



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:50 PM GMT

PDB ID : 1QU3  
Title : INSIGHTS INTO EDITING FROM AN ILE-TRNA SYNTHETASE STRUCTURE WITH TRNA(ILE) AND MUPIROCIN  
Authors : Silvian, L.F.; Wang, J.; Steitz, T.A.  
Deposited on : 1999-07-06  
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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

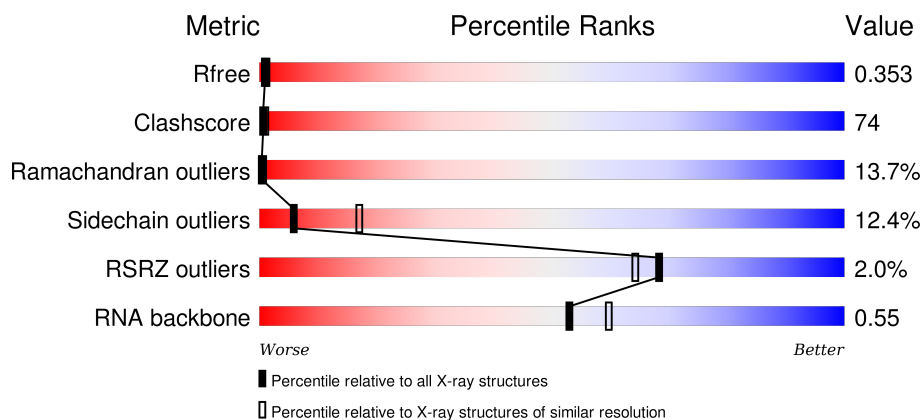
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

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

Mol	Chain	Length	Quality of chain
1	T	75	<div> <div>15%</div> <div>55%</div> <div>29%</div> <div>•</div> </div>
2	A	917	<div> <div>19%</div> <div>58%</div> <div>17%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MRC	A	993	X	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8870 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 ISOLEUCYL-TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	75	Total	C	N	O	P	24	0	0
			1603	715	289	525	74			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	880	Total	C	N	O	S	0	0	0
			7113	4537	1198	1358	20			

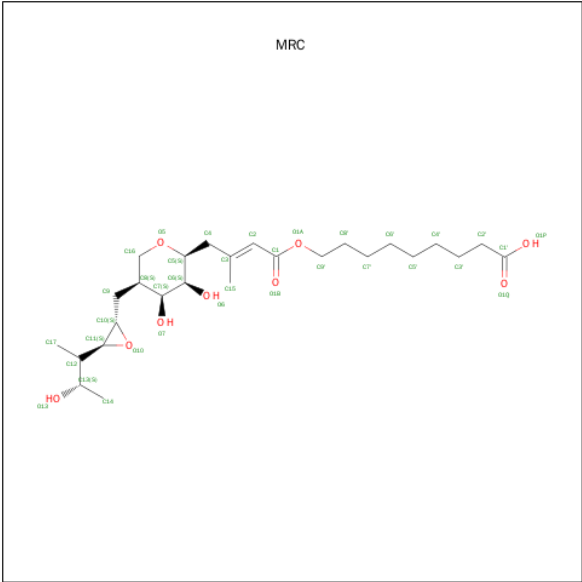
There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	GLU	LYS	CONFLICT	UNP P41972
A	5	LYS	GLU	CONFLICT	UNP P41972
A	295	TRP	TYR	CONFLICT	UNP P41972
A	340	GLN	LYS	CONFLICT	UNP P41972
A	644	ASP	VAL	CONFLICT	UNP P41972

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MUPIROCIN (three-letter code: MRC) (formula: C<sub>26</sub>H<sub>44</sub>O<sub>9</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	26	9		

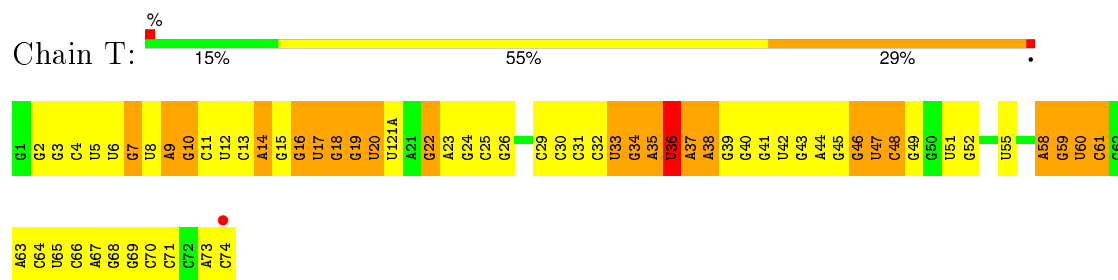
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total	O	0	0
			82	82		
5	T	36	Total	O	0	0
			36	36		

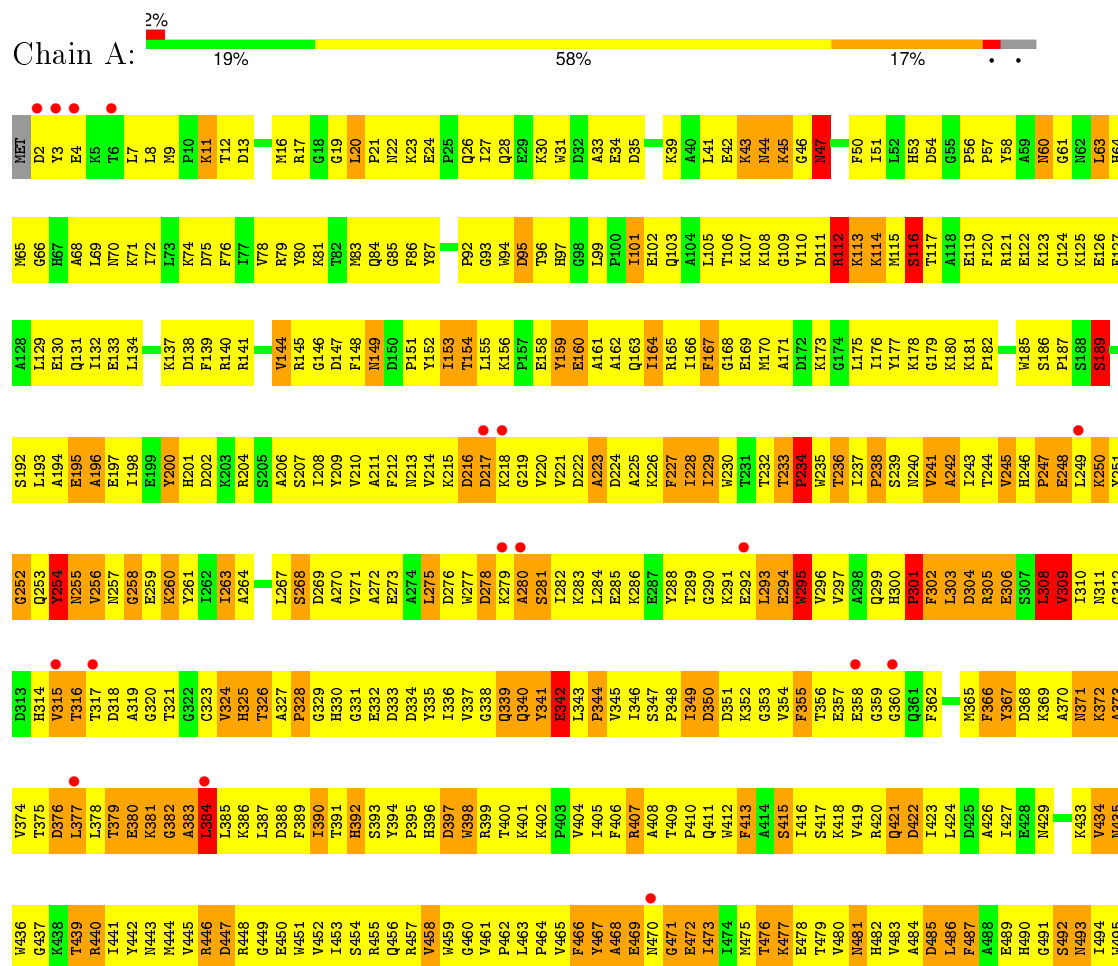
### 3 Residue-property plots

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

#### • Molecule 1: ISOLEUCYL-TRNA



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



ARG	K823	A757	R686	M621	R660	F496
CYS	S824	P758	S691	V622	G561	E497
TRP	L825	I759		S623	M662	R498
ASN	E826	L760	M694	S624	F663	E499
TYR	A827	L761	M695	T625	M664	A500
SER	K828	H762		D626	K501	K501
GLU	V829			Y627	I567	D502
ASP	T830			L628	T568	L503
LEU	I831	E765	M698	A629	T569	L504
GLY	A832	E766	F699	D630	S570	P505
ALA	S833	V767	Y701	V631	V571	P506
VAL	N834	H768	L702	R632	A572	G507
ASP	D835	S769	M703	L633	T573	F508
GLU	K836	H770	I704	S634	R574	T509
LEU	F837	I771	Y705	D635	G575	H510
THR	N838	P772	Q706	E636	V576	P511
HIS	A839	H773	E707	L637	S577	G512
LEU	S840	V774	V708	L638	P578	S513
CYS	F841	K775	Q709		Y579	P514
PRO	F842	E776	M710	S642	K580	N515
ARG	L843	E777	F711	D643	F581	
CYS	T844	S778	I712	D644	L582	F518
GLN		V779	M713	V645	L583	T519
GLN	A848	H780	V714	R646	S584	K520
VAL	L849	L781	E715	M647	H585	E521
VAL	H850	M784	L716	L648	G586	
LYS	Q851		S717	R649	F587	L524
SER	L852	D791	M718	N650	V588	M525
LEU	F853	Q792	F719	T651	M589	D526
	I854	A793	Y720	L652	D590	V527
	V855	L794	L721	R653	G591	M528
	S856	L795	Y722	F654	E592	F529
	Q857	L796	Y723	M655	G593	D530
	V858	D797	G724	L656	K594	
	K859	K797		G657	K595	S533
	V860	H798	I727	N658	M596	S534
	V861	R799	L728	L659	S597	H535
	D862	T800	Y729	R660	K598	R536
		F801	I730	D661	S599	G537
	D865	N802	E731		L600	V538
	D866	L803	R732	P664	G601	L539
	Q867	L804	R733	D665	N602	
	A868	R805		T666	V603	R542
	T869	D806	H736	D667	I604	P543
	A870	D807	I737	S668	V605	E544
	Y871	N808	R738	L669	P606	L545
	E872	N809	R739	P670	D607	S546
	H873	R810	S740	E671	Q608	F547
	G874	A811	M741	S672	V609	P548
	D875	L812	Q742	E673	V610	A549
	I876	E813	T743		K611	D550
	V877	T814	V744	E676	Q612	R551
		R815	L745		K613	M552
ASP	A881	R816	Y746	R679	G614	L553
GLY		N817	Q747	Y680	A615	P554
GLU		E818	I748	L681	D616	G555
LYS		K819	L749	L682	I617	S556
CYS		N820	V750	R683	A618	D557
GLU		I821	D751	R684	R619	Q558
		G822	M752	L685	L620	Y559

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.00Å 100.00Å 180.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.90 19.93 – 2.75	Depositor EDS
% Data completeness (in resolution range)	85.9 (10.00-2.90) 55.5 (19.93-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.76 (at 2.75Å)	Xtriage
Refinement program	unknown	Depositor
R, $R_{free}$	0.234 , 0.345 0.235 , 0.353	Depositor DCC
$R_{free}$ test set	813 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.7	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 42.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 19777 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	8870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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, MRC

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	T	0.53	0/1792	0.80	1/2794 (0.0%)
2	A	0.44	0/7287	0.72	3/9879 (0.0%)
All	All	0.46	0/9079	0.74	4/12673 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	471	GLY	N-CA-C	-6.82	96.06	113.10
2	A	681	LEU	CA-CB-CG	-5.37	102.94	115.30
1	T	36	U	N1-C1'-C2'	5.28	120.86	114.00
2	A	255	ASN	N-CA-C	5.25	125.18	111.00

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	T	1603	0	811	99	1
2	A	7113	0	6935	1135	1
3	A	1	0	0	0	0
4	A	35	0	40	5	0
5	A	82	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	T	36	0	0	2	0
All	All	8870	0	7786	1212	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 74.

