



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2024 – 01:38 PM EST

PDB ID : 1EFW  
Title : Crystal structure of aspartyl-tRNA synthetase from *Thermus thermophilus* complexed to tRNA<sup>asp</sup> from *Escherichia coli*  
Authors : Briand, C.; Poterszman, A.; Eiler, S.; Webster, G.; Thierry, J.-C.; Moras, D.  
Deposited on : 2000-02-10  
Resolution : 3.00 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

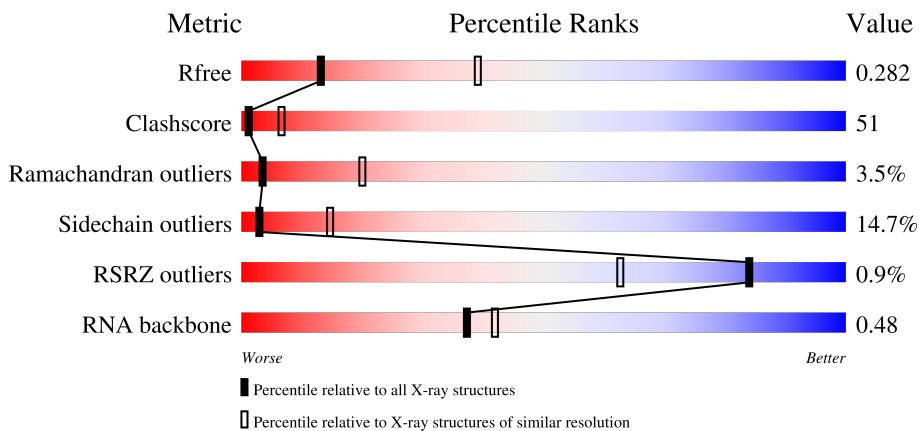
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



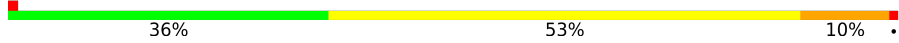

The reported resolution of this entry is 3.00 Å.

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))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	C	73	 59% 32% 5%
1	D	73	 8% 55% 29% 8%
2	A	580	 36% 53% 10%
2	B	580	 29% 57% 12%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12572 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 ASPARTYL-TRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	C	73	Total	C	N	O	P	S	0	0	0
			1570	703	274	519	73	1			
1	D	73	Total	C	N	O	P	S	0	0	0
			1570	703	274	519	73	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	580	Total	C	N	O	S	0	0	0
			4668	2980	840	837	11			
2	B	580	Total	C	N	O	S	0	0	0
			4668	2980	840	837	11			

- Molecule 3 is water.

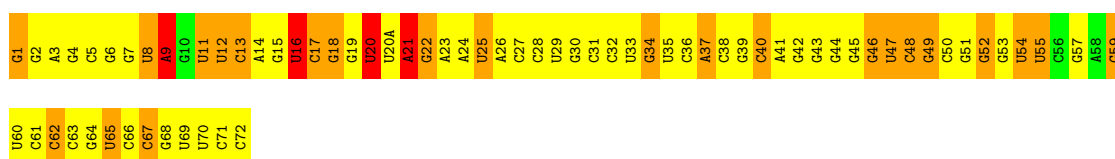
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	12	Total	O	0	0
			12	12		
3	D	10	Total	O	0	0
			10	10		
3	A	43	Total	O	0	0
			43	43		
3	B	31	Total	O	0	0
			31	31		

### 3 Residue-property plots

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

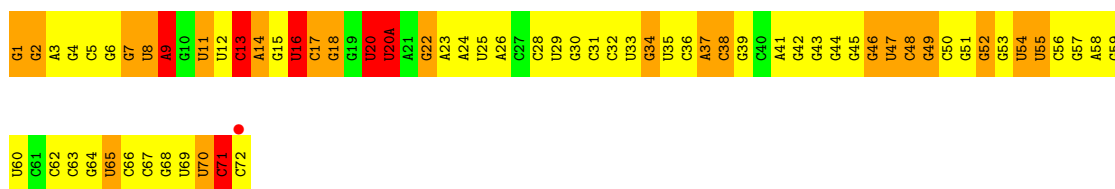
- Molecule 1: ASPARTYL-TRNA

Chain C: 



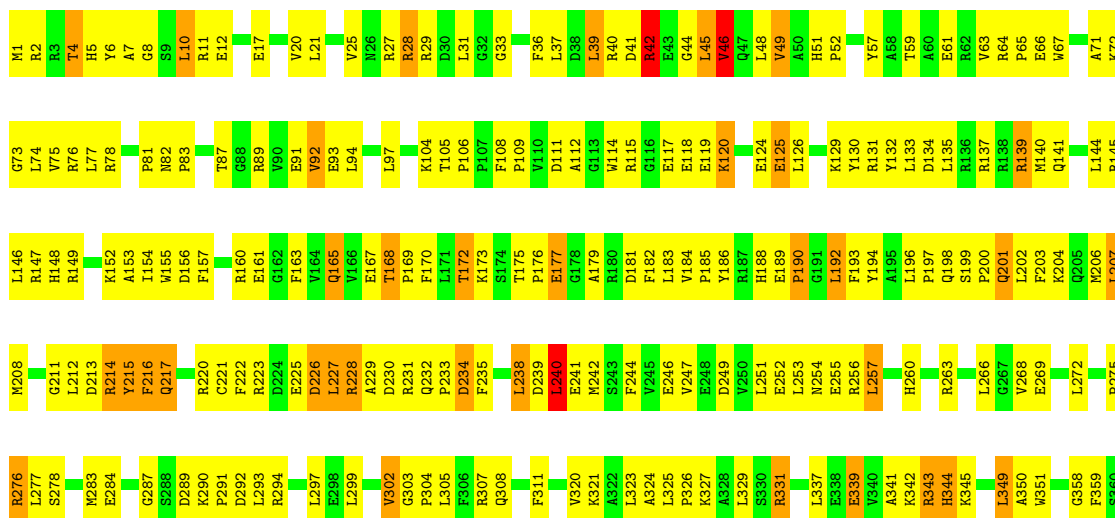
- Molecule 1: ASPARTYL-TRNA

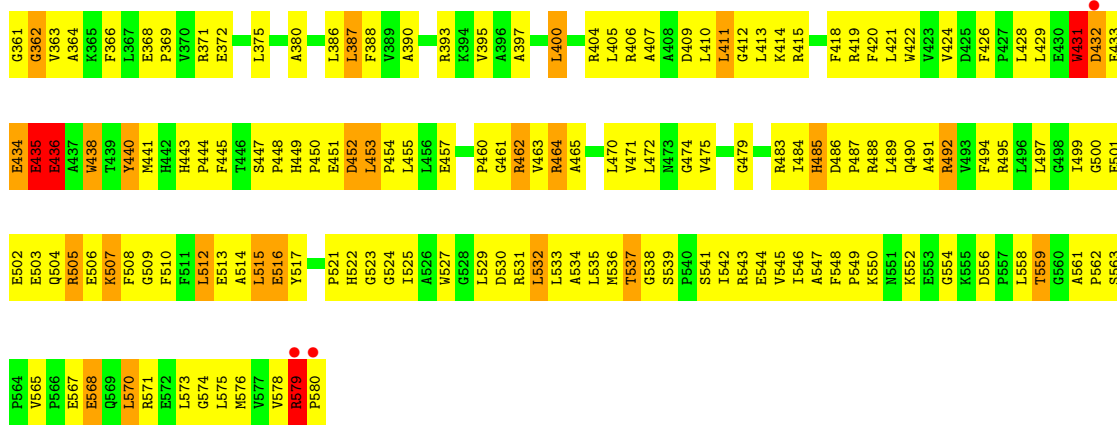
Chain D: 



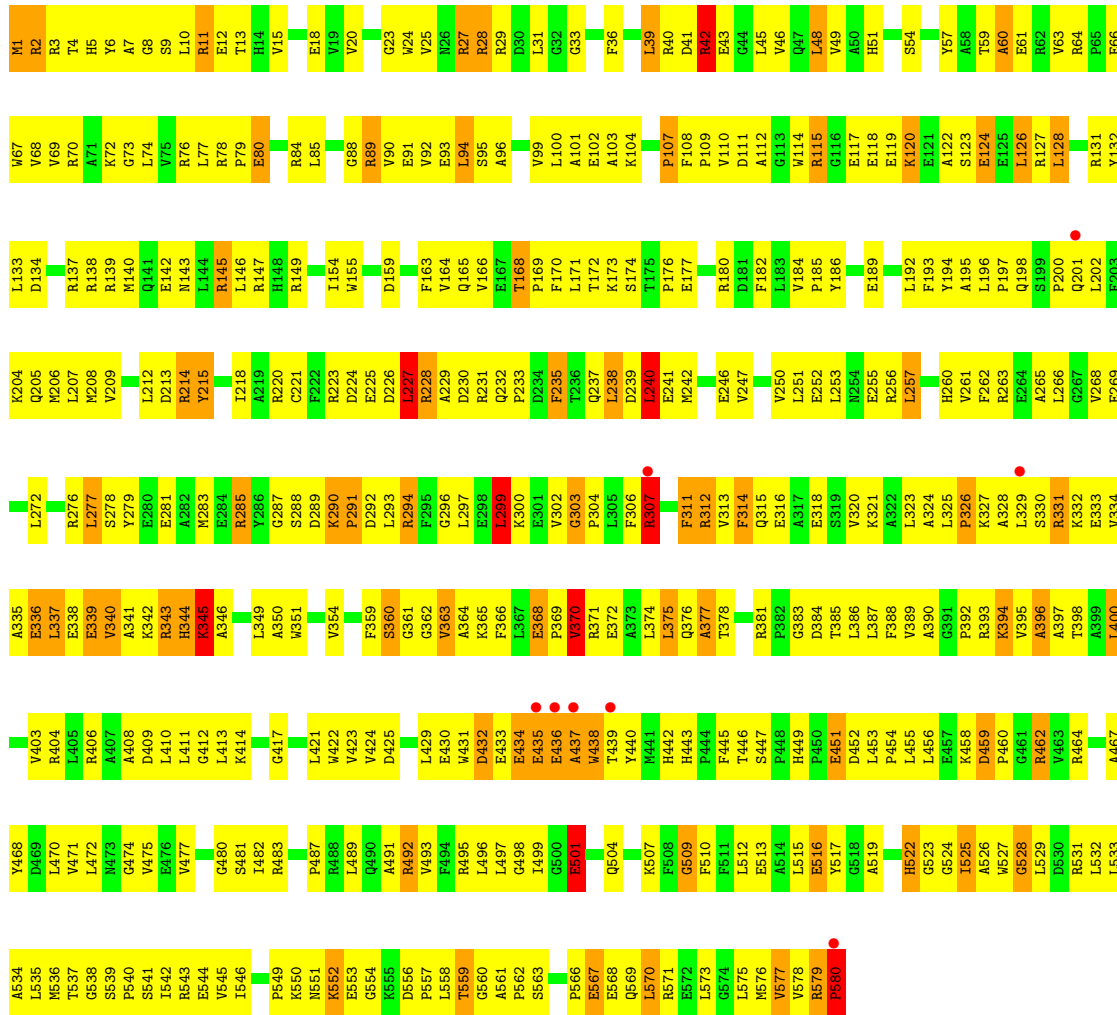
- Molecule 2: ASPARTYL-TRNA SYNTHETASE

Chain A: 





• Molecule 2: ASPARTYL-TRNA SYNTHETASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	251.45Å 251.45Å 88.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 14.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (15.00-3.00) 91.8 (14.99-3.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.87 (at 3.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.248 , 0.293 0.238 , 0.282	Depositor DCC
$R_{free}$ test set	2969 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 16.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12572	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 5MU, H2U, 4SU, PSU, QUO, G7M, 2MA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.98	6/1506 (0.4%)	1.08	10/2343 (0.4%)
1	D	0.74	1/1506 (0.1%)	0.98	8/2343 (0.3%)
2	A	0.55	2/4780 (0.0%)	1.01	16/6467 (0.2%)
2	B	0.59	6/4780 (0.1%)	1.03	18/6467 (0.3%)
All	All	0.65	15/12572 (0.1%)	1.02	52/17620 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	4
1	D	0	4
All	All	0	8

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	580	PRO	C-OXT	15.85	1.53	1.23
1	C	1	G	O3 <sup>1</sup> -P	-15.47	1.42	1.61
1	C	59	G	O3 <sup>1</sup> -P	12.60	1.76	1.61
2	A	495	ARG	CZ-NH1	11.61	1.48	1.33
2	A	495	ARG	CZ-NH2	10.79	1.47	1.33
2	B	580	PRO	CA-C	9.90	1.72	1.52
1	C	11	U	O3 <sup>1</sup> -P	-8.11	1.51	1.61
2	B	307	ARG	NE-CZ	7.48	1.42	1.33
2	B	580	PRO	C-O	6.65	1.36	1.23
1	C	62	C	O3 <sup>1</sup> -P	-6.63	1.53	1.61
2	B	307	ARG	CD-NE	6.39	1.57	1.46
1	C	12	U	O3 <sup>1</sup> -P	6.21	1.68	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	67	C	O3'-P	5.74	1.68	1.61
2	B	307	ARG	CG-CD	5.58	1.65	1.51
1	D	70	U	O3'-P	-5.07	1.55	1.61

