



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:48 PM UTC

PDB ID : 2ZM5 / pdb_00002zm5
Title : Crystal structure of tRNA modification enzyme MiaA in the complex with tRNA(Phe)
Authors : Sakai, J.; Yao, M.; Chimnaronk, S.; Tanaka, I.
Deposited on : 2008-04-11
Resolution : 2.55 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

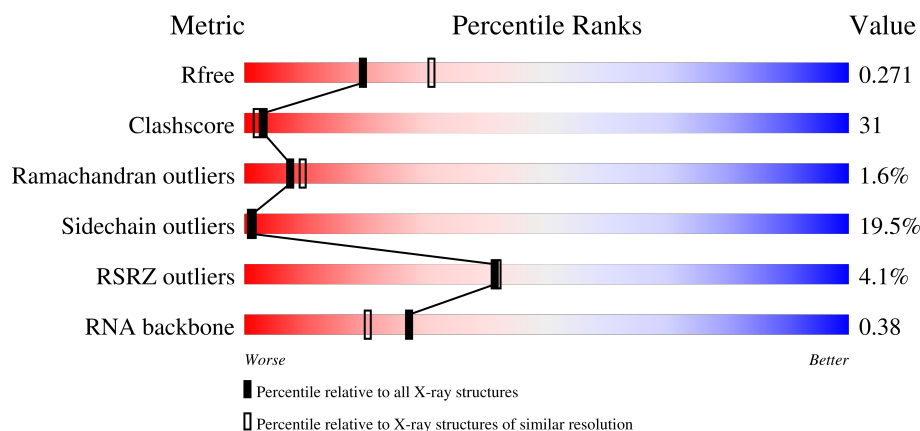
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)
RNA backbone	3983	1112 (2.80-2.28)

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	A	316	2% 59% 27% 11% .
1	B	316	4% 41% 38% 15% . .
2	C	76	% 37% 29% 20% 12% .
2	D	76	14% 29% 33% 16% 13% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8015 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 protein called tRNA delta(2)-isopentenylpyrophosphate transferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	Se	0	0	0
			2403	1523	428	443	2	7			
1	B	305	Total	C	N	O	S	Se	0	0	0
			2397	1518	427	443	2	7			

- Molecule 2 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	74	Total	C	N	O	P	0	0	0
			1577	704	282	518	73			
2	D	69	Total	C	N	O	P	0	0	0
			1469	656	261	484	68			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	6	Total	Mg	0	0
			6	6		
3	D	1	Total	Mg	0	0
			1	1		

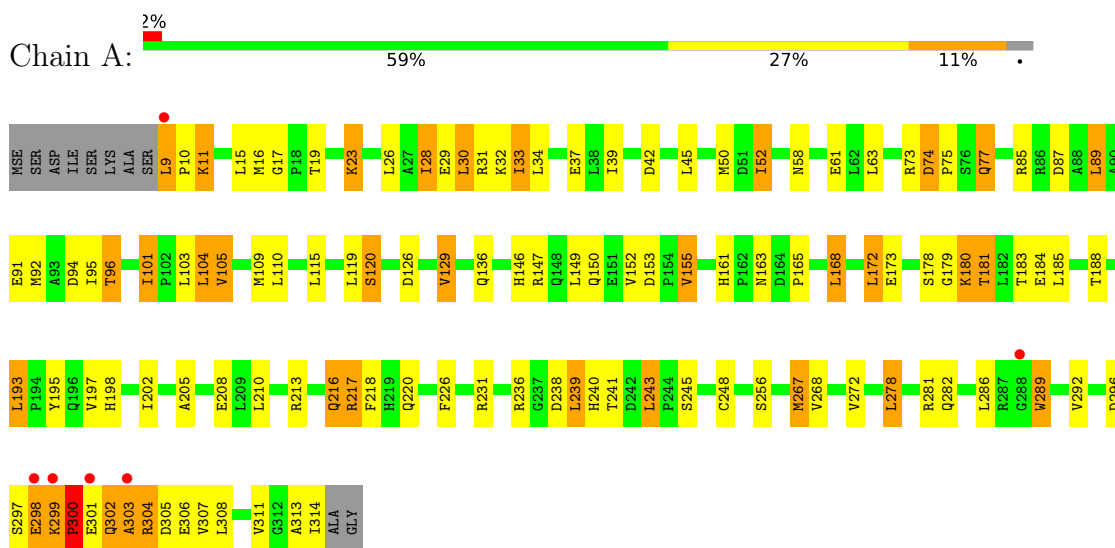
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	31	Total	O	0	0
			31	31		
4	C	57	Total	O	0	0
			57	57		
4	D	21	Total	O	0	0
			21	21		

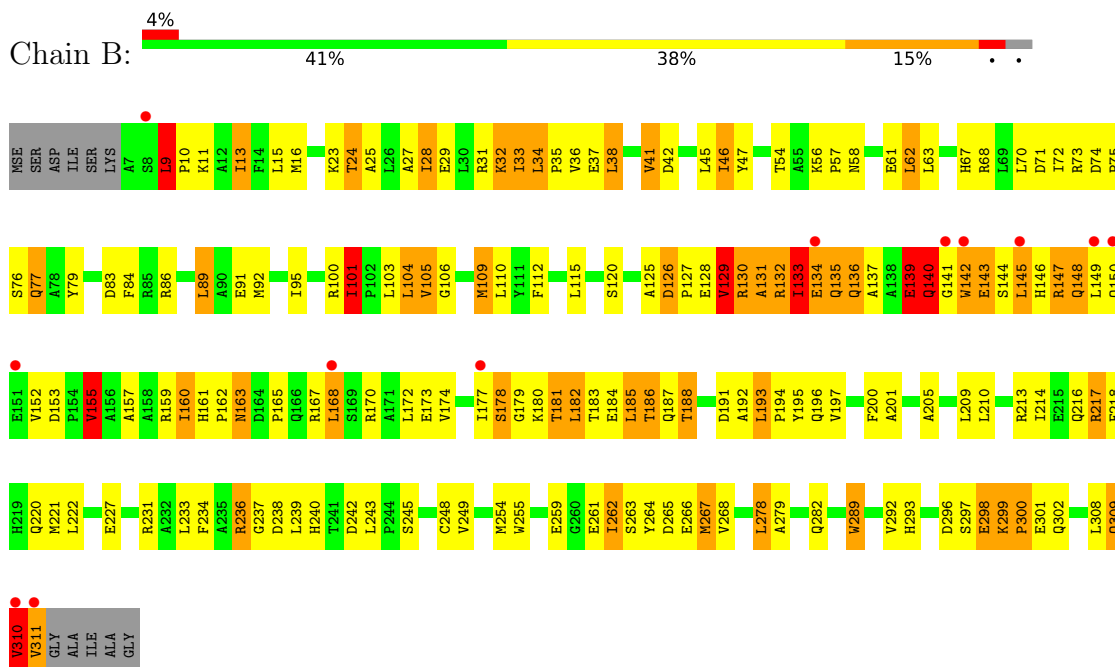
3 Residue-property plots

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.