All (1212) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:13:C:H2'	1:T:14:A:H5''	1.32	1.10
2:A:366:PHE:H	2:A:370:ALA:HB3	1.18	1.07
2:A:53:HIS:NE2	2:A:534:SER:HB3	1.73	1.02
2:A:250:LYS:HG2	2:A:290:GLY:N	1.77	1.00
2:A:302:PHE:HA	2:A:378:LEU:HD13	1.43	0.99
2:A:821:ILE:HD13	2:A:822:GLY:N	1.77	0.98
2:A:481:ASN:HD22	2:A:481:ASN:H	1.10	0.98
1:T:37:A:H2'	2:A:17:ARG:HD2	1.45	0.98
2:A:250:LYS:NZ	2:A:289:THR:HG23	1.78	0.97
2:A:469:GLU:HA	2:A:513:SER:N	1.79	0.97
2:A:70:ASN:HD22	2:A:585:HIS:HE1	1.10	0.97
2:A:250:LYS:HD3	2:A:289:THR:HA	1.45	0.97
2:A:589:MET:HE3	2:A:595:LYS:HA	1.46	0.96
2:A:596:MET:HB3	2:A:603:VAL:HG12	1.46	0.96
2:A:821:ILE:HD13	2:A:822:GLY:H	1.30	0.96
2:A:539:LEU:HD23	2:A:545:LEU:HD13	1.49	0.95
2:A:481:ASN:N	2:A:481:ASN:HD22	1.61	0.94
1:T:23:A:H2'	1:T:24:G:C8	2.03	0.94
2:A:23:LYS:HE3	2:A:27:ILE:HD11	1.47	0.94
2:A:467:TYR:HB3	2:A:472:GLU:CB	1.98	0.93
2:A:116:SER:HB3	2:A:119:GLU:HG3	1.50	0.93
2:A:487:PHE:CE1	2:A:492:SER:HA	2.02	0.93
2:A:704:ILE:O	2:A:708:VAL:HG12	1.68	0.93
2:A:411:GLN:HE22	2:A:456:GLN:NE2	1.65	0.93
2:A:481:ASN:H	2:A:481:ASN:ND2	1.66	0.93
2:A:857:GLN:NE2	2:A:858:VAL:H	1.67	0.93
2:A:237:ILE:HA	2:A:325:HIS:NE2	1.85	0.92
2:A:102:GLU:HA	2:A:105:LEU:HD12	1.50	0.92
2:A:390:ILE:HG12	2:A:391:THR:H	1.33	0.92
2:A:336:ILE:HG13	2:A:337:VAL:N	1.85	0.92
2:A:857:GLN:HE21	2:A:858:VAL:H	1.11	0.92
2:A:253:GLN:O	2:A:254:TYR:HB2	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:749:LEU:HD22	2:A:750:VAL:N	1.85	0.91
2:A:200:TYR:CE2	2:A:395:PRO:HG3	2.05	0.91
2:A:296:VAL:HG12	2:A:297:VAL:H	1.35	0.91
2:A:597:SER:H	2:A:602:ASN:HD21	1.18	0.91
2:A:105:LEU:HB3	2:A:110:VAL:HG21	1.53	0.90
2:A:602:ASN:HD22	2:A:602:ASN:H	1.20	0.90
2:A:250:LYS:HZ2	2:A:289:THR:HG23	1.37	0.89
2:A:4:GLU:HG3	2:A:7:LEU:HD23	1.54	0.89
2:A:649:ARG:HH11	2:A:649:ARG:HG3	1.34	0.89
2:A:355:PHE:HE1	2:A:365:MET:HB2	1.38	0.89
2:A:121:ARG:HD2	2:A:496:PHE:HD1	1.37	0.89
2:A:60:ASN:HD22	2:A:61:GLY:N	1.71	0.88
2:A:551:MET:HB3	2:A:581:PHE:HB3	1.55	0.88
2:A:467:TYR:HB3	2:A:472:GLU:HB3	1.57	0.87
2:A:324:VAL:O	2:A:325:HIS:HB3	1.75	0.87
2:A:829:VAL:HB	2:A:858:VAL:HG12	1.56	0.87
2:A:218:LYS:HD2	2:A:218:LYS:H	1.40	0.87
2:A:723:TYR:HA	2:A:854:ILE:HD11	1.55	0.87
2:A:349:ILE:HG12	2:A:355:PHE:HB3	1.55	0.86
2:A:749:LEU:HD13	2:A:750:VAL:H	1.38	0.86
2:A:71:LYS:HG3	2:A:139:PHE:CE2	2.10	0.86
2:A:578:PRO:HD2	5:A:1048:HOH:O	1.74	0.86
2:A:237:ILE:HB	2:A:238:PRO:HD3	1.58	0.86
1:T:33:U:H4'	1:T:34:G:O5'	1.73	0.86
2:A:105:LEU:HD13	2:A:124:CYS:SG	2.16	0.85
2:A:290:GLY:HA2	2:A:293:LEU:HB3	1.59	0.85
2:A:469:GLU:HA	2:A:513:SER:H	1.38	0.84
2:A:745:LEU:HA	2:A:748:ILE:HG22	1.57	0.84
2:A:434:VAL:HG13	2:A:435:ASN:H	1.43	0.84
2:A:240:ASN:ND2	2:A:308:LEU:HD21	1.93	0.84
2:A:289:THR:HG22	2:A:292:GLU:H	1.42	0.84
2:A:355:PHE:HD1	2:A:355:PHE:H	1.24	0.83
2:A:244:THR:HG22	2:A:311:ASN:HB2	1.58	0.83
2:A:741:MET:HE2	2:A:745:LEU:HD11	1.58	0.83
2:A:275:LEU:HG	2:A:386:LYS:HE3	1.61	0.83
2:A:482:HIS:O	2:A:486:LEU:HB2	1.78	0.83
1:T:13:C:C2'	1:T:14:A:H5''	2.09	0.83
2:A:384:LEU:O	2:A:385:LEU:HD23	1.79	0.82
2:A:379:THR:HG23	2:A:385:LEU:HB2	1.60	0.82
2:A:30:LYS:O	2:A:34:GLU:HG2	1.80	0.81
2:A:749:LEU:HD13	2:A:750:VAL:HG23	1.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:23:LYS:O	2:A:26:GLN:HG2	1.81	0.81
2:A:301:PRO:O	2:A:303:LEU:N	2.14	0.81
2:A:250:LYS:HG2	2:A:290:GLY:H	1.39	0.80
2:A:167:PHE:CE1	2:A:464:PRO:HD2	2.16	0.80
1:T:63:A:H2'	1:T:64:C:C6	2.16	0.80
2:A:212:PHE:CD2	2:A:301:PRO:HD2	2.17	0.80
2:A:834:ASN:HB2	2:A:874:GLY:HA2	1.64	0.80
2:A:536:ARG:HH12	2:A:574:ARG:CZ	1.95	0.79
1:T:33:U:H1'	1:T:36:U:H3	1.45	0.79
2:A:803:ASN:HB3	2:A:873:HIS:CE1	2.16	0.79
2:A:708:VAL:HG13	2:A:709:GLN:N	1.97	0.79
1:T:46:G:H2'	1:T:47:U:H5'	1.65	0.79
2:A:570:SER:CB	2:A:578:PRO:HG3	2.13	0.79
2:A:247:PRO:HB3	2:A:291:LYS:HA	1.65	0.78
2:A:390:ILE:HG12	2:A:391:THR:N	1.98	0.78
2:A:210:VAL:O	2:A:229:ILE:HG22	1.83	0.78
2:A:341:TYR:O	2:A:343:LEU:HG	1.82	0.78
2:A:535:HIS:HD1	2:A:536:ARG:N	1.81	0.78
2:A:272:ALA:HA	2:A:277:TRP:HB2	1.65	0.78
2:A:486:LEU:HD11	5:A:1020:HOH:O	1.83	0.78
2:A:323:CYS:O	2:A:324:VAL:HB	1.82	0.78
2:A:411:GLN:HE22	2:A:456:GLN:HE22	1.30	0.78
2:A:831:ILE:HA	2:A:875:ASP:O	1.83	0.78
2:A:857:GLN:HE21	2:A:858:VAL:N	1.81	0.77
2:A:154:THR:HA	2:A:159:TYR:CD1	2.19	0.77
2:A:164:ILE:HD11	2:A:484:ALA:HB2	1.65	0.77
2:A:501:LYS:CD	2:A:501:LYS:H	1.98	0.77
2:A:468:ALA:H	2:A:472:GLU:HB3	1.50	0.77
2:A:234:PRO:HG2	2:A:235:TRP:H	1.50	0.77
2:A:466:PHE:HA	2:A:520:LYS:HA	1.67	0.77
2:A:469:GLU:N	2:A:472:GLU:HG2	1.99	0.76
2:A:198:ILE:HG23	2:A:396:HIS:O	1.84	0.76
2:A:164:ILE:CD1	2:A:484:ALA:HB2	2.15	0.76
2:A:181:LYS:HG2	2:A:182:PRO:HD2	1.68	0.76
2:A:349:ILE:O	2:A:350:ASP:O	2.03	0.76
2:A:228:ILE:HD12	2:A:263:ILE:CG2	2.16	0.76
2:A:570:SER:HB2	2:A:578:PRO:HG3	1.68	0.76
1:T:43:G:O2'	1:T:44:A:H5'	1.86	0.76
2:A:164:ILE:HG13	2:A:165:ARG:N	2.01	0.75
2:A:161:ALA:HB1	2:A:165:ARG:HH12	1.51	0.75
1:T:19:G:O2'	1:T:20:U:OP1	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:823:LYS:O	2:A:825:LEU:N	2.19	0.75
2:A:229:ILE:HD12	2:A:323:CYS:HB2	1.69	0.75
2:A:178:LYS:HZ2	2:A:412:TRP:HE1	1.32	0.75
2:A:433:LYS:HB2	2:A:583:LEU:HG	1.69	0.75
2:A:240:ASN:HB2	2:A:308:LEU:HD11	1.69	0.75
1:T:37:A:H4'	1:T:38:A:OP2	1.87	0.74
2:A:462:PRO:HA	2:A:524:ILE:HA	1.67	0.74
1:T:47:U:O2'	1:T:48:C:OP2	2.05	0.74
2:A:309:VAL:C	2:A:310:ILE:HD12	2.08	0.74
2:A:336:ILE:HG13	2:A:337:VAL:H	1.50	0.74
1:T:63:A:H2'	1:T:64:C:H6	1.53	0.74
2:A:420:ARG:NH2	2:A:449:GLY:H	1.86	0.74
2:A:255:ASN:O	2:A:260:LYS:HA	1.86	0.74
2:A:602:ASN:HD22	2:A:602:ASN:N	1.84	0.74
2:A:650:ASN:O	2:A:653:ARG:HB3	1.87	0.74
2:A:54:ASP:OD1	2:A:92:PRO:HA	1.88	0.74
2:A:64:HIS:CD2	2:A:66:GLY:H	2.05	0.74
2:A:539:LEU:HD11	2:A:549:ALA:HB2	1.70	0.74
1:T:41:G:N2	5:T:156:HOH:O	2.20	0.74
2:A:807:ASP:OD2	2:A:871:TYR:HB3	1.88	0.73
2:A:653:ARG:HH11	2:A:653:ARG:HG2	1.52	0.73
2:A:604:ILE:HD12	2:A:633:ILE:HG23	1.70	0.73
2:A:459:TRP:H	2:A:524:ILE:HD13	1.51	0.73
2:A:469:GLU:C	2:A:471:GLY:H	1.89	0.73
2:A:300:HIS:O	2:A:304:ASP:HB3	1.87	0.73
2:A:293:LEU:O	2:A:295:TRP:N	2.20	0.73
2:A:468:ALA:N	2:A:472:GLU:HB3	2.04	0.73
2:A:70:ASN:HD22	2:A:585:HIS:CE1	2.02	0.73
2:A:58:TYR:CE2	2:A:101:ILE:HG13	2.23	0.73
2:A:220:VAL:HG22	2:A:224:ASP:OD1	1.89	0.72
2:A:681:LEU:HD13	2:A:720:TYR:CD1	2.23	0.72
2:A:745:LEU:HA	2:A:748:ILE:CG2	2.19	0.72
2:A:362:PHE:HA	2:A:365:MET:CG	2.20	0.72
1:T:13:C:H4'	2:A:702:LEU:HD11	1.70	0.72
2:A:289:THR:CG2	2:A:291:LYS:HB3	2.19	0.72
2:A:865:ASP:HB3	2:A:867:GLN:HE21	1.54	0.72
2:A:355:PHE:N	2:A:355:PHE:CD1	2.58	0.72
2:A:437:GLY:O	2:A:441:ILE:HG22	1.90	0.72
2:A:120:PHE:CD1	2:A:124:CYS:SG	2.83	0.72
2:A:293:LEU:O	2:A:296:VAL:HG23	1.90	0.72
2:A:632:ARG:HH11	2:A:632:ARG:HG3	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:289:THR:HG23	2:A:291:LYS:HB3	1.72	0.71
2:A:256:VAL:HG21	2:A:282:ILE:HD12	1.72	0.71
2:A:501:LYS:HD2	2:A:501:LYS:H	1.55	0.71
2:A:250:LYS:CG	2:A:290:GLY:H	2.03	0.71
2:A:163:GLN:HG2	2:A:461:VAL:HG11	1.71	0.71
2:A:597:SER:H	2:A:602:ASN:ND2	1.89	0.71
1:T:9:A:H5'	1:T:10:G:OP2	1.90	0.71
2:A:233:THR:HG23	2:A:236:THR:HG21	1.71	0.71
1:T:40:G:OP1	2:A:717:SER:HB3	1.90	0.71
2:A:247:PRO:CB	2:A:291:LYS:HA	2.20	0.71
2:A:229:ILE:CD1	2:A:323:CYS:HB2	2.20	0.71
2:A:757:ALA:HB3	2:A:758:PRO:HD3	1.73	0.71
2:A:255:ASN:ND2	2:A:256:VAL:HG23	2.06	0.70
2:A:185:TRP:O	2:A:404:VAL:HG13	1.92	0.70
2:A:499:GLU:HA	2:A:520:LYS:NZ	2.06	0.70
2:A:250:LYS:HZ1	2:A:289:THR:HG23	1.57	0.70
2:A:163:GLN:HG2	2:A:461:VAL:HG21	1.71	0.70
2:A:20:LEU:HD12	2:A:20:LEU:H	1.56	0.70
2:A:20:LEU:CD1	2:A:20:LEU:H	2.04	0.70
2:A:239:SER:O	2:A:346:ILE:HG12	1.90	0.70
2:A:250:LYS:CD	2:A:289:THR:HA	2.21	0.70
2:A:296:VAL:HG12	2:A:297:VAL:N	2.04	0.69
2:A:44:ASN:C	2:A:47:ASN:HD21	1.94	0.69
2:A:181:LYS:HG2	2:A:182:PRO:CD	2.23	0.69
2:A:493:ASN:O	2:A:497:GLU:HG2	1.93	0.69
2:A:494:ILE:HA	2:A:497:GLU:HG3	1.74	0.69
2:A:65:MET:HE3	2:A:606:PRO:HG3	1.72	0.69
2:A:706:GLN:HA	2:A:706:GLN:HE21	1.56	0.69
2:A:247:PRO:HA	2:A:291:LYS:HA	1.73	0.69
2:A:247:PRO:O	2:A:248:GLU:HB2	1.90	0.69
2:A:421:GLN:HA	2:A:424:LEU:HD12	1.75	0.69
2:A:473:ILE:HG22	2:A:473:ILE:O	1.90	0.69
2:A:121:ARG:HD2	2:A:496:PHE:CD1	2.24	0.69
2:A:749:LEU:CD1	2:A:750:VAL:H	2.06	0.69
2:A:434:VAL:HG13	2:A:435:ASN:N	2.08	0.69
2:A:821:ILE:CD1	2:A:822:GLY:H	2.01	0.69
1:T:69:G:H5''	2:A:589:MET:CE	2.23	0.69
2:A:246:HIS:CD2	2:A:315:VAL:H	2.11	0.69
2:A:362:PHE:HA	2:A:365:MET:HG3	1.72	0.69
2:A:469:GLU:N	2:A:513:SER:HB2	2.08	0.69
2:A:649:ARG:HG3	2:A:649:ARG:NH1	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:23:LYS:HA	2:A:26:GLN:HE21	1.57	0.68
1:T:43:G:H2'	1:T:44:A:C8	2.28	0.68