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	307	ARG	NE-CZ-NH1	35.08	137.84	120.30
2	A	495	ARG	NE-CZ-NH2	-31.89	104.36	120.30
2	A	495	ARG	NH1-CZ-NH2	19.00	140.31	119.40
2	B	307	ARG	NE-CZ-NH2	-17.90	111.35	120.30
2	B	307	ARG	CG-CD-NE	17.16	147.83	111.80
2	B	307	ARG	CD-NE-CZ	13.53	142.55	123.60
2	A	495	ARG	NE-CZ-NH1	-10.91	114.84	120.30
2	B	307	ARG	NH1-CZ-NH2	-9.35	109.11	119.40
1	D	70	U	N1-C1'-C2'	-8.57	102.57	112.00
2	B	307	ARG	CB-CG-CD	8.52	133.75	111.60
2	B	307	ARG	CA-CB-CG	-8.48	94.74	113.40
2	A	344	HIS	N-CA-C	-8.41	88.28	111.00
1	C	59	G	O3'-P-O5'	8.35	119.86	104.00
2	A	240	LEU	CA-CB-CG	7.31	132.12	115.30
2	A	431	TRP	N-CA-C	7.31	130.74	111.00
1	D	13	C	O4'-C1'-N1	7.12	113.89	108.20
1	D	1	G	P-O3'-C3'	-7.04	111.25	119.70
1	C	22	G	O3'-P-O5'	6.92	117.15	104.00
2	A	432	ASP	N-CA-C	6.88	129.59	111.00
1	C	21	A	P-O3'-C3'	6.67	127.70	119.70
2	A	435	GLU	N-CA-C	-6.42	93.68	111.00
2	B	417	GLY	N-CA-C	6.41	129.13	113.10
2	A	512	LEU	CA-CB-CG	6.24	129.65	115.30
1	D	14	A	O4'-C1'-N9	6.13	113.11	108.20
2	B	240	LEU	CA-CB-CG	6.06	129.23	115.30
2	B	434	GLU	N-CA-C	-5.92	95.02	111.00
1	C	22	G	P-O5'-C5'	-5.90	111.46	120.90
2	B	42	ARG	NE-CZ-NH2	-5.83	117.38	120.30
2	B	344	HIS	N-CA-C	-5.81	95.31	111.00
2	B	345	LYS	N-CA-C	5.81	126.68	111.00
1	C	52	G	N9-C1'-C2'	-5.68	105.75	112.00
1	C	9	A	C5'-C4'-C3'	-5.68	106.91	116.00
2	A	238	LEU	N-CA-C	-5.67	95.69	111.00
1	D	71	C	O4'-C1'-N1	-5.66	103.67	108.20
2	B	218	ILE	N-CA-C	-5.66	95.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	46	VAL	CB-CA-C	-5.63	100.70	111.40
2	A	436	GLU	N-CA-C	5.60	126.11	111.00
1	C	12	U	N1-C1'-C2'	-5.58	105.86	112.00
1	D	2	G	P-O5'-C5'	-5.58	111.97	120.90
1	C	60	U	OP1-P-OP2	-5.50	111.35	119.60
2	B	212	LEU	CA-CB-CG	-5.44	102.78	115.30
2	A	431	TRP	C-N-CA	-5.43	108.12	121.70
2	A	46	VAL	N-CA-C	-5.38	96.48	111.00
2	B	238	LEU	N-CA-C	-5.36	96.54	111.00
1	C	60	U	O5'-P-OP2	5.30	117.06	110.70
2	B	528	GLY	N-CA-C	-5.20	100.10	113.10
2	A	532	LEU	CA-CB-CG	5.17	127.19	115.30
2	A	45	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	52	G	N9-C1'-C2'	-5.14	106.34	112.00
1	D	41	A	N9-C1'-C2'	-5.08	106.41	112.00
2	B	570	LEU	CA-CB-CG	5.04	126.88	115.30
1	C	13	C	OP1-P-OP2	-5.02	112.08	119.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	21	A	Sidechain
1	C	25	U	Sidechain
1	C	40	C	Sidechain
1	C	9	A	Sidechain
1	D	11	U	Sidechain
1	D	42	G	Sidechain
1	D	7	G	Sidechain
1	D	9	A	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1570	0	807	111	0
1	D	1570	0	805	132	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4668	0	4679	469	0
2	B	4668	0	4679	548	0
3	A	43	0	0	3	0
3	B	31	0	0	7	0
3	C	12	0	0	1	0
3	D	10	0	0	0	0
All	All	12572	0	10970	1183	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (1183) 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:D:2:G:H1	1:D:71:C:N4	1.40	1.20
2:B:27:ARG:HH21	2:B:29:ARG:NH1	1.42	1.17
1:D:37:2MA:H5''	2:B:27:ARG:HH12	1.01	1.11
1:D:68:G:H2'	1:D:69:U:C6	1.88	1.08
1:D:34:QUO:H4'	1:D:35:U:H5'	1.35	1.08
2:B:408:ALA:HA	2:B:413:LEU:HD13	1.35	1.07
2:B:10:LEU:HD12	2:B:10:LEU:H	1.18	1.07
2:A:168:THR:HB	2:A:217:GLN:HE22	1.16	1.07
2:B:28:ARG:HG2	2:B:28:ARG:HH11	1.14	1.07
1:D:48:C:H4'	1:D:49:G:OP2	1.54	1.06
1:D:1:G:H2'	1:D:2:G:O4'	1.55	1.04
2:A:479:GLY:O	2:A:525:ILE:HG13	1.60	1.02
2:B:331:ARG:HE	2:B:331:ARG:HA	1.21	1.01
2:B:546:ILE:O	2:B:549:PRO:HD3	1.57	1.01
2:B:227:LEU:H	2:B:227:LEU:HD22	1.23	1.00
1:C:17:C:H4'	1:C:18:G:OP2	1.60	1.00
2:B:323:LEU:HB2	2:B:400:LEU:HD11	1.42	1.00
2:B:329:LEU:HD12	2:B:385:THR:HG21	1.43	1.00
1:C:61:C:O2'	1:C:62:C:H5'	1.61	1.00
2:B:127:ARG:NH2	2:B:137:ARG:HH22	1.58	1.00
2:B:349:LEU:HD12	2:B:350:ALA:H	1.24	1.00
2:A:226:ASP:HB2	2:A:228:ARG:HG2	1.44	0.99
2:B:27:ARG:NH2	2:B:29:ARG:HH11	1.61	0.99
2:A:299:LEU:HD22	2:A:400:LEU:HD13	1.40	0.98
1:D:68:G:H2'	1:D:69:U:H6	1.23	0.98
2:A:421:LEU:CD2	2:A:471:VAL:HG22	1.94	0.97
2:B:263:ARG:HD3	2:B:269:GLU:OE1	1.64	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:227:LEU:HA	2:A:231:ARG:HB2	1.48	0.95
1:D:3:A:H2'	1:D:4:G:C8	2.01	0.95
2:B:475:VAL:HG21	2:B:535:LEU:HD11	1.50	0.94
2:B:27:ARG:HH11	2:B:115:ARG:NE	1.65	0.93
2:B:27:ARG:CD	2:B:115:ARG:HE	1.81	0.93
2:A:254:ASN:HD21	2:A:525:ILE:HG21	1.33	0.93
1:D:37:2MA:H5''	2:B:27:ARG:NH1	1.82	0.93
2:B:147:ARG:HG3	2:B:533:LEU:CD1	1.98	0.93
2:A:231:ARG:HG3	2:A:231:ARG:HH11	1.34	0.93
2:A:331:ARG:H	2:A:331:ARG:HE	1.09	0.92
2:B:172:THR:HG22	2:B:195:ALA:O	1.69	0.92
2:A:421:LEU:HD21	2:A:471:VAL:HG22	1.50	0.91
2:B:202:LEU:HD21	2:B:445:PHE:HE1	1.33	0.91
2:A:147:ARG:HD2	2:A:533:LEU:CD1	2.02	0.90
2:B:166:VAL:HG11	2:B:207:LEU:HD21	1.53	0.89
1:C:34:QUO:H4'	1:C:35:U:H5'	1.55	0.88
2:B:146:LEU:HD12	2:B:149:ARG:NH1	1.87	0.88
2:A:42:ARG:HD3	2:A:145:ARG:NH2	1.89	0.88
2:A:78:ARG:HG3	2:A:91:GLU:HG2	1.54	0.87
2:B:349:LEU:HD11	2:B:387:LEU:HB3	1.56	0.87
1:C:22:G:O2'	1:C:23:A:H5'	1.75	0.86
2:B:120:LYS:H	2:B:120:LYS:HD2	1.40	0.86
1:D:37:2MA:C5'	2:B:27:ARG:HH12	1.86	0.86
1:D:1:G:C2'	1:D:2:G:H5'	2.05	0.86
2:B:281:GLU:HG3	2:B:285:ARG:HD3	1.57	0.86
2:B:290:LYS:O	2:B:474:GLY:HA2	1.75	0.85
2:B:28:ARG:HG2	2:B:28:ARG:NH1	1.90	0.85
2:A:431:TRP:HH2	2:A:436:GLU:HB3	1.39	0.84
2:B:27:ARG:NH2	2:B:29:ARG:NH1	2.23	0.83
1:D:3:A:H2'	1:D:4:G:H8	1.44	0.83
1:D:8:4SU:H5''	1:D:49:G:OP2	1.77	0.83
2:A:192:LEU:HD22	2:B:562:PRO:HG2	1.59	0.83
2:A:170:PHE:O	2:A:197:PRO:HD3	1.78	0.83
2:B:201:GLN:O	2:B:204:LYS:HG2	1.78	0.83
2:B:28:ARG:HH11	2:B:28:ARG:CG	1.90	0.82
2:A:220:ARG:HG2	2:B:170:PHE:CD1	2.15	0.82
2:A:546:ILE:O	2:A:549:PRO:HD3	1.80	0.82
2:B:127:ARG:NH2	2:B:137:ARG:NH2	2.27	0.82
2:B:226:ASP:OD1	2:B:228:ARG:HG2	1.80	0.81
2:A:213:ASP:CG	2:B:3:ARG:HH22	1.83	0.81
2:A:277:LEU:HD12	2:A:421:LEU:HD12	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:G:H2'	1:C:3:A:C8	2.16	0.81
2:A:203:PHE:O	2:A:207:LEU:HD22	1.81	0.80
2:B:307:ARG:HD3	2:B:315:GLN:HA	1.62	0.80
2:B:147:ARG:HG3	2:B:533:LEU:HD13	1.61	0.80
2:B:456:LEU:HD23	2:B:492:ARG:HD2	1.64	0.80
2:B:537:THR:HG23	2:B:539:SER:OG	1.81	0.80
2:A:168:THR:HG23	2:A:169:PRO:HD2	1.64	0.80
2:B:146:LEU:HD12	2:B:149:ARG:HH12	1.46	0.80
2:B:323:LEU:HB2	2:B:400:LEU:CD1	2.12	0.79
2:B:411:LEU:HB2	2:B:413:LEU:CD1	2.13	0.79
2:A:201:GLN:O	2:A:204:LYS:HG2	1.83	0.79
2:A:537:THR:CG2	2:A:539:SER:H	1.95	0.79
1:D:2:G:H1	1:D:71:C:H42	0.81	0.79
2:B:127:ARG:HH21	2:B:137:ARG:NH2	1.81	0.79
2:B:202:LEU:HD21	2:B:445:PHE:CE1	2.18	0.79
2:A:10:LEU:HD23	2:A:46:VAL:HG11	1.65	0.78
2:A:537:THR:HG22	2:A:539:SER:H	1.48	0.78
2:B:204:LYS:HE2	2:B:241:GLU:OE1	1.84	0.78
2:A:345:LYS:O	2:A:395:VAL:HG13	1.83	0.78
2:A:290:LYS:O	2:A:474:GLY:HA2	1.83	0.78
2:B:411:LEU:HB2	2:B:413:LEU:HD12	1.65	0.78
2:A:568:GLU:OE1	2:A:571:ARG:HD2	1.82	0.78
2:B:277:LEU:HD11	2:B:281:GLU:HG2	1.65	0.78
2:B:326:PRO:HA	2:B:384:ASP:OD1	1.83	0.78
2:B:112:ALA:HB3	2:B:119:GLU:HG2	1.66	0.77
2:B:393:ARG:HG2	3:B:2039:HOH:O	1.83	0.77
2:B:449:HIS:CD2	2:B:464:ARG:NH1	2.51	0.77
2:B:452:ASP:HA	2:B:455:LEU:HD23	1.66	0.77
2:A:568:GLU:OE1	2:A:571:ARG:CD	2.31	0.77
2:A:254:ASN:ND2	2:A:525:ILE:HG21	2.00	0.77
2:A:292:ASP:OD1	2:A:294:ARG:HD3	1.84	0.77
2:B:499:ILE:HD12	2:B:499:ILE:H	1.50	0.77
2:A:228:ARG:NH1	2:A:228:ARG:HA	1.99	0.77
1:C:1:G:O2'	1:C:2:G:H5'	1.85	0.77
1:C:71:C:H2'	1:C:72:C:C6	2.20	0.76
1:D:6:G:O2'	1:D:7:G:H5'	1.84	0.76
2:A:447:SER:HA	2:A:484:ILE:CD1	2.16	0.76
2:B:343:ARG:NH1	2:B:343:ARG:HA	1.99	0.76
2:B:10:LEU:H	2:B:10:LEU:CD1	1.98	0.76
2:A:297:LEU:O	2:A:404:ARG:HD2	1.85	0.76
2:B:276:ARG:HG3	2:B:422:TRP:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:431:TRP:CH2	2:A:436:GLU:HB3	2.21	0.75
2:A:443:HIS:CG	2:A:444:PRO:HD2	2.21	0.75
1:D:2:G:N1	1:D:71:C:N4	2.25	0.75
2:A:559:THR:HG23	2:B:173:LYS:HB2	1.69	0.75
1:C:15:G:H5''	1:C:16:H2U:H5'	1.68	0.75
1:D:69:U:H2'	1:D:70:U:C6	2.22	0.75
2:A:228:ARG:HA	2:A:228:ARG:CZ	2.16	0.75
1:D:36:C:N4	2:B:80:GLU:HB3	2.00	0.75
2:A:59:THR:O	2:A:63:VAL:HG23	1.86	0.75
2:A:109:PRO:CG	2:A:120:LYS:HE2	2.17	0.75
2:A:240:LEU:HD22	2:A:525:ILE:HG22	1.69	0.75
2:A:429:LEU:HD13	2:A:438:TRP:HB3	1.68	0.74
1:D:34:QUO:H4'	1:D:35:U:C5'	2.16	0.74
2:A:25:VAL:HG21	2:A:63:VAL:HG11	1.69	0.74
2:A:321:LYS:HD2	2:A:397:ALA:HB2	1.69	0.74
2:A:241:GLU:HA	2:A:241:GLU:OE1	1.86	0.74
2:B:220:ARG:HD3	2:B:235:PHE:O	1.87	0.74
2:B:27:ARG:HD3	2:B:115:ARG:HE	1.49	0.74
2:B:343:ARG:HA	2:B:343:ARG:CZ	2.18	0.74
2:B:349:LEU:HD12	2:B:350:ALA:N	2.01	0.74
1:C:42:G:O2'	1:C:43:G:H5'	1.88	0.74
2:B:318:GLU:OE2	2:B:393:ARG:HB2	1.88	0.74
2:A:7:ALA:N	2:A:41:ASP:OD2	2.21	0.73
2:A:147:ARG:HD2	2:A:533:LEU:HD13	1.67	0.73
2:A:326:PRO:HD2	2:A:411:LEU:HD21	1.71	0.73
2:B:10:LEU:HD12	2:B:10:LEU:N	1.97	0.73
2:B:299:LEU:N	2:B:299:LEU:HD23	2.03	0.73
2:B:475:VAL:CG2	2:B:535:LEU:HD11	2.18	0.72
1:D:62:C:H2'	1:D:63:C:C6	2.25	0.72
2:A:421:LEU:HD23	2:A:471:VAL:HG22	1.70	0.72
2:A:4:THR:HG1	2:A:5:HIS:HD1	1.38	0.72
2:A:220:ARG:HG2	2:B:170:PHE:CE1	2.25	0.72
2:A:226:ASP:CB	2:A:228:ARG:HG2	2.19	0.72
1:C:3:A:H2'	1:C:4:G:C8	2.25	0.72
2:B:49:VAL:HG21	2:B:91:GLU:OE2	1.89	0.71
2:A:238:LEU:HB3	2:A:527:TRP:HB2	1.72	0.71
2:B:307:ARG:HD2	2:B:315:GLN:O	1.90	0.71
1:C:36:C:O2	2:A:78:ARG:NH2	2.23	0.71
2:B:27:ARG:HD2	2:B:115:ARG:HE	1.55	0.71
2:B:78:ARG:HD3	2:B:88:GLY:O	1.91	0.71
2:B:120:LYS:HD2	2:B:120:LYS:N	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:C:H2'	1:C:67:C:H6	1.55	0.71
1:C:72:C:O3'	2:A:343:ARG:HD2	1.90	0.71
2:B:4:THR:HG23	2:B:20:VAL:HB	1.71	0.71
2:B:266:LEU:HB3	2:B:268:VAL:HG23	1.72	0.71
1:C:11:U:O2'	1:C:12:U:H5'	1.90	0.70
2:B:1:MET:N	2:B:70:ARG:HD3	2.04	0.70
2:A:165:GLN:HE21	2:A:165:GLN:C	1.94	0.70
1:D:3:A:C2	1:D:71:C:N4	2.60	0.70
1:D:70:U:H6	1:D:70:U:O5'	1.73	0.70
2:A:227:LEU:HD22	2:A:227:LEU:H	1.56	0.70
1:D:38:C:OP2	2:B:27:ARG:NH2	2.25	0.70
2:A:440:TYR:HB3	2:A:497:LEU:HD11	1.73	0.70
2:B:27:ARG:HH21	2:B:29:ARG:HH11	0.75	0.70
2:B:147:ARG:HG3	2:B:533:LEU:HD11	1.71	0.70
2:B:561:ALA:HA	2:B:562:PRO:C	2.11	0.70
2:A:129:LYS:HG3	2:A:129:LYS:O	1.90	0.70
2:A:550:LYS:HD2	2:A:554:GLY:O	1.91	0.70
2:A:76:ARG:HG2	2:A:76:ARG:HH11	1.57	0.69
2:B:266:LEU:CB	2:B:268:VAL:HG23	2.22	0.69
2:A:139:ARG:HH22	2:A:537:THR:HG23	1.55	0.69
2:B:394:LYS:O	2:B:398:THR:HG23	1.92	0.69
1:D:1:G:H2'	1:D:2:G:C4'	2.22	0.69
2:A:226:ASP:C	2:A:228:ARG:H	1.96	0.69
2:A:575:LEU:HD23	2:B:577:VAL:HA	1.73	0.69
2:A:500:GLY:O	2:A:504:GLN:HB2	1.91	0.69
2:B:198:GLN:O	2:B:221:CYS:HB3	1.92	0.69
2:B:251:LEU:O	2:B:255:GLU:HG3	1.93	0.69
2:B:111:ASP:OD1	2:B:115:ARG:NH2	2.26	0.69
1:D:48:C:C4'	1:D:49:G:OP2	2.36	0.69
2:A:173:LYS:HB2	2:B:559:THR:HG23	1.74	0.69
1:D:65:PSU:H2'	1:D:66:C:C6	2.28	0.69
2:B:386:LEU:HB3	2:B:388:PHE:CE1	2.27	0.69
1:C:2:G:H1	1:C:71:C:H42	1.40	0.69
2:A:371:ARG:HG3	2:A:375:LEU:CD2	2.23	0.69
2:B:299:LEU:O	2:B:300:LYS:HG2	1.93	0.69
2:B:389:VAL:HG23	2:B:400:LEU:HD23	1.74	0.68
2:A:351:TRP:HA	2:A:386:LEU:O	1.92	0.68
2:A:421:LEU:HD21	2:A:471:VAL:CG2	2.23	0.68
2:B:533:LEU:O	2:B:537:THR:HG22	1.94	0.68
2:B:561:ALA:HA	2:B:562:PRO:O	1.93	0.68
2:A:231:ARG:HG3	2:A:231:ARG:NH1	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:4SU:H1'	1:D:48:C:H1'	1.75	0.68
2:A:263:ARG:HD3	2:A:269:GLU:OE1	1.94	0.68
2:A:483:ARG:HE	2:A:523:GLY:HA2	1.58	0.68
2:B:27:ARG:HH11	2:B:115:ARG:HE	1.42	0.68
2:B:558:LEU:HD12	2:B:558:LEU:O	1.94	0.68
1:D:65:PSU:H2'	1:D:66:C:H6	1.59	0.68
2:A:488:ARG:O	2:A:491:ALA:HB3	1.93	0.68
2:B:368:GLU:N	2:B:369:PRO:HD2	2.09	0.68
2:A:184:VAL:HB	2:A:194:TYR:HB2	1.75	0.68
2:A:345:LYS:O	2:A:395:VAL:CG1	2.42	0.67
2:B:255:GLU:HG2	2:B:422:TRP:HE1	1.59	0.67
1:C:21:A:H2'	1:C:46:G7M:O6	1.94	0.67
1:C:22:G:O2'	1:C:23:A:C5'	2.42	0.67
2:A:445:PHE:HD2	2:A:490:GLN:OE1	1.77	0.67
1:D:36:C:O2	2:B:78:ARG:NH2	2.27	0.67
2:A:440:TYR:CE1	2:A:444:PRO:HD3	2.28	0.67
2:B:7:ALA:N	2:B:41:ASP:OD2	2.28	0.67
2:A:447:SER:HA	2:A:484:ILE:HD13	1.75	0.67
2:A:578:VAL:HG11	2:B:576:MET:SD	2.34	0.67
1:D:17:C:H4'	1:D:18:G:OP2	1.93	0.67
2:B:277:LEU:HB2	2:B:421:LEU:HD11	1.77	0.67
2:B:48:LEU:HB3	2:B:94:LEU:HD21	1.74	0.67
2:A:451:GLU:O	2:A:454:PRO:HD2	1.95	0.67
1:D:1:G:C2'	1:D:2:G:C5'	2.72	0.67
1:D:63:C:O2'	1:D:64:G:H5'	1.95	0.66
2:A:109:PRO:HG3	2:A:120:LYS:HE2	1.76	0.66
2:B:296:GLY:O	2:B:404:ARG:NH1	2.29	0.66
2:B:429:LEU:HB3	2:B:438:TRP:HB3	1.78	0.66
2:B:168:THR:HG23	2:B:169:PRO:HD2	1.76	0.66
1:C:66:C:H2'	1:C:67:C:C6	2.29	0.66
1:D:70:U:H2'	1:D:71:C:C6	2.30	0.66
2:B:329:LEU:HA	2:B:333:GLU:OE1	1.94	0.66
1:C:48:C:H4'	1:C:49:G:OP2	1.96	0.66
2:A:302:VAL:HG12	2:A:305:LEU:HD12	1.76	0.66
2:B:354:VAL:HG21	2:B:381:ARG:O	1.96	0.66
1:D:12:U:H2'	1:D:13:C:O4'	1.95	0.66
1:D:30:G:H2'	1:D:31:C:H6	1.60	0.66
2:A:443:HIS:CD2	2:A:444:PRO:HD2	2.31	0.66
1:D:1:G:H2'	1:D:2:G:C5'	2.25	0.66
2:B:127:ARG:CZ	2:B:137:ARG:HH22	2.09	0.66
2:B:268:VAL:HG12	2:B:269:GLU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:LYS:CG	2:B:328:ALA:H	2.09	0.66
1:D:9:A:H5''	1:D:46:G7M:H22	1.60	0.65
2:B:497:LEU:HB3	2:B:499:ILE:CD1	2.26	0.65
1:D:30:G:H2'	1:D:31:C:C6	2.31	0.65
2:A:115:ARG:HH11	2:A:117:GLU:CD	1.99	0.65
2:B:221:CYS:SG	2:B:237:GLN:HG3	2.37	0.65
2:B:487:PRO:HG3	2:B:515:LEU:HB3	1.78	0.65
1:D:11:U:H2'	1:D:12:U:C6	2.31	0.65
2:A:227:LEU:CA	2:A:231:ARG:HB2	2.26	0.65
1:D:34:QUO:H14	2:B:51:HIS:CE1	2.32	0.65
1:D:63:C:H2'	1:D:64:G:C8	2.32	0.65
2:A:115:ARG:HD2	2:A:117:GLU:OE2	1.97	0.65
1:C:71:C:H2'	1:C:72:C:H6	1.60	0.64
2:B:214:ARG:NH1	3:B:2066:HOH:O	2.30	0.64