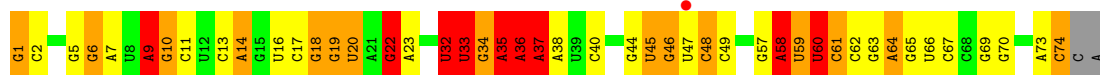
- Molecule 1: tRNA delta(2)-isopentenylpyrophosphate transferase



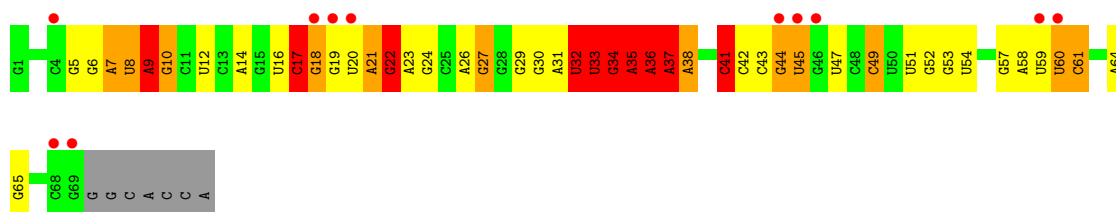
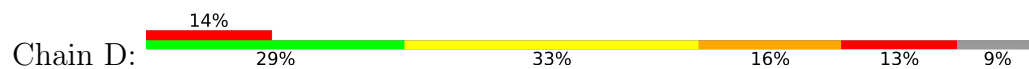
- Molecule 1: tRNA delta(2)-isopentenylpyrophosphate transferase



● Molecule 2: tRNA(Phe)



● Molecule 2: tRNA(Phe)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.20Å 89.40Å 150.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55 20.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-2.55) 98.7 (20.00-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.270 0.240 , 0.271	Depositor DCC
R_{free} test set	2763 reflections (7.05%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8015	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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 [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/2447	1.01	11/3308 (0.3%)
1	B	0.46	0/2441	1.09	21/3300 (0.6%)
2	C	0.53	0/1762	1.32	31/2746 (1.1%)
2	D	0.41	0/1641	1.12	27/2557 (1.1%)
All	All	0.48	0/8291	1.13	90/11911 (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
2	C	1	2
2	D	0	4
All	All	1	6

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	64	A	C2'-C3'-O3'	14.79	135.88	113.70
2	C	35	A	OP2-P-O3'	-14.32	65.04	108.00
2	C	35	A	OP1-P-O3'	-12.73	69.81	108.00
1	B	179	GLY	N-CA-C	-11.22	101.34	114.69
2	D	35	A	C3'-C2'-O2'	10.68	130.62	114.60
2	C	9	A	C4'-C3'-O3'	10.39	124.99	109.40
2	C	35	A	C2'-C3'-O3'	9.55	123.82	109.50
1	A	179	GLY	N-CA-C	-9.27	103.66	114.69
2	C	32	U	C2'-C3'-O3'	-9.22	95.67	109.50
2	C	60	U	C4'-C3'-O3'	9.00	122.90	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	34	G	C2'-C3'-O3'	8.91	122.87	109.50
2	D	32	U	C2'-C3'-O3'	8.83	122.75	109.50
2	D	32	U	C4'-C3'-O3'	8.59	122.28	109.40
2	C	36	A	O5'-P-OP1	-8.44	82.68	108.00
2	D	33	U	C2'-C3'-O3'	8.31	121.97	109.50
1	B	139	GLU	N-CA-C	-8.09	100.16	110.19
1	B	155	VAL	N-CA-C	-7.79	102.51	111.00
1	A	101	ILE	N-CA-C	7.71	116.78	107.61
2	D	22	G	N9-C1'-C2'	7.52	123.28	112.00
2	D	33	U	C5'-C4'-C3'	-7.39	104.12	115.20
1	B	100	ARG	N-CA-C	7.36	120.59	109.41
2	D	32	U	C3'-C2'-O2'	7.29	125.54	114.60
2	D	35	A	C2'-C3'-O3'	7.08	120.13	109.50
2	C	32	U	O3'-P-O5'	-7.01	93.49	104.00
1	B	9	LEU	N-CA-C	6.95	116.13	108.14
2	D	35	A	O3'-P-O5'	6.92	114.38	104.00
2	C	60	U	C2'-C3'-O3'	6.91	119.87	109.50
2	C	16	U	C2'-C3'-O3'	-6.83	103.46	113.70
1	A	289	TRP	N-CA-C	-6.81	99.96	110.10
2	D	33	U	C3'-C2'-O2'	6.80	124.80	114.60
1	B	145	LEU	N-CA-C	-6.69	104.06	111.36
1	B	129	VAL	N-CA-C	-6.69	105.11	112.80
1	B	47	TYR	N-CA-C	6.69	120.39	109.76
1	B	197	VAL	N-CA-C	6.51	117.98	108.53
2	D	36	A	C2'-C3'-O3'	6.48	119.22	109.50
1	B	148	GLN	N-CA-C	-6.47	105.10	112.87
2	C	1	G	O5'-C5'-C4'	6.39	121.08	111.50
1	B	299	LYS	CA-C-N	6.36	127.80	119.84
1	B	299	LYS	C-N-CA	6.36	127.80	119.84
1	A	197	VAL	N-CA-C	6.34	117.72	108.53
1	B	310	VAL	N-CA-C	-6.21	96.42	109.34
2	D	9	A	C2'-C3'-O3'	6.19	118.79	109.50
2	C	58	A	C3'-C2'-O2'	6.11	123.76	114.60
2	D	18	G	C4'-C3'-O3'	-6.08	103.88	113.00
1	B	302	GLN	N-CA-C	-6.07	104.77	111.82
2	C	69	G	C5'-C4'-C3'	-6.07	106.90	116.00
2	D	7	A	C4'-C3'-O3'	-6.06	103.91	113.00
2	C	32	U	C4'-C3'-O3'	6.04	118.46	109.40
2	D	36	A	C4'-C3'-O3'	5.99	118.39	109.40
1	B	126	ASP	CA-C-N	5.98	127.31	119.84
1	B	126	ASP	C-N-CA	5.98	127.31	119.84
2	C	37	A	C4'-C3'-C2'	5.96	108.56	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	19	G	C4'-C3'-O3'	-5.93	100.51	109.40
2	D	37	A	C4'-C3'-O3'	5.86	118.18	109.40
2	D	7	A	N9-C1'-C2'	5.85	120.78	112.00
1	B	205	ALA	N-CA-C	5.82	118.41	111.71
2	C	9	A	C4'-C3'-C2'	5.81	108.41	102.60
2	C	22	G	C2'-C3'-O3'	5.77	118.15	109.50
2	C	10	G	O5'-P-OP1	-5.74	90.78	108.00
2	C	19	G	C5'-C4'-C3'	5.71	123.77	115.20
2	D	35	A	C4'-C3'-O3'	-5.71	100.84	109.40
1	A	241	THR	N-CA-C	5.65	119.91	113.19
1	B	131	ALA	N-CA-C	-5.64	98.78	110.80
2	C	36	A	O5'-P-OP2	-5.62	91.13	108.00
1	B	289	TRP	N-CA-C	-5.60	101.76	110.10
2	D	41	C	C5'-C4'-O4'	-5.58	101.42	109.80
2	C	64	A	C3'-C2'-O2'	5.57	119.06	110.70
1	A	304	ARG	N-CA-C	-5.43	105.91	112.54
2	C	60	U	C4'-C3'-C2'	5.42	108.02	102.60
1	A	306	GLU	N-CA-C	-5.35	105.53	111.36
2	D	18	G	N9-C1'-C2'	5.35	120.02	112.00
1	A	74	ASP	N-CA-C	-5.29	103.41	110.07
2	C	5	G	C5'-C4'-C3'	-5.29	108.07	116.00
1	A	155	VAL	N-CA-C	-5.26	105.41	110.72
2	C	37	A	C2'-C3'-O3'	5.24	117.35	109.50
2	C	19	G	O4'-C1'-C2'	5.23	111.03	105.80
2	D	32	U	C4'-C3'-C2'	5.19	107.79	102.60
2	D	32	U	C1'-C2'-O2'	5.17	119.56	111.80
2	D	21	A	N9-C1'-C2'	5.17	119.75	112.00
2	C	33	U	O4'-C4'-C3'	5.15	109.15	104.00
2	C	58	A	C4'-C3'-O3'	-5.11	101.74	109.40
2	D	60	U	N1-C1'-C2'	5.10	119.66	112.00
1	A	303	ALA	N-CA-C	-5.09	106.75	113.17
2	D	36	A	OP1-P-O3'	-5.08	92.75	108.00
1	B	109	MSE	N-CA-C	5.07	116.81	111.28
2	C	37	A	O4'-C1'-C2'	5.07	110.87	105.80
2	C	35	A	C3'-C2'-O2'	5.03	122.15	114.60
1	B	101	ILE	N-CA-C	5.03	113.46	107.73
2	D	38	A	C4'-C3'-O3'	-5.03	105.46	113.00
1	A	205	ALA	N-CA-C	5.02	118.51	112.38

