



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:58 PM GMT

PDB ID : 3HTX
Title : Crystal structure of small RNA methyltransferase HEN1
Authors : Huang, Y.; Ji, L.-J.; Huang, Q.-C.; Vassylyev, D.G.; Chen, X.-M.; Ma, J.-B.
Deposited on : 2009-06-12
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

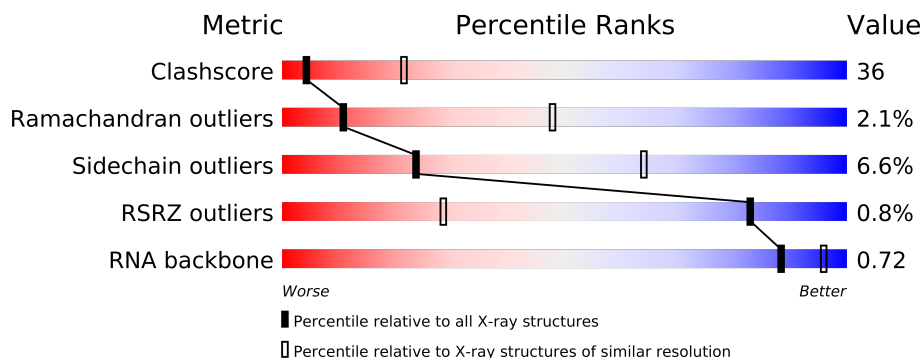
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	950	
1	D	950	
2	B	22	
2	E	22	
3	C	22	
3	F	22	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14269 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HEN1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	779	Total	C	N	O	S	0	0	0
			6093	3847	1046	1170	30			
1	D	795	Total	C	N	O	S	0	0	0
			6217	3928	1065	1194	30			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	EXPRESSION TAG	UNP Q945R3
A	-6	GLY	-	EXPRESSION TAG	UNP Q945R3
A	-5	HIS	-	EXPRESSION TAG	UNP Q945R3
A	-4	HIS	-	EXPRESSION TAG	UNP Q945R3
A	-3	HIS	-	EXPRESSION TAG	UNP Q945R3
A	-2	HIS	-	EXPRESSION TAG	UNP Q945R3
A	-1	HIS	-	EXPRESSION TAG	UNP Q945R3
A	0	HIS	-	EXPRESSION TAG	UNP Q945R3
A	604	PRO	LEU	ENGINEERED	UNP Q945R3
A	640	LYS	ARG	ENGINEERED	UNP Q945R3
D	-7	MET	-	EXPRESSION TAG	UNP Q945R3
D	-6	GLY	-	EXPRESSION TAG	UNP Q945R3
D	-5	HIS	-	EXPRESSION TAG	UNP Q945R3
D	-4	HIS	-	EXPRESSION TAG	UNP Q945R3
D	-3	HIS	-	EXPRESSION TAG	UNP Q945R3
D	-2	HIS	-	EXPRESSION TAG	UNP Q945R3
D	-1	HIS	-	EXPRESSION TAG	UNP Q945R3
D	0	HIS	-	EXPRESSION TAG	UNP Q945R3
D	604	PRO	LEU	ENGINEERED	UNP Q945R3
D	640	LYS	ARG	ENGINEERED	UNP Q945R3

- Molecule 2 is a RNA chain called 5'-R(*GP*AP*UP*UP*UP*CP*UP*CP*UP*CP*UP*GP*CP*AP*AP*GP*CP*GP*AP*AP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	22	Total	C	N	O	P	0	0	0
			464	209	82	152	21			
2	E	22	Total	C	N	O	P	0	0	0
			464	209	82	152	21			

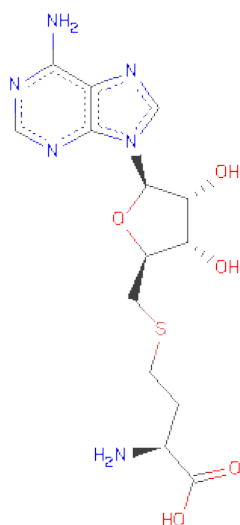
- Molecule 3 is a RNA chain called 5'-R(P*UP*UP*CP*GP*CP*UP*UP*GP*CP*AP*GP*AP*GP*AP*GP*AP*AP*UP*CP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	22	Total	C	N	O	P	0	0	0
			470	210	85	153	22			
3	F	22	Total	C	N	O	P	0	0	0
			470	210	85	153	22			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

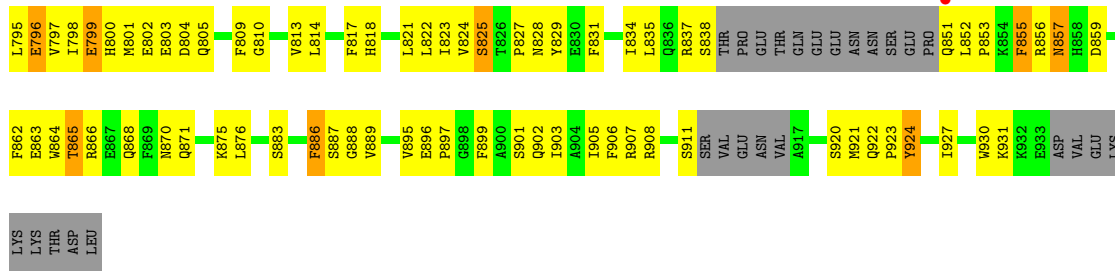
- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
5	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

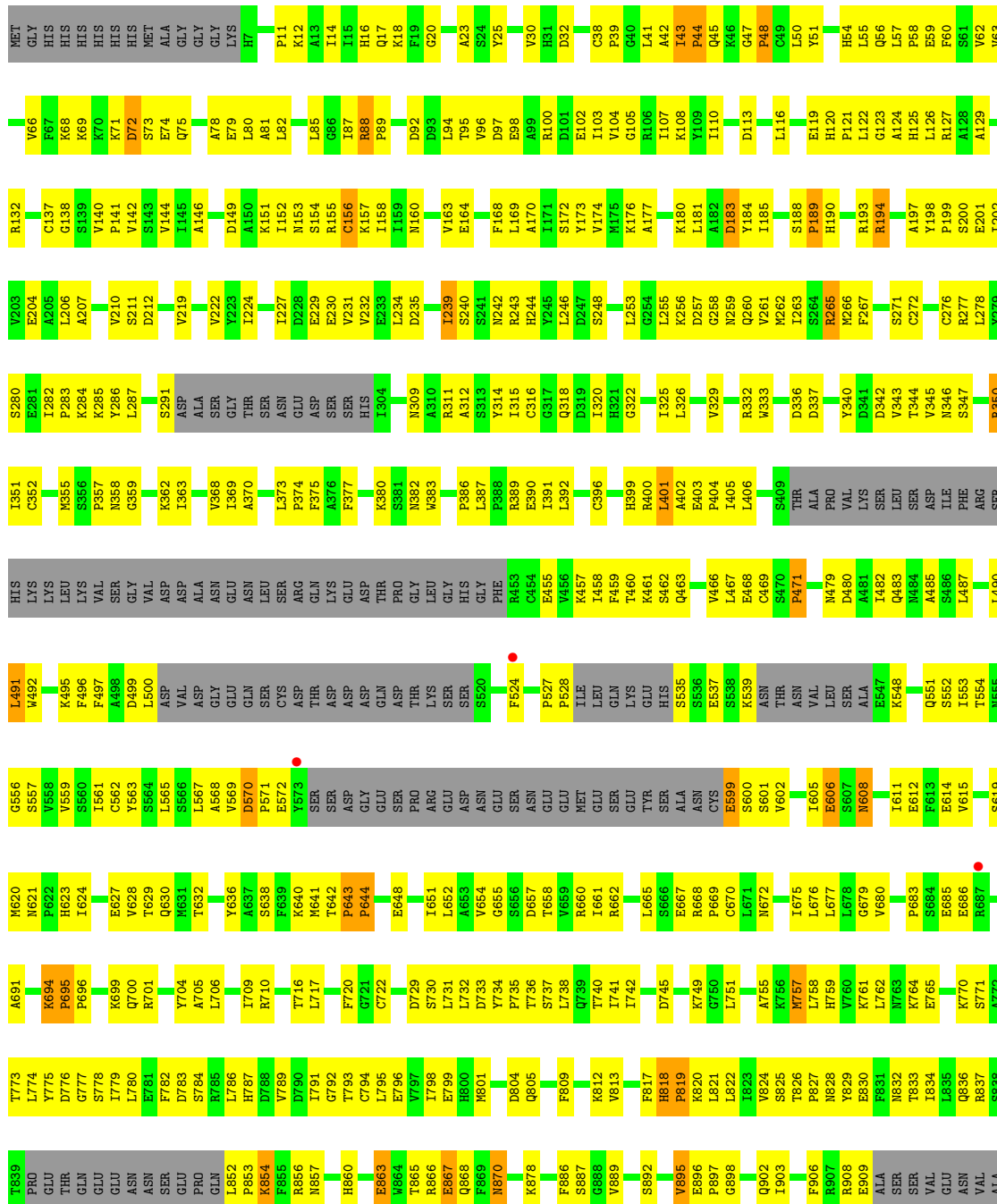
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	2	Total	O	0	0
			2	2		
6	C	2	Total	O	0	0
			2	2		
6	D	16	Total	O	0	0
			16	16		
6	E	1	Total	O	0	0
			1	1		
6	F	2	Total	O	0	0
			2	2		



• Molecule 1: HEN1

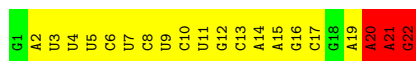
Chain D:





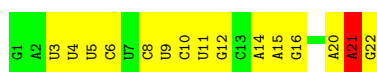
- Molecule 2: 5'-R(*GP*AP*UP*UP*UP*CP*UP*CP*UP*CP*UP*GP*CP*AP*AP*GP*CP*GP*AP*AP*AP*G)-3'

Chain B:



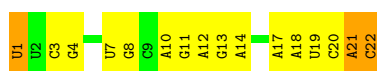
- Molecule 2: 5'-R(*GP*AP*UP*UP*UP*CP*UP*CP*UP*CP*UP*GP*CP*AP*AP*GP*CP*GP*AP*AP*AP*G)-3'

Chain E:



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

Chain C:



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

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.00Å 124.35Å 101.38Å 90.00° 93.47° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-3.10) 78.0 (19.99-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.288 0.248 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	72.0	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 8.9	EDS
Estimated twinning fraction	0.054 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 40951 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14269	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.51	0/6214	0.75	4/8395 (0.0%)
1	D	0.52	0/6343	0.76	5/8573 (0.1%)
2	B	0.46	0/518	0.92	3/805 (0.4%)
2	E	0.46	0/518	0.78	1/805 (0.1%)
3	C	0.55	1/525 (0.2%)	0.69	0/814
3	F	0.58	1/525 (0.2%)	0.84	1/814 (0.1%)
All	All	0.51	2/14643 (0.0%)	0.77	14/20206 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	U	OP3-P	-6.77	1.53	1.61
3	F	1	U	OP3-P	-6.57	1.53	1.61

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20	A	C2'-C3'-O3'	9.92	131.33	109.50
3	F	19	U	C2'-C3'-O3'	8.29	127.75	109.50
1	A	789	VAL	CB-CA-C	-7.54	97.08	111.40
1	D	20	GLY	N-CA-C	-7.19	95.12	113.10
1	D	818	HIS	C-N-CD	-7.07	105.05	120.60
1	D	695	PRO	N-CA-C	-6.44	95.36	112.10
2	B	21	A	C5'-C4'-C3'	-6.41	105.74	116.00
2	B	22	G	C2'-C3'-O3'	5.88	123.10	113.70
1	D	499	ASP	N-CA-C	-5.69	95.64	111.00
2	E	21	A	N9-C1'-C2'	5.44	121.07	114.00
1	A	764	LYS	N-CA-C	-5.43	96.33	111.00
1	A	695	PRO	N-CA-C	-5.15	98.71	112.10
1	D	819	PRO	N-CA-C	-5.06	98.95	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	562	CYS	N-CA-C	-5.03	97.43	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6093	0	6031	434	0
1	D	6217	0	6139	493	0
2	B	464	0	236	35	0
2	E	464	0	236	21	0
3	C	470	0	238	20	0
3	F	470	0	238	17	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	26	0	19	2	0
5	D	26	0	19	1	0
6	A	14	0	0	5	0
6	B	2	0	0	2	0
6	C	2	0	0	0	0
6	D	16	0	0	2	0
6	E	1	0	0	0	0
6	F	2	0	0	1	0
All	All	14269	0	13156	987	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 36.

