



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:35 PM UTC

PDB ID : 1EFW / pdb_00001efw
Title : Crystal structure of aspartyl-tRNA synthetase from *Thermus thermophilus* complexed to tRNA^{asp} 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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

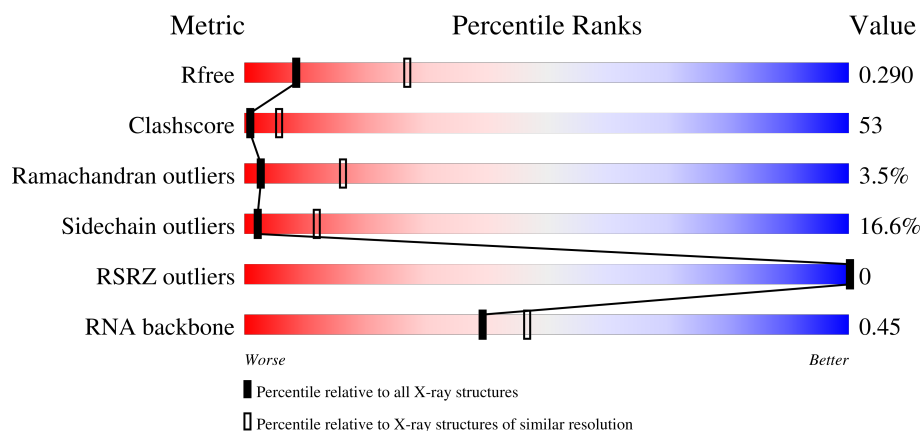
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

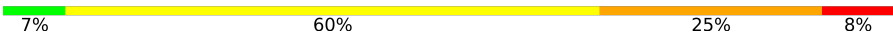
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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 ≥ 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	
1	D	73	
2	A	580	
2	B	580	

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
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
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			

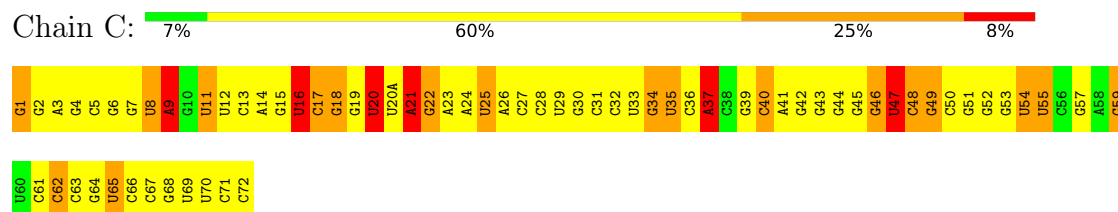
- Molecule 3 is water.

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		

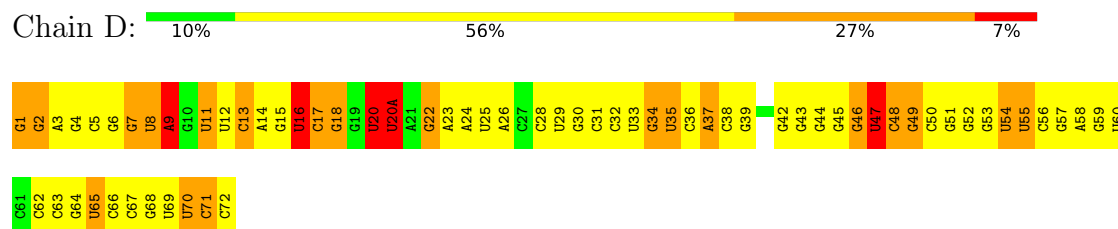
3 Residue-property plots

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.

