



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:06 am BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

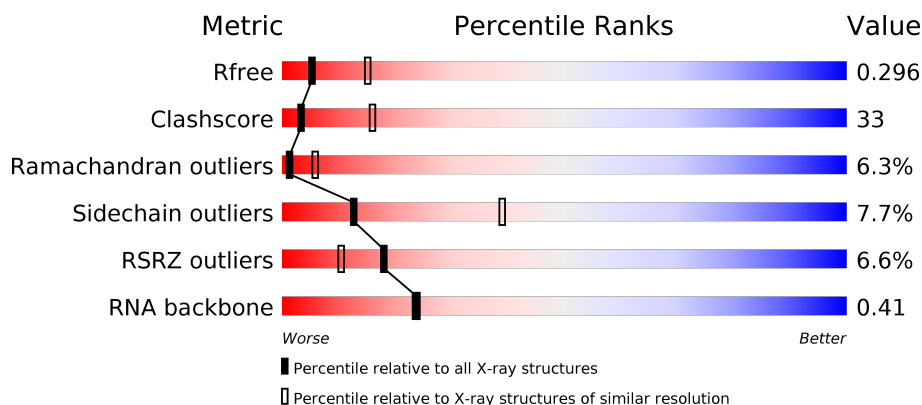
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	<div> <div>5%</div> <div>46%</div> <div>47%</div> <div>7%</div> </div>
1	B	336	<div> <div>6%</div> <div>38%</div> <div>51%</div> <div>11%</div> </div>
2	C	75	<div> <div>12%</div> <div>31%</div> <div>41%</div> <div>23%</div> <div>5%</div> </div>
2	D	75	<div> <div>11%</div> <div>36%</div> <div>31%</div> <div>25%</div> <div>5%</div> </div>

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
4	MG	C	102	-	-	-	X



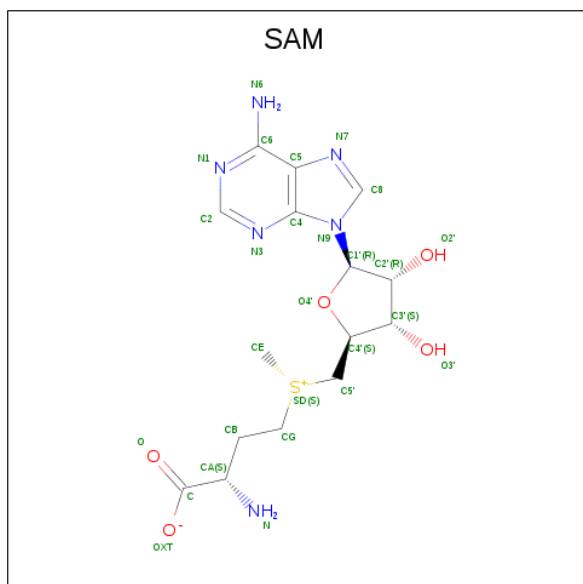
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ).



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		

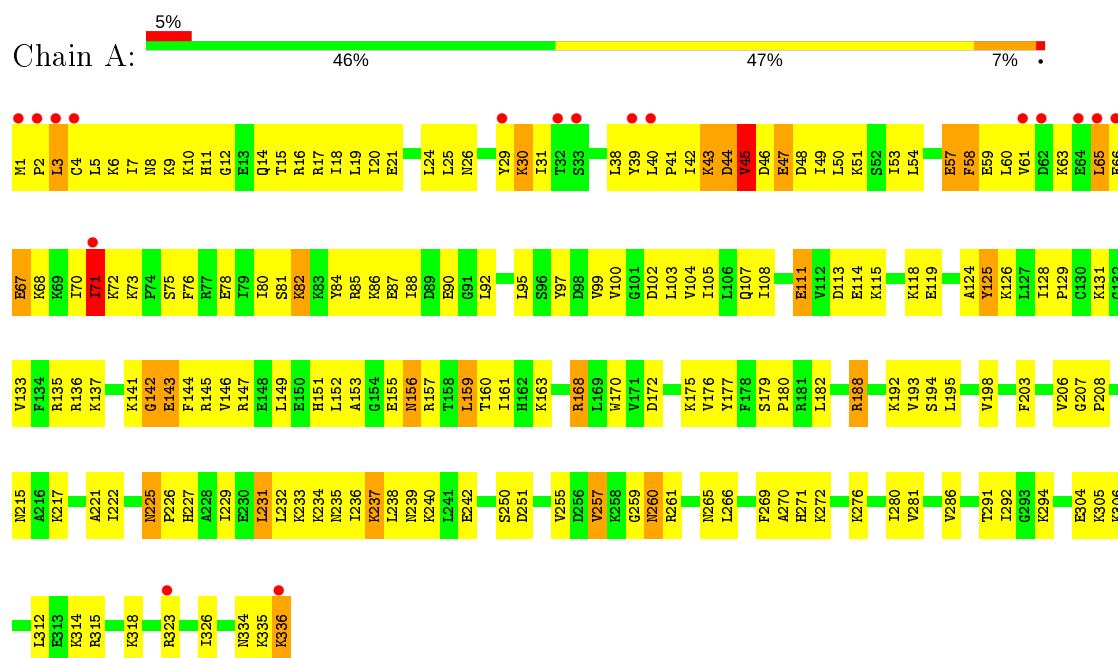
- Molecule 5 is water.

