2.78	0.42
2:B:103:HIS:O	2:B:104:ASP:O	2.38	0.42
2:B:148:LYS:O	2:B:148:LYS:HG3	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
2:B:313:ASP:CG	2:B:314:ARG:H	2.23	0.42
2:B:558:LEU:HD23	5:B:2020:HOH:O	2.20	0.42
2:B:649:TYR:CE2	2:B:668:LEU:HD23	2.55	0.42
2:B:38:ILE:HG22	2:B:76:TRP:CD1	2.55	0.42
2:B:837:VAL:O	2:B:841:GLU:HG3	2.20	0.42
1:C:971:C:H2'	1:C:972:A:C5'	2.32	0.42
2:A:155:TYR:OH	2:A:159:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:201:ARG:CZ	2:A:332:VAL:HG21	2.50	0.42
2:B:644:GLU:O	2:B:645:PHE:C	2.58	0.42
2:B:736:ALA:CB	2:B:738:LEU:HD13	2.49	0.42
2:B:778:ALA:HA	2:B:792:LEU:HB2	2.01	0.42
2:A:692:GLN:O	2:A:696:GLY:N	2.41	0.41
2:A:73:GLU:O	2:A:75:VAL:HG23	2.19	0.41
2:B:168:ARG:HA	2:B:358:GLN:O	2.20	0.41
2:B:416:TYR:N	2:B:447:LYS:O	2.36	0.41
2:B:469:TRP:CG	2:B:469:TRP:O	2.72	0.41
2:B:516:LEU:CD1	2:B:628:LEU:HD13	2.48	0.41
2:B:640:LEU:O	2:B:644:GLU:HB2	2.20	0.41
1:C:941:A:H2'	1:C:942:G:O5'	2.20	0.41
2:A:438:CYS:C	2:A:440:ALA:H	2.23	0.41
2:A:489:TYR:CD1	2:A:490:ASP:N	2.88	0.41
2:A:540:LEU:O	2:A:543:VAL:HG22	2.20	0.41
2:A:717:ARG:NH1	2:A:717:ARG:HB2	2.33	0.41
2:A:859:SER:OG	2:A:860:GLN:N	2.53	0.41
2:B:202:TYR:CD2	2:B:203:GLU:HB2	2.56	0.41
2:B:809:LEU:HD13	2:B:813:LEU:HG	2.02	0.41
2:B:42:PRO:HB2	2:B:80:THR:C	2.40	0.41
2:B:83:ALA:HA	2:B:455:THR:CG2	2.49	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:146:ASP:OD1	2:A:149:ARG:HB2	2.20	0.41
2:A:193:THR:CG2	2:A:194:PRO:HD2	2.49	0.41
2:A:666:ARG:CG	2:A:666:ARG:NH1	2.80	0.41
2:A:724:GLN:HE22	2:A:785:ARG:HB2	1.85	0.41
2:A:732:LEU:CD1	2:A:781:LYS:HB2	2.40	0.41
2:B:161:TYR:O	2:B:163:GLU:N	2.53	0.41
2:B:165:LEU:O	2:B:361:LEU:HA	2.19	0.41
2:B:210:ILE:HD12	2:B:210:ILE:HA	1.90	0.41
2:B:221:PHE:O	2:B:304:ARG:HG3	2.21	0.41
2:B:64:ILE:HG23	2:B:74:ALA:HB1	2.01	0.41
2:A:210:ILE:HA	2:A:210:ILE:HD12	1.86	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:170:PRO:C	2:B:171:ARG:O	2.56	0.41
2:B:199:THR:O	2:B:332:VAL:HG22	2.21	0.41
2:B:297:GLU:HB2	2:B:299:ARG:HG2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:PHE:CD2	2:B:457:PHE:CD2	3.09	0.41
2:B:611:ARG:HE	2:B:667:THR:HG23	1.86	0.41
2:B:680:HIS:CD2	2:B:687:THR:HG21	2.56	0.41
2:B:745:ARG:HG2	2:B:745:ARG:H	1.74	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