2:A:129:LEU:HA	2:A:132:ILE:HG12	1.75	0.68
2:A:129:LEU:O	2:A:132:ILE:HG12	1.93	0.68
2:A:247:PRO:CA	2:A:291:LYS:HA	2.23	0.68
1:T:32:C:H5'	2:A:823:LYS:HB3	1.75	0.68
2:A:278:ASP:C	2:A:280:ALA:H	1.97	0.68
2:A:354:VAL:HG22	2:A:365:MET:O	1.94	0.68
2:A:634:SER:OG	2:A:637:ILE:HG13	1.93	0.68
2:A:120:PHE:CE1	2:A:124:CYS:SG	2.87	0.68
2:A:469:GLU:CB	2:A:512:GLY:HA3	2.23	0.68
2:A:500:ALA:O	2:A:504:LEU:HD23	1.94	0.68
2:A:848:ALA:HB1	2:A:851:GLN:HB2	1.76	0.68
2:A:23:LYS:HG3	2:A:27:ILE:HD11	1.75	0.68
1:T:23:A:H2'	1:T:24:G:H8	1.58	0.68
2:A:840:SER:HA	2:A:860:VAL:CG1	2.23	0.68
2:A:237:ILE:C	2:A:239:SER:H	1.98	0.68
1:T:58:A:O2'	1:T:60:U:H5	1.77	0.68
2:A:214:VAL:HG22	2:A:227:PHE:CD1	2.29	0.67
2:A:829:VAL:O	2:A:858:VAL:HA	1.94	0.67
2:A:831:ILE:HG22	2:A:876:ILE:HG12	1.77	0.67
2:A:70:ASN:ND2	2:A:585:HIS:HE1	1.89	0.67
2:A:228:ILE:HD12	2:A:263:ILE:HG21	1.74	0.67
2:A:802:MET:HE2	2:A:802:MET:HA	1.76	0.67
1:T:74:C:H6	1:T:74:C:O5'	1.77	0.67
2:A:132:ILE:HG13	2:A:133:GLU:N	2.08	0.67
2:A:71:LYS:HG3	2:A:139:PHE:HE2	1.57	0.67
2:A:349:ILE:HA	2:A:355:PHE:HA	1.76	0.67
2:A:105:LEU:HD13	2:A:120:PHE:CZ	2.30	0.67
2:A:622:VAL:O	2:A:625:THR:HG22	1.94	0.67
2:A:220:VAL:HG13	2:A:224:ASP:OD2	1.93	0.67
2:A:351:ASP:HA	2:A:407:ARG:NH2	2.08	0.67
2:A:366:PHE:H	2:A:370:ALA:CB	2.03	0.67
2:A:57:PRO:HD2	2:A:93:GLY:O	1.95	0.67
2:A:808:VAL:O	2:A:812:LEU:HG	1.95	0.67
1:T:4:C:HO2'	2:A:436:TRP:HE3	1.40	0.67
1:T:4:C:O2'	2:A:436:TRP:HE3	1.77	0.67
2:A:484:ALA:C	2:A:486:LEU:H	1.98	0.66
2:A:467:TYR:HB3	2:A:472:GLU:HB2	1.77	0.66
2:A:766:GLU:O	2:A:770:HIS:HD2	1.79	0.66
2:A:175:LEU:HD23	2:A:418:LYS:HD2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:681:LEU:HD13	2:A:720:TYR:CG	2.30	0.66
2:A:708:VAL:HG13	2:A:709:GLN:H	1.59	0.66
2:A:237:ILE:O	2:A:239:SER:N	2.28	0.66
2:A:69:LEU:HD12	2:A:622:VAL:HG13	1.78	0.66
2:A:453:ILE:HD12	2:A:463:LEU:HD21	1.77	0.66
2:A:148:PHE:O	2:A:151:PRO:HD3	1.96	0.66
2:A:294:GLU:HA	2:A:310:ILE:HG22	1.77	0.66
2:A:275:LEU:HD21	2:A:386:LYS:HG3	1.76	0.66
2:A:371:ASN:HD22	2:A:371:ASN:N	1.93	0.66
2:A:544:GLU:H	2:A:544:GLU:CD	1.96	0.66
2:A:745:LEU:CA	2:A:748:ILE:HG22	2.26	0.65
2:A:275:LEU:HG	2:A:386:LYS:CE	2.26	0.65
2:A:499:GLU:HB2	2:A:501:LYS:HD2	1.79	0.65
2:A:653:ARG:HG2	2:A:653:ARG:NH1	2.11	0.65
2:A:606:PRO:O	2:A:609:VAL:HG12	1.95	0.65
2:A:736:HIS:HA	5:A:1007:HOH:O	1.95	0.65
2:A:254:TYR:CD2	2:A:286:LYS:HE3	2.32	0.65
2:A:861:VAL:O	2:A:862:ASP:HB2	1.96	0.65
2:A:96:THR:H	2:A:154:THR:CG2	2.09	0.65
2:A:256:VAL:HG12	2:A:257:ASN:N	2.11	0.65
2:A:491:GLY:C	2:A:493:ASN:H	1.98	0.65
2:A:368:ASP:OD1	2:A:372:LYS:HE3	1.97	0.65
1:T:69:G:H5''	2:A:589:MET:HE1	1.79	0.65
2:A:834:ASN:CB	2:A:874:GLY:HA2	2.27	0.65
2:A:667:ASP:O	2:A:668:SER:O	2.14	0.65
2:A:706:GLN:HA	2:A:706:GLN:NE2	2.12	0.65
2:A:300:HIS:CD2	2:A:308:LEU:HD12	2.31	0.65
2:A:210:VAL:HG13	2:A:385:LEU:HD22	1.79	0.65
2:A:469:GLU:H	2:A:472:GLU:HG2	1.61	0.65
2:A:390:ILE:CG1	2:A:391:THR:H	2.09	0.64
2:A:825:LEU:O	2:A:856:SER:HB2	1.96	0.64
2:A:451:TRP:O	2:A:453:ILE:HG23	1.97	0.64
2:A:644:ASP:HA	5:A:1040:HOH:O	1.97	0.64
2:A:64:HIS:HB2	5:A:1071:HOH:O	1.97	0.64
2:A:747:GLN:C	2:A:749:LEU:N	2.48	0.64
2:A:201:HIS:HB2	2:A:396:HIS:CD2	2.32	0.64
1:T:18:G:O2'	1:T:19:G:OP1	2.12	0.64
2:A:64:HIS:NE2	2:A:66:GLY:HA3	2.13	0.64
1:T:5:U:H2'	1:T:6:U:C6	2.32	0.64
2:A:413:PHE:CD1	2:A:413:PHE:N	2.65	0.64
2:A:316:THR:HG22	2:A:316:THR:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:538:VAL:HG23	2:A:542:ARG:HD3	1.81	0.63
2:A:167:PHE:HD2	2:A:167:PHE:C	2.01	0.63
2:A:548:PRO:HB2	2:A:580:LYS:HE3	1.79	0.63
2:A:813:GLU:OE2	2:A:813:GLU:HA	1.98	0.63
2:A:400:THR:HG22	2:A:402:LYS:HG2	1.80	0.63
2:A:831:ILE:CG2	2:A:876:ILE:HG12	2.28	0.63
2:A:876:ILE:HG22	2:A:877:VAL:N	2.14	0.63
2:A:84:GLN:OE1	2:A:84:GLN:HA	1.97	0.63
2:A:132:ILE:HG13	2:A:133:GLU:H	1.63	0.63
2:A:745:LEU:O	2:A:748:ILE:HG22	1.98	0.63
2:A:81:LYS:HE3	2:A:86:PHE:CE2	2.33	0.63
2:A:481:ASN:O	2:A:484:ALA:N	2.32	0.63
2:A:8:LEU:HD13	2:A:738:ARG:NE	2.14	0.63
2:A:244:THR:CG2	2:A:311:ASN:HB2	2.29	0.62
2:A:424:LEU:HD22	2:A:442:TYR:CE1	2.34	0.62
2:A:158:GLU:O	2:A:161:ALA:HB3	1.99	0.62
1:T:37:A:H8	1:T:37:A:OP2	1.82	0.62
2:A:535:HIS:CD2	2:A:570:SER:HB2	2.34	0.62
2:A:141:ARG:HG3	2:A:141:ARG:HH11	1.64	0.62
2:A:11:LYS:O	2:A:12:THR:HG23	1.99	0.62
2:A:16:MET:O	2:A:649:ARG:HD2	1.99	0.62
2:A:854:ILE:O	2:A:854:ILE:HG22	1.99	0.62
2:A:41:LEU:HB3	2:A:87:TYR:CE1	2.33	0.62
2:A:701:TYR:O	2:A:704:ILE:N	2.29	0.62
2:A:171:ALA:HA	2:A:176:ILE:HG22	1.82	0.62
2:A:500:ALA:HB3	2:A:501:LYS:HE3	1.81	0.62
2:A:17:ARG:HG2	2:A:646:ARG:HH22	1.65	0.62
2:A:749:LEU:C	2:A:749:LEU:HD22	2.20	0.62
1:T:47:U:O2'	1:T:48:C:P	2.58	0.62
1:T:19:G:OP1	1:T:60:U:N3	2.33	0.62
2:A:810:ARG:O	2:A:814:THR:HG23	2.00	0.62
2:A:235:TRP:HB3	2:A:371:ASN:HB3	1.81	0.62
2:A:166:ILE:HD12	2:A:533:SER:OG	2.00	0.62
2:A:212:PHE:CE2	2:A:300:HIS:HB3	2.35	0.62
2:A:379:THR:HA	2:A:385:LEU:CD1	2.30	0.62
2:A:397:ASP:OD2	2:A:400:THR:HB	1.99	0.62
1:T:41:G:O2'	2:A:813:GLU:HG2	2.00	0.61
2:A:676:GLU:HG2	2:A:798:TRP:HZ2	1.64	0.61
2:A:718:ASN:HB3	5:A:1060:HOH:O	1.98	0.61
2:A:267:LEU:HG	2:A:320:GLY:O	1.99	0.61
2:A:228:ILE:HG22	2:A:229:ILE:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:120:PHE:HA	2:A:123:LYS:HB2	1.82	0.61
1:T:58:A:O2'	1:T:59:G:O5'	2.17	0.61
2:A:821:ILE:HG12	2:A:826:GLU:HB2	1.81	0.61
2:A:80:TYR:O	2:A:83:MET:HB2	2.00	0.61
2:A:467:TYR:CB	2:A:472:GLU:HB3	2.29	0.61
2:A:367:TYR:O	2:A:371:ASN:OD1	2.18	0.61
2:A:124:CYS:O	2:A:459:TRP:CZ2	2.54	0.61
2:A:332:GLU:O	2:A:335:TYR:HB3	2.00	0.61
2:A:256:VAL:CG1	2:A:257:ASN:N	2.63	0.61
2:A:60:ASN:HD22	2:A:60:ASN:C	1.99	0.61
2:A:424:LEU:HB3	2:A:442:TYR:HE1	1.65	0.61
2:A:167:PHE:C	2:A:167:PHE:CD2	2.74	0.61
2:A:708:VAL:CG1	2:A:709:GLN:N	2.64	0.61
2:A:420:ARG:O	2:A:421:GLN:CB	2.48	0.61
2:A:105:LEU:CD1	2:A:124:CYS:SG	2.87	0.61
2:A:125:LYS:HG2	2:A:125:LYS:O	1.99	0.61
2:A:318:ASP:CG	2:A:319:ALA:H	2.03	0.61
2:A:64:HIS:CD2	2:A:66:GLY:N	2.69	0.61
2:A:263:ILE:HD12	2:A:271:VAL:HG21	1.83	0.60
2:A:536:ARG:HH12	2:A:574:ARG:NE	1.98	0.60
2:A:434:VAL:HG22	2:A:435:ASN:N	2.16	0.60
2:A:702:LEU:O	2:A:706:GLN:HG2	2.00	0.60
2:A:218:LYS:C	2:A:220:VAL:H	2.04	0.60
2:A:476:THR:O	2:A:479:THR:OG1	2.17	0.60
2:A:733:ARG:HG3	2:A:733:ARG:HH11	1.65	0.60
2:A:366:PHE:N	2:A:366:PHE:CD2	2.67	0.60
2:A:366:PHE:N	2:A:370:ALA:HB3	2.03	0.60
2:A:398:TRP:CD1	2:A:399:ARG:HG3	2.35	0.60
2:A:251:TYR:O	2:A:253:GLN:N	2.34	0.60
2:A:250:LYS:O	2:A:264:ALA:HA	2.01	0.60
2:A:373:ALA:HA	2:A:376:ASP:OD1	2.01	0.60
2:A:382:GLY:O	2:A:383:ALA:HB2	2.01	0.60
2:A:50:PHE:HZ	2:A:551:MET:HG2	1.67	0.60
2:A:832:ALA:HB2	2:A:861:VAL:CG1	2.31	0.60
2:A:397:ASP:OD1	2:A:400:THR:HB	2.02	0.60
2:A:239:SER:HB3	2:A:346:ILE:HD13	1.83	0.60
2:A:251:TYR:C	2:A:253:GLN:H	2.04	0.60
2:A:336:ILE:CG1	2:A:337:VAL:N	2.62	0.60
2:A:4:GLU:HG3	2:A:7:LEU:CD2	2.30	0.60
2:A:605:VAL:HG13	2:A:606:PRO:HD2	1.84	0.60
2:A:244:THR:HG21	2:A:337:VAL:CG2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:367:TYR:CE1	2:A:405:ILE:HG21	2.37	0.60
2:A:164:ILE:CG1	2:A:484:ALA:HB2	2.31	0.60
2:A:536:ARG:HH12	2:A:574:ARG:NH2	2.00	0.60
2:A:232:THR:HG21	2:A:392:HIS:HE1	1.67	0.60
2:A:494:ILE:HA	2:A:497:GLU:CG	2.31	0.59
2:A:545:LEU:O	2:A:546:SER:HB3	2.01	0.59
2:A:548:PRO:O	2:A:580:LYS:HE3	2.02	0.59
2:A:659:ILE:C	2:A:659:ILE:HD12	2.23	0.59
2:A:749:LEU:CD2	2:A:750:VAL:N	2.63	0.59
2:A:625:THR:OG1	2:A:631:VAL:HG12	2.03	0.59
2:A:218:LYS:CD	2:A:218:LYS:H	2.14	0.59
2:A:223:ALA:HB3	2:A:254:TYR:OH	2.02	0.59
2:A:470:ASN:N	2:A:472:GLU:HG2	2.17	0.59
2:A:126:GLU:O	2:A:130:GLU:HG3	2.02	0.59
2:A:510:HIS:CE1	2:A:511:PRO:HG2	2.37	0.59
2:A:539:LEU:CD1	2:A:549:ALA:HB2	2.33	0.59
2:A:215:LYS:HG2	2:A:216:ASP:H	1.66	0.59
2:A:228:ILE:CG2	2:A:321:THR:HG21	2.32	0.59
2:A:235:TRP:O	2:A:238:PRO:HD2	2.02	0.59
2:A:823:LYS:HG2	2:A:826:GLU:OE2	2.02	0.59
2:A:830:THR:HB	2:A:877:VAL:HG22	1.83	0.59
2:A:745:LEU:HD23	2:A:748:ILE:HG21	1.83	0.59
2:A:41:LEU:HB3	2:A:87:TYR:HE1	1.66	0.59
2:A:220:VAL:HG12	2:A:220:VAL:O	2.02	0.59
2:A:234:PRO:HG2	2:A:235:TRP:N	2.17	0.59
2:A:289:THR:O	2:A:289:THR:HG22	2.02	0.59
2:A:484:ALA:C	2:A:486:LEU:N	2.56	0.59
2:A:600:LEU:HD23	2:A:600:LEU:O	2.03	0.59
1:T:38:A:H2'	1:T:39:G:H5'	1.85	0.59
2:A:499:GLU:HA	2:A:520:LYS:HZ2	1.68	0.59
2:A:257:ASN:O	2:A:258:GLY:C	2.41	0.59
2:A:338:GLY:O	2:A:343:LEU:HD12	2.01	0.59
2:A:535:HIS:HB2	2:A:547:PHE:CE1	2.38	0.59
2:A:411:GLN:NE2	2:A:456:GLN:HE22	1.97	0.59
2:A:558:GLN:O	2:A:563:PHE:HB2	2.03	0.59
2:A:46:GLY:O	2:A:47:ASN:O	2.20	0.58
2:A:613:LYS:HD3	2:A:642:SER:OG	2.03	0.58
2:A:178:LYS:NZ	2:A:412:TRP:HE1	2.01	0.58
2:A:453:ILE:O	2:A:453:ILE:HD12	2.02	0.58
2:A:589:MET:HB3	2:A:594:LYS:O	2.04	0.58
