



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:52 pm BST

PDB ID : 5HR7  
Title : X-ray crystal structure of C118A RlmN from Escherichia coli with cross-linked in vitro transcribed tRNA  
Authors : Schwalm, E.L.; Grove, T.L.; Booker, S.J.; Boal, A.K.  
Deposited on : 2016-01-22  
Resolution : 2.40 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.

---

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

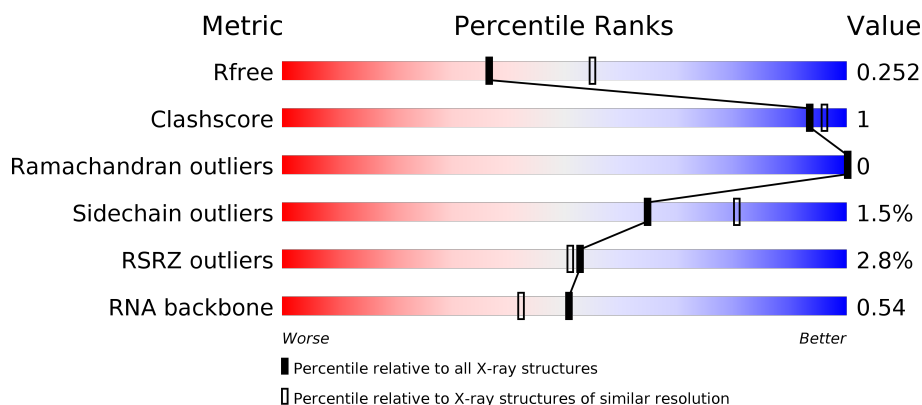
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	C	76	<div> <div>5%</div> <div> <div></div> <div>74%</div> <div>18%</div> <div>8%</div> </div> </div>
1	D	76	<div> <div>3%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>8%</div> </div> </div>
2	A	404	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>11%</div> </div> </div>
2	B	404	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>•</div> <div>11%</div> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8837 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called tRNA Glu.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	70	Total	C	N	O	P	0	0	0
			1486	663	264	489	70			
1	C	70	Total	C	N	O	P	0	0	0
			1486	663	264	489	70			

- Molecule 2 is a protein called Dual-specificity RNA methyltransferase RlmN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	360	Total	As	C	N	O	S	0	1	0
			2847	1	1783	511	532	20			
2	A	360	Total	As	C	N	O	S	0	1	0
			2847	1	1783	511	532	20			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	118	ALA	CYS	conflict	UNP A7ZPW0
B	385	GLY	-	expression tag	UNP A7ZPW0
B	386	ASN	-	expression tag	UNP A7ZPW0
B	387	SER	-	expression tag	UNP A7ZPW0
B	388	SER	-	expression tag	UNP A7ZPW0
B	389	SER	-	expression tag	UNP A7ZPW0
B	390	VAL	-	expression tag	UNP A7ZPW0
B	391	ASP	-	expression tag	UNP A7ZPW0
B	392	LYS	-	expression tag	UNP A7ZPW0
B	393	LEU	-	expression tag	UNP A7ZPW0
B	394	ALA	-	expression tag	UNP A7ZPW0
B	395	ALA	-	expression tag	UNP A7ZPW0
B	396	ALA	-	expression tag	UNP A7ZPW0
B	397	LEU	-	expression tag	UNP A7ZPW0
B	398	GLU	-	expression tag	UNP A7ZPW0
B	399	HIS	-	expression tag	UNP A7ZPW0
B	400	HIS	-	expression tag	UNP A7ZPW0