All (1) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
2	C	64	A	C3'

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	20	U	Sidechain
2	C	37	A	Sidechain
2	D	17	C	Sidechain
2	D	22	G	Sidechain
2	D	34	G	Sidechain
2	D	37	A	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2403	0	2408	122	0
1	B	2397	0	2399	240	0
2	C	1577	0	800	41	0
2	D	1469	0	745	48	0
3	C	6	0	0	0	0
3	D	1	0	0	0	0
4	A	53	0	0	1	2
4	B	31	0	0	0	0
4	C	57	0	0	1	0
4	D	21	0	0	1	2
All	All	8015	0	6352	439	2

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 31.

All (439) 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:B:136:GLN:HE22	1:B:145:LEU:HD11	1.09	1.15
1:B:147:ARG:HH11	1:B:147:ARG:HB3	1.02	1.10
2:D:41:C:H5'	2:D:41:C:H6	1.13	1.08
1:B:37:GLU:HB3	1:B:95:ILE:HD13	1.38	1.05
1:B:92:MSE:HE1	1:B:115:LEU:HD11	1.39	1.03
1:A:92:MSE:HE1	1:A:115:LEU:HD11	1.42	1.01
1:A:89:LEU:HA	1:A:92:MSE:HE3	1.43	0.99
1:B:147:ARG:HB3	1:B:147:ARG:NH1	1.76	0.99
1:B:133:ILE:N	1:B:133:ILE:HD12	1.75	0.99
1:B:147:ARG:HH11	1:B:147:ARG:CB	1.76	0.99
1:B:129:VAL:O	1:B:133:ILE:HD11	1.62	0.97
2:C:13:C:H2'	2:C:14:A:H5''	1.44	0.96
1:A:311:VAL:HG22	1:A:314:ILE:HD11	1.50	0.94
1:A:50:MSE:HE1	1:A:245:SER:HB2	1.50	0.94
1:A:52:ILE:HD11	1:A:226:PHE:HB2	1.48	0.94
2:D:41:C:H5'	2:D:41:C:C6	2.04	0.93
1:B:9:LEU:HB2	1:B:10:PRO:HD2	1.52	0.91
1:B:149:LEU:HD22	1:B:172:LEU:HD23	1.51	0.91
1:B:213:ARG:O	1:B:217:ARG:HG3	1.72	0.89
2:C:74:C:H6	2:C:74:C:H5'	1.37	0.89
1:A:193:LEU:HD13	1:A:195:TYR:HB2	1.56	0.86
1:A:307:VAL:O	1:A:311:VAL:HG12	1.76	0.86
1:A:73:ARG:HG3	1:A:73:ARG:HH11	1.40	0.85
1:B:181:THR:O	1:B:185:LEU:HD23	1.75	0.85
1:B:130:ARG:HA	1:B:133:ILE:HD11	1.58	0.85
2:D:17:C:H5'	2:D:18:G:H5''	1.59	0.83
1:A:155:VAL:HB	1:A:183:THR:HG21	1.60	0.83
1:B:136:GLN:NE2	1:B:145:LEU:HD11	1.92	0.83
1:A:11:LYS:HD3	1:A:11:LYS:N	1.93	0.83
1:B:131:ALA:O	1:B:134:GLU:HB3	1.76	0.83
1:B:137:ALA:HA	1:B:141:GLY:HA3	1.61	0.82
1:B:133:ILE:HD12	1:B:133:ILE:H	1.39	0.82
1:B:298:GLU:C	1:B:300:PRO:HD3	2.02	0.82
1:B:218:PHE:HA	1:B:221:MSE:HE2	1.60	0.82
1:A:33:ILE:O	1:A:33:ILE:HG13	1.80	0.82
1:A:299:LYS:C	1:A:301:GLU:H	1.88	0.82
2:C:13:C:C2'	2:C:14:A:H5''	2.09	0.81
1:A:101:ILE:HD11	1:A:314:ILE:HG21	1.61	0.81
1:B:163:ASN:OD1	1:B:163:ASN:N	2.13	0.81
1:B:161:HIS:HD2	1:B:163:ASN:OD1	1.62	0.81
1:B:155:VAL:HG12	1:B:183:THR:OG1	1.83	0.79
2:C:45:U:H5''	4:C:87:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ARG:HA	1:B:133:ILE:CD1	2.13	0.78
1:B:236:ARG:O	1:B:238:ASP:N	2.17	0.77
1:A:92:MSE:O	1:A:96:THR:HG23	1.84	0.77
1:B:126:ASP:CG	1:B:129:VAL:HG12	2.09	0.77
1:B:298:GLU:O	1:B:299:LYS:HD2	1.85	0.77
2:D:18:G:H2'	2:D:57:G:N2	1.99	0.77
1:A:17:GLY:O	1:A:23:LYS:HE2	1.85	0.76
1:B:130:ARG:CA	1:B:133:ILE:HD11	2.15	0.76
1:B:68:ARG:HD3	1:B:91:GLU:HG3	1.67	0.76
1:A:120:SER:HB3	1:A:188:THR:O	1.85	0.76
2:D:18:G:H2'	2:D:57:G:H22	1.51	0.76
1:A:9:LEU:N	1:A:10:PRO:HD3	2.00	0.75
2:D:17:C:C5'	2:D:18:G:H5''	2.15	0.75
2:D:34:G:O2'	2:D:35:A:OP2	2.03	0.75
1:B:240:HIS:CE1	1:B:242:ASP:HB2	2.23	0.74
2:D:37:A:H8	2:D:37:A:OP1	1.69	0.74
1:A:248:CYS:HA	2:C:37:A:O2'	1.88	0.74
1:A:50:MSE:HE3	1:A:75:PRO:HB3	1.70	0.74
1:A:92:MSE:CE	1:A:115:LEU:HD11	2.18	0.74
1:A:161:HIS:HD2	1:A:163:ASN:H	1.36	0.74
1:B:16:MSE:HE3	1:B:112:PHE:CB	2.18	0.73
1:B:132:ARG:O	1:B:136:GLN:HG3	1.86	0.73
1:A:153:ASP:OD2	1:A:183:THR:HG23	1.88	0.72
1:A:302:GLN:H	1:A:302:GLN:NE2	1.86	0.72
1:A:299:LYS:O	1:A:301:GLU:N	2.22	0.72
1:B:137:ALA:HA	1:B:141:GLY:CA	2.19	0.72
1:B:259:GLU:HG2	1:B:261:GLU:OE1	1.88	0.72
1:B:16:MSE:HE2	1:B:109:MSE:HG3	1.70	0.72
2:C:35:A:O2'	2:C:36:A:OP1	2.07	0.72
1:B:222:LEU:HD21	1:B:267:MSE:HE1	1.72	0.72
1:B:32:LYS:HE2	1:B:32:LYS:N	2.05	0.71
1:B:262:ILE:HG13	1:B:266:GLU:HG2	1.72	0.71
1:B:16:MSE:HE3	1:B:112:PHE:CG	2.25	0.71
1:B:136:GLN:C	1:B:136:GLN:HE21	1.98	0.71
1:B:133:ILE:HA	1:B:136:GLN:OE1	1.91	0.70
1:B:161:HIS:CD2	1:B:163:ASN:OD1	2.45	0.70
1:B:299:LYS:N	1:B:300:PRO:HD3	2.05	0.70
1:A:50:MSE:CE	1:A:75:PRO:HB3	2.22	0.70
1:B:16:MSE:HE1	1:B:289:TRP:CH2	2.26	0.70
1:B:92:MSE:CE	1:B:115:LEU:HD11	2.18	0.69
1:B:16:MSE:HB3	1:B:109:MSE:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:HIS:CE1	1:B:157:ALA:HB1	2.26	0.69
1:B:89:LEU:HA	1:B:92:MSE:HE3	1.75	0.68
1:B:126:ASP:HB3	1:B:129:VAL:CG1	2.24	0.68
1:B:16:MSE:HE1	1:B:289:TRP:CZ2	2.28	0.68
1:B:147:ARG:HA	1:B:150:GLN:HG2	1.75	0.68
2:D:60:U:H5'	2:D:61:C:OP2	1.94	0.67
1:B:129:VAL:O	1:B:129:VAL:HG22	1.95	0.66
1:A:85:ARG:HG3	1:A:115:LEU:HA	1.78	0.66
1:B:27:ALA:HB1	1:B:38:LEU:HD11	1.78	0.66
1:B:37:GLU:CB	1:B:95:ILE:HD13	2.22	0.66
1:B:103:LEU:CD2	1:B:105:VAL:HG22	2.26	0.66
1:B:146:HIS:CD2	1:B:162:PRO:HG3	2.31	0.66
2:D:5:G:H2'	2:D:6:G:H8	1.61	0.66
1:B:46:ILE:HG22	1:B:73:ARG:HB2	1.77	0.65
1:B:149:LEU:HB2	1:B:172:LEU:CD2	2.27	0.65
1:A:50:MSE:HE1	1:A:245:SER:CB	2.27	0.65
1:A:89:LEU:HA	1:A:92:MSE:CE	2.25	0.65
1:B:134:GLU:O	1:B:137:ALA:N	2.29	0.65
1:A:298:GLU:O	1:A:300:PRO:N	2.30	0.64