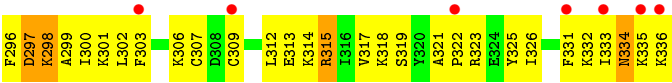
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	5	Total	O	0	0
			5	5		
5	C	6	Total	O	0	0
			6	6		
5	D	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

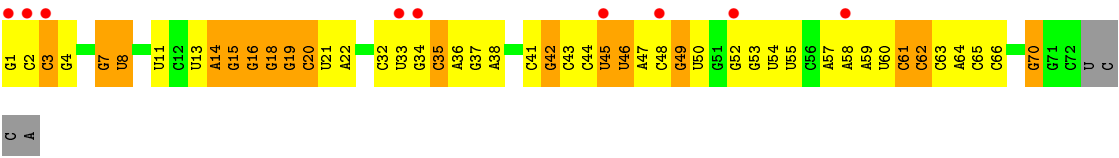
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Uncharacterized protein MJ0883

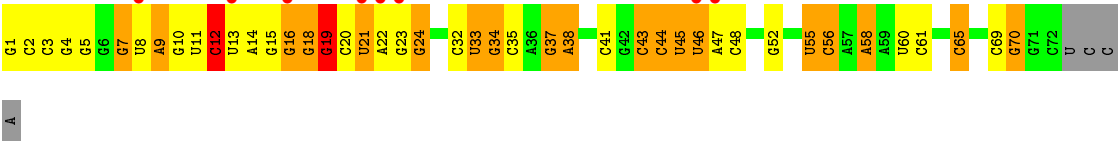




● Molecule 2: RNA (71-MER)



● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 2.96Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.226 , 0.295 0.223 , 0.296	Depositor DCC
$R_{free}$ test set	1303 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 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 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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

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 33.