*Continued on next page...*

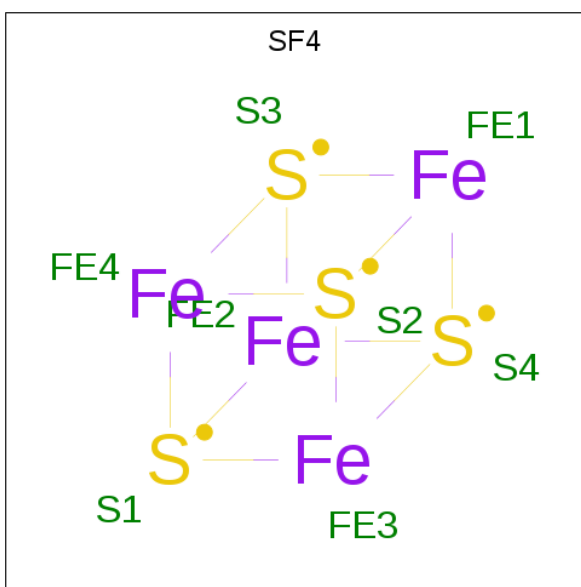
*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	401	HIS	-	expression tag	UNP A7ZPW0
B	402	HIS	-	expression tag	UNP A7ZPW0
B	403	HIS	-	expression tag	UNP A7ZPW0
B	404	HIS	-	expression tag	UNP A7ZPW0
A	118	ALA	CYS	conflict	UNP A7ZPW0
A	385	GLY	-	expression tag	UNP A7ZPW0
A	386	ASN	-	expression tag	UNP A7ZPW0
A	387	SER	-	expression tag	UNP A7ZPW0
A	388	SER	-	expression tag	UNP A7ZPW0
A	389	SER	-	expression tag	UNP A7ZPW0
A	390	VAL	-	expression tag	UNP A7ZPW0
A	391	ASP	-	expression tag	UNP A7ZPW0
A	392	LYS	-	expression tag	UNP A7ZPW0
A	393	LEU	-	expression tag	UNP A7ZPW0
A	394	ALA	-	expression tag	UNP A7ZPW0
A	395	ALA	-	expression tag	UNP A7ZPW0
A	396	ALA	-	expression tag	UNP A7ZPW0
A	397	LEU	-	expression tag	UNP A7ZPW0
A	398	GLU	-	expression tag	UNP A7ZPW0
A	399	HIS	-	expression tag	UNP A7ZPW0
A	400	HIS	-	expression tag	UNP A7ZPW0
A	401	HIS	-	expression tag	UNP A7ZPW0
A	402	HIS	-	expression tag	UNP A7ZPW0
A	403	HIS	-	expression tag	UNP A7ZPW0
A	404	HIS	-	expression tag	UNP A7ZPW0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

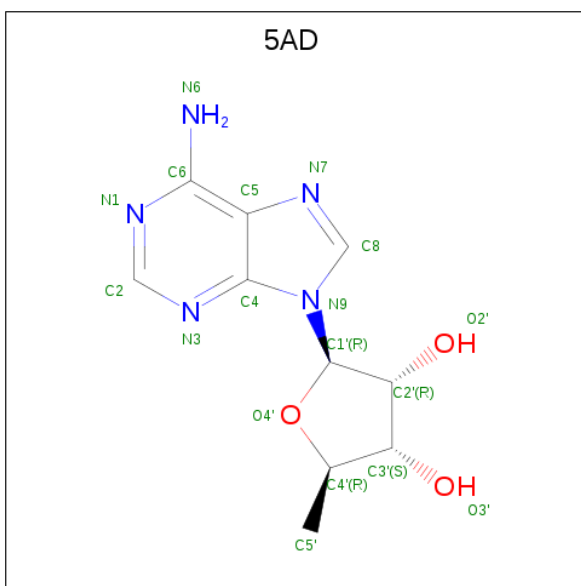
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	3	Total Mg 3 3	0	0
3	C	4	Total Mg 4 4	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



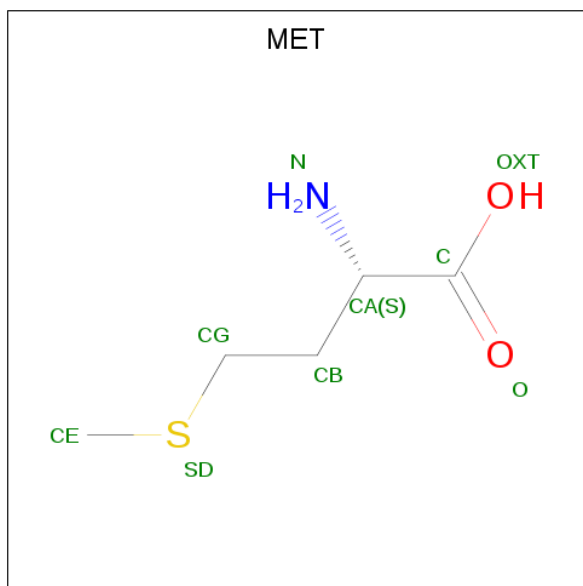
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	A	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula:  $C_{10}H_{13}N_5O_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			18	10	5	3		
5	A	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 6 is METHIONINE (three-letter code: MET) (formula:  $C_5H_{11}NO_2S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			9	5	1	2	1		
6	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