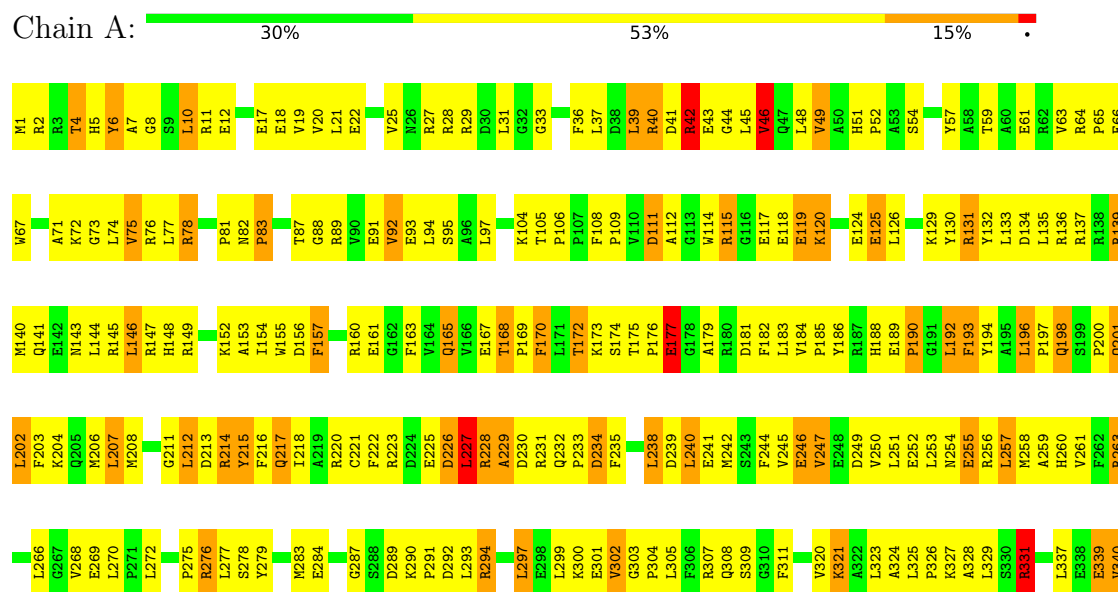
• Molecule 1: ASPARTYL-TRNA

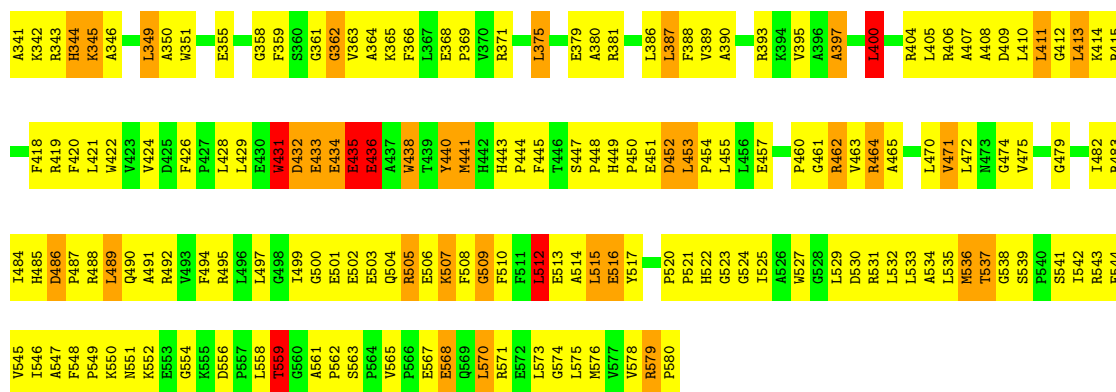


• Molecule 1: ASPARTYL-TRNA

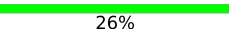


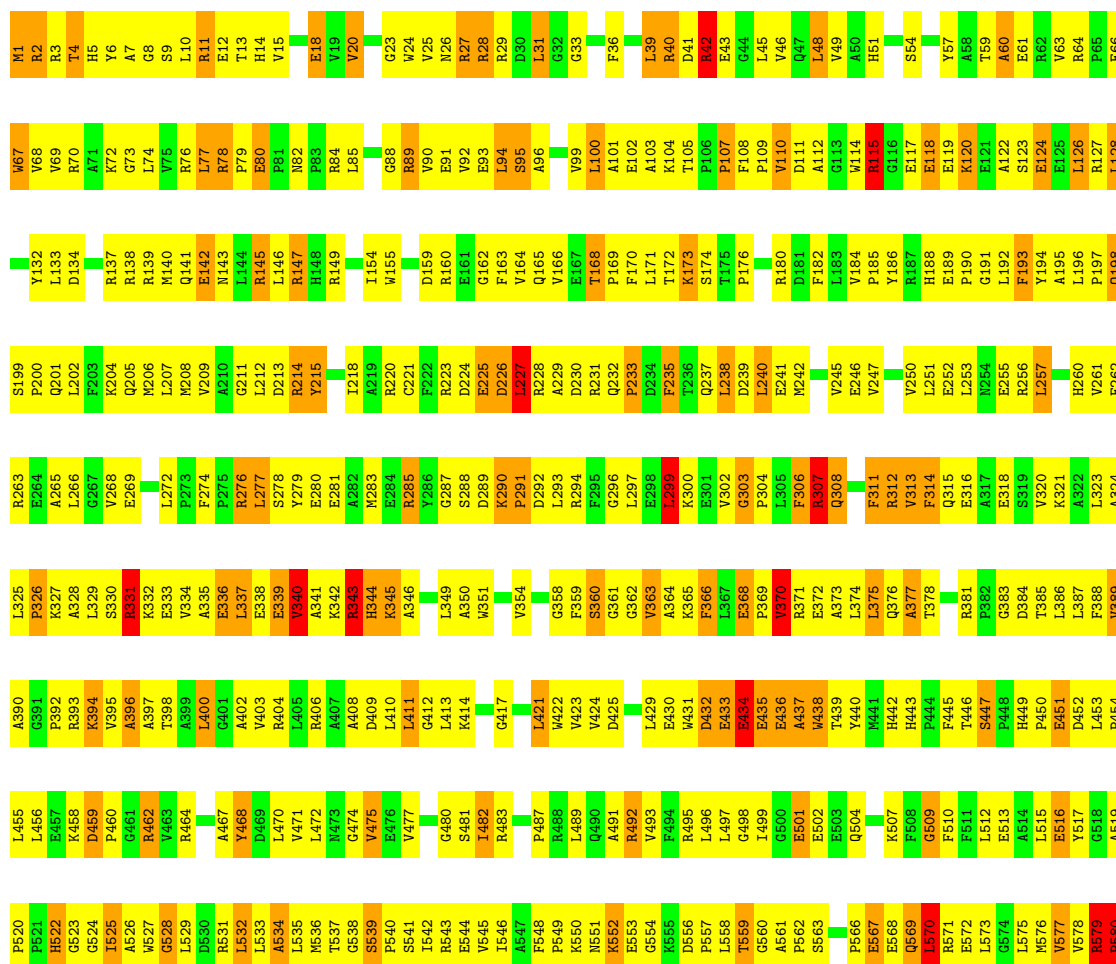
• Molecule 2: ASPARTYL-TRNA SYNTHETASE





● Molecule 2: ASPARTYL-TRNA SYNTHETASE

Chain B:  26%  55%  18% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	251.45Å 251.45Å 88.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (15.00-3.00) 91.8 (15.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.293 0.249 , 0.290	Depositor DCC
R_{free} test set	2969 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12572	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: QUO, G7M, PSU, H2U, 4SU, 5MU, 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	0.80	4/1506 (0.3%)	0.97	7/2343 (0.3%)
1	D	0.62	1/1506 (0.1%)	0.90	5/2343 (0.2%)
2	A	0.65	2/4780 (0.0%)	1.32	64/6467 (1.0%)
2	B	0.68	7/4780 (0.1%)	1.29	68/6467 (1.1%)
All	All	0.67	14/12572 (0.1%)	1.22	144/17620 (0.8%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	580	PRO	C-OXT	14.96	1.53	1.23
1	C	1	G	O3'-P	-12.38	1.42	1.61
2	A	495	ARG	CZ-NH1	10.99	1.48	1.32
2	A	495	ARG	CZ-NH2	10.48	1.47	1.33
1	C	59	G	O3'-P	10.08	1.76	1.61
2	B	580	PRO	CA-C	9.38	1.72	1.52
2	B	307	ARG	NE-CZ	8.84	1.42	1.33
2	B	307	ARG	CD-NE	7.90	1.57	1.46
2	B	579	ARG	CA-C	7.81	1.62	1.53
1	D	46	G7M	O3'-P	6.52	1.62	1.56
2	B	580	PRO	C-O	6.50	1.36	1.23
1	C	11	U	O3'-P	-6.49	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	307	ARG	CA-C	-5.91	1.44	1.52
1	C	62	C	O3'-P	-5.30	1.53	1.61