2:A:239:SER:HB3	2:A:346:ILE:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:834:ASN:HD22	2:A:874:GLY:C	2.05	0.58
2:A:792:GLN:O	2:A:795:LEU:N	2.37	0.58
2:A:739:ARG:HD3	2:A:742:GLN:NE2	2.19	0.58
2:A:419:VAL:HA	2:A:422:ASP:OD1	2.03	0.58
2:A:469:GLU:HB2	2:A:512:GLY:HA3	1.83	0.58
2:A:314:HIS:O	2:A:315:VAL:HB	2.03	0.58
2:A:247:PRO:CD	2:A:312:GLY:HA2	2.34	0.58
2:A:379:THR:HG23	2:A:385:LEU:CB	2.31	0.58
2:A:234:PRO:CG	2:A:235:TRP:H	2.17	0.58
2:A:821:ILE:CD1	2:A:822:GLY:N	2.61	0.58
2:A:792:GLN:HE22	2:A:799:ARG:NH1	2.00	0.58
2:A:315:VAL:O	2:A:316:THR:OG1	2.22	0.58
2:A:616:ASP:OD1	2:A:762:HIS:HB2	2.04	0.58
2:A:490:HIS:HB2	2:A:494:ILE:HB	1.84	0.58
2:A:247:PRO:O	2:A:248:GLU:CB	2.51	0.58
2:A:328:PRO:HA	2:A:335:TYR:HA	1.86	0.58
2:A:299:GLN:HB3	2:A:304:ASP:HB2	1.86	0.57
2:A:724:GLY:HA3	2:A:741:MET:HE1	1.85	0.57
2:A:225:ALA:HB2	2:A:254:TYR:CE2	2.39	0.57
2:A:387:LEU:C	2:A:387:LEU:HD23	2.24	0.57
2:A:552:TYR:CD1	2:A:579:TYR:HB3	2.39	0.57
2:A:192:SER:O	2:A:193:LEU:HD23	2.04	0.57
2:A:243:ILE:HG23	2:A:323:CYS:O	2.03	0.57
2:A:250:LYS:HD2	2:A:251:TYR:H	1.69	0.57
2:A:588:VAL:HG12	2:A:596:MET:SD	2.44	0.57
2:A:185:TRP:C	2:A:404:VAL:HG13	2.24	0.57
2:A:69:LEU:CD1	2:A:622:VAL:HG13	2.34	0.57
1:T:71:C:O2'	2:A:560:ARG:NH1	2.38	0.57
2:A:209:TYR:O	2:A:386:LYS:HB2	2.04	0.57
2:A:821:ILE:HD11	2:A:824:SER:N	2.20	0.57
2:A:469:GLU:C	2:A:471:GLY:N	2.58	0.57
2:A:625:THR:OG1	2:A:631:VAL:CG1	2.53	0.57
2:A:809:ASN:O	2:A:812:LEU:N	2.37	0.57
2:A:163:GLN:NE2	2:A:529:PHE:CD2	2.73	0.57
2:A:228:ILE:O	2:A:229:ILE:HB	2.05	0.57
1:T:42:U:O2'	1:T:43:G:H5'	2.05	0.57
2:A:218:LYS:O	2:A:221:VAL:HG23	2.05	0.57
2:A:35:ASP:O	2:A:39:LYS:HG2	2.04	0.57
2:A:708:VAL:CG1	2:A:709:GLN:H	2.18	0.57
2:A:164:ILE:HG12	2:A:484:ALA:HB2	1.86	0.57
2:A:23:LYS:HA	2:A:26:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:741:MET:CE	2:A:745:LEU:HD11	2.34	0.57
2:A:469:GLU:CG	2:A:512:GLY:HA3	2.35	0.57
2:A:747:GLN:C	2:A:749:LEU:H	2.06	0.57
2:A:397:ASP:CG	2:A:400:THR:HB	2.24	0.57
2:A:336:ILE:CG1	2:A:337:VAL:H	2.17	0.57
2:A:416:ILE:HD11	2:A:451:TRP:HB2	1.85	0.57
2:A:842:PHE:C	2:A:844:THR:H	2.09	0.57
2:A:217:ASP:O	2:A:220:VAL:HB	2.05	0.56
2:A:296:VAL:O	2:A:310:ILE:HD13	2.05	0.56
2:A:382:GLY:O	2:A:383:ALA:CB	2.53	0.56
2:A:385:LEU:O	2:A:386:LYS:HG2	2.05	0.56
2:A:472:GLU:O	2:A:473:ILE:HB	2.05	0.56
2:A:201:HIS:HB2	2:A:396:HIS:NE2	2.20	0.56
2:A:160:GLU:O	2:A:163:GLN:HB3	2.05	0.56
1:T:47:U:HO2'	1:T:48:C:P	2.28	0.56
2:A:832:ALA:HB2	2:A:861:VAL:HG13	1.86	0.56
2:A:302:PHE:CD1	2:A:303:LEU:N	2.74	0.56
2:A:461:VAL:O	2:A:525:MET:HG3	2.05	0.56
2:A:424:LEU:HB3	2:A:442:TYR:CE1	2.41	0.56
2:A:553:LEU:O	2:A:554:GLU:CD	2.44	0.56
2:A:212:PHE:HD2	2:A:301:PRO:HD2	1.67	0.56
2:A:487:PHE:CD1	2:A:492:SER:HA	2.40	0.56
1:T:66:C:O2'	1:T:67:A:H5'	2.05	0.56
2:A:865:ASP:HB3	2:A:867:GLN:NE2	2.21	0.56
2:A:713:ASN:O	2:A:718:ASN:HB2	2.05	0.56
2:A:263:ILE:CD1	2:A:271:VAL:HG21	2.36	0.56
2:A:8:LEU:HD21	2:A:733:ARG:NH1	2.21	0.56
1:T:43:G:O2'	1:T:44:A:C5'	2.54	0.56
2:A:79:ARG:HH12	2:A:780:HIS:CG	2.23	0.56
2:A:218:LYS:HD2	2:A:218:LYS:N	2.15	0.56
2:A:219:GLY:HA2	2:A:297:VAL:H	1.70	0.56
2:A:327:ALA:C	2:A:329:GLY:H	2.08	0.56
2:A:816:ARG:HD2	2:A:822:GLY:O	2.06	0.56
2:A:468:ALA:HA	2:A:472:GLU:OE2	2.06	0.56
2:A:749:LEU:O	2:A:752:MET:N	2.30	0.56
2:A:194:ALA:O	2:A:195:GLU:C	2.44	0.56
2:A:664:PRO:O	2:A:665:ASP:C	2.45	0.56
2:A:212:PHE:CE1	2:A:229:ILE:HG21	2.40	0.56
2:A:254:TYR:HD2	2:A:286:LYS:HE3	1.69	0.56
2:A:57:PRO:HG3	5:A:1013:HOH:O	2.06	0.56
2:A:419:VAL:O	2:A:420:ARG:C	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:487:PHE:O	2:A:491:GLY:N	2.37	0.56
2:A:120:PHE:CG	2:A:124:CYS:SG	2.99	0.56
1:T:51:U:C2	1:T:52:G:C8	2.94	0.56
2:A:618:ALA:O	2:A:621:TRP:HB3	2.06	0.56
2:A:64:HIS:HD2	2:A:66:GLY:H	1.54	0.56
2:A:237:ILE:C	2:A:239:SER:N	2.58	0.55
2:A:747:GLN:O	2:A:749:LEU:N	2.39	0.55
2:A:24:GLU:HG2	2:A:762:HIS:CD2	2.41	0.55
2:A:219:GLY:HA3	2:A:297:VAL:O	2.06	0.55
2:A:484:ALA:O	2:A:486:LEU:N	2.39	0.55
2:A:842:PHE:O	2:A:844:THR:N	2.39	0.55
2:A:212:PHE:CE2	2:A:301:PRO:HD2	2.40	0.55
2:A:212:PHE:N	2:A:227:PHE:O	2.37	0.55
2:A:470:ASN:H	2:A:472:GLU:HG2	1.71	0.55
1:T:63:A:O2'	1:T:64:C:H5'	2.05	0.55
2:A:293:LEU:HD23	2:A:296:VAL:HG23	1.89	0.55
2:A:371:ASN:N	2:A:371:ASN:ND2	2.54	0.55
1:T:31:C:H2'	1:T:32:C:H6	1.72	0.55
2:A:477:LYS:O	2:A:478:GLU:HB3	2.06	0.55
2:A:536:ARG:HH22	2:A:574:ARG:NH2	2.04	0.55
1:T:19:G:HO2'	1:T:20:U:P	2.28	0.55
2:A:324:VAL:O	2:A:325:HIS:CB	2.52	0.55
2:A:469:GLU:HB3	2:A:472:GLU:H	1.72	0.55
2:A:765:GLU:OE1	2:A:778:SER:HA	2.05	0.55
2:A:535:HIS:HB2	2:A:547:PHE:HE1	1.70	0.55
1:T:4:C:O2'	1:T:5:U:H5'	2.07	0.55
2:A:81:LYS:HE3	2:A:86:PHE:HE2	1.72	0.55
2:A:272:ALA:CA	2:A:277:TRP:HB2	2.36	0.55
2:A:350:ASP:OD2	2:A:351:ASP:N	2.38	0.55
2:A:23:LYS:HE3	2:A:27:ILE:CD1	2.31	0.55
2:A:212:PHE:CD1	2:A:229:ILE:HG21	2.41	0.55
2:A:74:LYS:O	2:A:78:VAL:HG23	2.07	0.55
2:A:590:ASP:C	2:A:590:ASP:OD1	2.44	0.55
2:A:446:ARG:CG	2:A:446:ARG:O	2.55	0.55
2:A:741:MET:HB2	5:A:1063:HOH:O	2.07	0.55
2:A:294:GLU:O	2:A:295:TRP:HB2	2.05	0.54
2:A:290:GLY:HA2	2:A:293:LEU:CB	2.34	0.54
2:A:164:ILE:HD11	2:A:484:ALA:CB	2.35	0.54
2:A:494:ILE:HG13	2:A:494:ILE:O	2.06	0.54
2:A:505:PRO:HB2	2:A:508:PHE:HB2	1.88	0.54
1:T:2:G:H2'	1:T:3:G:C8	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:362:PHE:HE2	2:A:374:VAL:CG2	2.20	0.54
2:A:453:ILE:CD1	2:A:463:LEU:HD21	2.36	0.54
2:A:491:GLY:C	2:A:493:ASN:N	2.60	0.54
2:A:463:LEU:CD1	2:A:525:MET:HG2	2.36	0.54
2:A:466:PHE:CE1	2:A:504:LEU:HD11	2.41	0.54
2:A:602:ASN:ND2	2:A:602:ASN:N	2.54	0.54
2:A:380:GLU:HA	2:A:384:LEU:HA	1.88	0.54
2:A:23:LYS:CE	2:A:27:ILE:HD11	2.30	0.54
2:A:415:SER:O	2:A:419:VAL:HG22	2.08	0.54
2:A:491:GLY:O	2:A:494:ILE:HG22	2.08	0.54
2:A:595:LYS:NZ	4:A:993:MRC:H8'1	2.21	0.54
2:A:121:ARG:NH1	2:A:496:PHE:CE1	2.76	0.54
2:A:81:LYS:HG3	2:A:86:PHE:CD2	2.42	0.54
2:A:707:GLU:O	2:A:708:VAL:C	2.46	0.54
2:A:163:GLN:OE1	2:A:530:ASP:HA	2.08	0.54
1:T:22:G:N7	1:T:46:G:N2	2.50	0.54
2:A:250:LYS:CD	2:A:251:TYR:H	2.20	0.54
2:A:372:LYS:C	2:A:374:VAL:N	2.60	0.54
2:A:374:VAL:HG12	2:A:375:THR:N	2.23	0.54
2:A:486:LEU:CD2	2:A:494:ILE:HG12	2.38	0.54
2:A:598:LYS:O	2:A:600:LEU:N	2.41	0.54
1:T:33:U:H1'	1:T:36:U:N3	2.19	0.54
2:A:551:MET:HE3	2:A:699:PHE:CZ	2.43	0.54
2:A:278:ASP:C	2:A:280:ALA:N	2.60	0.54
2:A:621:TRP:O	2:A:624:SER:N	2.40	0.54
2:A:706:GLN:CA	2:A:706:GLN:HE21	2.21	0.53
2:A:321:THR:C	2:A:323:CYS:H	2.10	0.53
2:A:433:LYS:HG2	2:A:583:LEU:HD21	1.90	0.53
2:A:768:TRP:HB2	2:A:779:VAL:HG22	1.89	0.53
2:A:327:ALA:N	2:A:334:ASP:OD1	2.41	0.53
2:A:420:ARG:HH21	2:A:448:ARG:HB3	1.71	0.53
2:A:632:ARG:CG	2:A:632:ARG:HH11	2.21	0.53
2:A:175:LEU:CD2	2:A:418:LYS:HD2	2.37	0.53
2:A:739:ARG:HA	2:A:742:GLN:HE21	1.73	0.53
2:A:24:GLU:HG2	2:A:762:HIS:CG	2.43	0.53
2:A:773:HIS:O	2:A:774:VAL:C	2.45	0.53
2:A:294:GLU:HA	2:A:310:ILE:CG2	2.39	0.53
2:A:348:PRO:O	2:A:407:ARG:HD3	2.09	0.53
2:A:44:ASN:O	2:A:45:LYS:O	2.25	0.53
2:A:818:GLU:O	2:A:819:LYS:HB2	2.09	0.53
2:A:243:ILE:O	2:A:310:ILE:HA	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:357:GLU:O	2:A:359:GLY:N	2.39	0.53
2:A:685:LEU:HD13	2:A:748:ILE:HA	1.89	0.53
2:A:555:GLY:O	2:A:557:ASP:N	2.42	0.53
2:A:116:SER:N	2:A:119:GLU:HB2	2.24	0.53
2:A:551:MET:HA	2:A:581:PHE:O	2.09	0.53
2:A:96:THR:HB	2:A:155:LEU:HD23	1.91	0.53
2:A:207:SER:HB3	2:A:388:ASP:HB2	1.90	0.53
2:A:204:ARG:HG3	2:A:204:ARG:O	2.07	0.53
2:A:331:GLY:HA3	2:A:334:ASP:HB3	1.90	0.53
1:T:69:G:H5'	2:A:589:MET:HE2	1.90	0.53
2:A:676:GLU:HG2	2:A:798:TRP:CZ2	2.44	0.53
2:A:733:ARG:NH1	2:A:733:ARG:HG3	2.24	0.53
2:A:818:GLU:HB2	2:A:820:VAL:HG23	1.90	0.53
2:A:661:ASP:C	2:A:661:ASP:OD2	2.45	0.53
2:A:482:HIS:CD2	2:A:486:LEU:HD12	2.44	0.53
2:A:547:PHE:HB3	2:A:548:PRO:HD3	1.91	0.53
2:A:501:LYS:H	2:A:501:LYS:CE	2.21	0.53
2:A:711:PHE:CE2	2:A:752:MET:HE1	2.44	0.53
2:A:649:ARG:CG	2:A:649:ARG:NH1	2.72	0.53
2:A:225:ALA:HB2	2:A:254:TYR:CZ	2.44	0.53
2:A:350:ASP:HB3	2:A:352:LYS:O	2.08	0.53
2:A:350:ASP:O	2:A:407:ARG:CZ	2.57	0.53
2:A:423:ILE:O	2:A:426:ALA:N	2.42	0.53
2:A:469:GLU:OE1	2:A:510:HIS:HE1	1.92	0.53
2:A:372:LYS:C	2:A:374:VAL:H	2.12	0.52
2:A:597:SER:HB2	5:A:1021:HOH:O	2.09	0.52
2:A:58:TYR:CZ	2:A:101:ILE:HG13	2.44	0.52
2:A:439:THR:O	2:A:440:ARG:C	2.48	0.52
2:A:166:ILE:O	2:A:170:MET:HG3	2.10	0.52
2:A:749:LEU:CG	2:A:750:VAL:H	2.20	0.52
2:A:182:PRO:HA	2:A:407:ARG:O	2.09	0.52
2:A:380:GLU:O	2:A:382:GLY:N	2.41	0.52
2:A:120:PHE:CZ	2:A:124:CYS:SG	3.03	0.52
2:A:12:THR:HG23	2:A:657:GLY:HA2	1.91	0.52
2:A:229:ILE:O	2:A:229:ILE:HG23	2.09	0.52
2:A:823:LYS:HG2	2:A:826:GLU:HG3	1.91	0.52
2:A:2:ASP:OD2	2:A:4:GLU:HB3	2.09	0.52
2:A:267:LEU:O	2:A:268:SER:C	2.47	0.52
2:A:638:LEU:O	2:A:642:SER:N	2.42	0.52