All (987) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:802:GLU:HB2	1:A:805:GLN:HG3	1.21	1.20
3:F:21:A:H2'	6:F:226:HOH:O	1.45	1.12
1:A:262:MET:HE3	1:A:263:ILE:H	1.16	1.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:776:ASP:HB2	1:D:927:ILE:HD11	1.34	1.07
1:A:45:GLN:HE21	1:A:752:ALA:HB1	1.18	1.07
1:A:401:LEU:HD22	1:A:461:LYS:HB2	1.39	1.03
1:A:142:VAL:HG11	1:A:171:ILE:HG23	1.43	1.01
1:A:15:ILE:HG21	1:A:82:LEU:HD11	1.43	1.00
1:D:537:GLU:HA	1:D:641:MET:HE2	1.42	1.00
1:D:570:ASP:H	1:D:571:PRO:HD2	1.27	0.98
1:D:457:LYS:HA	1:D:457:LYS:HE2	1.46	0.97
1:A:183:ASP:HA	6:A:947:HOH:O	1.66	0.95
1:D:43:ILE:N	1:D:44:PRO:HD3	1.82	0.94
1:D:836:GLN:HE22	1:D:854:LYS:HB2	1.29	0.94
1:A:45:GLN:NE2	1:A:752:ALA:HB1	1.82	0.93
1:D:401:LEU:HD22	1:D:461:LYS:HD3	1.51	0.93
1:A:82:LEU:HD23	1:A:85:LEU:HD12	1.50	0.92
1:D:262:MET:HB2	1:D:282:ILE:HG12	1.52	0.92
1:A:405:ILE:HB	1:A:458:ILE:HG12	1.53	0.91
1:D:757:MET:HG3	1:D:758:LEU:N	1.85	0.89
1:D:116:LEU:HG	1:D:206:LEU:HD11	1.53	0.89
1:D:265:ARG:H	1:D:318:GLN:NE2	1.71	0.88
1:D:244:HIS:CD2	1:D:246:LEU:HB2	2.09	0.88
1:A:244:HIS:HD2	1:A:246:LEU:H	1.18	0.88
1:A:400:ARG:O	1:A:401:LEU:HD23	1.74	0.87
1:D:570:ASP:H	1:D:571:PRO:CD	1.88	0.87
1:D:716:THR:HG22	1:D:740:THR:HB	1.56	0.87
1:A:810:GLY:HA3	1:A:876:LEU:HD21	1.57	0.86
1:A:457:LYS:HZ3	1:A:486:SER:HA	1.41	0.86
1:A:401:LEU:HD22	1:A:461:LYS:CB	2.04	0.86
1:D:88:ARG:HG2	1:D:89:PRO:HD2	1.57	0.86
1:D:262:MET:HB2	1:D:282:ILE:CG1	2.06	0.86
1:D:817:PHE:O	1:D:819:PRO:HD2	1.77	0.85
1:D:43:ILE:N	1:D:44:PRO:CD	2.39	0.84
1:A:831:PHE:O	1:A:834:ILE:HG22	1.76	0.83
1:D:265:ARG:H	1:D:318:GLN:HE22	1.21	0.83
1:A:365:ARG:HH11	1:A:365:ARG:HG3	1.44	0.83
1:D:729:ASP:HB2	1:D:757:MET:SD	2.19	0.83
1:D:776:ASP:HB2	1:D:927:ILE:CD1	2.07	0.83
1:D:710:ARG:NH2	1:D:734:TYR:HB2	1.92	0.83
1:A:255:LEU:HD11	1:A:281:GLU:HB2	1.62	0.82
1:A:88:ARG:HG3	1:A:89:PRO:HD3	1.59	0.82
1:A:742:ILE:HD13	1:A:786:LEU:HD22	1.62	0.82
1:D:387:LEU:HB3	1:D:483:GLN:HE22	1.45	0.82
1:D:23:ALA:CB	1:D:57:LEU:HD23	2.09	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:405:ILE:HD12	1:A:458:ILE:HD11	1.61	0.81
1:D:124:ALA:HA	1:D:127:ARG:NH1	1.96	0.81
1:A:127:ARG:HG3	1:A:206:LEU:HD21	1.63	0.81
1:D:621:ASN:HD22	1:D:624:ILE:HG13	1.45	0.81
1:D:548:LYS:O	1:D:552:SER:HB2	1.80	0.81
1:D:892:SER:HB2	1:D:895:VAL:HG23	1.62	0.80
1:A:126:LEU:HD23	1:A:140:VAL:HG21	1.63	0.80
1:D:43:ILE:HD11	1:D:927:ILE:HD13	1.64	0.80
1:D:817:PHE:C	1:D:819:PRO:HD2	2.02	0.80
1:A:865:THR:H	1:A:868:GLN:NE2	1.80	0.80
1:A:569:VAL:HG23	1:A:601:SER:HB2	1.61	0.80
1:A:624:ILE:HG23	1:A:675:ILE:HD11	1.65	0.79
1:D:57:LEU:HB3	1:D:58:PRO:HD2	1.62	0.79
1:D:105:GLY:O	1:D:108:LYS:HG2	1.82	0.79
1:D:570:ASP:N	1:D:571:PRO:HD2	1.96	0.79
1:D:387:LEU:HB3	1:D:483:GLN:NE2	1.98	0.79
1:A:895:VAL:HG12	1:A:897:PRO:HD2	1.64	0.79
1:D:559:VAL:HG12	1:D:561:ILE:HG23	1.63	0.79
1:A:537:GLU:HB3	1:A:641:MET:CE	2.12	0.79
1:D:799:GLU:HG3	1:D:860:HIS:CD2	2.18	0.79
1:A:537:GLU:HB3	1:A:641:MET:HE1	1.64	0.78
1:D:740:THR:HG23	1:D:771:SER:HB3	1.66	0.78
1:D:829:TYR:HD1	1:D:832:ASN:HD21	1.29	0.78
1:D:266:MET:HB3	1:D:277:ARG:HE	1.47	0.78
1:A:457:LYS:NZ	1:A:486:SER:HA	1.98	0.78
1:D:405:ILE:HB	1:D:458:ILE:HG13	1.66	0.78
2:E:8:C:H2'	2:E:9:U:C6	2.20	0.77
1:A:108:LYS:HD2	1:A:181:LEU:HD21	1.66	0.77
1:A:151:LYS:O	1:A:155:ARG:HG2	1.85	0.77
1:D:557:SER:O	1:D:615:VAL:HG23	1.84	0.77
1:D:461:LYS:HG3	1:D:466:VAL:HG21	1.65	0.77
1:A:123:GLY:O	1:A:127:ARG:HB2	1.86	0.76
1:D:552:SER:HA	1:D:629:THR:O	1.86	0.76
1:A:852:LEU:HB2	1:A:855:PHE:CE1	2.20	0.76
1:A:865:THR:H	1:A:868:GLN:HE21	1.30	0.76
3:F:19:U:O2'	3:F:20:C:H5'	1.86	0.76
1:D:164:GLU:HB3	1:D:400:ARG:HH12	1.48	0.75
1:A:318:GLN:HG3	1:A:400:ARG:HH22	1.50	0.75
1:D:895:VAL:HG12	1:D:897:PRO:HD2	1.67	0.75
1:A:827:PRO:HA	1:A:901:SER:HA	1.68	0.75
3:F:18:A:H2'	3:F:19:U:C6	2.21	0.75
1:D:568:ALA:HB1	1:D:601:SER:O	1.85	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:553:ILE:HD12	1:A:629:THR:HA	1.68	0.75
1:D:830:GLU:HG3	1:D:865:THR:HG23	1.69	0.75
1:D:181:LEU:HG	1:D:184:TYR:HB2	1.68	0.74
1:A:704:TYR:HA	1:A:707:LYS:HE3	1.69	0.74
1:D:41:LEU:HD21	1:D:755:ALA:HB1	1.69	0.74
1:D:606:GLU:HB3	1:D:654:VAL:HG11	1.70	0.74
1:A:650:LEU:O	1:A:654:VAL:HG23	1.86	0.74
1:D:552:SER:HA	1:D:629:THR:HG22	1.68	0.74
1:D:12:LYS:HG3	1:D:79:GLU:HB2	1.69	0.74
1:A:368:VAL:HB	1:A:650:LEU:HD11	1.68	0.74
1:D:16:HIS:NE2	1:D:82:LEU:HG	2.03	0.74
3:F:19:U:H2'	3:F:20:C:H6	1.53	0.73
1:D:283:PRO:HG2	1:D:286:TYR:HD1	1.54	0.73
1:A:47:GLY:HA2	2:B:15:A:H4'	1.69	0.73
1:D:627:GLU:HB2	6:D:955:HOH:O	1.86	0.73
1:D:731:LEU:HD21	1:D:738:LEU:HD13	1.71	0.73
1:A:392:LEU:HD22	1:A:457:LYS:HZ2	1.54	0.73
1:D:866:ARG:NH1	1:D:898:GLY:HA3	2.03	0.73
1:A:864:TRP:HA	1:A:868:GLN:NE2	2.03	0.73
1:A:10:THR:HG21	1:A:90:GLN:HG2	1.69	0.72
1:D:836:GLN:NE2	1:D:854:LYS:HB2	2.04	0.72
1:A:569:VAL:O	1:A:571:PRO:HD3	1.88	0.72
1:A:94:LEU:HD23	1:A:99:ALA:HB2	1.72	0.72
1:D:710:ARG:CZ	1:D:734:TYR:HB2	2.19	0.72
1:D:88:ARG:CG	1:D:89:PRO:HD2	2.20	0.72
1:A:364:SER:HB3	1:A:386:PRO:HG2	1.70	0.72
1:D:784:SER:HB3	1:D:920:SER:HA	1.73	0.71
1:D:731:LEU:HD11	1:D:738:LEU:HD12	1.72	0.71
1:D:628:VAL:CG2	1:D:675:ILE:HD12	2.21	0.71
1:D:164:GLU:HB3	1:D:400:ARG:NH1	2.05	0.71
1:A:253:LEU:HD21	1:A:325:ILE:HG12	1.72	0.71
1:D:244:HIS:HD2	1:D:246:LEU:HB2	1.54	0.71
1:D:402:ALA:HB3	1:D:460:THR:O	1.91	0.71
1:D:283:PRO:HG2	1:D:286:TYR:CD1	2.26	0.71
1:D:553:ILE:H	1:D:629:THR:HG23	1.56	0.71
1:A:364:SER:CB	1:A:386:PRO:HG2	2.21	0.71
1:D:278:LEU:HD21	1:D:312:ALA:HB1	1.73	0.70
1:A:262:MET:HE3	1:A:263:ILE:N	2.00	0.70
1:D:742:ILE:HG21	1:D:786:LEU:HD21	1.73	0.70
1:D:628:VAL:HG22	1:D:675:ILE:HD12	1.72	0.70
1:D:232:VAL:HG23	1:D:311:ARG:NH2	2.07	0.70
1:D:160:ASN:O	1:D:163:VAL:HG23	1.92	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:392:LEU:HD11	1:A:459:PHE:HE1	1.57	0.70
1:A:332:ARG:HG2	1:A:333:TRP:H	1.57	0.70
1:D:567:LEU:HB2	1:D:605:ILE:HD11	1.72	0.70
1:D:827:PRO:HB3	1:D:856:ARG:HD2	1.72	0.69
1:A:367:ALA:HB1	1:A:370:ALA:HB3	1.74	0.69
1:A:255:LEU:HB3	1:A:260:GLN:OE1	1.92	0.69
1:A:887:SER:O	1:A:903:ILE:HB	1.93	0.69
1:A:667:GLU:O	1:A:669:PRO:HD3	1.93	0.69
1:A:369:ILE:HG21	1:A:565:LEU:HD11	1.74	0.69
1:D:81:ALA:O	1:D:85:LEU:HG	1.93	0.69
1:A:809:PHE:O	1:A:813:VAL:HG23	1.93	0.69
1:A:108:LYS:HB2	1:A:181:LEU:HD21	1.74	0.69
3:C:7:U:H2'	3:C:8:G:C8	2.28	0.69
3:F:21:A:H1'	3:F:22:C:H5	1.57	0.68
1:A:110:ILE:HG22	1:A:126:LEU:HD11	1.74	0.68
1:D:731:LEU:HD21	1:D:738:LEU:CD1	2.23	0.68
1:D:219:VAL:HG21	1:D:239:ILE:HD11	1.74	0.68
1:A:244:HIS:CD2	1:A:246:LEU:H	2.06	0.68
1:D:809:PHE:O	1:D:813:VAL:HG23	1.93	0.68
1:D:257:ASP:H	1:D:260:GLN:HE21	1.42	0.68
1:D:559:VAL:CG1	1:D:561:ILE:HG23	2.23	0.68
1:A:721:GLY:HA3	1:A:797:VAL:HG21	1.75	0.68
1:D:406:LEU:HD13	1:D:457:LYS:HE3	1.74	0.68
1:A:362:LYS:HB3	1:A:368:VAL:HA	1.76	0.67
1:D:43:ILE:HG22	1:D:43:ILE:O	1.91	0.67
1:D:265:ARG:HH12	1:D:400:ARG:HE	1.42	0.67
1:A:117:SER:HB3	1:A:206:LEU:HD13	1.77	0.67
1:A:18:LYS:HE2	3:C:19:U:H4'	1.75	0.67
1:D:152:ILE:O	1:D:156:CYS:HB2	1.94	0.67
1:D:828:ASN:HA	1:D:902:GLN:NE2	2.10	0.67
1:D:124:ALA:HA	1:D:127:ARG:HH12	1.57	0.67
1:D:30:VAL:HG12	1:D:32:ASP:H	1.58	0.67
1:D:344:THR:H	1:D:347:SER:HB2	1.60	0.67