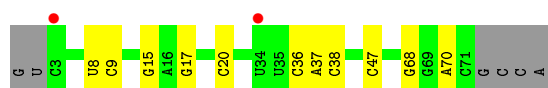
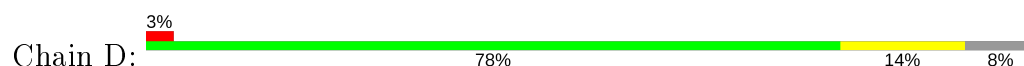
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	16	Total	O	0	0
			16	16		
7	C	14	Total	O	0	0
			14	14		
7	B	24	Total	O	0	0
			24	24		
7	A	40	Total	O	0	0
			40	40		

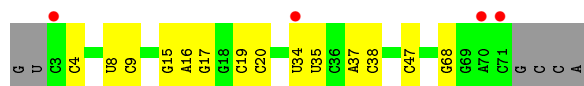
### 3 Residue-property plots [i](#)

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.

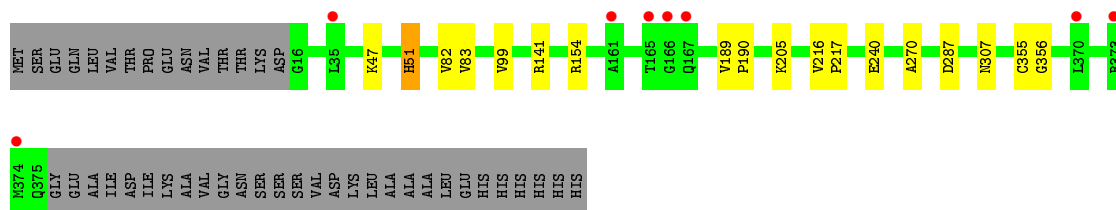
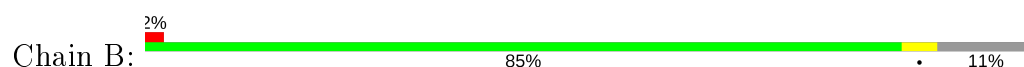
- Molecule 1: tRNA Glu



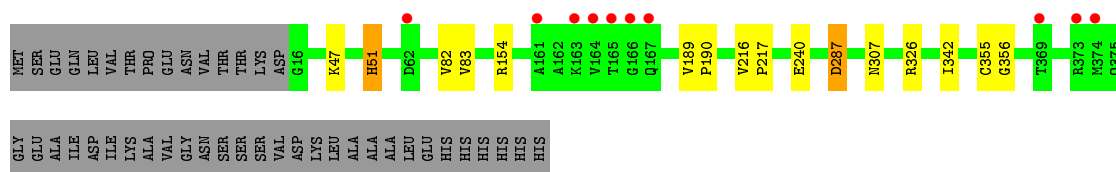
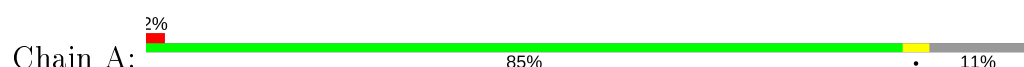
- Molecule 1: tRNA Glu



- Molecule 2: Dual-specificity RNA methyltransferase RlmN



- Molecule 2: Dual-specificity RNA methyltransferase RlmN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.72Å 70.38Å 151.81Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 44.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.40) 99.4 (44.83-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.216 , 0.247 0.221 , 0.252	Depositor DCC
$R_{free}$ test set	3788 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.7	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 18.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8837	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CAS, MG, SMC, SF4, 5AD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	C	0.24	0/1658	0.66	0/2581
1	D	0.24	0/1658	0.66	0/2581
2	A	0.31	0/2875	0.53	0/3878
2	B	0.31	0/2875	0.54	0/3878
All	All	0.28	0/9066	0.59	0/12918

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1486	0	759	2	0
1	D	1486	0	759	3	0
2	A	2847	0	2861	11	0
2	B	2847	0	2861	10	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	18	0	12	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	18	0	13	1	0
6	A	9	0	8	0	0
6	B	9	0	8	0	0
7	A	40	0	0	0	0
7	B	24	0	0	0	0
7	C	14	0	0	0	0
7	D	16	0	0	0	0
All	All	8837	0	7281	23	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 1.

