Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 04:04 AM EDT

PDB ID	:	2DER
Title	:	Cocrystal structure of an RNA sulfuration enzyme MnmA and tRNA-Glu in the initial tRNA binding state
Authors	:	Numata, T.; Ikeuchi, Y.; Fukai, S.; Suzuki, T.; Nureki, O.
Deposited on	:	2006-02-17
Resolution	:	3.10 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:

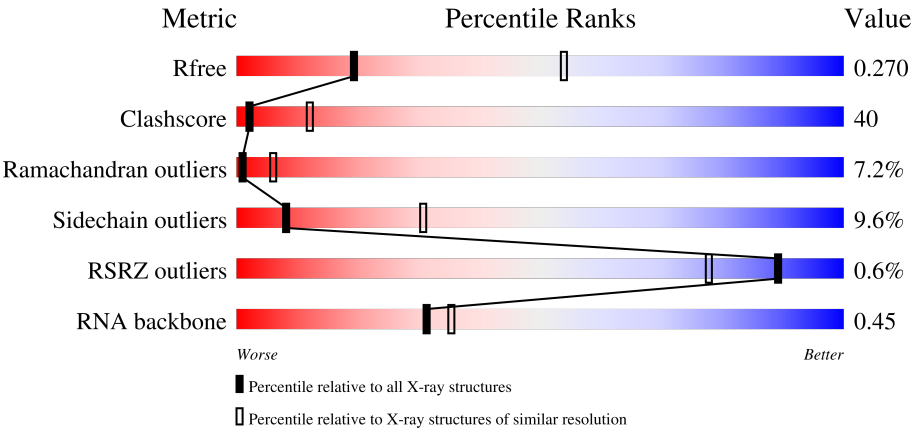
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 <=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	76	17% 46% 30% • •
1	D	76	21% 43% 25% • 7%
2	A	380	36% 47% 8% • 8%
2	B	380	% 34% 53% 7% • 6%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	1002	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8675 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	74	Total	C	N	O	P	0	0	0
			1573	701	279	519	74			
1	D	71	Total	C	N	O	P	0	0	0
			1509	673	269	496	71			

- Molecule 2 is a protein called tRNA-specific 2-thiouridylase mnmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	348	Total	C	N	O	S	0	0	0
			2733	1735	463	524	11			
2	B	359	Total	C	N	O	S	0	0	0
			2815	1786	477	540	12			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P25745
A	-10	ARG	-	expression tag	UNP P25745
A	-9	GLY	-	expression tag	UNP P25745
A	-8	SER	-	expression tag	UNP P25745
A	-7	HIS	-	expression tag	UNP P25745
A	-6	HIS	-	expression tag	UNP P25745
A	-5	HIS	-	expression tag	UNP P25745
A	-4	HIS	-	expression tag	UNP P25745
A	-3	HIS	-	expression tag	UNP P25745
A	-2	HIS	-	expression tag	UNP P25745
A	-1	GLY	-	expression tag	UNP P25745
A	0	SER	-	expression tag	UNP P25745
B	-11	MET	-	expression tag	UNP P25745
B	-10	ARG	-	expression tag	UNP P25745
B	-9	GLY	-	expression tag	UNP P25745
B	-8	SER	-	expression tag	UNP P25745
B	-7	HIS	-	expression tag	UNP P25745

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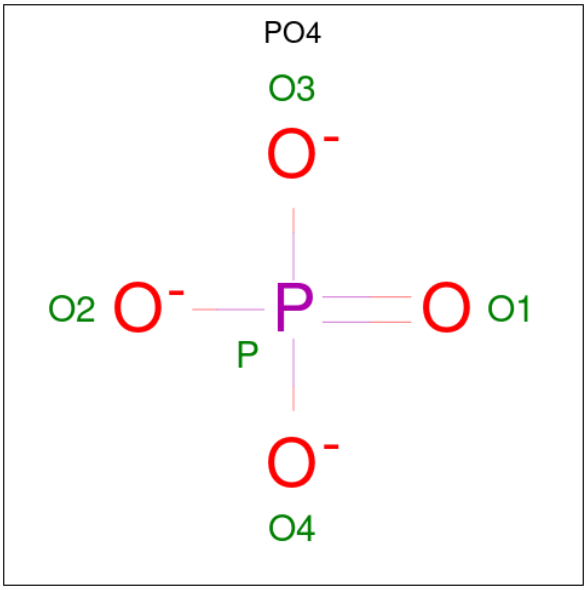
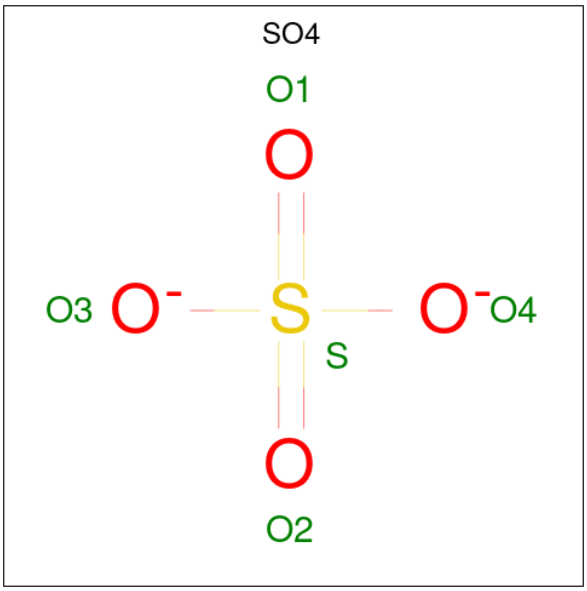
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP P25745
B	-5	HIS	-	expression tag	UNP P25745
B	-4	HIS	-	expression tag	UNP P25745
B	-3	HIS	-	expression tag	UNP P25745
B	-2	HIS	-	expression tag	UNP P25745
B	-1	GLY	-	expression tag	UNP P25745
B	0	SER	-	expression tag	UNP P25745

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



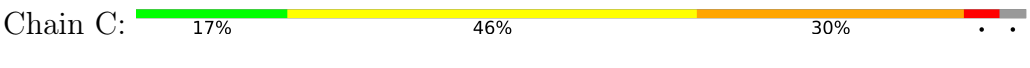
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

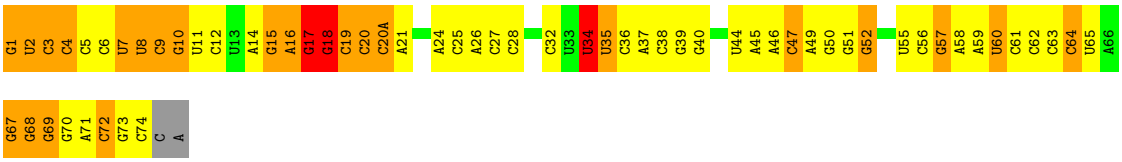
3 Residue-property plots (i)

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: tRNA

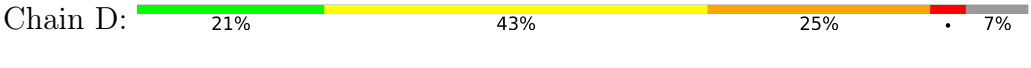
Chain C:

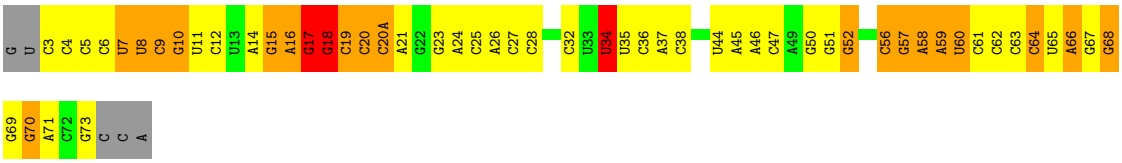




• Molecule 1: tRNA

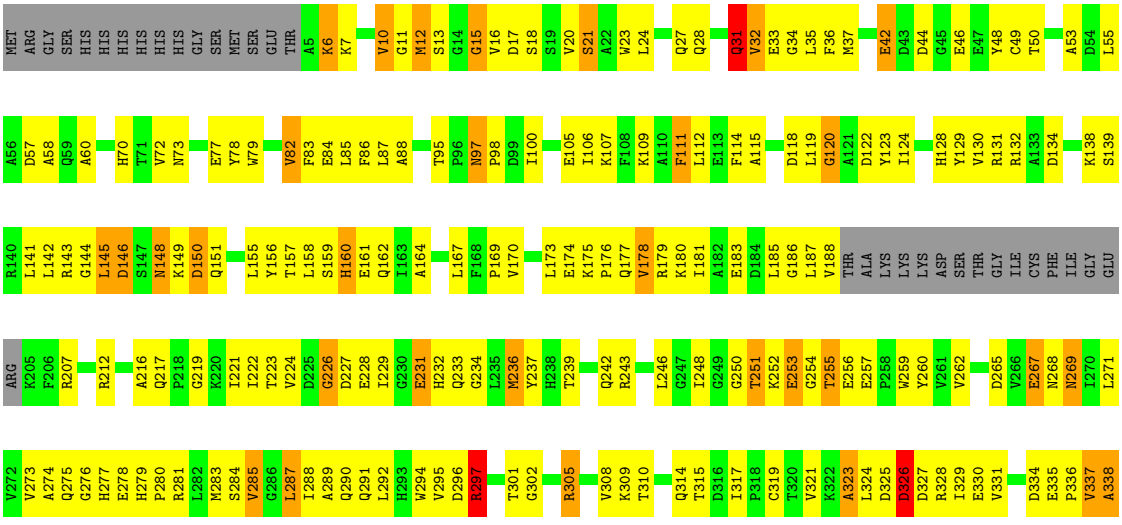
Chain D:





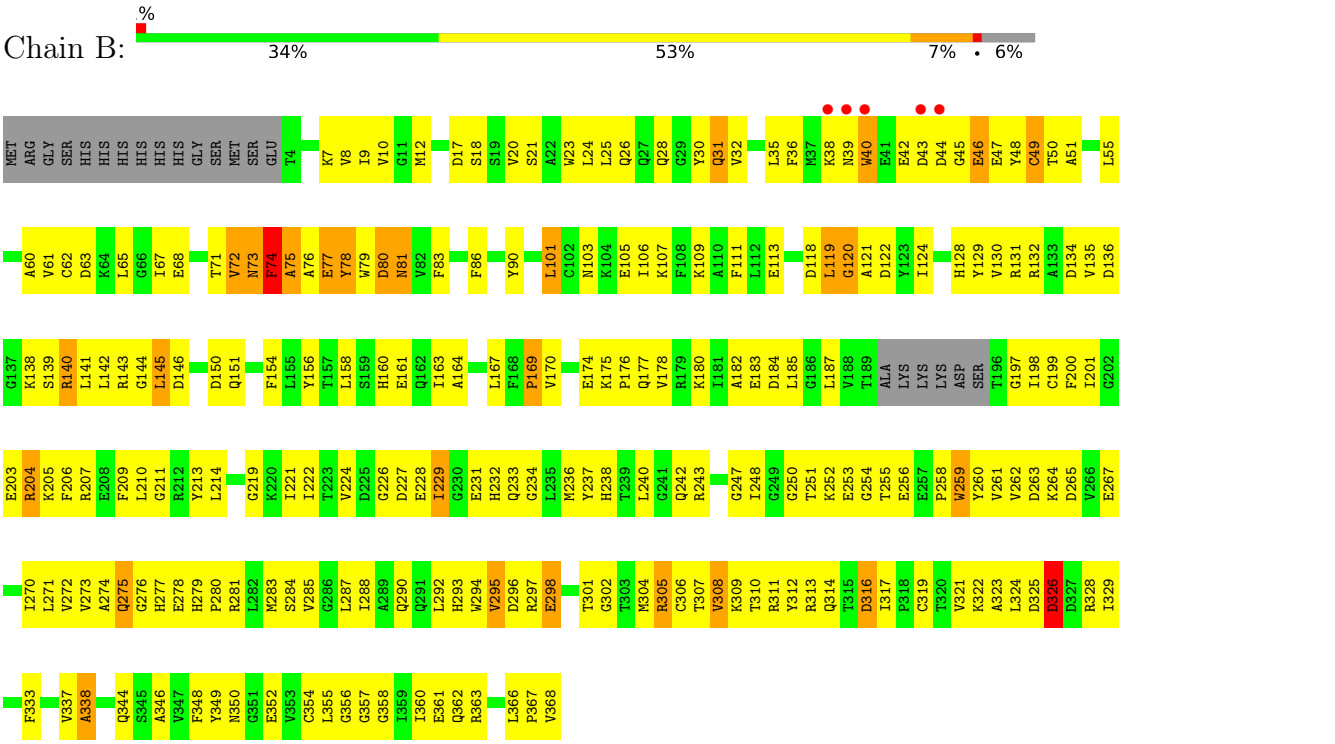
• Molecule 2: tRNA-specific 2-thiouridylase mnmA

Chain A:



• Molecule 2: tRNA-specific 2-thiouridylase mnmA

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	225.39Å 175.84Å 52.97Å 90.00° 101.62° 90.00°	Depositor
Resolution (Å)	46.75 – 3.10 46.75 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.9 (46.75-3.10) 83.5 (46.75-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.269 0.225 , 0.270	Depositor DCC
R_{free} test set	2924 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.055 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8675	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, SO4

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	0.46	1/1755 (0.1%)	0.79	3/2731 (0.1%)
1	D	0.43	0/1684	0.81	3/2622 (0.1%)
2	A	0.43	0/2790	0.70	1/3777 (0.0%)
2	B	0.40	0/2873	0.65	1/3889 (0.0%)
All	All	0.43	1/9102 (0.0%)	0.73	8/13019 (0.1%)

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	2
1	D	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	G	OP3-P	-7.33	1.52	1.61

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	34	U	C2'-C3'-O3'	8.18	127.48	109.50
1	C	34	U	C2'-C3'-O3'	8.06	127.23	109.50
1	C	18	G	N9-C1'-C2'	7.81	124.15	114.00
1	D	18	G	N9-C1'-C2'	7.73	124.05	114.00
1	C	47	C	N1-C1'-C2'	5.93	121.71	114.00
2	A	31	GLN	N-CA-C	-5.65	95.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	58	A	N9-C1'-C2'	5.35	120.95	114.00
2	B	31	GLN	N-CA-C	-5.14	97.13	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	17	G	Sidechain
1	C	18	G	Sidechain
1	D	17	G	Sidechain
1	D	18	G	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	1573	0	802	85	0
1	D	1509	0	770	78	0
2	A	2733	0	2670	225	0
2	B	2815	0	2750	246	0
3	A	5	0	0	3	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
All	All	8675	0	6992	624	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 40.