1:C:901:G:N2	1:C:972:A:H1'	2.36	0.41
1:C:975:A:OP2	2:A:337:TYR:OH	2.28	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: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:242:ARG:NH1	2:A:242:ARG:CG	2.82	0.41
2:A:55:LEU:HD11	2:A:559:ALA:HB2	2.03	0.41
2:A:599:LYS:HE2	2:A:599:LYS:HA	2.01	0.41
1:C:918:G:H21	1:C:956:A:H1'	1.84	0.41
2:A:415:TRP:HZ3	2:A:448:ARG:HD2	1.81	0.41
2:B:520:LEU:HA	4:B:1990:VAA:C2	2.51	0.41
2:B:233:GLU:C	2:B:235:TYR:N	2.73	0.41
2:B:487:THR:OG1	2:B:488:GLY:N	2.53	0.41
2:B:49:LEU:HD22	2:B:53:HIS:ND1	2.35	0.41
2:B:587:ARG:NH1	2:B:587:ARG:CG	2.79	0.41
2:B:600:GLU:O	2:B:661:ASN:HA	2.20	0.41
2:B:83:ALA:HB1	2:B:86:ALA:HB3	2.02	0.41
2:A:15:LYS:HG3	2:A:16:TRP:N	2.36	0.41
2:A:157:PHE:CD2	2:A:413:PRO:CG	3.04	0.41
2:B:15:LYS:HG3	2:B:16:TRP:N	2.36	0.41
2:B:161:TYR:C	2:B:163:GLU:H	2.24	0.41
2:B:611:ARG:NE	2:B:667:THR:HG23	2.36	0.41
1:D:973:C:O2	1:D:973:C:C2'	2.69	0.41
2:A:154:ARG:HG3	2:A:154:ARG:NH1	2.36	0.41
2:A:779:LEU:HD13	2:A:792:LEU:CD2	2.51	0.41
2:B:736:ALA:HB3	2:B:738:LEU:HD13	2.02	0.41
2:B:745:ARG:HB2	2:B:771:LEU:CD2	2.41	0.41
2:B:27:ALA:CB	2:B:75:VAL:HG13	2.51	0.41
1:C:943:A:H2'	1:C:944:G:O4'	2.20	0.41
1:D:907:C:H5''	1:D:908:U:OP2	2.20	0.41
1:D:903:G:N2	1:D:970:C:H1'	2.36	0.41
2:A:225:ALA:CA	2:A:252:ILE:CG2	2.94	0.41
2:A:358:GLN:HB2	2:A:360:TRP:NE1	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:397:VAL:HG12	2:A:398:LYS:N	2.36	0.41
2:A:408:TRP:HE3	2:A:408:TRP:HA	1.86	0.41
2:B:231:GLU:C	2:B:233:GLU:H	2.24	0.41
2:B:510:ARG:CZ	2:B:513:LYS:HG2	2.51	0.41
2:B:5:LYS:N	2:B:5:LYS:HD2	2.13	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
2:B:46:THR:HG22	2:B:87:THR:HA	2.03	0.41
1:C:946:U:H3'	1:C:946:U:H6	1.85	0.41
1:D:909:A:O2'	1:D:910:G:N7	2.39	0.41
2:A:273:PRO:HA	2:A:280:TYR:HA	2.02	0.41
2:A:373:GLY:O	2:A:376:ARG:N	2.54	0.41
2:A:448:ARG:NH1	2:A:448:ARG:HG2	2.36	0.41
2:A:7:TYR:HB2	2:A:583:TYR:CG	2.56	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:B:63:LEU:O	2:B:67:LYS:HB2	2.21	0.41
2:B:804:ARG:O	2:B:807:LYS:N	2.54	0.41
2:A:401:ASN:HD22	2:A:401:ASN:C	2.24	0.40
2:A:523:ASP:OD2	2:A:527:GLN:HG3	2.22	0.40
2:A:76:TRP:O	2:A:78:PRO:HD3	2.21	0.40
2:B:228:VAL:CG2	2:B:268:ALA:HB2	2.51	0.40
2:B:312:LEU:HD12	2:B:313:ASP:H	1.86	0.40
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.86	0.40