2:A:309:VAL:HG12	2:A:310:ILE:H	1.75	0.52
2:A:348:PRO:O	2:A:349:ILE:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:691:SER:O	2:A:695:ASN:ND2	2.43	0.52
2:A:229:ILE:HD11	2:A:324:VAL:C	2.30	0.52
2:A:372:LYS:O	2:A:374:VAL:N	2.42	0.52
2:A:176:ILE:O	2:A:176:ILE:HG23	2.10	0.52
2:A:398:TRP:HA	2:A:401:LYS:HD3	1.92	0.52
2:A:163:GLN:NE2	2:A:529:PHE:HD2	2.07	0.52
2:A:278:ASP:OD1	2:A:281:SER:HB3	2.10	0.52
2:A:802:MET:CE	2:A:805:ARG:HD3	2.40	0.52
2:A:245:VAL:HG12	2:A:246:HIS:H	1.74	0.52
2:A:571:VAL:C	2:A:573:THR:H	2.13	0.52
2:A:226:LYS:HD2	2:A:259:GLU:HB2	1.91	0.51
2:A:420:ARG:O	2:A:421:GLN:HB2	2.09	0.51
2:A:107:LYS:O	2:A:107:LYS:HG2	2.10	0.51
2:A:300:HIS:HD2	2:A:308:LEU:HD12	1.74	0.51
2:A:802:MET:HA	2:A:802:MET:CE	2.40	0.51
2:A:560:ARG:HB2	2:A:560:ARG:NH1	2.25	0.51
2:A:250:LYS:HD2	2:A:251:TYR:N	2.25	0.51
2:A:280:ALA:O	2:A:282:ILE:N	2.40	0.51
2:A:377:LEU:O	2:A:381:LYS:HB2	2.10	0.51
2:A:200:TYR:CD1	2:A:200:TYR:N	2.79	0.51
2:A:200:TYR:HE2	2:A:395:PRO:HG3	1.70	0.51
2:A:560:ARG:CB	2:A:560:ARG:NH1	2.74	0.51
2:A:244:THR:HG21	2:A:337:VAL:HG21	1.91	0.51
2:A:837:PHE:HD2	2:A:873:HIS:O	1.94	0.51
2:A:257:ASN:CG	2:A:258:GLY:H	2.14	0.51
1:T:35:A:C2	2:A:654:PHE:HB2	2.45	0.51
2:A:876:ILE:CG2	2:A:877:VAL:N	2.73	0.51
2:A:292:GLU:C	2:A:294:GLU:N	2.64	0.51
2:A:416:ILE:O	2:A:420:ARG:HG2	2.10	0.51
2:A:417:SER:HA	2:A:420:ARG:HD2	1.92	0.51
2:A:470:ASN:N	2:A:472:GLU:CG	2.73	0.51
2:A:330:HIS:HA	2:A:406:PHE:HB3	1.92	0.51
2:A:229:ILE:HA	2:A:321:THR:OG1	2.10	0.51
1:T:4:C:C2'	1:T:5:U:H5'	2.40	0.51
2:A:129:LEU:CA	2:A:132:ILE:HG12	2.40	0.51
2:A:328:PRO:HB3	2:A:335:TYR:HA	1.93	0.51
2:A:194:ALA:O	2:A:196:ALA:N	2.44	0.51
2:A:777:GLU:O	2:A:778:SER:HB3	2.11	0.51
2:A:567:ILE:O	2:A:571:VAL:HG23	2.11	0.51
2:A:417:SER:HA	2:A:420:ARG:HG2	1.91	0.51
2:A:861:VAL:O	2:A:862:ASP:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:679:ARG:HH22	2:A:791:ASP:CG	2.13	0.51
2:A:195:GLU:O	2:A:197:GLU:N	2.44	0.51
2:A:768:TRP:CG	2:A:779:VAL:HG22	2.46	0.51
2:A:250:LYS:HZ2	2:A:289:THR:CG2	2.18	0.51
2:A:56:PRO:HD3	2:A:152:TYR:OH	2.10	0.51
2:A:805:ARG:O	2:A:808:VAL:N	2.44	0.51
2:A:468:ALA:HB2	2:A:518:PHE:CD2	2.46	0.51
2:A:664:PRO:HG2	2:A:746:TYR:CE2	2.46	0.51
2:A:279:LYS:O	2:A:280:ALA:CB	2.58	0.51
2:A:350:ASP:HB2	2:A:354:VAL:O	2.11	0.51
2:A:809:ASN:C	2:A:811:ALA:N	2.63	0.51
2:A:512:GLY:O	2:A:513:SER:C	2.49	0.51
2:A:309:VAL:O	2:A:310:ILE:HD12	2.11	0.50
2:A:348:PRO:O	2:A:407:ARG:HG2	2.11	0.50
2:A:181:LYS:HD3	2:A:452:VAL:HG21	1.92	0.50
2:A:719:PHE:HD1	2:A:805:ARG:NH2	2.09	0.50
2:A:468:ALA:H	2:A:472:GLU:CB	2.22	0.50
2:A:110:VAL:O	2:A:111:ASP:HB3	2.11	0.50
2:A:120:PHE:O	2:A:124:CYS:SG	2.69	0.50
1:T:58:A:O2'	1:T:59:G:P	2.68	0.50
1:T:11:C:H5'	2:A:636:GLU:OE2	2.11	0.50
2:A:218:LYS:HA	2:A:221:VAL:HG23	1.92	0.50
2:A:213:ASN:ND2	2:A:226:LYS:HE3	2.26	0.50
2:A:719:PHE:HD1	2:A:805:ARG:CZ	2.24	0.50
2:A:469:GLU:HG3	2:A:512:GLY:HA3	1.91	0.50
2:A:727:ILE:HD13	2:A:737:ILE:CG1	2.41	0.50
1:T:60:U:O2'	1:T:61:C:OP1	2.26	0.50
1:T:55:U:O5'	1:T:55:U:H6	1.95	0.50
2:A:366:PHE:HD1	2:A:369:LYS:HB3	1.75	0.50
2:A:420:ARG:HH22	2:A:449:GLY:H	1.59	0.50
2:A:652:LEU:HA	2:A:655:MET:CE	2.42	0.50
2:A:409:THR:HG23	2:A:410:PRO:HD2	1.92	0.50
2:A:775:LYS:C	2:A:776:GLU:HG2	2.31	0.50
2:A:223:ALA:CB	2:A:254:TYR:OH	2.60	0.50
2:A:178:LYS:NZ	2:A:412:TRP:NE1	2.57	0.50
2:A:443:ASN:ND2	2:A:446:ARG:CZ	2.74	0.50
2:A:589:MET:HE3	2:A:595:LYS:CA	2.31	0.50
2:A:603:VAL:HG11	4:A:993:MRC:H3'1	1.92	0.50
2:A:50:PHE:CZ	2:A:551:MET:HG2	2.45	0.50
2:A:39:LYS:HA	2:A:42:GLU:HB2	1.94	0.50
2:A:267:LEU:O	2:A:270:ALA:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:20:LEU:N	2:A:20:LEU:HD12	2.24	0.50
1:T:43:G:H2'	1:T:44:A:H8	1.73	0.50
2:A:186:SER:HB2	2:A:404:VAL:HG22	1.93	0.50
2:A:230:TRP:CE3	2:A:319:ALA:HB1	2.47	0.50
2:A:303:LEU:O	2:A:305:ARG:N	2.45	0.50
2:A:467:TYR:N	2:A:519:THR:O	2.34	0.50
2:A:112:ARG:NH2	2:A:458:VAL:HG21	2.27	0.50
1:T:5:U:H2'	1:T:6:U:H6	1.75	0.50
2:A:292:GLU:O	2:A:294:GLU:N	2.45	0.50
2:A:510:HIS:CG	2:A:511:PRO:HD2	2.46	0.50
2:A:359:GLY:HA3	2:A:362:PHE:HB2	1.92	0.50
2:A:711:PHE:HE2	2:A:752:MET:HE1	1.76	0.50
2:A:58:TYR:HA	2:A:95:ASP:HB2	1.94	0.50
2:A:247:PRO:HA	2:A:291:LYS:CA	2.41	0.49
2:A:277:TRP:C	2:A:279:LYS:H	2.15	0.49
2:A:116:SER:HB3	2:A:119:GLU:CG	2.31	0.49
2:A:8:LEU:HB2	2:A:729:TYR:O	2.11	0.49
2:A:861:VAL:O	2:A:861:VAL:CG2	2.60	0.49
2:A:853:PHE:O	2:A:855:VAL:HG13	2.11	0.49
2:A:719:PHE:CD1	2:A:805:ARG:CZ	2.95	0.49
2:A:805:ARG:O	2:A:807:ASP:N	2.45	0.49
2:A:476:THR:O	2:A:480:VAL:HG23	2.12	0.49
2:A:141:ARG:HG3	2:A:141:ARG:NH1	2.27	0.49
2:A:861:VAL:O	2:A:861:VAL:HG22	2.11	0.49
2:A:339:GLN:O	2:A:341:TYR:N	2.46	0.49
2:A:373:ALA:O	2:A:376:ASP:HB2	2.12	0.49
2:A:451:TRP:CD1	2:A:453:ILE:HG22	2.46	0.49
2:A:112:ARG:HD2	2:A:113:LYS:HD2	1.95	0.49
2:A:65:MET:HA	2:A:606:PRO:HG3	1.93	0.49
2:A:204:ARG:CG	2:A:204:ARG:O	2.59	0.49
2:A:338:GLY:HA2	2:A:343:LEU:HD12	1.94	0.49
2:A:341:TYR:CD1	2:A:341:TYR:N	2.80	0.49
2:A:113:LYS:O	2:A:114:LYS:HB2	2.11	0.49
2:A:279:LYS:O	2:A:280:ALA:HB3	2.13	0.49
2:A:443:ASN:ND2	2:A:446:ARG:NH1	2.60	0.49
2:A:176:ILE:CG2	2:A:475:MET:HE3	2.43	0.49
2:A:81:LYS:HG3	2:A:86:PHE:HD2	1.75	0.49
2:A:206:ALA:O	2:A:208:ILE:HG23	2.11	0.49
1:T:12:U:H5''	5:A:1033:HOH:O	2.12	0.49
2:A:472:GLU:O	2:A:473:ILE:CB	2.61	0.49
2:A:255:ASN:CG	2:A:256:VAL:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:327:ALA:O	2:A:329:GLY:N	2.45	0.49
2:A:656:LEU:HD21	2:A:771:THR:HG23	1.95	0.49
2:A:222:ASP:HB3	2:A:288:TYR:CE2	2.48	0.49
2:A:289:THR:HG21	2:A:292:GLU:HG3	1.95	0.49
2:A:368:ASP:O	2:A:372:LYS:HG3	2.13	0.49
2:A:500:ALA:HB3	2:A:501:LYS:CE	2.41	0.49
2:A:658:ASN:HB3	2:A:728:LEU:HD13	1.94	0.49
1:T:13:C:O3'	2:A:702:LEU:HD21	2.13	0.49
2:A:333:ASP:O	2:A:337:VAL:HG12	2.12	0.49
2:A:833:SER:CB	2:A:840:SER:HG	2.26	0.49
2:A:44:ASN:C	2:A:47:ASN:ND2	2.65	0.49
2:A:443:ASN:HD22	2:A:446:ARG:NH1	2.11	0.49
2:A:411:GLN:HE22	2:A:456:GLN:HE21	1.56	0.49
2:A:504:LEU:HB3	2:A:505:PRO:HD2	1.95	0.49
2:A:229:ILE:HA	2:A:323:CYS:SG	2.53	0.48
2:A:451:TRP:CE2	2:A:453:ILE:HG22	2.47	0.48
2:A:469:GLU:O	2:A:471:GLY:N	2.45	0.48
2:A:8:LEU:HD13	2:A:738:ARG:HE	1.77	0.48
2:A:230:TRP:CZ3	2:A:319:ALA:HB1	2.46	0.48
2:A:300:HIS:HB2	2:A:302:PHE:CE2	2.48	0.48
2:A:64:HIS:HD2	4:A:993:MRC:H9'2	1.78	0.48
2:A:711:PHE:HE2	2:A:752:MET:CE	2.26	0.48
2:A:65:MET:HE3	2:A:65:MET:HA	1.94	0.48
2:A:296:VAL:CG1	2:A:297:VAL:N	2.76	0.48
2:A:719:PHE:O	2:A:720:TYR:C	2.50	0.48
2:A:807:ASP:O	2:A:809:ASN:N	2.46	0.48
2:A:416:ILE:HB	2:A:449:GLY:O	2.13	0.48
2:A:495:TRP:O	2:A:520:LYS:HE3	2.13	0.48
2:A:466:PHE:HB3	2:A:520:LYS:HA	1.96	0.48
2:A:739:ARG:HD3	2:A:742:GLN:HE22	1.78	0.48
2:A:220:VAL:CG1	2:A:220:VAL:O	2.62	0.48
2:A:23:LYS:HG3	2:A:27:ILE:CD1	2.40	0.48
2:A:500:ALA:H	2:A:501:LYS:HZ2	1.62	0.48
2:A:465:VAL:O	2:A:521:GLU:CB	2.62	0.48
2:A:282:ILE:HG13	2:A:282:ILE:O	2.14	0.48
2:A:589:MET:CE	2:A:595:LYS:HA	2.31	0.48
2:A:469:GLU:O	2:A:469:GLU:HG2	2.13	0.48
2:A:470:ASN:H	2:A:472:GLU:CG	2.26	0.48
2:A:627:TYR:C	2:A:629:ALA:H	2.17	0.48
2:A:152:TYR:CD2	2:A:538:VAL:HG21	2.48	0.48
2:A:840:SER:HA	2:A:860:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:668:SER:HA	2:A:743:THR:OG1	2.14	0.48
2:A:547:PHE:O	2:A:549:ALA:N	2.46	0.48
2:A:711:PHE:CE2	2:A:752:MET:CE	2.96	0.48
2:A:632:ARG:CZ	2:A:632:ARG:HB2	2.42	0.48
2:A:254:TYR:CE2	2:A:260:LYS:HE2	2.49	0.48
2:A:327:ALA:H	2:A:334:ASP:CG	2.17	0.48
2:A:165:ARG:O	2:A:169:GLU:HG3	2.14	0.48
2:A:99:LEU:O	2:A:103:GLN:HG3	2.13	0.48
2:A:749:LEU:O	2:A:751:ASP:N	2.46	0.48
2:A:138:ASP:O	2:A:141:ARG:N	2.47	0.48
1:T:16:G:H5'	1:T:17:U:OP2	2.14	0.48
2:A:332:GLU:O	2:A:335:TYR:N	2.45	0.48
1:T:65:U:O2'	1:T:66:C:H5'	2.14	0.48
2:A:180:LYS:HD3	2:A:408:ALA:HB1	1.96	0.48
2:A:350:ASP:CB	2:A:354:VAL:O	2.62	0.48
2:A:357:GLU:C	2:A:359:GLY:H	2.18	0.48
2:A:800:THR:O	2:A:803:ASN:HB2	2.14	0.48
1:T:69:G:O2'	2:A:630:ASP:OD2	2.25	0.48
2:A:849:LEU:HB2	2:A:858:VAL:HG21	1.96	0.48
2:A:243:ILE:HD11	2:A:300:HIS:NE2	2.28	0.47
2:A:504:LEU:O	2:A:506:GLU:N	2.47	0.47
2:A:840:SER:OG	2:A:862:ASP:HA	2.14	0.47
2:A:106:THR:HG21	2:A:399:ARG:HH12	1.79	0.47
2:A:194:ALA:O	2:A:197:GLU:N	2.42	0.47
2:A:369:LYS:HA	2:A:372:LYS:HD2	1.96	0.47
2:A:481:ASN:O	2:A:483:VAL:N	2.47	0.47
2:A:569:THR:CG2	2:A:570:SER:N	2.76	0.47
2:A:153:ILE:HG13	2:A:156:LYS:HG2	1.94	0.47
1:T:2:G:H2'	1:T:3:G:H8	1.78	0.47
2:A:241:VAL:O	2:A:242:ALA:HB2	2.14	0.47
2:A:248:GLU:C	2:A:249:LEU:HG	2.34	0.47
2:A:293:LEU:HD23	2:A:293:LEU:O	2.14	0.47
2:A:366:PHE:O	2:A:371:ASN:ND2	2.44	0.47
2:A:724:GLY:HA3	2:A:741:MET:CE	2.44	0.47
2:A:722:ASP:O	2:A:723:TYR:C	2.53	0.47
2:A:398:TRP:C	2:A:400:THR:H	2.17	0.47
2:A:321:THR:O	2:A:323:CYS:N	2.42	0.47
