



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 11:43 PM GMT

PDB ID : 2ZZN
Title : The complex structure of aTrm5 and tRNACys
Authors : Goto-Ito, S.; Ito, T.; Yokoyama, S.
Deposited on : 2009-02-19
Resolution : 2.95 Å(reported)

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

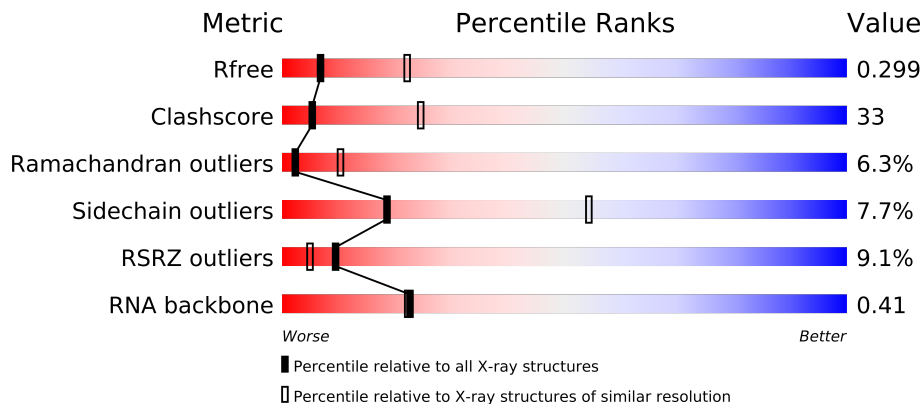
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.95 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}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)
RNA backbone	1838	1019 (3.46-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	
2	C	75	
2	D	75	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SAM	B	402	-	X
4	MG	C	101	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	MG	C	102	-	X
4	MG	C	103	-	X
4	MG	C	105	-	X
4	MG	D	201	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8606 atoms, of which 0 are hydrogen and 0 are deuterium.

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

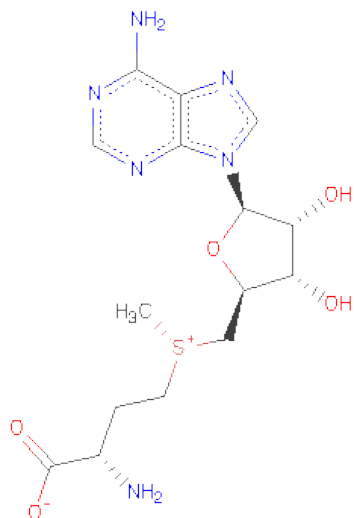
- Molecule 1 is a protein called Uncharacterized protein MJ0883.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2747	1774	470	494	9			
1	B	335	Total	C	N	O	S	0	0	0
			2739	1769	469	493	8			

- Molecule 2 is a RNA chain called RNA (71-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	71	Total	C	N	O	P	0	0	0
			1517	675	273	498	71			
2	D	71	Total	C	N	O	P	0	0	0
			1517	675	273	498	71			

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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

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

- Molecule 5 is water.

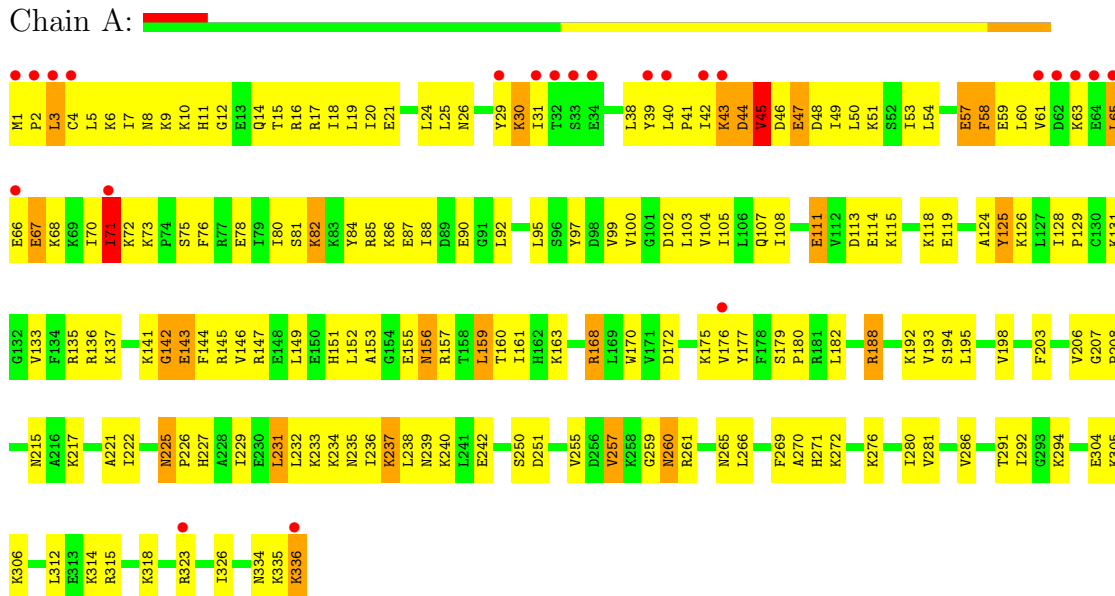
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	5	Total	O	0	0
			5	5		
5	C	6	Total	O	0	0
			6	6		
5	D	3	Total	O	0	0
			3	3		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

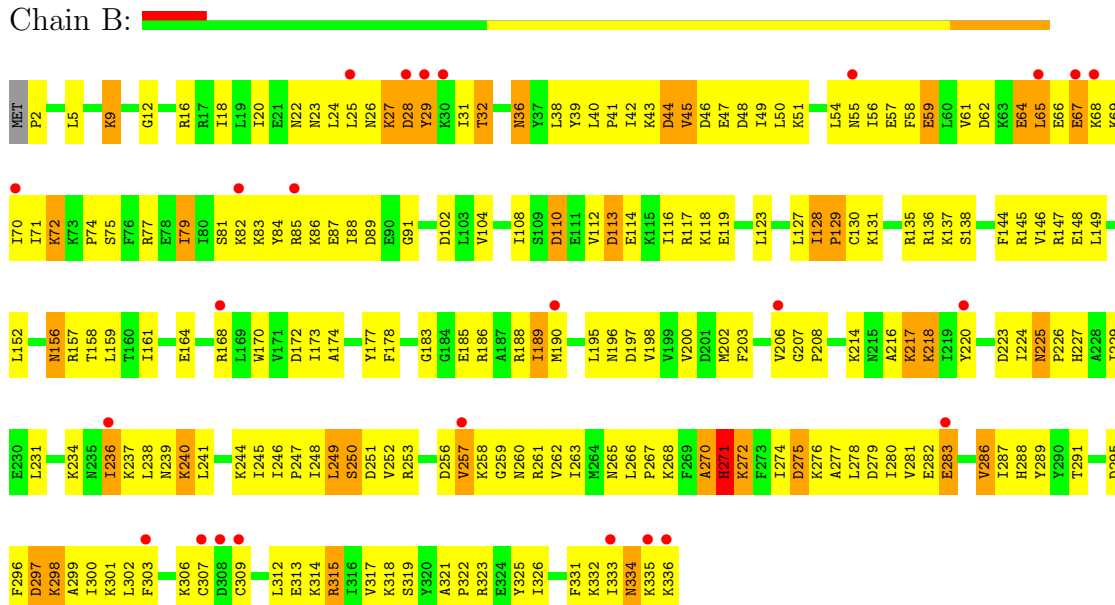
• Molecule 1: Uncharacterized protein MJ0883

Chain A:

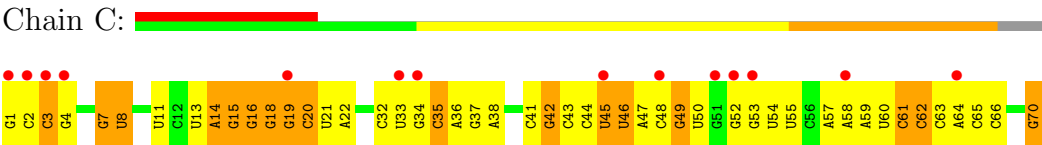


• Molecule 1: Uncharacterized protein MJ0883

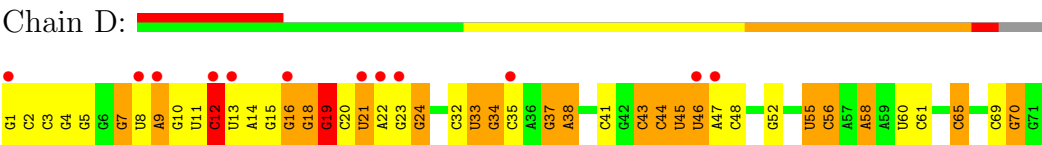
Chain B:



● Molecule 2: RNA (71-MER)



● Molecule 2: RNA (71-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.84Å 106.54Å 134.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.69 – 2.95 46.69 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.69-2.95) 99.2 (46.69-2.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.226 , 0.295 0.227 , 0.299	Depositor DCC
R_{free} test set	1303 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25578 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8606	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.47	0/2790	0.71	0/3737
1	B	0.41	0/2782	0.65	0/3726
2	C	0.55	1/1694 (0.1%)	0.79	0/2638
2	D	0.54	1/1694 (0.1%)	0.79	3/2638 (0.1%)
All	All	0.48	2/8960 (0.0%)	0.73	3/12739 (0.0%)

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	0	2
2	D	0	2
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	G	OP3-P	-6.92	1.52	1.61
2	C	1	G	OP3-P	-6.42	1.53	1.61

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	19	G	N9-C1'-C2'	8.02	124.43	114.00
2	D	7	G	N9-C1'-C2'	6.43	122.36	114.00
2	D	12	C	C5'-C4'-O4'	-5.10	102.97	109.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	11	U	Sidechain
2	C	15	G	Sidechain
2	D	19	G	Sidechain
2	D	52	G	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2747	0	2905	205	0
1	B	2739	0	2894	222	0
2	C	1517	0	770	55	0
2	D	1517	0	770	59	0
3	A	27	0	22	5	0
3	B	27	0	22	8	0
4	C	6	0	0	0	0
4	D	1	0	0	0	0
5	A	11	0	0	0	0
5	B	5	0	0	2	0
5	C	6	0	0	0	0
5	D	3	0	0	0	0
All	All	8606	0	7383	522	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 33.