All (624) 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:C:56:C:H2'	1:C:57:G:H5"	1.32	1.06
1:D:56:C:H2'	1:D:57:G:H5"	1.33	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:35:LEU:HD11	2:A:72:VAL:HG23	1.40	1.03
1:D:51:G:H2'	1:D:52:G:H5"	1.45	0.98
1:C:51:G:H2'	1:C:52:G:H5"	1.49	0.95
1:D:24:A:O2'	2:B:256:GLU:HB3	1.67	0.93
2:B:254:GLY:HA2	2:B:259:TRP:HH2	1.32	0.92
1:C:56:C:C2'	1:C:57:G:H5"	2.00	0.92
2:B:35:LEU:HD11	2:B:72:VAL:HG22	1.53	0.90
2:A:274:ALA:HB1	2:A:279:HIS:ND1	1.87	0.90
2:B:310:THR:HB	2:B:314:GLN:HE22	1.35	0.90
1:D:19:C:OP2	1:D:20:C:H3'	1.70	0.89
1:D:56:C:C2'	1:D:57:G:H5"	2.02	0.88
2:B:38:LYS:NZ	2:B:71:THR:HB	1.88	0.88
1:C:1:G:H1'	1:C:73:G:H22	1.39	0.88
2:A:17:ASP:O	2:A:21:SER:HB2	1.74	0.86
1:D:9:C:O2'	1:D:45:A:H2'	1.77	0.85
1:D:57:G:H5'	1:D:57:G:H8	1.40	0.84
2:A:287:LEU:HD12	2:A:331:VAL:HB	1.57	0.84
2:B:321:VAL:HG12	2:B:329:ILE:HD11	1.59	0.84
1:C:57:G:H8	1:C:57:G:H5'	1.41	0.84
2:B:259:TRP:CZ3	2:B:275:GLN:HB3	2.14	0.83
2:A:251:THR:HG22	2:A:252:LYS:N	1.92	0.83
2:A:251:THR:HG22	2:A:252:LYS:H	1.42	0.82
1:C:9:C:O2'	1:C:45:A:H2'	1.79	0.82
2:B:40:TRP:HB2	2:B:205:LYS:HE2	1.62	0.81
2:B:197:GLY:O	2:B:201:ILE:HG12	1.81	0.81
1:D:57:G:H5'	1:D:57:G:C8	2.16	0.81
1:D:51:G:C2'	1:D:52:G:H5"	2.10	0.81
2:A:262:VAL:HG13	2:A:281:ARG:O	1.80	0.81
1:C:19:C:OP2	1:C:20:C:H3'	1.81	0.80
1:C:25:C:H5'	2:A:256:GLU:O	1.82	0.80
1:D:60:U:H5"	1:D:61:C:OP2	1.82	0.80
2:A:138:LYS:HD2	2:A:160:HIS:HB2	1.63	0.80
1:D:5:C:H42	1:D:68:G:H1	1.28	0.79
1:C:6:C:H2'	1:C:6:C:O2	1.82	0.79
2:A:219:GLY:H	2:A:232:HIS:HB2	1.48	0.79
2:A:143:ARG:HA	2:A:150:ASP:OD2	1.83	0.79
2:B:74:PHE:HD1	2:B:78:TYR:HB2	1.46	0.79
2:B:284:SER:OG	2:B:363:ARG:HD2	1.82	0.79
1:C:51:G:C2'	1:C:52:G:H5"	2.13	0.78
1:D:9:C:H5'	1:D:10:G:OP2	1.83	0.78
1:C:57:G:H5'	1:C:57:G:C8	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:U:H5”	1:C:61:C:OP2	1.85	0.76
2:A:173:LEU:HB3	2:A:177:GLN:NE2	2.01	0.76
2:A:308:VAL:HG23	2:A:319:CYS:SG	2.25	0.76
2:B:262:VAL:HG11	2:B:281:ARG:HB3	1.68	0.75
2:A:128:HIS:CD2	2:A:155:LEU:HD21	2.22	0.75
1:C:17:G:H2’	1:C:57:G:H22	1.52	0.74
2:B:131:ARG:NE	2:B:144:GLY:HA2	2.02	0.74
2:B:48:TYR:HB3	2:B:204:ARG:HH22	1.51	0.74
2:B:103:ASN:OD1	2:B:107:LYS:HD2	1.88	0.74
2:B:252:LYS:O	2:B:252:LYS:HD3	1.87	0.74
1:C:17:G:H2’	1:C:57:G:N2	2.03	0.74
2:A:37:MET:SD	2:A:111:PHE:HD1	2.11	0.73
1:C:14:A:H2’	1:C:15:G:O4’	1.89	0.72
1:D:5:C:N4	1:D:68:G:H1	1.87	0.72
2:A:287:LEU:HD22	2:A:360:ILE:HG12	1.72	0.72
1:C:9:C:H5’	1:C:10:G:OP2	1.89	0.72
2:A:308:VAL:HG22	2:A:348:PHE:CD2	2.24	0.72
2:B:74:PHE:CD1	2:B:78:TYR:HB2	2.24	0.72
1:D:68:G:H2’	1:D:69:G:H8	1.55	0.71
2:A:6:LYS:HA	2:A:122:ASP:OD2	1.91	0.70
2:B:308:VAL:HG12	2:B:309:LYS:H	1.56	0.70
1:D:24:A:H2’	1:D:25:C:C6	2.26	0.70
2:B:254:GLY:HA2	2:B:259:TRP:CH2	2.22	0.70
2:B:75:ALA:HB3	2:B:77:GLU:HG3	1.73	0.69
2:B:38:LYS:HZ2	2:B:71:THR:HB	1.57	0.69
2:A:174:GLU:C	2:A:176:PRO:HD2	2.12	0.69
2:A:222:ILE:CG2	2:A:226:GLY:HA2	2.23	0.69
1:D:21:A:H61	1:D:46:A:H2’	1.58	0.69
1:D:25:C:H5’	2:B:256:GLU:O	1.92	0.69
2:A:7:LYS:HD2	2:A:120:GLY:O	1.92	0.69
2:A:287:LEU:CD1	2:A:331:VAL:HB	2.22	0.69
2:B:232:HIS:O	2:B:233:GLN:HB2	1.91	0.69
2:B:325:ASP:HB3	2:B:326:ASP:OD1	1.93	0.69
2:A:279:HIS:HD2	2:A:280:PRO:N	1.89	0.68
1:C:34:U:H2’	1:C:34:U:O2	1.94	0.68
2:B:243:ARG:HE	2:B:258:PRO:CB	2.07	0.68
2:A:236:MET:HG2	2:A:237:TYR:CD1	2.28	0.68
2:A:337:VAL:CG1	2:A:340:VAL:HG23	2.24	0.68
2:A:324:LEU:HD13	2:A:330:GLU:HB2	1.74	0.68
1:C:20:C:H1’	1:C:21:A:O4’	1.94	0.68
2:A:265:ASP:CG	2:A:268:ASN:HD22	1.95	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:308:VAL:HG12	2:A:309:LYS:N	2.08	0.67
1:C:24:A:O2'	2:A:256:GLU:HB3	1.94	0.67
2:A:143:ARG:HG3	2:A:352:GLU:HA	1.77	0.67
2:A:243:ARG:HB2	2:A:260:TYR:CE1	2.29	0.67
2:A:321:VAL:HG11	2:A:329:ILE:HD11	1.75	0.67
1:D:17:G:H2'	1:D:57:G:N2	2.10	0.67
2:B:366:LEU:HD12	2:B:367:PRO:HD2	1.76	0.67
1:D:34:U:H2'	1:D:34:U:O2	1.95	0.67
2:A:224:VAL:HG21	2:A:279:HIS:CE1	2.31	0.66
2:A:224:VAL:HG21	2:A:279:HIS:HE1	1.59	0.66
2:A:254:GLY:HA2	2:A:275:GLN:OE1	1.94	0.66
2:A:232:HIS:HB3	2:A:234:GLY:H	1.60	0.66
2:B:322:LYS:O	2:B:329:ILE:HD12	1.94	0.66
2:A:363:ARG:HD2	2:A:365:PRO:HG3	1.76	0.66
1:C:21:A:H61	1:C:46:A:H2'	1.61	0.65
1:C:16:A:O2'	1:C:60:U:O2'	2.15	0.65
2:A:105:GLU:O	2:A:109:LYS:HB3	1.97	0.65
2:A:130:VAL:HG11	2:A:141:LEU:HD11	1.77	0.65
2:A:222:ILE:HG23	2:A:226:GLY:HA2	1.77	0.65
2:A:290:GLN:HG3	2:A:291:GLN:HG3	1.78	0.65
2:B:224:VAL:HG13	2:B:281:ARG:NH1	2.12	0.64
1:C:57:G:H8	1:C:57:G:C5'	2.10	0.64
1:C:2:U:H5"	1:C:3:C:C5	2.32	0.64
2:B:279:HIS:CD2	2:B:281:ARG:HB2	2.31	0.64
1:D:17:G:H2'	1:D:57:G:H22	1.62	0.64
1:D:57:G:H8	1:D:57:G:C5'	2.08	0.64
2:A:289:ALA:HB3	2:A:329:ILE:CG2	2.28	0.64
2:B:38:LYS:HZ1	2:B:71:THR:HB	1.59	0.64
2:B:26:GLN:HB3	2:B:32:VAL:HG11	1.80	0.64
2:B:243:ARG:HE	2:B:258:PRO:HB2	1.62	0.64
2:A:310:THR:HB	2:A:314:GLN:OE1	1.98	0.64
2:A:207:ARG:HE	2:A:237:TYR:HD2	1.46	0.63
1:D:20:C:H1'	1:D:21:A:O4'	1.97	0.63
2:A:363:ARG:O	2:A:365:PRO:HD3	1.98	0.63
2:B:219:GLY:H	2:B:232:HIS:HB2	1.63	0.63
1:C:51:G:C3'	1:C:52:G:H5"	2.29	0.63
1:C:56:C:C3'	1:C:57:G:H5"	2.27	0.63
1:D:11:U:H2'	1:D:12:C:C6	2.34	0.63
2:B:75:ALA:C	2:B:77:GLU:H	2.02	0.63
2:A:146:ASP:OD1	2:A:174:GLU:HG2	1.99	0.63
1:D:51:G:C3'	1:D:52:G:H5"	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:276:GLY:C	2:A:278:GLU:H	1.99	0.63
2:A:279:HIS:CD2	2:A:281:ARG:H	2.17	0.62
2:A:321:VAL:CG1	2:A:329:ILE:HD11	2.29	0.62
2:B:283:MET:HE1	2:B:338:ALA:HA	1.81	0.62
2:B:288:ILE:HG22	2:B:361:GLU:HG2	1.80	0.62
1:D:56:C:C3'	1:D:57:G:H5"	2.28	0.62
1:C:61:C:H2'	1:C:62:C:C6	2.35	0.62
1:D:6:C:H2'	1:D:7:U:C6	2.35	0.62
2:A:131:ARG:CD	2:A:144:GLY:HA2	2.30	0.62
1:D:24:A:H2'	1:D:25:C:H6	1.65	0.62
1:C:6:C:H2'	1:C:7:U:H5'	1.81	0.61
2:B:45:GLY:C	2:B:47:GLU:H	2.01	0.61
2:B:154:PHE:HE1	2:B:312:TYR:CG	2.18	0.61
2:B:292:LEU:HD23	2:B:358:GLY:HA3	1.82	0.61
2:B:174:GLU:C	2:B:176:PRO:HD2	2.20	0.61
1:C:6:C:O2	1:C:6:C:C2'	2.48	0.61
1:C:16:A:H4'	1:C:16:A:OP1	2.01	0.61
2:A:174:GLU:HB3	2:A:176:PRO:HD2	1.83	0.61
2:B:86:PHE:HE1	2:B:210:LEU:HD11	1.65	0.61
2:A:123:TYR:C	2:A:124:ILE:HD12	2.21	0.61
2:A:236:MET:HG2	2:A:237:TYR:HD1	1.65	0.61
2:A:252:LYS:O	2:A:253:GLU:HB3	2.00	0.61
1:C:20:C:H5'	1:C:20(A):C:OP1	2.01	0.60
2:A:42:GLU:CD	2:A:42:GLU:H	2.04	0.60
2:B:46:GLU:O	2:B:47:GLU:HB2	2.02	0.60
1:D:11:U:H2'	1:D:12:C:H6	1.66	0.60
1:D:16:A:H4'	1:D:16:A:OP1	2.01	0.59
2:B:283:MET:CE	2:B:338:ALA:HA	2.32	0.59
2:B:290:GLN:HE21	2:B:328:ARG:CD	2.15	0.59
1:C:18:G:H5"	1:C:19:C:H5	1.67	0.59
2:A:129:TYR:HD1	2:A:175:LYS:HZ3	1.50	0.59