1:A:101:ILE:CD1	1:A:314:ILE:HG21	2.25	0.64
1:B:216:GLN:O	1:B:220:GLN:HG3	1.97	0.64
1:A:218:PHE:HE2	1:A:267:MSE:HE1	1.63	0.64
1:A:73:ARG:HG3	1:A:73:ARG:NH1	2.12	0.64
1:B:139:GLU:O	1:B:140:GLN:C	2.40	0.64
1:B:298:GLU:C	1:B:299:LYS:HD2	2.22	0.64
1:A:11:LYS:N	1:A:11:LYS:CD	2.59	0.64
2:D:6:G:H2'	2:D:7:A:O4'	1.97	0.64
1:A:50:MSE:CE	1:A:245:SER:HB2	2.27	0.63
2:D:9:A:O2'	2:D:10:G:OP1	2.16	0.63
1:B:193:LEU:HD13	1:B:195:TYR:HB2	1.79	0.63
1:B:68:ARG:HD3	1:B:91:GLU:CG	2.28	0.63
1:B:91:GLU:O	1:B:95:ILE:HG13	1.98	0.63
2:D:14:A:N6	2:D:21:A:H2	1.97	0.63
1:B:227:GLU:O	1:B:231:ARG:HG3	1.98	0.63
1:B:134:GLU:CD	1:B:134:GLU:C	2.67	0.63
1:B:36:VAL:HG12	1:B:101:ILE:HG12	1.81	0.62
1:B:130:ARG:CA	1:B:133:ILE:CD1	2.76	0.62
2:D:51:U:H2'	2:D:52:G:C8	2.34	0.62
1:B:25:ALA:O	1:B:29:GLU:HG2	1.98	0.62
1:B:248:CYS:HA	2:D:37:A:O2'	2.00	0.62
1:A:11:LYS:HD3	1:A:11:LYS:H	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:PHE:CE2	1:A:267:MSE:HE1	2.35	0.62
2:C:6:G:H5''	2:C:6:G:H8	1.64	0.62
1:A:126:ASP:HB3	1:A:129:VAL:HG13	1.82	0.61
1:A:267:MSE:HE2	1:A:268:VAL:HA	1.82	0.61
1:B:160:ILE:N	1:B:160:ILE:HD13	2.13	0.61
2:C:74:C:H5'	2:C:74:C:C6	2.28	0.61
2:D:23:A:H2'	2:D:24:G:C8	2.35	0.61
1:A:181:THR:HG22	1:A:184:GLU:H	1.64	0.61
1:B:236:ARG:C	1:B:238:ASP:H	2.08	0.61
1:B:155:VAL:HG11	1:B:183:THR:CG2	2.30	0.61
1:B:139:GLU:OE2	1:B:140:GLN:HB3	2.00	0.61
1:B:173:GLU:O	1:B:177:ILE:HG22	2.00	0.61
1:A:153:ASP:CG	1:A:183:THR:HG23	2.25	0.61
2:D:43:C:H2'	2:D:44:G:H5''	1.82	0.61
1:B:129:VAL:C	1:B:133:ILE:HD11	2.26	0.60
1:B:136:GLN:HE21	1:B:137:ALA:N	1.98	0.60
1:B:217:ARG:O	1:B:221:MSE:HG3	2.00	0.60
2:D:51:U:H2'	2:D:52:G:H8	1.65	0.60
1:B:181:THR:HG22	1:B:184:GLU:H	1.67	0.60
1:B:129:VAL:O	1:B:129:VAL:CG2	2.50	0.60
1:B:141:GLY:C	1:B:143:GLU:H	2.09	0.60
1:B:132:ARG:O	1:B:134:GLU:N	2.35	0.59
2:C:60:U:H3'	2:C:61:C:C5	2.37	0.59
2:D:5:G:H2'	2:D:6:G:C8	2.37	0.59
1:B:58:ASN:OD1	1:B:61:GLU:HG3	2.01	0.59
2:D:14:A:H61	2:D:21:A:H2	1.50	0.59
1:B:161:HIS:CD2	1:B:162:PRO:HD2	2.38	0.59
1:A:161:HIS:CD2	1:A:163:ASN:HB2	2.38	0.59
1:A:299:LYS:O	1:A:302:GLN:NE2	2.35	0.59
1:B:134:GLU:CD	1:B:135:GLN:N	2.61	0.59
1:B:142:TRP:HE3	1:B:168:LEU:HD13	1.67	0.59
2:D:26:A:C2'	2:D:27:G:H5'	2.33	0.58
1:B:41:VAL:HG11	1:B:112:PHE:CZ	2.37	0.58
2:D:6:G:O2'	2:D:7:A:H5'	2.02	0.58
1:B:9:LEU:N	1:B:9:LEU:CD2	2.67	0.58
2:C:60:U:H3'	2:C:61:C:H5	1.69	0.58
1:A:58:ASN:OD1	1:A:61:GLU:HG3	2.04	0.58
1:B:133:ILE:H	1:B:133:ILE:CD1	2.03	0.58
1:B:13:ILE:HG23	1:B:101:ILE:HD11	1.86	0.58
2:D:33:U:O2'	2:D:34:G:OP2	2.20	0.58
1:B:149:LEU:HD22	1:B:172:LEU:CD2	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HB	1:A:104:LEU:HD13	1.86	0.57
1:B:131:ALA:O	1:B:134:GLU:N	2.30	0.57
1:B:234:PHE:HA	1:B:255:TRP:CH2	2.39	0.57
1:A:50:MSE:HE3	1:A:75:PRO:CB	2.34	0.57
1:B:296:ASP:HB3	1:B:299:LYS:HB2	1.87	0.57
1:B:147:ARG:HA	1:B:150:GLN:CG	2.34	0.57
1:A:193:LEU:CD1	1:A:195:TYR:HB2	2.32	0.57
1:B:13:ILE:CG2	1:B:101:ILE:HD11	2.35	0.57
1:B:126:ASP:CG	1:B:129:VAL:CG1	2.77	0.56
1:B:147:ARG:C	1:B:149:LEU:N	2.60	0.56
2:C:35:A:C2'	2:C:36:A:OP1	2.46	0.56
2:C:73:A:H2'	2:C:74:C:H5'	1.85	0.56
1:A:33:ILE:C	1:A:34:LEU:HD12	2.29	0.56
2:C:74:C:H6	2:C:74:C:C5'	2.14	0.56
1:A:92:MSE:O	1:A:96:THR:CG2	2.54	0.56
1:B:142:TRP:CE3	1:B:168:LEU:HD13	2.40	0.56
1:B:130:ARG:C	1:B:133:ILE:CD1	2.79	0.56
1:A:161:HIS:CD2	1:A:163:ASN:H	2.20	0.56
1:B:142:TRP:HE3	1:B:168:LEU:CD1	2.19	0.56
1:B:261:GLU:O	1:B:262:ILE:HD12	2.06	0.56
1:B:41:VAL:HG22	1:B:41:VAL:O	2.05	0.55
1:B:147:ARG:HA	1:B:150:GLN:HB3	1.87	0.55
1:B:222:LEU:HD11	1:B:268:VAL:HG22	1.88	0.55
2:C:33:U:O2'	2:C:34:G:N2	2.35	0.55
1:A:301:GLU:C	1:A:303:ALA:H	2.14	0.55
1:B:161:HIS:CE1	2:D:41:C:H4'	2.41	0.55
1:B:155:VAL:HG11	1:B:183:THR:HG23	1.87	0.55
1:B:143:GLU:CA	1:B:143:GLU:OE2	2.55	0.55
1:B:132:ARG:C	1:B:134:GLU:N	2.60	0.55
1:B:153:ASP:OD1	1:B:181:THR:HG23	2.07	0.55
2:C:20:U:H6	2:C:20:U:O5'	1.89	0.55
1:B:149:LEU:CD2	1:B:172:LEU:HD23	2.32	0.54
2:C:61:C:H2'	2:C:62:C:C6	2.42	0.54
2:D:41:C:H6	2:D:41:C:C5'	2.02	0.54
1:B:227:GLU:OE2	1:B:231:ARG:NH1	2.35	0.54
1:A:11:LYS:CD	1:A:11:LYS:H	2.19	0.54
1:A:37:GLU:HB2	1:A:95:ILE:HD13	1.90	0.54
1:A:9:LEU:N	1:A:10:PRO:CD	2.69	0.53
1:A:218:PHE:HE2	1:A:267:MSE:CE	2.22	0.53
1:B:126:ASP:O	1:B:130:ARG:HB2	2.08	0.53
1:B:147:ARG:CA	1:B:150:GLN:HG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:SER:C	1:A:298:GLU:O	2.50	0.53
1:B:147:ARG:C	1:B:150:GLN:H	2.16	0.53
1:B:149:LEU:HB2	1:B:172:LEU:HD21	1.90	0.53
1:B:181:THR:O	1:B:185:LEU:CD2	2.52	0.53
2:C:1:G:C8	2:C:1:G:H5''	2.44	0.53
1:A:218:PHE:CE2	1:A:267:MSE:CE	2.92	0.53
1:B:174:VAL:HG21	1:B:182:LEU:HD23	1.89	0.53
1:B:310:VAL:O	1:B:311:VAL:O	2.27	0.53
1:A:87:ASP:O	1:A:91:GLU:HG2	2.09	0.52
1:B:103:LEU:C	1:B:103:LEU:HD23	2.34	0.52
1:A:240:HIS:CE1	1:A:243:LEU:HD13	2.45	0.52
1:B:9:LEU:HB2	1:B:10:PRO:CD	2.34	0.52
1:B:58:ASN:CG	1:B:61:GLU:HG3	2.34	0.52
1:B:143:GLU:OE2	1:B:143:GLU:HA	2.10	0.52