All (522) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:23:G:H2'	2:D:24:G:H5''	1.30	1.13
1:A:50:LEU:HD23	1:A:53:ILE:HD11	1.38	1.01
1:A:71:ILE:HG12	1:A:72:LYS:H	1.22	1.01
1:B:135:ARG:HB2	1:B:152:LEU:HD11	1.50	0.93
1:A:198:VAL:H	1:A:260:ASN:HD21	1.17	0.91
1:A:44:ASP:O	1:A:45:VAL:HG13	1.72	0.89
1:A:88:ILE:HD11	1:A:95:LEU:HD21	1.52	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:27:LYS:HE2	1:B:71:ILE:HD13	1.52	0.89
1:A:85:ARG:HH11	1:A:85:ARG:HG3	1.38	0.89
1:B:198:VAL:HB	1:B:260:ASN:H	1.38	0.86
2:D:55:U:H5'	2:D:56:C:OP2	1.75	0.86
1:A:234:LYS:O	1:A:237:LYS:HD3	1.75	0.86
2:C:42:G:H5'	2:C:42:G:H8	1.44	0.83
1:B:36:ASN:N	1:B:36:ASN:HD22	1.77	0.83
1:A:71:ILE:HD13	1:A:71:ILE:H	1.44	0.82
1:B:248:ILE:HG22	1:B:249:LEU:H	1.44	0.82
1:B:298:LYS:HE2	1:B:298:LYS:HA	1.60	0.82
2:D:34:G:H5'	2:D:35:C:OP2	1.79	0.82
2:C:41:C:H2'	2:C:42:G:H5''	1.62	0.81
2:D:23:G:C2'	2:D:24:G:H5''	2.10	0.80
1:A:163:LYS:HE2	1:A:168:ARG:HD3	1.64	0.80
2:C:41:C:C2'	2:C:42:G:H5''	2.11	0.80
1:A:115:LYS:O	1:A:119:GLU:HG2	1.82	0.80
1:B:118:LYS:HE2	1:B:152:LEU:O	1.82	0.79
1:B:307:CYS:HA	1:B:336:LYS:HD2	1.65	0.79
1:B:186:ARG:NE	1:B:208:PRO:HB2	1.98	0.78
1:B:177:TYR:HD2	3:B:402:SAM:HB1	1.48	0.78
1:A:294:LYS:NZ	2:C:34:G:H21	1.82	0.78
1:A:294:LYS:HZ1	2:C:34:G:H21	1.32	0.77
1:B:281:VAL:HG11	1:B:333:ILE:HG13	1.65	0.77
1:A:163:LYS:HD2	2:C:13:U:OP1	1.85	0.77
2:D:20:C:H3'	2:D:21:U:H5''	1.68	0.75
2:D:60:U:H5''	2:D:61:C:H5	1.50	0.75
2:D:11:U:H2'	2:D:12:C:H5''	1.70	0.74
2:D:45:U:H2'	2:D:46:U:H1'	1.68	0.74
1:A:168:ARG:NH1	1:A:238:LEU:HD11	2.03	0.74
1:B:49:ILE:HG13	1:B:50:LEU:N	2.02	0.73
1:A:188:ARG:HH21	1:A:315:ARG:HE	1.36	0.73
2:D:34:G:H2'	2:D:34:G:N3	2.03	0.73
1:B:197:ASP:HA	1:B:260:ASN:HD22	1.52	0.73
1:B:323:ARG:H	2:D:32:C:N4	1.86	0.73
1:B:158:THR:O	1:B:172:ASP:HA	1.88	0.73
1:A:45:VAL:HB	1:A:49:ILE:HD11	1.71	0.72
1:B:29:TYR:HE1	1:B:65:LEU:HB3	1.53	0.72
1:B:61:VAL:HG12	1:B:62:ASP:N	2.05	0.72
1:A:159:LEU:HD13	1:A:160:THR:H	1.51	0.72
1:A:318:LYS:HD3	1:A:326:ILE:HD12	1.70	0.72
1:B:246:ILE:HG22	1:B:248:ILE:HD11	1.72	0.72
1:A:135:ARG:HB2	1:A:152:LEU:HD11	1.69	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:218:LYS:HE3	1:B:218:LYS:HA	1.70	0.72
1:A:16:ARG:O	1:A:20:ILE:HG22	1.90	0.71
1:A:143:GLU:HG2	1:A:144:PHE:CD1	2.24	0.71
1:A:225:ASN:ND2	1:A:227:HIS:H	1.88	0.71
1:B:70:ILE:O	1:B:70:ILE:HG13	1.91	0.71
1:B:104:VAL:HG11	1:B:128:ILE:HD11	1.71	0.71
1:A:72:LYS:HG3	1:A:73:LYS:O	1.91	0.70
1:B:186:ARG:HD3	1:B:208:PRO:O	1.90	0.70
1:B:217:LYS:H	1:B:217:LYS:HD3	1.57	0.70
1:A:335:LYS:O	1:A:336:LYS:HB2	1.91	0.70
2:D:69:C:H5'	2:D:70:G:OP2	1.92	0.70
1:A:198:VAL:H	1:A:260:ASN:ND2	1.88	0.70
1:B:177:TYR:CD2	3:B:402:SAM:HB1	2.27	0.69
1:A:179:SER:HB3	1:A:182:LEU:HD12	1.73	0.69
1:A:6:LYS:HD3	1:A:61:VAL:HG21	1.74	0.69
1:A:265:ASN:ND2	3:A:401:SAM:N	2.39	0.69
1:B:9:LYS:HA	1:B:38:LEU:HB2	1.74	0.69
1:A:71:ILE:HG12	1:A:72:LYS:N	2.02	0.69
1:B:20:ILE:HD11	1:B:25:LEU:HD23	1.74	0.69
2:C:34:G:C8	2:C:34:G:H3'	2.28	0.68
1:B:16:ARG:CZ	2:D:19:G:O2'	2.42	0.68
1:A:71:ILE:CD1	1:A:71:ILE:H	2.06	0.68
2:C:62:C:H6	2:C:62:C:H5'	1.58	0.68
1:B:271:HIS:CD2	1:B:272:LYS:H	2.11	0.68
1:B:189:ILE:HD12	1:B:189:ILE:H	1.59	0.68
1:B:287:ILE:HG23	1:B:331:PHE:HB2	1.76	0.67
2:C:61:C:H2'	2:C:62:C:H5'	1.76	0.67
1:B:315:ARG:HD3	1:B:315:ARG:N	2.10	0.67
2:D:46:U:H2'	2:D:46:U:O2	1.94	0.67
1:A:260:ASN:H	1:A:260:ASN:HD22	1.43	0.67
1:A:71:ILE:CG1	1:A:72:LYS:H	2.05	0.66
1:A:159:LEU:HD13	1:A:160:THR:N	2.11	0.66
1:B:295:ASP:OD1	1:B:297:ASP:HB2	1.95	0.66
2:C:63:C:O2'	2:C:64:A:H5'	1.95	0.66
2:C:34:G:H8	2:C:34:G:H3'	1.61	0.66
1:A:4:CYS:CB	1:A:41:PRO:HA	2.26	0.66
1:B:202:MET:HB3	1:B:252:VAL:HG21	1.78	0.66
1:B:271:HIS:HD2	1:B:272:LYS:H	1.42	0.65
1:B:186:ARG:HE	1:B:208:PRO:HB2	1.58	0.65
1:A:85:ARG:NH1	1:A:85:ARG:HG3	2.10	0.65
1:B:274:ILE:HG21	1:B:306:LYS:HD2	1.78	0.65
1:A:168:ARG:HH12	1:A:238:LEU:HD11	1.62	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:38:LEU:HD12	1:B:40:LEU:HG	1.79	0.65
2:D:55:U:H6	2:D:55:U:H5''	1.61	0.65
2:C:41:C:H2'	2:C:42:G:C5'	2.26	0.65
1:B:253:ARG:NH1	2:C:44:C:H4'	2.12	0.65
1:B:189:ILE:O	1:B:189:ILE:HG22	1.96	0.65
1:B:312:LEU:HD11	1:B:332:LYS:HB2	1.77	0.65
1:A:142:GLY:HA2	1:A:145:ARG:HH11	1.60	0.64
2:D:3:C:H2'	2:D:4:G:H8	1.61	0.64
1:B:196:ASN:HA	1:B:217:LYS:HE3	1.80	0.64
1:A:125:TYR:HD2	1:A:125:TYR:O	1.81	0.64
1:A:229:ILE:CG2	1:A:233:LYS:HE3	2.26	0.64
1:A:71:ILE:N	1:A:71:ILE:HD13	2.11	0.64
1:A:276:LYS:O	1:A:280:ILE:HG13	1.97	0.64
1:A:141:LYS:O	1:A:142:GLY:O	2.14	0.64
1:B:61:VAL:HG12	1:B:62:ASP:H	1.63	0.64
1:B:26:ASN:HB3	1:B:41:PRO:HB2	1.79	0.64
1:B:46:ASP:HB2	1:B:48:ASP:OD2	1.97	0.64
1:A:114:GLU:N	1:A:114:GLU:OE1	2.23	0.63
1:B:198:VAL:HB	1:B:260:ASN:N	2.10	0.63
1:A:49:ILE:O	1:A:53:ILE:HG12	1.99	0.63
1:A:159:LEU:HD11	1:A:170:TRP:HE3	1.62	0.62
1:B:271:HIS:HA	1:B:274:ILE:HG13	1.81	0.62
1:B:206:VAL:HG22	1:B:208:PRO:HD3	1.80	0.62
2:D:11:U:C2'	2:D:12:C:H5''	2.29	0.62
2:D:45:U:H2'	2:D:46:U:C1'	2.28	0.62
1:A:42:ILE:HG12	1:A:43:LYS:N	2.14	0.62
1:A:47:GLU:HB3	1:A:60:LEU:HD11	1.81	0.62
1:A:102:ASP:C	1:A:103:LEU:HD23	2.20	0.62
1:B:159:LEU:HD11	1:B:170:TRP:CZ3	2.34	0.62
1:B:188:ARG:C	1:B:190:MET:H	2.03	0.62
1:A:143:GLU:HG2	1:A:144:PHE:HD1	1.63	0.61
1:B:164:GLU:OE2	1:B:186:ARG:HD2	2.00	0.61
1:A:81:SER:HA	1:A:88:ILE:HD12	1.82	0.61
2:D:20:C:H2'	2:D:21:U:C6	2.36	0.61
1:A:198:VAL:N	1:A:260:ASN:HD21	1.95	0.61
2:D:14:A:O2'	2:D:15:G:H5'	2.01	0.61
1:A:159:LEU:HD11	1:A:170:TRP:CE3	2.36	0.61
1:A:323:ARG:NH1	2:C:33:U:OP2	2.33	0.61
1:A:208:PRO:HG3	3:A:401:SAM:OXT	2.01	0.60