2:B:276:ARG:HG3	2:B:422:TRP:CB	2.27	0.64
2:A:76:ARG:HG2	2:A:76:ARG:NH1	2.11	0.64
2:B:206:MET:HE1	2:B:510:PHE:HD1	1.62	0.64
2:B:313:VAL:HG12	2:B:314:PHE:N	2.12	0.64
1:C:61:C:HO2'	1:C:62:C:H5'	1.62	0.64
1:D:8:4SU:C5'	1:D:49:G:OP2	2.45	0.64
2:A:42:ARG:HD3	2:A:145:ARG:HH22	1.59	0.64
2:B:27:ARG:NH1	2:B:115:ARG:NE	2.43	0.64
1:C:21:A:O2'	1:C:22:G:C8	2.48	0.64
2:B:227:LEU:HA	2:B:231:ARG:HB2	1.78	0.64
1:C:1:G:H2'	1:C:2:G:H8	1.62	0.64
2:B:281:GLU:CG	2:B:285:ARG:HD3	2.28	0.64
2:B:321:LYS:O	2:B:388:PHE:HA	1.98	0.64
2:B:325:LEU:O	2:B:384:ASP:HB3	1.96	0.64
1:C:28:C:H2'	1:C:29:U:C6	2.33	0.64
2:A:39:LEU:HB3	2:A:46:VAL:HG23	1.80	0.64
2:B:6:TYR:HB2	2:B:9:SER:OG	1.98	0.64
1:C:28:C:H2'	1:C:29:U:H6	1.62	0.63
1:D:2:G:C2	1:D:3:A:C4	2.85	0.63
2:A:36:PHE:CD2	2:A:49:VAL:HG23	2.32	0.63
2:B:68:VAL:HB	2:B:101:ALA:HB3	1.81	0.63
1:C:2:G:N1	1:C:72:C:N4	2.46	0.63
2:B:77:LEU:HD23	2:B:89:ARG:O	1.98	0.63
2:B:226:ASP:C	2:B:228:ARG:H	2.01	0.63
2:A:455:LEU:HB2	2:A:463:VAL:HG22	1.78	0.63
2:B:109:PRO:HG2	2:B:120:LYS:HD3	1.78	0.63
2:A:359:PHE:HB2	2:A:364:ALA:HB1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:LEU:HD23	2:B:471:VAL:HG21	1.80	0.63
2:B:293:LEU:HD11	2:B:421:LEU:HD13	1.80	0.63
1:C:24:A:H2'	1:C:25:U:O4'	1.99	0.63
2:B:312:ARG:HH11	2:B:312:ARG:HA	1.63	0.63
2:A:576:MET:HB2	2:B:578:VAL:HG21	1.81	0.62
1:D:38:C:OP2	2:B:27:ARG:CZ	2.47	0.62
2:A:240:LEU:HD22	2:A:525:ILE:CG2	2.29	0.62
2:B:41:ASP:O	2:B:43:GLU:N	2.32	0.62
2:A:168:THR:HG23	2:A:169:PRO:CD	2.29	0.62
2:A:172:THR:HG22	2:A:173:LYS:H	1.64	0.62
2:A:534:ALA:O	2:A:537:THR:HG22	2.00	0.62
1:C:4:G:N2	1:C:70:U:O2	2.33	0.62
1:D:2:G:C6	1:D:3:A:C6	2.88	0.62
2:A:277:LEU:HD12	2:A:421:LEU:CD1	2.30	0.62
2:B:166:VAL:CG1	2:B:207:LEU:HD21	2.28	0.62
2:A:251:LEU:HD12	2:A:276:ARG:NH2	2.14	0.62
2:A:266:LEU:HD11	2:A:536:MET:HB3	1.82	0.62
2:A:579:ARG:CB	2:A:580:PRO:HD3	2.29	0.62
2:B:329:LEU:HD22	2:B:333:GLU:HB3	1.82	0.62
2:A:302:VAL:HG12	2:A:305:LEU:CD1	2.30	0.62
2:B:323:LEU:CB	2:B:400:LEU:HD11	2.25	0.62
2:A:109:PRO:HG2	2:A:120:LYS:HE2	1.80	0.62
2:A:326:PRO:HD2	2:A:411:LEU:CD2	2.30	0.62
2:A:490:GLN:HG3	2:A:494:PHE:CE1	2.35	0.61
1:C:12:U:H5	3:C:2011:HOH:O	1.83	0.61
2:A:244:PHE:CE2	2:A:521:PRO:HD2	2.34	0.61
2:A:168:THR:HB	2:A:217:GLN:NE2	2.01	0.61
2:B:327:LYS:CG	2:B:328:ALA:N	2.63	0.61
2:B:332:LYS:O	2:B:335:ALA:HB3	2.01	0.61
2:B:354:VAL:CG2	2:B:384:ASP:H	2.13	0.61
2:B:354:VAL:HG23	2:B:383:GLY:H	1.63	0.61
1:C:30:G:O2'	1:C:31:C:H5'	2.00	0.61
2:A:533:LEU:O	2:A:537:THR:HB	2.00	0.61
1:D:28:C:O2'	1:D:29:U:H5'	2.01	0.61
1:D:70:U:C6	1:D:70:U:H3'	2.35	0.61
2:A:155:TRP:CH2	2:A:165:GLN:HG3	2.35	0.61
2:B:336:GLU:O	2:B:339:GLU:N	2.32	0.61
2:B:556:ASP:CG	2:B:559:THR:HB	2.20	0.61
2:B:74:LEU:HD23	2:B:76:ARG:HH21	1.64	0.61
2:B:155:TRP:CZ2	2:B:165:GLN:HG3	2.35	0.61
2:A:483:ARG:NE	2:A:523:GLY:HA2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:HIS:HB2	2:B:446:THR:OG1	2.00	0.61
2:B:320:VAL:HG22	2:B:390:ALA:HB1	1.81	0.61
2:B:226:ASP:OD1	2:B:228:ARG:CG	2.48	0.60
2:B:290:LYS:N	2:B:291:PRO:HD3	2.16	0.60
2:A:25:VAL:HG21	2:A:63:VAL:CG1	2.31	0.60
2:B:139:ARG:NH2	2:B:544:GLU:HB3	2.15	0.60
2:B:440:TYR:HD1	2:B:442:HIS:O	1.83	0.60
2:B:525:ILE:HG12	2:B:526:ALA:H	1.65	0.60
2:A:7:ALA:HA	2:A:21:LEU:HD13	1.83	0.60
2:B:313:VAL:HG12	2:B:314:PHE:HD1	1.65	0.60
2:B:566:PRO:O	2:B:569:GLN:N	2.32	0.60
2:A:17:GLU:O	2:A:75:VAL:HG23	2.00	0.60
2:B:372:GLU:O	2:B:376:GLN:HB2	2.02	0.60
2:A:81:PRO:O	2:A:83:PRO:HD3	2.01	0.60
2:A:213:ASP:OD1	2:B:3:ARG:NH1	2.31	0.60
2:A:215:TYR:CE1	2:A:217:GLN:HB3	2.37	0.60
2:B:311:PHE:HB2	2:B:366:PHE:CD2	2.35	0.60
2:B:369:PRO:O	2:B:370:VAL:HG13	2.02	0.60
1:C:7:G:C2	1:C:49:G:C8	2.90	0.60
1:D:1:G:O2'	1:D:2:G:H5'	2.02	0.60
1:D:5:C:O2'	1:D:6:G:H5'	2.01	0.60
2:B:108:PHE:HD2	2:B:126:LEU:HD13	1.67	0.60
2:B:262:PHE:CZ	2:B:536:MET:HG2	2.36	0.60
2:B:202:LEU:CD2	2:B:445:PHE:HE1	2.09	0.60
2:B:205:GLN:HE22	2:B:445:PHE:HD1	1.48	0.60
2:A:499:ILE:HG23	2:A:503:GLU:HG3	1.84	0.59
2:A:501:GLU:O	2:A:505:ARG:HD3	2.01	0.59
2:A:132:TYR:CD2	2:B:206:MET:HE2	2.37	0.59
2:A:452:ASP:OD1	2:A:464:ARG:NE	2.35	0.59
2:B:1:MET:H1	2:B:70:ARG:HD3	1.65	0.59
2:B:51:HIS:O	2:B:57:TYR:HB2	2.03	0.59
2:B:336:GLU:O	2:B:337:LEU:C	2.39	0.59
2:B:57:TYR:HA	2:B:60:ALA:HB3	1.82	0.59
2:B:315:GLN:HE21	2:B:316:GLU:HG2	1.68	0.59
1:C:4:G:H2'	1:C:5:C:O4'	2.02	0.59
1:D:2:G:H2'	1:D:3:A:H8	1.67	0.59
2:B:299:LEU:HD23	2:B:299:LEU:H	1.67	0.59
2:A:154:ILE:HG21	2:A:238:LEU:HD13	1.83	0.59
2:A:568:GLU:OE1	2:A:571:ARG:NH1	2.33	0.59
1:D:49:G:O2'	1:D:50:C:H5'	2.03	0.59
2:A:497:LEU:O	2:A:499:ILE:HG13	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:ARG:HG2	2:B:91:GLU:OE1	2.03	0.59
2:B:331:ARG:HA	2:B:331:ARG:NE	2.02	0.59
2:B:491:ALA:O	2:B:495:ARG:HG3	2.02	0.59
2:A:254:ASN:HD21	2:A:525:ILE:CG2	2.13	0.59
2:B:39:LEU:HG	2:B:48:LEU:HD11	1.85	0.59
2:B:354:VAL:HG23	2:B:384:ASP:H	1.68	0.59
1:C:2:G:H2'	1:C:3:A:H8	1.64	0.58
1:D:1:G:C3'	1:D:2:G:H5'	2.25	0.58
2:A:146:LEU:HD12	2:A:149:ARG:NH1	2.18	0.58
2:B:483:ARG:HG2	2:B:523:GLY:HA2	1.83	0.58
2:A:331:ARG:H	2:A:331:ARG:NE	1.91	0.58
2:B:119:GLU:OE2	2:B:137:ARG:HD2	2.02	0.58
2:B:386:LEU:HD13	2:B:388:PHE:CZ	2.37	0.58
1:D:2:G:H2'	1:D:3:A:C8	2.39	0.58
2:B:330:SER:OG	2:B:331:ARG:N	2.36	0.58
1:D:38:C:N3	2:B:31:LEU:HD13	2.18	0.58
2:A:371:ARG:HG3	2:A:375:LEU:HD23	1.85	0.58
2:B:201:GLN:HG3	2:B:202:LEU:H	1.67	0.58
1:C:1:G:H2'	1:C:2:G:C8	2.38	0.58
2:B:235:PHE:CD1	2:B:235:PHE:N	2.71	0.58
2:A:135:LEU:HD23	2:A:140:MET:HB3	1.86	0.58
2:A:220:ARG:NH1	2:A:234:ASP:OD1	2.35	0.58
2:B:238:LEU:HB3	2:B:527:TRP:HB2	1.85	0.58
2:B:277:LEU:CD1	2:B:281:GLU:HG2	2.31	0.58
1:D:3:A:C2	1:D:4:G:C5	2.92	0.58
2:A:155:TRP:CZ2	2:A:165:GLN:HG3	2.39	0.58
2:A:186:TYR:CG	2:B:562:PRO:HG3	2.38	0.58
2:A:440:TYR:H	2:A:440:TYR:HD2	1.50	0.58
2:B:180:ARG:NH1	2:B:224:ASP:O	2.36	0.58
1:D:37:2MA:C5'	2:B:27:ARG:NH1	2.55	0.58
2:B:556:ASP:OD1	2:B:559:THR:HB	2.03	0.58
1:D:8:4SU:C4'	1:D:49:G:OP2	2.52	0.58
1:D:15:G:H5''	1:D:16:H2U:H5'	1.86	0.58
1:D:36:C:H41	2:B:80:GLU:HB3	1.65	0.58
1:D:71:C:H2'	1:D:72:C:O4'	2.04	0.58
2:A:139:ARG:NH2	2:A:537:THR:HG23	2.18	0.58
2:A:290:LYS:HD3	3:A:2048:HOH:O	2.03	0.58
2:B:39:LEU:HB2	2:B:48:LEU:HD21	1.85	0.58
2:A:438:TRP:CZ3	2:A:460:PRO:HG2	2.39	0.57
2:B:184:VAL:HB	2:B:194:TYR:HB2	1.86	0.57
2:B:276:ARG:NH1	3:B:2081:HOH:O	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:VAL:HG22	2:B:390:ALA:CB	2.34	0.57
2:A:303:GLY:N	2:A:304:PRO:HD2	2.19	0.57
2:A:252:GLU:OE1	2:A:256:ARG:HD3	2.03	0.57
2:B:7:ALA:O	2:B:10:LEU:HD13	2.04	0.57
2:A:109:PRO:HG3	2:A:120:LYS:CE	2.34	0.57
2:A:532:LEU:O	2:A:536:MET:HG3	2.04	0.57
2:B:227:LEU:O	2:B:229:ALA:O	2.23	0.57
2:B:341:ALA:O	2:B:344:HIS:O	2.22	0.57
2:B:449:HIS:CD2	2:B:464:ARG:HH12	2.22	0.57
2:B:499:ILE:HG22	2:B:504:GLN:HG3	1.86	0.57
2:A:428:LEU:HD22	2:A:448:PRO:HB3	1.87	0.57
2:B:205:GLN:HB3	2:B:522:HIS:HE2	1.69	0.57
2:B:432:ASP:HB2	2:B:439:THR:OG1	2.04	0.57
2:B:499:ILE:HD12	2:B:499:ILE:N	2.18	0.57
2:B:176:PRO:HB2	2:B:507:LYS:HE2	1.87	0.57
2:B:257:LEU:HD13	2:B:527:TRP:CH2	2.39	0.57
1:D:47:U:H1'	1:D:48:C:OP1	2.05	0.57
2:A:40:ARG:HG2	2:A:41:ASP:N	2.19	0.57
2:A:556:ASP:OD1	2:A:559:THR:HB	2.04	0.57
2:B:421:LEU:HD23	2:B:471:VAL:CG2	2.35	0.57
2:A:7:ALA:CB	2:A:21:LEU:HD13	2.35	0.57
2:A:176:PRO:HD2	2:A:507:LYS:HG2	1.86	0.57
2:B:458:LYS:C	2:B:460:PRO:HD3	2.25	0.57
1:C:31:C:H2'	1:C:32:C:C6	2.40	0.57
1:C:70:U:H2'	1:C:71:C:C6	2.40	0.57
2:A:278:SER:HA	2:A:424:VAL:O	2.05	0.57
2:A:341:ALA:O	2:A:344:HIS:O	2.22	0.57
2:B:289:ASP:C	2:B:291:PRO:HD3	2.25	0.57
2:B:525:ILE:HG12	2:B:526:ALA:N	2.19	0.57
2:B:556:ASP:O	2:B:560:GLY:N	2.28	0.57
1:D:63:C:H6	1:D:63:C:O5'	1.87	0.56
2:A:106:PRO:HB2	2:A:108:PHE:O	2.05	0.56
1:D:70:U:H2'	1:D:71:C:C5	2.40	0.56
2:A:104:LYS:HD3	2:B:516:GLU:HG2	1.87	0.56
2:A:447:SER:HA	2:A:484:ILE:HD11	1.87	0.56
2:A:452:ASP:HA	2:A:455:LEU:HD12	1.87	0.56
2:B:27:ARG:HD2	2:B:115:ARG:HH21	1.70	0.56
2:B:36:PHE:CE2	2:B:49:VAL:HG22	2.40	0.56
2:B:40:ARG:HG3	2:B:45:LEU:HD23	1.87	0.56
2:B:421:LEU:HB3	2:B:471:VAL:CG2	2.36	0.56
2:B:166:VAL:HB	2:B:215:TYR:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:G:O2'	1:C:53:G:H5'	2.04	0.56
2:A:563:SER:O	2:B:193:PHE:N	2.31	0.56
2:B:108:PHE:CD2	2:B:126:LEU:HD13	2.40	0.56
1:D:34:QUO:C4'	1:D:35:U:H5'	2.22	0.56
2:B:230:ASP:HB3	2:B:531:ARG:HH22	1.69	0.56
1:C:44:G:O2'	1:C:45:G:H5'	2.06	0.56
1:C:34:QUO:H4'	1:C:35:U:C5'	2.34	0.56
2:A:45:LEU:O	2:A:87:THR:OG1	2.23	0.56
2:B:112:ALA:CB	2:B:119:GLU:HG2	2.35	0.56
1:D:13:C:O2'	1:D:14:A:H5'	2.06	0.56
1:D:36:C:O2'	2:B:27:ARG:NH2	2.39	0.56
2:B:227:LEU:HB3	2:B:231:ARG:O	2.05	0.56
2:B:306:PHE:CD2	2:B:314:PHE:HD2	2.24	0.56
2:B:359:PHE:CE1	2:B:371:ARG:HG2	2.40	0.56
1:D:4:G:H2'	1:D:5:C:O4'	2.06	0.56
2:A:235:PHE:HB2	2:A:530:ASP:OD2	2.05	0.56
2:A:419:ARG:HG3	2:A:419:ARG:HH11	1.71	0.56
2:A:554:GLY:O	2:B:194:TYR:OH	2.22	0.56
2:B:331:ARG:O	2:B:335:ALA:HB2	2.05	0.56
2:B:374:LEU:O	2:B:378:THR:HG23	2.05	0.56
1:C:8:4SU:H5''	1:C:49:G:OP2	2.04	0.55
2:A:6:TYR:CE2	2:B:213:ASP:OD1	2.59	0.55
2:A:154:ILE:HD13	2:A:238:LEU:HD13	1.89	0.55
2:B:268:VAL:HG12	2:B:269:GLU:N	2.21	0.55
2:B:344:HIS:O	2:B:346:ALA:N	2.39	0.55
1:D:51:G:O2'	1:D:52:G:H5'	2.06	0.55
2:A:42:ARG:CD	2:A:145:ARG:NH2	2.65	0.55
2:B:532:LEU:O	2:B:536:MET:HG3	2.06	0.55
2:B:12:GLU:O	2:B:15:VAL:HG23	2.06	0.55
1:D:59:G:H2'	1:D:60:U:H5'	1.88	0.55
2:B:2:ARG:HG2	3:B:2085:HOH:O	2.06	0.55
2:B:299:LEU:C	2:B:300:LYS:HG2	2.26	0.55
2:B:315:GLN:HG3	2:B:316:GLU:N	2.20	0.55
2:B:483:ARG:HH21	2:B:524:GLY:N	2.03	0.55
1:D:43:G:H2'	1:D:44:G:C8	2.42	0.55
2:A:293:LEU:O	2:A:419:ARG:NH1	2.39	0.55
2:A:176:PRO:HD2	2:A:507:LYS:HE2	1.88	0.55
2:A:462:ARG:O	2:A:462:ARG:HG3	2.07	0.55
2:B:155:TRP:HH2	2:B:165:GLN:HE21	1.55	0.55
2:B:302:VAL:O	2:B:303:GLY:C	2.45	0.55
1:C:20(A):H2U:H3'	1:C:21:A:H5'	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:292:ASP:OD2	2:A:294:ARG:NH1	2.40	0.55
2:A:198:GLN:O	2:A:221:CYS:HB3	2.06	0.55
2:A:325:LEU:HD12	2:A:329:LEU:HD11	1.87	0.55
1:D:11:U:H2'	1:D:12:U:H6	1.72	0.55
2:A:173:LYS:HB2	2:B:559:THR:CG2	2.37	0.55
2:B:227:LEU:H	2:B:227:LEU:CD2	1.94	0.55
2:B:361:GLY:O	2:B:364:ALA:N	2.35	0.54
2:A:168:THR:CB	2:A:217:GLN:HE22	2.05	0.54
2:A:251:LEU:HD22	2:A:422:TRP:CD2	2.42	0.54
2:A:433:GLU:O	2:A:435:GLU:N	2.40	0.54
2:B:209:VAL:HG22	2:B:519:ALA:CB	2.38	0.54
1:C:39:G:O2'	1:C:40:C:H5'	2.08	0.54
2:B:537:THR:HG23	2:B:539:SER:HG	1.72	0.54
2:A:450:PRO:O	2:A:453:LEU:HB2	2.07	0.54
2:B:208:MET:HG3	2:B:522:HIS:CD2	2.42	0.54
2:B:311:PHE:CE1	2:B:313:VAL:HB	2.42	0.54
2:B:411:LEU:HB2	2:B:413:LEU:HD11	1.88	0.54
2:A:222:PHE:CD1	2:A:222:PHE:N	2.75	0.54
2:B:307:ARG:CD	2:B:315:GLN:O	2.54	0.54
2:B:323:LEU:HD12	2:B:324:ALA:H	1.71	0.54
1:C:3:A:H2'	1:C:4:G:H8	1.72	0.54
1:D:59:G:C2'	1:D:60:U:H5'	2.37	0.54
2:A:111:ASP:OD1	2:A:115:ARG:NH2	2.41	0.54
2:B:277:LEU:O	2:B:423:VAL:HA	2.06	0.54
2:B:542:ILE:O	2:B:545:VAL:HG22	2.07	0.54
2:A:508:PHE:HB2	2:A:512:LEU:CD2	2.38	0.54
2:B:551:ASN:O	2:B:553:GLU:N	2.40	0.54
2:A:146:LEU:CD1	2:A:149:ARG:HH12	2.21	0.54
2:A:457:GLU:OE2	2:A:492:ARG:HD3	2.07	0.54
2:A:505:ARG:N	2:A:505:ARG:CD	2.71	0.54
2:B:163:PHE:HA	2:B:214:ARG:CG	2.37	0.54
2:B:449:HIS:ND1	2:B:451:GLU:HB2	2.22	0.54
2:A:419:ARG:HG3	2:A:419:ARG:NH1	2.22	0.54
2:A:578:VAL:HG11	2:B:576:MET:CB	2.38	0.54
1:C:53:G:O2'	1:C:54:5MU:H5''	2.08	0.54
2:B:326:PRO:HD2	2:B:411:LEU:CD1	2.38	0.54
1:C:68:G:H4'	2:A:125:GLU:OE1	2.08	0.53
2:A:71:ALA:HB1	2:A:94:LEU:CD2	2.38	0.53
2:A:440:TYR:HB3	2:A:497:LEU:CD1	2.38	0.53
2:B:292:ASP:CG	2:B:294:ARG:HE	2.12	0.53
2:A:418:PHE:O	2:A:419:ARG:HD2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:451:GLU:O	2:A:453:LEU:N	2.42	0.53
2:A:568:GLU:OE1	2:A:571:ARG:HD3	2.08	0.53
2:B:182:PHE:CZ	2:B:233:PRO:HB3	2.43	0.53
2:B:228:ARG:HG2	2:B:228:ARG:HH11	1.74	0.53
2:B:327:LYS:HG3	2:B:328:ALA:H	1.72	0.53
2:B:392:PRO:HB2	2:B:395:VAL:HG23	1.90	0.53
2:A:189:GLU:HB3	2:A:192:LEU:HD13	1.91	0.53
2:A:461:GLY:O	2:A:463:VAL:N	2.41	0.53
2:A:137:ARG:O	2:A:141:GLN:HG3	2.08	0.53
2:A:517:TYR:CZ	2:B:104:LYS:HE2	2.43	0.53
2:B:36:PHE:CD2	2:B:49:VAL:HG22	2.44	0.53
1:D:2:G:C2	1:D:3:A:C5	2.96	0.53
2:A:283:MET:O	2:A:287:GLY:HA2	2.08	0.53
2:A:543:ARG:HH21	2:A:552:LYS:HG3	1.73	0.53
2:B:109:PRO:CG	2:B:120:LYS:HD3	2.39	0.53
2:A:321:LYS:HB3	2:A:400:LEU:HD12	1.91	0.53
2:A:513:GLU:O	2:A:516:GLU:HB2	2.08	0.53
2:B:89:ARG:HG3	2:B:89:ARG:HH11	1.74	0.53
2:A:42:ARG:HD3	2:A:145:ARG:HH21	1.69	0.53
2:A:302:VAL:CG1	2:A:305:LEU:HD12	2.39	0.53
2:A:324:ALA:HB2	2:A:386:LEU:CD2	2.38	0.53
2:A:457:GLU:OE1	2:A:492:ARG:NH1	2.38	0.53
2:A:472:LEU:HD23	2:A:535:LEU:HD12	1.90	0.53
2:A:537:THR:HG23	2:A:539:SER:H	1.74	0.53
2:B:39:LEU:CB	2:B:48:LEU:HD21	2.39	0.53
2:B:551:ASN:ND2	2:B:557:PRO:HG3	2.24	0.53
2:A:63:VAL:HA	2:A:67:TRP:CE3	2.43	0.53
2:A:163:PHE:CD2	2:A:214:ARG:HB2	2.44	0.53
2:A:230:ASP:OD1	2:A:542:ILE:N	2.38	0.53
2:B:127:ARG:CZ	2:B:137:ARG:NH2	2.70	0.53
2:B:408:ALA:CA	2:B:413:LEU:HD13	2.25	0.53
2:A:112:ALA:HA	2:A:115:ARG:NH1	2.24	0.53
2:A:235:PHE:CD1	2:A:235:PHE:N	2.77	0.53
2:A:438:TRP:CZ2	2:A:460:PRO:HB2	2.44	0.53
2:B:223:ARG:CD	2:B:225:GLU:HG2	2.38	0.53
2:B:430:GLU:HG3	2:B:431:TRP:N	2.24	0.53
1:D:66:C:H2'	1:D:67:C:C6	2.43	0.52
2:B:72:LYS:HB3	2:B:96:ALA:HB3	1.91	0.52
2:B:290:LYS:HA	2:B:471:VAL:HG11	1.90	0.52
2:A:45:LEU:HD21	2:A:114:TRP:HB3	1.91	0.52