1:B:155:VAL:CG1	1:B:183:THR:OG1	2.57	0.52
1:B:249:VAL:HG22	2:D:37:A:C2	2.44	0.52
1:B:79:TYR:OH	1:B:84:PHE:HA	2.09	0.52
1:B:126:ASP:CB	1:B:129:VAL:CG1	2.88	0.52
1:B:132:ARG:C	1:B:134:GLU:H	2.17	0.52
1:B:126:ASP:O	1:B:129:VAL:HG13	2.10	0.52
1:B:38:LEU:N	1:B:38:LEU:CD2	2.73	0.52
1:B:27:ALA:HB1	1:B:38:LEU:CD1	2.40	0.52
1:B:170:ARG:HG2	2:D:34:G:OP1	2.09	0.52
1:A:153:ASP:OD2	1:A:181:THR:HG23	2.10	0.52
1:B:131:ALA:O	1:B:134:GLU:CB	2.54	0.52
2:D:64:A:H2'	2:D:65:G:H8	1.74	0.52
1:A:298:GLU:O	1:A:300:PRO:CD	2.58	0.51
2:D:26:A:H2'	2:D:27:G:H5'	1.91	0.51
1:B:309:GLN:HE21	1:B:309:GLN:HA	1.76	0.51
2:C:9:A:N6	2:C:22:G:C5	2.79	0.51
1:B:15:LEU:HB3	1:B:105:VAL:HG13	1.92	0.51
1:A:298:GLU:O	1:A:300:PRO:HD2	2.11	0.51
1:B:147:ARG:HA	1:B:150:GLN:CB	2.40	0.51
1:B:167:ARG:HH21	1:B:167:ARG:HG3	1.76	0.51
1:B:299:LYS:N	1:B:300:PRO:CD	2.74	0.51
2:D:49:C:H6	2:D:49:C:O5'	1.93	0.51
1:A:163:ASN:O	1:A:165:PRO:HD3	2.11	0.51
1:A:298:GLU:C	1:A:300:PRO:HD2	2.36	0.51
1:B:103:LEU:HD22	1:B:105:VAL:HG22	1.93	0.51
1:A:147:ARG:HA	1:A:150:GLN:HE21	1.75	0.51
1:B:147:ARG:HG2	1:B:150:GLN:CD	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:LYS:HA	1:A:301:GLU:HG3	1.91	0.51
1:A:161:HIS:HD2	1:A:163:ASN:HB2	1.77	0.51
1:A:268:VAL:O	1:A:272:VAL:HG23	2.11	0.51
1:B:34:LEU:HD12	1:B:35:PRO:HD2	1.93	0.51
1:B:89:LEU:CD1	1:B:92:MSE:HE3	2.40	0.51
1:B:140:GLN:HG2	1:B:143:GLU:HB2	1.93	0.51
2:D:36:A:H4'	2:D:37:A:O5'	2.10	0.50
2:D:52:G:O2'	2:D:53:G:H5'	2.11	0.50
1:A:161:HIS:HD2	1:A:163:ASN:N	2.06	0.50
1:A:304:ARG:NH1	1:A:305:ASP:OD1	2.44	0.50
1:B:46:ILE:HG23	1:B:72:ILE:HG13	1.92	0.50
1:B:57:PRO:HA	1:B:61:GLU:OE1	2.12	0.50
1:B:89:LEU:HD13	1:B:92:MSE:CE	2.42	0.50
1:B:134:GLU:O	1:B:137:ALA:HB3	2.11	0.50
1:B:136:GLN:OE1	1:B:145:LEU:HD21	2.12	0.50
1:A:289:TRP:HB3	1:A:292:VAL:HG21	1.93	0.50
1:B:45:LEU:HD12	1:B:54:THR:HB	1.94	0.50
1:B:145:LEU:HD22	1:B:172:LEU:CD1	2.42	0.50
1:B:147:ARG:C	1:B:149:LEU:H	2.19	0.50
1:A:28:ILE:C	1:A:28:ILE:HD12	2.37	0.49
1:B:131:ALA:O	1:B:132:ARG:C	2.55	0.49
1:B:309:GLN:C	1:B:309:GLN:NE2	2.70	0.49
1:B:16:MSE:HB3	1:B:109:MSE:CE	2.42	0.49
2:C:58:A:O2'	2:C:60:U:OP2	2.22	0.49
2:D:9:A:C2	2:D:44:G:H2'	2.47	0.49
1:A:73:ARG:NH1	1:A:73:ARG:CG	2.75	0.49
1:A:231:ARG:HD2	1:B:264:TYR:CE2	2.47	0.49
2:D:18:G:H4'	2:D:60:U:C2	2.47	0.49
2:C:45:U:O2'	2:C:46:G:OP2	2.30	0.49
1:A:149:LEU:HD13	1:A:172:LEU:HD13	1.94	0.49
1:B:160:ILE:N	1:B:160:ILE:CD1	2.76	0.49
1:A:231:ARG:HH12	1:B:265:ASP:CG	2.19	0.49
1:B:240:HIS:HE1	1:B:242:ASP:HB2	1.75	0.49
2:C:60:U:O3'	2:C:61:C:H6	1.96	0.49
1:B:129:VAL:O	1:B:133:ILE:CD1	2.49	0.48
1:B:133:ILE:CG2	1:B:172:LEU:HD12	2.43	0.48
2:C:32:U:O2'	2:C:36:A:N1	2.46	0.48
2:C:45:U:C6	2:C:45:U:OP1	2.67	0.48
1:A:302:GLN:H	1:A:302:GLN:CD	2.21	0.48
1:B:46:ILE:CG2	1:B:73:ARG:HB2	2.41	0.48
1:B:163:ASN:O	1:B:165:PRO:HD3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:MSE:HE2	1:B:109:MSE:HE2	1.95	0.48
1:B:191:ASP:N	1:B:191:ASP:OD1	2.47	0.48
1:B:144:SER:O	1:B:148:GLN:N	2.39	0.48
1:B:178:SER:HB3	1:B:180:LYS:H	1.79	0.48
1:B:83:ASP:HA	1:B:86:ARG:NH2	2.28	0.48
1:B:133:ILE:HA	1:B:136:GLN:CD	2.37	0.48
1:B:159:ARG:HH21	1:B:160:ILE:HD11	1.79	0.48
2:D:8:U:O2	2:D:21:A:C2	2.67	0.48
2:D:59:U:OP2	4:D:93:HOH:O	2.20	0.48
1:A:146:HIS:HA	1:A:168:LEU:HD21	1.95	0.47
1:A:42:ASP:CG	1:A:45:LEU:HG	2.38	0.47
2:C:45:U:OP1	2:C:45:U:H6	1.96	0.47
1:B:45:LEU:HD11	1:B:54:THR:O	2.13	0.47
2:C:73:A:H2'	2:C:74:C:C5'	2.43	0.47
1:B:75:PRO:HB3	1:B:245:SER:OG	2.13	0.47
1:B:109:MSE:HE3	1:B:112:PHE:CD2	2.49	0.47
1:B:130:ARG:HA	1:B:133:ILE:HD13	1.94	0.47
1:B:133:ILE:N	1:B:133:ILE:CD1	2.51	0.47
2:C:61:C:H2'	2:C:62:C:H6	1.79	0.47
2:C:6:G:H5''	2:C:6:G:C8	2.47	0.47
1:B:42:ASP:HB3	1:B:45:LEU:HB2	1.97	0.47
1:B:297:SER:O	1:B:300:PRO:HG3	2.14	0.47
1:A:198:HIS:CE1	1:A:311:VAL:HA	2.49	0.47
1:B:137:ALA:HA	1:B:141:GLY:HA2	1.97	0.46
1:A:163:ASN:O	2:C:40:C:C5'	2.64	0.46
1:A:298:GLU:C	1:A:300:PRO:CD	2.88	0.46
1:A:9:LEU:N	1:A:9:LEU:CD2	2.79	0.46
1:B:33:ILE:HD11	1:B:308:LEU:HD21	1.96	0.46
1:B:227:GLU:HG2	1:B:231:ARG:NH1	2.31	0.46
1:A:301:GLU:C	1:A:303:ALA:N	2.74	0.46
1:B:149:LEU:HB2	1:B:172:LEU:HD23	1.96	0.46
1:B:182:LEU:O	1:B:186:THR:OG1	2.29	0.46
1:B:57:PRO:HB2	1:B:62:LEU:HD13	1.97	0.46
1:A:52:ILE:HD11	1:A:226:PHE:CB	2.32	0.46
1:B:184:GLU:O	1:B:187:GLN:HG3	2.15	0.46
1:A:17:GLY:C	1:A:23:LYS:HE2	2.41	0.46
1:B:24:THR:O	1:B:28:ILE:HG23	2.16	0.46
1:B:34:LEU:HD21	1:B:308:LEU:CD2	2.45	0.46
1:A:153:ASP:OD1	1:A:183:THR:HG23	2.16	0.45
1:B:104:LEU:N	1:B:104:LEU:CD2	2.78	0.45
1:B:200:PHE:CD1	1:B:293:HIS:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LEU:HD21	1:B:279:ALA:HB1	1.98	0.45
1:B:89:LEU:HD12	1:B:92:MSE:HE3	1.97	0.45
1:B:126:ASP:HB3	1:B:129:VAL:HG11	1.99	0.45
1:B:34:LEU:HD21	1:B:308:LEU:HD22	1.98	0.45
1:B:74:ASP:O	1:B:77:GLN:HG3	2.17	0.45
1:A:103:LEU:HD22	1:A:105:VAL:HG22	1.99	0.45
1:A:216:GLN:O	1:A:220:GLN:HG3	2.15	0.45
1:A:299:LYS:C	1:A:301:GLU:HG3	2.41	0.45