1:B:240:LYS:O	1:B:241:LEU:HG	2.01	0.60
2:C:61:C:O2'	2:C:62:C:H5''	2.01	0.60
1:A:260:ASN:ND2	1:A:260:ASN:H	1.99	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:75:SER:HB2	1:A:78:GLU:HB2	1.82	0.60
1:B:178:PHE:HA	3:B:402:SAM:OXT	2.01	0.60
1:B:261:ARG:NH2	1:B:286:VAL:HG21	2.16	0.60
1:A:131:LYS:HG2	1:A:155:GLU:OE2	2.00	0.60
1:A:6:LYS:CD	1:A:61:VAL:HG21	2.31	0.60
1:A:7:ILE:HD13	1:A:15:THR:HG21	1.83	0.60
1:B:75:SER:O	1:B:79:ILE:HG23	2.02	0.59
1:B:322:PRO:HA	2:D:32:C:N3	2.17	0.59
2:C:61:C:H2'	2:C:62:C:C5'	2.33	0.59
1:A:4:CYS:HB3	1:A:41:PRO:HA	1.83	0.59
1:B:170:TRP:HB3	1:B:231:LEU:HD12	1.84	0.59
1:A:238:LEU:HD12	1:A:238:LEU:O	2.02	0.59
1:A:142:GLY:HA2	1:A:145:ARG:NH1	2.17	0.59
1:B:218:LYS:HD3	1:B:220:TYR:CE1	2.37	0.58
1:A:114:GLU:O	1:A:118:LYS:HG2	2.02	0.58
2:C:13:U:H2'	2:C:14:A:H5''	1.85	0.58
1:B:258:LYS:HB3	1:B:282:GLU:CG	2.32	0.58
1:B:336:LYS:HE3	1:B:336:LYS:HA	1.85	0.58
2:C:35:C:H4'	2:C:36:A:OP2	2.03	0.58
1:B:38:LEU:HD13	1:B:39:TYR:N	2.19	0.58
1:B:256:ASP:O	1:B:257:VAL:HG13	2.04	0.58
1:A:3:LEU:HD11	1:A:60:LEU:HD13	1.84	0.58
1:A:88:ILE:CD1	1:A:95:LEU:HD21	2.31	0.58
1:B:306:LYS:O	1:B:336:LYS:HG2	2.03	0.58
2:C:52:G:O2'	2:C:53:G:H5'	2.02	0.58
1:A:250:SER:OG	1:A:251:ASP:N	2.37	0.57
2:D:21:U:C2'	2:D:21:U:O2	2.53	0.57
1:A:104:VAL:CG2	1:A:133:VAL:HG22	2.34	0.57
1:A:126:LYS:NZ	1:A:126:LYS:HB2	2.20	0.57
2:C:65:C:O2'	2:C:66:C:H5'	2.05	0.57
1:B:146:VAL:HG12	1:B:147:ARG:N	2.18	0.57
1:A:1:MET:H2	1:A:26:ASN:HD22	1.53	0.57
1:A:42:ILE:CD1	1:A:50:LEU:HD21	2.35	0.56
1:A:145:ARG:O	1:A:177:TYR:HB2	2.05	0.56
1:B:26:ASN:O	1:B:28:ASP:N	2.38	0.56
1:B:307:CYS:HA	1:B:336:LYS:CD	2.35	0.56
2:C:46:U:C2'	2:C:47:A:OP2	2.53	0.56
2:C:2:C:C2'	2:C:3:C:H5''	2.35	0.56
1:B:77:ARG:NH2	2:D:41:C:OP2	2.39	0.56
2:C:42:G:H5'	2:C:42:G:C8	2.32	0.56
1:B:246:ILE:HG22	1:B:248:ILE:CD1	2.35	0.56
2:D:12:C:H2'	2:D:13:U:O4'	2.06	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:GLN:CG	1:A:136:ARG:HD2	2.36	0.56
2:C:46:U:H2'	2:C:47:A:OP2	2.06	0.55
1:A:107:GLN:HG2	1:A:136:ARG:HD2	1.88	0.55
1:A:147:ARG:O	1:A:149:LEU:HD13	2.06	0.55
1:A:156:ASN:O	1:A:156:ASN:ND2	2.39	0.55
1:A:44:ASP:C	1:A:45:VAL:HG22	2.26	0.55
1:A:161:ILE:HD11	1:A:170:TRP:CZ2	2.42	0.55
1:B:88:ILE:O	1:B:91:GLY:N	2.36	0.55
2:C:34:G:C8	2:C:34:G:C3'	2.90	0.55
1:B:218:LYS:HD3	1:B:220:TYR:HE1	1.72	0.55
1:A:259:GLY:O	1:A:281:VAL:HA	2.06	0.55
1:B:198:VAL:HB	1:B:259:GLY:CA	2.36	0.55
1:A:30:LYS:CD	1:A:31:ILE:H	2.20	0.55
1:B:267:PRO:HA	1:B:291:THR:HA	1.88	0.55
2:C:2:C:H2'	2:C:3:C:C5'	2.37	0.54
1:A:42:ILE:HD11	1:A:50:LEU:HD21	1.90	0.54
1:A:125:TYR:CD2	1:A:125:TYR:O	2.59	0.54
1:A:46:ASP:C	1:A:48:ASP:H	2.11	0.54
2:C:59:A:O2'	2:C:60:U:H5'	2.07	0.54
1:B:58:PHE:C	1:B:59:GLU:HG3	2.27	0.54
2:C:61:C:C2'	2:C:62:C:H5''	2.38	0.54
1:B:336:LYS:OXT	1:B:336:LYS:HG3	2.08	0.54
2:C:61:C:C2'	2:C:62:C:C5'	2.87	0.53
2:C:3:C:H5'	2:C:3:C:H6	1.72	0.53
1:A:136:ARG:HG2	1:A:147:ARG:HD3	1.89	0.53
1:A:312:LEU:HD22	1:B:110:ASP:OD2	2.08	0.53
1:B:44:ASP:O	1:B:45:VAL:HB	2.09	0.53
1:A:104:VAL:HG22	1:A:133:VAL:HG22	1.89	0.53
1:A:232:LEU:O	1:A:236:ILE:HG13	2.08	0.53
1:B:321:ALA:HB1	1:B:322:PRO:CD	2.39	0.53
1:B:81:SER:HA	1:B:88:ILE:HD12	1.90	0.53
1:B:188:ARG:O	1:B:190:MET:N	2.41	0.53
2:D:9:A:OP1	2:D:9:A:H4'	2.08	0.53
1:B:198:VAL:HB	1:B:259:GLY:HA2	1.90	0.53
1:A:237:LYS:HZ2	1:A:238:LEU:HB2	1.74	0.53
2:D:20:C:H3'	2:D:21:U:C5'	2.38	0.53
1:A:65:LEU:HD13	1:A:65:LEU:O	2.08	0.53
1:A:188:ARG:NH2	1:A:315:ARG:HE	2.04	0.53
1:B:61:VAL:CG1	1:B:62:ASP:N	2.71	0.53
1:B:189:ILE:N	1:B:189:ILE:HD12	2.22	0.53
1:A:104:VAL:C	1:A:105:ILE:HG13	2.28	0.53
1:B:335:LYS:O	1:B:336:LYS:HB2	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:318:LYS:HE2	1:B:326:ILE:HD12	1.91	0.52
1:A:237:LYS:NZ	1:A:238:LEU:HB2	2.23	0.52
2:C:2:C:O2'	2:C:3:C:H5''	2.09	0.52
2:C:16:G:OP2	2:C:16:G:H8	1.92	0.52
1:B:77:ARG:HH22	2:D:41:C:P	2.33	0.52
1:B:61:VAL:CG1	1:B:62:ASP:H	2.23	0.52
1:B:79:ILE:HD11	1:B:123:LEU:HD13	1.92	0.52
2:D:21:U:H2'	2:D:21:U:O2	2.09	0.51
2:D:2:C:O2'	2:D:3:C:H5'	2.10	0.51
1:B:136:ARG:HG2	1:B:147:ARG:HD3	1.92	0.51
1:A:84:TYR:HB3	1:A:87:GLU:HG2	1.92	0.51
1:A:4:CYS:HA	1:A:42:ILE:HG22	1.91	0.51
1:A:45:VAL:CB	1:A:49:ILE:HD11	2.39	0.51
1:A:82:LYS:NZ	1:A:85:ARG:HH21	2.09	0.51
1:B:250:SER:O	1:B:251:ASP:C	2.49	0.51
2:D:33:U:O2	2:D:34:G:N7	2.43	0.51
2:D:15:G:H2'	2:D:16:G:H5'	1.91	0.51
1:B:319:SER:HA	1:B:325:TYR:HD1	1.76	0.51
1:B:258:LYS:HB3	1:B:282:GLU:HG3	1.93	0.51
2:D:15:G:C2'	2:D:16:G:H5'	2.41	0.51
1:A:42:ILE:HG12	1:A:43:LYS:H	1.77	0.50
1:A:104:VAL:HG22	1:A:133:VAL:HA	1.93	0.50
1:B:42:ILE:HG12	1:B:43:LYS:N	2.25	0.50
1:A:172:ASP:O	1:A:176:VAL:HG22	2.11	0.50
1:A:17:ARG:O	1:A:21:GLU:HB2	2.11	0.50
1:A:24:LEU:O	1:A:42:ILE:HG13	2.11	0.50
1:A:17:ARG:NH2	1:B:336:LYS:HE2	2.26	0.50
1:B:2:PRO:HG3	1:B:65:LEU:HD12	1.92	0.50
1:A:86:LYS:O	1:A:90:GLU:HG3	2.11	0.50
1:A:100:VAL:HG22	1:A:180:PRO:HD3	1.92	0.50
1:A:59:GLU:HG2	1:A:60:LEU:H	1.76	0.50
1:B:217:LYS:H	1:B:217:LYS:CD	2.24	0.50
1:A:47:GLU:HA	1:A:50:LEU:HB2	1.92	0.50
1:B:206:VAL:CG2	1:B:208:PRO:HD3	2.40	0.50
1:B:265:ASN:ND2	3:B:402:SAM:N	2.60	0.50
1:B:200:VAL:HG13	1:B:220:TYR:HB2	1.93	0.50
1:A:334:ASN:O	1:A:335:LYS:HB3	2.11	0.50
1:A:260:ASN:N	1:A:260:ASN:HD22	2.01	0.50
1:B:271:HIS:HA	1:B:274:ILE:CD1	2.41	0.50
1:B:26:ASN:OD1	1:B:28:ASP:HB2	2.12	0.50
1:A:57:GLU:OE1	1:A:57:GLU:N	2.45	0.50
1:A:225:ASN:HD22	1:A:226:PRO:CD	2.25	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:2:C:H2'	2:C:3:C:H5'	1.94	0.49
1:A:84:TYR:HB3	1:A:87:GLU:CG	2.42	0.49