All (23) 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:A:287[A]:ASP:OD1	2:A:287[A]:ASP:O	2.11	0.67
2:B:287[A]:ASP:O	2:B:287[A]:ASP:OD1	2.20	0.59
1:D:8:U:C2	1:D:15:G:O6	2.59	0.56
1:C:8:U:C2	1:C:15:G:O6	2.63	0.51
2:B:82:VAL:HG23	2:B:154:ARG:HG2	1.92	0.50
2:A:287[A]:ASP:CG	2:A:287[A]:ASP:O	2.50	0.48
2:A:189:VAL:HB	2:A:190:PRO:HD3	1.96	0.48
2:B:205:LYS:HB3	2:B:270:ALA:HB2	1.97	0.47
2:B:189:VAL:HB	2:B:190:PRO:HD3	1.97	0.47
2:A:82:VAL:HG23	2:A:154:ARG:HG2	1.97	0.46
2:A:356:GLY:HA3	5:A:502:5AD:C5	2.45	0.46
2:A:47:LYS:O	2:A:51:HIS:HB2	2.16	0.45
2:B:83:VAL:O	2:B:83:VAL:HG12	2.17	0.45
2:B:356:GLY:HA3	5:B:502:5AD:C5	2.49	0.43
2:A:83:VAL:O	2:A:83:VAL:HG12	2.18	0.43
1:C:37:A:C6	2:B:355:SMC:SG	3.12	0.43
2:A:287[A]:ASP:OD2	2:A:326:ARG:NE	2.48	0.43
2:B:216:VAL:HG22	2:B:217:PRO:HD3	2.01	0.43
1:D:36:C:H2'	2:A:342:ILE:HG21	2.01	0.42
2:B:47:LYS:O	2:B:51:HIS:HB2	2.19	0.41
1:D:37:A:C6	2:A:355:SMC:SG	3.14	0.41
2:A:216:VAL:HG22	2:A:217:PRO:HD3	2.02	0.41
2:B:99:VAL:HG13	2:B:141:ARG:NH2	2.37	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	
2	A	357/404 (88%)	349 (98%)	8 (2%)	0	100	100
2	B	357/404 (88%)	346 (97%)	11 (3%)	0	100	100
All	All	714/808 (88%)	695 (97%)	19 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	308/344 (90%)	303 (98%)	5 (2%)	62	79
2	B	308/344 (90%)	305 (99%)	3 (1%)	76	88
All	All	616/688 (90%)	608 (99%)	8 (1%)	65	84

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	51	HIS
2	B	240	GLU
2	B	307	ASN
2	A	51	HIS
2	A	240	GLU
2	A	287[A]	ASP
2	A	287[B]	ASP
2	A	307	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	69/76 (90%)	11 (15%)	1 (1%)
1	D	69/76 (90%)	7 (10%)	1 (1%)
All	All	138/152 (90%)	18 (13%)	2 (1%)

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	9	C
1	D	17	G
1	D	20	C
1	D	38	C
1	D	47	C
1	D	68	G
1	D	70	A
1	C	4	C
1	C	9	C
1	C	16	A
1	C	17	G
1	C	19	C
1	C	20	C
1	C	34	U
1	C	35	U
1	C	38	C
1	C	47	C
1	C	68	G

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	9	C
1	C	9	C

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	CAS	A	53	2	5,8,9	1.07	0	1,9,11	1.03	0
2	CAS	B	53	2	5,8,9	1.08	0	1,9,11	1.01	0
2	SMC	A	355	1,2	5,6,7	1.34	1 (20%)	2,6,8	4.60	1 (50%)
2	SMC	B	355	1,2	5,6,7	1.35	1 (20%)	2,6,8	4.92	1 (50%)