1:D:194:ARG:HH12	1:D:198:TYR:HA	1.60	0.67
1:A:108:LYS:HB2	1:A:181:LEU:CD2	2.24	0.67
1:D:43:ILE:HD11	1:D:927:ILE:CD1	2.23	0.67
1:D:691:ALA:HB2	2:E:20:A:H5''	1.75	0.67
1:D:459:PHE:HB2	1:D:466:VAL:HB	1.76	0.67
1:A:742:ILE:HD13	1:A:786:LEU:CD2	2.24	0.67
1:D:347:SER:O	1:D:351:ILE:HG12	1.94	0.66
1:A:94:LEU:HB2	1:A:158:ILE:HD13	1.78	0.66
3:C:7:U:H2'	3:C:8:G:H8	1.59	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:21:A:H5'	3:C:22:C:OP1	1.96	0.66
1:A:753:ARG:O	1:A:756:LYS:HG2	1.94	0.66
1:D:23:ALA:HB1	1:D:56:GLN:O	1.95	0.66
1:D:458:ILE:HG22	1:D:468:GLU:HA	1.76	0.66
1:A:658:THR:O	1:A:662:ARG:CG	2.43	0.66
1:A:888:GLY:C	1:A:899:PHE:CD2	2.70	0.66
1:A:149:ASP:OD1	1:A:151:LYS:HB2	1.95	0.65
1:D:567:LEU:CB	1:D:605:ILE:HD11	2.26	0.65
1:A:829:TYR:HD1	1:A:863:GLU:HB3	1.61	0.65
1:A:561:ILE:HD11	1:A:613:PHE:HE1	1.62	0.65
1:A:888:GLY:O	1:A:899:PHE:CE2	2.50	0.65
1:D:467:LEU:HD13	1:D:492:TRP:CZ3	2.31	0.65
1:D:257:ASP:H	1:D:260:GLN:NE2	1.94	0.65
1:A:113:ASP:HB3	1:A:202:ILE:HD13	1.78	0.65
1:A:168:PHE:HE2	1:A:282:ILE:HA	1.62	0.65
1:A:57:LEU:HG	1:A:58:PRO:HD2	1.79	0.64
1:D:210:VAL:HG12	1:D:211:SER:N	2.12	0.64
1:D:655:GLY:HA3	1:D:661:ILE:HD11	1.78	0.64
1:A:639:PHE:HE1	1:A:641:MET:HE3	1.61	0.64
1:A:639:PHE:CE1	1:A:641:MET:HE3	2.33	0.64
1:D:362:LYS:HD3	1:D:368:VAL:O	1.97	0.64
1:A:85:LEU:HD22	1:A:88:ARG:NH2	2.12	0.64
1:D:798:ILE:HD11	1:D:826:THR:OG1	1.98	0.64
3:F:21:A:H1'	3:F:22:C:C5	2.33	0.64
1:D:168:PHE:CD2	1:D:282:ILE:HG23	2.32	0.64
1:D:265:ARG:HH12	1:D:400:ARG:NE	1.94	0.64
1:A:239:ILE:HD12	1:A:239:ILE:N	2.13	0.64
1:D:701:ARG:NH1	1:D:796:GLU:HG2	2.13	0.64
1:A:88:ARG:CG	1:A:89:PRO:HD3	2.28	0.63
1:A:392:LEU:HD13	1:A:457:LYS:HZ1	1.63	0.63
1:D:60:PHE:HE1	1:D:62:VAL:HG22	1.64	0.63
1:A:365:ARG:HH11	1:A:365:ARG:CG	2.12	0.63
1:A:624:ILE:HG23	1:A:675:ILE:CD1	2.28	0.63
1:A:12:LYS:HA	1:A:15:ILE:HD12	1.79	0.63
1:D:401:LEU:HA	1:D:461:LYS:HG2	1.78	0.63
1:D:627:GLU:N	6:D:955:HOH:O	2.31	0.63
1:A:658:THR:O	1:A:662:ARG:HG2	1.98	0.63
1:A:883:SER:HB3	1:A:907:ARG:HB2	1.78	0.63
1:D:14:ILE:HD11	2:E:5:U:H1'	1.81	0.63
1:D:50:LEU:HD22	1:D:68:LYS:HA	1.79	0.63
1:D:929:GLU:HG3	1:D:930:TRP:N	2.13	0.63
1:A:796:GLU:HA	1:A:825:SER:O	1.99	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:240:SER:HB2	1:D:242:ASN:OD1	1.98	0.63
1:A:795:LEU:O	1:A:796:GLU:HG3	1.99	0.63
1:D:243:ARG:HH11	1:D:248:SER:HB3	1.63	0.63
1:A:565:LEU:HD21	1:A:673:TYR:CE2	2.33	0.63
1:A:852:LEU:HB2	1:A:855:PHE:HE1	1.62	0.63
1:D:278:LEU:HD23	1:D:320:ILE:HG13	1.81	0.63
1:A:813:VAL:HA	1:A:817:PHE:HD1	1.64	0.63
1:A:69:LYS:HE3	3:C:8:G:OP1	1.98	0.62
1:D:455:GLU:HG2	1:D:482:ILE:HA	1.81	0.62
1:D:661:ILE:O	1:D:665:LEU:HG	1.99	0.62
1:D:710:ARG:HH22	1:D:734:TYR:HB2	1.65	0.62
1:D:102:GLU:HG3	1:D:155:ARG:HD2	1.81	0.62
1:A:329:VAL:HG12	1:A:340:TYR:HB3	1.82	0.62
1:D:751:LEU:HD13	1:D:927:ILE:HD13	1.81	0.62
1:A:717:LEU:HD12	1:A:718:VAL:N	2.14	0.62
2:B:2:A:H2'	2:B:3:U:O4'	1.99	0.62
1:D:373:LEU:HD12	1:D:374:PRO:HD2	1.81	0.62
1:A:255:LEU:HD22	1:A:260:GLN:NE2	2.15	0.62
1:D:23:ALA:HB2	1:D:57:LEU:HD23	1.81	0.62
1:A:238:TYR:HE1	1:A:252:ARG:HH22	1.46	0.62
1:D:256:LYS:H	1:D:260:GLN:HE22	1.46	0.62
1:D:729:ASP:HB2	1:D:757:MET:CE	2.30	0.62
1:D:169:LEU:HB3	1:D:173:TYR:CE1	2.34	0.62
1:A:182:ALA:O	6:A:947:HOH:O	2.16	0.62
1:D:283:PRO:C	1:D:285:LYS:H	2.02	0.62
1:D:467:LEU:HD22	1:D:492:TRP:CE3	2.34	0.62
1:A:368:VAL:CG2	1:A:654:VAL:HG22	2.30	0.62
1:D:45:GLN:HE22	1:D:749:LYS:HA	1.65	0.62
1:A:694:LYS:HB3	1:A:695:PRO:CD	2.29	0.61
1:D:43:ILE:H	1:D:44:PRO:HD3	1.63	0.61
1:D:387:LEU:O	1:D:391:ILE:HG13	2.00	0.61
1:D:716:THR:HA	1:D:740:THR:O	2.00	0.61
1:D:41:LEU:HD21	1:D:755:ALA:CB	2.29	0.61
1:A:710:ARG:HG2	1:A:711:GLU:N	2.11	0.61
1:A:60:PHE:HB2	6:A:948:HOH:O	2.01	0.61
3:C:19:U:O2'	3:C:20:C:H5'	2.01	0.61
1:D:95:THR:HG22	1:D:97:ASP:H	1.64	0.61
1:D:636:TYR:HD1	1:D:676:LEU:HD13	1.65	0.61
1:A:41:LEU:HG	1:A:43:ILE:H	1.66	0.61
1:A:17:GLN:NE2	2:B:4:U:O2'	2.28	0.61
1:D:309:ASN:HB2	1:D:322:GLY:O	2.00	0.61
1:A:757:MET:HE2	1:A:758:LEU:HD23	1.82	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:170:ALA:HA	1:D:173:TYR:HD1	1.66	0.61
1:A:856:ARG:HD3	2:B:21:A:O2'	2.01	0.60
1:D:219:VAL:CG2	1:D:239:ILE:HD11	2.30	0.60
2:B:22:G:H1'	3:C:1:U:O2	2.01	0.60
1:D:694:LYS:HB2	1:D:695:PRO:HD2	1.82	0.60
1:D:358:ASN:ND2	1:D:373:LEU:H	1.99	0.60
1:A:133:ASP:O	1:A:136:ARG:HB2	2.01	0.60
1:D:120:HIS:ND1	1:D:121:PRO:HD2	2.16	0.60
1:D:732:LEU:HD23	1:D:761:LYS:HB3	1.84	0.60
1:A:828:ASN:HA	1:A:902:GLN:NE2	2.16	0.60
1:A:308:ARG:HD3	1:A:321:HIS:CE1	2.36	0.60
1:D:642:THR:O	1:D:644:PRO:HD3	2.02	0.60
1:D:183:ASP:OD2	1:D:183:ASP:N	2.32	0.60
1:A:870:ASN:HA	1:A:886:PHE:CE2	2.36	0.60
1:A:103:ILE:O	1:A:107:ILE:HG13	2.00	0.60
1:D:11:PRO:HD2	1:D:14:ILE:HD12	1.83	0.60
1:D:113:ASP:HB3	1:D:202:ILE:HD13	1.83	0.60
3:F:19:U:H2'	3:F:20:C:C6	2.36	0.60
1:D:141:PRO:HB2	1:D:144:VAL:HG23	1.84	0.60
1:D:368:VAL:HB	1:D:654:VAL:CG2	2.32	0.60
1:A:921:MET:C	1:A:923:PRO:HD3	2.22	0.60
1:D:780:LEU:O	1:D:812:LYS:HD2	2.01	0.60
1:A:499:ASP:O	1:A:500:LEU:HB2	2.02	0.60
1:A:255:LEU:HD22	1:A:260:GLN:HE22	1.66	0.59
1:D:406:LEU:HD21	1:D:482:ILE:HD13	1.82	0.59
1:D:401:LEU:CD1	1:D:461:LYS:HE2	2.33	0.59
1:D:731:LEU:HD11	1:D:738:LEU:CD1	2.32	0.59
1:A:633:VAL:HG22	1:A:677:LEU:HD12	1.84	0.59
2:B:8:C:H2'	2:B:9:U:C6	2.38	0.59
1:A:266:MET:SD	1:A:275:GLU:HB3	2.43	0.59
1:D:716:THR:HG22	1:D:740:THR:CB	2.32	0.59
1:D:559:VAL:HG23	1:D:615:VAL:CG2	2.33	0.59
1:D:243:ARG:NH1	1:D:248:SER:HB3	2.18	0.59
1:D:404:PRO:HB3	1:D:459:PHE:CE2	2.38	0.59
1:A:697:LEU:HD23	2:B:22:G:OP2	2.03	0.59
1:D:764:LYS:HG3	1:D:765:GLU:HG3	1.83	0.59
1:D:386:PRO:HG2	1:D:391:ILE:HD11	1.85	0.59
3:C:18:A:H2'	3:C:19:U:C6	2.38	0.58
3:C:21:A:H5'	3:C:22:C:P	2.42	0.58
1:D:265:ARG:NH1	1:D:400:ARG:HH21	2.01	0.58
1:A:810:GLY:CA	1:A:876:LEU:HD21	2.32	0.58
3:F:2:U:H2'	3:F:3:C:C6	2.38	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:362:LYS:HB3	1:D:368:VAL:HA	1.85	0.58
1:A:392:LEU:HD22	1:A:457:LYS:NZ	2.18	0.58
1:A:818:HIS:O	1:A:908:ARG:NH1	2.36	0.58
1:A:560:SER:O	1:A:678:LEU:HB2	2.03	0.58
1:A:642:THR:HB	1:A:643:PRO:CD	2.33	0.58
1:A:473:LYS:HE3	1:A:484:ASN:ND2	2.18	0.58
1:D:559:VAL:O	1:D:612:GLU:HA	2.04	0.58
1:D:866:ARG:HD2	1:D:897:PRO:O	2.04	0.58
1:A:895:VAL:C	1:A:897:PRO:HD2	2.24	0.58
1:A:262:MET:CE	1:A:263:ILE:H	2.04	0.58
1:D:60:PHE:CE1	1:D:62:VAL:HG22	2.38	0.58
1:D:95:THR:HB	1:D:98:GLU:HG3	1.86	0.58
1:D:829:TYR:HA	1:D:832:ASN:ND2	2.18	0.58
1:D:777:GLY:HA3	1:D:924:TYR:CD1	2.39	0.58
1:A:567:LEU:HB2	1:A:605:ILE:HD11	1.85	0.58
1:D:16:HIS:CD2	1:D:78:ALA:HB1	2.38	0.57
1:A:642:THR:O	1:A:644:PRO:HD3	2.04	0.57
1:D:870:ASN:HA	1:D:886:PHE:CE2	2.39	0.57
1:A:835:LEU:HD13	2:B:21:A:H1'	1.87	0.57
1:D:210:VAL:HG12	1:D:211:SER:H	1.69	0.57
1:A:46:LYS:HE3	2:B:14:A:O3'	2.04	0.57
1:D:539:LYS:HG3	1:D:638:SER:O	2.04	0.57
2:B:15:A:H2'	2:B:16:G:H8	1.69	0.57
1:A:332:ARG:HB2	1:A:339:ASP:OD2	2.04	0.57
1:D:315:ILE:HD11	1:D:352:CYS:SG	2.45	0.57
1:A:207:ALA:HA	1:A:210:VAL:HG23	1.84	0.57
1:D:829:TYR:HA	1:D:832:ASN:HD21	1.69	0.57
1:D:813:VAL:O	1:D:817:PHE:O	2.21	0.57
1:A:460:THR:HG23	6:A:944:HOH:O	2.04	0.57
1:D:266:MET:HA	1:D:276:CYS:O	2.05	0.57