All (522) 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)
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ILE:HD11	1:A:95:LEU:HD21	1.52	0.89
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:158:THR:O	1:B:172:ASP:HA	1.88	0.73
1:B:323:ARG:H	2:D:32:C:N4	1.86	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:A:159:LEU:HD13	1:A:160:THR:H	1.51	0.72
1:B:61:VAL:HG12	1:B:62:ASP:N	2.05	0.72
1:A:318:LYS:HD3	1:A:326:ILE:HD12	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HB2	1:A:152:LEU:HD11	1.69	0.72
1:B:246:ILE:HG22	1:B:248:ILE:HD11	1.72	0.72
1:B:218:LYS:HE3	1:B:218:LYS:HA	1.70	0.72
1:A:143:GLU:HG2	1:A:144:PHE:CD1	2.24	0.71
1:A:16:ARG:O	1:A:20:ILE:HG22	1.90	0.71
1:A:225:ASN:ND2	1:A:227:HIS:H	1.88	0.71
1:B:104:VAL:HG11	1:B:128:ILE:HD11	1.71	0.71
1:B:70:ILE:O	1:B:70:ILE:HG13	1.91	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:A:179:SER:HB3	1:A:182:LEU:HD12	1.73	0.69
1:B:177:TYR:CD2	3:B:402:SAM:HB1	2.27	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
1:B:16:ARG:CZ	2:D:19:G:O2'	2.42	0.68
2:C:34:G:C8	2:C:34:G:H3'	2.28	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:N	1:B:315:ARG:HD3	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:186:ARG:HE	1:B:208:PRO:HB2	1.58	0.65
1:B:271:HIS:HD2	1:B:272:LYS:H	1.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:38:LEU:HD12	1:B:40:LEU:HG	1.79	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
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
2:D:55:U:H6	2:D:55:U:H5''	1.61	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: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:B:196:ASN:HA	1:B:217:LYS:HE3	1.80	0.64
1:A:276:LYS:O	1:A:280:ILE:HG13	1.97	0.64
1:A:71:ILE:HD13	1:A:71:ILE:N	2.11	0.64
1:A:141:LYS:O	1:A:142:GLY:O	2.14	0.64
1:B:26:ASN:HB3	1:B:41:PRO:HB2	1.79	0.64
1:B:61:VAL:HG12	1:B:62:ASP:H	1.63	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:206:VAL:HG22	1:B:208:PRO:HD3	1.80	0.62
1:B:271:HIS:HA	1:B:274:ILE:HG13	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:131:LYS:HG2	1:A:155:GLU:OE2	2.00	0.60
1:B:261:ARG:NH2	1:B:286:VAL:HG21	2.16	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:142:GLY:HA2	1:A:145:ARG:NH1	2.17	0.59
1:A:238:LEU:HD12	1:A:238:LEU:O	2.02	0.59
1:A:114:GLU:O	1:A:118:LYS:HG2	2.02	0.58
1:B:218:LYS:HD3	1:B:220:TYR:CE1	2.37	0.58
1:B:258:LYS:HB3	1:B:282:GLU:CG	2.32	0.58
2:C:13:U:H2'	2:C:14:A:H5''	1.85	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:256:ASP:O	1:B:257:VAL:HG13	2.04	0.58
1:B:38:LEU:HD13	1:B:39:TYR:N	2.19	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
1:A:126:LYS:NZ	1:A:126:LYS:HB2	2.20	0.57
1:A:104:VAL:CG2	1:A:133:VAL:HG22	2.34	0.57
2:D:21:U:C2'	2:D:21:U:O2	2.53	0.57
1:A:1:MET:H2	1:A:26:ASN:HD22	1.53	0.57
1:B:146:VAL:HG12	1:B:147:ARG:N	2.18	0.57
2:C:65:C:O2'	2:C:66:C:H5'	2.05	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:2:C:C2'	2:C:3:C:H5''	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:46:U:C2'	2:C:47:A:OP2	2.53	0.56
1:B:77:ARG:NH2	2:D:41:C:OP2	2.39	0.56
1:B:246:ILE:HG22	1:B:248:ILE:CD1	2.35	0.56
2:C:42:G:H5'	2:C:42:G:C8	2.32	0.56
2:D:12:C:H2'	2:D:13:U:O4'	2.06	0.56
1:A:107:GLN:CG	1:A:136:ARG:HD2	2.36	0.56
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
2:C:46:U:H2'	2:C:47:A:OP2	2.06	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
1:A:259:GLY:O	1:A:281:VAL:HA	2.06	0.55
1:B:218:LYS:HD3	1:B:220:TYR:HE1	1.72	0.55
2:C:34:G:C8	2:C:34:G:C3'	2.90	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:125:TYR:CD2	1:A:125:TYR:O	2.59	0.54
1:A:42:ILE:HD11	1:A:50:LEU:HD21	1.90	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
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
2:C:3:C:H5'	2:C:3:C:H6	1.72	0.53
1:A:104:VAL:HG22	1:A:133:VAL:HG22	1.89	0.53
1:B:44:ASP:O	1:B:45:VAL:HB	2.09	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
1:A:65:LEU:HD13	1:A:65:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:C:H3'	2:D:21:U:C5'	2.38	0.53
1:A:104:VAL:C	1:A:105:ILE:HG13	2.28	0.53
1:A:188:ARG:NH2	1:A:315:ARG:HE	2.04	0.53
1:B:189:ILE:N	1:B:189:ILE:HD12	2.22	0.53
1:B:61:VAL:CG1	1:B:62:ASP:N	2.71	0.53
1:B:318:LYS:HE2	1:B:326:ILE:HD12	1.91	0.52
1:B:335:LYS:O	1:B:336:LYS:HB2	2.08	0.52
1:A:237:LYS:NZ	1:A:238:LEU:HB2	2.23	0.52
2:C:16:G:OP2	2:C:16:G:H8	1.92	0.52
2:C:2:C:O2'	2:C:3:C:H5''	2.09	0.52
1:B:77:ARG:HH22	2:D:41:C:P	2.33	0.52
1:B:79:ILE:HD11	1:B:123:LEU:HD13	1.92	0.52
1:B:61:VAL:CG1	1:B:62:ASP:H	2.23	0.52
1:A:84:TYR:HB3	1:A:87:GLU:HG2	1.92	0.51
1:B:136:ARG:HG2	1:B:147:ARG:HD3	1.92	0.51
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: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:104:VAL:HG22	1:A:133:VAL:HA	1.93	0.50
1:A:172:ASP:O	1:A:176:VAL:HG22	2.11	0.50