1:B:113:ASP:OD2	1:B:113:ASP:N	2.36	0.49
1:B:36:ASN:N	1:B:36:ASN:ND2	2.49	0.49
2:D:13:U:O2'	2:D:14:A:H5'	2.12	0.49
1:B:177:TYR:CD2	1:B:177:TYR:C	2.86	0.49
1:A:84:TYR:O	1:A:87:GLU:HG2	2.11	0.49
1:B:276:LYS:O	1:B:280:ILE:HG13	2.12	0.49
1:B:137:LYS:HB3	1:B:148:GLU:C	2.32	0.49
1:B:258:LYS:HE2	1:B:279:ASP:O	2.13	0.49
1:A:146:VAL:CG1	1:A:147:ARG:N	2.75	0.49
1:A:30:LYS:HD2	1:A:31:ILE:H	1.77	0.49
1:A:76:PHE:CE1	1:A:124:ALA:HB2	2.48	0.49
1:B:138:SER:HB3	1:B:148:GLU:OE1	2.12	0.49
1:B:146:VAL:CG1	1:B:147:ARG:N	2.75	0.49
1:A:314:LYS:O	1:A:314:LYS:HG3	2.12	0.49
2:D:46:U:C2'	2:D:46:U:O2	2.59	0.49
1:B:298:LYS:HZ1	1:B:301:LYS:HD3	1.78	0.49
2:D:33:U:O2'	2:D:34:G:O5'	2.30	0.49
1:B:81:SER:C	1:B:83:LYS:H	2.16	0.49
2:D:65:C:O2	2:D:65:C:H2'	2.13	0.49
1:B:79:ILE:HG12	1:B:127:LEU:HD11	1.93	0.48
1:A:99:VAL:HG23	1:A:99:VAL:O	2.12	0.48
2:D:60:U:C5'	2:D:61:C:H5	2.22	0.48
1:B:188:ARG:HB3	1:B:188:ARG:CZ	2.42	0.48
1:A:4:CYS:HB2	1:A:40:LEU:O	2.13	0.48
1:A:45:VAL:O	1:A:46:ASP:C	2.51	0.48
1:B:223:ASP:HA	3:B:402:SAM:N3	2.28	0.48
2:C:46:U:O2	2:C:46:U:H2'	2.13	0.48
1:A:70:ILE:O	1:A:70:ILE:HG23	2.13	0.48
1:A:222:ILE:HD13	1:A:255:VAL:HG21	1.96	0.48
2:D:33:U:O2'	2:D:34:G:C5'	2.62	0.48
1:A:44:ASP:O	1:A:45:VAL:CG1	2.55	0.48
1:B:113:ASP:OD2	1:B:116:ILE:HD12	2.14	0.48
1:B:229:ILE:HG13	1:B:249:LEU:HG	1.95	0.48
2:C:3:C:H2'	2:C:4:G:O4'	2.13	0.48
1:B:47:GLU:O	1:B:51:LYS:HG3	2.13	0.48
1:B:112:VAL:HG23	1:B:117:ARG:CG	2.44	0.48
1:A:234:LYS:HA	1:A:237:LYS:HD2	1.95	0.48
1:B:218:LYS:CE	1:B:218:LYS:HA	2.39	0.48
1:A:225:ASN:ND2	1:A:225:ASN:C	2.67	0.48
1:A:82:LYS:HZ1	1:A:85:ARG:HH21	1.62	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:GLU:O	1:A:67:GLU:O	2.32	0.48
1:A:19:LEU:HD12	1:A:40:LEU:HD23	1.95	0.48
1:A:144:PHE:N	1:A:144:PHE:CD1	2.82	0.48
1:A:157:ARG:O	1:A:157:ARG:HG3	2.13	0.48
2:D:3:C:C2	2:D:4:G:C8	3.02	0.47
1:A:40:LEU:N	1:A:40:LEU:HD12	2.29	0.47
1:A:26:ASN:HD21	1:A:29:TYR:HE2	1.61	0.47
1:A:255:VAL:HG12	1:A:257:VAL:HG22	1.96	0.47
1:A:304:GLU:C	1:A:306:LYS:H	2.17	0.47
1:B:84:TYR:HD1	1:B:87:GLU:OE1	1.96	0.47
1:B:144:PHE:O	1:B:145:ARG:HB2	2.14	0.47
1:A:225:ASN:HD22	1:A:226:PRO:N	2.11	0.47
2:C:46:U:O4'	2:C:46:U:P	2.72	0.47
1:A:47:GLU:O	1:A:51:LYS:HG3	2.14	0.47
1:A:2:PRO:HB3	1:A:63:LYS:O	2.15	0.47
1:A:3:LEU:HD23	1:A:44:ASP:OD1	2.14	0.47
1:B:59:GLU:O	1:B:61:VAL:HG23	2.13	0.47
1:A:6:LYS:HD3	1:A:61:VAL:CG2	2.43	0.47
1:B:261:ARG:HH22	1:B:286:VAL:HG21	1.80	0.47
1:B:31:ILE:HG22	1:B:32:THR:N	2.29	0.47
1:A:115:LYS:HD2	1:A:115:LYS:HA	1.78	0.47
1:B:218:LYS:CA	1:B:218:LYS:HE3	2.43	0.47
1:B:275:ASP:O	1:B:278:LEU:N	2.48	0.47
1:A:99:VAL:HG12	1:A:104:VAL:HG12	1.97	0.47
1:A:1:MET:N	1:A:26:ASN:HD22	2.13	0.47
1:B:22:ASN:HD22	1:B:22:ASN:N	2.13	0.47
1:A:5:LEU:HD11	1:A:58:PHE:CD2	2.51	0.46
1:B:29:TYR:CE1	1:B:65:LEU:HB3	2.41	0.46
1:B:18:ILE:C	1:B:20:ILE:H	2.18	0.46
1:B:258:LYS:HG2	1:B:280:ILE:O	2.15	0.46
1:A:25:LEU:HD12	1:A:41:PRO:O	2.16	0.46
1:B:189:ILE:H	1:B:189:ILE:CD1	2.28	0.46
1:A:291:THR:OG1	1:A:292:ILE:N	2.48	0.46
1:B:16:ARG:NE	2:D:19:G:O2'	2.48	0.46
1:B:262:VAL:O	1:B:288:HIS:N	2.47	0.46
1:B:45:VAL:HG21	1:B:49:ILE:HD11	1.97	0.46
1:A:144:PHE:N	1:A:144:PHE:HD1	2.13	0.46
2:D:12:C:O2'	2:D:13:U:H5'	2.15	0.46
1:A:229:ILE:HG22	1:A:233:LYS:HE3	1.97	0.46
1:A:68:LYS:NZ	2:C:20:C:H42	2.13	0.46
1:B:271:HIS:HA	1:B:274:ILE:CG1	2.44	0.46
1:A:151:HIS:HE1	1:A:155:GLU:O	1.99	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111:GLU:OE1	1:A:111:GLU:N	2.49	0.46
1:A:240:LYS:HA	1:A:242:GLU:OE1	2.16	0.46
1:A:188:ARG:HH21	1:A:315:ARG:NE	2.10	0.46
1:B:81:SER:O	1:B:85:ARG:HD3	2.16	0.46
1:B:271:HIS:CD2	1:B:272:LYS:N	2.80	0.45
1:B:183:GLY:HA2	1:B:186:ARG:HH11	1.80	0.45
1:B:217:LYS:HG2	1:B:218:LYS:H	1.80	0.45
1:A:146:VAL:HG12	1:A:147:ARG:N	2.31	0.45
2:C:45:U:H4'	2:C:45:U:OP1	2.15	0.45
1:B:69:LYS:HD2	1:B:70:ILE:N	2.31	0.45
1:B:313:GLU:HG2	1:B:314:LYS:N	2.32	0.45
1:A:135:ARG:NH2	1:A:137:LYS:HD3	2.31	0.45
1:B:128:ILE:HA	1:B:129:PRO:HD3	1.80	0.45
1:B:104:VAL:HG13	1:B:130:CYS:HB3	1.97	0.45
1:B:258:LYS:HB3	1:B:282:GLU:HG2	1.98	0.45
2:C:7:G:H4'	2:C:8:U:OP2	2.17	0.45
1:A:221:ALA:HB1	1:A:232:LEU:HD21	1.98	0.45
1:A:103:LEU:HD23	1:A:103:LEU:N	2.32	0.45
1:B:227:HIS:O	1:B:231:LEU:HD23	2.16	0.45
1:B:149:LEU:HD12	1:B:174:ALA:HB2	1.98	0.45
1:A:175:LYS:HD2	1:A:227:HIS:CD2	2.52	0.45
1:B:25:LEU:HD12	1:B:41:PRO:O	2.16	0.45
1:A:206:VAL:O	1:A:235:ASN:ND2	2.50	0.45
1:B:258:LYS:HG2	1:B:280:ILE:HA	1.98	0.45
1:A:225:ASN:C	1:A:225:ASN:HD22	2.19	0.45
1:B:296:PHE:O	1:B:299:ALA:HB3	2.17	0.45
1:B:270:ALA:O	1:B:272:LYS:N	2.50	0.45
1:A:203:PHE:HB3	3:A:401:SAM:O4'	2.17	0.45
1:B:297:ASP:O	1:B:300:ILE:N	2.49	0.45
1:B:275:ASP:O	1:B:276:LYS:C	2.54	0.45
2:D:43:C:H5''	2:D:44:C:OP2	2.16	0.45
1:B:274:ILE:HD11	1:B:302:LEU:HD13	1.99	0.45
1:A:159:LEU:CD1	1:A:160:THR:N	2.78	0.45
1:A:235:ASN:O	1:A:239:ASN:ND2	2.40	0.45
1:B:207:GLY:N	1:B:208:PRO:CD	2.80	0.45
2:D:3:C:H2'	2:D:4:G:C8	2.48	0.45
2:C:8:U:O2	2:C:47:A:H2	2.00	0.45
1:A:39:TYR:N	1:A:39:TYR:CD1	2.85	0.45
1:A:2:PRO:O	1:A:4:CYS:N	2.49	0.44
1:A:323:ARG:NH2	2:C:32:C:OP2	2.50	0.44
1:A:151:HIS:CE1	1:A:153:ALA:O	2.70	0.44
2:C:2:C:C2'	2:C:3:C:C5'	2.94	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:18:G:H21	2:D:58:A:H5'	1.81	0.44
2:D:11:U:H2'	2:D:11:U:O2	2.16	0.44
1:B:188:ARG:C	1:B:190:MET:N	2.69	0.44
2:C:4:G:C2	2:C:70:G:C2	3.05	0.44
1:A:115:LYS:HE3	1:A:119:GLU:CD	2.38	0.44
1:B:265:ASN:HD21	3:B:402:SAM:HB2	1.82	0.44
2:D:21:U:OP1	2:D:21:U:C4'	2.66	0.44
1:A:269:PHE:HD1	1:A:272:LYS:HZ1	1.63	0.44
1:B:2:PRO:O	1:B:62:ASP:HA	2.17	0.44