2:A:324:VAL:CG1	2:A:326:THR:HG23	2.45	0.47
2:A:535:HIS:ND1	2:A:536:ARG:N	2.55	0.47
2:A:535:HIS:NE2	2:A:569:THR:CG2	2.77	0.47
2:A:848:ALA:HA	2:A:850:HIS:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:220:VAL:HG13	2:A:224:ASP:CG	2.34	0.47
2:A:717:SER:O	2:A:719:PHE:N	2.47	0.47
2:A:811:ALA:HA	2:A:871:TYR:OH	2.14	0.47
2:A:552:TYR:CD2	2:A:562:TRP:CZ3	3.03	0.47
2:A:567:ILE:HG23	2:A:568:THR:N	2.30	0.47
1:T:24:G:H2'	1:T:25:C:O4'	2.14	0.47
1:T:51:U:O2'	1:T:52:G:H5'	2.14	0.47
2:A:591:GLY:O	2:A:592:GLU:C	2.52	0.47
2:A:379:THR:HA	2:A:385:LEU:HD12	1.97	0.47
2:A:296:VAL:CG1	2:A:297:VAL:H	2.16	0.47
2:A:446:ARG:O	2:A:446:ARG:HG2	2.15	0.47
2:A:466:PHE:CD2	2:A:504:LEU:HD21	2.49	0.47
2:A:4:GLU:HA	2:A:7:LEU:HB2	1.96	0.47
2:A:551:MET:HE3	2:A:699:PHE:CE2	2.50	0.47
2:A:434:VAL:HG11	2:A:436:TRP:NE1	2.30	0.47
2:A:652:LEU:HD22	2:A:767:VAL:HG21	1.97	0.47
2:A:680:TYR:CE1	2:A:798:TRP:HB2	2.48	0.47
2:A:701:TYR:O	2:A:702:LEU:C	2.53	0.47
2:A:242:ALA:N	2:A:308:LEU:HD13	2.30	0.47
2:A:275:LEU:HD11	2:A:386:LYS:HD2	1.97	0.47
2:A:285:GLU:OE2	2:A:285:GLU:HA	2.15	0.47
1:T:46:G:C2'	1:T:47:U:H5'	2.39	0.47
2:A:433:LYS:O	2:A:433:LYS:HD2	2.14	0.47
2:A:366:PHE:CG	2:A:370:ALA:HB2	2.50	0.47
2:A:467:TYR:CA	2:A:472:GLU:HB3	2.44	0.47
2:A:23:LYS:HE2	2:A:766:GLU:OE2	2.14	0.47
2:A:849:LEU:CB	2:A:858:VAL:HG21	2.44	0.47
2:A:571:VAL:HG13	2:A:575:GLY:HA2	1.97	0.47
1:T:55:U:H3'	1:T:55:U:C6	2.50	0.47
2:A:587:PHE:HA	4:A:993:MRC:H152	1.96	0.47
2:A:596:MET:HB3	2:A:603:VAL:CG1	2.30	0.47
2:A:42:GLU:O	2:A:43:LYS:C	2.53	0.47
2:A:571:VAL:O	2:A:573:THR:N	2.42	0.47
2:A:239:SER:HB3	2:A:346:ILE:CG1	2.45	0.46
2:A:802:MET:O	2:A:805:ARG:HB3	2.15	0.46
2:A:831:ILE:CD1	2:A:839:ALA:HB1	2.44	0.46
2:A:96:THR:OG1	2:A:154:THR:HG23	2.15	0.46
2:A:632:ARG:NH1	2:A:632:ARG:HG3	2.28	0.46
2:A:127:PHE:O	2:A:130:GLU:HB2	2.15	0.46
2:A:598:LYS:C	2:A:600:LEU:H	2.19	0.46
2:A:229:ILE:HA	2:A:321:THR:HG1	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:163:GLN:HG2	2:A:461:VAL:CG1	2.44	0.46
2:A:549:ALA:O	2:A:580:LYS:HG3	2.15	0.46
2:A:749:LEU:O	2:A:750:VAL:C	2.53	0.46
2:A:63:LEU:HD12	2:A:138:ASP:HB2	1.96	0.46
1:T:9:A:H2'	1:T:11:C:H41	1.80	0.46
1:T:25:C:H2'	1:T:26:G:O4'	2.15	0.46
2:A:210:VAL:HG11	2:A:212:PHE:CE2	2.50	0.46
2:A:219:GLY:HA2	2:A:296:VAL:HG12	1.97	0.46
2:A:327:ALA:C	2:A:334:ASP:OD1	2.54	0.46
2:A:211:ALA:HB3	2:A:385:LEU:HD23	1.98	0.46
2:A:493:ASN:HA	2:A:493:ASN:HD22	1.59	0.46
2:A:500:ALA:N	2:A:501:LYS:HZ2	2.14	0.46
2:A:436:TRP:N	2:A:436:TRP:CD1	2.82	0.46
2:A:433:LYS:CB	2:A:583:LEU:HG	2.43	0.46
2:A:560:ARG:HB3	2:A:560:ARG:HH11	1.81	0.46
2:A:97:HIS:CG	2:A:460:GLY:HA2	2.50	0.46
2:A:216:ASP:O	2:A:220:VAL:HG23	2.15	0.46
2:A:228:ILE:O	2:A:229:ILE:CB	2.62	0.46
2:A:238:PRO:HB3	2:A:362:PHE:CE1	2.51	0.46
2:A:812:LEU:O	2:A:816:ARG:N	2.47	0.46
2:A:424:LEU:O	2:A:427:ILE:HB	2.15	0.46
2:A:504:LEU:HB3	2:A:505:PRO:CD	2.45	0.46
2:A:609:VAL:CG1	2:A:610:VAL:N	2.79	0.46
2:A:252:GLY:HA2	2:A:263:ILE:O	2.15	0.46
2:A:289:THR:CG2	2:A:292:GLU:HG3	2.46	0.46
2:A:53:HIS:HE1	2:A:152:TYR:CE2	2.32	0.46
2:A:200:TYR:HB3	2:A:393:SER:O	2.16	0.46
2:A:632:ARG:CG	2:A:632:ARG:NH1	2.77	0.46
2:A:397:ASP:O	2:A:397:ASP:CG	2.52	0.46
2:A:383:ALA:O	2:A:384:LEU:O	2.33	0.46
2:A:237:ILE:HB	2:A:238:PRO:CD	2.37	0.46
2:A:802:MET:HE2	2:A:805:ARG:HD3	1.97	0.46
2:A:805:ARG:O	2:A:806:ASP:C	2.54	0.46
2:A:160:GLU:O	2:A:161:ALA:C	2.54	0.46
2:A:170:MET:O	2:A:173:LYS:HB2	2.16	0.46
2:A:536:ARG:NH1	2:A:574:ARG:NH2	2.63	0.46
2:A:857:GLN:NE2	2:A:858:VAL:N	2.47	0.46
1:T:58:A:HO2'	1:T:59:G:P	2.38	0.46
2:A:240:ASN:ND2	2:A:302:PHE:HZ	2.14	0.46
2:A:293:LEU:HD23	2:A:296:VAL:CG2	2.45	0.46
2:A:329:GLY:HA3	2:A:346:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:542:ARG:O	2:A:544:GLU:N	2.49	0.46
2:A:102:GLU:O	2:A:105:LEU:HB2	2.16	0.46
2:A:323:CYS:O	2:A:324:VAL:CB	2.55	0.46
2:A:211:ALA:H	2:A:385:LEU:HD22	1.81	0.46
2:A:500:ALA:HB3	2:A:501:LYS:NZ	2.31	0.46
2:A:75:ASP:OD2	2:A:619:ARG:NH2	2.49	0.46
2:A:285:GLU:C	2:A:286:LYS:HG2	2.37	0.46
2:A:310:ILE:CG2	2:A:311:ASN:N	2.78	0.46
2:A:162:ALA:HB1	2:A:536:ARG:CG	2.47	0.46
1:T:18:G:O2'	1:T:19:G:P	2.74	0.46
2:A:397:ASP:O	2:A:401:LYS:N	2.42	0.46
2:A:255:ASN:HD21	2:A:256:VAL:HG23	1.81	0.45
2:A:362:PHE:O	2:A:365:MET:HG2	2.16	0.45
1:T:74:C:OP1	2:A:333:ASP:CG	2.55	0.45
2:A:160:GLU:O	2:A:163:GLN:N	2.50	0.45
2:A:481:ASN:O	2:A:482:HIS:C	2.53	0.45
2:A:176:ILE:HG23	2:A:475:MET:HE3	1.98	0.45
2:A:20:LEU:HA	2:A:23:LYS:HB3	1.97	0.45
2:A:120:PHE:O	2:A:124:CYS:N	2.50	0.45
1:T:34:G:H1'	2:A:9:MET:HE1	1.99	0.45
2:A:394:TYR:HA	2:A:395:PRO:HD3	1.85	0.45
2:A:840:SER:HA	2:A:860:VAL:HG13	1.96	0.45
1:T:67:A:H2'	1:T:68:G:O5'	2.15	0.45
2:A:240:ASN:ND2	2:A:302:PHE:CZ	2.84	0.45
2:A:121:ARG:NH1	2:A:496:PHE:HE1	2.14	0.45
2:A:198:ILE:HG21	2:A:395:PRO:HB3	1.98	0.45
2:A:609:VAL:HG13	2:A:610:VAL:N	2.30	0.45
2:A:792:GLN:O	2:A:794:LEU:N	2.50	0.45
2:A:679:ARG:NH2	2:A:794:LEU:HD22	2.32	0.45
2:A:684:ARG:NH1	2:A:684:ARG:HB3	2.31	0.45
1:T:14:A:H2'	1:T:15:G:O4'	2.16	0.45
1:T:24:G:H2'	1:T:25:C:C6	2.51	0.45
2:A:445:VAL:C	2:A:447:ASP:H	2.20	0.45
2:A:560:ARG:HB2	2:A:560:ARG:CZ	2.46	0.45
2:A:765:GLU:HA	2:A:765:GLU:OE1	2.17	0.45
1:T:24:G:H2'	1:T:25:C:H6	1.82	0.45
2:A:372:LYS:O	2:A:375:THR:N	2.50	0.45
2:A:451:TRP:NE1	2:A:453:ILE:HG22	2.32	0.45
2:A:494:ILE:O	2:A:503:LEU:HD21	2.16	0.45
2:A:60:ASN:C	2:A:60:ASN:ND2	2.67	0.45
2:A:865:ASP:CB	2:A:867:GLN:HE21	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:367:TYR:C	2:A:371:ASN:ND2	2.70	0.45
2:A:421:GLN:CA	2:A:424:LEU:HD12	2.45	0.45
2:A:831:ILE:HD11	2:A:843:LEU:HD11	1.99	0.45
2:A:46:GLY:O	2:A:47:ASN:C	2.55	0.45
2:A:64:HIS:CD2	4:A:993:MRC:H9'2	2.51	0.45
2:A:749:LEU:HD11	2:A:771:THR:CG2	2.45	0.45
1:T:17:U:C5'	1:T:18:G:H5'	2.47	0.45
2:A:240:ASN:HD21	2:A:306:GLU:CB	2.29	0.45
2:A:479:THR:O	2:A:483:VAL:HG23	2.17	0.45
2:A:683:ASN:O	2:A:686:ARG:HB2	2.17	0.45
2:A:257:ASN:ND2	2:A:258:GLY:H	2.15	0.45
2:A:749:LEU:HD11	2:A:771:THR:HG21	1.98	0.45
1:T:24:G:O2'	1:T:25:C:H5'	2.16	0.45
2:A:235:TRP:C	2:A:238:PRO:HD2	2.37	0.45
2:A:225:ALA:HB1	2:A:260:LYS:HB2	1.99	0.45
2:A:480:VAL:O	2:A:483:VAL:HB	2.17	0.45
2:A:467:TYR:N	2:A:467:TYR:CD1	2.85	0.45
2:A:71:LYS:NZ	5:A:1073:HOH:O	2.44	0.45
2:A:559:TYR:HA	2:A:563:PHE:HD1	1.82	0.45
2:A:616:ASP:OD1	2:A:762:HIS:ND1	2.48	0.45
2:A:560:ARG:CB	2:A:560:ARG:HH11	2.30	0.45
2:A:285:GLU:C	2:A:286:LYS:CG	2.86	0.45
2:A:500:ALA:N	2:A:520:LYS:HZ3	2.15	0.45
2:A:579:TYR:CD2	2:A:579:TYR:N	2.85	0.45
1:T:7:G:H1	1:T:66:C:H42	1.64	0.45
2:A:99:LEU:HD22	2:A:457:ARG:HD2	1.97	0.45
2:A:365:MET:HB3	2:A:370:ALA:CB	2.47	0.44
1:T:17:U:H5'	1:T:18:G:C5'	2.47	0.44
2:A:343:LEU:HA	2:A:344:PRO:HD3	1.88	0.44
2:A:681:LEU:O	2:A:682:LEU:C	2.54	0.44
2:A:417:SER:HA	2:A:420:ARG:CD	2.48	0.44
2:A:508:PHE:CD1	2:A:509:THR:N	2.86	0.44
1:T:34:G:H5''	1:T:36:U:C5	2.52	0.44
2:A:832:ALA:O	2:A:833:SER:C	2.54	0.44
2:A:813:GLU:O	2:A:817:ASN:N	2.46	0.44
2:A:605:VAL:HG13	2:A:606:PRO:CD	2.47	0.44
2:A:376:ASP:O	2:A:378:LEU:N	2.51	0.44
2:A:550:ASP:HA	2:A:580:LYS:HD2	1.99	0.44
2:A:810:ARG:NH1	2:A:814:THR:HG23	2.32	0.44
2:A:328:PRO:CA	2:A:335:TYR:HA	2.47	0.44
2:A:3:TYR:N	2:A:3:TYR:CD1	2.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:277:TRP:O	2:A:279:LYS:N	2.48	0.44
2:A:807:ASP:C	2:A:809:ASN:N	2.70	0.44
1:T:17:U:H5'	1:T:18:G:H5'	2.00	0.44
2:A:215:LYS:HG2	2:A:216:ASP:N	2.32	0.44
2:A:251:TYR:C	2:A:253:GLN:N	2.70	0.44
2:A:353:GLY:HA3	2:A:367:TYR:HB3	1.98	0.44
2:A:804:LEU:HD12	2:A:837:PHE:HE2	1.82	0.44
2:A:439:THR:O	2:A:442:TYR:N	2.50	0.44
2:A:749:LEU:CG	2:A:750:VAL:N	2.81	0.44
2:A:153:ILE:O	2:A:155:LEU:N	2.50	0.44
2:A:627:TYR:C	2:A:629:ALA:N	2.71	0.44
2:A:178:LYS:HG3	2:A:179:GLY:H	1.82	0.44
2:A:555:GLY:HA2	2:A:585:HIS:O	2.17	0.44
2:A:120:PHE:O	2:A:121:ARG:C	2.56	0.44
2:A:211:ALA:N	2:A:385:LEU:HD22	2.33	0.44
2:A:807:ASP:C	2:A:809:ASN:H	2.21	0.44
2:A:417:SER:CA	2:A:420:ARG:HG2	2.48	0.44
2:A:446:ARG:O	2:A:446:ARG:CD	2.65	0.44
2:A:481:ASN:C	2:A:483:VAL:N	2.72	0.44
2:A:13:ASP:OD1	2:A:770:HIS:CE1	2.71	0.44
2:A:598:LYS:C	2:A:600:LEU:N	2.71	0.44
2:A:362:PHE:HE2	2:A:374:VAL:HG22	1.83	0.44
2:A:423:ILE:O	2:A:424:LEU:C	2.55	0.44
2:A:13:ASP:OD2	2:A:770:HIS:HE1	2.01	0.44
2:A:737:ILE:HG23	2:A:738:ARG:N	2.32	0.44
2:A:768:TRP:HB2	2:A:779:VAL:CG2	2.48	0.44
2:A:694:ASN:O	2:A:698:ASN:ND2	2.50	0.44
2:A:229:ILE:HA	2:A:323:CYS:HB2	1.99	0.43
2:A:234:PRO:CG	2:A:235:TRP:N	2.75	0.43
2:A:355:PHE:CE1	2:A:365:MET:HB2	2.30	0.43
1:T:70:C:OP1	2:A:595:LYS:HD3	2.18	0.43
2:A:749:LEU:C	2:A:749:LEU:CD2	2.85	0.43
2:A:648:ILE:O	2:A:652:LEU:HD12	2.18	0.43
2:A:83:MET:HB3	2:A:784:MET:HG2	1.99	0.43
2:A:446:ARG:O	2:A:447:ASP:CG	2.57	0.43
1:T:70:C:O2	2:A:440:ARG:NH2	2.47	0.43