2:B:166:VAL:HB	2:B:215:TYR:HD1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:U:C2'	1:C:48:C:OP1	2.57	0.52
2:A:4:THR:HG23	2:A:20:VAL:HB	1.92	0.52
2:A:179:ALA:HA	2:A:225:GLU:OE2	2.08	0.52
2:A:226:ASP:C	2:A:228:ARG:N	2.61	0.52
2:A:475:VAL:HG11	2:A:531:ARG:HG2	1.92	0.52
2:B:108:PHE:HD2	2:B:126:LEU:CD1	2.22	0.52
2:B:237:GLN:HA	2:B:527:TRP:O	2.09	0.52
2:B:311:PHE:CD1	2:B:311:PHE:C	2.81	0.52
1:C:11:U:H2'	1:C:12:U:C6	2.45	0.52
1:D:2:G:N1	1:D:3:A:C5	2.78	0.52
2:A:194:TYR:OH	2:B:554:GLY:O	2.23	0.52
2:A:571:ARG:NE	2:B:580:PRO:O	2.43	0.52
1:D:46:G7M:H4'	1:D:47:U:OP1	2.09	0.52
2:A:452:ASP:OD2	2:A:464:ARG:HD3	2.10	0.52
2:B:409:ASP:O	2:B:412:GLY:N	2.29	0.52
1:C:37:2MA:H4'	2:A:27:ARG:NH1	2.25	0.52
1:D:70:U:C6	1:D:70:U:C3'	2.93	0.52
2:A:230:ASP:HB3	2:A:531:ARG:HH22	1.74	0.52
2:A:563:SER:CB	2:B:173:LYS:HE3	2.39	0.52
2:B:364:ALA:O	2:B:365:LYS:C	2.46	0.52
2:A:49:VAL:HG12	2:A:93:GLU:HA	1.91	0.52
2:B:115:ARG:NH1	2:B:117:GLU:CD	2.64	0.52
2:B:493:VAL:O	2:B:497:LEU:HD13	2.09	0.52
2:B:513:GLU:CG	3:B:2071:HOH:O	2.58	0.52
2:B:206:MET:HE1	2:B:510:PHE:CD1	2.45	0.51
2:B:406:ARG:HG3	2:B:410:LEU:HG	1.92	0.51
2:B:410:LEU:C	2:B:411:LEU:HD23	2.30	0.51
2:B:429:LEU:HA	2:B:439:THR:O	2.10	0.51
2:A:324:ALA:HB2	2:A:386:LEU:HD23	1.91	0.51
2:B:27:ARG:HD3	2:B:115:ARG:NE	2.24	0.51
2:B:59:THR:C	2:B:61:GLU:H	2.13	0.51
2:B:76:ARG:NH1	2:B:93:GLU:OE1	2.43	0.51
2:B:200:PRO:HG2	2:B:239:ASP:OD1	2.11	0.51
2:B:470:LEU:O	2:B:477:VAL:HG22	2.11	0.51
1:C:34:QUO:H5'	2:A:31:LEU:HD23	1.91	0.51
2:A:337:LEU:CD1	2:A:387:LEU:HD21	2.41	0.51
2:B:182:PHE:HZ	2:B:233:PRO:HB3	1.75	0.51
2:B:290:LYS:N	2:B:291:PRO:CD	2.72	0.51
2:B:368:GLU:N	2:B:369:PRO:CD	2.73	0.51
1:C:20:H2U:H5'	1:C:20(A):H2U:H5''	1.92	0.51
2:B:327:LYS:HG2	2:B:328:ALA:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:ASP:OD1	2:B:462:ARG:HB2	2.11	0.51
1:C:27:C:H2'	1:C:28:C:C6	2.46	0.51
1:C:64:G:H2'	1:C:65:PSU:O4'	2.11	0.51
2:B:28:ARG:NE	2:B:64:ARG:HE	2.08	0.51
2:B:163:PHE:HA	2:B:214:ARG:HG2	1.92	0.51
2:B:340:VAL:HG12	2:B:341:ALA:N	2.26	0.51
1:D:18:G:H21	1:D:58:A:H5'	1.76	0.51
1:D:44:G:O2'	1:D:45:G:H5'	2.11	0.51
2:A:440:TYR:HE1	2:A:444:PRO:HD3	1.72	0.51
2:B:48:LEU:HD23	2:B:48:LEU:N	2.25	0.51
2:B:227:LEU:HD13	2:B:227:LEU:N	2.24	0.51
2:A:252:GLU:OE1	2:A:256:ARG:CD	2.59	0.51
2:A:561:ALA:HA	2:A:562:PRO:C	2.31	0.51
1:C:53:G:H2'	1:C:54:5MU:H6	1.74	0.51
2:A:457:GLU:OE1	2:A:492:ARG:HD3	2.11	0.51
2:A:543:ARG:NH2	2:A:552:LYS:HG3	2.25	0.51
2:B:164:VAL:O	2:B:166:VAL:HG23	2.11	0.51
2:B:320:VAL:HG13	2:B:390:ALA:HB2	1.93	0.51
2:B:325:LEU:HD12	2:B:387:LEU:HD21	1.93	0.51
2:B:389:VAL:CG2	2:B:400:LEU:HD23	2.41	0.51
1:D:8:4SU:C1'	1:D:48:C:H1'	2.41	0.51
1:D:54:5MU:C5M	1:D:55:PSU:C2	2.94	0.51
2:A:182:PHE:HB2	2:A:196:LEU:HD12	1.93	0.51
2:A:449:HIS:CE1	2:A:451:GLU:HG3	2.46	0.51
2:A:567:GLU:HG3	2:A:568:GLU:N	2.25	0.51
2:B:451:GLU:O	2:B:454:PRO:HD2	2.11	0.51
2:B:456:LEU:HG	2:B:496:LEU:HD22	1.93	0.51
2:A:10:LEU:HD23	2:A:46:VAL:CG1	2.39	0.50
2:A:175:THR:HB	2:A:507:LYS:CE	2.41	0.50
2:B:566:PRO:O	2:B:567:GLU:C	2.50	0.50
2:B:566:PRO:O	2:B:568:GLU:N	2.45	0.50
2:B:7:ALA:O	2:B:10:LEU:CD1	2.59	0.50
2:B:168:THR:HG23	2:B:169:PRO:CD	2.41	0.50
2:B:209:VAL:HG22	2:B:519:ALA:HB2	1.94	0.50
1:C:2:G:H1	1:C:71:C:N4	2.08	0.50
2:A:154:ILE:HG21	2:A:238:LEU:CD1	2.42	0.50
1:C:27:C:H2'	1:C:28:C:H6	1.77	0.50
1:C:36:C:C2	2:A:78:ARG:NH2	2.79	0.50
2:A:39:LEU:HG	2:A:48:LEU:HD11	1.91	0.50
2:B:4:THR:C	2:B:5:HIS:ND1	2.65	0.50
2:B:7:ALA:O	2:B:46:VAL:HB	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:TRP:CH2	2:B:102:GLU:HG2	2.46	0.50
2:B:172:THR:OG1	2:B:173:LYS:N	2.42	0.50
2:B:311:PHE:O	2:B:312:ARG:C	2.48	0.50
2:B:361:GLY:O	2:B:363:VAL:N	2.45	0.50
1:C:12:U:H2'	1:C:13:C:O4'	2.10	0.50
1:D:63:C:H2'	1:D:64:G:H8	1.74	0.50
2:A:186:TYR:CD2	2:B:562:PRO:HG3	2.46	0.50
2:B:201:GLN:HA	2:B:204:LYS:CD	2.42	0.50
1:C:4:G:N2	1:C:70:U:C2	2.80	0.50
1:D:2:G:N3	1:D:3:A:C8	2.79	0.50
2:A:42:ARG:CD	2:A:145:ARG:HH21	2.25	0.50
2:A:558:LEU:HD21	2:B:206:MET:SD	2.52	0.50
2:B:115:ARG:NH1	2:B:117:GLU:OE2	2.45	0.50
2:B:354:VAL:HG23	2:B:383:GLY:N	2.27	0.50
2:B:435:GLU:O	2:B:436:GLU:OE1	2.29	0.50
2:B:483:ARG:HH21	2:B:524:GLY:CA	2.24	0.50
2:A:1:MET:HG2	2:A:1:MET:O	2.11	0.50
1:C:20(A):H2U:H3'	1:C:21:A:C5'	2.42	0.50
1:D:29:U:H2'	1:D:30:G:H8	1.75	0.50
2:A:290:LYS:N	2:A:291:PRO:HD3	2.27	0.50
2:B:147:ARG:NH1	2:B:533:LEU:HD12	2.26	0.50
2:B:429:LEU:HB3	2:B:438:TRP:CB	2.40	0.50
1:C:53:G:C2	1:C:62:C:C2	3.00	0.50
2:A:4:THR:CG2	2:A:20:VAL:HB	2.42	0.49
2:A:112:ALA:HB1	2:A:117:GLU:HB2	1.94	0.49
2:A:562:PRO:HG3	2:B:186:TYR:CG	2.47	0.49
2:B:223:ARG:HD2	2:B:225:GLU:HG2	1.93	0.49
2:B:255:GLU:CG	2:B:422:TRP:HE1	2.22	0.49
2:B:266:LEU:HB2	2:B:268:VAL:HG23	1.93	0.49
2:B:334:VAL:HG11	2:B:351:TRP:CD1	2.47	0.49
1:C:3:A:H2'	1:C:4:G:O4'	2.12	0.49
2:A:7:ALA:HB1	2:A:46:VAL:HG22	1.94	0.49
2:B:351:TRP:HA	2:B:386:LEU:O	2.12	0.49
2:B:18:GLU:HA	2:B:74:LEU:HA	1.94	0.49
2:A:326:PRO:CD	2:A:411:LEU:HD21	2.41	0.49
2:A:358:GLY:HA2	2:A:371:ARG:HD3	1.93	0.49
2:A:499:ILE:HA	2:A:503:GLU:OE1	2.12	0.49
2:B:325:LEU:HD22	2:B:411:LEU:HD11	1.95	0.49
2:B:570:LEU:HD13	2:B:575:LEU:O	2.12	0.49
2:B:325:LEU:O	2:B:384:ASP:CB	2.60	0.49
1:C:47:U:H2'	1:C:50:C:OP1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:LEU:HB2	2:A:48:LEU:HG	1.95	0.49
2:A:77:LEU:HD23	2:A:89:ARG:O	2.12	0.49
2:A:251:LEU:HD22	2:A:422:TRP:CE3	2.48	0.49
2:A:457:GLU:CD	2:A:492:ARG:HD3	2.33	0.49
2:B:331:ARG:HE	2:B:331:ARG:CA	2.08	0.49
2:A:539:SER:OG	2:A:544:GLU:HB2	2.13	0.49
2:B:299:LEU:N	2:B:299:LEU:CD2	2.74	0.49
2:B:323:LEU:HD12	2:B:324:ALA:N	2.27	0.49
2:B:543:ARG:HD3	2:B:550:LYS:O	2.13	0.49
2:A:213:ASP:OD1	2:A:214:ARG:HD3	2.12	0.49
2:B:472:LEU:O	2:B:475:VAL:HG23	2.13	0.49
1:C:61:C:C2'	1:C:62:C:H5'	2.43	0.49
2:B:89:ARG:HH11	2:B:89:ARG:CG	2.26	0.49
2:B:291:PRO:HB2	2:B:421:LEU:HD22	1.94	0.49
2:A:455:LEU:CB	2:A:463:VAL:HG22	2.42	0.49
2:B:312:ARG:HH12	2:B:316:GLU:CG	2.26	0.49
2:B:341:ALA:HB2	2:B:403:VAL:CG2	2.43	0.49
2:B:537:THR:O	2:B:538:GLY:C	2.51	0.49
1:D:43:G:H2'	1:D:44:G:H8	1.77	0.48
2:A:21:LEU:HD12	2:A:39:LEU:HD12	1.94	0.48
2:A:155:TRP:O	2:A:156:ASP:C	2.52	0.48
2:A:283:MET:O	2:A:287:GLY:N	2.46	0.48
2:A:490:GLN:HG3	2:A:494:PHE:CD1	2.48	0.48
2:A:514:ALA:HB2	2:B:132:TYR:CZ	2.48	0.48
2:A:546:ILE:O	2:A:547:ALA:C	2.51	0.48
2:B:4:THR:CG2	2:B:20:VAL:HB	2.43	0.48
2:B:119:GLU:OE2	2:B:137:ARG:CD	2.61	0.48
2:B:497:LEU:CB	2:B:499:ILE:CD1	2.91	0.48
2:B:513:GLU:HG2	3:B:2071:HOH:O	2.13	0.48
2:A:241:GLU:OE1	2:A:524:GLY:N	2.46	0.48
2:A:268:VAL:HG12	2:A:269:GLU:N	2.29	0.48
2:A:558:LEU:HD11	2:B:206:MET:CE	2.42	0.48
2:B:134:ASP:CG	2:B:137:ARG:HH21	2.17	0.48
1:D:70:U:C6	1:D:70:U:O5'	2.62	0.48
2:A:74:LEU:HD21	2:A:76:ARG:NH2	2.29	0.48
2:A:311:PHE:HB2	2:A:366:PHE:CD2	2.49	0.48
2:A:359:PHE:HB2	2:A:364:ALA:CB	2.43	0.48
2:B:39:LEU:HD22	2:B:40:ARG:H	1.78	0.48
2:B:69:VAL:HG12	2:B:99:VAL:HA	1.95	0.48
2:B:123:SER:O	2:B:124:GLU:C	2.51	0.48
2:B:155:TRP:O	2:B:159:ASP:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:GLU:O	2:B:343:ARG:N	2.43	0.48
1:D:33:U:C6	2:B:33:GLY:O	2.67	0.48
2:A:36:PHE:CE2	2:A:49:VAL:HG23	2.48	0.48
2:A:63:VAL:HG12	2:A:64:ARG:N	2.29	0.48
2:A:559:THR:CG2	2:B:173:LYS:HB2	2.41	0.48
2:B:120:LYS:H	2:B:120:LYS:CD	2.18	0.48
2:B:434:GLU:O	2:B:436:GLU:N	2.43	0.48
2:A:204:LYS:O	2:A:208:MET:HG2	2.13	0.48
2:B:146:LEU:CD1	2:B:149:ARG:HH12	2.20	0.48
2:B:449:HIS:HD2	2:B:464:ARG:NH1	2.10	0.48
1:C:20:H2U:H5'	1:C:20(A):H2U:C5'	2.43	0.48
1:D:34:QUO:N2	2:B:91:GLU:OE1	2.42	0.48
2:A:452:ASP:O	2:A:455:LEU:HB2	2.14	0.48
2:B:312:ARG:HH12	2:B:316:GLU:HG3	1.77	0.48
2:B:452:ASP:CA	2:B:455:LEU:HD23	2.40	0.48
1:D:66:C:H2'	1:D:67:C:H6	1.78	0.48
2:A:198:GLN:NE2	2:A:223:ARG:HB2	2.29	0.48
2:A:200:PRO:O	2:A:201:GLN:C	2.51	0.48
2:B:28:ARG:NH1	2:B:28:ARG:CG	2.59	0.48
2:B:321:LYS:HG3	2:B:397:ALA:HA	1.96	0.48
2:A:7:ALA:CA	2:A:21:LEU:HD13	2.43	0.48
2:B:78:ARG:HD2	2:B:90:VAL:O	2.13	0.48
2:B:173:LYS:HD3	2:B:174:SER:N	2.29	0.48
1:D:52:G:H2'	1:D:53:G:O4'	2.14	0.48
2:A:105:THR:HA	2:A:106:PRO:HD3	1.77	0.48
2:A:234:ASP:OD1	2:A:234:ASP:O	2.32	0.48
2:A:428:LEU:HA	2:A:465:ALA:HB2	1.96	0.48
2:A:503:GLU:O	2:A:507:LYS:HB2	2.14	0.48
2:B:28:ARG:NE	2:B:64:ARG:NE	2.61	0.48
2:B:202:LEU:HD23	2:B:202:LEU:HA	1.61	0.48
2:B:235:PHE:HE2	2:B:237:GLN:NE2	2.11	0.48
2:B:246:GLU:O	2:B:247:VAL:C	2.52	0.48
1:C:15:G:C5'	1:C:16:H2U:H5'	2.42	0.48
1:C:35:U:O2'	2:A:29:ARG:HD2	2.14	0.48
1:C:49:G:H2'	1:C:50:C:C6	2.49	0.48
1:C:49:G:N2	1:C:50:C:C2	2.81	0.48
1:C:53:G:H2'	1:C:54:5MU:C6	2.49	0.48
1:C:65:PSU:H2'	1:C:66:C:H6	1.78	0.48
1:D:9:A:H5''	1:D:46:G7M:N2	2.28	0.48
1:D:28:C:H2'	1:D:29:U:H6	1.76	0.48
2:A:431:TRP:CD1	2:A:438:TRP:NE1	2.82	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:SER:O	2:B:126:LEU:N	2.45	0.48
1:D:29:U:H2'	1:D:30:G:C8	2.48	0.47
2:A:182:PHE:HB3	2:B:184:VAL:CG1	2.44	0.47
2:A:230:ASP:HB3	2:A:531:ARG:HH12	1.79	0.47
2:A:508:PHE:O	2:A:512:LEU:HD22	2.14	0.47
2:B:39:LEU:HD22	2:B:40:ARG:N	2.28	0.47
1:D:22:G:O2'	1:D:23:A:H5'	2.13	0.47
2:A:64:ARG:O	2:A:67:TRP:HB2	2.14	0.47
2:A:133:LEU:HD11	2:B:517:TYR:CG	2.50	0.47
2:B:128:LEU:O	2:B:558:LEU:HB2	2.15	0.47
2:A:4:THR:HG1	2:A:5:HIS:CE1	2.32	0.47
2:B:139:ARG:HH21	2:B:544:GLU:HB3	1.79	0.47
2:B:140:MET:O	2:B:143:ASN:HB2	2.14	0.47
2:B:534:ALA:O	2:B:537:THR:HG22	2.14	0.47
2:B:551:ASN:HD22	2:B:557:PRO:HG3	1.77	0.47
1:D:34:QUO:HN22	2:B:91:GLU:CD	2.18	0.47
2:A:505:ARG:N	2:A:505:ARG:HD2	2.28	0.47
2:B:63:VAL:HA	2:B:67:TRP:CE3	2.49	0.47
2:B:77:LEU:HD23	2:B:78:ARG:N	2.29	0.47
1:D:24:A:H2'	1:D:25:U:O4'	2.14	0.47
2:A:147:ARG:HD2	2:A:533:LEU:HD11	1.94	0.47
2:A:339:GLU:O	2:A:339:GLU:HG3	2.15	0.47
2:A:371:ARG:HG3	2:A:375:LEU:HD21	1.96	0.47
2:A:461:GLY:C	2:A:463:VAL:H	2.17	0.47
2:A:579:ARG:HB2	2:A:580:PRO:HD3	1.95	0.47
2:B:114:TRP:CZ2	2:B:138:ARG:HA	2.49	0.47
2:B:120:LYS:O	2:B:120:LYS:HG2	2.14	0.47
2:B:260:HIS:HA	2:B:263:ARG:NH2	2.30	0.47
2:B:361:GLY:H	2:B:364:ALA:CB	2.28	0.47
2:A:139:ARG:HH21	2:A:539:SER:HG	1.61	0.47
2:A:212:LEU:HD23	2:A:212:LEU:HA	1.71	0.47
2:A:517:TYR:CG	2:B:133:LEU:HD11	2.50	0.47
2:B:171:LEU:HB3	2:B:194:TYR:CD1	2.50	0.47
2:B:226:ASP:O	2:B:228:ARG:N	2.42	0.47
1:D:70:U:OP2	1:D:70:U:H5	1.98	0.47
2:A:433:GLU:C	2:A:435:GLU:H	2.18	0.47
2:A:494:PHE:HD2	2:A:499:ILE:HB	1.80	0.47
2:B:250:VAL:HG11	2:B:468:TYR:OH	2.14	0.47
2:B:287:GLY:O	2:B:398:THR:HA	2.15	0.47
2:B:354:VAL:CG2	2:B:381:ARG:O	2.62	0.47
2:B:372:GLU:HA	2:B:375:LEU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:284:GLU:OE1	2:A:284:GLU:HA	2.14	0.47
2:A:449:HIS:HE1	2:A:451:GLU:HG3	1.79	0.47
3:A:2016:HOH:O	2:B:147:ARG:HD3	2.14	0.47
2:B:386:LEU:HD13	2:B:388:PHE:HZ	1.80	0.47
1:C:22:G:H2'	1:C:23:A:H8	1.80	0.47
2:A:10:LEU:O	2:A:87:THR:HG22	2.14	0.47
2:A:303:GLY:HA2	2:A:320:VAL:HG23	1.97	0.47
2:A:426:PHE:CD2	2:A:441:MET:HE2	2.50	0.47
2:B:435:GLU:HA	2:B:435:GLU:OE1	2.15	0.47
1:D:2:G:C6	1:D:3:A:C5	3.03	0.47
2:A:349:LEU:HD22	2:A:350:ALA:O	2.15	0.47
2:A:275:PRO:HD2	2:A:420:PHE:O	2.14	0.46
2:A:320:VAL:HG13	2:A:390:ALA:HB2	1.98	0.46
2:A:517:TYR:CE2	2:B:107:PRO:HD3	2.50	0.46
2:B:205:GLN:O	2:B:208:MET:HB2	2.15	0.46
2:B:300:LYS:HE2	2:B:377:ALA:O	2.15	0.46
2:A:204:LYS:HE3	2:A:241:GLU:HB2	1.97	0.46
2:A:409:ASP:O	2:A:410:LEU:C	2.53	0.46
2:A:576:MET:HB2	2:B:578:VAL:CG2	2.45	0.46
2:B:73:GLY:HA2	2:B:95:SER:H	1.81	0.46
2:B:296:GLY:O	2:B:297:LEU:HB2	2.15	0.46
1:C:15:G:H2'	1:C:59:G:C6	2.49	0.46
2:A:179:ALA:HB1	2:A:198:GLN:NE2	2.29	0.46
2:A:289:ASP:C	2:A:291:PRO:HD3	2.36	0.46
2:A:361:GLY:O	2:A:362:GLY:C	2.54	0.46
2:B:115:ARG:HH11	2:B:117:GLU:CD	2.18	0.46
2:A:517:TYR:HB3	2:B:133:LEU:HD21	1.97	0.46
2:B:452:ASP:OD1	2:B:464:ARG:NE	2.49	0.46
2:A:111:ASP:CG	2:A:115:ARG:NH2	2.69	0.46
2:A:539:SER:CB	2:A:544:GLU:HB2	2.45	0.46
1:C:65:PSU:H2'	1:C:66:C:C6	2.50	0.46
2:A:406:ARG:O	2:A:409:ASP:HB2	2.15	0.46
2:A:534:ALA:O	2:A:538:GLY:N	2.47	0.46
2:B:242:MET:O	2:B:522:HIS:HB2	2.14	0.46
2:A:175:THR:HB	2:A:507:LYS:HE2	1.97	0.46
2:A:426:PHE:HD2	2:A:441:MET:HE1	1.81	0.46
2:A:147:ARG:NH1	2:A:545:VAL:O	2.49	0.46
2:A:311:PHE:HB2	2:A:366:PHE:CG	2.51	0.46
2:B:170:PHE:O	2:B:197:PRO:HD3	2.16	0.46
2:B:297:LEU:O	2:B:404:ARG:HD2	2.16	0.46
2:B:360:SER:O	2:B:360:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:429:LEU:HD13	2:B:438:TRP:HB2	1.98	0.46
1:D:2:G:C4	1:D:3:A:N7	2.84	0.46
1:D:48:C:H5''	1:D:49:G:H5''	1.98	0.46
2:B:311:PHE:O	2:B:313:VAL:N	2.49	0.46
1:C:33:U:C6	2:A:33:GLY:HA3	2.51	0.46
1:C:18:G:H1'	1:C:57:G:N2	2.32	0.45
1:D:49:G:H2'	1:D:50:C:H6	1.80	0.45
2:A:165:GLN:HE22	2:A:167:GLU:HG3	1.80	0.45
2:A:169:PRO:HG2	2:A:203:PHE:CE2	2.51	0.45
2:A:185:PRO:HA	2:A:193:PHE:CD1	2.52	0.45
2:A:331:ARG:HE	2:A:331:ARG:N	1.92	0.45
2:A:405:LEU:HD22	2:A:415:ARG:NH2	2.31	0.45
2:A:426:PHE:HD2	2:A:441:MET:CE	2.28	0.45
2:B:292:ASP:OD1	2:B:294:ARG:NE	2.47	0.45
2:B:327:LYS:HE2	2:B:333:GLU:OE1	2.16	0.45
1:C:13:C:O2'	1:C:14:A:H5'	2.17	0.45
2:A:130:TYR:O	2:A:132:TYR:N	2.50	0.45
2:A:409:ASP:O	2:A:412:GLY:N	2.45	0.45
2:A:501:GLU:OE2	2:A:505:ARG:CZ	2.64	0.45
2:B:147:ARG:NH1	2:B:533:LEU:CD1	2.79	0.45
2:B:155:TRP:CH2	2:B:165:GLN:HG3	2.51	0.45
2:A:182:PHE:CB	2:A:196:LEU:HD12	2.47	0.45
2:A:208:MET:HG3	2:A:241:GLU:HG3	1.99	0.45
2:A:232:GLN:O	2:A:233:PRO:C	2.55	0.45
2:A:433:GLU:C	2:A:435:GLU:N	2.70	0.45
2:A:445:PHE:O	2:A:484:ILE:HG12	2.17	0.45