1:B:65:LEU:N	1:B:65:LEU:HD22	2.32	0.44
1:B:104:VAL:CG1	1:B:128:ILE:HD11	2.42	0.44
1:A:82:LYS:HD2	1:A:82:LYS:N	2.32	0.44
1:A:16:ARG:CZ	2:C:19:G:O2'	2.66	0.44
1:B:66:GLU:O	1:B:67:GLU:O	2.36	0.44
2:C:13:U:C2'	2:C:14:A:H5''	2.46	0.44
3:B:402:SAM:HE1	2:D:37:G:H1	1.83	0.44
1:B:286:VAL:HG11	1:B:312:LEU:HD22	2.00	0.44
1:B:137:LYS:HB3	1:B:148:GLU:O	2.18	0.44
2:D:20:C:C2'	2:D:21:U:C6	3.01	0.44
1:B:217:LYS:O	1:B:244:LYS:HG3	2.17	0.44
1:B:104:VAL:HG13	1:B:130:CYS:CB	2.47	0.44
1:B:159:LEU:HD11	1:B:170:TRP:HZ3	1.79	0.44
1:B:312:LEU:HD12	1:B:312:LEU:N	2.33	0.44
1:A:85:ARG:NH1	1:A:85:ARG:CG	2.77	0.43
1:B:283:GLU:HA	1:B:333:ILE:O	2.18	0.43
1:A:47:GLU:HB3	1:A:60:LEU:CD1	2.48	0.43
2:D:60:U:H3'	2:D:61:C:C6	2.53	0.43
1:B:317:VAL:O	1:B:318:LYS:HB3	2.18	0.43
1:B:22:ASN:CB	1:B:24:LEU:HD13	2.48	0.43
1:A:193:VAL:HG12	1:A:194:SER:N	2.34	0.43
2:C:49:G:H2'	2:C:50:U:C6	2.53	0.43
1:B:195:LEU:HD22	1:B:195:LEU:H	1.83	0.43
1:B:112:VAL:HG23	1:B:117:ARG:HG3	2.01	0.43
1:B:203:PHE:N	5:B:601:HOH:O	2.43	0.43
1:B:9:LYS:HG2	1:B:36:ASN:C	2.39	0.43
1:A:17:ARG:HH22	1:B:336:LYS:CE	2.31	0.43
2:D:21:U:OP1	2:D:21:U:H4'	2.19	0.43
1:A:225:ASN:HD22	1:A:226:PRO:HD2	1.83	0.43
1:B:286:VAL:HA	1:B:331:PHE:O	2.19	0.43
1:B:280:ILE:HG22	1:B:280:ILE:O	2.19	0.43
1:A:8:ASN:O	1:A:9:LYS:C	2.56	0.43
1:B:102:ASP:OD1	1:B:157:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:270:ALA:HB1	1:B:289:TYR:CE2	2.54	0.43
1:B:23:ASN:HB2	5:B:604:HOH:O	2.18	0.43
1:B:168:ARG:O	1:B:239:ASN:ND2	2.52	0.43
1:A:59:GLU:HG2	1:A:60:LEU:N	2.33	0.43
1:B:71:ILE:O	1:B:72:LYS:O	2.37	0.43
1:B:249:LEU:O	1:B:250:SER:HB2	2.18	0.43
1:B:274:ILE:O	1:B:277:ALA:HB3	2.18	0.43
1:B:68:LYS:HG3	1:B:69:LYS:N	2.33	0.43
1:A:125:TYR:CD2	1:A:125:TYR:C	2.92	0.43
2:C:2:C:H2'	2:C:3:C:H5''	1.97	0.43
1:B:64:GLU:HG3	1:B:65:LEU:N	2.34	0.43
1:B:74:PRO:HB2	1:B:79:ILE:HG22	2.01	0.43
1:B:112:VAL:CG2	1:B:117:ARG:HG2	2.48	0.43
1:A:4:CYS:HB2	1:A:41:PRO:HA	1.99	0.42
1:A:42:ILE:HD13	1:A:50:LEU:HD11	2.00	0.42
2:D:11:U:C3'	2:D:12:C:H5''	2.49	0.42
1:B:240:LYS:C	1:B:241:LEU:HG	2.40	0.42
2:C:54:U:C5	2:C:55:U:C5	3.07	0.42
1:B:214:LYS:C	1:B:216:ALA:H	2.21	0.42
1:B:236:ILE:CG2	1:B:245:ILE:HB	2.48	0.42
1:B:27:LYS:HG2	1:B:27:LYS:O	2.19	0.42
1:B:303:PHE:O	1:B:309:CYS:SG	2.77	0.42
1:A:168:ARG:HB2	1:A:168:ARG:HH11	1.84	0.42
1:A:294:LYS:NZ	2:C:34:G:N2	2.60	0.42
2:D:60:U:H3'	2:D:61:C:H6	1.83	0.42
1:B:65:LEU:H	1:B:65:LEU:HD22	1.85	0.42
2:D:56:C:H6	2:D:56:C:O5'	2.02	0.42
1:A:163:LYS:HG2	1:A:168:ARG:HD3	2.01	0.42
1:A:108:ILE:HB	1:A:135:ARG:HD2	2.01	0.42
1:A:97:TYR:CZ	1:A:128:ILE:HD13	2.54	0.42
2:D:34:G:C2'	2:D:34:G:N3	2.78	0.42
1:B:183:GLY:HA2	1:B:186:ARG:NH1	2.35	0.42
1:B:297:ASP:O	1:B:299:ALA:N	2.53	0.42
1:A:30:LYS:HD3	1:A:31:ILE:H	1.85	0.42
1:A:266:LEU:O	1:A:270:ALA:HB2	2.19	0.42
1:B:283:GLU:HB3	1:B:334:ASN:O	2.20	0.42
1:B:18:ILE:C	1:B:20:ILE:N	2.72	0.42
2:C:20:C:H5'	2:C:21:U:C5	2.55	0.42
2:C:15:G:H22	2:C:48:C:H42	1.67	0.42
1:A:63:LYS:HE2	1:A:63:LYS:HB2	1.88	0.42
3:A:401:SAM:CE	2:C:37:G:H1	2.33	0.42
1:B:185:GLU:O	1:B:188:ARG:HB2	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:LYS:HB2	1:A:131:LYS:HE2	1.61	0.42
1:B:319:SER:HA	1:B:325:TYR:CD1	2.54	0.42
1:A:58:PHE:CD2	1:A:59:GLU:N	2.87	0.42
1:B:280:ILE:O	1:B:280:ILE:CG2	2.68	0.42
1:A:144:PHE:CE2	1:A:226:PRO:HD2	2.54	0.42
1:A:90:GLU:HB2	1:A:92:LEU:HG	2.02	0.41
1:A:242:GLU:CD	1:A:242:GLU:H	2.23	0.41
1:B:224:ILE:HG23	1:B:225:ASN:N	2.34	0.41
1:A:14:GLN:O	1:A:18:ILE:HG13	2.19	0.41
1:B:46:ASP:C	1:B:48:ASP:H	2.23	0.41
1:B:263:ILE:HA	1:B:288:HIS:HB2	2.01	0.41
1:A:54:LEU:HD12	1:A:54:LEU:C	2.40	0.41
1:A:72:LYS:HG3	1:A:73:LYS:N	2.35	0.41
1:B:251:ASP:OD1	1:B:253:ARG:HG3	2.19	0.41
1:B:195:LEU:CD2	1:B:195:LEU:H	2.32	0.41
1:A:260:ASN:HD22	1:A:261:ARG:N	2.18	0.41
1:B:248:ILE:HG22	1:B:249:LEU:N	2.22	0.41
1:B:54:LEU:C	1:B:56:ILE:H	2.23	0.41
1:A:195:LEU:HA	1:A:215:ASN:O	2.20	0.41
2:C:42:G:O2'	2:C:43:C:H5'	2.21	0.41
2:D:45:U:C2'	2:D:46:U:H1'	2.45	0.41
3:B:402:SAM:CE	2:D:37:G:H1	2.34	0.41
1:A:102:ASP:O	1:A:103:LEU:HD23	2.19	0.41
1:B:159:LEU:HD13	1:B:159:LEU:C	2.41	0.41
1:A:156:ASN:HD22	1:A:156:ASN:C	2.24	0.41
1:B:225:ASN:HD22	1:B:226:PRO:CD	2.34	0.41
2:D:20:C:O2'	2:D:21:U:H6	2.03	0.41
1:A:7:ILE:HG22	1:A:58:PHE:HB3	2.03	0.41
1:B:246:ILE:HA	1:B:247:PRO:HD2	1.87	0.41
1:A:135:ARG:NH2	1:A:137:LYS:CD	2.84	0.41
1:B:195:LEU:O	1:B:217:LYS:HD3	2.21	0.41
1:A:80:ILE:HG23	1:A:84:TYR:HD2	1.86	0.41
1:B:237:LYS:CG	1:B:238:LEU:N	2.83	0.41
1:B:108:ILE:HB	1:B:135:ARG:HD2	2.03	0.41
1:B:22:ASN:O	1:B:24:LEU:CD1	2.69	0.40
2:C:18:G:HO2'	2:C:57:A:H2	1.68	0.40
1:A:54:LEU:HD11	1:A:58:PHE:CE1	2.56	0.40
1:B:5:LEU:HD11	1:B:58:PHE:HB2	2.02	0.40
1:B:267:PRO:O	1:B:291:THR:HA	2.21	0.40
2:D:43:C:H3'	2:D:44:C:C6	2.56	0.40
1:A:170:TRP:HB3	1:A:231:LEU:CD1	2.51	0.40
1:B:136:ARG:NH2	2:D:38:A:OP1	2.54	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:234:LYS:HE2	1:B:234:LYS:HB3	1.85	0.40
2:C:41:C:C2'	2:C:42:G:C5'	2.91	0.40
1:B:251:ASP:C	1:B:253:ARG:N	2.74	0.40
1:A:207:GLY:N	1:A:208:PRO:CD	2.84	0.40
1:B:46:ASP:C	1:B:48:ASP:N	2.75	0.40
1:B:161:ILE:HG21	1:B:168:ARG:CZ	2.52	0.40
1:B:225:ASN:HD22	1:B:226:PRO:HD2	1.86	0.40
1:B:119:GLU:HA	1:B:119:GLU:OE1	2.21	0.40
1:B:156:ASN:C	1:B:156:ASN:HD22	2.25	0.40
1:A:265:ASN:HD22	3:A:401:SAM:HN1	1.59	0.40
2:D:3:C:O5'	2:D:3:C:H6	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	334/336 (99%)	289 (86%)	30 (9%)	15 (4%)	4	20
1	B	333/336 (99%)	259 (78%)	47 (14%)	27 (8%)	1	6
All	All	667/672 (99%)	548 (82%)	77 (12%)	42 (6%)	2	10