1:A:42:ILE:HG12	1:A:43:LYS:H	1.77	0.50
1:B:42:ILE:HG12	1:B:43:LYS:N	2.25	0.50
1:A:17:ARG:O	1:A:21:GLU:HB2	2.11	0.50
1:A:17:ARG:NH2	1:B:336:LYS:HE2	2.26	0.50
1:A:100:VAL:HG22	1:A:180:PRO:HD3	1.92	0.50
1:A:24:LEU:O	1:A:42:ILE:HG13	2.11	0.50
1:A:86:LYS:O	1:A:90:GLU:HG3	2.11	0.50
1:B:2:PRO:HG3	1:B:65:LEU:HD12	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:200:VAL:HG13	1:B:220:TYR:HB2	1.93	0.50
1:B:206:VAL:CG2	1:B:208:PRO:HD3	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ASN:ND2	3:B:402:SAM:N	2.60	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:A:57:GLU:OE1	1:A:57:GLU:N	2.45	0.50
1:B:26:ASN:OD1	1:B:28:ASP:HB2	2.12	0.50
1:A:225:ASN:HD22	1:A:226:PRO:CD	2.25	0.49
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:A:84:TYR:O	1:A:87:GLU:HG2	2.11	0.49
1:B:177:TYR:CD2	1:B:177:TYR:C	2.86	0.49
1:B:137:LYS:HB3	1:B:148:GLU:C	2.32	0.49
1:B:276:LYS:O	1:B:280:ILE:HG13	2.12	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:258:LYS:HE2	1:B:279:ASP:O	2.13	0.49
1:B:138:SER:HB3	1:B:148:GLU:OE1	2.12	0.49
1:A:314:LYS:HG3	1:A:314:LYS:O	2.12	0.49
1:B:146:VAL:CG1	1:B:147:ARG:N	2.75	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
1:B:81:SER:C	1:B:83:LYS:H	2.16	0.49
2:D:33:U:O2'	2:D:34:G:O5'	2.30	0.49
2:D:65:C:O2	2:D:65:C:H2'	2.13	0.49
1:A:99:VAL:HG23	1:A:99:VAL:O	2.12	0.48
1:B:79:ILE:HG12	1:B:127:LEU:HD11	1.93	0.48
1:B:188:ARG:HB3	1:B:188:ARG:CZ	2.42	0.48
2:D:60:U:C5'	2:D:61:C:H5	2.22	0.48
1:A:222:ILE:HD13	1:A:255:VAL:HG21	1.96	0.48
1:A:45:VAL:O	1:A:46:ASP:C	2.51	0.48
1:A:4:CYS:HB2	1:A:40:LEU:O	2.13	0.48
1:A:70:ILE:O	1:A:70:ILE:HG23	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:HG23	1:B:117:ARG:CG	2.44	0.48
1:B:229:ILE:HG13	1:B:249:LEU:HG	1.95	0.48
1:B:47:GLU:O	1:B:51:LYS:HG3	2.13	0.48
2:C:3:C:H2'	2:C:4:G:O4'	2.13	0.48
1:A:225:ASN:ND2	1:A:225:ASN:C	2.67	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:66:GLU:O	1:A:67:GLU:O	2.32	0.48
1:A:82:LYS:HZ1	1:A:85:ARG:HH21	1.62	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
1:A:19:LEU:HD12	1:A:40:LEU:HD23	1.95	0.48
2:D:3:C:C2	2:D:4:G:C8	3.02	0.47
1:A:255:VAL:HG12	1:A:257:VAL:HG22	1.96	0.47
1:A:26:ASN:HD21	1:A:29:TYR:HE2	1.61	0.47
1:A:304:GLU:C	1:A:306:LYS:H	2.17	0.47
1:A:40:LEU:HD12	1:A:40:LEU:N	2.29	0.47
1:B:144:PHE:O	1:B:145:ARG:HB2	2.14	0.47
1:B:84:TYR:HD1	1:B:87:GLU:OE1	1.96	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:B:261:ARG:HH22	1:B:286:VAL:HG21	1.80	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:A:6:LYS:HD3	1:A:61:VAL:CG2	2.43	0.47
1:B:31:ILE:HG22	1:B:32:THR:N	2.29	0.47
1:B:59:GLU:O	1:B:61:VAL:HG23	2.13	0.47
1:A:115:LYS:HD2	1:A:115:LYS:HA	1.78	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:218:LYS:CA	1:B:218:LYS:HE3	2.43	0.47
1:B:22:ASN:HD22	1:B:22:ASN:N	2.13	0.47
1:B:275:ASP:O	1:B:278:LEU:N	2.48	0.47
1:A:5:LEU:HD11	1:A:58:PHE:CD2	2.51	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:B:29:TYR:CE1	1:B:65:LEU:HB3	2.41	0.46
1:A:25:LEU:HD12	1:A:41:PRO:O	2.16	0.46
1:A:291:THR:OG1	1:A:292:ILE:N	2.48	0.46
1:B:189:ILE:H	1:B:189:ILE:CD1	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:O	1:B:288:HIS:N	2.47	0.46
1:B:16:ARG:NE	2:D:19:G:O2'	2.48	0.46
1:A:144:PHE:N	1:A:144:PHE:HD1	2.13	0.46
1:B:45:VAL:HG21	1:B:49:ILE:HD11	1.97	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
2:D:12:C:O2'	2:D:13:U:H5'	2.15	0.46
1:A:111:GLU:OE1	1:A:111:GLU:N	2.49	0.46
1:A:151:HIS:HE1	1:A:155:GLU:O	1.99	0.46
1:A:240:LYS:HA	1:A:242:GLU:OE1	2.16	0.46
1:B:271:HIS:HA	1:B:274:ILE:CG1	2.44	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:A:146:VAL:HG12	1:A:147:ARG:N	2.31	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:B:271:HIS:CD2	1:B:272:LYS:N	2.80	0.45
2:C:45:U:H4'	2:C:45:U:OP1	2.15	0.45
1:B:313:GLU:HG2	1:B:314:LYS:N	2.32	0.45
1:B:69:LYS:HD2	1:B:70:ILE:N	2.31	0.45
1:A:135:ARG:NH2	1:A:137:LYS:HD3	2.31	0.45
1:A:221:ALA:HB1	1:A:232:LEU:HD21	1.98	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:103:LEU:HD23	1:A:103:LEU:N	2.32	0.45
1:B:149:LEU:HD12	1:B:174:ALA:HB2	1.98	0.45
1:B:227:HIS:O	1:B:231:LEU:HD23	2.16	0.45
1:A:175:LYS:HD2	1:A:227:HIS:CD2	2.52	0.45
1:A:206:VAL:O	1:A:235:ASN:ND2	2.50	0.45
1:B:25:LEU:HD12	1:B:41:PRO:O	2.16	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:A:203:PHE:HB3	3:A:401:SAM:O4'	2.17	0.45
1:B:270:ALA:O	1:B:272:LYS:N	2.50	0.45
1:B:275:ASP:O	1:B:276:LYS:C	2.54	0.45
1:B:297:ASP:O	1:B:300:ILE:N	2.49	0.45
2:D:43:C:H5''	2:D:44:C:OP2	2.16	0.45
1:A:159:LEU:CD1	1:A:160:THR:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASN:O	1:A:239:ASN:ND2	2.40	0.45
1:B:274:ILE:HD11	1:B:302:LEU:HD13	1.99	0.45
1:A:39:TYR:CD1	1:A:39:TYR:N	2.85	0.45
1:B:207:GLY:N	1:B:208:PRO:CD	2.80	0.45
2:C:8:U:O2	2:C:47:A:H2	2.00	0.45
2:D:3:C:H2'	2:D:4:G:C8	2.48	0.45