1:C:909:A:H61	1:C:921:G:H3'	1.85	0.40
1:D:934:A:N3	2:B:584:ASN:HB3	2.36	0.40
1:D:973:C:C2'	1:D:974:C:H5''	2.51	0.40
2:A:223:ASP:HA	2:A:271:VAL:O	2.22	0.40
2:A:431:TYR:CD1	2:A:431:TYR:C	2.94	0.40
2:A:641:VAL:HG22	2:A:675:LEU:HD13	2.02	0.40
2:A:735:GLU:HG2	2:A:804:ARG:NH1	2.36	0.40
2:A:859:SER:O	2:A:860:GLN:C	2.60	0.40
2:B:281:GLU:O	2:B:285:ARG:CG	2.62	0.40
2:B:201:ARG:CG	2:B:332:VAL:HG11	2.51	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:B:416:TYR:CE2	2:B:423:VAL:HG22	2.56	0.40
2:B:607:ASP:O	2:B:609:PHE:N	2.54	0.40
2:B:684:PRO:HG2	2:B:685:PHE:CD1	2.56	0.40
1:D:931:C:O5'	1:D:931:C:H6	2.03	0.40
2:A:220:VAL:HA	2:A:270:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:156:ALA:CB	2:A:461:LEU:HD21	2.51	0.40
2:A:624:LEU:HD12	2:A:633:ALA:CA	2.51	0.40
2:A:846:GLU:HA	2:A:849:GLU:HG3	2.02	0.40
2:B:211:GLU:H	2:B:211:GLU:HG2	1.61	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
2:B:657:LEU:HD21	2:B:664:THR:HG22	2.03	0.40
1:C:923:G:H2'	1:C:924:C:O4'	2.21	0.40
1:C:961:C:C2'	1:C:962:U:H5'	2.51	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:A:12:VAL:O	2:A:15:LYS:HG2	2.22	0.40
2:A:231:GLU:C	2:A:233:GLU:H	2.24	0.40
2:A:790:MET:HA	2:A:791:PRO:HD3	1.97	0.40
2:B:264:PHE:O	2:B:265:GLY:C	2.60	0.40
2:B:363:MET:C	2:B:365:PRO:HD2	2.42	0.40
2:B:3:LEU:HD11	2:B:590:LEU:CB	2.52	0.40
2:B:92:GLU:O	2:B:96:LEU:HB2	2.22	0.40
2:A:242:ARG:O	2:A:243:ALA:CB	2.69	0.40
2:A:287:GLY:O	2:A:288:LEU:HD23	2.21	0.40
2:A:28:ASN:HD22	2:A:29:PRO:CD	2.34	0.40
2:A:326:ARG:O	2:A:329:GLY:N	2.45	0.40
2:A:430:ARG:HB3	2:A:433:GLU:OE2	2.22	0.40
2:A:674:VAL:O	2:A:677:LYS:HB2	2.21	0.40
2:A:767:ARG:HG2	2:A:767:ARG:HH11	1.87	0.40
2:A:789:ARG:HG2	2:A:789:ARG:NH1	2.37	0.40
2:A:837:VAL:CG1	2:A:838:GLU:N	2.82	0.40
2:B:301:GLU:HA	2:B:310:ARG:HG3	2.04	0.40
2:B:89:VAL:HG21	2:B:346:ARG:HG3	2.04	0.40
2:B:358:GLN:HB3	2:B:359:TRP:H	1.76	0.40
2:B:430:ARG:HB3	2:B:433:GLU:OE2	2.20	0.40
2:B:448:ARG:HH11	2:B:448:ARG:HG2	1.87	0.40
2:B:582:LEU:O	2:B:583:TYR:C	2.59	0.40
1:C:918:G:N2	1:C:956:A:C1'	2.84	0.40
1:D:947:C:C5	1:D:958:G:H5''	2.56	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%)	2	6
2	B	860/862 (100%)	652 (76%)	156 (18%)	52 (6%)	1	4
All	All	1720/1724 (100%)	1328 (77%)	295 (17%)	97 (6%)	2	5