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	67	GLU
1	A	142	GLY
1	B	27	LYS
1	B	45	VAL
1	B	67	GLU
1	B	72	LYS
1	B	189	ILE
1	B	270	ALA

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Mol	Chain	Res	Type
1	B	271	HIS
1	B	283	GLU
1	B	297	ASP
1	A	3	LEU
1	A	71	ILE
1	B	28	ASP
1	B	29	TYR
1	B	268	LYS
1	B	275	ASP
1	A	10	LYS
1	A	217	LYS
1	B	64	GLU
1	A	43	LYS
1	A	47	GLU
1	A	58	PHE
1	A	143	GLU
1	A	305	LYS
1	B	173	ILE
1	B	240	LYS
1	B	249	LEU
1	B	250	SER
1	A	44	ASP
1	B	9	LYS
1	B	55	ASN
1	B	86	LYS
1	B	272	LYS
1	B	298	LYS
1	B	89	ASP
1	B	12	GLY
1	B	266	LEU
1	A	129	PRO
1	B	129	PRO
1	A	12	GLY

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	305/305 (100%)	281 (92%)	24 (8%)	18	52
1	B	304/305 (100%)	281 (92%)	23 (8%)	19	55
All	All	609/610 (100%)	562 (92%)	47 (8%)	18	54