2:A:212:PHE:O	2:A:227:PHE:N	2.42	0.43
2:A:250:LYS:O	2:A:251:TYR:HB2	2.19	0.43
2:A:723:TYR:CE1	2:A:852:LEU:HD23	2.53	0.43
2:A:606:PRO:O	2:A:607:ASP:C	2.56	0.43
2:A:134:LEU:HA	2:A:134:LEU:HD23	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:233:THR:HG23	2:A:236:THR:CG2	2.44	0.43
2:A:241:VAL:HG11	2:A:343:LEU:HB3	2.00	0.43
2:A:804:LEU:HD23	2:A:808:VAL:HG23	2.00	0.43
2:A:4:GLU:O	2:A:4:GLU:HG2	2.18	0.43
2:A:275:LEU:O	2:A:276:ASP:C	2.56	0.43
2:A:162:ALA:HB1	2:A:536:ARG:HG3	2.01	0.43
1:T:13:C:H4'	2:A:702:LEU:HD21	1.99	0.43
2:A:240:ASN:O	2:A:241:VAL:HG23	2.18	0.43
2:A:275:LEU:HA	2:A:275:LEU:HD12	1.81	0.43
2:A:318:ASP:OD2	2:A:319:ALA:N	2.49	0.43
2:A:670:PRO:HG2	2:A:673:GLU:OE2	2.18	0.43
1:T:22:G:OP2	5:T:152:HOH:O	2.22	0.43
2:A:832:ALA:CB	2:A:861:VAL:HG13	2.47	0.43
2:A:795:LEU:HA	2:A:795:LEU:HD23	1.81	0.43
2:A:259:GLU:O	2:A:260:LYS:HB2	2.19	0.43
2:A:240:ASN:HD21	2:A:306:GLU:HB2	1.84	0.43
2:A:324:VAL:HG12	2:A:325:HIS:N	2.32	0.43
2:A:161:ALA:HB1	2:A:165:ARG:NH1	2.27	0.43
2:A:79:ARG:NH1	2:A:780:HIS:ND1	2.66	0.43
2:A:842:PHE:C	2:A:844:THR:N	2.71	0.43
2:A:777:GLU:O	2:A:778:SER:CB	2.66	0.43
2:A:240:ASN:HD22	2:A:308:LEU:HD21	1.77	0.43
2:A:422:ASP:OD2	2:A:422:ASP:N	2.41	0.43
2:A:129:LEU:C	2:A:132:ILE:HG12	2.39	0.43
2:A:68:ALA:O	2:A:72:ILE:HG13	2.18	0.43
2:A:338:GLY:C	2:A:343:LEU:HD12	2.39	0.43
2:A:166:ILE:O	2:A:167:PHE:C	2.58	0.43
2:A:466:PHE:CA	2:A:520:LYS:HA	2.44	0.43
2:A:830:THR:HB	2:A:877:VAL:CG2	2.48	0.43
2:A:187:PRO:C	2:A:189:SER:H	2.22	0.43
2:A:654:PHE:HE1	2:A:729:TYR:HH	1.65	0.42
2:A:727:ILE:HD13	2:A:737:ILE:HG12	2.01	0.42
2:A:727:ILE:CG2	2:A:738:ARG:HA	2.48	0.42
2:A:434:VAL:HG22	2:A:435:ASN:H	1.83	0.42
2:A:324:VAL:HG11	2:A:326:THR:HG23	2.01	0.42
2:A:821:ILE:HG13	2:A:827:ALA:HB2	2.01	0.42
2:A:632:ARG:HD3	5:A:1074:HOH:O	2.19	0.42
2:A:81:LYS:HE3	2:A:86:PHE:CD2	2.54	0.42
2:A:76:PHE:CE2	2:A:759:ILE:HA	2.54	0.42
2:A:379:THR:HG23	2:A:385:LEU:CG	2.50	0.42
2:A:809:ASN:C	2:A:811:ALA:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:525:MET:SD	2:A:529:PHE:CD2	3.13	0.42
2:A:577:SER:HA	2:A:578:PRO:HD3	1.89	0.42
2:A:129:LEU:O	2:A:132:ILE:CG1	2.65	0.42
2:A:144:VAL:CG1	2:A:145:ARG:N	2.81	0.42
2:A:454:SER:O	2:A:455:ARG:HD3	2.19	0.42
2:A:816:ARG:CD	2:A:822:GLY:O	2.67	0.42
2:A:417:SER:HA	2:A:420:ARG:CG	2.49	0.42
2:A:491:GLY:O	2:A:493:ASN:N	2.53	0.42
2:A:111:ASP:O	2:A:112:ARG:O	2.36	0.42
2:A:731:GLU:HG3	2:A:737:ILE:HG21	2.02	0.42
2:A:71:LYS:HE2	2:A:139:PHE:CE2	2.54	0.42
2:A:830:THR:O	2:A:877:VAL:HG22	2.20	0.42
1:T:55:U:C3'	1:T:55:U:C6	3.02	0.42
2:A:218:LYS:C	2:A:220:VAL:N	2.71	0.42
2:A:339:GLN:O	2:A:340:GLN:C	2.57	0.42
2:A:177:TYR:HD1	2:A:178:LYS:O	2.03	0.42
2:A:413:PHE:HA	2:A:451:TRP:O	2.20	0.42
2:A:513:SER:O	2:A:515:ASN:N	2.47	0.42
2:A:115:MET:HB3	2:A:119:GLU:HB3	2.01	0.42
2:A:122:GLU:C	2:A:124:CYS:H	2.23	0.42
2:A:434:VAL:HG21	2:A:436:TRP:CD1	2.55	0.42
2:A:436:TRP:HD1	2:A:436:TRP:H	1.64	0.42
2:A:30:LYS:O	2:A:33:ALA:HB3	2.19	0.42
1:T:45:G:H5'	1:T:46:G:OP2	2.20	0.42
2:A:644:ASP:O	2:A:648:ILE:HG13	2.20	0.42
2:A:84:GLN:OE1	2:A:784:MET:HB2	2.19	0.42
2:A:664:PRO:O	2:A:666:THR:N	2.53	0.42
2:A:821:ILE:CG1	2:A:822:GLY:H	2.32	0.42
1:T:38:A:C2'	1:T:39:G:H5'	2.49	0.42
2:A:501:LYS:N	2:A:501:LYS:HE3	2.35	0.42
2:A:792:GLN:NE2	2:A:796:ASP:OD1	2.51	0.42
2:A:775:LYS:O	2:A:776:GLU:CB	2.67	0.42
2:A:289:THR:HG22	2:A:292:GLU:N	2.21	0.42
2:A:832:ALA:HB2	2:A:861:VAL:HG12	1.99	0.42
1:T:41:G:O2'	1:T:42:U:H5'	2.20	0.42
2:A:44:ASN:OD1	2:A:85:GLY:HA2	2.20	0.42
2:A:56:PRO:HA	2:A:57:PRO:HD2	1.97	0.42
2:A:178:LYS:HG3	2:A:179:GLY:N	2.35	0.42
2:A:548:PRO:HB2	2:A:580:LYS:CE	2.49	0.42
2:A:462:PRO:HG3	2:A:496:PHE:CZ	2.55	0.42
2:A:623:SER:O	2:A:702:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:228:ILE:HD11	2:A:261:TYR:HB3	2.02	0.42
2:A:326:THR:HA	2:A:334:ASP:OD2	2.20	0.42
2:A:365:MET:HB3	2:A:370:ALA:HB1	2.01	0.42
1:T:29:C:H2'	1:T:30:C:C6	2.55	0.42
2:A:226:LYS:HD2	2:A:259:GLU:CB	2.50	0.42
2:A:325:HIS:C	2:A:325:HIS:ND1	2.73	0.42
2:A:350:ASP:OD1	2:A:352:LYS:HD3	2.19	0.42
2:A:376:ASP:O	2:A:377:LEU:C	2.57	0.42
2:A:163:GLN:HG2	2:A:461:VAL:CG2	2.44	0.42
2:A:110:VAL:HG11	2:A:120:PHE:CZ	2.55	0.42
2:A:8:LEU:CD2	2:A:733:ARG:NH1	2.81	0.42
2:A:292:GLU:C	2:A:294:GLU:H	2.22	0.41
2:A:179:GLY:HA3	2:A:413:PHE:CE1	2.55	0.41
2:A:116:SER:O	2:A:117:THR:C	2.59	0.41
2:A:43:LYS:HG2	2:A:44:ASN:N	2.35	0.41
2:A:269:ASP:O	2:A:270:ALA:C	2.58	0.41
1:T:51:U:H2'	1:T:52:G:H8	1.85	0.41
2:A:256:VAL:CG1	2:A:257:ASN:H	2.32	0.41
2:A:296:VAL:C	2:A:310:ILE:HD13	2.40	0.41
2:A:152:TYR:HB2	5:A:1041:HOH:O	2.20	0.41
2:A:163:GLN:CG	2:A:461:VAL:HG21	2.44	0.41
2:A:477:LYS:O	2:A:479:THR:N	2.45	0.41
2:A:469:GLU:O	2:A:470:ASN:HB2	2.20	0.41
2:A:141:ARG:HH21	2:A:611:LYS:NZ	2.18	0.41
2:A:831:ILE:HG13	2:A:832:ALA:N	2.33	0.41
2:A:131:GLN:O	2:A:132:ILE:C	2.57	0.41
2:A:146:GLY:O	2:A:148:PHE:N	2.50	0.41
2:A:106:THR:C	2:A:108:LYS:H	2.23	0.41
2:A:216:ASP:O	2:A:219:GLY:N	2.53	0.41
2:A:538:VAL:HG23	2:A:542:ARG:CD	2.50	0.41
2:A:469:GLU:O	2:A:469:GLU:CG	2.68	0.41
2:A:536:ARG:NH2	2:A:574:ARG:NH2	2.66	0.41
2:A:539:LEU:HD23	2:A:539:LEU:HA	1.85	0.41
2:A:505:PRO:O	2:A:506:GLU:C	2.58	0.41
2:A:51:ILE:HD12	2:A:51:ILE:N	2.36	0.41
2:A:325:HIS:C	2:A:325:HIS:HD1	2.23	0.41
2:A:170:MET:O	2:A:171:ALA:C	2.59	0.41
2:A:79:ARG:O	2:A:80:TYR:C	2.58	0.41
2:A:318:ASP:CG	2:A:319:ALA:N	2.72	0.41
2:A:300:HIS:C	2:A:304:ASP:HB3	2.40	0.41
2:A:341:TYR:O	2:A:342:GLU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:745:LEU:C	2:A:748:ILE:HG22	2.39	0.41
2:A:138:ASP:O	2:A:139:PHE:C	2.58	0.41
2:A:798:TRP:HA	2:A:801:PHE:HB3	2.02	0.41
2:A:214:VAL:HG12	2:A:219:GLY:O	2.21	0.41
2:A:236:THR:HG23	2:A:237:ILE:H	1.86	0.41
2:A:327:ALA:C	2:A:329:GLY:N	2.73	0.41
2:A:367:TYR:CD1	2:A:405:ILE:HD13	2.54	0.41
2:A:466:PHE:N	2:A:466:PHE:CD1	2.87	0.41
2:A:749:LEU:HD13	2:A:750:VAL:CG2	2.41	0.41
2:A:443:ASN:HD21	2:A:446:ARG:NH2	2.18	0.41
2:A:463:LEU:HG	2:A:525:MET:HE3	2.02	0.41
2:A:162:ALA:O	2:A:166:ILE:HG13	2.20	0.41
2:A:170:MET:O	2:A:173:LYS:N	2.53	0.41
2:A:828:LYS:HG3	2:A:857:GLN:HB2	2.02	0.41
2:A:137:LYS:O	2:A:141:ARG:HB2	2.21	0.41
2:A:664:PRO:CG	2:A:746:TYR:CE2	3.03	0.41
2:A:564:ASN:HA	2:A:567:ILE:HG22	2.03	0.41
2:A:75:ASP:O	2:A:76:PHE:C	2.58	0.41
1:T:12:U:H2'	1:T:13:C:O4'	2.21	0.41
2:A:239:SER:HB3	2:A:346:ILE:CD1	2.48	0.41
2:A:539:LEU:HA	2:A:545:LEU:CD1	2.51	0.41
2:A:583:LEU:HD23	2:A:584:SER:H	1.85	0.41
2:A:328:PRO:CB	2:A:335:TYR:HA	2.50	0.41
2:A:765:GLU:HA	2:A:779:VAL:HG23	2.02	0.41
2:A:28:GLN:O	2:A:31:TRP:N	2.54	0.41
2:A:301:PRO:O	2:A:302:PHE:C	2.58	0.41
2:A:348:PRO:O	2:A:407:ARG:CD	2.68	0.41
2:A:210:VAL:HG22	2:A:385:LEU:HD13	2.03	0.41
2:A:367:TYR:CD1	2:A:367:TYR:O	2.74	0.41
1:T:73:A:H2'	1:T:74:C:H5'	2.03	0.41
2:A:823:LYS:HG2	2:A:826:GLU:CD	2.40	0.41
2:A:445:VAL:HA	2:A:448:ARG:HB2	2.02	0.41
2:A:171:ALA:C	2:A:173:LYS:H	2.25	0.41
2:A:539:LEU:HA	2:A:545:LEU:HD12	2.02	0.41
2:A:747:GLN:O	2:A:748:ILE:C	2.59	0.41
2:A:185:TRP:H	2:A:404:VAL:CG1	2.34	0.41
2:A:740:SER:O	2:A:743:THR:HB	2.20	0.41
2:A:80:TYR:O	2:A:83:MET:N	2.51	0.41
1:T:67:A:C2'	1:T:68:G:O5'	2.69	0.41
2:A:684:ARG:HB3	2:A:684:ARG:CZ	2.51	0.41
2:A:140:ARG:NH2	2:A:149:ASN:HD22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:338:GLY:CA	2:A:343:LEU:HD12	2.50	0.41
2:A:477:LYS:HB2	2:A:477:LYS:HE3	1.87	0.41
2:A:116:SER:O	2:A:119:GLU:N	2.54	0.41
2:A:79:ARG:HH11	2:A:79:ARG:HG2	1.86	0.41
2:A:482:HIS:HE1	5:A:1014:HOH:O	2.05	0.40
2:A:495:TRP:HD1	2:A:496:PHE:CD2	2.39	0.40
2:A:727:ILE:HD12	5:A:1063:HOH:O	2.20	0.40
2:A:24:GLU:CD	2:A:615:ALA:H	2.24	0.40
1:T:71:C:O3'	2:A:560:ARG:HD2	2.21	0.40
2:A:229:ILE:HD13	2:A:323:CYS:CB	2.51	0.40
2:A:251:TYR:N	2:A:251:TYR:CD1	2.88	0.40
2:A:304:ASP:C	2:A:306:GLU:H	2.24	0.40
2:A:327:ALA:HB1	2:A:346:ILE:HD11	2.03	0.40
2:A:168:GLY:O	2:A:169:GLU:C	2.59	0.40
2:A:476:THR:C	2:A:477:LYS:O	2.59	0.40
2:A:120:PHE:HD1	2:A:123:LYS:CB	2.34	0.40
1:T:35:A:C2'	1:T:36:U:OP1	2.70	0.40
1:T:5:U:H5'	2:A:436:TRP:CE3	2.56	0.40
2:A:426:ALA:O	2:A:429:ASN:N	2.54	0.40
2:A:120:PHE:CD2	2:A:124:CYS:SG	3.15	0.40
2:A:44:ASN:CA	2:A:47:ASN:HD21	2.35	0.40
2:A:74:LYS:HE2	2:A:553:LEU:O	2.21	0.40
2:A:367:TYR:C	2:A:371:ASN:HD21	2.25	0.40
2:A:367:TYR:CD1	2:A:405:ILE:HG21	2.56	0.40
1:T:51:U:H2'	1:T:52:G:C8	2.57	0.40
2:A:180:LYS:HG2	2:A:409:THR:C	2.41	0.40
2:A:781:LEU:HD23	2:A:781:LEU:HA	1.91	0.40
2:A:19:GLY:C	2:A:21:PRO:HD2	2.42	0.40
2:A:171:ALA:HB1	2:A:475:MET:HE3	2.03	0.40
2:A:112:ARG:HB3	2:A:113:LYS:H	1.47	0.40
2:A:867:GLN:HG3	2:A:868:ALA:N	2.36	0.40
2:A:610:VAL:O	2:A:614:GLY:HA2	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:19:G:O2'	2:A:672:SER:O[4_576]	2.19	0.01