2:B:6:TYR:O	2:B:7:ALA:C	2.55	0.45
2:B:27:ARG:NH1	2:B:115:ARG:CD	2.79	0.45
2:B:114:TRP:CE2	2:B:138:ARG:HB2	2.51	0.45
2:B:226:ASP:C	2:B:228:ARG:N	2.69	0.45
2:B:307:ARG:HG3	2:B:315:GLN:HB2	1.99	0.45
2:B:449:HIS:CE1	2:B:451:GLU:HB2	2.51	0.45
2:B:454:PRO:HG2	2:B:455:LEU:HD22	1.98	0.45
1:C:52:G:N2	1:C:63:C:C2	2.85	0.45
1:D:9:A:C5'	1:D:46:G7M:H22	2.29	0.45
2:A:41:ASP:OD1	2:A:41:ASP:C	2.54	0.45
2:A:508:PHE:HB2	2:A:512:LEU:HD22	1.99	0.45
2:B:84:ARG:O	2:B:85:LEU:HD23	2.17	0.45
2:A:7:ALA:HB1	2:A:46:VAL:CG2	2.46	0.45
2:A:57:TYR:O	2:A:61:GLU:HG3	2.16	0.45
2:A:165:GLN:C	2:A:165:GLN:NE2	2.67	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:177:GLU:H	2:A:507:LYS:HE3	1.81	0.45
2:A:206:MET:HE1	2:A:510:PHE:HD1	1.81	0.45
2:A:558:LEU:HD11	2:B:206:MET:HE1	1.99	0.45
2:B:163:PHE:HA	2:B:214:ARG:O	2.16	0.45
2:B:437:ALA:HB1	2:B:496:LEU:O	2.16	0.45
2:A:112:ALA:HA	2:A:115:ARG:CZ	2.46	0.45
2:A:244:PHE:CD2	2:A:521:PRO:HD2	2.52	0.45
2:A:257:LEU:HD13	2:A:527:TRP:CH2	2.52	0.45
1:C:11:U:H2'	1:C:12:U:H6	1.81	0.45
1:C:35:U:O2	2:A:29:ARG:NE	2.39	0.45
2:A:240:LEU:CD2	2:A:525:ILE:HG22	2.42	0.45
2:A:453:LEU:HD12	2:A:453:LEU:HA	1.81	0.45
2:A:490:GLN:CG	2:A:494:PHE:HE1	2.30	0.45
2:B:185:PRO:HG3	2:B:193:PHE:HE1	1.82	0.45
2:B:499:ILE:H	2:B:499:ILE:CD1	2.26	0.45
1:D:22:G:H2'	1:D:23:A:C8	2.50	0.45
2:A:165:GLN:HA	2:A:216:PHE:O	2.17	0.45
2:A:214:ARG:H	2:A:214:ARG:HG2	1.63	0.45
2:A:297:LEU:HB3	2:A:323:LEU:HD11	1.99	0.45
2:A:371:ARG:O	2:A:375:LEU:HD23	2.17	0.45
2:B:335:ALA:O	2:B:338:GLU:HB3	2.17	0.45
1:C:71:C:N4	1:C:72:C:N4	2.65	0.45
1:D:30:G:O2'	1:D:31:C:H5'	2.17	0.45
2:A:297:LEU:H	2:A:404:ARG:NH1	2.15	0.45
2:B:371:ARG:O	2:B:375:LEU:HB2	2.16	0.45
1:D:38:C:OP2	2:B:29:ARG:HD3	2.17	0.44
2:A:230:ASP:OD1	2:A:541:SER:HA	2.17	0.44
2:A:246:GLU:O	2:A:249:ASP:HB2	2.17	0.44
2:B:513:GLU:O	2:B:516:GLU:HB2	2.17	0.44
1:C:34:QUO:O6	1:C:34:QUO:H101	2.17	0.44
2:A:8:GLY:HA3	2:A:44:GLY:N	2.33	0.44
2:A:192:LEU:HD23	2:B:563:SER:N	2.32	0.44
2:A:351:TRP:HB3	2:A:387:LEU:HD12	1.99	0.44
2:B:1:MET:H2	2:B:70:ARG:HD3	1.81	0.44
2:B:23:GLY:HA3	2:B:40:ARG:O	2.16	0.44
2:B:74:LEU:CD2	2:B:76:ARG:HE	2.30	0.44
2:B:321:LYS:HA	2:B:321:LYS:HD3	1.69	0.44
2:B:371:ARG:O	2:B:375:LEU:N	2.40	0.44
2:B:480:GLY:HA3	2:B:525:ILE:HA	1.99	0.44
2:B:561:ALA:CA	2:B:562:PRO:O	2.64	0.44
1:C:3:A:O2'	1:C:4:G:O4'	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:350:ALA:HB3	2:A:388:PHE:HB2	1.99	0.44
2:A:375:LEU:HD12	2:A:380:ALA:O	2.17	0.44
2:A:487:PRO:HG3	2:A:515:LEU:HB3	1.99	0.44
2:B:532:LEU:HD13	2:B:536:MET:SD	2.57	0.44
2:B:551:ASN:O	2:B:554:GLY:N	2.50	0.44
1:C:64:G:O2'	1:C:65:PSU:H5''	2.17	0.44
2:A:52:PRO:HA	2:A:57:TYR:CG	2.52	0.44
2:A:193:PHE:N	2:B:563:SER:O	2.45	0.44
2:B:509:GLY:O	2:B:510:PHE:C	2.56	0.44
1:C:61:C:H2'	1:C:62:C:H6	1.83	0.44
2:A:20:VAL:HG13	2:A:72:LYS:HG2	1.99	0.44
2:A:82:ASN:C	2:A:82:ASN:OD1	2.54	0.44
2:A:504:GLN:HB2	2:A:504:GLN:HE21	1.68	0.44
2:B:67:TRP:CZ3	2:B:102:GLU:HG2	2.52	0.44
2:B:287:GLY:HA3	2:B:397:ALA:O	2.18	0.44
2:B:306:PHE:CB	2:B:314:PHE:HB3	2.47	0.44
2:B:482:ILE:HA	2:B:523:GLY:HA3	1.99	0.44
2:A:157:PHE:HD1	2:A:160:ARG:HH12	1.62	0.44
2:A:443:HIS:CD2	2:A:445:PHE:H	2.35	0.44
2:B:261:VAL:C	2:B:263:ARG:H	2.19	0.44
2:B:536:MET:HE2	2:B:536:MET:HB3	1.66	0.44
2:A:140:MET:O	2:A:141:GLN:C	2.55	0.44
2:A:189:GLU:OE2	2:A:192:LEU:HD11	2.18	0.44
2:A:216:PHE:HA	2:A:239:ASP:O	2.16	0.44
2:A:451:GLU:C	2:A:453:LEU:H	2.21	0.44
2:A:508:PHE:HB2	2:A:512:LEU:HD21	1.98	0.44
2:B:337:LEU:HB3	2:B:349:LEU:CD2	2.48	0.44
2:B:495:ARG:O	2:B:498:GLY:N	2.50	0.44
2:A:20:VAL:O	2:A:21:LEU:HD23	2.18	0.44
2:A:73:GLY:HA3	2:A:92:VAL:HG12	1.99	0.44
2:A:327:LYS:HG2	2:A:329:LEU:HD23	2.00	0.44
2:B:48:LEU:HB3	2:B:94:LEU:CD2	2.47	0.44
1:D:3:A:O2'	1:D:4:G:H5'	2.18	0.43
2:A:144:LEU:O	2:A:147:ARG:HB3	2.17	0.43
2:A:490:GLN:HG3	2:A:494:PHE:HE1	1.82	0.43
2:B:127:ARG:NE	2:B:137:ARG:NH2	2.65	0.43
2:B:313:VAL:CG1	2:B:314:PHE:N	2.81	0.43
1:C:40:C:O2'	1:C:41:A:H5'	2.17	0.43
2:A:115:ARG:NH1	2:A:117:GLU:OE1	2.50	0.43
2:B:154:ILE:HD13	2:B:238:LEU:HD22	1.99	0.43
2:B:543:ARG:HH21	2:B:552:LYS:HG3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:U:H2'	1:C:71:C:C5	2.52	0.43
1:D:46:G7M:O2'	1:D:47:U:H3'	2.18	0.43
2:B:72:LYS:HB2	2:B:72:LYS:HE3	1.68	0.43
2:B:110:VAL:O	2:B:110:VAL:HG13	2.18	0.43
2:B:279:TYR:O	2:B:283:MET:HB2	2.16	0.43
2:B:350:ALA:O	2:B:388:PHE:HD1	2.01	0.43
2:B:361:GLY:N	2:B:364:ALA:HB2	2.33	0.43
2:B:552:LYS:HB2	2:B:552:LYS:HE3	1.74	0.43
1:D:16:H2U:H3'	1:D:17:C:C5'	2.48	0.43
2:A:12:GLU:CD	2:A:89:ARG:HD3	2.39	0.43
2:A:182:PHE:HB3	2:B:184:VAL:HG11	2.00	0.43
2:A:211:GLY:HA2	2:B:24:TRP:CH2	2.53	0.43
2:A:216:PHE:CD1	2:A:216:PHE:C	2.92	0.43
2:A:308:GLN:HE21	2:A:308:GLN:HB3	1.54	0.43
2:B:361:GLY:H	2:B:364:ALA:HB2	1.83	0.43
1:C:2:G:H1	1:C:72:C:N4	2.16	0.43
2:A:192:LEU:CD2	2:B:562:PRO:HG2	2.39	0.43
2:B:8:GLY:O	2:B:11:ARG:NH2	2.52	0.43
2:B:483:ARG:HB2	2:B:522:HIS:CE1	2.54	0.43
1:C:26:A:C6	1:C:27:C:C4	3.07	0.43
2:A:543:ARG:HH22	2:A:552:LYS:HE3	1.83	0.43
2:B:117:GLU:O	2:B:118:GLU:C	2.57	0.43
2:B:540:PRO:HG2	2:B:541:SER:H	1.83	0.43
1:C:19:G:N2	1:C:57:G:H1'	2.34	0.43
1:C:68:G:H2'	1:C:69:U:C6	2.53	0.43
2:A:71:ALA:HB1	2:A:94:LEU:HD21	2.01	0.43
2:A:148:HIS:CD2	2:A:148:HIS:C	2.92	0.43
2:A:227:LEU:HD22	2:A:227:LEU:N	2.30	0.43
2:A:579:ARG:HB3	2:A:580:PRO:HD3	2.00	0.43
2:B:76:ARG:CZ	2:B:93:GLU:OE1	2.66	0.43
2:A:6:TYR:HE2	2:B:213:ASP:OD1	2.00	0.43
2:A:40:ARG:HG3	2:A:45:LEU:HD23	2.00	0.43
2:A:71:ALA:HB2	2:A:97:LEU:CD1	2.49	0.43
2:A:170:PHE:HD1	2:B:220:ARG:NH1	2.16	0.43
2:B:443:HIS:C	2:B:445:PHE:N	2.72	0.43
2:B:556:ASP:OD2	2:B:559:THR:N	2.51	0.43
1:C:8:4SU:HO2'	1:C:21:A:H2	1.63	0.43
1:C:20(A):H2U:C3'	1:C:21:A:C5'	2.97	0.43
2:A:152:LYS:HD3	2:B:155:TRP:CE3	2.54	0.43
2:A:202:LEU:HD23	2:A:202:LEU:HA	1.67	0.43
2:A:266:LEU:HB3	2:A:268:VAL:HG23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:349:LEU:HD22	2:A:349:LEU:C	2.39	0.43
2:A:368:GLU:N	2:A:369:PRO:HD2	2.33	0.43
2:A:494:PHE:CD2	2:A:499:ILE:HG21	2.53	0.43
2:B:278:SER:HA	2:B:424:VAL:O	2.19	0.43
2:B:381:ARG:O	2:B:384:ASP:OD2	2.37	0.43
2:A:343:ARG:HA	2:A:343:ARG:NE	2.33	0.43
2:A:407:ALA:O	2:A:411:LEU:HB2	2.18	0.43
2:A:529:LEU:HD12	2:A:529:LEU:HA	1.90	0.43
2:B:409:ASP:C	2:B:411:LEU:N	2.72	0.43
2:B:443:HIS:C	2:B:445:PHE:H	2.22	0.43
2:B:528:GLY:O	2:B:529:LEU:C	2.57	0.43
2:B:543:ARG:HG2	2:B:549:PRO:HB2	2.00	0.43
1:C:30:G:C6	1:C:31:C:C4	3.06	0.42
2:A:351:TRP:O	2:A:363:VAL:HG12	2.18	0.42
2:A:426:PHE:CD2	2:A:441:MET:CE	3.02	0.42
2:A:443:HIS:HD2	2:A:445:PHE:H	1.67	0.42
2:B:294:ARG:NH1	2:B:294:ARG:HG2	2.34	0.42
2:B:570:LEU:HD22	2:B:575:LEU:HB2	2.01	0.42
1:D:34:QUO:H14	2:B:51:HIS:ND1	2.34	0.42
2:A:42:ARG:NE	2:A:145:ARG:HH21	2.17	0.42
2:A:242:MET:O	2:A:522:HIS:HB2	2.19	0.42
2:A:299:LEU:N	2:A:299:LEU:HD23	2.33	0.42
2:B:330:SER:H	2:B:333:GLU:HB2	1.84	0.42
2:A:74:LEU:N	2:A:92:VAL:HG12	2.34	0.42
2:A:443:HIS:CG	2:A:444:PRO:CD	2.99	0.42
2:A:486:ASP:C	2:A:486:ASP:OD1	2.57	0.42
2:B:25:VAL:HG21	2:B:63:VAL:HG22	2.02	0.42
1:C:14:A:C2	1:C:22:G:C4	3.08	0.42
1:D:18:G:N2	1:D:57:G:H2'	2.35	0.42
1:D:71:C:C2'	1:D:72:C:H5'	2.49	0.42
2:A:97:LEU:HD12	2:A:97:LEU:HA	1.88	0.42
2:A:225:GLU:O	2:A:226:ASP:C	2.57	0.42
2:A:241:GLU:OE1	2:A:524:GLY:HA3	2.19	0.42
2:A:571:ARG:O	2:A:574:GLY:N	2.42	0.42
2:B:107:PRO:HD2	2:B:133:LEU:HD13	2.00	0.42
2:B:163:PHE:CE1	2:B:253:LEU:HD11	2.54	0.42
2:B:201:GLN:HA	2:B:204:LYS:HD3	2.01	0.42
2:B:240:LEU:C	2:B:240:LEU:HD23	2.39	0.42
2:B:410:LEU:O	2:B:411:LEU:HD23	2.19	0.42
2:B:512:LEU:HD12	2:B:512:LEU:HA	1.76	0.42
1:C:63:C:O2'	1:C:64:G:H5'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:C:C4	1:C:72:C:N4	2.87	0.42
2:B:483:ARG:HE	2:B:523:GLY:HA2	1.84	0.42
2:A:190:PRO:HB3	2:B:577:VAL:HG12	2.02	0.42
2:A:292:ASP:CG	2:A:294:ARG:HH11	2.22	0.42
2:A:432:ASP:O	2:A:433:GLU:OE2	2.37	0.42
2:A:452:ASP:HB3	2:A:463:VAL:HG13	2.02	0.42
2:A:570:LEU:O	2:A:573:LEU:HB2	2.19	0.42
2:B:70:ARG:NH2	2:B:100:LEU:HD22	2.33	0.42
2:B:235:PHE:HE2	2:B:237:GLN:HE21	1.66	0.42
2:B:294:ARG:HG2	2:B:294:ARG:HH11	1.83	0.42
2:B:453:LEU:N	2:B:454:PRO:HD2	2.35	0.42
2:B:579:ARG:HA	2:B:580:PRO:HD3	1.88	0.42
1:C:2:G:O2'	1:C:3:A:O4'	2.34	0.42
1:D:20:H2U:O2'	1:D:20(A):H2U:OP1	2.34	0.42
1:D:52:G:C2	1:D:53:G:H1'	2.54	0.42
1:D:70:U:C2	1:D:71:C:C5	3.07	0.42
2:A:8:GLY:HA3	2:A:44:GLY:CA	2.49	0.42
2:A:226:ASP:CG	2:A:228:ARG:HG2	2.40	0.42
2:A:283:MET:O	2:A:287:GLY:CA	2.67	0.42
2:B:59:THR:C	2:B:61:GLU:N	2.73	0.42
2:B:232:GLN:HG2	2:B:542:ILE:HD11	2.01	0.42
1:C:4:G:C2	1:C:70:U:O2	2.72	0.42
1:C:22:G:C2	1:C:23:A:C5	3.07	0.42
1:C:29:U:O2'	1:C:30:G:H5'	2.20	0.42
1:D:31:C:O2'	1:D:32:C:H5'	2.19	0.42
2:A:153:ALA:HB1	2:A:260:HIS:CD2	2.55	0.42
2:A:548:PHE:HB2	2:B:169:PRO:HG3	2.02	0.42
1:D:25:U:H2'	1:D:26:A:C8	2.55	0.42
2:A:192:LEU:HD23	2:B:562:PRO:C	2.39	0.42
2:A:486:ASP:HA	2:A:487:PRO:HD3	1.86	0.42
1:C:39:G:H2'	1:C:40:C:C6	2.55	0.42
1:D:37:2MA:H4'	2:B:27:ARG:NH1	2.34	0.42
1:D:48:C:O2'	1:D:49:G:P	2.77	0.42
1:D:57:G:H2'	1:D:58:A:H5'	2.01	0.42
2:A:20:VAL:C	2:A:21:LEU:HD23	2.40	0.42
2:A:183:LEU:HD12	2:B:573:LEU:HD11	2.01	0.42
2:A:246:GLU:O	2:A:249:ASP:N	2.52	0.42
2:A:405:LEU:HA	2:A:405:LEU:HD23	1.70	0.42
1:C:33:U:O2	1:C:34:QUO:H14	2.20	0.41
1:D:38:C:C2'	1:D:39:G:H5'	2.50	0.41
1:D:53:G:C5	1:D:54:5MU:C5	3.07	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:326:PRO:HG2	2:A:411:LEU:CD2	2.49	0.41
2:A:342:LYS:O	2:A:344:HIS:O	2.37	0.41
2:A:447:SER:CA	2:A:484:ILE:HD13	2.46	0.41
2:B:77:LEU:HA	2:B:90:VAL:HG12	2.01	0.41
2:B:182:PHE:HB3	2:B:196:LEU:HD12	2.01	0.41
2:B:189:GLU:HB3	2:B:192:LEU:HD22	2.01	0.41
2:B:414:LYS:HD2	2:B:414:LYS:HA	1.80	0.41
2:B:513:GLU:HG3	3:B:2071:HOH:O	2.17	0.41
1:C:3:A:C2'	1:C:4:G:O4'	2.68	0.41
2:A:263:ARG:HA	2:A:268:VAL:O	2.19	0.41
2:A:452:ASP:OD2	2:A:464:ARG:CD	2.69	0.41
2:B:149:ARG:HD2	2:B:265:ALA:HA	2.02	0.41
2:B:302:VAL:O	2:B:304:PRO:N	2.53	0.41
2:A:28:ARG:HA	2:A:37:LEU:HD23	2.01	0.41
2:A:160:ARG:NH2	2:A:161:GLU:OE2	2.53	0.41
2:A:326:PRO:O	2:A:327:LYS:HB2	2.20	0.41
2:A:512:LEU:O	2:A:515:LEU:HB2	2.19	0.41
2:B:66:GLU:O	2:B:103:ALA:HB2	2.20	0.41
2:B:424:VAL:O	2:B:425:ASP:HB2	2.21	0.41
1:D:6:G:C2'	1:D:7:G:H5'	2.51	0.41
2:A:541:SER:OG	2:A:543:ARG:HG3	2.20	0.41
1:C:67:C:O2'	1:C:68:G:H5'	2.19	0.41
2:A:172:THR:CG2	2:A:173:LYS:H	2.25	0.41
2:A:485:HIS:O	2:A:515:LEU:HD23	2.20	0.41
2:B:68:VAL:HG12	2:B:100:LEU:HD12	2.01	0.41
2:B:73:GLY:HA3	2:B:92:VAL:HG12	2.02	0.41
2:B:110:VAL:O	2:B:110:VAL:CG1	2.68	0.41
2:B:252:GLU:OE1	2:B:256:ARG:HD3	2.20	0.41
2:B:430:GLU:O	2:B:438:TRP:CD1	2.73	0.41
2:B:537:THR:CG2	2:B:539:SER:OG	2.61	0.41
1:C:34:QUO:H13	2:A:51:HIS:ND1	2.36	0.41
2:B:163:PHE:HA	2:B:214:ARG:HG3	2.02	0.41
2:B:333:GLU:C	2:B:335:ALA:N	2.73	0.41
2:B:421:LEU:HB3	2:B:471:VAL:HG22	2.02	0.41
1:C:24:A:C6	1:C:25:U:N3	2.89	0.41
2:A:512:LEU:HA	2:A:515:LEU:HD12	2.02	0.41
2:B:522:HIS:ND1	2:B:522:HIS:N	2.68	0.41
1:D:2:G:N1	1:D:3:A:C6	2.89	0.41
1:D:31:C:H2'	1:D:32:C:O4'	2.21	0.41
1:D:70:U:OP2	1:D:70:U:C5	2.74	0.41
2:A:299:LEU:HD13	2:A:400:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:504:GLN:HB3	2:A:505:ARG:HH11	1.86	0.41
2:A:578:VAL:HG11	2:B:576:MET:HB3	2.03	0.41
2:B:440:TYR:CD2	2:B:440:TYR:N	2.88	0.41
1:D:47:U:C1'	1:D:48:C:OP1	2.69	0.41
1:D:49:G:N3	1:D:50:C:C6	2.89	0.41
2:A:39:LEU:HD22	2:A:40:ARG:N	2.36	0.41
2:A:48:LEU:HB3	2:A:94:LEU:HD11	2.03	0.41
2:A:134:ASP:O	2:A:137:ARG:HG3	2.21	0.41
2:A:206:MET:CE	2:A:510:PHE:HD1	2.34	0.41
2:A:371:ARG:O	2:A:375:LEU:CD2	2.68	0.41
2:A:579:ARG:CB	2:A:580:PRO:CD	2.97	0.41
2:B:27:ARG:HD2	2:B:115:ARG:NE	2.28	0.41
2:B:42:ARG:HD3	2:B:145:ARG:HH21	1.86	0.41
2:B:330:SER:O	2:B:334:VAL:HG23	2.20	0.41
2:B:409:ASP:C	2:B:411:LEU:H	2.23	0.41
2:A:206:MET:HE1	2:A:510:PHE:CD1	2.56	0.40
2:A:363:VAL:O	2:A:363:VAL:HG22	2.21	0.40
2:A:517:TYR:HE2	2:B:107:PRO:HD3	1.85	0.40
2:B:154:ILE:HG21	2:B:238:LEU:HD13	2.03	0.40
2:B:208:MET:HG3	2:B:522:HIS:CB	2.51	0.40
1:C:51:G:H2'	1:C:52:G:O4'	2.21	0.40
1:C:52:G:H1	1:C:62:C:H42	1.68	0.40
1:D:22:G:H2'	1:D:23:A:H8	1.85	0.40
1:D:56:C:H6	1:D:56:C:O5'	2.04	0.40
2:A:77:LEU:HD23	2:A:78:ARG:N	2.37	0.40
2:A:118:GLU:HG3	2:A:118:GLU:O	2.22	0.40
2:B:237:GLN:HB3	2:B:527:TRP:O	2.22	0.40
2:B:392:PRO:HB2	2:B:395:VAL:CG2	2.51	0.40
2:B:440:TYR:CD1	2:B:442:HIS:O	2.70	0.40
1:C:51:G:C4	1:C:64:G:N2	2.89	0.40
1:D:5:C:O5'	1:D:5:C:H6	2.04	0.40
1:D:69:U:H2'	1:D:70:U:C5	2.55	0.40
2:A:414:LYS:HA	2:A:414:LYS:HD3	1.99	0.40
2:A:422:TRP:CZ3	2:A:470:LEU:HB2	2.56	0.40
2:A:429:LEU:HD13	2:A:438:TRP:CB	2.46	0.40
2:A:486:ASP:OD1	2:A:488:ARG:N	2.55	0.40
2:B:78:ARG:HA	2:B:79:PRO:HD3	1.88	0.40
2:B:118:GLU:HG2	2:B:119:GLU:N	2.35	0.40
2:B:395:VAL:O	2:B:396:ALA:C	2.57	0.40
1:C:6:G:C2	1:C:7:G:C4	3.09	0.40
2:A:287:GLY:HA3	2:A:397:ALA:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:386:LEU:HD23	2:A:386:LEU:HA	1.98	0.40
1:C:48:C:C4'	1:C:49:G:OP2	2.68	0.40
1:D:28:C:H2'	1:D:29:U:C6	2.54	0.40
2:A:27:ARG:HB2	3:A:2026:HOH:O	2.22	0.40
2:A:168:THR:CG2	2:A:169:PRO:N	2.85	0.40
2:A:175:THR:HB	2:A:507:LYS:NZ	2.37	0.40
2:B:467:ALA:HA	2:B:481:SER:CB	2.52	0.40
2:B:501:GLU:O	2:B:504:GLN:N	2.53	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	578/580 (100%)	499 (86%)	64 (11%)	15 (3%)	5	27
2	B	578/580 (100%)	459 (79%)	93 (16%)	26 (4%)	2	14
All	All	1156/1160 (100%)	958 (83%)	157 (14%)	41 (4%)	3	20