1:A:368:VAL:HG23	1:A:369:ILE:N	2.20	0.57
1:D:255:LEU:HD13	1:D:260:GLN:HB2	1.85	0.57
1:D:98:GLU:O	1:D:102:GLU:HG2	2.03	0.57
1:D:113:ASP:HB3	1:D:202:ILE:CD1	2.35	0.57
1:D:368:VAL:HB	1:D:654:VAL:HG21	1.86	0.57
1:D:374:PRO:HG3	1:D:619:SER:HA	1.86	0.57
1:A:374:PRO:HG3	1:A:619:SER:HB3	1.87	0.57
3:F:21:A:OP2	3:F:21:A:C2	2.58	0.57
1:A:142:VAL:CG1	1:A:171:ILE:HG23	2.26	0.57
1:A:94:LEU:CB	1:A:158:ILE:HD13	2.34	0.57
1:D:94:LEU:HD12	1:D:158:ILE:HD13	1.87	0.57
1:A:658:THR:O	1:A:662:ARG:HG3	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:81:ALA:O	1:A:85:LEU:HG	2.05	0.56
1:A:694:LYS:CB	1:A:695:PRO:CD	2.83	0.56
1:A:762:LEU:HD13	1:A:930:TRP:CE3	2.40	0.56
2:B:20:A:O2'	2:B:21:A:H5''	2.05	0.56
1:D:720:PHE:HB3	1:D:779:ILE:HG21	1.86	0.56
1:A:798:ILE:O	1:A:801:MET:HG2	2.06	0.56
3:F:18:A:H2'	3:F:19:U:H6	1.70	0.56
1:D:694:LYS:HB2	1:D:695:PRO:CD	2.36	0.56
1:A:360:ILE:HD11	1:A:398:GLN:NE2	2.20	0.56
1:D:142:VAL:HG23	1:D:259:ASN:OD1	2.05	0.56
1:D:390:GLU:HA	1:D:390:GLU:OE1	2.06	0.56
1:D:467:LEU:HG	1:D:468:GLU:N	2.20	0.56
1:A:43:ILE:CD1	1:A:927:ILE:HD13	2.35	0.56
2:B:4:U:H2'	2:B:5:U:C6	2.40	0.56
1:A:603:GLU:HG3	1:A:604:PRO:HD2	1.88	0.56
1:A:400:ARG:C	1:A:401:LEU:HD23	2.26	0.56
1:A:405:ILE:CD1	1:A:458:ILE:HD11	2.35	0.56
1:D:624:ILE:HG22	1:D:624:ILE:O	2.05	0.56
1:A:46:LYS:NZ	2:B:14:A:H5''	2.20	0.56
1:D:567:LEU:HB2	1:D:605:ILE:CD1	2.35	0.56
2:B:15:A:H2'	2:B:16:G:C8	2.40	0.56
1:D:570:ASP:HB3	1:D:640:LYS:NZ	2.21	0.56
1:D:570:ASP:N	1:D:571:PRO:CD	2.51	0.56
1:A:365:ARG:NH1	1:A:365:ARG:CG	2.67	0.56
1:D:865:THR:HG22	1:D:866:ARG:N	2.21	0.56
1:D:11:PRO:HD2	1:D:14:ILE:CD1	2.35	0.56
1:D:563:TYR:CE2	1:D:608:ASN:HB2	2.41	0.56
1:D:551:GLN:O	1:D:629:THR:O	2.24	0.56
1:D:122:LEU:O	1:D:125:HIS:HB2	2.06	0.56
1:A:493:PHE:HA	1:A:496:PHE:CD1	2.41	0.56
1:A:814:LEU:HD12	1:A:876:LEU:HG	1.86	0.56
1:A:568:ALA:HA	1:A:601:SER:O	2.06	0.56
1:D:568:ALA:HB2	1:D:602:VAL:HA	1.88	0.55
1:A:719:ASP:HB3	1:A:722:CYS:HB3	1.89	0.55
1:D:369:ILE:HG21	1:D:565:LEU:CD2	2.36	0.55
1:D:401:LEU:HD13	1:D:461:LYS:HE2	1.88	0.55
1:A:725:GLY:O	1:A:729:ASP:N	2.38	0.55
1:D:222:VAL:HB	1:D:326:LEU:HB3	1.87	0.55
1:A:169:LEU:O	1:A:173:TYR:CD1	2.59	0.55
1:D:455:GLU:O	1:D:471:PRO:HD2	2.06	0.55
1:A:405:ILE:HB	1:A:458:ILE:CG1	2.32	0.55
1:A:387:LEU:O	1:A:391:ILE:HG22	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:369:ILE:CG2	1:A:565:LEU:HD11	2.35	0.55
1:D:253:LEU:HD13	1:D:325:ILE:HG12	1.87	0.55
1:A:283:PRO:O	1:A:285:LYS:N	2.39	0.55
1:A:392:LEU:O	1:A:395:PHE:HB3	2.07	0.55
1:A:852:LEU:HB2	1:A:855:PHE:CD1	2.42	0.55
1:D:606:GLU:CB	1:D:654:VAL:HG11	2.35	0.55
1:A:908:ARG:HE	1:A:911:SER:HB3	1.71	0.55
1:A:160:ASN:HD21	1:A:169:LEU:HD13	1.71	0.55
1:A:146:ALA:HB2	1:A:174:VAL:HG21	1.88	0.55
1:D:821:LEU:HD12	1:D:906:PHE:O	2.06	0.55
1:D:553:ILE:H	1:D:629:THR:CG2	2.20	0.55
1:D:345:VAL:CG1	1:D:658:THR:HG21	2.37	0.55
1:A:864:TRP:HA	1:A:868:GLN:HE22	1.72	0.55
1:A:865:THR:N	1:A:868:GLN:HE21	2.04	0.55
1:A:360:ILE:HD11	1:A:398:GLN:HE22	1.72	0.55
1:A:27:VAL:HG11	1:A:70:LYS:HE2	1.89	0.55
1:A:132:ARG:NH2	1:A:257:ASP:OD1	2.39	0.55
1:D:570:ASP:O	1:D:572:GLU:HG3	2.07	0.55
1:D:829:TYR:OH	1:D:853:PRO:HG2	2.07	0.55
1:A:365:ARG:HG3	1:A:365:ARG:NH1	2.18	0.55
1:D:103:ILE:HG23	1:D:152:ILE:HD12	1.87	0.55
1:D:496:PHE:CD2	1:D:496:PHE:N	2.74	0.55
2:B:13:C:O2'	2:B:14:A:H5'	2.07	0.55
1:D:168:PHE:HD2	1:D:282:ILE:HG23	1.71	0.54
1:D:12:LYS:HD2	1:D:82:LEU:HD12	1.90	0.54
1:D:568:ALA:CB	1:D:601:SER:O	2.53	0.54
1:D:392:LEU:HD13	1:D:490:LEU:HG	1.89	0.54
1:D:710:ARG:NH1	1:D:734:TYR:HB2	2.22	0.54
1:A:851:GLN:O	1:A:852:LEU:HG	2.08	0.54
1:A:358:ASN:HA	1:A:373:LEU:HB2	1.90	0.54
1:A:558:VAL:CG1	1:A:681:LYS:HD3	2.37	0.54
1:D:569:VAL:HG22	1:D:668:ARG:O	2.08	0.54
1:D:88:ARG:CB	1:D:89:PRO:HD2	2.37	0.54
1:A:365:ARG:HD2	1:A:385:GLY:HA3	1.89	0.54
1:A:537:GLU:HB3	1:A:641:MET:HE2	1.90	0.54
1:A:855:PHE:HZ	1:A:862:PHE:HA	1.73	0.54
1:D:829:TYR:HB2	1:D:863:GLU:O	2.07	0.54
1:D:736:THR:HG22	1:D:737:SER:N	2.23	0.54
1:D:11:PRO:HB2	1:D:75:GLN:HE22	1.72	0.54
1:D:17:GLN:HG3	1:D:17:GLN:O	2.07	0.54
1:A:374:PRO:HG3	1:A:619:SER:CB	2.38	0.54
1:A:171:ILE:HD13	1:A:282:ILE:HD13	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:255:LEU:HD13	1:A:260:GLN:HB3	1.90	0.54
1:A:168:PHE:CE2	1:A:282:ILE:HA	2.42	0.54
1:A:62:VAL:HG11	1:A:80:LEU:HB2	1.90	0.54
1:A:700:GLN:HB2	1:A:889:VAL:HG11	1.90	0.54
1:D:571:PRO:HD3	1:D:670:CYS:HB2	1.88	0.54
1:D:121:PRO:HD3	1:D:333:TRP:CD2	2.43	0.54
1:D:895:VAL:HG12	1:D:896:GLU:N	2.22	0.54
1:D:627:GLU:O	1:D:630:GLN:HG2	2.07	0.54
1:D:257:ASP:N	1:D:260:GLN:HE21	2.03	0.54
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.73	0.54
1:A:871:GLN:O	1:A:875:LYS:HG3	2.08	0.54
1:A:12:LYS:HB3	1:A:78:ALA:CB	2.39	0.53
2:B:10:C:H2'	2:B:11:U:C6	2.43	0.53
1:A:392:LEU:HD21	1:A:404:PRO:HG3	1.90	0.53
1:D:704:TYR:HH	1:D:887:SER:HG	1.55	0.53
1:A:12:LYS:HE3	1:A:79:GLU:CD	2.29	0.53
1:D:265:ARG:N	1:D:318:GLN:HE22	1.98	0.53
1:D:18:LYS:HD3	3:F:19:U:O2'	2.08	0.53
1:D:392:LEU:HD21	1:D:459:PHE:HZ	1.74	0.53
1:D:857:ASN:OD1	3:F:2:U:H4'	2.08	0.53
1:A:23:ALA:HB2	1:A:57:LEU:CD1	2.38	0.53
1:D:685:GLU:HG3	1:D:686:GLU:H	1.73	0.53
1:D:257:ASP:OD1	1:D:258:GLY:N	2.42	0.53
1:D:188:SER:O	1:D:190:HIS:N	2.41	0.53
1:D:551:GLN:O	1:D:553:ILE:HG13	2.08	0.53
1:D:896:GLU:HB2	1:D:897:PRO:HD3	1.91	0.53
1:D:194:ARG:HH12	1:D:198:TYR:CA	2.20	0.53
1:A:677:LEU:HD13	1:A:678:LEU:N	2.23	0.53
1:A:278:LEU:HD23	1:A:320:ILE:HD12	1.90	0.53
1:D:39:PRO:HD2	1:D:759:HIS:CD2	2.44	0.53
1:D:201:GLU:HA	1:D:204:GLU:OE1	2.09	0.53
1:D:119:GLU:OE1	1:D:119:GLU:HA	2.08	0.53
1:D:828:ASN:HA	1:D:902:GLN:HE21	1.74	0.53
1:D:146:ALA:HB2	1:D:174:VAL:HG21	1.91	0.53
1:A:246:LEU:HD22	1:A:261:VAL:HG11	1.90	0.53
3:F:19:U:H2'	3:F:20:C:O4'	2.09	0.53
1:A:392:LEU:HA	1:A:490:LEU:HD21	1.91	0.53
1:D:818:HIS:N	1:D:819:PRO:HD2	2.11	0.53
1:D:50:LEU:CD2	1:D:68:LYS:HG3	2.39	0.53
1:A:160:ASN:ND2	1:A:169:LEU:HD13	2.24	0.53
1:A:407:SER:HB2	1:A:456:VAL:HB	1.90	0.53
1:A:8:THR:O	1:A:10:THR:N	2.42	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:813:VAL:HG11	1:A:822:LEU:HD11	1.92	0.52
1:D:357:PRO:HB3	1:D:490:LEU:HD22	1.90	0.52
1:A:365:ARG:NH2	1:A:612:GLU:O	2.42	0.52
1:A:368:VAL:HG21	1:A:654:VAL:HG22	1.90	0.52
1:D:655:GLY:HA3	1:D:661:ILE:CD1	2.38	0.52
1:A:642:THR:HB	1:A:643:PRO:HD2	1.90	0.52
1:A:793:THR:CG2	1:A:795:LEU:HG	2.39	0.52
1:A:278:LEU:HD21	1:A:312:ALA:HB1	1.90	0.52
1:D:375:PHE:HA	1:D:491:LEU:HD11	1.92	0.52
1:D:123:GLY:HA2	1:D:126:LEU:HB2	1.91	0.52
1:A:221:ALA:O	1:A:234:LEU:HD12	2.09	0.52
1:D:829:TYR:HD1	1:D:832:ASN:ND2	2.04	0.52
1:D:265:ARG:NH1	1:D:400:ARG:HE	2.07	0.52
1:D:14:ILE:CD1	2:E:5:U:H1'	2.39	0.52
1:A:267:PHE:CE1	1:A:315:ILE:HG22	2.45	0.52
1:D:359:GLY:O	1:D:363:ILE:HG13	2.09	0.52
1:D:621:ASN:HD21	1:D:623:HIS:HB2	1.73	0.52
1:D:679:GLY:O	1:D:680:VAL:HG23	2.10	0.52
1:A:318:GLN:HG3	1:A:400:ARG:NH2	2.24	0.52
1:A:391:ILE:HG23	1:A:490:LEU:HD11	1.90	0.52
1:D:789:VAL:O	1:D:819:PRO:HA	2.10	0.52
1:A:155:ARG:O	1:A:159:ILE:HG13	2.10	0.52
1:D:132:ARG:O	1:D:137:CYS:HB2	2.10	0.52
2:E:14:A:H2'	2:E:15:A:C8	2.44	0.52
1:D:570:ASP:O	1:D:572:GLU:N	2.39	0.52
1:D:358:ASN:HD21	1:D:373:LEU:H	1.58	0.52
1:D:778:SER:HA	5:D:951:SAH:N1	2.24	0.52