1:B:127:PRO:O	1:B:130:ARG:N	2.45	0.45
2:C:45:U:C2'	2:C:46:G:OP2	2.65	0.45
2:D:7:A:N6	2:D:49:C:N4	2.64	0.45
1:B:184:GLU:O	1:B:187:GLN:CG	2.64	0.45
2:D:32:U:O2'	2:D:36:A:C2	2.68	0.45
1:A:30:LEU:HD12	1:A:30:LEU:HA	1.78	0.45
1:A:300:PRO:O	1:A:303:ALA:HB2	2.16	0.45
2:C:9:A:N6	2:C:22:G:C8	2.85	0.45
1:A:94:ASP:OD1	1:A:94:ASP:C	2.61	0.44
1:B:89:LEU:HA	1:B:89:LEU:HD12	1.87	0.44
1:A:217:ARG:HE	1:A:217:ARG:HB3	1.53	0.44
1:A:202:ILE:HD11	1:A:297:SER:HA	1.99	0.44
1:B:32:LYS:HE2	1:B:32:LYS:CA	2.46	0.44
1:B:126:ASP:HA	1:B:127:PRO:HD2	1.75	0.44
1:B:309:GLN:HE21	1:B:309:GLN:CA	2.30	0.44
2:C:48:C:H2'	2:C:59:U:H1'	2.00	0.44
1:A:136:GLN:O	1:A:136:GLN:HG2	2.17	0.44
1:B:141:GLY:C	1:B:143:GLU:N	2.74	0.44
2:C:66:U:H2'	2:C:67:C:C6	2.52	0.44
1:A:163:ASN:O	2:C:40:C:H5''	2.17	0.44
1:A:297:SER:O	1:A:298:GLU:C	2.60	0.44
1:B:125:ALA:HB2	2:D:35:A:OP2	2.17	0.44
1:B:146:HIS:NE2	1:B:157:ALA:O	2.51	0.44
1:A:77:GLN:HE21	1:A:77:GLN:HB3	1.57	0.44
1:B:76:SER:HA	1:B:243:LEU:HD13	2.00	0.44
1:A:153:ASP:OD1	1:A:183:THR:CG2	2.66	0.43
1:A:299:LYS:C	1:A:301:GLU:N	2.56	0.43
1:B:120:SER:OG	1:B:188:THR:O	2.27	0.43
1:B:139:GLU:O	1:B:141:GLY:N	2.51	0.43
1:B:149:LEU:HD12	1:B:152:VAL:HB	1.99	0.43
2:D:58:A:H1'	2:D:60:U:C5	2.53	0.43
1:A:313:ALA:O	1:A:314:ILE:HD13	2.18	0.43
1:B:67:HIS:HB2	1:B:70:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:A:N6	2:D:49:C:H42	2.16	0.43
1:B:262:ILE:HG23	1:B:263:SER:O	2.19	0.43
1:A:9:LEU:N	1:A:9:LEU:HD23	2.33	0.43
1:B:141:GLY:O	1:B:143:GLU:N	2.51	0.43
1:B:278:LEU:O	1:B:282:GLN:HG3	2.19	0.43
1:A:297:SER:O	1:A:298:GLU:O	2.35	0.43
1:B:167:ARG:HG3	1:B:167:ARG:NH2	2.34	0.43
1:B:23:LYS:HE3	1:B:106:GLY:C	2.44	0.43
2:D:16:U:H5''	2:D:17:C:OP2	2.18	0.43
1:B:177:ILE:HG23	1:B:178:SER:N	2.33	0.43
1:A:267:MSE:HE2	1:A:267:MSE:C	2.44	0.43
1:B:130:ARG:HD2	1:B:173:GLU:OE2	2.18	0.43
1:B:145:LEU:HD22	1:B:172:LEU:HD11	2.01	0.43
1:B:192:ALA:O	1:B:194:PRO:HD3	2.18	0.43
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.84	0.43
2:D:29:G:O2'	2:D:30:G:H5'	2.19	0.43
1:B:249:VAL:HG11	1:B:278:LEU:HD12	2.00	0.42
2:C:18:G:O2'	2:C:57:G:N2	2.39	0.42
1:B:227:GLU:HA	1:B:254:MSE:HE3	2.02	0.42
2:D:41:C:C6	2:D:41:C:C5'	2.89	0.42
1:A:238:ASP:OD1	1:A:239:LEU:HD13	2.19	0.42
1:B:58:ASN:OD1	1:B:58:ASN:C	2.62	0.42
1:B:210:LEU:O	1:B:214:ILE:HG13	2.19	0.42
1:A:278:LEU:O	1:A:282:GLN:HG3	2.20	0.42
1:A:16:MSE:HE1	1:A:289:TRP:CD1	2.55	0.42
1:A:74:ASP:O	1:A:77:GLN:HG2	2.19	0.42
1:A:147:ARG:HA	1:A:147:ARG:HD2	1.90	0.42
1:B:38:LEU:N	1:B:38:LEU:HD23	2.34	0.42
1:B:146:HIS:ND1	1:B:146:HIS:C	2.78	0.42
1:A:236:ARG:HH21	1:A:238:ASP:CG	2.27	0.42
1:B:9:LEU:N	1:B:9:LEU:HD22	2.34	0.42
1:B:222:LEU:CD2	1:B:267:MSE:HE1	2.45	0.42
1:B:104:LEU:N	1:B:104:LEU:HD22	2.34	0.42
2:C:45:U:O2'	2:C:46:G:P	2.78	0.42
2:D:58:A:O2'	2:D:60:U:H5	2.02	0.42
1:A:181:THR:HG23	1:A:183:THR:H	1.84	0.42
1:B:240:HIS:ND1	1:B:242:ASP:HB2	2.33	0.41
1:A:281:ARG:NH1	4:A:369:HOH:O	2.53	0.41
1:A:296:ASP:HB3	1:A:300:PRO:HB2	2.02	0.41
1:B:147:ARG:NH1	1:B:147:ARG:CB	2.56	0.41
1:B:201:ALA:HB2	1:B:292:VAL:HG21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:A:N6	2:C:22:G:C4	2.89	0.41
2:C:74:C:C6	2:C:74:C:C3'	3.03	0.41
1:A:89:LEU:HD12	1:A:92:MSE:HE3	2.02	0.41
1:A:129:VAL:HG22	1:A:173:GLU:HG3	2.01	0.41
1:B:109:MSE:HE3	1:B:112:PHE:HD2	1.85	0.41
1:B:132:ARG:O	1:B:133:ILE:C	2.64	0.41
1:B:133:ILE:HG22	1:B:172:LEU:HD12	2.02	0.41
1:B:142:TRP:CE2	1:B:165:PRO:HB3	2.56	0.41
1:A:299:LYS:O	1:A:301:GLU:HG3	2.20	0.41
1:B:33:ILE:HG12	1:B:34:LEU:HD22	2.03	0.41
1:B:309:GLN:NE2	1:B:309:GLN:CA	2.84	0.41
2:D:44:G:H4'	2:D:45:U:OP1	2.21	0.41
1:B:56:LYS:NZ	1:B:71:ASP:OD2	2.51	0.41
1:B:29:GLU:O	1:B:32:LYS:HB2	2.21	0.41
1:B:181:THR:O	1:B:184:GLU:HB2	2.21	0.41
2:C:62:C:O2'	2:C:63:G:H5'	2.21	0.41
2:D:53:G:H2'	2:D:54:U:O4'	2.21	0.41
1:A:165:PRO:HD2	2:C:40:C:H5'	2.02	0.41
1:A:178:SER:C	1:A:180:LYS:H	2.28	0.41
1:A:110:LEU:HD22	2:C:36:A:C4	2.56	0.40
1:B:213:ARG:O	1:B:217:ARG:CG	2.56	0.40
2:D:23:A:H2'	2:D:24:G:H8	1.83	0.40
1:A:28:ILE:HD12	1:A:28:ILE:O	2.21	0.40
1:A:29:GLU:O	1:A:32:LYS:HB2	2.21	0.40
1:B:140:GLN:CG	1:B:143:GLU:HB2	2.50	0.40
2:C:73:A:C2'	2:C:74:C:C5'	3.00	0.40
1:B:147:ARG:O	1:B:150:GLN:N	2.52	0.40
1:B:137:ALA:O	1:B:139:GLU:O	2.40	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:329:HOH:O	4:D:86:HOH:O[1_565]	2.14	0.06
4:A:329:HOH:O	4:D:97:HOH:O[1_565]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/316 (96%)	294 (97%)	7 (2%)	3 (1%)	12	17
1	B	303/316 (96%)	284 (94%)	12 (4%)	7 (2%)	5	4
All	All	607/632 (96%)	578 (95%)	19 (3%)	10 (2%)	7	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	LYS
1	B	237	GLY
1	B	132	ARG
1	B	133	ILE
1	B	142	TRP
1	A	298	GLU
1	B	140	GLN
1	A	300	PRO
1	B	300	PRO
1	B	310	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	
1	A	249/248 (100%)	207 (83%)	42 (17%)	2	2
1	B	249/248 (100%)	194 (78%)	55 (22%)	1	1
All	All	498/496 (100%)	401 (80%)	97 (20%)	1	1