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	HIS
1	A	30	LYS
1	A	38	LEU
1	A	45	VAL
1	A	57	GLU
1	A	65	LEU
1	A	71	ILE
1	A	82	LYS
1	A	111	GLU
1	A	113	ASP
1	A	125	TYR
1	A	156	ASN
1	A	159	LEU
1	A	168	ARG
1	A	188	ARG
1	A	192	LYS
1	A	225	ASN
1	A	231	LEU
1	A	237	LYS
1	A	257	VAL
1	A	260	ASN
1	A	271	HIS
1	A	286	VAL
1	A	336	LYS
1	B	32	THR
1	B	36	ASN
1	B	44	ASP
1	B	57	GLU
1	B	59	GLU
1	B	65	LEU
1	B	79	ILE
1	B	82	LYS
1	B	110	ASP
1	B	113	ASP
1	B	114	GLU

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Mol	Chain	Res	Type
1	B	128	ILE
1	B	131	LYS
1	B	156	ASN
1	B	217	LYS
1	B	218	LYS
1	B	225	ASN
1	B	236	ILE
1	B	257	VAL
1	B	271	HIS
1	B	286	VAL
1	B	315	ARG
1	B	334	ASN

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

Mol	Chain	Res	Type
1	A	23	ASN
1	A	151	HIS
1	A	156	ASN
1	A	215	ASN
1	A	225	ASN
1	A	260	ASN
1	A	265	ASN
1	A	271	HIS
1	A	334	ASN
1	B	22	ASN
1	B	36	ASN
1	B	55	ASN
1	B	107	GLN
1	B	151	HIS
1	B	156	ASN
1	B	215	ASN
1	B	225	ASN
1	B	260	ASN
1	B	265	ASN
1	B	271	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	70/75 (93%)	18 (25%)	2 (2%)
2	D	70/75 (93%)	25 (35%)	3 (4%)
All	All	140/150 (93%)	43 (30%)	5 (3%)

All (43) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	3	C
2	C	7	G
2	C	8	U
2	C	14	A
2	C	16	G
2	C	18	G
2	C	20	C
2	C	22	A
2	C	35	C
2	C	38	A
2	C	42	G
2	C	45	U
2	C	46	U
2	C	49	G
2	C	58	A
2	C	61	C
2	C	62	C
2	C	70	G
2	D	5	G
2	D	8	U
2	D	9	A
2	D	10	G
2	D	12	C
2	D	16	G
2	D	18	G
2	D	19	G
2	D	21	U
2	D	22	A
2	D	24	G
2	D	34	G
2	D	37	G
2	D	38	A
2	D	43	C
2	D	44	C
2	D	45	U
2	D	46	U

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Mol	Chain	Res	Type
2	D	47	A
2	D	48	C
2	D	55	U
2	D	56	C
2	D	58	A
2	D	65	C
2	D	70	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	7	G
2	C	19	G
2	D	7	G
2	D	19	G
2	D	33	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SAM	A	401	-	26,29,29	1.07	1 (3%)	38,42,42	2.23	10 (26%)
3	SAM	B	402	-	26,29,29	1.12	2 (7%)	38,42,42	2.23	9 (23%)

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
3	SAM	A	401	-	-	0/13/33/33	0/1/3/3
3	SAM	B	402	-	-	0/13/33/33	0/1/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	SAM	CG-CB	3.47	1.56	1.52
3	A	401	SAM	CG-CB	3.32	1.56	1.52
3	B	402	SAM	C8-N7	-2.03	1.30	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	SAM	N3-C2-N1	-8.89	121.28	128.71
3	B	402	SAM	N3-C2-N1	-8.83	121.33	128.71
3	B	402	SAM	N3-C4-N9	5.17	134.77	125.43
3	A	401	SAM	N3-C4-N9	4.80	134.10	125.43
3	A	401	SAM	CG-CB-CA	3.56	117.46	112.22
3	B	402	SAM	CG-CB-CA	3.35	117.15	112.22
3	B	402	SAM	CB-CG-SD	-3.34	105.22	112.49
3	A	401	SAM	CB-CG-SD	-3.23	105.46	112.49
3	A	401	SAM	CB-CA-C	-3.23	106.57	111.44
3	B	402	SAM	C5'-SD-CG	2.86	111.64	102.90
3	B	402	SAM	C5-C4-N3	-2.83	119.54	125.70
3	A	401	SAM	C5-C4-N3	-2.59	120.07	125.70
3	B	402	SAM	C2-N3-C4	2.54	121.25	114.01
3	B	402	SAM	C4-C5-N7	-2.50	107.38	109.52
3	B	402	SAM	C3'-C2'-C1'	2.48	104.79	100.91
3	A	401	SAM	C2-N3-C4	2.34	120.69	114.01
3	A	401	SAM	C5'-SD-CG	2.34	110.05	102.90
3	A	401	SAM	C4-C5-N7	-2.23	107.61	109.52
3	A	401	SAM	C5'-C4'-C3'	-2.08	111.43	116.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/336 (100%)	0.32	23 (6%) 17 9	29, 55, 100, 124	0
1	B	335/336 (99%)	0.41	25 (7%) 14 7	48, 79, 108, 121	0
2	C	71/75 (94%)	1.30	15 (21%) 1 1	35, 77, 110, 123	0
2	D	71/75 (94%)	1.11	12 (16%) 2 2	49, 73, 119, 133	0
All	All	813/822 (98%)	0.51	75 (9%) 9 4	29, 68, 108, 133	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	12.9
1	A	65	LEU	9.3
1	A	3	LEU	6.4
1	A	64	GLU	5.8
1	B	70	ILE	5.8
1	B	336	LYS	5.3
1	A	2	PRO	5.2
2	D	22	A	5.1
2	C	33	U	5.1
1	A	29	TYR	5.0
1	A	39	TYR	5.0
1	B	206	VAL	4.7
2	C	34	G	4.7
1	A	336	LYS	4.7
1	B	29	TYR	4.5
1	B	67	GLU	4.4
1	A	62	ASP	4.2
1	B	257	VAL	4.1
2	D	46	U	4.1
2	C	52	G	3.8
2	D	16	G	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	8	U	3.8
2	C	3	C	3.7
2	C	2	C	3.7
1	B	335	LYS	3.6
2	C	45	U	3.6
2	D	9	A	3.5
1	B	55	ASN	3.4
1	B	65	LEU	3.4
2	D	13	U	3.4
1	B	28	ASP	3.3
1	B	283	GLU	3.3
2	C	1	G	3.3
1	B	303	PHE	3.3
2	D	47	A	3.3
1	B	168	ARG	3.3
1	B	333	ILE	3.2
1	B	308	ASP	3.2
1	A	71	ILE	3.2
2	C	48	C	3.2
1	B	85	ARG	3.0
1	A	323	ARG	3.0
2	D	21	U	3.0
1	B	309	CYS	2.9
2	D	23	G	2.9
1	A	66	GLU	2.9
1	A	61	VAL	2.8
1	A	32	THR	2.7
1	A	63	LYS	2.7
1	B	30	LYS	2.6
2	D	12	C	2.6
1	A	33	SER	2.5
1	B	82	LYS	2.5
2	D	1	G	2.5
1	B	307	CYS	2.4
2	C	51	G	2.4
2	C	72	C	2.4
2	C	58	A	2.3
2	D	35	C	2.3
1	A	4	CYS	2.2
1	B	190	MET	2.2
1	A	40	LEU	2.2
1	A	34	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	19	G	2.2
1	A	42	ILE	2.1
2	C	64	A	2.1
1	B	68	LYS	2.1
1	B	25	LEU	2.1
1	A	43	LYS	2.1
1	B	220	TYR	2.1
1	A	31	ILE	2.1
1	B	236	ILE	2.1
2	C	53	G	2.1
2	C	4	G	2.0
1	A	176	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	MG	C	105	1/1	0.53	11.91	61,61,61,61	0
4	MG	C	102	1/1	0.36	9.04	52,52,52,52	0
4	MG	C	103	1/1	0.27	7.33	48,48,48,48	0
4	MG	C	101	1/1	0.43	6.07	66,66,66,66	0
3	SAM	B	402	27/27	0.38	4.57	78,84,86,86	0
4	MG	D	201	1/1	0.21	3.01	58,58,58,58	0
4	MG	C	106	1/1	0.30	1.45	53,53,53,53	0
3	SAM	A	401	27/27	0.27	1.08	42,49,68,72	0
4	MG	C	104	1/1	0.24	0.41	59,59,59,59	0

6.5 Other polymers ⓘ

There are no such residues in this entry.