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
2	CAS	A	53	2	-	0/0/7/9	-
2	CAS	B	53	2	-	0/0/7/9	-
2	SMC	A	355	1,2	-	0/3/5/7	-
2	SMC	B	355	1,2	-	0/3/5/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	355	SMC	CB-SG	-2.85	1.76	1.80
2	A	355	SMC	CB-SG	-2.85	1.76	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	355	SMC	CS-SG-CB	6.87	113.94	101.30
2	A	355	SMC	CS-SG-CB	6.45	113.16	101.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	355	SMC	1	0
2	B	355	SMC	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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	$\# Z  > 2$
4	SF4	A	501	2,6	0,12,12	0.00	-	-		
5	5AD	B	502	-	17,20,20	1.07	1 (5%)	15,30,30	1.87	4 (26%)
4	SF4	B	501	2,6	0,12,12	0.00	-	-		
5	5AD	A	502	-	17,20,20	1.06	1 (5%)	15,30,30	2.79	8 (53%)

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
4	SF4	A	501	2,6	-	-	0/6/5/5
5	5AD	B	502	-	-	0/0/20/20	0/3/3/3
4	SF4	B	501	2,6	-	-	0/6/5/5
5	5AD	A	502	-	-	0/0/20/20	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	502	5AD	C5-C4	2.41	1.47	1.40
5	A	502	5AD	C5-C4	2.37	1.47	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	5AD	O2'-C2'-C1'	4.48	127.41	110.85
5	A	502	5AD	C3'-C2'-C1'	4.32	107.48	100.98
5	B	502	5AD	C5'-C4'-C3'	-4.16	111.33	115.70
5	A	502	5AD	C5'-C4'-C3'	-4.06	111.44	115.70
5	A	502	5AD	N3-C2-N1	-3.60	123.05	128.68
5	A	502	5AD	O4'-C1'-C2'	-3.54	101.76	106.93
5	A	502	5AD	C4-C5-N7	-3.43	105.83	109.40
5	B	502	5AD	N3-C2-N1	-3.42	123.34	128.68
5	A	502	5AD	O2'-C2'-C3'	3.32	122.57	111.82
5	B	502	5AD	C4-C5-N7	-2.93	106.34	109.40
5	A	502	5AD	C1'-N9-C4	-2.48	122.28	126.64
5	B	502	5AD	O4'-C1'-C2'	-2.31	103.55	106.93

There are no chirality outliers.