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

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Mol	Chain	Res	Type
2	A	45	VAL
2	A	100	LYS
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

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Mol	Chain	Res	Type
2	B	462	TRP
2	B	685	PHE
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%)	5 17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	724/724 (100%)	630 (87%)	94 (13%)	4	12
All	All	1448/1448 (100%)	1271 (88%)	177 (12%)	5	15

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

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Mol	Chain	Res	Type
2	A	388	LYS
2	A	390	ASN
2	A	396	ASN
2	A	400	TRP
2	A	401	ASN
2	A	403	SER
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

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Mol	Chain	Res	Type
2	A	800	GLU
2	A	805	GLN
2	A	834	LYS
2	A	838	GLU
2	A	845	LYS
2	B	2	ASP
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

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Mol	Chain	Res	Type
2	B	288	LEU
2	B	289	LYS
2	B	291	VAL
2	B	339	ILE
2	B	347	CYS
2	B	356	PHE
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

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Mol	Chain	Res	Type
2	B	732	LEU
2	B	733	LYS
2	B	745	ARG
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	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

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Mol	Chain	Res	Type
2	B	174	ASN
2	B	229	HIS
2	B	275	HIS
2	B	330	HIS
2	B	358	GLN
2	B	396	ASN
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

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Mol	Chain	Res	Type
1	C	932	U
1	C	933	C
1	C	934	A
1	C	936	A
1	C	937	C
1	C	938	G
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
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 [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](#)

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	B	1990	-	27,32,32	3.05	9 (33%)	30,48,48	1.69	5 (16%)
4	VAA	A	990	-	27,32,32	3.18	10 (37%)	30,48,48	1.87	5 (16%)

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	B	1990	-	-	1/19/39/39	0/3/3/3
4	VAA	A	990	-	-	5/19/39/39	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	990	VAA	C5'-N5'	-9.33	1.31	1.47
4	B	1990	VAA	C5'-N5'	-8.38	1.33	1.47
4	B	1990	VAA	S-N5'	7.13	1.69	1.61
4	A	990	VAA	S-N5'	6.44	1.69	1.61
4	A	990	VAA	O1S-S	6.27	1.52	1.43
4	B	1990	VAA	O1S-S	5.45	1.51	1.43
4	A	990	VAA	O4'-C1'	5.06	1.48	1.41
4	B	1990	VAA	O4'-C1'	4.95	1.48	1.41
4	A	990	VAA	C5'-C4'	-4.64	1.41	1.52
4	B	1990	VAA	C5'-C4'	-3.96	1.42	1.52
4	A	990	VAA	C8-N7	-3.82	1.27	1.34
4	B	1990	VAA	C4-N3	3.34	1.40	1.35
4	B	1990	VAA	C8-N7	-3.30	1.28	1.34
4	A	990	VAA	C4-N3	3.28	1.40	1.35
4	B	1990	VAA	C2-N3	2.67	1.36	1.32
4	A	990	VAA	C2-N3	2.54	1.36	1.32
4	B	1990	VAA	CA-C	-2.24	1.51	1.53
4	A	990	VAA	C3'-C4'	-2.13	1.47	1.53
4	A	990	VAA	O2S-S	2.07	1.46	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	990	VAA	O2S-S-O1S	-6.27	111.01	120.40
4	B	1990	VAA	O2S-S-O1S	-5.46	112.23	120.40
4	A	990	VAA	C-N3S-S	-3.83	117.87	124.23
4	B	1990	VAA	C-N3S-S	-3.05	119.18	124.23
4	B	1990	VAA	O1S-S-N5'	-2.84	101.73	106.73
4	A	990	VAA	O-C-CA	-2.64	118.65	120.73
4	A	990	VAA	O1S-S-N5'	-2.56	102.22	106.73
4	B	1990	VAA	C1'-N9-C4	-2.52	122.21	126.64
4	B	1990	VAA	O-C-CA	-2.30	118.92	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	990	VAA	C-CA-N	2.06	113.42	110.28

There are no chirality outliers.