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	188	HIS
2	A	462	ARG
2	A	579	ARG
2	B	42	ARG
2	B	227	LEU
2	B	312	ARG
2	B	345	LYS
2	B	362	GLY
2	B	435	GLU
2	B	501	GLU

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Mol	Chain	Res	Type
2	B	552	LYS
2	A	42	ARG
2	A	131	ARG
2	A	434	GLU
2	A	452	ASP
2	A	509	GLY
2	B	370	VAL
2	B	377	ALA
2	B	433	GLU
2	B	437	ALA
2	B	509	GLY
2	B	567	GLU
2	A	362	GLY
2	A	413	LEU
2	B	60	ALA
2	B	94	LEU
2	B	303	GLY
2	B	336	GLU
2	B	438	TRP
2	A	229	ALA
2	A	502	GLU
2	B	299	LEU
2	B	314	PHE
2	B	337	LEU
2	B	396	ALA
2	B	525	ILE
2	A	226	ASP
2	A	255	GLU
2	B	122	ALA
2	B	291	PRO
2	A	247	VAL

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	483/483 (100%)	410 (85%)	73 (15%)	3	14
2	B	483/483 (100%)	414 (86%)	69 (14%)	3	15
All	All	966/966 (100%)	824 (85%)	142 (15%)	3	15