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	11	LYS
1	A	15	LEU
1	A	19	THR
1	A	23	LYS
1	A	26	LEU
1	A	28	ILE
1	A	30	LEU
1	A	31	ARG
1	A	33	ILE
1	A	52	ILE
1	A	63	LEU
1	A	77	GLN
1	A	89	LEU
1	A	96	THR
1	A	104	LEU
1	A	105	VAL
1	A	109	MSE
1	A	119	LEU
1	A	120	SER
1	A	129	VAL
1	A	152	VAL
1	A	168	LEU
1	A	172	LEU
1	A	180	LYS
1	A	181	THR
1	A	185	LEU
1	A	193	LEU
1	A	208	GLU
1	A	210	LEU
1	A	213	ARG
1	A	216	GLN
1	A	217	ARG
1	A	239	LEU
1	A	243	LEU
1	A	256	SER
1	A	267	MSE
1	A	278	LEU
1	A	286	LEU
1	A	300	PRO
1	A	302	GLN
1	A	308	LEU

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Mol	Chain	Res	Type
1	B	9	LEU
1	B	11	LYS
1	B	13	ILE
1	B	24	THR
1	B	28	ILE
1	B	31	ARG
1	B	32	LYS
1	B	33	ILE
1	B	34	LEU
1	B	38	LEU
1	B	41	VAL
1	B	46	ILE
1	B	62	LEU
1	B	63	LEU
1	B	77	GLN
1	B	89	LEU
1	B	101	ILE
1	B	104	LEU
1	B	105	VAL
1	B	110	LEU
1	B	128	GLU
1	B	129	VAL
1	B	130	ARG
1	B	133	ILE
1	B	134	GLU
1	B	135	GLN
1	B	136	GLN
1	B	139	GLU
1	B	140	GLN
1	B	143	GLU
1	B	147	ARG
1	B	155	VAL
1	B	160	ILE
1	B	163	ASN
1	B	168	LEU
1	B	178	SER
1	B	181	THR
1	B	182	LEU
1	B	185	LEU
1	B	186	THR
1	B	188	THR
1	B	193	LEU