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	495	ARG	NE-CZ-NH2	-16.49	104.36	119.20
2	B	307	ARG	NE-CZ-NH1	16.34	137.84	121.50
2	B	307	ARG	CG-CD-NE	16.29	147.83	112.00
2	A	495	ARG	NH1-CZ-NH2	16.16	140.31	119.30
2	A	344	HIS	N-CA-C	-15.03	88.28	110.52
2	A	432	ASP	N-CA-C	13.60	129.59	109.59
2	B	307	ARG	CD-NE-CZ	12.96	142.55	124.40
1	C	59	G	O3'-P-O5'	10.58	119.86	104.00
2	B	306	PHE	N-CA-C	9.89	124.00	112.72
2	B	307	ARG	CB-CG-CD	9.76	133.75	111.30
2	B	307	ARG	CA-CB-CG	-9.68	94.74	114.10
2	A	95	SER	N-CA-C	-9.55	101.39	113.23
2	A	146	LEU	N-CA-C	-9.48	101.03	111.36
2	A	431	TRP	N-CA-C	9.36	130.74	110.80
2	A	227	LEU	N-CA-C	-9.22	100.66	113.20
2	A	431	TRP	CA-C-N	-9.11	108.12	121.24
2	A	431	TRP	C-N-CA	-9.11	108.12	121.24
1	C	22	G	O3'-P-O5'	8.76	117.15	104.00
2	B	307	ARG	NE-CZ-NH2	-8.72	111.35	119.20
2	A	212	LEU	N-CA-C	-8.47	98.56	110.50
2	B	331	ARG	N-CA-C	-8.34	103.04	113.55
2	B	358	GLY	N-CA-C	8.27	123.23	110.91
2	B	402	ALA	N-CA-C	-8.27	102.21	111.14
2	B	373	ALA	N-CA-C	-8.19	100.68	111.24
2	B	198	GLN	N-CA-C	-8.18	101.42	111.40
2	A	482	ILE	N-CA-C	-8.07	98.24	109.21
2	A	196	LEU	CA-C-N	8.03	129.88	119.84
2	A	196	LEU	C-N-CA	8.03	129.88	119.84
2	A	46	VAL	N-CA-C	-8.02	96.48	108.99
2	B	4	THR	N-CA-C	-8.01	103.72	113.97
2	A	238	LEU	N-CA-C	-8.00	95.69	108.73
2	B	307	ARG	NH1-CZ-NH2	-7.84	109.11	119.30
2	B	238	LEU	N-CA-C	-7.81	96.54	108.96
2	A	345	LYS	N-CA-C	7.71	121.49	108.23
2	B	520	PRO	CA-C-N	-7.57	111.95	119.90
2	B	520	PRO	C-N-CA	-7.57	111.95	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	435	GLU	N-CA-C	-7.57	93.68	107.75
2	B	212	LEU	N-CA-C	-7.52	99.35	110.48
2	B	345	LYS	N-CA-C	7.46	126.68	110.80
2	B	434	GLU	N-CA-C	-7.41	95.02	110.80
2	B	40	ARG	N-CA-C	7.37	121.14	109.50
2	B	447	SER	N-CA-C	7.34	118.90	109.65
1	D	47	U	C2'-C3'-O3'	7.33	120.49	109.50
2	B	274	PHE	N-CA-C	-7.21	100.13	110.08
2	A	436	GLU	N-CA-C	7.19	126.11	110.80
2	A	198	GLN	N-CA-C	-7.14	103.58	111.36
2	B	579	ARG	N-CA-C	7.13	119.84	109.71
2	A	46	VAL	CB-CA-C	-7.08	100.70	110.90
2	B	95	SER	N-CA-C	-7.03	104.70	113.28
2	B	482	ILE	N-CA-C	-6.95	100.56	109.80
2	B	570	LEU	N-CA-C	-6.92	104.98	113.50
2	A	381	ARG	CA-C-N	-6.90	112.88	119.85
2	A	381	ARG	C-N-CA	-6.90	112.88	119.85
2	A	246	GLU	N-CA-C	-6.84	99.07	109.95
2	B	105	THR	N-CA-C	6.82	118.72	109.24
2	A	279	TYR	N-CA-C	-6.82	103.85	111.28
2	A	328	ALA	N-CA-C	-6.75	99.66	109.59
2	B	417	GLY	N-CA-C	6.73	129.13	113.18
2	B	225	GLU	N-CA-C	-6.70	100.29	110.14
2	B	548	PHE	CA-C-N	6.70	126.64	120.21
2	B	548	PHE	C-N-CA	6.70	126.64	120.21
2	B	344	HIS	N-CA-C	-6.69	95.31	107.75
2	B	147	ARG	N-CA-C	-6.66	103.12	111.11
2	A	495	ARG	NE-CZ-NH1	-6.66	114.84	121.50
2	B	218	ILE	N-CA-C	-6.58	95.72	106.32
2	A	196	LEU	N-CA-C	-6.56	101.38	109.65
2	A	6	TYR	N-CA-C	-6.53	100.16	109.96
2	B	389	VAL	N-CA-C	-6.45	98.85	108.46
2	B	162	GLY	N-CA-C	6.44	123.58	115.21
2	A	170	PHE	N-CA-C	-6.39	106.11	114.04
2	B	225	GLU	CA-C-N	-6.38	112.65	122.09
2	B	225	GLU	C-N-CA	-6.38	112.65	122.09
2	B	343	ARG	N-CA-C	-6.35	104.41	111.71
2	A	344	HIS	CA-C-N	-6.31	111.95	122.17
2	A	344	HIS	C-N-CA	-6.31	111.95	122.17
2	A	40	ARG	N-CA-C	6.31	119.46	109.50
1	C	22	G	P-O5'-C5'	-6.29	111.46	120.90
1	D	70	U	N1-C1'-C2'	-6.29	102.57	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	355	GLU	N-CA-C	-6.26	100.67	109.69
2	A	111	ASP	N-CA-C	6.22	121.75	114.04
2	B	534	ALA	N-CA-C	-6.18	104.46	111.14
2	B	14	HIS	N-CA-C	6.15	120.25	112.87
2	A	18	GLU	N-CA-C	-6.14	101.20	110.28
2	A	193	PHE	N-CA-C	6.12	118.59	108.99
2	A	397	ALA	N-CA-C	6.11	118.02	111.36
2	A	301	GLU	N-CA-C	-6.08	100.66	110.32
2	A	88	GLY	N-CA-C	6.03	121.09	114.40
2	B	571	ARG	N-CA-C	-6.00	104.66	112.23
2	B	31	LEU	N-CA-C	-5.98	104.58	112.72
1	D	1	G	P-O3'-C3'	-5.96	111.25	120.20
1	D	2	G	P-O5'-C5'	-5.96	111.97	120.90
2	A	331	ARG	N-CA-C	-5.93	104.82	111.28
2	B	340	VAL	N-CA-C	-5.93	104.07	110.23
2	A	512	LEU	N-CA-C	-5.92	104.91	111.71
2	A	400	LEU	N-CA-C	-5.91	104.91	111.71
2	B	193	PHE	N-CA-C	5.90	118.37	109.23
1	C	11	U	O3'-P-O5'	-5.88	95.17	104.00
2	B	191	GLY	N-CA-C	-5.75	107.13	114.37
2	B	226	ASP	N-CA-C	5.72	119.57	109.96
1	D	70	U	C4'-C3'-O3'	5.71	121.57	113.00
2	A	346	ALA	N-CA-C	5.71	117.74	108.26
2	A	408	ALA	N-CA-C	-5.63	105.23	111.36
2	B	211	GLY	N-CA-C	5.62	123.08	115.32
2	B	67	TRP	N-CA-C	-5.61	102.19	110.48
2	B	366	PHE	N-CA-C	5.60	119.73	113.01
2	B	18	GLU	N-CA-C	-5.58	101.38	110.20
2	A	202	LEU	N-CA-C	5.58	117.16	111.14
2	A	340	VAL	N-CA-C	-5.56	105.30	110.53
2	A	115	ARG	N-CA-C	-5.53	106.57	113.38
1	C	9	A	C5'-C4'-C3'	-5.53	106.91	115.20
2	B	528	GLY	N-CA-C	-5.52	100.10	113.18
2	B	539	SER	CA-C-N	5.48	124.94	119.24
2	B	539	SER	C-N-CA	5.48	124.94	119.24
2	A	520	PRO	CA-C-N	-5.47	114.15	119.90
2	A	520	PRO	C-N-CA	-5.47	114.15	119.90
2	B	569	GLN	N-CA-C	-5.42	106.84	113.50
2	A	559	THR	N-CA-C	5.41	120.15	113.50
2	A	54	SER	N-CA-C	5.41	116.63	109.93
2	A	486	ASP	CA-C-N	5.40	125.48	119.32
2	A	486	ASP	C-N-CA	5.40	125.48	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	218	ILE	N-CA-C	-5.39	98.13	109.34
1	C	47	U	N1-C1'-C2'	5.38	120.07	112.00
2	A	177	GLU	N-CA-C	5.37	117.42	109.69
2	B	233	PRO	N-CA-C	-5.33	106.91	113.84
2	A	389	VAL	N-CA-C	-5.32	100.82	108.48
2	B	105	THR	CA-C-N	5.31	125.85	120.38
2	B	105	THR	C-N-CA	5.31	125.85	120.38
2	A	297	LEU	N-CA-C	-5.30	97.64	107.71
2	B	274	PHE	CA-C-N	-5.29	114.80	120.03
2	B	274	PHE	C-N-CA	-5.29	114.80	120.03
2	B	459	ASP	CA-C-N	5.28	124.73	119.24
2	B	459	ASP	C-N-CA	5.28	124.73	119.24
2	A	536	MET	N-CA-C	-5.23	105.76	111.82
2	A	136	ARG	N-CA-C	-5.21	106.43	112.89
2	B	308	GLN	N-CA-C	-5.18	99.76	110.80
2	B	411	LEU	N-CA-C	-5.18	105.64	112.94
2	A	270	LEU	CA-C-N	-5.18	114.62	119.85
2	A	270	LEU	C-N-CA	-5.18	114.62	119.85
2	B	115	ARG	N-CA-C	-5.16	107.01	113.72
2	A	157	PHE	N-CA-C	5.14	116.73	111.03
2	B	188	HIS	N-CA-C	5.07	118.56	112.38
2	A	309	SER	N-CA-C	5.06	117.64	110.50
2	B	468	TYR	N-CA-C	5.06	116.75	108.55
1	C	21	A	P-O3'-C3'	5.00	127.70	120.20