2:B:4:U:H5'	6:B:23:HOH:O	2.10	0.52
1:D:176:LYS:O	1:D:180:LYS:HG3	2.10	0.51
1:D:121:PRO:HD3	1:D:333:TRP:CE2	2.45	0.51
1:A:621:ASN:HD22	1:A:622:PRO:N	2.08	0.51
1:A:353:CYS:O	1:A:359:GLY:HA3	2.09	0.51
1:D:459:PHE:CB	1:D:466:VAL:HB	2.41	0.51
1:A:895:VAL:HG12	1:A:897:PRO:CD	2.37	0.51
1:D:18:LYS:HD3	3:F:20:C:H5'	1.92	0.51
1:A:23:ALA:HA	1:A:56:GLN:O	2.09	0.51
1:D:867:GLU:HG3	1:D:868:GLN:N	2.25	0.51
1:A:35:GLN:NE2	1:A:47:GLY:HA3	2.25	0.51
1:A:829:TYR:OH	1:A:853:PRO:O	2.26	0.51
1:A:828:ASN:CG	1:A:866:ARG:HG3	2.30	0.51
1:D:921:MET:O	1:D:923:PRO:HD3	2.11	0.51
1:A:389:ARG:O	1:A:392:LEU:HB3	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:704:TYR:CD2	1:A:903:ILE:HD13	2.46	0.51
1:A:886:PHE:CD1	1:A:886:PHE:N	2.78	0.51
1:A:160:ASN:ND2	1:A:173:TYR:OH	2.42	0.51
1:D:921:MET:O	1:D:921:MET:HG2	2.10	0.51
1:A:378:THR:CG2	1:A:382:ASN:HD22	2.24	0.51
1:A:43:ILE:HG22	1:A:44:PRO:N	2.25	0.51
1:D:406:LEU:HD11	1:D:482:ILE:HG23	1.91	0.51
1:D:373:LEU:HD12	1:D:374:PRO:CD	2.41	0.51
1:A:57:LEU:O	1:A:58:PRO:C	2.49	0.51
1:D:701:ARG:NH1	1:D:796:GLU:CG	2.73	0.51
1:D:224:ILE:HG22	1:D:309:ASN:HD21	1.76	0.51
1:D:479:ASN:O	1:D:483:GLN:HG2	2.11	0.51
1:D:401:LEU:HD13	1:D:461:LYS:CG	2.41	0.50
1:D:496:PHE:HB3	1:D:524:PHE:CD1	2.46	0.50
1:D:48:PRO:HD2	1:D:48:PRO:O	2.12	0.50
1:D:780:LEU:CD1	1:D:805:GLN:HB3	2.41	0.50
1:A:558:VAL:HG12	1:A:681:LYS:HB2	1.92	0.50
1:D:605:ILE:HD13	1:D:651:ILE:HG23	1.94	0.50
1:A:258:GLY:HA2	1:A:261:VAL:HG23	1.94	0.50
1:D:818:HIS:N	1:D:819:PRO:CD	2.69	0.50
1:A:7:HIS:C	1:A:9:PRO:HD2	2.32	0.50
1:D:819:PRO:HB2	1:D:821:LEU:O	2.12	0.50
1:A:697:LEU:HD23	2:B:22:G:P	2.50	0.50
1:A:12:LYS:O	1:A:15:ILE:HB	2.11	0.50
1:A:865:THR:N	1:A:868:GLN:NE2	2.55	0.50
1:A:22:LYS:HG3	1:A:22:LYS:O	2.10	0.50
1:A:920:SER:O	1:A:921:MET:HG3	2.11	0.50
1:D:47:GLY:HA2	2:E:14:A:O2'	2.11	0.50
3:F:8:G:H2'	3:F:9:C:C6	2.46	0.50
1:D:706:LEU:HD11	1:D:730:SER:HB2	1.94	0.50
1:A:369:ILE:HG21	1:A:565:LEU:CD1	2.41	0.50
1:D:643:PRO:O	1:D:644:PRO:C	2.48	0.50
1:A:769:VAL:HG12	1:A:770:LYS:N	2.27	0.50
1:D:396:CYS:O	1:D:401:LEU:HB2	2.11	0.50
1:D:553:ILE:HG22	1:D:557:SER:HB2	1.94	0.50
1:D:25:TYR:CD2	1:D:55:LEU:HD13	2.47	0.50
1:A:567:LEU:HB2	1:A:605:ILE:CD1	2.42	0.50
1:A:706:LEU:HA	1:A:709:ILE:HD12	1.94	0.50
1:D:640:LYS:HD2	1:D:670:CYS:SG	2.51	0.50
1:D:262:MET:HE3	1:D:263:ILE:H	1.76	0.50
1:D:103:ILE:O	1:D:107:ILE:HG13	2.12	0.50
1:D:621:ASN:ND2	1:D:624:ILE:HG13	2.23	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:7:HIS:NE2	3:C:17:A:H4'	2.27	0.49
1:D:770:LYS:O	1:D:931:LYS:HA	2.12	0.49
1:D:403:GLU:HG3	1:D:404:PRO:HD2	1.93	0.49
1:D:246:LEU:HD22	1:D:261:VAL:HB	1.92	0.49
1:A:694:LYS:HB3	1:A:695:PRO:HD3	1.93	0.49
1:A:188:SER:C	1:A:190:HIS:H	2.15	0.49
1:A:487:LEU:O	1:A:491:LEU:HG	2.12	0.49
1:D:42:ALA:C	1:D:44:PRO:HD3	2.33	0.49
1:D:567:LEU:O	1:D:568:ALA:HB2	2.12	0.49
1:A:18:LYS:CE	3:C:19:U:H4'	2.42	0.49
1:D:262:MET:HA	1:D:282:ILE:HD11	1.94	0.49
1:A:396:CYS:SG	1:A:459:PHE:CZ	3.02	0.49
1:D:16:HIS:HD2	1:D:78:ALA:HB1	1.78	0.49
1:A:87:ILE:O	1:A:91:ASN:HB2	2.13	0.49
1:A:329:VAL:HG12	1:A:340:TYR:CB	2.43	0.49
1:A:798:ILE:HG13	1:A:799:GLU:N	2.28	0.49
1:A:315:ILE:HD11	1:A:348:PHE:HE1	1.77	0.49
1:A:565:LEU:HD21	1:A:673:TYR:CZ	2.48	0.49
1:A:803:GLU:HG2	1:A:862:PHE:CD2	2.48	0.49
1:A:43:ILE:CG2	1:A:44:PRO:CD	2.91	0.49
1:A:265:ARG:HG2	1:A:266:MET:N	2.28	0.49
1:A:642:THR:CB	1:A:643:PRO:CD	2.91	0.49
1:D:704:TYR:CE2	1:D:903:ILE:HD11	2.47	0.49
1:D:43:ILE:HD11	1:D:927:ILE:CG1	2.43	0.49
1:A:358:ASN:ND2	1:A:373:LEU:H	2.11	0.49
1:A:106:ARG:HD3	1:A:151:LYS:HD2	1.95	0.48
1:D:242:ASN:OD1	1:D:243:ARG:N	2.46	0.48
1:A:265:ARG:HG2	1:A:266:MET:H	1.76	0.48
1:A:401:LEU:CD2	1:A:461:LYS:HB2	2.26	0.48
1:D:757:MET:HG3	1:D:758:LEU:H	1.73	0.48
1:D:467:LEU:HD22	1:D:492:TRP:HE3	1.76	0.48
1:D:887:SER:O	1:D:903:ILE:HG12	2.13	0.48
1:D:462:SER:O	1:D:463:GLN:HB2	2.13	0.48
1:D:287:LEU:O	1:D:291:SER:HB3	2.13	0.48
1:A:357:PRO:HB3	1:A:490:LEU:HD22	1.95	0.48
1:D:780:LEU:HD21	1:D:801:MET:SD	2.53	0.48
1:A:700:GLN:HB2	1:A:889:VAL:CG1	2.44	0.48
1:A:392:LEU:CD2	1:A:404:PRO:HG3	2.44	0.48
1:A:110:ILE:HG23	1:A:115:PHE:CE2	2.48	0.48
1:D:189:PRO:O	1:D:259:ASN:ND2	2.46	0.48
1:D:138:GLY:O	1:D:193:ARG:HG3	2.12	0.48
1:D:820:LYS:HG2	1:D:908:ARG:NH2	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:832:ASN:HB3	1:D:856:ARG:HE	1.79	0.48
1:D:357:PRO:CB	1:D:490:LEU:HD22	2.44	0.48
1:D:278:LEU:HD22	1:D:316:CYS:SG	2.54	0.48
2:E:15:A:H2'	2:E:16:G:C8	2.49	0.48
1:D:567:LEU:HD12	1:D:670:CYS:O	2.13	0.48
1:A:779:ILE:HD12	1:A:809:PHE:CE1	2.48	0.48
1:A:905:ILE:HD12	1:A:905:ILE:N	2.29	0.48
1:A:907:ARG:HG3	6:A:952:HOH:O	2.13	0.48
1:D:87:ILE:HG22	1:D:87:ILE:O	2.13	0.48
2:B:19:A:O2'	2:B:20:A:H5'	2.14	0.48
1:A:170:ALA:O	1:A:174:VAL:HG23	2.13	0.48
1:D:181:LEU:HD11	1:D:184:TYR:CD1	2.49	0.48
1:D:107:ILE:HG22	1:D:185:ILE:HD13	1.96	0.48
1:A:23:ALA:HB2	1:A:57:LEU:HD12	1.95	0.48
1:D:50:LEU:HB3	1:D:66:VAL:CG1	2.43	0.48
1:A:43:ILE:HD11	1:A:927:ILE:HD13	1.96	0.48
1:D:188:SER:O	1:D:189:PRO:C	2.52	0.48
2:E:11:U:H2'	2:E:12:G:H8	1.78	0.48
1:D:852:LEU:N	1:D:853:PRO:CD	2.77	0.48
1:A:822:LEU:HD23	1:A:823:ILE:N	2.29	0.48
1:D:315:ILE:HG23	1:D:351:ILE:HG21	1.95	0.48
1:A:35:GLN:HE22	1:A:47:GLY:HA3	1.79	0.47
1:A:380:LYS:O	1:A:380:LYS:HG2	2.14	0.47
1:D:43:ILE:HG13	1:D:927:ILE:HG23	1.96	0.47
2:E:9:U:C2	3:F:13:G:N2	2.82	0.47
3:F:19:U:O2'	3:F:20:C:C5'	2.61	0.47
1:D:345:VAL:HG12	1:D:658:THR:HG21	1.96	0.47
1:D:825:SER:HA	1:D:903:ILE:HG22	1.96	0.47
1:A:462:SER:O	1:A:463:GLN:HB2	2.13	0.47
1:A:467:LEU:HD22	1:A:492:TRP:HE3	1.79	0.47
1:A:461:LYS:HE2	1:A:466:VAL:HG21	1.97	0.47
1:D:71:LYS:HD2	2:E:6:C:OP2	2.14	0.47
1:A:834:ILE:HG23	1:A:835:LEU:N	2.29	0.47
1:D:552:SER:CA	1:D:629:THR:O	2.61	0.47
1:A:59:GLU:HB3	1:A:60:PHE:HD1	1.79	0.47
1:A:467:LEU:HD13	1:A:492:TRP:CE3	2.50	0.47
1:D:642:THR:HB	1:D:643:PRO:HD3	1.97	0.47
1:A:680:VAL:C	1:A:681:LYS:HD2	2.35	0.47
3:C:10:A:O2'	3:C:11:G:H5'	2.14	0.47
1:A:365:ARG:NH2	1:A:384:ARG:HB3	2.29	0.47
1:A:538:SER:O	1:A:639:PHE:HB2	2.14	0.47
1:D:272:CYS:HB2	1:D:351:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:709:ILE:O	1:A:712:SER:O	2.33	0.47
1:D:856:ARG:HB3	2:E:21:A:O2'	2.13	0.47
1:D:392:LEU:HD11	1:D:459:PHE:CZ	2.50	0.47
1:A:693:PHE:O	1:A:694:LYS:C	2.51	0.47
1:A:160:ASN:O	1:A:163:VAL:HG23	2.15	0.47
1:A:382:ASN:HD21	1:A:684:SER:HB2	1.79	0.47
1:A:383:TRP:HH2	1:A:487:LEU:HD21	1.79	0.47
1:A:821:LEU:HD11	1:A:905:ILE:CG2	2.45	0.47
1:A:22:LYS:HE2	1:A:22:LYS:HA	1.97	0.47
1:D:210:VAL:CG1	1:D:211:SER:N	2.77	0.47
1:D:795:LEU:HA	1:D:825:SER:HB3	1.95	0.47
1:A:739:GLN:HE22	1:A:770:LYS:NZ	2.12	0.47
1:D:382:ASN:O	1:D:614:GLU:HG3	2.14	0.47
1:A:190:HIS:HA	1:A:257:ASP:OD2	2.15	0.47
1:A:383:TRP:CH2	1:A:487:LEU:HD21	2.50	0.47
2:E:10:C:O2'	2:E:11:U:H5'	2.15	0.47
1:A:745:ASP:HB3	1:A:751:LEU:HD21	1.96	0.47
1:D:691:ALA:CB	2:E:20:A:H5"	2.45	0.47
1:D:210:VAL:CG1	1:D:211:SER:H	2.28	0.47
1:A:43:ILE:HD12	1:A:927:ILE:HD13	1.97	0.47
1:D:764:LYS:HG3	1:D:765:GLU:N	2.30	0.47
1:D:401:LEU:HD22	1:D:461:LYS:CD	2.33	0.46
1:A:392:LEU:HD11	1:A:459:PHE:CE1	2.45	0.46
2:B:8:C:H2'	2:B:9:U:H6	1.80	0.46
1:A:160:ASN:ND2	1:A:162:SER:OG	2.47	0.46
1:A:22:LYS:HG2	1:A:58:PRO:HG3	1.97	0.46