2:A:143:ARG:HG3	2:A:352:GLU:OE1	2.02	0.59
2:B:48:TYR:HB3	2:B:204:ARG:NH2	2.16	0.59
2:A:279:HIS:HD2	2:A:280:PRO:CD	2.15	0.59
1:C:73:G:H2'	1:D:73:G:O6	2.02	0.59
2:A:276:GLY:O	2:A:278:GLU:N	2.35	0.59
2:B:290:GLN:NE2	2:B:328:ARG:HD3	2.18	0.59
2:A:279:HIS:CD2	2:A:280:PRO:HD2	2.37	0.59
2:A:7:LYS:HE3	2:A:31:GLN:HE22	1.66	0.59
2:B:262:VAL:CG1	2:B:281:ARG:HB3	2.33	0.59
2:A:160:HIS:CD2	2:A:161:GLU:H	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:LEU:HD23	2:B:111:PHE:CE1	2.37	0.58
2:A:7:LYS:HA	2:A:31:GLN:O	2.04	0.58
2:A:48:TYR:C	2:A:50:THR:H	2.07	0.58
1:C:24:A:H2'	1:C:25:C:C6	2.39	0.58
2:A:289:ALA:HB3	2:A:329:ILE:HG21	1.84	0.58
2:B:366:LEU:CD1	2:B:367:PRO:HD2	2.34	0.58
2:A:129:TYR:HB3	2:A:151:GLN:HG3	1.85	0.58
2:A:279:HIS:CD2	2:A:280:PRO:N	2.71	0.58
2:B:174:GLU:H	2:B:177:GLN:NE2	2.00	0.58
2:B:307:THR:HG21	2:B:316:ASP:HB3	1.85	0.58
2:A:274:ALA:CB	2:A:279:HIS:ND1	2.66	0.58
2:A:289:ALA:O	2:A:329:ILE:HG22	2.04	0.58
2:B:106:ILE:HG22	2:B:107:LYS:N	2.18	0.58
2:B:23:TRP:CE2	2:B:185:LEU:HD11	2.38	0.58
2:B:243:ARG:HH21	2:B:258:PRO:HG3	1.69	0.58
1:C:68:G:N3	1:C:68:G:H2'	2.17	0.57
2:A:207:ARG:NE	2:A:237:TYR:HD2	2.02	0.57
2:B:74:PHE:C	2:B:76:ALA:H	2.07	0.57
2:A:15:GLY:O	2:A:188:VAL:HG21	2.04	0.57
2:B:20:VAL:O	2:B:24:LEU:HG	2.03	0.57
2:B:26:GLN:HB3	2:B:32:VAL:CG1	2.35	0.57
2:B:43:ASP:OD1	2:B:204:ARG:NH1	2.38	0.57
2:A:44:ASP:HB3	2:A:46:GLU:HG2	1.86	0.57
2:B:38:LYS:HB2	2:B:73:ASN:HA	1.86	0.57
2:B:107:LYS:O	2:B:111:PHE:HB3	2.05	0.57
2:A:262:VAL:HG11	2:A:281:ARG:HB3	1.87	0.57
2:A:325:ASP:HB2	2:A:326:ASP:OD1	2.05	0.57
2:B:261:VAL:HG13	2:B:271:LEU:HD21	1.87	0.57
1:C:67:G:C2	1:C:68:G:N7	2.73	0.57
2:A:232:HIS:NE2	2:A:271:LEU:HB2	2.19	0.57
2:B:61:VAL:O	2:B:65:LEU:HD13	2.04	0.57
1:C:37:A:C2'	1:C:38:C:H5'	2.35	0.56
2:A:85:LEU:HD22	2:B:324:LEU:O	2.05	0.56
1:C:15:G:O2'	1:C:16:A:P	2.63	0.56
2:A:175:LYS:N	2:A:176:PRO:HD2	2.20	0.56
2:B:40:TRP:CB	2:B:205:LYS:HE2	2.33	0.56
2:B:263:ASP:OD1	2:B:264:LYS:N	2.38	0.56
1:C:56:C:H2'	1:C:57:G:C5'	2.21	0.56
2:A:287:LEU:C	2:A:288:ILE:HD12	2.25	0.56
2:B:311:ARG:H	2:B:314:GLN:NE2	2.03	0.56
2:A:305:ARG:CG	2:A:305:ARG:HH11	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:U:H2'	1:C:12:C:C6	2.41	0.56
2:A:95:THR:HG22	2:A:344:GLN:HE21	1.69	0.56
2:B:10:VAL:O	2:B:10:VAL:HG13	2.05	0.56
2:B:138:LYS:HE2	2:B:160:HIS:CD2	2.41	0.56
1:D:14:A:H2'	1:D:15:G:O4'	2.06	0.56
2:A:138:LYS:HG3	2:A:160:HIS:ND1	2.21	0.56
2:A:111:PHE:C	2:A:111:PHE:CD2	2.80	0.56
2:A:134:ASP:HA	2:A:139:SER:HA	1.87	0.56
2:B:86:PHE:CE1	2:B:210:LEU:HD11	2.41	0.56
2:A:276:GLY:C	2:A:278:GLU:N	2.60	0.55
2:B:43:ASP:CG	2:B:44:ASP:H	2.08	0.55
1:C:73:G:H2'	1:D:73:G:C6	2.42	0.55
1:D:51:G:H2'	1:D:52:G:C5'	2.28	0.55
2:A:111:PHE:C	2:A:111:PHE:HD2	2.09	0.55
2:A:129:TYR:CD1	2:A:175:LYS:HG3	2.42	0.55
1:C:9:C:O2'	1:C:45:A:C2'	2.53	0.55
2:B:236:MET:HG3	2:B:237:TYR:CD2	2.41	0.55
1:C:37:A:H2'	1:C:38:C:H5'	1.87	0.55
2:A:243:ARG:HB2	2:A:260:TYR:HE1	1.68	0.55
1:C:51:G:H2'	1:C:52:G:C5'	2.32	0.55
1:D:15:G:O2'	1:D:16:A:P	2.64	0.55
2:B:140:ARG:CB	2:B:140:ARG:HH11	2.19	0.55
2:A:337:VAL:HG12	2:A:340:VAL:HG23	1.89	0.54
2:B:129:TYR:CE2	2:B:145:LEU:O	2.61	0.54
2:B:276:GLY:C	2:B:278:GLU:H	2.10	0.54
2:A:23:TRP:O	2:A:27:GLN:HG2	2.07	0.54
2:B:131:ARG:CD	2:B:144:GLY:HA2	2.38	0.54
2:B:308:VAL:HG12	2:B:309:LYS:N	2.23	0.54
2:A:232:HIS:O	2:A:233:GLN:HB2	2.08	0.54
2:A:308:VAL:HG12	2:A:309:LYS:H	1.70	0.54
2:A:324:LEU:HD23	2:A:328:ARG:CD	2.38	0.54
1:D:8:U:H5'	1:D:9:C:OP2	2.08	0.54
1:D:9:C:O2'	1:D:45:A:C2'	2.54	0.54
2:A:216:ALA:HB1	2:A:233:GLN:O	2.07	0.54
1:D:63:C:H2'	1:D:64:C:C6	2.43	0.54
2:B:40:TRP:CG	2:B:205:LYS:HG3	2.43	0.54
2:B:232:HIS:O	2:B:233:GLN:CB	2.56	0.53
2:A:53:ALA:O	2:A:57:ASP:OD2	2.26	0.53
2:A:24:LEU:O	2:A:28:GLN:HG3	2.08	0.53
2:A:251:THR:CG2	2:A:252:LYS:H	2.09	0.53
2:A:305:ARG:HH11	2:A:305:ARG:HG2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:ILE:CD1	2:B:119:LEU:HB3	2.39	0.53
2:B:290:GLN:HE21	2:B:328:ARG:HG2	1.74	0.53
2:A:305:ARG:NH2	2:A:334:ASP:OD2	2.41	0.53
2:A:155:LEU:HB3	2:A:158:LEU:HD22	1.91	0.53
2:A:159:SER:OG	2:A:162:GLN:HG3	2.08	0.53
2:B:46:GLU:H	2:B:46:GLU:CD	2.12	0.53
2:A:118:ASP:O	2:A:120:GLY:N	2.42	0.53
2:B:198:ILE:C	2:B:200:PHE:H	2.12	0.53
2:B:296:ASP:O	2:B:298:GLU:N	2.42	0.53
2:A:217:GLN:HB3	2:B:368:VAL:HG12	1.90	0.53
2:B:140:ARG:HH11	2:B:140:ARG:HB2	1.74	0.53
1:D:69:G:H2'	1:D:70:G:H5'	1.91	0.53
2:A:254:GLY:C	2:A:256:GLU:N	2.61	0.53
2:B:276:GLY:O	2:B:278:GLU:N	2.42	0.53
2:B:254:GLY:CA	2:B:259:TRP:HH2	2.12	0.53
2:B:150:ASP:OD2	2:B:151:GLN:N	2.41	0.52
2:A:131:ARG:HD3	2:A:144:GLY:HA2	1.90	0.52
2:A:231:GLU:CD	2:A:231:GLU:H	2.11	0.52
2:B:143:ARG:HH21	2:B:349:TYR:HB3	1.75	0.52
2:B:294:TRP:O	2:B:296:ASP:N	2.43	0.52
1:D:15:G:O3'	1:D:16:A:O4'	2.28	0.52
1:D:16:A:N3	1:D:16:A:H2'	2.24	0.52
1:C:7:U:O4	1:C:49:A:N6	2.43	0.52
2:A:279:HIS:HD2	2:A:280:PRO:HD2	1.75	0.52
2:A:294:TRP:O	2:A:297:ARG:N	2.39	0.52
2:B:9:ILE:HD11	2:B:119:LEU:HB3	1.91	0.52
2:B:142:LEU:HA	2:B:352:GLU:O	2.10	0.52
1:D:59:A:H2'	1:D:60:U:O4'	2.09	0.52
2:A:48:TYR:O	2:A:50:THR:N	2.43	0.52
1:D:18:G:H5"	1:D:19:C:H5	1.74	0.52
2:A:131:ARG:HG3	2:A:144:GLY:HA2	1.92	0.52
1:D:20:C:H5'	1:D:20(A):C:OP1	2.09	0.52
2:A:37:MET:CE	2:A:111:PHE:HD1	2.23	0.52
1:D:8:U:H2'	1:D:46:A:N3	2.25	0.52
1:D:44:U:H2'	1:D:45:A:O4'	2.10	0.52
2:A:20:VAL:O	2:A:24:LEU:HG	2.10	0.52
2:A:251:THR:CG2	2:A:252:LYS:N	2.61	0.52
2:A:12:MET:HE3	2:A:34:GLY:HA3	1.92	0.51
2:A:129:TYR:CE1	2:A:175:LYS:HG3	2.45	0.51
2:B:17:ASP:O	2:B:21:SER:HB2	2.10	0.51
2:B:296:ASP:OD2	2:B:298:GLU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:SER:O	2:A:162:GLN:N	2.40	0.51
1:D:16:A:O2'	1:D:60:U:O2'	2.27	0.51
1:D:23:G:O2'	1:D:24:A:H5'	2.11	0.51
2:A:77:GLU:OE1	2:A:77:GLU:N	2.38	0.51
2:A:118:ASP:C	2:A:120:GLY:H	2.14	0.51
2:A:17:ASP:OD1	2:A:178:VAL:HG11	2.10	0.51
2:B:47:GLU:O	2:B:48:TYR:C	2.48	0.51
2:B:296:ASP:OD2	2:B:296:ASP:C	2.48	0.51
2:B:366:LEU:CG	2:B:367:PRO:HD2	2.41	0.51
2:A:350:ASN:CG	2:A:350:ASN:O	2.48	0.51
2:B:229:ILE:HG12	2:B:229:ILE:O	2.09	0.51
1:D:57:G:C8	1:D:57:G:C5'	2.88	0.51
2:A:279:HIS:CD2	2:A:280:PRO:CD	2.94	0.51
2:A:308:VAL:CG1	2:A:309:LYS:N	2.73	0.51
2:B:86:PHE:CG	2:B:206:PHE:HD2	2.28	0.51
2:B:214:LEU:HD21	2:B:236:MET:HE3	1.93	0.51
1:D:56:C:H2'	1:D:57:G:C5'	2.23	0.51
2:B:305:ARG:HH11	2:B:305:ARG:CG	2.24	0.50
2:B:337:VAL:CG1	2:B:338:ALA:N	2.74	0.50
2:A:305:ARG:CG	2:A:305:ARG:NH1	2.74	0.50
2:A:290:GLN:O	2:A:291:GLN:HB2	2.11	0.50
2:B:73:ASN:O	2:B:74:PHE:O	2.29	0.50
1:D:52:G:O6	1:D:62:C:N3	2.44	0.50
2:B:175:LYS:N	2:B:176:PRO:HD2	2.26	0.50