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 ⓘ

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	110	0
1	D	1570	0	805	132	0
2	A	4668	0	4679	492	0
2	B	4668	0	4679	575	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	1230	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 53.

All (1230) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:213:ASP:CG	2:B:3:ARG:HH22	1.83	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:277:LEU:HD12	2:A:421:LEU:HD12	1.63	0.81
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:165:GLN:HE21	2:A:165:GLN:C	1.94	0.75
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
2:B:576:MET:HE3	2:B:578:VAL:HG11	1.69	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:B:561:ALA:HA	2:B:562:PRO:C	2.11	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:B:283:MET:HE3	2:B:398:THR:HG22	1.69	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:A:226:ASP:C	2:A:228:ARG:H	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:220:ARG:HG2	2:B:170:PHE:CE1	2.25	0.72
2:B:576:MET:HE3	2:B:578:VAL:CG1	2.20	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:558:LEU:HD11	2:B:206:MET:HE1	1.71	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
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
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:A:115:ARG:HH11	2:A:117:GLU:CD	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:226:ASP:C	2:B:228:ARG:H	2.01	0.68
2:A:231:ARG:HG3	2:A:231:ARG:NH1	2.00	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:426:PHE:CD2	2:A:441:MET:HE2	2.31	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
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:556:ASP:CG	2:B:559:THR:HB	2.20	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: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: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
2:B:336:GLU:O	2:B:337:LEU:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:132:TYR:CD2	2:B:206:MET:HE2	2.32	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: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
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:B:458:LYS:C	2:B:460:PRO:HD3	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:ASP:C	2:B:291:PRO:HD3	2.25	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: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
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:299:LEU:C	2:B:300:LYS:HG2	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:302:VAL:O	2:B:303:GLY:C	2.45	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: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: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
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:B:292:ASP:CG	2:B:294:ARG:HE	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:PHE:CD1	2:B:311:PHE:C	2.81	0.57
2:A:341:ALA:O	2:A:344:HIS:O	2.22	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:554:GLY:O	2:B:194:TYR:OH	2.22	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:115:ARG:NH1	2:B:117:GLU:CD	2.64	0.56
2:B:364:ALA:O	2:B:365:LYS:C	2.46	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
2:B:410:LEU:C	2:B:411:LEU:HD23	2.30	0.56
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:A:561:ALA:HA	2:A:562:PRO:C	2.31	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: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:127:ARG:NH2	2:B:140:MET:HE2	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:59:THR:C	2:B:61:GLU:H	2.13	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
2:B:566:PRO:O	2:B:567:GLU:C	2.50	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:311:PHE:O	2:B:312:ARG:C	2.48	0.55
1:C:20(A):H2U:H3'	1:C:21:A:H5'	1.88	0.55
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:4:THR:C	2:B:5:HIS:ND1	2.65	0.54
2:B:266:LEU:CD1	2:B:536:MET:HE3	2.38	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:226:ASP:C	2:A:228:ARG:N	2.61	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:45:LEU:O	2:A:87:THR:OG1	2.23	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:537:THR:O	2:B:538:GLY:C	2.51	0.53
2:A:4:THR:OG1	2:A:5:HIS:ND1	2.40	0.53
2:A:155:TRP:O	2:A:156:ASP:C	2.52	0.53
2:A:418:PHE:O	2:A:419:ARG:HD2	2.07	0.53
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:B:134:ASP:CG	2:B:137:ARG:HH21	2.17	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
2:B:123:SER:O	2:B:124:GLU:C	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:457:GLU:CD	2:A:492:ARG:HD3	2.33	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:200:PRO:O	2:A:201:GLN:C	2.51	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
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
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: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
1:C:11:U:H2'	1:C:12:U:C6	2.45	0.52
1:D:34:QUO:HN22	2:B:91:GLU:CD	2.18	0.52
2:B:430:GLU:HG3	2:B:431:TRP:N	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:G7M:H4'	1:D:47:U:OP1	2.09	0.52
2:A:426:PHE:HD2	2:A:441:MET:HE2	1.74	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:433:GLU:C	2:A:435:GLU:H	2.18	0.52
2:A:461:GLY:C	2:A:463:VAL:H	2.17	0.52
2:A:563:SER:CB	2:B:173:LYS:HE3	2.39	0.52
2:A:49:VAL:HG12	2:A:93:GLU:HA	1.91	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:406:ARG:HG3	2:B:410:LEU:HG	1.92	0.51
2:B:429:LEU:HA	2:B:439:THR:O	2.10	0.51
1:C:3:A:O2'	1:C:4:G:O4'	2.28	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: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:A:409:ASP:O	2:A:410:LEU:C	2.53	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
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:A:289:ASP:C	2:A:291:PRO:HD3	2.36	0.51
2:A:361:GLY:O	2:A:362:GLY:C	2.54	0.51
2:B:28:ARG:NE	2:B:64:ARG:HE	2.08	0.51
2:B:115:ARG:HH11	2:B:117:GLU:CD	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:546:ILE:O	2:A:547:ALA:C	2.51	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:111:ASP:CG	2:A:115:ARG:NH2	2.69	0.51
2:A:252:GLU:OE1	2:A:256:ARG:CD	2.59	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: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
2:B:67:TRP:CD1	2:B:103:ALA:H	2.29	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:7:ALA:O	2:B:46:VAL:HB	2.11	0.50
2:B:67:TRP:CH2	2:B:102:GLU:HG2	2.46	0.50
2:B:127:ARG:HH21	2:B:140:MET:HE2	1.77	0.50
2:B:172:THR:OG1	2:B:173:LYS:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:41:ASP:OD1	2:A:41:ASP:C	2.54	0.50
2:A:232:GLN:O	2:A:233:PRO:C	2.55	0.50
2:B:6:TYR:O	2:B:7:ALA:C	2.55	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:226:ASP:C	2:B:228:ARG:N	2.69	0.50
2:B:261:VAL:C	2:B:263:ARG:H	2.19	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:A:165:GLN:C	2:A:165:GLN:NE2	2.67	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:433:GLU:C	2:A:435:GLU:N	2.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:251:LEU:HD22	2:A:422:TRP:CE3	2.48	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
2:B:509:GLY:O	2:B:510:PHE:C	2.56	0.49
1:C:61:C:C2'	1:C:62:C:H5'	2.43	0.49
2:A:82:ASN:C	2:A:82:ASN:OD1	2.54	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
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: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: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:246:GLU:O	2:B:247:VAL:C	2.52	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:140:MET:O	2:A:141:GLN:C	2.55	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
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:266:LEU:HG	2:A:536:MET:HE2	1.94	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:A:451:GLU:C	2:A:453:LEU:H	2.21	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:155:TRP:O	2:B:159:ASP:HB2	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:42:G:HO2'	1:C:43:G:H5'	1.79	0.48