1:A:151:HIS:CE1	1:A:153:ALA:O	2.70	0.44
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
2:C:2:C:C2'	2:C:3:C:C5'	2.94	0.44
2:D:18:G:H21	2:D:58:A:H5'	1.81	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
2:D:11:U:H2'	2:D:11:U:O2	2.16	0.44
1:A:115:LYS:HE3	1:A:119:GLU:CD	2.38	0.44
1:A:269:PHE:HD1	1:A:272:LYS:HZ1	1.63	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:B:104:VAL:CG1	1:B:128:ILE:HD11	2.42	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:A:82:LYS:HD2	1:A:82:LYS:N	2.32	0.44
1:B:66:GLU:O	1:B:67:GLU:O	2.36	0.44
1:A:16:ARG:CZ	2:C:19:G:O2'	2.66	0.44
1:B:137:LYS:HB3	1:B:148:GLU:O	2.18	0.44
1:B:286:VAL:HG11	1:B:312:LEU:HD22	2.00	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
2:D:20:C:C2'	2:D:21:U:C6	3.01	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:217:LYS:O	1:B:244:LYS:HG3	2.17	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:A:193:VAL:HG12	1:A:194:SER:N	2.34	0.43
1:B:22:ASN:CB	1:B:24:LEU:HD13	2.48	0.43
1:B:317:VAL:O	1:B:318:LYS:HB3	2.18	0.43
2:C:49:G:H2'	2:C:50:U:C6	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:HG23	1:B:117:ARG:HG3	2.01	0.43
1:B:195:LEU:HD22	1:B:195:LEU:H	1.83	0.43
1:B:203:PHE:N	5:B:601:HOH:O	2.43	0.43
1:A:17:ARG:HH22	1:B:336:LYS:CE	2.31	0.43
1:A:225:ASN:HD22	1:A:226:PRO:HD2	1.83	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
1:B:280:ILE:HG22	1:B:280:ILE:O	2.19	0.43
1:B:286:VAL:HA	1:B:331:PHE:O	2.19	0.43
1:B:9:LYS:HG2	1:B:36:ASN:C	2.39	0.43
2:D:21:U:OP1	2:D:21:U:H4'	2.19	0.43
1:B:168:ARG:O	1:B:239:ASN:ND2	2.52	0.43
1:B:23:ASN:HB2	5:B:604:HOH:O	2.18	0.43
1:B:270:ALA:HB1	1:B:289:TYR:CE2	2.54	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:A:125:TYR:CD2	1:A:125:TYR:C	2.92	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
2:C:2:C:H2'	2:C:3:C:H5''	1.97	0.43
1:B:112:VAL:CG2	1:B:117:ARG:HG2	2.48	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: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
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: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
2:D:11:U:C3'	2:D:12:C:H5''	2.49	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
1:B:65:LEU:H	1:B:65:LEU:HD22	1.85	0.42
2:D:60:U:H3'	2:D:61:C:H6	1.83	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
1:A:163:LYS:HG2	1:A:168:ARG:HD3	2.01	0.42
2:D:56:C:O5'	2:D:56:C:H6	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:O	1:A:270:ALA:HB2	2.19	0.42
1:A:30:LYS:HD3	1:A:31:ILE:H	1.85	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
2:D:34:G:C2'	2:D:34:G:N3	2.78	0.42
1:B:18:ILE:C	1:B:20:ILE:N	2.72	0.42
1:B:283:GLU:HB3	1:B:334:ASN:O	2.20	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:131:LYS:HB2	1:A:131:LYS:HE2	1.61	0.42
3:A:401:SAM:CE	2:C:37:G:H1	2.33	0.42
1:A:63:LYS:HE2	1:A:63:LYS:HB2	1.88	0.42
1:B:185:GLU:O	1:B:188:ARG:HB2	2.19	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:14:GLN:O	1:A:18:ILE:HG13	2.19	0.41
1:A:242:GLU:CD	1:A:242:GLU:H	2.23	0.41
1:A:90:GLU:HB2	1:A:92:LEU:HG	2.02	0.41
1:B:224:ILE:HG23	1:B:225:ASN:N	2.34	0.41
1:B:263:ILE:HA	1:B:288:HIS:HB2	2.01	0.41
1:B:46:ASP:C	1:B:48:ASP:H	2.23	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:195:LEU:CD2	1:B:195:LEU:H	2.32	0.41
1:B:251:ASP:OD1	1:B:253:ARG:HG3	2.19	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:A:195:LEU:HA	1:A:215:ASN:O	2.20	0.41
1:B:54:LEU:C	1:B:56:ILE:H	2.23	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
1:A:102:ASP:O	1:A:103:LEU:HD23	2.19	0.41
1:A:156:ASN:HD22	1:A:156:ASN:C	2.24	0.41
1:B:159:LEU:HD13	1:B:159:LEU:C	2.41	0.41
1:B:225:ASN:HD22	1:B:226:PRO:CD	2.34	0.41
3:B:402:SAM:CE	2:D:37:G:H1	2.34	0.41
2:D:20:C:O2'	2:D:21:U:H6	2.03	0.41
1:A:135:ARG:NH2	1:A:137:LYS:CD	2.84	0.41
1:B:237:LYS:CG	1:B:238:LEU:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG22	1:A:58:PHE:HB3	2.03	0.41
1:A:80:ILE:HG23	1:A:84:TYR:HD2	1.86	0.41
1:B:195:LEU:O	1:B:217:LYS:HD3	2.21	0.41
1:B:246:ILE:HA	1:B:247:PRO:HD2	1.87	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:267:PRO:O	1:B:291:THR:HA	2.21	0.40
1:B:5:LEU:HD11	1:B:58:PHE:HB2	2.02	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
1:B:234:LYS:HE2	1:B:234:LYS:HB3	1.85	0.40
1:A:207:GLY:N	1:A:208:PRO:CD	2.84	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: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:251:ASP:C	1:B:253:ARG:N	2.74	0.40
1:B:46:ASP:C	1:B:48:ASP:N	2.75	0.40
2:C:41:C:C2'	2:C:42:G:C5'	2.91	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 [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
1	A	334/336 (99%)	289 (86%)	30 (9%)	15 (4%)	<b>2</b> <b>12</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	333/336 (99%)	259 (78%)	47 (14%)	27 (8%)	1	3
All	All	667/672 (99%)	548 (82%)	77 (12%)	42 (6%)	1	6