1:C:73:G:H5'	1:C:74:C:O5'	2.11	0.50
2:A:129:TYR:HD1	2:A:175:LYS:NZ	2.09	0.50
2:A:285:VAL:HG23	2:A:364:LEU:O	2.11	0.50
2:B:222:ILE:HD13	2:B:270:ILE:HG21	1.93	0.50
1:C:52:G:O6	1:C:62:C:N3	2.44	0.50
2:B:81:ASN:H	2:B:81:ASN:ND2	2.10	0.50
2:B:350:ASN:HB2	2:B:355:LEU:HD21	1.94	0.50
2:B:25:LEU:O	2:B:28:GLN:HB3	2.12	0.50
1:D:61:C:H2'	1:D:62:C:C6	2.47	0.50
1:C:65:U:H6	1:C:65:U:O5'	1.95	0.50
2:B:204:ARG:HB3	2:B:204:ARG:HH11	1.76	0.50
2:B:307:THR:HG21	2:B:316:ASP:OD2	2.11	0.50
2:B:9:ILE:HD13	2:B:119:LEU:HD13	1.93	0.49
2:B:134:ASP:HA	2:B:139:SER:HA	1.93	0.49
1:C:8:U:H5'	1:C:9:C:OP2	2.11	0.49
2:B:71:THR:O	2:B:72:VAL:HG13	2.13	0.49
1:D:6:C:H2'	1:D:7:U:H6	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:13:SER:OG	3:A:1002:PO4:O2	2.30	0.49
2:A:227:ASP:O	2:A:228:GLU:C	2.51	0.49
2:B:183:GLU:C	2:B:185:LEU:H	2.15	0.49
1:D:34:U:O2	1:D:34:U:C2'	2.58	0.49
2:A:246:LEU:HD13	2:A:273:VAL:HG11	1.95	0.49
1:D:50:G:H2'	1:D:51:G:C8	2.48	0.49
2:B:81:ASN:ND2	2:B:81:ASN:N	2.61	0.49
2:B:279:HIS:ND1	2:B:280:PRO:HD2	2.27	0.49
2:B:290:GLN:NE2	2:B:328:ARG:CD	2.75	0.49
2:B:311:ARG:O	2:B:314:GLN:HB3	2.12	0.49
1:C:68:G:N2	1:C:69:G:C8	2.81	0.49
2:B:224:VAL:HG23	2:B:273:VAL:O	2.12	0.49
1:C:15:G:HO2'	1:C:16:A:P	2.35	0.49
1:D:8:U:C5'	1:D:9:C:OP2	2.61	0.49
2:A:33:GLU:OE1	2:A:70:HIS:HE1	1.95	0.48
2:A:348:PHE:N	2:A:348:PHE:CD1	2.81	0.48
2:B:74:PHE:O	2:B:76:ALA:N	2.39	0.48
1:C:72:C:H2'	1:C:73:G:O4'	2.13	0.48
1:D:50:G:H2'	1:D:51:G:H8	1.78	0.48
2:B:305:ARG:HH11	2:B:305:ARG:HG2	1.78	0.48
2:B:283:MET:HB2	2:B:366:LEU:HD22	1.94	0.48
1:D:9:C:C5'	1:D:10:G:OP2	2.58	0.48
2:B:103:ASN:HA	2:B:107:LYS:HB2	1.94	0.48
1:D:37:A:C2'	1:D:38:C:H5'	2.44	0.48
2:A:36:PHE:CE1	2:A:55:LEU:HA	2.48	0.48
2:A:145:LEU:O	2:A:146:ASP:HB2	2.13	0.48
2:B:49:CYS:C	2:B:51:ALA:H	2.17	0.48
2:B:154:PHE:HE1	2:B:312:TYR:CD2	2.31	0.48
2:B:227:ASP:O	2:B:228:GLU:C	2.51	0.48
2:A:265:ASP:OD1	2:A:268:ASN:ND2	2.38	0.48
2:B:45:GLY:O	2:B:47:GLU:N	2.37	0.48
2:B:130:VAL:HG21	2:B:141:LEU:HD11	1.95	0.48
2:B:337:VAL:HG12	2:B:338:ALA:N	2.29	0.48
1:C:8:U:C5'	1:C:9:C:OP2	2.62	0.48
1:D:11:U:C2	1:D:12:C:C5	3.01	0.48
2:B:35:LEU:HD23	2:B:111:PHE:HE1	1.78	0.48
2:B:274:ALA:HB1	2:B:279:HIS:CD2	2.49	0.48
1:C:15:G:O3'	1:C:16:A:O4'	2.32	0.47
1:C:57:G:C8	1:C:57:G:C5'	2.91	0.47
2:B:271:LEU:HD23	2:B:272:VAL:O	2.13	0.47
2:B:132:ARG:NH1	2:B:164:ALA:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:254:GLY:C	2:A:256:GLU:H	2.17	0.47
2:B:308:VAL:CG2	2:B:319:CYS:SG	3.02	0.47
2:B:312:TYR:CZ	2:B:313:ARG:HD3	2.49	0.47
2:B:78:TYR:HA	2:B:106:ILE:HD11	1.97	0.47
2:B:83:PHE:HA	2:B:206:PHE:CE2	2.49	0.47
2:B:243:ARG:HH21	2:B:258:PRO:CG	2.27	0.47
2:B:283:MET:HE2	2:B:283:MET:HA	1.95	0.47
1:C:2:U:N3	1:C:72:C:N4	2.63	0.47
1:C:19:C:OP2	1:C:20:C:H5"	2.15	0.47
2:A:88:ALA:CB	2:B:324:LEU:HD11	2.45	0.47
2:A:337:VAL:HG13	2:A:338:ALA:N	2.30	0.47
2:B:75:ALA:C	2:B:77:GLU:N	2.68	0.47
2:B:344:GLN:O	2:B:360:ILE:HG13	2.15	0.47
1:D:9:C:HO2'	1:D:45:A:H2'	1.79	0.47
1:D:69:G:H2'	1:D:70:G:C5'	2.44	0.47
2:A:132:ARG:NH1	2:A:164:ALA:O	2.47	0.47
2:B:158:LEU:O	2:B:295:VAL:HG12	2.14	0.47
1:C:34:U:O2	1:C:34:U:C2'	2.58	0.47
2:A:72:VAL:HG12	2:A:73:ASN:H	1.80	0.47
2:A:308:VAL:CG1	2:A:309:LYS:H	2.27	0.47
2:B:81:ASN:H	2:B:81:ASN:HD22	1.62	0.47
2:B:298:GLU:OE1	2:B:298:GLU:HA	2.15	0.46
2:A:287:LEU:CD2	2:A:360:ILE:HG12	2.43	0.46
2:A:325:ASP:OD2	2:A:326:ASP:OD1	2.33	0.46
2:B:74:PHE:HD2	2:B:74:PHE:N	2.13	0.46
1:C:3:C:H5"	1:C:4:C:OP1	2.15	0.46
2:A:252:LYS:O	2:A:252:LYS:HG3	2.15	0.46
2:B:254:GLY:CA	2:B:259:TRP:CH2	2.95	0.46
2:A:23:TRP:CE2	2:A:185:LEU:HD11	2.49	0.46
2:A:100:ILE:HD12	2:A:156:TYR:CE2	2.51	0.46
2:A:221:ILE:HG13	2:A:231:GLU:O	2.16	0.46
2:A:23:TRP:CD2	2:A:185:LEU:HD11	2.51	0.46
2:A:129:TYR:HE1	2:A:175:LYS:CB	2.29	0.46
2:A:180:LYS:O	2:A:181:ILE:C	2.54	0.46
2:A:265:ASP:O	2:A:269:ASN:N	2.48	0.46
2:B:74:PHE:N	2:B:74:PHE:CD2	2.83	0.46
2:A:83:PHE:CE1	2:A:87:LEU:HD11	2.51	0.46
2:A:185:LEU:O	2:A:187:LEU:HG	2.16	0.46
2:A:368:VAL:OXT	2:A:368:VAL:HG13	2.14	0.46
2:B:366:LEU:HG	2:B:367:PRO:HD2	1.97	0.46
1:C:6:C:N4	1:C:67:G:H1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:PHE:C	2:B:211:GLY:N	2.69	0.46
2:B:290:GLN:HE21	2:B:328:ARG:CG	2.29	0.46
2:B:293:HIS:O	2:B:356:GLY:HA3	2.15	0.46
1:C:2:U:H2'	1:C:3:C:OP1	2.16	0.46
2:A:10:VAL:O	2:A:12:MET:HE2	2.16	0.46
2:A:138:LYS:HA	2:A:138:LYS:HD3	1.60	0.46
2:A:158:LEU:HA	2:A:162:GLN:OE1	2.16	0.46
2:A:267:GLU:CD	2:A:267:GLU:H	2.19	0.46
2:B:35:LEU:HD21	2:B:72:VAL:HG21	1.97	0.46
2:B:74:PHE:C	2:B:76:ALA:N	2.70	0.46
2:B:287:LEU:HD23	2:B:333:PHE:HZ	1.80	0.46
2:B:279:HIS:HD2	2:B:281:ARG:HB2	1.79	0.45
2:A:44:ASP:C	2:A:46:GLU:N	2.70	0.45
2:B:73:ASN:O	2:B:74:PHE:C	2.54	0.45
2:B:276:GLY:C	2:B:278:GLU:N	2.69	0.45
2:B:322:LYS:HB2	2:B:322:LYS:HE3	1.71	0.45
1:D:7:U:O2'	1:D:8:U:OP1	2.31	0.45
1:D:51:G:N2	1:D:63:C:O2	2.38	0.45
2:A:86:PHE:CD1	2:A:98:PRO:HB3	2.52	0.45
2:A:232:HIS:NE2	2:A:271:LEU:CB	2.78	0.45
2:B:86:PHE:CZ	2:B:90:TYR:HE1	2.34	0.45
2:B:240:LEU:N	2:B:240:LEU:HD23	2.32	0.45
1:C:58:A:HO2'	1:C:59:A:H3'	1.81	0.45
1:C:59:A:H2'	1:C:60:U:O4'	2.16	0.45
1:D:37:A:H2'	1:D:38:C:H5'	1.98	0.45
2:A:284:SER:O	2:A:336:PRO:HA	2.16	0.45
2:B:304:MET:HE2	2:B:306:CYS:HB3	1.97	0.45
1:C:9:C:HO2'	1:C:45:A:H2'	1.77	0.45
2:A:7:LYS:HE3	2:A:31:GLN:NE2	2.30	0.45
1:D:6:C:O2'	1:D:7:U:H5'	2.17	0.45
2:A:105:GLU:HA	2:A:105:GLU:OE1	2.16	0.45
2:B:154:PHE:CE1	2:B:312:TYR:CG	3.03	0.45
2:B:287:LEU:HD23	2:B:333:PHE:CZ	2.52	0.45
2:A:10:VAL:O	2:A:10:VAL:HG22	2.17	0.45
2:B:301:THR:HG22	2:B:302:GLY:N	2.31	0.45
2:B:312:TYR:CD1	2:B:313:ARG:HG2	2.51	0.45
2:A:11:GLY:HA3	2:A:111:PHE:HE1	1.82	0.45
2:A:78:TYR:CE1	2:A:82:VAL:HG21	2.51	0.45
2:A:97:ASN:HD22	2:A:97:ASN:C	2.18	0.45
1:C:63:C:H2'	1:C:64:C:C6	2.52	0.45
2:A:317:ILE:CG1	2:A:317:ILE:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:TYR:C	2:B:50:THR:H	2.20	0.45
2:B:144:GLY:O	2:B:145:LEU:O	2.35	0.45
2:B:183:GLU:O	2:B:185:LEU:N	2.50	0.45
1:D:38:C:H3'	1:D:38:C:O2	2.16	0.45
2:A:79:TRP:O	2:A:84:GLU:HG2	2.17	0.45
2:A:359:ILE:N	2:A:359:ILE:HD12	2.31	0.45
2:B:222:ILE:O	2:B:272:VAL:HA	2.17	0.45
1:D:15:G:HO2'	1:D:16:A:P	2.40	0.44
2:B:174:GLU:HB2	2:B:177:GLN:HE21	1.80	0.44
1:D:65:U:H2'	1:D:66:A:O4'	2.18	0.44
2:B:183:GLU:C	2:B:185:LEU:N	2.70	0.44
2:A:144:GLY:O	2:A:145:LEU:O	2.35	0.44
2:B:236:MET:HG3	2:B:237:TYR:HD2	1.82	0.44
2:B:368:VAL:OXT	2:B:368:VAL:HG13	2.17	0.44
1:D:25:C:C4	1:D:26:A:N7	2.86	0.44
1:D:38:C:O2	1:D:38:C:O5'	2.35	0.44
2:A:148:ASN:ND2	2:A:148:ASN:O	2.50	0.44
2:A:232:HIS:O	2:A:233:GLN:CB	2.65	0.44
2:B:46:GLU:O	2:B:47:GLU:CB	2.65	0.44