1:D:66:C:H2'	1:D:67:C:H6	1.78	0.48
2:A:12:GLU:CD	2:A:89:ARG:HD3	2.39	0.48
2:A:198:GLN:NE2	2:A:223:ARG:HB2	2.29	0.48
2:A:216:PHE:CD1	2:A:216:PHE:C	2.92	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:349:LEU:C	2:A:349:LEU:HD22	2.39	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:117:GLU:O	2:B:118:GLU:C	2.57	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:148:HIS:C	2:A:148:HIS:CD2	2.92	0.48
2:A:431:TRP:CD1	2:A:438:TRP:NE1	2.82	0.48
2:A:576:MET:HB3	2:B:576:MET:HE2	1.95	0.48
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: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:409:ASP:C	2:B:411:LEU:N	2.72	0.47
2:B:528:GLY:O	2:B:529:LEU:C	2.57	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
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
2:B:443:HIS:C	2:B:445:PHE:H	2.22	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:371:ARG:HG3	2:A:375:LEU:HD21	1.96	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: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:486:ASP:C	2:A:486:ASP:OD1	2.57	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:225:GLU:O	2:A:226:ASP:C	2.57	0.47
2:A:494:PHE:HD2	2:A:499:ILE:HB	1.80	0.47
2:B:240:LEU:C	2:B:240:LEU:HD23	2.39	0.47
2:B:250:VAL:HG11	2:B:468:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:443:HIS:C	2:B:445:PHE:N	2.72	0.47
2:A:284:GLU:OE1	2:A:284:GLU:HA	2.14	0.47
2:A:292:ASP:CG	2:A:294:ARG:HH11	2.22	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:59:THR:C	2:B:61:GLU:N	2.73	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:140:MET:HE1	2:A:544:GLU:HA	1.96	0.47
2:A:226:ASP:CG	2:A:228:ARG:HG2	2.40	0.47
2:A:303:GLY:HA2	2:A:320:VAL:HG23	1.97	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:20:VAL:C	2:A:21:LEU:HD23	2.40	0.46
2:A:192:LEU:HD23	2:B:562:PRO:C	2.39	0.46
2:A:204:LYS:HE3	2:A:241:GLU:HB2	1.97	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:B:120:LYS:O	2:B:120:LYS:HG2	2.14	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: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:67:TRP:NE1	2:B:103:ALA:H	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:429:LEU:HD13	2:B:438:TRP:HB2	1.98	0.46
2:B:561:ALA:CA	2:B:562:PRO:C	2.88	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
2:B:333:GLU:C	2:B:335:ALA:N	2.73	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:B:208:MET:HE2	2:B:208:MET:HA	1.97	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:445:PHE:O	2:A:484:ILE:HG12	2.17	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:307:ARG:HG3	2:B:315:GLN:HB2	1.99	0.45
2:B:409:ASP:C	2:B:411:LEU:H	2.23	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:508:PHE:HB2	2:A:512:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:177:GLU:H	2:A:507:LYS:HE3	1.81	0.45
2:B:163:PHE:HA	2:B:214:ARG:O	2.16	0.45
2:B:395:VAL:O	2:B:396:ALA:C	2.57	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:246:GLU:CD	2:B:1:MET:HE1	2.41	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:41:ASP:C	2:B:43:GLU:H	2.24	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:342:LYS:C	2:A:344:HIS:O	2.60	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:118:GLU:O	2:A:119:GLU:C	2.60	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:302:VAL:O	2:A:303:GLY:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:307:ARG:C	2:B:308:GLN:HG2	2.42	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
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
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:349:LEU:C	2:A:349:LEU:CD2	2.91	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:141:GLN:O	2:B:142:GLU:C	2.61	0.44
2:B:449:HIS:O	2:B:450:PRO:C	2.61	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: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
1:C:40:C:O2'	1:C:41:A:H5'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:PRO:HG2	2:B:239:ASP:CG	2.43	0.43
2:B:543:ARG:HH21	2:B:552:LYS:HG3	1.83	0.43
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: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:308:GLN:HE21	2:A:308:GLN:HB3	1.54	0.43
2:A:451:GLU:C	2:A:453:LEU:N	2.76	0.43
2:B:339:GLU:O	2:B:340:VAL:C	2.61	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:A:206:MET:HE1	2:A:510:PHE:HD1	1.84	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:260:HIS:O	2:A:261:VAL:C	2.61	0.43
2:A:489:LEU:O	2:A:490:GLN:C	2.61	0.43
2:A:543:ARG:HH22	2:A:552:LYS:HE3	1.83	0.43
2:B:146:LEU:O	2:B:147:ARG:C	2.61	0.43
2:B:199:SER:C	2:B:201:GLN:H	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:GLU:O	2:B:190:PRO:C	2.62	0.43
2:B:556:ASP:OD2	2:B:559:THR:N	2.51	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
2:A:368:GLU:N	2:A:369:PRO:HD2	2.33	0.43
2:A:412:GLY:O	2:A:413:LEU:C	2.61	0.43
2:A:494:PHE:CD2	2:A:499:ILE:HG21	2.53	0.43
2:B:26:ASN:C	2:B:27:ARG:HG3	2.44	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:B:432:ASP:O	2:B:433:GLU:C	2.61	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: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: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:551:ASN:O	2:B:552:LYS:C	2.61	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:11:ARG:O	2:B:12:GLU:C	2.61	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:204:LYS:HE2	2:A:241:GLU:CD	2.45	0.42
2:A:242:MET:HE2	2:A:245:VAL:HG11	2.00	0.42
2:A:443:HIS:CG	2:A:444:PRO:CD	2.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:71:C:C4	1:C:72:C:N4	2.87	0.42
2:A:258:MET:O	2:A:259:ALA:C	2.62	0.42
2:A:339:GLU:O	2:A:339:GLU:HG3	2.15	0.42
2:A:364:ALA:O	2:A:365:LYS:C	2.62	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: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: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:283:MET:O	2:A:287:GLY:CA	2.67	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
2:B:261:VAL:C	2:B:263:ARG:N	2.77	0.42
2:B:278:SER:C	2:B:280:GLU:N	2.77	0.42
1:D:25:U:H2'	1:D:26:A:C8	2.55	0.42
2:A:486:ASP:HA	2:A:487:PRO:HD3	1.86	0.42
2:A:551:ASN:C	2:A:551:ASN:OD1	2.62	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:183:LEU:HD12	2:B:573:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:130:TYR:O	2:A:131:ARG:C	2.63	0.41
2:A:246:GLU:O	2:A:247:VAL:C	2.62	0.41
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:508:PHE:O	2:A:509:GLY:C	2.63	0.41
2:A:8:GLY:HA3	2:A:43:GLU:C	2.45	0.41
2:A:228:ARG:C	2:A:229:ALA:O	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:PHE:HA	2:B:214:ARG:HG3	2.02	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:143:ASN:O	2:A:144:LEU:C	2.63	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:C	2:A:300:LYS:HG2	2.46	0.41
2:A:299:LEU:HD13	2:A:400:LEU:HB3	2.02	0.41
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:252:GLU:CD	2:A:256:ARG:HD3	2.46	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: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:O	2:A:118:GLU:HG3	2.22	0.40
2:B:237:GLN:HB3	2:B:527:TRP:O	2.22	0.40
2:B:278:SER:O	2:B:279:TYR:C	2.65	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:6:G:C2	1:C:7:G:C4	3.09	0.40
2:A:111:ASP:CG	2:A:115:ARG:HH21	2.27	0.40
2:A:287:GLY:HA3	2:A:397:ALA:O	2.21	0.40
2:A:386:LEU:HD23	2:A:386:LEU:HA	1.98	0.40
2:B:82:ASN:OD1	2:B:82:ASN:C	2.64	0.40
2:B:312:ARG:HH12	2:B:316:GLU:CD	2.29	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:173:LYS:O	2:A:174:SER:C	2.65	0.40
2:A:175:THR:HB	2:A:507:LYS:NZ	2.37	0.40
2:B:159:ASP:O	2:B:160:ARG:C	2.64	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%)	4	23
2	B	578/580 (100%)	459 (79%)	93 (16%)	26 (4%)	2	12
All	All	1156/1160 (100%)	958 (83%)	157 (14%)	41 (4%)	3	16