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	2	ARG
2	A	4	THR
2	A	10	LEU
2	A	11	ARG
2	A	28	ARG
2	A	39	LEU
2	A	42	ARG
2	A	46	VAL
2	A	49	VAL
2	A	65	PRO
2	A	66	GLU
2	A	92	VAL
2	A	119	GLU
2	A	120	LYS
2	A	124	GLU
2	A	125	GLU
2	A	126	LEU
2	A	139	ARG
2	A	165	GLN
2	A	168	THR
2	A	172	THR
2	A	177	GLU
2	A	181	ASP
2	A	190	PRO
2	A	192	LEU
2	A	199	SER
2	A	201	GLN
2	A	207	LEU
2	A	214	ARG
2	A	215	TYR
2	A	216	PHE
2	A	217	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	A	227	LEU
2	A	228	ARG
2	A	234	ASP
2	A	240	LEU
2	A	253	LEU
2	A	257	LEU
2	A	272	LEU
2	A	276	ARG
2	A	302	VAL
2	A	307	ARG
2	A	331	ARG
2	A	339	GLU
2	A	343	ARG
2	A	349	LEU
2	A	372	GLU
2	A	387	LEU
2	A	393	ARG
2	A	400	LEU
2	A	411	LEU
2	A	431	TRP
2	A	434	GLU
2	A	435	GLU
2	A	436	GLU
2	A	438	TRP
2	A	440	TYR
2	A	453	LEU
2	A	464	ARG
2	A	485	HIS
2	A	489	LEU
2	A	492	ARG
2	A	505	ARG
2	A	506	GLU
2	A	507	LYS
2	A	515	LEU
2	A	516	GLU
2	A	537	THR
2	A	559	THR
2	A	565	VAL
2	A	568	GLU
2	A	570	LEU
2	A	579	ARG
2	B	1	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	2	ARG
2	B	11	ARG
2	B	13	THR
2	B	27	ARG
2	B	28	ARG
2	B	39	LEU
2	B	42	ARG
2	B	48	LEU
2	B	54	SER
2	B	80	GLU
2	B	89	ARG
2	B	107	PRO
2	B	115	ARG
2	B	120	LYS
2	B	124	GLU
2	B	126	LEU
2	B	128	LEU
2	B	131	ARG
2	B	142	GLU
2	B	145	ARG
2	B	168	THR
2	B	177	GLU
2	B	214	ARG
2	B	215	TYR
2	B	227	LEU
2	B	228	ARG
2	B	235	PHE
2	B	240	LEU
2	B	257	LEU
2	B	272	LEU
2	B	277	LEU
2	B	285	ARG
2	B	288	SER
2	B	290	LYS
2	B	294	ARG
2	B	299	LEU
2	B	307	ARG
2	B	311	PHE
2	B	326	PRO
2	B	331	ARG
2	B	339	GLU
2	B	340	VAL