2:B:243:ARG:HB2	2:B:260:TYR:CE2	2.52	0.44
1:C:55:U:H5"	1:C:55:U:H6	1.81	0.44
2:A:185:LEU:O	2:A:186:GLY:C	2.55	0.44
1:C:50:G:H2'	1:C:51:G:C8	2.53	0.44
2:A:144:GLY:O	2:A:145:LEU:C	2.56	0.44
2:A:288:ILE:HD12	2:A:288:ILE:N	2.33	0.44
2:B:271:LEU:HD23	2:B:271:LEU:C	2.38	0.44
2:A:35:LEU:HD11	2:A:72:VAL:CG2	2.29	0.44
1:C:50:G:H2'	1:C:51:G:H8	1.82	0.44
1:D:27:C:H2'	1:D:28:C:C6	2.52	0.44
2:A:12:MET:CE	2:A:34:GLY:HA3	2.47	0.44
2:B:324:LEU:HD12	2:B:324:LEU:HA	1.87	0.44
2:B:135:VAL:O	2:B:136:ASP:HB3	2.17	0.43
2:B:198:ILE:C	2:B:200:PHE:N	2.71	0.43
2:B:222:ILE:HG23	2:B:270:ILE:HG23	2.00	0.43
2:A:131:ARG:CG	2:A:144:GLY:HA2	2.48	0.43
2:B:238:HIS:HA	2:B:242:GLN:NE2	2.32	0.43
2:A:16:VAL:HG22	2:A:188:VAL:HB	1.99	0.43
2:B:107:LYS:HE2	2:B:199:CYS:SG	2.58	0.43
2:B:129:TYR:HE2	2:B:145:LEU:O	2.01	0.43
2:B:243:ARG:NH2	2:B:258:PRO:HG3	2.33	0.43
2:B:265:ASP:OD2	2:B:267:GLU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:U:O2	1:D:21:A:H2	2.01	0.43
2:A:124:ILE:HD12	2:A:124:ILE:N	2.32	0.43
2:A:156:TYR:CE2	2:A:345:SER:HB3	2.54	0.43
2:A:337:VAL:HG11	2:A:340:VAL:CG2	2.49	0.43
2:B:45:GLY:C	2:B:47:GLU:N	2.68	0.43
2:B:128:HIS:O	2:B:170:VAL:HG23	2.17	0.43
2:B:305:ARG:CG	2:B:305:ARG:NH1	2.81	0.43
2:B:307:THR:HG21	2:B:316:ASP:CB	2.48	0.43
1:C:62:C:H6	1:C:62:C:O5'	2.02	0.43
2:A:72:VAL:HG12	2:A:73:ASN:N	2.33	0.43
2:A:294:TRP:O	2:A:296:ASP:N	2.52	0.43
2:A:112:LEU:HD12	2:A:124:ILE:HG12	2.01	0.43
2:A:302:GLY:H	2:A:323:ALA:HB3	1.84	0.43
2:B:101:LEU:O	2:B:105:GLU:HB2	2.18	0.43
2:B:118:ASP:O	2:B:120:GLY:N	2.52	0.43
2:B:247:GLY:O	2:B:248:ILE:HD12	2.19	0.43
2:B:361:GLU:HG3	2:B:362:GLN:N	2.33	0.43
1:C:20:C:C4'	1:C:20(A):C:OP1	2.67	0.43
2:A:337:VAL:HG11	2:A:340:VAL:HG23	1.98	0.43
2:B:9:ILE:HD12	2:B:121:ALA:HB2	2.01	0.43
2:B:203:GLU:O	2:B:207:ARG:HG2	2.19	0.43
2:B:307:THR:O	2:B:348:PHE:HA	2.18	0.43
2:B:323:ALA:HA	2:B:329:ILE:HD13	2.00	0.43
2:A:138:LYS:HD2	2:A:160:HIS:CB	2.40	0.43
2:B:141:LEU:HB2	2:B:163:ILE:CD1	2.48	0.43
2:B:221:ILE:HG13	2:B:231:GLU:O	2.18	0.43
2:B:275:GLN:O	2:B:275:GLN:NE2	2.43	0.43
2:B:118:ASP:C	2:B:120:GLY:H	2.21	0.43
2:B:325:ASP:O	2:B:326:ASP:C	2.57	0.43
1:C:44:U:H2'	1:C:45:A:O4'	2.18	0.43
2:A:37:MET:SD	2:A:111:PHE:CD1	3.01	0.43
2:A:138:LYS:HE3	2:A:160:HIS:ND1	2.34	0.43
2:B:198:ILE:HG23	2:B:199:CYS:N	2.34	0.43
2:B:309:LYS:NZ	2:B:316:ASP:OD1	2.49	0.43
2:A:48:TYR:C	2:A:50:THR:N	2.72	0.42
2:A:128:HIS:NE2	2:A:155:LEU:HD21	2.34	0.42
2:A:239:THR:HG22	2:A:242:GLN:OE1	2.19	0.42
2:A:308:VAL:HG22	2:A:348:PHE:CE2	2.54	0.42
2:A:324:LEU:HD23	2:A:328:ARG:HG2	2.00	0.42
2:B:12:MET:SD	2:B:62:CYS:SG	3.17	0.42
2:B:36:PHE:CG	2:B:55:LEU:HD13	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:C:O5'	1:D:32:C:H6	2.02	0.42
1:D:58:A:O2'	1:D:60:U:OP2	2.28	0.42
1:C:32:C:H6	1:C:32:C:O5'	2.03	0.42
1:D:56:C:H6	1:D:56:C:O5'	2.02	0.42
2:A:55:LEU:O	2:A:58:ALA:HB3	2.19	0.42
2:A:142:LEU:CD2	2:A:353:VAL:HG22	2.49	0.42
1:C:52:G:N2	1:C:63:C:H1'	2.34	0.42
1:C:73:G:H4'	1:C:74:C:H5"	2.01	0.42
2:A:32:VAL:O	2:A:32:VAL:HG22	2.19	0.42
2:A:248:ILE:HG21	2:A:259:TRP:CE2	2.54	0.42
2:A:325:ASP:O	2:A:326:ASP:C	2.56	0.42
2:B:7:LYS:HA	2:B:31:GLN:O	2.19	0.42
2:B:224:VAL:O	2:B:224:VAL:HG12	2.18	0.42
2:B:236:MET:HE2	2:B:236:MET:HB3	1.82	0.42
2:A:150:ASP:OD1	2:A:150:ASP:C	2.58	0.42
2:A:222:ILE:HG22	2:A:223:THR:O	2.19	0.42
2:A:279:HIS:CD2	2:A:279:HIS:C	2.92	0.42
2:B:32:VAL:O	2:B:32:VAL:HG13	2.19	0.42
2:A:88:ALA:HB1	2:B:324:LEU:HD11	2.02	0.42
2:B:141:LEU:HD23	2:B:354:CYS:HB3	2.01	0.42
2:B:237:TYR:CD2	2:B:237:TYR:N	2.87	0.42
1:C:35:U:H2'	1:C:36:C:C6	2.54	0.42
1:D:3:C:O2	1:D:71:A:H3'	2.20	0.42
2:B:60:ALA:O	2:B:63:ASP:HB2	2.20	0.42
2:B:221:ILE:HG22	2:B:229:ILE:CG2	2.50	0.42
1:C:20:C:H4'	1:C:20(A):C:OP1	2.20	0.42
2:A:160:HIS:HD2	2:A:161:GLU:H	1.67	0.42
2:A:324:LEU:HA	2:A:324:LEU:HD12	1.80	0.42
2:B:18:SER:O	2:B:21:SER:HB3	2.20	0.42
2:B:174:GLU:CB	2:B:177:GLN:HE21	2.32	0.42
2:B:304:MET:CE	2:B:306:CYS:HB3	2.49	0.42
2:A:301:THR:HA	2:A:323:ALA:CB	2.49	0.42
1:C:3:C:O5'	1:C:3:C:H6	2.03	0.41
2:B:9:ILE:O	2:B:124:ILE:HA	2.20	0.41
2:B:210:LEU:O	2:B:214:LEU:O	2.38	0.41
1:C:16:A:N3	1:C:16:A:H2'	2.35	0.41
2:A:243:ARG:HB2	2:A:260:TYR:CD1	2.54	0.41
2:B:42:GLU:OE2	2:B:47:GLU:HG2	2.20	0.41
2:B:76:ALA:O	2:B:80:ASP:OD1	2.38	0.41
2:B:73:ASN:ND2	2:B:74:PHE:CD2	2.88	0.41
1:C:20:C:C5'	1:C:20(A):C:OP1	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:G:O2'	1:C:40:G:H5'	2.20	0.41
2:A:142:LEU:HD23	2:A:353:VAL:HA	2.02	0.41
2:A:257:GLU:H	2:A:257:GLU:HG2	1.67	0.41
2:B:304:MET:HG2	2:B:321:VAL:HB	2.02	0.41
1:C:9:C:C5'	1:C:10:G:OP2	2.63	0.41
1:C:27:C:H2'	1:C:28:C:C6	2.55	0.41
2:A:179:ARG:O	2:A:183:GLU:HG3	2.21	0.41
2:A:292:LEU:HG	2:A:327:ASP:O	2.20	0.41
2:B:8:VAL:HG12	2:B:30:TYR:HB3	2.02	0.41
2:B:232:HIS:HB3	2:B:234:GLY:H	1.85	0.41
1:D:36:C:O5'	1:D:36:C:H6	2.04	0.41
1:C:25:C:C4	1:C:26:A:N7	2.88	0.41
2:B:35:LEU:HD23	2:B:111:PHE:CD1	2.56	0.41
2:B:346:ALA:O	2:B:357:GLY:HA3	2.20	0.41
2:A:15:GLY:HA3	3:A:1002:PO4:O2	2.20	0.41
2:B:32:VAL:O	2:B:67:ILE:HG23	2.21	0.41
2:B:75:ALA:O	2:B:77:GLU:N	2.54	0.41
2:A:118:ASP:C	2:A:120:GLY:N	2.74	0.41
2:A:129:TYR:CE2	2:A:145:LEU:O	2.74	0.41
2:A:142:LEU:HD21	2:A:353:VAL:HG22	2.01	0.41
2:A:149:LYS:HB3	2:A:175:LYS:HD2	2.03	0.41
2:A:279:HIS:HA	2:A:280:PRO:HD3	1.95	0.41
2:B:43:ASP:CG	2:B:44:ASP:N	2.75	0.41
2:B:237:TYR:HD2	2:B:237:TYR:N	2.18	0.41
2:A:18:SER:HB3	3:A:1002:PO4:O2	2.20	0.41
2:A:283:MET:HB2	2:A:366:LEU:CD1	2.51	0.41
2:A:324:LEU:C	2:A:325:ASP:OD1	2.60	0.41
2:B:368:VAL:OXT	2:B:368:VAL:CG1	2.70	0.41
1:C:58:A:O2'	1:C:59:A:H3'	2.21	0.40
2:B:86:PHE:CE1	2:B:206:PHE:HB3	2.55	0.40
2:B:182:ALA:O	2:B:187:LEU:HB2	2.22	0.40
2:B:275:GLN:HE21	2:B:275:GLN:C	2.24	0.40
1:C:5:C:C2	1:C:6:C:H6	2.39	0.40
2:B:86:PHE:HE1	2:B:210:LEU:CD1	2.31	0.40
2:B:169:PRO:HG2	2:B:170:VAL:H	1.87	0.40
2:B:180:LYS:O	2:B:183:GLU:N	2.53	0.40
1:D:70:G:HO2'	1:D:71:A:C4'	2.34	0.40
2:A:254:GLY:C	2:A:255:THR:HG1	2.24	0.40
2:A:324:LEU:HD23	2:A:328:ARG:CG	2.52	0.40
2:B:48:TYR:O	2:B:50:THR:N	2.55	0.40
2:B:50:THR:HG22	2:B:50:THR:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:HIS:HA	2:B:242:GLN:HE22	1.87	0.40
2:A:180:LYS:O	2:A:183:GLU:N	2.49	0.40
2:A:212:ARG:HG2	2:A:212:ARG:NH1	2.37	0.40
2:B:17:ASP:OD1	2:B:175:LYS:NZ	2.54	0.40
2:B:324:LEU:O	2:B:325:ASP:CG	2.60	0.40
1:C:2:U:H5"	1:C:3:C:C4	2.56	0.40
2:B:274:ALA:CB	2:B:279:HIS:CD2	3.04	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	344/380 (90%)	275 (80%)	44 (13%)	25 (7%)	1 6
2	B	355/380 (93%)	275 (78%)	55 (16%)	25 (7%)	1 7
All	All	699/760 (92%)	550 (79%)	99 (14%)	50 (7%)	1 6