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
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 ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	483/483 (100%)	401 (83%)	82 (17%)	2	11
2	B	483/483 (100%)	405 (84%)	78 (16%)	2	12
All	All	966/966 (100%)	806 (83%)	160 (17%)	2	12

All (160) 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	19	VAL
2	A	22	GLU
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	75	VAL
2	A	78	ARG
2	A	83	PRO
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

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Mol	Chain	Res	Type
2	A	190	PRO
2	A	192	LEU
2	A	201	GLN
2	A	207	LEU
2	A	214	ARG
2	A	215	TYR
2	A	217	GLN
2	A	227	LEU
2	A	228	ARG
2	A	234	ASP
2	A	240	LEU
2	A	250	VAL
2	A	253	LEU
2	A	255	GLU
2	A	257	LEU
2	A	263	ARG
2	A	272	LEU
2	A	276	ARG
2	A	294	ARG
2	A	302	VAL
2	A	307	ARG
2	A	321	LYS
2	A	331	ARG
2	A	339	GLU
2	A	340	VAL
2	A	349	LEU
2	A	375	LEU
2	A	379	GLU
2	A	387	LEU
2	A	393	ARG
2	A	400	LEU
2	A	411	LEU
2	A	431	TRP
2	A	433	GLU
2	A	434	GLU
2	A	435	GLU
2	A	436	GLU
2	A	438	TRP
2	A	440	TYR
2	A	441	MET
2	A	453	LEU
2	A	464	ARG