All (6) torsion outliers are listed below:

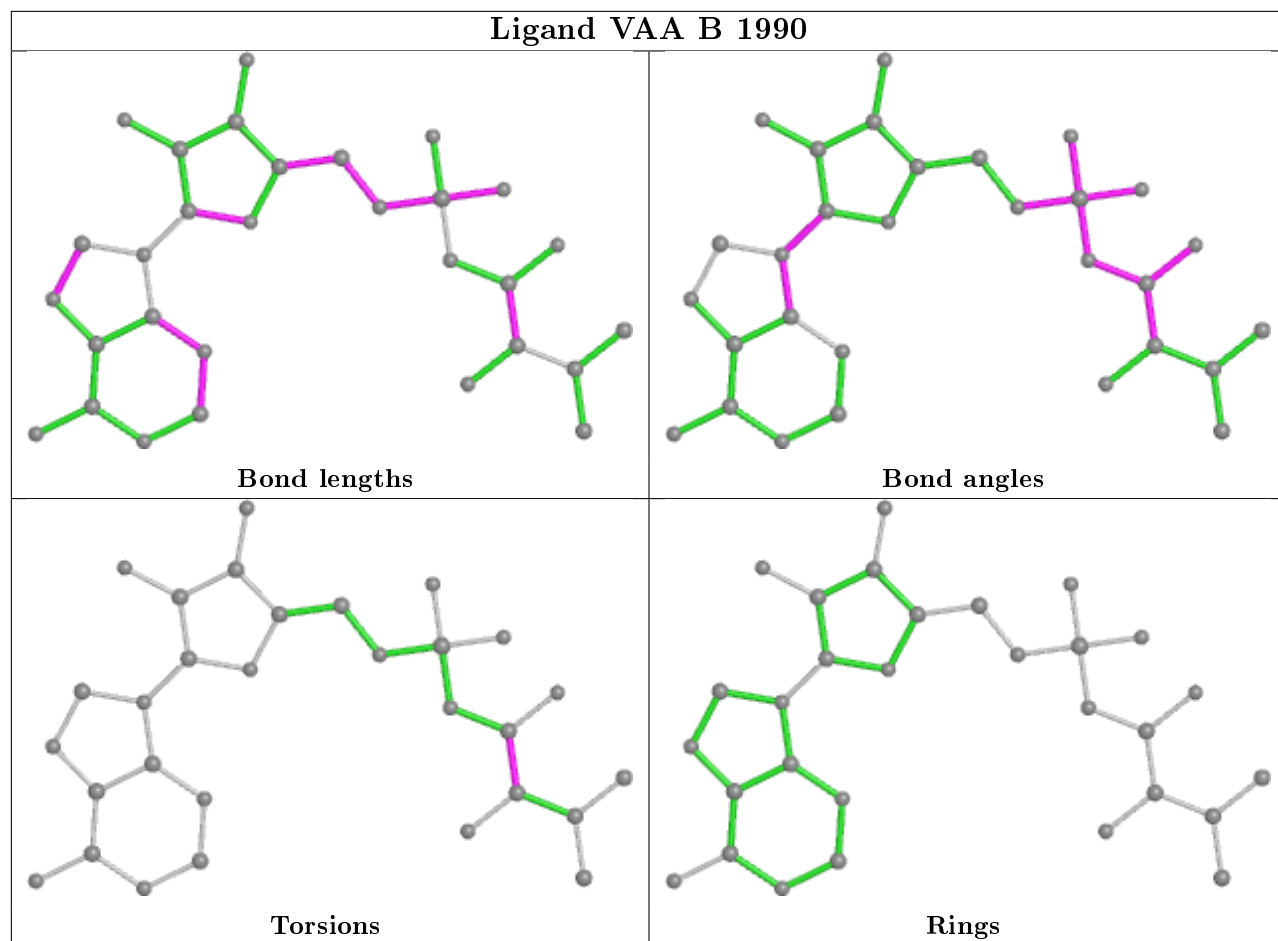
Mol	Chain	Res	Type	Atoms
4	A	990	VAA	C5'-N5'-S-O1S
4	A	990	VAA	C3'-C4'-C5'-N5'
4	A	990	VAA	O4'-C4'-C5'-N5'
4	A	990	VAA	C5'-N5'-S-O2S
4	A	990	VAA	C5'-N5'-S-N3S
4	B	1990	VAA	N3S-C-CA-CB