1:D:932:LYS:C	1:D:932:LYS:HD3	2.35	0.46
1:A:365:ARG:O	1:A:366:GLN:HB2	2.15	0.46
1:A:199:PRO:HD2	1:A:202:ILE:HD12	1.96	0.46
1:D:181:LEU:CG	1:D:184:TYR:HB2	2.42	0.46
1:A:223:TYR:HB2	1:A:235:ASP:HB2	1.97	0.46
1:A:59:GLU:HB3	1:A:60:PHE:CD1	2.51	0.46
1:A:557:SER:HB2	1:A:681:LYS:O	2.15	0.46
1:D:599:GLU:HG2	1:D:600:SER:N	2.31	0.46
1:D:190:HIS:O	1:D:259:ASN:HB2	2.15	0.46
1:A:486:SER:O	1:A:490:LEU:HG	2.16	0.46
1:A:110:ILE:CG2	1:A:126:LEU:HD11	2.44	0.46
1:A:46:LYS:CE	2:B:14:A:H4'	2.45	0.46
1:A:797:VAL:O	1:A:800:HIS:HB2	2.16	0.46
1:D:642:THR:N	1:D:643:PRO:CD	2.78	0.46
1:A:372:GLN:O	1:A:374:PRO:HD3	2.15	0.46
1:D:54:HIS:ND1	1:D:63:VAL:HG22	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:199:PRO:HG2	1:D:202:ILE:HD12	1.98	0.46
1:A:106:ARG:O	1:A:110:ILE:HG13	2.16	0.46
1:D:741:ILE:C	1:D:742:ILE:HG13	2.35	0.46
1:A:931:LYS:HG3	1:A:931:LYS:O	2.16	0.46
1:A:305:VAL:HG12	1:A:306:LYS:N	2.31	0.46
1:D:396:CYS:O	1:D:399:HIS:O	2.33	0.46
1:D:55:LEU:HD23	1:D:81:ALA:HB2	1.97	0.46
1:A:870:ASN:HA	1:A:886:PHE:HE2	1.78	0.46
1:D:705:ALA:O	1:D:709:ILE:HG13	2.16	0.46
1:A:689:GLU:OE2	3:C:3:C:H1'	2.16	0.46
1:A:636:TYR:HA	1:A:675:ILE:O	2.16	0.46
1:D:12:LYS:HD2	1:D:79:GLU:HA	1.97	0.46
1:A:221:ALA:HB1	1:A:326:LEU:O	2.16	0.46
1:D:232:VAL:HG23	1:D:311:ARG:HH21	1.79	0.45
1:A:796:GLU:OE2	5:A:951:SAH:HB2	2.16	0.45
1:A:315:ILE:HD11	1:A:348:PHE:CE1	2.51	0.45
1:D:773:THR:C	1:D:774:LEU:HD23	2.36	0.45
1:D:282:ILE:HG23	1:D:283:PRO:HD2	1.98	0.45
2:B:14:A:O2'	2:B:15:A:H5'	2.17	0.45
1:D:265:ARG:HH12	1:D:400:ARG:CZ	2.29	0.45
1:A:368:VAL:CG2	1:A:654:VAL:CG2	2.94	0.45
1:A:565:LEU:HD21	1:A:673:TYR:CD2	2.52	0.45
1:D:107:ILE:HG22	1:D:185:ILE:CD1	2.46	0.45
1:A:17:GLN:NE2	2:B:4:U:H4'	2.31	0.45
1:A:237:LEU:CD2	1:A:249:ILE:HG12	2.46	0.45
1:D:783:ASP:H	1:D:817:PHE:HZ	1.65	0.45
1:A:283:PRO:C	1:A:285:LYS:H	2.20	0.45
1:D:524:PHE:CD1	1:D:524:PHE:O	2.70	0.45
1:A:271:SER:HB3	1:A:351:ILE:HA	1.98	0.45
1:A:714:ALA:O	1:A:737:SER:O	2.34	0.45
1:D:100:ARG:O	1:D:104:VAL:HG23	2.16	0.45
1:D:104:VAL:HG22	1:D:177:ALA:HB1	1.99	0.45
1:D:826:THR:HG23	1:D:827:PRO:HD2	1.98	0.45
1:D:88:ARG:HG2	1:D:89:PRO:CD	2.38	0.45
1:A:46:LYS:HZ1	2:B:14:A:H5''	1.81	0.45
1:D:700:GLN:HB3	1:D:889:VAL:HG11	1.97	0.45
1:D:628:VAL:HG23	1:D:675:ILE:HD12	1.98	0.45
1:A:231:VAL:HG12	1:A:232:VAL:N	2.32	0.45
1:A:12:LYS:HB3	1:A:78:ALA:HB1	1.99	0.45
1:D:116:LEU:HG	1:D:206:LEU:CD1	2.36	0.45
1:A:255:LEU:CD1	1:A:281:GLU:HB2	2.40	0.45
1:D:553:ILE:HG22	1:D:554:THR:N	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:821:LEU:HD11	1:A:905:ILE:HG23	1.99	0.45
1:A:822:LEU:HB3	1:A:906:PHE:HB2	1.99	0.45
1:A:169:LEU:O	1:A:173:TYR:HD1	1.97	0.45
1:A:379:THR:C	1:A:381:SER:H	2.20	0.45
1:D:717:LEU:HD12	1:D:791:ILE:O	2.16	0.45
3:C:13:G:H2'	3:C:14:A:C8	2.52	0.45
1:D:792:GLY:O	1:D:822:LEU:HD12	2.16	0.45
1:A:719:ASP:OD2	1:A:727:LEU:HD23	2.17	0.45
1:A:727:LEU:CD2	1:A:793:THR:HG21	2.46	0.45
1:D:11:PRO:HG3	2:E:5:U:O2'	2.17	0.45
1:D:775:TYR:HB3	1:D:924:TYR:HB3	1.97	0.45
1:D:696:PRO:O	1:D:699:LYS:HB2	2.17	0.45
1:A:108:LYS:CD	1:A:181:LEU:HD21	2.43	0.45
1:A:235:ASP:OD1	1:A:252:ARG:HD2	2.18	0.45
2:E:20:A:O2'	2:E:21:A:H5''	2.17	0.44
1:D:401:LEU:HD11	1:D:461:LYS:HE2	1.99	0.44
1:A:896:GLU:N	1:A:897:PRO:HD2	2.31	0.44
1:D:267:PHE:CE1	1:D:315:ILE:HG22	2.52	0.44
1:D:169:LEU:O	1:D:173:TYR:CD1	2.70	0.44
1:D:733:ASP:OD1	1:D:761:LYS:HE2	2.17	0.44
1:D:358:ASN:ND2	1:D:373:LEU:N	2.65	0.44
1:D:278:LEU:CD2	1:D:320:ILE:HG13	2.46	0.44
1:D:59:GLU:HB3	1:D:60:PHE:HD2	1.82	0.44
1:A:347:SER:O	1:A:351:ILE:HG13	2.18	0.44
1:D:570:ASP:HB3	1:D:640:LYS:HZ3	1.81	0.44
1:D:396:CYS:HA	1:D:401:LEU:HG	1.99	0.44
1:D:283:PRO:C	1:D:285:LYS:N	2.68	0.44
1:D:127:ARG:NH1	1:D:336:ASP:OD1	2.50	0.44
1:A:219:VAL:HG23	1:A:239:ILE:HD13	1.99	0.44
1:D:47:GLY:HA2	2:E:14:A:HO2'	1.80	0.44
1:A:621:ASN:ND2	1:A:621:ASN:C	2.70	0.44
1:D:745:ASP:O	1:D:776:ASP:HA	2.18	0.44
1:A:113:ASP:HB3	1:A:202:ILE:CD1	2.46	0.44
1:D:648:GLU:OE1	1:D:665:LEU:HD13	2.18	0.44
1:D:487:LEU:HD23	1:D:491:LEU:HD12	2.00	0.44
1:D:556:GLY:HA3	1:D:683:PRO:HB3	1.99	0.44
1:A:837:ARG:O	1:A:838:SER:HB3	2.17	0.44
1:A:759:HIS:O	1:A:763:ASN:ND2	2.51	0.44
2:B:7:U:O2	2:B:7:U:H2'	2.18	0.44
1:A:48:PRO:HD3	2:B:15:A:O2'	2.18	0.44
1:A:222:VAL:CG1	1:A:223:TYR:N	2.81	0.44
1:D:778:SER:C	1:D:780:LEU:H	2.20	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:11:U:O2'	2:B:12:G:H5'	2.17	0.44
1:A:94:LEU:HB3	1:A:158:ILE:HG21	2.00	0.44
1:D:559:VAL:HG23	1:D:615:VAL:HG22	1.99	0.44
3:C:19:U:H2'	3:C:20:C:H6	1.83	0.44
1:D:172:SER:O	1:D:176:LYS:HG3	2.18	0.44
1:A:8:THR:N	1:A:9:PRO:CD	2.81	0.43
1:D:262:MET:CE	1:D:263:ILE:H	2.31	0.43
1:A:696:PRO:HD2	1:A:699:LYS:HD2	2.00	0.43
1:D:110:ILE:HD13	1:D:122:LEU:HD13	2.00	0.43
1:A:188:SER:C	1:A:190:HIS:N	2.70	0.43
3:C:11:G:H2'	3:C:12:A:H8	1.83	0.43
1:D:121:PRO:O	1:D:124:ALA:HB3	2.18	0.43
1:A:467:LEU:HD22	1:A:492:TRP:CE3	2.53	0.43
1:A:50:LEU:HD23	1:A:50:LEU:N	2.32	0.43
1:D:153:ASN:O	1:D:157:LYS:HG3	2.18	0.43
1:A:120:HIS:O	1:A:121:PRO:C	2.56	0.43
1:A:318:GLN:CG	1:A:400:ARG:HH22	2.24	0.43
1:D:461:LYS:HG3	1:D:466:VAL:CG2	2.41	0.43
1:D:164:GLU:CB	1:D:400:ARG:HH12	2.24	0.43
2:B:16:G:O2'	2:B:17:C:H5'	2.19	0.43
1:D:652:LEU:HD23	1:D:661:ILE:HG21	1.99	0.43
2:E:4:U:H2'	2:E:5:U:C6	2.53	0.43
1:A:217:ARG:HD3	1:A:340:TYR:CE2	2.53	0.43
1:D:695:PRO:HG2	1:D:700:GLN:NE2	2.33	0.43
1:A:356:SER:O	1:A:360:ILE:HG13	2.18	0.43
1:D:496:PHE:N	1:D:496:PHE:HD2	2.14	0.43
1:A:407:SER:HB2	1:A:456:VAL:O	2.18	0.43
1:A:121:PRO:HB2	1:A:148:VAL:CG1	2.48	0.43
1:D:389:ARG:HD2	1:D:389:ARG:O	2.18	0.43
1:D:406:LEU:HD13	1:D:457:LYS:CE	2.44	0.43
1:D:391:ILE:HB	1:D:490:LEU:HD11	2.00	0.43
1:D:257:ASP:N	1:D:260:GLN:NE2	2.65	0.43
1:D:824:VAL:HG12	1:D:825:SER:N	2.33	0.43
1:D:126:LEU:O	1:D:129:ALA:HB3	2.18	0.43
3:C:10:A:H2'	3:C:11:G:C8	2.53	0.43
1:A:71:LYS:HE2	2:B:6:C:P	2.58	0.43
1:D:832:ASN:O	1:D:836:GLN:HG3	2.18	0.43
1:D:234:LEU:HB2	1:D:345:VAL:HG23	1.99	0.43
1:D:227:ILE:HB	1:D:230:GLU:OE2	2.18	0.43
1:D:667:GLU:O	1:D:669:PRO:HD3	2.19	0.43
1:A:57:LEU:CG	1:A:58:PRO:HD2	2.48	0.43
1:A:920:SER:C	1:A:921:MET:HG3	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:680:VAL:HG12	1:A:681:LYS:N	2.34	0.43
1:A:785:ARG:NH2	1:A:922:GLN:HB3	2.34	0.43
1:D:537:GLU:HA	1:D:641:MET:CE	2.31	0.43
1:D:265:ARG:HH12	1:D:400:ARG:NH2	2.17	0.43
1:D:895:VAL:HG12	1:D:896:GLU:H	1.83	0.43
1:D:732:LEU:HD21	1:D:762:LEU:HD23	2.00	0.43
1:A:694:LYS:CB	1:A:695:PRO:HD2	2.48	0.43
1:D:158:ILE:HG13	1:D:158:ILE:H	1.66	0.43
1:D:657:ASP:CG	1:D:660:ARG:HE	2.22	0.43
1:D:12:LYS:CD	1:D:82:LEU:HD12	2.48	0.43
1:D:69:LYS:HB2	1:D:72:ASP:HB2	2.00	0.43
1:D:329:VAL:HG12	1:D:340:TYR:HB3	2.00	0.43
1:D:314:TYR:CE2	1:D:355:MET:HG3	2.54	0.43
1:A:11:PRO:O	1:A:12:LYS:C	2.57	0.43
1:A:624:ILE:O	1:A:628:VAL:HG23	2.18	0.43
1:D:492:TRP:CD1	1:D:495:LYS:HD3	2.53	0.43
1:D:742:ILE:HD13	1:D:786:LEU:CD2	2.48	0.43
1:D:92:ASP:O	1:D:94:LEU:HG	2.19	0.43
1:A:160:ASN:HB2	1:A:173:TYR:OH	2.19	0.43
1:A:120:HIS:HD2	1:A:122:LEU:HB2	1.84	0.43
1:D:729:ASP:HB2	1:D:757:MET:HE3	1.98	0.43
1:A:834:ILE:CG2	1:A:835:LEU:N	2.82	0.43
1:A:742:ILE:HG21	1:A:786:LEU:CD2	2.49	0.43
1:A:126:LEU:HD23	1:A:140:VAL:CG2	2.42	0.43
1:D:762:LEU:HD13	1:D:930:TRP:CE3	2.54	0.43