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Mol	Chain	Res	Type
1	B	196	GLN
1	B	209	LEU
1	B	217	ARG
1	B	233	LEU
1	B	236	ARG
1	B	239	LEU
1	B	262	ILE
1	B	267	MSE
1	B	278	LEU
1	B	298	GLU
1	B	301	GLU
1	B	309	GLN
1	B	311	VAL

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

Mol	Chain	Res	Type
1	A	77	GLN
1	A	150	GLN
1	A	161	HIS
1	A	163	ASN
1	A	196	GLN
1	A	198	HIS
1	A	212	GLN
1	A	216	GLN
1	A	220	GLN
1	A	302	GLN
1	B	136	GLN
1	B	161	HIS
1	B	166	GLN
1	B	196	GLN
1	B	211	HIS
1	B	216	GLN
1	B	220	GLN
1	B	277	GLN
1	B	302	GLN
1	B	309	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	73/76 (96%)	29 (39%)	16 (21%)
2	D	68/76 (89%)	22 (32%)	10 (14%)
All	All	141/152 (92%)	51 (36%)	26 (18%)

All (51) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	C
2	C	6	G
2	C	7	A
2	C	10	G
2	C	11	C
2	C	14	A
2	C	17	C
2	C	18	G
2	C	19	G
2	C	22	G
2	C	23	A
2	C	33	U
2	C	34	G
2	C	36	A
2	C	37	A
2	C	38	A
2	C	44	G
2	C	45	U
2	C	46	G
2	C	47	U
2	C	48	C
2	C	49	C
2	C	58	A
2	C	59	U
2	C	61	C
2	C	64	A
2	C	65	G
2	C	70	G
2	C	74	C
2	D	8	U
2	D	9	A
2	D	10	G
2	D	12	U
2	D	17	C
2	D	20	U
2	D	22	G

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Mol	Chain	Res	Type
2	D	27	G
2	D	31	A
2	D	33	U
2	D	34	G
2	D	35	A
2	D	36	A
2	D	37	A
2	D	38	A
2	D	41	C
2	D	42	C
2	D	44	G
2	D	45	U
2	D	47	U
2	D	49	C
2	D	61	C

All (26) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	6	G
2	C	7	A
2	C	9	A
2	C	18	G
2	C	22	G
2	C	32	U
2	C	33	U
2	C	35	A
2	C	37	A
2	C	44	G
2	C	45	U
2	C	46	G
2	C	48	C
2	C	58	A
2	C	60	U
2	C	64	A
2	D	9	A
2	D	19	G
2	D	32	U
2	D	33	U
2	D	34	G
2	D	35	A
2	D	36	A

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Mol	Chain	Res	Type
2	D	37	A
2	D	41	C
2	D	44	G

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/316 (94%)	0.05	6 (2%) 65 65	29, 49, 70, 95	0
1	B	298/316 (94%)	0.30	12 (4%) 42 43	37, 57, 95, 98	0
2	C	74/76 (97%)	-0.24	1 (1%) 73 74	34, 49, 69, 91	0
2	D	69/76 (90%)	1.16	11 (15%) 5 4	46, 88, 98, 98	0
All	All	740/784 (94%)	0.23	30 (4%) 41 42	29, 53, 97, 98	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	44	G	4.1
1	B	311	VAL	3.8
1	B	168	LEU	3.6
1	B	150	GLN	3.5
2	D	18	G	3.1
2	D	69	G	3.0
2	D	60	U	3.0
1	B	134	GLU	2.9
2	D	46	G	2.8
1	A	303	ALA	2.8
1	B	8	SER	2.7
1	B	149	LEU	2.7
1	A	9	LEU	2.7
1	A	301	GLU	2.6
2	D	4	C	2.6
2	D	20	U	2.6
2	D	19	G	2.5
1	B	177	ILE	2.4
2	D	45	U	2.3
1	A	298	GLU	2.3
1	B	141	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	288	GLY	2.2
2	D	68	C	2.2
1	B	310	VAL	2.1
2	C	47	U	2.1
1	B	142	TRP	2.1
1	B	151	GLU	2.1
1	A	299	LYS	2.1
1	B	145	LEU	2.0
2	D	59	U	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	MG	C	81	1/1	0.81	0.23	35,35,35,35	0
3	MG	C	78	1/1	0.88	0.26	33,33,33,33	0
3	MG	D	77	1/1	0.89	0.16	41,41,41,41	0
3	MG	C	80	1/1	0.91	0.33	45,45,45,45	0
3	MG	C	79	1/1	0.93	0.18	31,31,31,31	0
3	MG	C	82	1/1	0.93	0.19	49,49,49,49	0
3	MG	C	77	1/1	0.93	0.14	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.