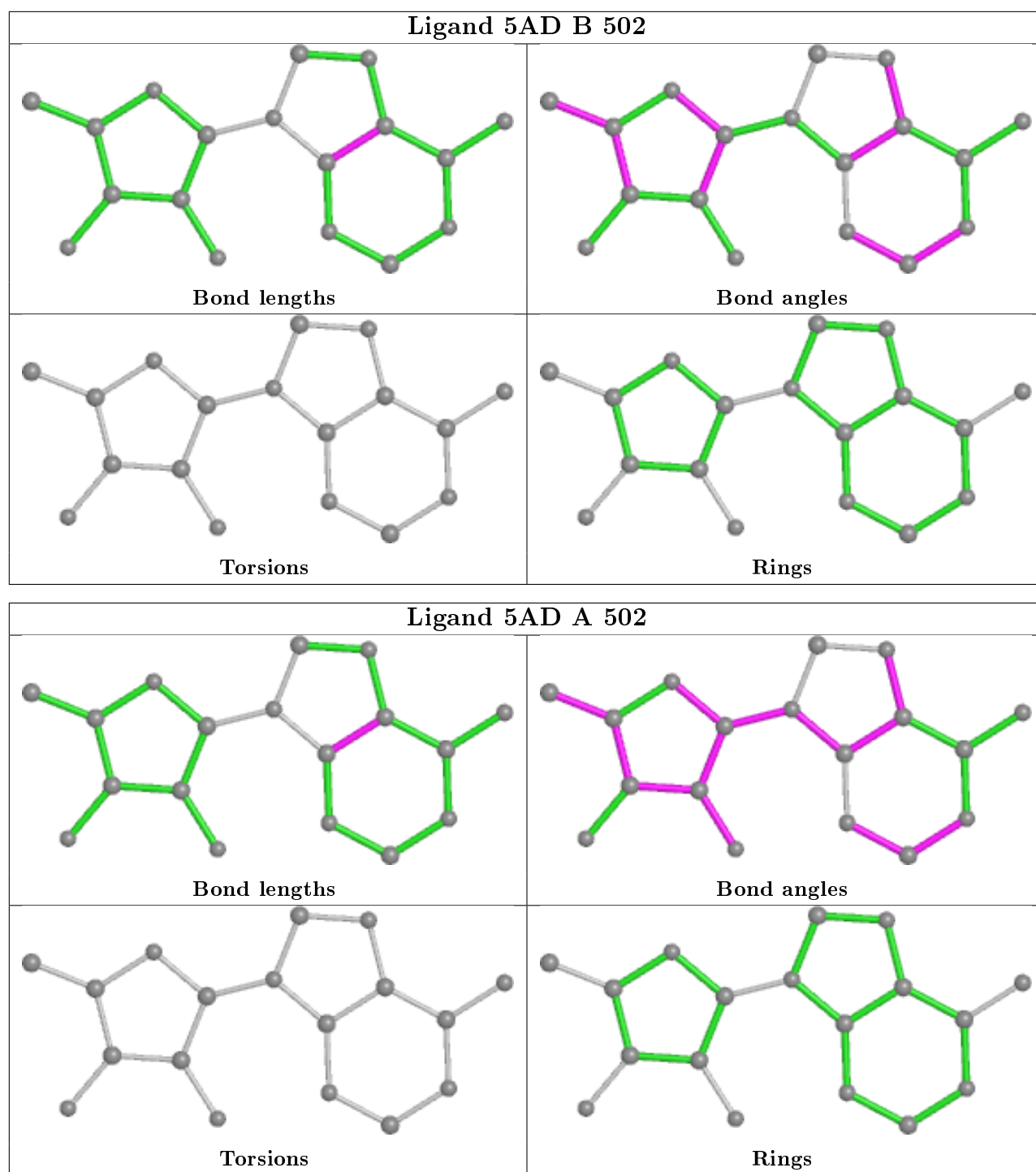
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	502	5AD	1	0
5	A	502	5AD	1	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(Å²)	Q<0.9	
1	C	70/76 (92%)	-0.30	4 (5%)	23	22	44, 63, 116, 136	0
1	D	70/76 (92%)	-0.47	2 (2%)	51	50	46, 64, 105, 134	0
2	A	358/404 (88%)	-0.17	10 (2%)	53	51	43, 55, 98, 128	0
2	B	358/404 (88%)	-0.09	8 (2%)	62	60	41, 53, 96, 129	0
All	All	856/960 (89%)	-0.17	24 (2%)	53	51	41, 56, 99, 136	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	165	THR	6.0
2	A	165	THR	5.6
2	A	373	ARG	5.1
2	A	166	GLY	4.8
2	B	373	ARG	4.7
2	A	161	ALA	3.8
1	C	34	U	3.7
2	B	161	ALA	3.3
1	D	34	U	3.1
2	A	167	GLN	3.1
2	B	166	GLY	3.0
1	C	70	A	2.9
1	C	71	C	2.8
2	B	167	GLN	2.7
2	B	35	LEU	2.7
1	D	3	C	2.7
1	C	3	C	2.6
2	A	62	ASP	2.6
2	A	163	LYS	2.3
2	A	164	VAL	2.2
2	B	374	MET	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	374	MET	2.1
2	B	370	LEU	2.1
2	A	369	THR	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
2	CAS	A	53	9/10	0.83	0.15	69,71,97,104	0
2	CAS	B	53	9/10	0.83	0.16	71,72,95,102	0
2	SMC	B	355	7/8	0.95	0.12	41,43,44,45	0
2	SMC	A	355	7/8	0.97	0.10	42,44,46,46	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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
3	MG	D	103	1/1	0.75	0.19	76,76,76,76	0
3	MG	D	101	1/1	0.79	0.08	63,63,63,63	0
3	MG	C	103	1/1	0.80	0.17	74,74,74,74	0
3	MG	C	101	1/1	0.89	0.10	66,66,66,66	0
3	MG	C	104	1/1	0.92	0.09	83,83,83,83	0
6	MET	A	503	9/9	0.93	0.20	57,58,62,62	0
5	5AD	A	502	18/18	0.94	0.13	50,53,56,56	0
6	MET	B	503	9/9	0.95	0.28	57,58,60,60	0
4	SF4	B	501	8/8	0.95	0.19	44,47,48,49	0
4	SF4	A	501	8/8	0.96	0.11	47,51,51,52	0
3	MG	C	102	1/1	0.97	0.10	46,46,46,46	0