1:D:326:LEU:HG	1:D:343:VAL:HG11	2.01	0.43
1:A:796:GLU:HB3	1:A:825:SER:OG	2.19	0.42
1:D:11:PRO:HB2	1:D:75:GLN:NE2	2.34	0.42
1:A:120:HIS:O	1:A:122:LEU:N	2.52	0.42
1:D:329:VAL:HG12	1:D:340:TYR:CB	2.49	0.42
1:A:741:ILE:HG13	1:A:772:ALA:HA	2.00	0.42
1:A:10:THR:CG2	1:A:90:GLN:HG2	2.45	0.42
1:D:624:ILE:O	1:D:624:ILE:CG2	2.66	0.42
1:D:255:LEU:HD13	1:D:260:GLN:CB	2.48	0.42
1:A:695:PRO:HA	1:A:696:PRO:HD3	1.88	0.42
1:A:225:PRO:HG3	1:A:230:GLU:HG2	2.01	0.42
1:A:250:ALA:HB2	1:A:261:VAL:CG2	2.49	0.42
2:B:20:A:O2'	2:B:21:A:C5'	2.68	0.42
1:A:127:ARG:CG	1:A:206:LEU:HD21	2.42	0.42
1:A:864:TRP:CA	1:A:868:GLN:NE2	2.78	0.42
5:A:951:SAH:HG2	2:B:22:G:N2	2.34	0.42
1:A:924:TYR:CD2	1:A:924:TYR:N	2.86	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:818:HIS:HA	1:D:819:PRO:HD2	1.34	0.42
1:D:632:THR:C	1:D:677:LEU:HD23	2.39	0.42
1:D:12:LYS:HE3	1:D:79:GLU:OE2	2.19	0.42
1:A:796:GLU:CD	1:A:796:GLU:O	2.58	0.42
2:B:4:U:O2'	2:B:5:U:H5'	2.19	0.42
1:D:94:LEU:HD12	1:D:158:ILE:CD1	2.49	0.42
1:A:8:THR:HG22	1:A:8:THR:O	2.19	0.42
1:D:262:MET:CA	1:D:282:ILE:HD11	2.49	0.42
1:D:895:VAL:CG1	1:D:897:PRO:HD2	2.43	0.42
1:D:742:ILE:HD13	1:D:786:LEU:HD23	2.01	0.42
1:A:795:LEU:C	1:A:796:GLU:HG3	2.40	0.42
1:D:870:ASN:C	1:D:870:ASN:OD1	2.56	0.42
1:D:608:ASN:ND2	1:D:611:ILE:HD11	2.35	0.42
1:A:621:ASN:HD22	1:A:622:PRO:CD	2.33	0.42
3:C:11:G:H2'	3:C:12:A:C8	2.54	0.42
2:E:3:U:H2'	2:E:4:U:O4'	2.20	0.42
1:D:694:LYS:CB	1:D:695:PRO:CD	2.97	0.42
1:D:227:ILE:HG22	1:D:229:GLU:H	1.84	0.42
1:D:271:SER:O	1:D:350:ARG:NH1	2.52	0.42
2:B:6:C:H2'	2:B:7:U:O4'	2.19	0.42
1:A:218:GLU:OE1	1:A:236:THR:HG21	2.20	0.42
1:D:834:ILE:HD12	1:D:897:PRO:HB3	2.01	0.42
1:D:14:ILE:O	1:D:17:GLN:HB3	2.20	0.42
1:D:151:LYS:O	1:D:155:ARG:HG2	2.19	0.42
1:D:126:LEU:HD23	1:D:140:VAL:HG21	2.02	0.42
1:A:39:PRO:HD2	1:A:759:HIS:NE2	2.34	0.42
1:A:857:ASN:HB3	1:A:859:ASP:H	1.84	0.42
1:D:377:PHE:CD2	1:D:377:PHE:C	2.93	0.42
1:D:833:THR:O	1:D:837:ARG:HG3	2.19	0.42
1:D:387:LEU:CB	1:D:483:GLN:HE22	2.24	0.42
1:D:283:PRO:O	1:D:285:LYS:N	2.52	0.42
1:D:908:ARG:HG2	1:D:909:GLU:H	1.84	0.42
1:D:836:GLN:HG2	2:E:21:A:N1	2.34	0.42
1:A:391:ILE:HG12	1:A:391:ILE:O	2.20	0.42
1:D:559:VAL:HG13	1:D:677:LEU:HD11	2.01	0.42
1:A:822:LEU:CD2	1:A:824:VAL:HG23	2.50	0.42
1:A:693:PHE:N	1:A:693:PHE:CD1	2.88	0.42
1:D:535:SER:N	1:D:643:PRO:HB2	2.35	0.42
3:C:13:G:H2'	3:C:14:A:H8	1.85	0.42
1:D:383:TRP:HZ2	1:D:386:PRO:O	2.03	0.41
1:D:387:LEU:HD13	1:D:483:GLN:NE2	2.35	0.41
1:D:817:PHE:C	1:D:819:PRO:CD	2.81	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:368:VAL:HG22	1:A:654:VAL:HG22	1.99	0.41
1:D:62:VAL:HG11	1:D:80:LEU:HB3	2.02	0.41
1:A:745:ASP:OD1	1:A:746:ILE:N	2.53	0.41
1:D:96:VAL:O	1:D:100:ARG:HD2	2.19	0.41
1:A:39:PRO:HD2	1:A:759:HIS:CD2	2.55	0.41
1:A:559:VAL:HG23	1:A:615:VAL:CG2	2.50	0.41
1:A:12:LYS:CB	1:A:78:ALA:HB3	2.51	0.41
1:D:658:THR:O	1:D:662:ARG:HG3	2.20	0.41
1:D:524:PHE:CG	1:D:524:PHE:O	2.74	0.41
1:A:30:VAL:HG12	1:A:31:HIS:N	2.34	0.41
1:A:209:HIS:CG	1:A:209:HIS:O	2.71	0.41
1:D:18:LYS:O	1:D:18:LYS:HG3	2.19	0.41
1:D:47:GLY:HA3	1:D:48:PRO:HD3	1.91	0.41
1:A:168:PHE:HD2	1:A:282:ILE:HG23	1.84	0.41
1:D:380:LYS:HD2	1:D:479:ASN:ND2	2.35	0.41
1:A:246:LEU:HD22	1:A:261:VAL:CG1	2.50	0.41
1:D:783:ASP:OD1	1:D:922:GLN:HA	2.19	0.41
1:A:864:TRP:CA	1:A:868:GLN:HE21	2.32	0.41
1:A:368:VAL:CG2	1:A:369:ILE:N	2.82	0.41
1:D:857:ASN:HB3	1:D:860:HIS:CE1	2.56	0.41
2:B:13:C:H2'	2:B:14:A:H8	1.85	0.41
1:D:599:GLU:C	1:D:601:SER:H	2.22	0.41
1:D:482:ILE:O	1:D:485:ALA:HB3	2.20	0.41
1:D:38:CYS:HB3	1:D:41:LEU:CD1	2.50	0.41
1:D:231:VAL:HG12	1:D:232:VAL:O	2.21	0.41
1:D:272:CYS:HB2	1:D:351:ILE:CD1	2.51	0.41
1:A:356:SER:HA	1:A:497:PHE:CE1	2.55	0.41
1:D:773:THR:O	1:D:774:LEU:HD23	2.20	0.41
1:A:32:ASP:HB2	1:A:50:LEU:CD1	2.50	0.41
1:A:52:ARG:HB2	1:A:64:SER:O	2.21	0.41
1:D:793:THR:HG22	1:D:795:LEU:HG	2.02	0.41
1:A:631:MET:HA	1:A:635:GLU:OE1	2.20	0.41
1:D:527:PRO:N	1:D:528:PRO:CD	2.84	0.41
1:D:561:ILE:HG22	1:D:677:LEU:HD12	2.02	0.41
1:D:358:ASN:HA	1:D:373:LEU:HB2	2.02	0.41
2:E:11:U:O2'	2:E:12:G:H5'	2.21	0.41
3:C:3:C:H2'	3:C:4:G:C8	2.55	0.41
1:D:370:ALA:O	1:D:620:MET:HB2	2.20	0.41
1:D:43:ILE:O	1:D:44:PRO:C	2.58	0.41
1:D:168:PHE:HE2	1:D:282:ILE:HG12	1.86	0.41
1:D:262:MET:N	1:D:280:SER:O	2.46	0.41
1:A:244:HIS:HD2	1:A:246:LEU:N	2.01	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:667:GLU:O	1:A:669:PRO:CD	2.64	0.41
1:D:154:SER:O	1:D:158:ILE:HG13	2.20	0.41
1:A:263:ILE:HG12	1:A:279:TYR:CE2	2.56	0.41
1:A:392:LEU:HD21	1:A:404:PRO:CG	2.51	0.41
1:D:782:PHE:HD1	1:D:817:PHE:CE1	2.39	0.41
1:D:857:ASN:HB3	1:D:860:HIS:ND1	2.36	0.41
1:D:18:LYS:O	1:D:18:LYS:CG	2.69	0.41
1:A:753:ARG:HA	1:A:756:LYS:HE2	2.03	0.41
1:D:199:PRO:HB2	1:D:201:GLU:OE1	2.20	0.41
1:A:237:LEU:HD22	1:A:249:ILE:HG12	2.03	0.41
1:A:186:VAL:CG2	1:A:195:LYS:HG3	2.50	0.41
1:A:470:SER:HA	1:A:471:PRO:HD3	1.83	0.41
1:A:401:LEU:HD22	1:A:461:LYS:HB3	1.98	0.41
1:D:401:LEU:CD2	1:D:461:LYS:HD3	2.37	0.41
1:A:827:PRO:HB2	1:A:856:ARG:CZ	2.50	0.41
1:A:887:SER:O	1:A:903:ILE:N	2.54	0.41
1:A:821:LEU:HD12	1:A:906:PHE:O	2.21	0.41
1:D:780:LEU:HD11	1:D:805:GLN:HB3	2.03	0.41
2:E:11:U:H2'	2:E:12:G:C8	2.55	0.41
1:A:783:ASP:OD1	1:A:922:GLN:HA	2.21	0.41
1:A:728:LEU:HD22	1:A:741:ILE:HD12	2.03	0.41
1:D:212:ASP:HB3	1:D:337:ASP:OD1	2.21	0.41
1:D:43:ILE:CG2	1:D:43:ILE:O	2.62	0.40
1:A:624:ILE:HD11	1:A:673:TYR:CE2	2.55	0.40
1:A:719:ASP:O	1:A:721:GLY:N	2.54	0.40
1:A:160:ASN:CB	1:A:173:TYR:OH	2.69	0.40
1:A:211:SER:O	1:A:212:ASP:C	2.60	0.40
1:A:12:LYS:HE2	1:A:90:GLN:HE22	1.85	0.40
1:A:82:LEU:CD2	1:A:85:LEU:HD12	2.37	0.40
1:D:570:ASP:OD2	1:D:672:ASN:OD1	2.38	0.40
1:D:483:GLN:HA	1:D:483:GLN:OE1	2.21	0.40
1:A:361:TYR:HB2	1:A:391:ILE:CD1	2.52	0.40
1:A:457:LYS:NZ	1:A:489:ALA:HB3	2.36	0.40
2:B:20:A:C2'	2:B:21:A:H5''	2.51	0.40
1:A:252:ARG:CG	1:A:252:ARG:HH11	2.33	0.40
1:D:695:PRO:HG2	1:D:700:GLN:CG	2.50	0.40
1:A:798:ILE:HA	1:A:801:MET:CE	2.51	0.40
1:A:493:PHE:HA	1:A:496:PHE:HD1	1.84	0.40
1:A:621:ASN:HD22	1:A:621:ASN:C	2.25	0.40
1:A:120:HIS:CD2	1:A:122:LEU:H	2.38	0.40
1:D:73:SER:OG	1:D:74:GLU:N	2.53	0.40
1:D:38:CYS:HA	1:D:39:PRO:HD3	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:62:VAL:HG21	1:D:81:ALA:HA	2.02	0.40
1:D:373:LEU:HA	1:D:374:PRO:HD3	1.80	0.40
1:A:605:ILE:HD13	1:A:651:ILE:HG23	2.03	0.40
1:A:493:PHE:HA	1:A:496:PHE:CE1	2.55	0.40
1:D:824:VAL:O	1:D:903:ILE:HB	2.21	0.40
1:D:392:LEU:HD11	1:D:459:PHE:HZ	1.87	0.40
1:D:736:THR:CG2	1:D:738:LEU:HG	2.52	0.40
1:D:149:ASP:OD2	1:D:152:ILE:HG12	2.21	0.40
1:D:648:GLU:OE1	1:D:665:LEU:HD22	2.22	0.40
1:A:17:GLN:HG2	6:B:23:HOH:O	2.22	0.40
1:A:757:MET:HE2	1:A:758:LEU:CD2	2.48	0.40
1:A:100:ARG:O	1:A:104:VAL:HG23	2.22	0.40
1:A:12:LYS:HB3	1:A:78:ALA:HB3	2.04	0.40
1:A:457:LYS:HZ3	1:A:489:ALA:HB3	1.87	0.40
1:A:333:TRP:C	1:A:335:SER:H	2.25	0.40
1:A:813:VAL:HA	1:A:817:PHE:CD1	2.50	0.40
1:A:217:ARG:HD3	1:A:340:TYR:HE2	1.85	0.40
1:D:777:GLY:HA3	1:D:924:TYR:CE1	2.57	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	
1	A	761/950 (80%)	671 (88%)	72 (10%)	18 (2%)	9	43
1	D	777/950 (82%)	692 (89%)	70 (9%)	15 (2%)	12	51
All	All	1538/1900 (81%)	1363 (89%)	142 (9%)	33 (2%)	11	48