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
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

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Mol	Chain	Res	Type
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%)	12	37
1	B	304/305 (100%)	281 (92%)	23 (8%)	13	39
All	All	609/610 (100%)	562 (92%)	47 (8%)	13	39

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

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Mol	Chain	Res	Type
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
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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	-	21,29,29	0.92	1 (4%)	18,42,42	1.64	2 (11%)
3	SAM	B	402	-	21,29,29	0.99	2 (9%)	18,42,42	1.74	3 (16%)

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	-	-	0/8/33/33	0/3/3/3
3	SAM	B	402	-	-	2/8/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	SAM	C8-N7	-2.29	1.30	1.34
3	B	402	SAM	O4'-C1'	2.26	1.44	1.41
3	A	401	SAM	C8-N7	-2.01	1.31	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	SAM	N3-C2-N1	-4.74	121.28	128.68
3	B	402	SAM	N3-C2-N1	-4.70	121.33	128.68
3	B	402	SAM	C5'-SD-CG	3.23	111.64	103.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	SAM	C5'-SD-CG	2.61	110.05	103.40
3	B	402	SAM	C3'-C2'-C1'	2.53	104.79	100.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

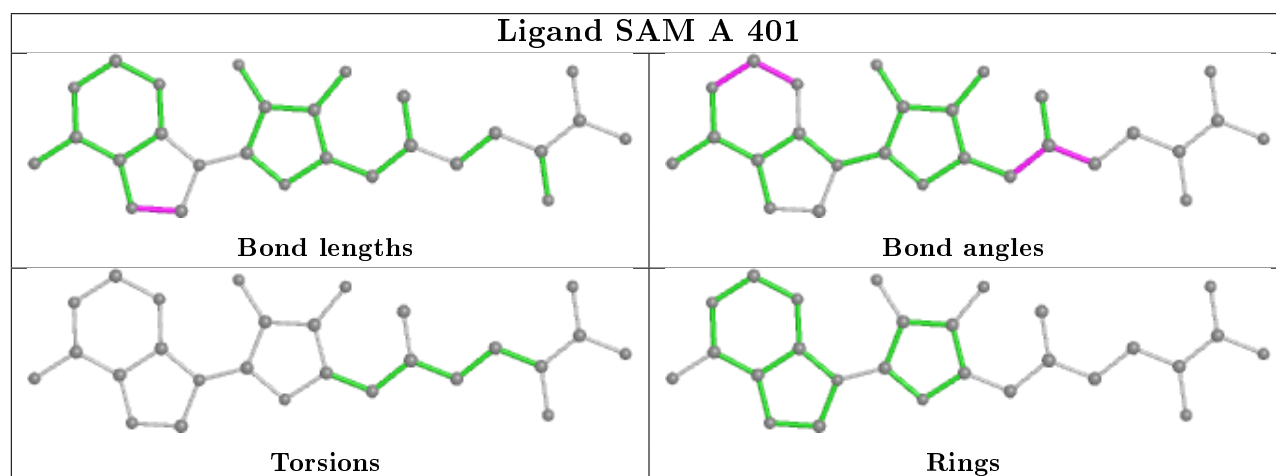
Mol	Chain	Res	Type	Atoms
3	B	402	SAM	O4'-C4'-C5'-SD
3	B	402	SAM	C3'-C4'-C5'-SD