*Continued on next page...*

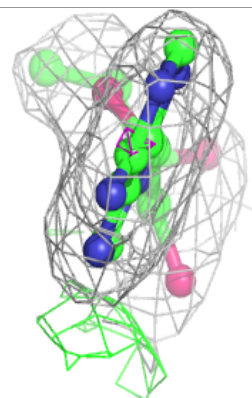
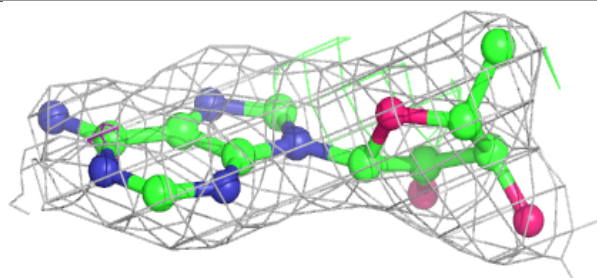
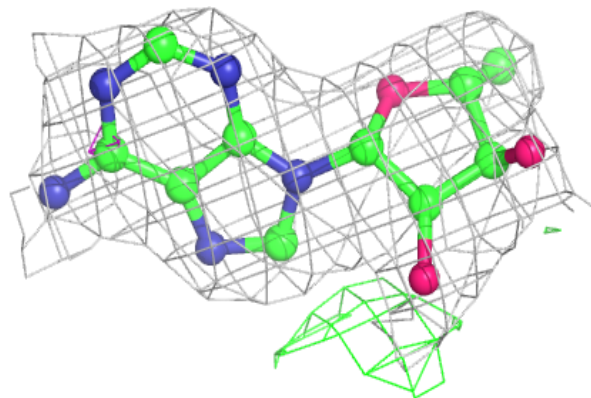
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	5AD	B	502	18/18	0.98	0.14	46,49,52,52	0
3	MG	D	102	1/1	0.99	0.05	48,48,48,48	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.

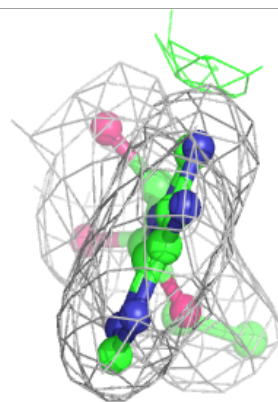
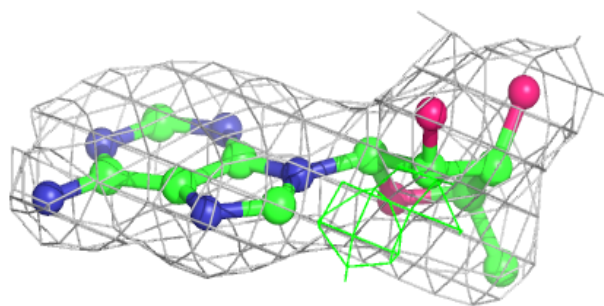
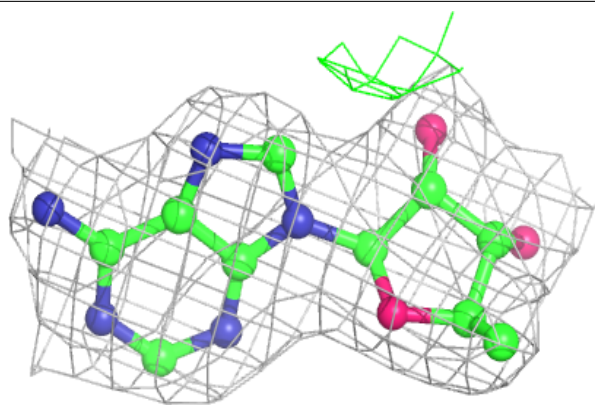
**Electron density around 5AD A 502:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around 5AD B 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.