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PRO
1	A	59	GLU

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Mol	Chain	Res	Type
1	A	284	LYS
1	D	48	PRO
1	D	854	LYS
1	A	682	GLY
1	A	687	ARG
1	A	720	PHE
1	A	924	TYR
1	D	644	PRO
1	A	58	PRO
1	A	694	LYS
1	A	722	CYS
1	A	723	GLY
1	D	44	PRO
1	D	284	LYS
1	A	310	ALA
1	A	380	LYS
1	D	197	ALA
1	D	207	ALA
1	D	895	VAL
1	A	121	PRO
1	A	334	LYS
1	A	669	PRO
1	D	189	PRO
1	A	8	THR
1	D	570	ASP
1	D	643	PRO
1	D	694	LYS
1	A	735	PRO
1	D	43	ILE
1	D	471	PRO
1	D	735	PRO

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
1	A	676/828 (82%)	621 (92%)	55 (8%)	17 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	689/828 (83%)	654 (95%)	35 (5%)	33	74
All	All	1365/1656 (82%)	1275 (93%)	90 (7%)	24	64

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	49	CYS
1	A	58	PRO
1	A	63	VAL
1	A	64	SER
1	A	91	ASN
1	A	92	ASP
1	A	121	PRO
1	A	143	SER
1	A	167	PRO
1	A	173	TYR
1	A	175	MET
1	A	183	ASP
1	A	184	TYR
1	A	193	ARG
1	A	209	HIS
1	A	218	GLU
1	A	230	GLU
1	A	251	GLU
1	A	311	ARG
1	A	336	ASP
1	A	339	ASP
1	A	365	ARG
1	A	392	LEU
1	A	396	CYS
1	A	458	ILE
1	A	459	PHE
1	A	462	SER
1	A	473	LYS
1	A	497	PHE
1	A	537	GLU
1	A	541	THR
1	A	560	SER
1	A	621	ASN
1	A	660	ARG
1	A	667	GLU

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Mol	Chain	Res	Type
1	A	677	LEU
1	A	695	PRO
1	A	701	ARG
1	A	703	GLU
1	A	710	ARG
1	A	715	SER
1	A	717	LEU
1	A	738	LEU
1	A	757	MET
1	A	776	ASP
1	A	784	SER
1	A	796	GLU
1	A	799	GLU
1	A	804	ASP
1	A	825	SER
1	A	855	PHE
1	A	857	ASN
1	A	865	THR
1	A	886	PHE
1	D	51	TYR
1	D	72	ASP
1	D	88	ARG
1	D	156	CYS
1	D	183	ASP
1	D	194	ARG
1	D	200	SER
1	D	235	ASP
1	D	239	ILE
1	D	265	ARG
1	D	332	ARG
1	D	342	ASP
1	D	346	ASN
1	D	350	ARG
1	D	401	LEU
1	D	469	CYS
1	D	480	ASP
1	D	491	LEU
1	D	497	PHE
1	D	500	LEU
1	D	562	CYS
1	D	599	GLU
1	D	606	GLU

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Mol	Chain	Res	Type
1	D	608	ASN
1	D	722	CYS
1	D	757	MET
1	D	787	HIS
1	D	794	CYS
1	D	804	ASP
1	D	863	GLU
1	D	867	GLU
1	D	870	ASN
1	D	878	LYS
1	D	921	MET
1	D	929	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	35	GLN
1	A	45	GLN
1	A	90	GLN
1	A	120	HIS
1	A	244	HIS
1	A	321	HIS
1	A	358	ASN
1	A	382	ASN
1	A	398	GLN
1	A	484	ASN
1	A	621	ASN
1	A	739	GLN
1	A	857	ASN
1	A	868	GLN
1	A	870	ASN
1	D	45	GLN
1	D	244	HIS
1	D	260	GLN
1	D	318	GLN
1	D	346	ASN
1	D	358	ASN
1	D	479	ASN
1	D	484	ASN
1	D	608	ASN
1	D	621	ASN

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Mol	Chain	Res	Type
1	D	672	ASN
1	D	832	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	21/22 (95%)	3 (14%)	2 (9%)
2	E	21/22 (95%)	2 (9%)	0
3	C	21/22 (95%)	2 (9%)	0
3	F	21/22 (95%)	4 (19%)	1 (4%)
All	All	84/88 (95%)	11 (13%)	3 (3%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	20	A
2	B	21	A
2	B	22	G
3	C	21	A
3	C	22	C
2	E	21	A
2	E	22	G
3	F	19	U
3	F	20	C
3	F	21	A
3	F	22	C

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	20	A
2	B	21	A
3	F	19	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
5	SAH	A	951	-	28,28,28	0.95	2 (7%)	40,40,40	1.09	4 (10%)
5	SAH	D	951	-	28,28,28	0.90	1 (3%)	40,40,40	0.91	2 (5%)

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
5	SAH	A	951	-	-	0/15/31/31	0/1/3/3
5	SAH	D	951	-	-	0/15/31/31	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	951	SAH	C8-N9	2.17	1.39	1.36
5	A	951	SAH	O-C	2.07	1.29	1.22
5	A	951	SAH	C8-N9	2.04	1.39	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	951	SAH	O4'-C1'-C2'	-3.62	101.23	106.77
5	A	951	SAH	C8-N9-C4	-2.64	104.89	106.90
5	A	951	SAH	O4'-C1'-N9	-2.58	106.04	108.44
5	D	951	SAH	O4'-C1'-N9	-2.15	106.44	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	951	SAH	O4'-C1'-C2'	-2.05	103.63	106.77
5	A	951	SAH	C4-C5-N7	2.04	111.27	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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, 95th 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 ²)	Q<0.9
1	A	779/950 (82%)	-0.10	11 (1%)	72 17	60, 96, 160, 193	0
1	D	795/950 (83%)	-0.12	3 (0%)	90 45	55, 98, 154, 188	0
2	B	22/22 (100%)	-0.72	0	100 100	91, 120, 146, 151	0
2	E	22/22 (100%)	-0.71	0	100 100	99, 114, 123, 130	0
3	C	22/22 (100%)	-0.65	0	100 100	89, 137, 168, 199	0
3	F	22/22 (100%)	-0.66	0	100 100	91, 125, 144, 186	0
All	All	1662/1988 (83%)	-0.14	14 (0%)	83 28	55, 98, 159, 199	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	573	TYR	4.6
1	A	7	HIS	3.3
1	A	851	GLN	3.2
1	A	89	PRO	2.9
1	A	32	ASP	2.8
1	A	406	LEU	2.5
1	D	687	ARG	2.3
1	A	92	ASP	2.3
1	A	90	GLN	2.3
1	D	524	PHE	2.3
1	A	475	TYR	2.2
1	A	468	GLU	2.1
1	A	687	ARG	2.0
1	A	23	ALA	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SAH	A	951	26/26	0.21	0.48	62,68,85,86	0
5	SAH	D	951	26/26	0.14	-0.85	70,74,86,87	0
4	MG	D	950	1/1	0.10	-1.78	36,36,36,36	0
4	MG	A	950	1/1	0.04	-4.21	60,60,60,60	0

6.5 Other polymers

There are no such residues in this entry.