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Mol	Chain	Res	Type
2	B	342	LYS
2	B	343	ARG
2	B	345	LYS
2	B	360	SER
2	B	363	VAL
2	B	368	GLU
2	B	370	VAL
2	B	375	LEU
2	B	394	LYS
2	B	400	LEU
2	B	432	ASP
2	B	436	GLU
2	B	447	SER
2	B	451	GLU
2	B	459	ASP
2	B	462	ARG
2	B	489	LEU
2	B	492	ARG
2	B	501	GLU
2	B	516	GLU
2	B	522	HIS
2	B	559	THR
2	B	571	ARG
2	B	577	VAL
2	B	579	ARG
2	B	580	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	143	ASN
2	A	165	GLN
2	A	198	GLN
2	A	205	GLN
2	A	217	GLN
2	A	254	ASN
2	A	308	GLN
2	A	443	HIS
2	A	504	GLN
2	B	143	ASN
2	B	237	GLN
2	B	260	HIS

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Mol	Chain	Res	Type
2	B	315	GLN
2	B	443	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	70/73 (95%)	9 (12%)	3 (4%)
1	D	70/73 (95%)	13 (18%)	3 (4%)
All	All	140/146 (95%)	22 (15%)	6 (4%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	9	A
1	C	16	H2U
1	C	17	C
1	C	18	G
1	C	20	H2U
1	C	38	C
1	C	48	C
1	C	49	G
1	C	55	PSU
1	D	9	A
1	D	13	C
1	D	16	H2U
1	D	17	C
1	D	18	G
1	D	20	H2U
1	D	20(A)	H2U
1	D	22	G
1	D	38	C
1	D	47	U
1	D	48	C
1	D	49	G
1	D	71	C

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	17	C
1	C	47	U

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Mol	Chain	Res	Type
1	C	48	C
1	D	17	C
1	D	47	U
1	D	48	C

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

20 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	4SU	D	8	1	18,21,22	5.28	1 (5%)	26,30,33	0.43	0
1	H2U	D	16	1	18,21,22	0.66	1 (5%)	21,30,33	0.81	0
1	G7M	C	46	1	20,26,27	0.92	1 (5%)	17,39,42	0.50	0
1	2MA	C	37	1	17,25,26	1.00	2 (11%)	17,37,40	1.24	2 (11%)
1	QUO	D	34	1	29,35,36	0.97	2 (6%)	31,52,55	2.39	9 (29%)
1	5MU	C	54	1	19,22,23	0.29	0	28,32,35	0.65	1 (3%)
1	H2U	D	20(A)	1	18,21,22	0.81	1 (5%)	21,30,33	0.82	0
1	PSU	C	55	1	18,21,22	1.77	1 (5%)	22,30,33	0.71	0
1	G7M	D	46	1	20,26,27	0.84	1 (5%)	17,39,42	0.94	1 (5%)
1	QUO	C	34	1	29,35,36	1.12	3 (10%)	31,52,55	2.44	9 (29%)
1	4SU	C	8	1	18,21,22	5.22	1 (5%)	26,30,33	0.44	0
1	H2U	D	20	1	18,21,22	0.70	1 (5%)	21,30,33	0.83	1 (4%)
1	2MA	D	37	1	17,25,26	0.95	1 (5%)	17,37,40	1.23	2 (11%)
1	H2U	C	20	1	18,21,22	0.90	1 (5%)	21,30,33	0.71	0
1	H2U	C	20(A)	1	18,21,22	0.53	0	21,30,33	0.79	0
1	PSU	D	65	1	18,21,22	1.78	1 (5%)	22,30,33	0.73	1 (4%)
1	PSU	C	65	1	18,21,22	1.86	1 (5%)	22,30,33	0.84	1 (4%)
1	H2U	C	16	1	18,21,22	0.93	1 (5%)	21,30,33	0.82	1 (4%)
1	PSU	D	55	1	18,21,22	1.73	1 (5%)	22,30,33	0.74	1 (4%)
1	5MU	D	54	1	19,22,23	1.95	4 (21%)	28,32,35	13.47	10 (35%)

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
1	4SU	D	8	1	-	0/7/25/26	0/2/2/2
1	H2U	D	16	1	-	2/7/38/39	0/2/2/2
1	G7M	C	46	1	-	0/3/25/26	0/3/3/3
1	2MA	C	37	1	-	1/3/25/26	0/3/3/3
1	QUO	D	34	1	-	1/6/43/44	0/4/4/4
1	5MU	C	54	1	-	0/7/25/26	0/2/2/2
1	H2U	D	20(A)	1	-	3/7/38/39	0/2/2/2
1	PSU	C	55	1	-	0/7/25/26	0/2/2/2
1	G7M	D	46	1	-	0/3/25/26	0/3/3/3
1	QUO	C	34	1	-	2/6/43/44	0/4/4/4
1	4SU	C	8	1	-	1/7/25/26	0/2/2/2
1	H2U	D	20	1	-	7/7/38/39	0/2/2/2
1	2MA	D	37	1	-	1/3/25/26	0/3/3/3
1	H2U	C	20	1	-	0/7/38/39	0/2/2/2
1	H2U	C	20(A)	1	-	1/7/38/39	0/2/2/2
1	PSU	D	65	1	-	1/7/25/26	0/2/2/2
1	PSU	C	65	1	-	0/7/25/26	0/2/2/2
1	H2U	C	16	1	-	2/7/38/39	0/2/2/2
1	PSU	D	55	1	-	2/7/25/26	0/2/2/2
1	5MU	D	54	1	-	0/7/25/26	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	4SU	C4-S4	-22.32	1.26	1.68
1	C	8	4SU	C4-S4	-22.05	1.26	1.68
1	C	65	PSU	C6-N1	-7.39	1.23	1.36
1	D	65	PSU	C6-N1	-7.25	1.24	1.36
1	C	55	PSU	C6-N1	-7.09	1.24	1.36
1	D	55	PSU	C6-N1	-7.01	1.24	1.36
1	D	54	5MU	C6-N1	-4.73	1.30	1.38
1	D	54	5MU	C4-C5	-4.53	1.37	1.44
1	D	54	5MU	C2-N3	3.99	1.45	1.38
1	C	34	QUO	C5-C6	-3.17	1.40	1.47
1	C	16	H2U	C2-N1	3.17	1.40	1.35
1	C	20	H2U	C2-N1	3.15	1.40	1.35
1	C	34	QUO	C5-C4	-2.91	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	34	QUO	C5-C4	-2.88	1.37	1.40
1	D	20(A)	H2U	C2-N1	2.77	1.39	1.35
1	D	46	G7M	C8-N9	2.69	1.38	1.33
1	C	46	G7M	C8-N9	2.64	1.38	1.33
1	D	34	QUO	C5-C6	-2.41	1.42	1.47
1	C	34	QUO	C5-C7	-2.37	1.35	1.39
1	D	20	H2U	C2-N1	2.36	1.39	1.35
1	C	37	2MA	C8-N7	-2.05	1.31	1.35
1	D	54	5MU	C2-N1	2.04	1.41	1.38
1	D	16	H2U	C2-N1	2.01	1.38	1.35
1	C	37	2MA	CM2-C2	-2.01	1.43	1.49
1	D	37	2MA	C8-N7	-2.01	1.31	1.35

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	5MU	C5M-C5-C4	-66.62	45.44	118.77
1	D	54	5MU	C6-N1-C2	-18.29	102.78	121.30
1	D	54	5MU	C5-C4-N3	-13.45	103.83	115.31
1	C	34	QUO	C10-N11-C12	8.44	132.63	114.90
1	D	34	QUO	C10-N11-C12	7.69	131.06	114.90
1	D	54	5MU	C1'-N1-C6	5.89	130.92	121.12
1	D	34	QUO	C5-C6-N1	-5.51	110.69	115.36
1	C	34	QUO	C5-C6-N1	-5.51	110.70	115.36
1	D	54	5MU	C5-C6-N1	-5.25	117.94	123.34
1	D	54	5MU	O4-C4-N3	4.93	129.56	120.12
1	D	34	QUO	C7-C10-N11	4.43	125.29	112.65
1	C	34	QUO	C8-N9-C1'	3.92	128.96	125.48
1	C	34	QUO	O14-C14-C13	3.81	118.48	111.27
1	D	34	QUO	C8-N9-C1'	3.78	128.83	125.48
1	C	37	2MA	N1-C2-N3	3.72	129.23	123.06
1	D	34	QUO	O14-C14-C15	3.72	120.39	111.54
1	D	37	2MA	N1-C2-N3	3.68	129.16	123.06
1	D	34	QUO	C16-C15-C14	-3.67	99.40	105.68
1	C	34	QUO	C16-C15-C14	-3.60	99.51	105.68
1	C	34	QUO	C7-C10-N11	3.58	122.88	112.65
1	D	54	5MU	N3-C2-N1	3.01	118.88	114.89
1	D	54	5MU	O2-C2-N1	-2.75	119.13	122.79
1	D	34	QUO	O14-C14-C13	2.65	116.28	111.27
1	C	34	QUO	O14-C14-C15	2.53	117.57	111.54
1	D	34	QUO	O6-C6-C5	2.52	129.26	123.98
1	C	54	5MU	C2'-C1'-N1	-2.51	106.11	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	20	H2U	N3-C2-N1	-2.44	114.07	116.65
1	D	34	QUO	C16-C12-C13	2.44	106.81	103.18
1	D	65	PSU	C5-C6-N1	2.37	125.65	122.11
1	C	34	QUO	O6-C6-C5	2.34	128.87	123.98
1	D	54	5MU	C4-N3-C2	-2.29	124.39	127.35
1	D	54	5MU	C5M-C5-C6	-2.26	119.82	122.85
1	C	37	2MA	C5-C6-N1	2.24	117.88	114.02
1	D	55	PSU	C5-C6-N1	2.23	125.44	122.11
1	C	65	PSU	C5-C6-N1	2.19	125.39	122.11
1	C	34	QUO	C16-C12-C13	2.19	106.43	103.18
1	D	37	2MA	C5-C6-N1	2.19	117.79	114.02
1	D	46	G7M	O4'-C1'-C2'	2.14	110.06	106.93
1	C	16	H2U	C4-N3-C2	2.11	127.54	125.79

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	16	H2U	O4'-C1'-N1-C2
1	C	16	H2U	O4'-C1'-N1-C6
1	C	34	QUO	C13-C12-N11-C10
1	C	34	QUO	C16-C12-N11-C10
1	D	16	H2U	O4'-C1'-N1-C6
1	D	20	H2U	O4'-C1'-N1-C6
1	D	20	H2U	C2'-C1'-N1-C2
1	D	20	H2U	C2'-C1'-N1-C6
1	D	20	H2U	O4'-C4'-C5'-O5'
1	D	20(A)	H2U	C2'-C1'-N1-C6
1	D	16	H2U	O4'-C1'-N1-C2
1	D	20	H2U	C4'-C5'-O5'-P
1	D	20	H2U	O4'-C1'-N1-C2
1	D	20	H2U	C3'-C4'-C5'-O5'
1	D	55	PSU	O4'-C1'-C5-C4
1	D	20(A)	H2U	O4'-C1'-N1-C2
1	D	37	2MA	C4'-C5'-O5'-P
1	D	20(A)	H2U	C2'-C1'-N1-C2
1	D	55	PSU	O4'-C1'-C5-C6
1	D	65	PSU	O4'-C1'-C5-C6
1	D	34	QUO	C16-C12-N11-C10
1	C	8	4SU	C2'-C1'-N1-C2
1	C	20(A)	H2U	C4'-C5'-O5'-P
1	C	37	2MA	C4'-C5'-O5'-P

There are no ring outliers.

19 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	8	4SU	5	0
1	D	16	H2U	2	0
1	C	46	G7M	1	0
1	C	37	2MA	1	0
1	D	34	QUO	7	0
1	C	54	5MU	3	0
1	D	20(A)	H2U	1	0
1	D	46	G7M	5	0
1	C	34	QUO	6	0
1	C	8	4SU	2	0
1	D	20	H2U	1	0
1	D	37	2MA	5	0
1	C	20	H2U	2	0
1	C	20(A)	H2U	5	0
1	D	65	PSU	2	0
1	C	65	PSU	4	0
1	C	16	H2U	2	0
1	D	55	PSU	1	0
1	D	54	5MU	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	59:G	O3'	60:U	P	1.76

## 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	C	63/73 (86%)	-0.15	0 <b>100</b> <b>100</b>	26, 56, 90, 102	0
1	D	63/73 (86%)	-0.13	1 (1%) 72 44	32, 52, 96, 101	0
2	A	580/580 (100%)	0.01	3 (0%) 91 75	7, 26, 64, 102	0
2	B	580/580 (100%)	0.08	8 (1%) 75 49	6, 34, 68, 102	0
All	All	1286/1306 (98%)	0.03	12 (0%) 84 63	6, 31, 71, 102	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	437	ALA	5.7
2	A	432	ASP	5.0
2	B	580	PRO	5.0
2	B	435	GLU	4.9
1	D	72	C	2.6
2	B	307	ARG	2.5
2	B	439	THR	2.5
2	B	436	GLU	2.5
2	A	580	PRO	2.5
2	B	201	GLN	2.4
2	A	579	ARG	2.2
2	B	329	LEU	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PSU	D	65	20/21	0.86	0.15	76,79,82,83	0
1	H2U	C	20	20/21	0.88	0.24	61,72,77,77	0
1	5MU	D	54	21/22	0.89	0.15	54,60,64,65	0
1	H2U	D	20	20/21	0.89	0.20	49,68,72,73	0
1	4SU	C	8	20/21	0.90	0.19	52,56,60,61	0
1	QUO	D	34	32/33	0.90	0.23	48,63,72,73	0
1	5MU	C	54	21/22	0.91	0.16	79,81,81,82	0
1	PSU	C	55	20/21	0.93	0.10	74,75,82,82	0
1	H2U	C	16	20/21	0.93	0.14	60,66,70,73	0
1	PSU	D	55	20/21	0.93	0.15	48,53,65,65	0
1	H2U	D	20(A)	20/21	0.93	0.15	57,61,66,67	0
1	PSU	C	65	20/21	0.94	0.12	72,75,80,82	0
1	QUO	C	34	32/33	0.94	0.25	23,35,51,53	0
1	G7M	D	46	24/25	0.94	0.16	43,47,49,53	0
1	2MA	D	37	23/24	0.95	0.17	50,60,67,68	0
1	H2U	D	16	20/21	0.95	0.18	51,65,67,71	0
1	G7M	C	46	24/25	0.95	0.18	36,42,48,50	0
1	H2U	C	20(A)	20/21	0.95	0.14	57,63,73,73	0
1	4SU	D	8	20/21	0.95	0.20	39,43,47,48	0
1	2MA	C	37	23/24	0.96	0.18	25,41,44,64	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.