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Mol	Chain	Res	Type
2	A	471	VAL
2	A	489	LEU
2	A	505	ARG
2	A	506	GLU
2	A	507	LYS
2	A	512	LEU
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	B	1	MET
2	B	2	ARG
2	B	11	ARG
2	B	13	THR
2	B	20	VAL
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	77	LEU
2	B	78	ARG
2	B	80	GLU
2	B	89	ARG
2	B	100	LEU
2	B	107	PRO
2	B	110	VAL
2	B	115	ARG
2	B	118	GLU
2	B	120	LYS
2	B	124	GLU
2	B	126	LEU
2	B	128	LEU
2	B	142	GLU
2	B	145	ARG
2	B	168	THR
2	B	173	LYS
2	B	214	ARG

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Mol	Chain	Res	Type
2	B	215	TYR
2	B	227	LEU
2	B	235	PHE
2	B	240	LEU
2	B	245	VAL
2	B	257	LEU
2	B	272	LEU
2	B	276	ARG
2	B	277	LEU
2	B	285	ARG
2	B	288	SER
2	B	290	LYS
2	B	299	LEU
2	B	307	ARG
2	B	311	PHE
2	B	313	VAL
2	B	326	PRO
2	B	331	ARG
2	B	339	GLU
2	B	340	VAL
2	B	342	LYS
2	B	343	ARG
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	421	LEU
2	B	432	ASP
2	B	434	GLU
2	B	436	GLU
2	B	447	SER
2	B	451	GLU
2	B	462	ARG
2	B	475	VAL
2	B	489	LEU
2	B	492	ARG
2	B	502	GLU
2	B	516	GLU
2	B	522	HIS

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Mol	Chain	Res	Type
2	B	532	LEU
2	B	559	THR
2	B	570	LEU
2	B	572	GLU
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 (15) 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	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
2	B	315	GLN
2	B	443	HIS
2	B	490	GLN
2	B	551	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	72/73 (98%)	10 (13%)	3 (4%)
1	D	72/73 (98%)	14 (19%)	3 (4%)
All	All	144/146 (98%)	24 (16%)	6 (4%)

All (24) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	9	A
1	C	16	H2U
1	C	17	C

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Mol	Chain	Res	Type
1	C	18	G
1	C	20	H2U
1	C	35	U
1	C	37	2MA
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	35	U
1	D	37	2MA
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
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	H2U	D	20	1	18,21,22	0.73	1 (5%)	19,30,33	0.87	1 (5%)
1	PSU	D	55	1	18,21,22	1.77	1 (5%)	21,30,33	0.79	1 (4%)
1	G7M	C	46	1	23,26,27	0.69	1 (4%)	34,39,42	0.80	2 (5%)
1	H2U	C	16	1	18,21,22	0.95	1 (5%)	19,30,33	0.73	0
1	H2U	D	20(A)	1	18,21,22	0.83	1 (5%)	19,30,33	0.86	0
1	QUO	C	34	1	32,35,36	0.95	2 (6%)	36,52,55	2.00	6 (16%)
1	H2U	C	20	1	18,21,22	0.91	1 (5%)	19,30,33	0.68	0
1	4SU	C	8	1	18,21,22	5.56	1 (5%)	25,30,33	0.47	0
1	QUO	D	34	1	32,35,36	0.87	2 (6%)	36,52,55	1.91	6 (16%)
1	PSU	C	65	1	18,21,22	1.90	1 (5%)	21,30,33	0.89	1 (4%)
1	PSU	D	65	1	18,21,22	1.82	1 (5%)	21,30,33	0.77	1 (4%)
1	4SU	D	8	1	18,21,22	5.62	1 (5%)	25,30,33	0.46	0
1	5MU	D	54	1	19,22,23	1.97	4 (21%)	27,32,35	14.09	10 (37%)
1	H2U	C	20(A)	1	18,21,22	0.54	0	19,30,33	0.83	0
1	5MU	C	54	1	19,22,23	0.29	0	27,32,35	0.67	1 (3%)
1	H2U	D	16	1	18,21,22	0.67	1 (5%)	19,30,33	0.85	1 (5%)
1	2MA	D	37	1	22,25,26	0.43	0	32,37,40	0.76	0
1	PSU	C	55	1	18,21,22	1.81	1 (5%)	21,30,33	0.75	1 (4%)
1	G7M	D	46	1	23,26,27	0.45	0	34,39,42	0.99	2 (5%)
1	2MA	C	37	1	22,25,26	0.56	1 (4%)	32,37,40	0.80	1 (3%)