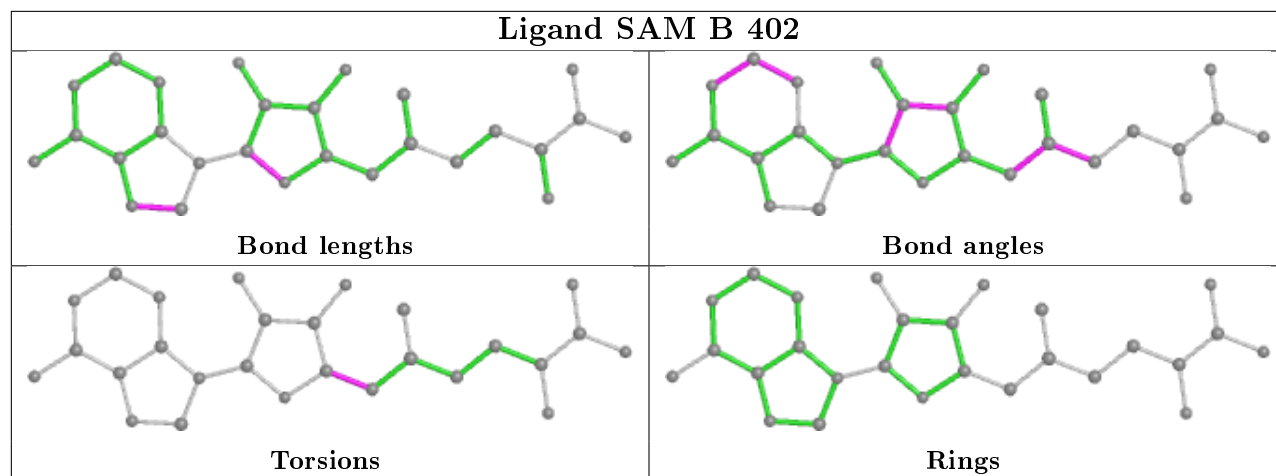
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	SAM	5	0
3	B	402	SAM	8	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	336/336 (100%)	0.22	17 (5%) 28 17	29, 55, 100, 124	0
1	B	335/336 (99%)	0.31	20 (5%) 21 13	48, 79, 108, 121	0
2	C	71/75 (94%)	0.88	9 (12%) 3 2	35, 77, 110, 123	0
2	D	71/75 (94%)	0.65	8 (11%) 5 3	49, 73, 119, 133	0
All	All	813/822 (98%)	0.35	54 (6%) 18 10	29, 68, 108, 133	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	11.2
1	A	65	LEU	7.3
1	A	3	LEU	6.4
1	A	2	PRO	5.1
1	B	336	LYS	5.0
1	A	64	GLU	4.5
1	A	39	TYR	4.4
2	C	33	U	4.4
1	B	206	VAL	4.3
1	B	70	ILE	4.3
1	A	29	TYR	4.3
1	B	29	TYR	3.8
2	D	22	A	3.6
1	B	335	LYS	3.6
1	A	62	ASP	3.5
2	C	34	G	3.5
2	D	46	U	3.3
1	B	67	GLU	3.2
1	B	65	LEU	3.2
1	B	333	ILE	3.0
2	C	45	U	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	283	GLU	3.0
1	B	303	PHE	3.0
2	D	16	G	2.9
2	C	52	G	2.8
1	B	55	ASN	2.8
1	A	71	ILE	2.7
2	C	2	C	2.7
2	C	1	G	2.6
1	A	336	LYS	2.6
1	A	33	SER	2.6
2	D	8	U	2.5
1	B	85	ARG	2.5
1	B	257	VAL	2.5
2	D	21	U	2.5
1	A	323	ARG	2.4
1	B	168	ARG	2.4
2	C	3	C	2.4
2	D	47	A	2.4
1	B	28	ASP	2.4
2	D	13	U	2.3
1	B	309	CYS	2.2
1	A	32	THR	2.2
1	A	61	VAL	2.2
1	A	4	CYS	2.2
2	D	23	G	2.2
1	B	190	MET	2.1
2	C	58	A	2.1
1	A	66	GLU	2.1
1	B	322	PRO	2.0
1	B	331	PHE	2.0
1	A	40	LEU	2.0
1	B	236	ILE	2.0
2	C	48	C	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 ⓘ

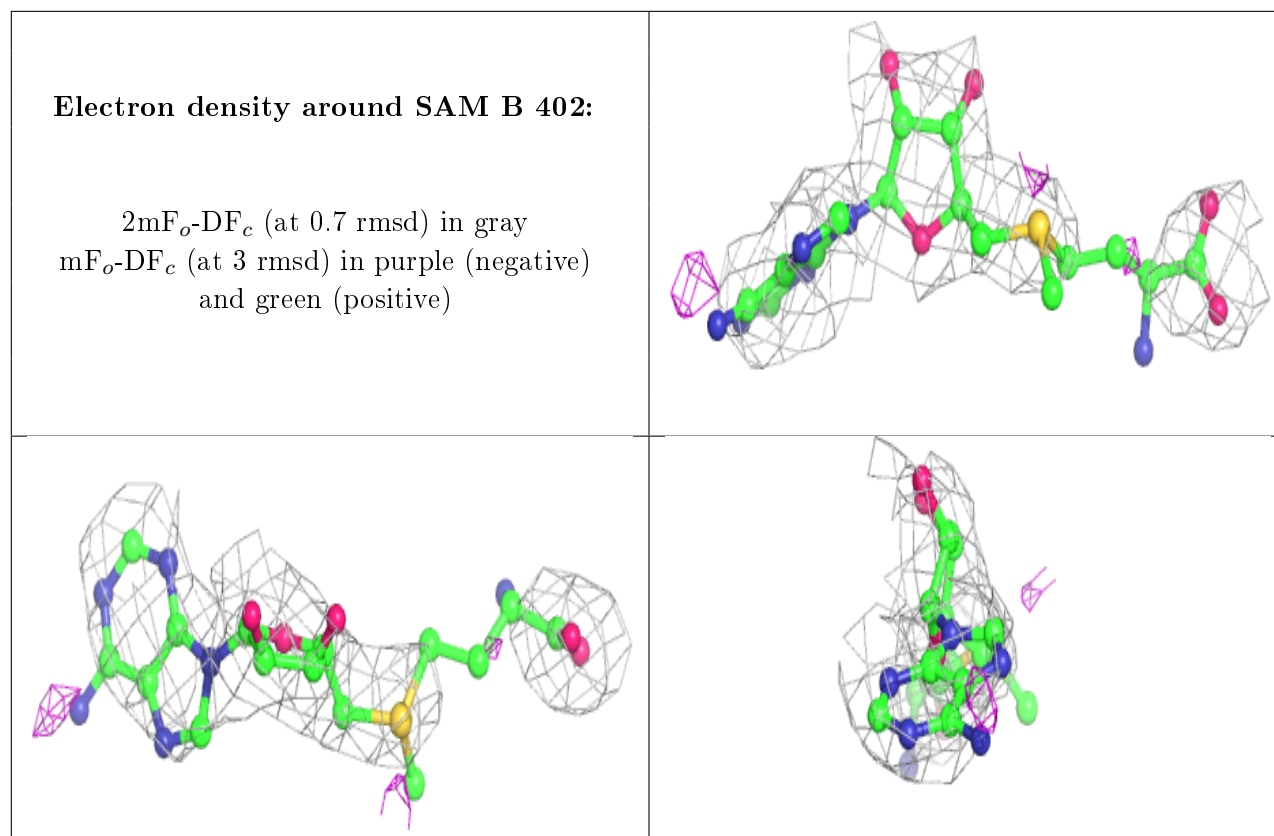
There are no carbohydrates in this entry.