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	49	CYS
2	A	145	LEU
2	A	326	ASP
2	A	338	ALA
2	B	74	PHE
2	B	80	ASP
2	B	145	LEU
2	B	213	TYR
2	B	297	ARG
2	B	338	ALA
2	A	6	LYS

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Mol	Chain	Res	Type
2	A	107	LYS
2	A	119	LEU
2	A	178	VAL
2	A	226	GLY
2	A	229	ILE
2	A	250	GLY
2	A	253	GLU
2	A	277	HIS
2	A	295	VAL
2	A	297	ARG
2	B	40	TRP
2	B	46	GLU
2	B	49	CYS
2	B	119	LEU
2	B	120	GLY
2	B	178	VAL
2	B	229	ILE
2	B	253	GLU
2	B	277	HIS
2	B	295	VAL
2	B	326	ASP
2	A	42	GLU
2	A	114	PHE
2	A	120	GLY
2	A	323	ALA
2	B	77	GLU
2	B	184	ASP
2	A	60	ALA
2	A	115	ALA
2	B	75	ALA
2	B	226	GLY
2	A	169	PRO
2	B	78	TYR
2	B	109	LYS
2	B	169	PRO
2	A	251	THR
2	A	15	GLY
2	A	106	ILE
2	B	250	GLY