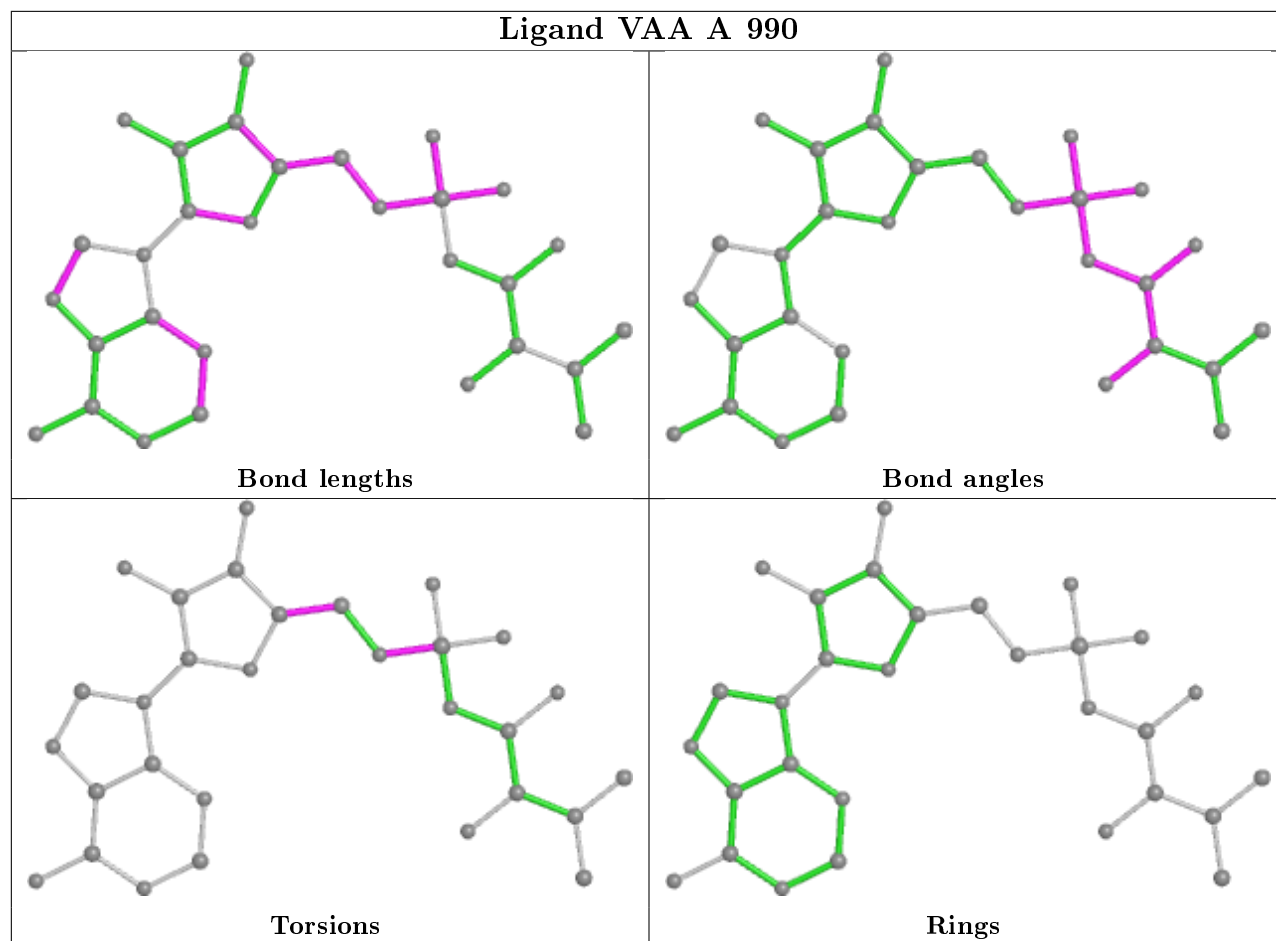
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1990	VAA	4	0
4	A	990	VAA	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.