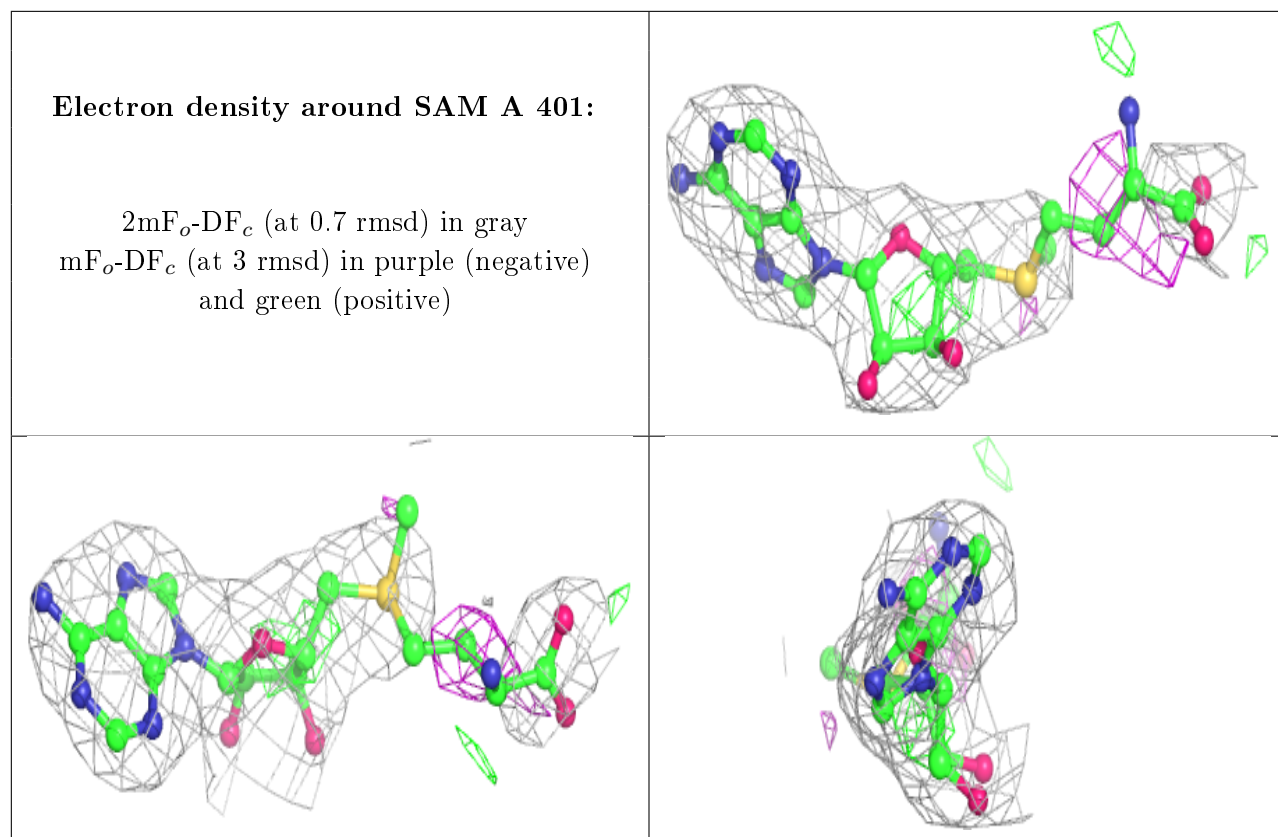
## 6.4 Ligands ⓘ

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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	MG	C	102	1/1	0.68	0.42	52,52,52,52	0
4	MG	C	104	1/1	0.84	0.28	59,59,59,59	0
3	SAM	B	402	27/27	0.87	0.40	78,84,86,86	0
4	MG	C	105	1/1	0.88	0.51	61,61,61,61	0
4	MG	D	201	1/1	0.89	0.20	58,58,58,58	0
4	MG	C	101	1/1	0.90	0.43	66,66,66,66	0
3	SAM	A	401	27/27	0.92	0.28	42,49,68,72	0
4	MG	C	103	1/1	0.92	0.31	48,48,48,48	0
4	MG	C	106	1/1	0.92	0.33	53,53,53,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.