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	H2U	D	20	1	-	7/7/38/39	0/2/2/2
1	PSU	D	55	1	-	1/7/25/26	0/2/2/2
1	G7M	C	46	1	-	0/7/25/26	0/3/3/3
1	H2U	C	16	1	-	2/7/38/39	0/2/2/2
1	H2U	D	20(A)	1	-	3/7/38/39	0/2/2/2
1	QUO	C	34	1	-	3/12/43/44	0/4/4/4
1	H2U	C	20	1	-	0/7/38/39	0/2/2/2
1	4SU	C	8	1	-	0/7/25/26	0/2/2/2
1	QUO	D	34	1	-	1/12/43/44	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	C	65	1	-	0/7/25/26	0/2/2/2
1	PSU	D	65	1	-	1/7/25/26	0/2/2/2
1	4SU	D	8	1	-	0/7/25/26	0/2/2/2
1	5MU	D	54	1	-	0/7/25/26	0/2/2/2
1	H2U	C	20(A)	1	-	1/7/38/39	0/2/2/2
1	5MU	C	54	1	-	0/7/25/26	0/2/2/2
1	H2U	D	16	1	-	2/7/38/39	0/2/2/2
1	2MA	D	37	1	-	2/7/25/26	0/3/3/3
1	PSU	C	55	1	-	0/7/25/26	0/2/2/2
1	G7M	D	46	1	-	0/7/25/26	0/3/3/3
1	2MA	C	37	1	-	2/7/25/26	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	4SU	C4-S4	-23.77	1.26	1.68
1	C	8	4SU	C4-S4	-23.49	1.26	1.68
1	C	65	PSU	C6-N1	-7.55	1.23	1.36
1	D	65	PSU	C6-N1	-7.40	1.24	1.36
1	C	55	PSU	C6-N1	-7.25	1.24	1.36
1	D	55	PSU	C6-N1	-7.16	1.24	1.36
1	D	54	5MU	C6-N1	-4.72	1.30	1.38
1	D	54	5MU	C4-C5	-4.65	1.37	1.44
1	D	54	5MU	C2-N3	4.08	1.45	1.38
1	C	16	H2U	C2-N1	3.28	1.40	1.35
1	C	20	H2U	C2-N1	3.25	1.40	1.35
1	C	34	QUO	C8-C7	-3.23	1.31	1.37
1	D	34	QUO	C8-C7	-3.13	1.31	1.37
1	D	20(A)	H2U	C2-N1	2.87	1.39	1.35
1	C	46	G7M	CN7-N7	2.59	1.51	1.46
1	D	20	H2U	C2-N1	2.44	1.39	1.35
1	C	34	QUO	C5-C4	-2.19	1.37	1.44
1	C	37	2MA	CM2-C2	-2.18	1.43	1.49
1	D	34	QUO	C5-C4	-2.18	1.37	1.44
1	D	16	H2U	C2-N1	2.09	1.38	1.35
1	D	54	5MU	C2-N1	2.08	1.41	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	5MU	C5M-C5-C4	-68.69	45.44	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	54	5MU	C6-N1-C2	-18.60	102.78	121.30
1	D	54	5MU	C5-C4-N3	-13.23	103.83	115.32
1	C	34	QUO	C10-N11-C12	8.73	132.63	114.83
1	D	34	QUO	C10-N11-C12	7.95	131.06	114.83
1	D	54	5MU	C1'-N1-C6	5.93	130.92	121.15
1	D	54	5MU	O4-C4-N3	5.02	129.56	120.11
1	D	54	5MU	C5-C6-N1	-4.94	117.94	123.31
1	D	34	QUO	O14-C14-C15	3.82	120.39	111.43
1	C	34	QUO	O14-C14-C13	3.58	118.48	111.43
1	D	34	QUO	C7-C10-N11	3.47	125.29	111.84
1	D	34	QUO	C16-C15-C14	-3.35	99.40	105.67
1	C	34	QUO	C16-C15-C14	-3.29	99.51	105.67
1	D	54	5MU	N3-C2-N1	3.06	118.88	114.89
1	C	34	QUO	C1'-N9-C8	2.85	128.96	125.72
1	C	34	QUO	C7-C10-N11	2.85	122.88	111.84
1	D	54	5MU	O2-C2-N1	-2.82	119.13	122.80
1	C	46	G7M	C8-N7-C5	-2.80	104.28	107.78
1	D	34	QUO	C1'-N9-C8	2.74	128.83	125.72
1	D	46	G7M	C8-N7-C5	-2.62	104.51	107.78
1	C	34	QUO	O14-C14-C15	2.62	117.57	111.43
1	C	54	5MU	C2'-C1'-N1	-2.57	106.11	113.25
1	D	20	H2U	N3-C2-N1	-2.57	114.07	116.65
1	D	65	PSU	C5-C6-N1	2.53	125.65	122.14
1	D	34	QUO	O14-C14-C13	2.46	116.28	111.43
1	D	55	PSU	C5-C6-N1	2.38	125.44	122.14
1	C	65	PSU	C5-C6-N1	2.34	125.39	122.14
1	D	54	5MU	C4-N3-C2	-2.25	124.39	127.34
1	D	54	5MU	C5M-C5-C6	-2.24	119.82	122.85
1	D	46	G7M	C2'-C1'-N9	2.18	119.32	113.25
1	C	46	G7M	CN7-N7-C8	2.14	128.03	124.79
1	C	55	PSU	C5-C6-N1	2.10	125.06	122.14
1	D	16	H2U	N3-C2-N1	-2.07	114.56	116.65
1	C	37	2MA	CM2-C2-N1	-2.01	114.11	117.13

There are no chirality outliers.

All (25) 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	N11-C10-C7-C5
1	C	34	QUO	C13-C12-N11-C10

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Mol	Chain	Res	Type	Atoms
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	34	QUO	C16-C12-N11-C10
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	55	PSU	O4'-C1'-C5-C4
1	D	20	H2U	C3'-C4'-C5'-O5'
1	C	37	2MA	C2'-C1'-N9-C8
1	D	37	2MA	C2'-C1'-N9-C8
1	D	37	2MA	C4'-C5'-O5'-P
1	D	65	PSU	O4'-C1'-C5-C6
1	D	20(A)	H2U	O4'-C1'-N1-C2
1	D	20(A)	H2U	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 52 short contacts:

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	37	2MA	5	0
1	D	46	G7M	5	0
1	C	37	2MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

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	C	63/73 (86%)	-2.11	0 100 100	26, 56, 90, 102	0
1	D	63/73 (86%)	-2.08	0 100 100	32, 52, 96, 101	0
2	A	580/580 (100%)	-1.79	0 100 100	7, 26, 64, 102	0
2	B	580/580 (100%)	-1.74	0 100 100	6, 34, 68, 102	0
All	All	1286/1306 (98%)	-1.79	0 100 100	6, 31, 71, 102	0

There are no RSRZ outliers to report.

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

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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PSU	C	55	20/21	0.98	0.04	74,75,82,82	0
1	H2U	C	20	20/21	0.99	0.04	61,72,77,77	0
1	H2U	C	20(A)	20/21	0.99	0.03	57,63,73,73	0
1	5MU	C	54	21/22	0.99	0.04	79,81,81,82	0
1	H2U	C	16	20/21	0.99	0.03	60,66,70,73	0
1	PSU	C	65	20/21	0.99	0.04	72,75,80,82	0
1	H2U	D	16	20/21	0.99	0.03	51,65,67,71	0
1	H2U	D	20	20/21	0.99	0.04	49,68,72,73	0
1	H2U	D	20(A)	20/21	0.99	0.04	57,61,66,67	0
1	QUO	D	34	32/33	0.99	0.04	48,63,72,73	0
1	G7M	D	46	24/25	0.99	0.03	43,47,49,53	0
1	5MU	D	54	21/22	0.99	0.03	54,60,64,65	0
1	PSU	D	55	20/21	0.99	0.03	48,53,65,65	0
1	PSU	D	65	20/21	0.99	0.04	76,79,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	2MA	C	37	23/24	1.00	0.02	25,41,44,64	0
1	2MA	D	37	23/24	1.00	0.03	50,60,67,68	0
1	4SU	D	8	20/21	1.00	0.03	39,43,47,48	0
1	G7M	C	46	24/25	1.00	0.02	36,42,48,50	0
1	4SU	C	8	20/21	1.00	0.03	52,56,60,61	0
1	QUO	C	34	32/33	1.00	0.03	23,35,51,53	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.