## 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	878/917 (96%)	572 (65%)	186 (21%)	120 (14%)	<b>0</b> <b>0</b>

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	45	LYS
2	A	47	ASN
2	A	112	ARG
2	A	114	LYS
2	A	195	GLU
2	A	229	ILE
2	A	248	GLU
2	A	254	TYR
2	A	256	VAL
2	A	263	ILE
2	A	268	SER
2	A	283	LYS
2	A	294	GLU
2	A	295	TRP
2	A	301	PRO
2	A	302	PHE
2	A	304	ASP
2	A	316	THR
2	A	344	PRO
2	A	347	SER
2	A	350	ASP
2	A	376	ASP
2	A	377	LEU
2	A	383	ALA
2	A	421	GLN
2	A	439	THR
2	A	469	GLU
2	A	473	ILE

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Mol	Chain	Res	Type
2	A	506	GLU
2	A	556	SER
2	A	668	SER
2	A	750	VAL
2	A	776	GLU
2	A	824	SER
2	A	843	LEU
2	A	43	LYS
2	A	44	ASN
2	A	116	SER
2	A	147	ASP
2	A	154	THR
2	A	196	ALA
2	A	223	ALA
2	A	234	PRO
2	A	258	GLY
2	A	280	ALA
2	A	281	SER
2	A	293	LEU
2	A	303	LEU
2	A	315	VAL
2	A	340	GLN
2	A	360	GLY
2	A	372	LYS
2	A	379	THR
2	A	381	LYS
2	A	384	LEU
2	A	390	ILE
2	A	472	GLU
2	A	546	SER
2	A	561	GLY
2	A	572	ALA
2	A	599	SER
2	A	606	PRO
2	A	731	GLU
2	A	793	ALA
2	A	840	SER
2	A	113	LYS
2	A	189	SER
2	A	216	ASP
2	A	238	PRO
2	A	308	LEU

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Mol	Chain	Res	Type
2	A	324	VAL
2	A	342	GLU
2	A	349	ILE
2	A	358	GLU
2	A	382	GLY
2	A	415	SER
2	A	440	ARG
2	A	447	ASP
2	A	468	ALA
2	A	485	ASP
2	A	505	PRO
2	A	527	VAL
2	A	543	PRO
2	A	665	ASP
2	A	718	ASN
2	A	778	SER
2	A	806	ASP
2	A	822	GLY
2	A	833	SER
2	A	63	LEU
2	A	260	LYS
2	A	278	ASP
2	A	328	PRO
2	A	356	THR
2	A	373	ALA
2	A	434	VAL
2	A	435	ASN
2	A	446	ARG
2	A	477	LYS
2	A	489	GLU
2	A	497	GLU
2	A	664	PRO
2	A	773	HIS
2	A	808	VAL
2	A	862	ASP
2	A	109	GLY
2	A	217	ASP
2	A	242	ALA
2	A	252	GLY
2	A	380	GLU
2	A	492	SER
2	A	228	ILE

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Mol	Chain	Res	Type
2	A	241	VAL
2	A	339	GLN
2	A	501	LYS
2	A	309	VAL
2	A	101	ILE
2	A	761	VAL
2	A	247	PRO
2	A	245	VAL

### 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	772/806 (96%)	676 (88%)	96 (12%)	6 17

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	11	LYS
2	A	20	LEU
2	A	22	ASN
2	A	47	ASN
2	A	60	ASN
2	A	94	TRP
2	A	95	ASP
2	A	112	ARG
2	A	116	SER
2	A	144	VAL
2	A	149	ASN
2	A	153	ILE
2	A	159	TYR
2	A	160	GLU
2	A	164	ILE
2	A	167	PHE
2	A	189	SER
2	A	200	TYR

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Mol	Chain	Res	Type
2	A	202	ASP
2	A	227	PHE
2	A	233	THR
2	A	234	PRO
2	A	236	THR
2	A	250	LYS
2	A	254	TYR
2	A	273	GLU
2	A	275	LEU
2	A	284	LEU
2	A	295	TRP
2	A	301	PRO
2	A	305	ARG
2	A	306	GLU
2	A	308	LEU
2	A	309	VAL
2	A	317	THR
2	A	325	HIS
2	A	326	THR
2	A	341	TYR
2	A	342	GLU
2	A	345	VAL
2	A	355	PHE
2	A	366	PHE
2	A	367	TYR
2	A	371	ASN
2	A	384	LEU
2	A	389	PHE
2	A	392	HIS
2	A	397	ASP
2	A	398	TRP
2	A	407	ARG
2	A	413	PHE
2	A	422	ASP
2	A	444	MET
2	A	450	GLU
2	A	458	VAL
2	A	466	PHE
2	A	467	TYR
2	A	476	THR
2	A	481	ASN
2	A	485	ASP

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Mol	Chain	Res	Type
2	A	486	LEU
2	A	487	PHE
2	A	493	ASN
2	A	499	GLU
2	A	501	LYS
2	A	526	ASP
2	A	527	VAL
2	A	535	HIS
2	A	544	GLU
2	A	551	MET
2	A	560	ARG
2	A	569	THR
2	A	573	THR
2	A	583	LEU
2	A	602	ASN
2	A	616	ASP
2	A	630	ASP
2	A	644	ASP
2	A	646	ARG
2	A	649	ARG
2	A	666	THR
2	A	681	LEU
2	A	715	GLU
2	A	723	TYR
2	A	732	GLN
2	A	749	LEU
2	A	773	HIS
2	A	807	ASP
2	A	813	GLU
2	A	821	ILE
2	A	830	THR
2	A	831	ILE
2	A	836	LYS
2	A	857	GLN
2	A	869	THR
2	A	875	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	26	GLN
2	A	36	GLN

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Mol	Chain	Res	Type
2	A	38	HIS
2	A	47	ASN
2	A	53	HIS
2	A	60	ASN
2	A	62	ASN
2	A	131	GLN
2	A	149	ASN
2	A	240	ASN
2	A	246	HIS
2	A	299	GLN
2	A	339	GLN
2	A	371	ASN
2	A	392	HIS
2	A	396	HIS
2	A	443	ASN
2	A	456	GLN
2	A	481	ASN
2	A	482	HIS
2	A	490	HIS
2	A	493	ASN
2	A	585	HIS
2	A	602	ASN
2	A	612	GLN
2	A	650	ASN
2	A	698	ASN
2	A	706	GLN
2	A	713	ASN
2	A	732	GLN
2	A	736	HIS
2	A	742	GLN
2	A	770	HIS
2	A	773	HIS
2	A	792	GLN
2	A	809	ASN
2	A	851	GLN
2	A	857	GLN
2	A	867	GLN

### 5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	T	74/75 (98%)	21 (28%)	12 (16%)

All (21) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	T	8	U
1	T	9	A
1	T	10	G
1	T	14	A
1	T	16	G
1	T	17	U
1	T	18	G
1	T	19	G
1	T	20	U
1	T	121(A)	U
1	T	22	G
1	T	34	G
1	T	35	A
1	T	36	U
1	T	37	A
1	T	38	A
1	T	46	G
1	T	48	C
1	T	49	G
1	T	59	G
1	T	61	C

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	T	7	G
1	T	9	A
1	T	18	G
1	T	19	G
1	T	33	U
1	T	34	G
1	T	36	U
1	T	37	A
1	T	47	U
1	T	48	C

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Mol	Chain	Res	Type
1	T	58	A
1	T	60	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 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	MRC	A	993	-	33,36,36	2.30	11 (33%)	35,48,48	2.04	7 (20%)

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	MRC	A	993	-	1/1/11/12	0/30/54/54	0/1/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	993	MRC	C11-C10	-7.50	1.36	1.46
4	A	993	MRC	C2-C1	-2.88	1.39	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	993	MRC	C9-C10	2.07	1.56	1.52
4	A	993	MRC	C4-C3	2.30	1.54	1.51
4	A	993	MRC	C12-C13	2.35	1.58	1.54
4	A	993	MRC	C16-C8	2.60	1.55	1.51
4	A	993	MRC	C4-C5	2.71	1.58	1.53
4	A	993	MRC	C2-C3	2.89	1.39	1.33
4	A	993	MRC	C9-C8	3.29	1.60	1.53
4	A	993	MRC	O1A-C1	3.92	1.43	1.34
4	A	993	MRC	C8-C7	4.46	1.59	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	993	MRC	C11-O10-C10	-5.63	57.39	60.59
4	A	993	MRC	C9'-O1A-C1	-3.38	110.72	116.66
4	A	993	MRC	C5-C4-C3	2.91	120.99	113.47
4	A	993	MRC	C17-C12-C13	3.58	120.10	112.82
4	A	993	MRC	C17-C12-C11	3.72	118.34	111.38
4	A	993	MRC	O1A-C1-C2	4.09	118.98	110.65
4	A	993	MRC	C11-C12-C13	5.23	120.59	110.78

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	993	MRC	C12

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	993	MRC	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	T	75/75 (100%)	-0.23	1 (1%) 79 78	5, 30, 78, 100	2 (2%)
2	A	880/917 (95%)	-0.38	18 (2%) 68 64	3, 32, 70, 83	0
All	All	955/992 (96%)	-0.37	19 (1%) 68 64	3, 32, 70, 100	2 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	2	ASP	4.2
1	T	74	C	4.1
2	A	4	GLU	4.0
2	A	3	TYR	3.7
2	A	280	ALA	3.7
2	A	377	LEU	3.5
2	A	217	ASP	3.3
2	A	279	LYS	3.0
2	A	384	LEU	3.0
2	A	249	LEU	2.9
2	A	218	LYS	2.8
2	A	866	ASP	2.7
2	A	6	THR	2.4
2	A	360	GLY	2.4
2	A	317	THR	2.3
2	A	358	GLU	2.2
2	A	315	VAL	2.2
2	A	470	ASN	2.1
2	A	292	GLU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MRC	A	993	35/35	0.90	0.21	2.49	22,29,57,58	0
3	ZN	A	992	1/1	1.00	0.04	-1.35	35,35,35,35	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.