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	288/315 (91%)	259 (90%)	29 (10%)	7 28
2	B	297/315 (94%)	270 (91%)	27 (9%)	9 33
All	All	585/630 (93%)	529 (90%)	56 (10%)	8 31

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	10	VAL
2	A	12	MET
2	A	21	SER
2	A	31	GLN
2	A	32	VAL
2	A	82	VAL
2	A	97	ASN
2	A	111	PHE
2	A	146	ASP
2	A	148	ASN
2	A	150	ASP
2	A	157	THR
2	A	160	HIS
2	A	167	LEU
2	A	170	VAL
2	A	231	GLU
2	A	236	MET
2	A	255	THR
2	A	267	GLU
2	A	269	ASN
2	A	285	VAL
2	A	287	LEU
2	A	297	ARG
2	A	305	ARG
2	A	315	THR
2	A	326	ASP
2	A	335	GLU

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Mol	Chain	Res	Type
2	A	337	VAL
2	A	362	GLN
2	B	39	ASN
2	B	68	GLU
2	B	72	VAL
2	B	73	ASN
2	B	74	PHE
2	B	79	TRP
2	B	81	ASN
2	B	101	LEU
2	B	113	GLU
2	B	122	ASP
2	B	140	ARG
2	B	146	ASP
2	B	156	TYR
2	B	161	GLU
2	B	167	LEU
2	B	204	ARG
2	B	251	THR
2	B	255	THR
2	B	259	TRP
2	B	275	GLN
2	B	285	VAL
2	B	298	GLU
2	B	305	ARG
2	B	308	VAL
2	B	316	ASP
2	B	317	ILE
2	B	326	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	31	GLN
2	A	70	HIS
2	A	97	ASN
2	A	148	ASN
2	A	177	GLN
2	A	268	ASN
2	A	269	ASN
2	A	279	HIS
2	B	31	GLN

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Mol	Chain	Res	Type
2	B	70	HIS
2	B	73	ASN
2	B	81	ASN
2	B	177	GLN
2	B	242	GLN
2	B	269	ASN
2	B	275	GLN
2	B	279	HIS
2	B	290	GLN
2	B	314	GLN
2	B	362	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	73/76 (96%)	23 (31%)	9 (12%)
1	D	70/76 (92%)	20 (28%)	10 (14%)
All	All	143/152 (94%)	43 (30%)	19 (13%)

All (43) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	U
1	C	3	C
1	C	4	C
1	C	8	U
1	C	9	C
1	C	10	G
1	C	16	A
1	C	17	G
1	C	18	G
1	C	19	C
1	C	20	C
1	C	20(A)	C
1	C	34	U
1	C	35	U
1	C	52	G
1	C	57	G
1	C	64	C
1	C	67	G
1	C	68	G

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Mol	Chain	Res	Type
1	C	69	G
1	C	70	G
1	C	71	A
1	C	72	C
1	D	4	C
1	D	8	U
1	D	9	C
1	D	10	G
1	D	16	A
1	D	17	G
1	D	18	G
1	D	19	C
1	D	20	C
1	D	20(A)	C
1	D	34	U
1	D	35	U
1	D	52	G
1	D	57	G
1	D	59	A
1	D	64	C
1	D	66	A
1	D	67	G
1	D	68	G
1	D	70	G

All (19) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	7	U
1	C	9	C
1	C	15	G
1	C	18	G
1	C	20	C
1	C	34	U
1	C	47	C
1	C	57	G
1	C	60	U
1	D	7	U
1	D	9	C
1	D	15	G
1	D	18	G
1	D	20	C

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Mol	Chain	Res	Type
1	D	34	U
1	D	47	C
1	D	56	C
1	D	57	G
1	D	60	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 ligands 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	$\#\|Z\| > 2$
3	PO4	B	1001	-	4,4,4	1.74	1 (25%)	6,6,6	0.43	0
4	SO4	A	2003	-	4,4,4	0.25	0	6,6,6	0.08	0
4	SO4	B	2004	-	4,4,4	0.26	0	6,6,6	0.07	0
3	PO4	A	1002	-	4,4,4	1.59	0	6,6,6	0.44	0
4	SO4	A	2005	-	4,4,4	0.24	0	6,6,6	0.10	0
3	PO4	B	1003	-	4,4,4	1.65	0	6,6,6	0.43	0
4	SO4	B	2002	-	4,4,4	0.25	0	6,6,6	0.11	0
3	PO4	C	1004	-	4,4,4	1.59	0	6,6,6	0.44	0
4	SO4	A	2001	-	4,4,4	0.30	0	6,6,6	0.17	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	PO4	P-O4	-2.03	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	PO4	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	74/76 (97%)	-0.46	0	100	100	32, 71, 172, 188	0
1	D	71/76 (93%)	-0.59	0	100	100	42, 73, 145, 185	0
2	A	348/380 (91%)	-0.37	0	100	100	11, 43, 80, 104	0
2	B	359/380 (94%)	-0.20	5 (1%)	75	56	19, 57, 110, 166	0
All	All	852/912 (93%)	-0.32	5 (0%)	89	78	11, 53, 111, 188	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	40	TRP	7.0
2	B	39	ASN	4.6
2	B	38	LYS	3.1
2	B	44	ASP	2.4
2	B	43	ASP	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95^{th} 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
3	PO4	C	1004	5/5	0.76	0.16	141,149,151,152	0
4	SO4	B	2004	5/5	0.87	0.15	116,118,120,120	0
4	SO4	A	2003	5/5	0.88	0.15	140,141,143,144	0
4	SO4	B	2002	5/5	0.90	0.15	130,131,134,134	0
4	SO4	A	2001	5/5	0.91	0.15	82,90,97,102	0
4	SO4	A	2005	5/5	0.94	0.13	89,92,93,99	0
3	PO4	B	1003	5/5	0.98	0.10	72,73,78,81	0
3	PO4	A	1002	5/5	0.98	0.16	53,54,63,69	0
3	PO4	B	1001	5/5	0.99	0.14	47,56,64,68	0

6.5 Other polymers (i)

There are no such residues in this entry.