Full wwPDB X-ray Structure Validation Report (i)

Oct 10, 2023 – 10:33 PM EDT

PDB ID	:	6WKS
Title	:	Structure of SARS-CoV-2 nsp16/nsp10 in complex with RNA cap analogue (m7GpppA) and S-adenosylmethionine
Authors	:	Gupta, Y.K.; Viswanathan, T.; Arya, S.; Qi, S.; Misra, A.; Chan, S.-H.
Deposited on	:	2020-04-16
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

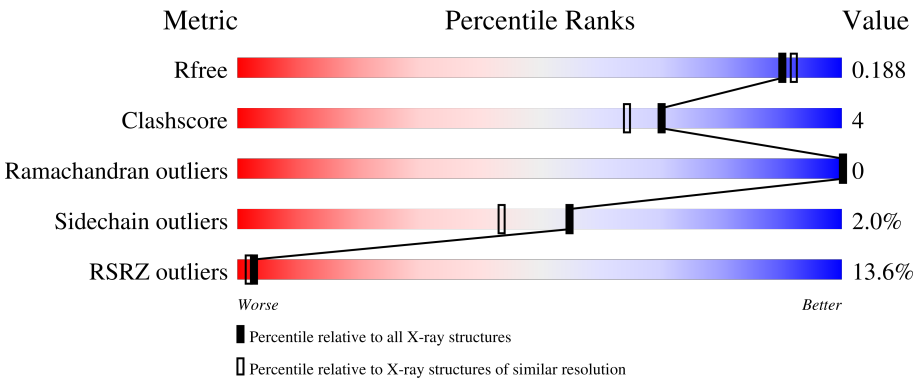
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	AAA	298	11% 95% • •
2	BBB	139	16% 76% 6% • 18%

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	ADN	AAA	302	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 3516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

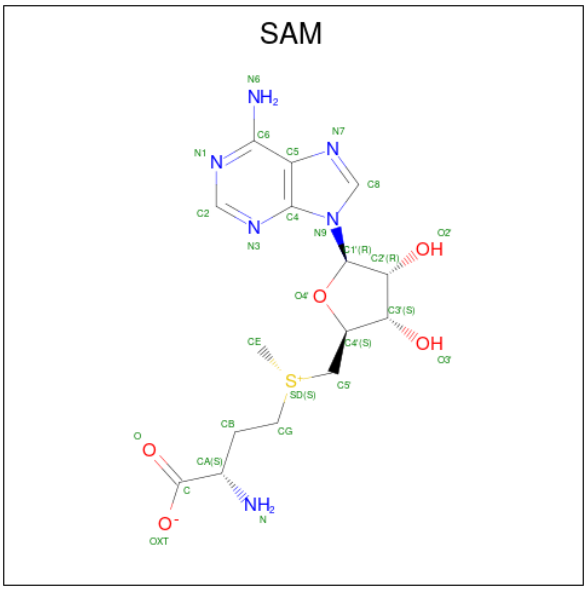
- Molecule 1 is a protein called 2'-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AAA	298	2331	1487	391	436	17	0	0	0

- Molecule 2 is a protein called Non-structural protein 10.

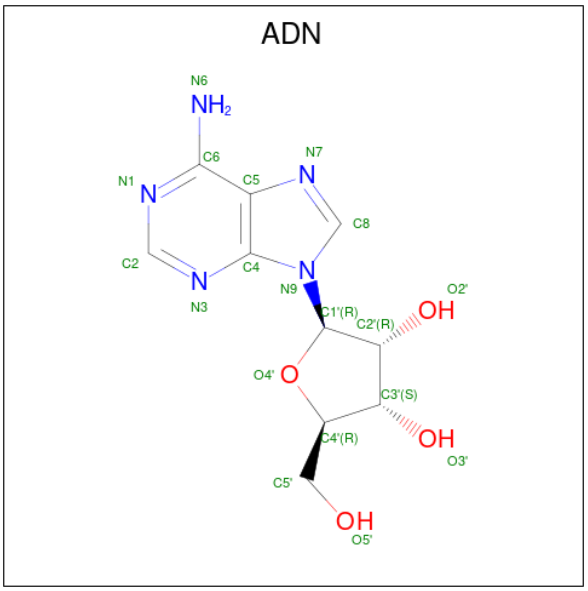
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	BBB	114	832	519	140	158	15	0	0	0

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



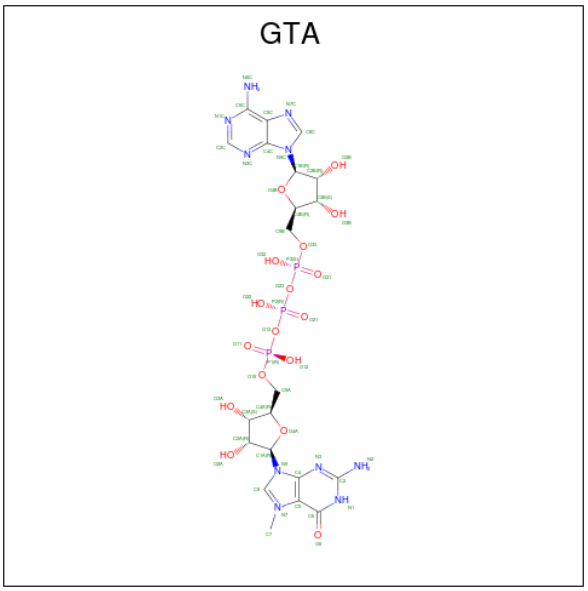
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	AAA	1	27	15	6	5	1	0	0

- Molecule 4 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	AAA	1	19	10	5	4	0	0

- Molecule 5 is P1-7-METHYLGUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHATE (three-letter code: GTA) (formula: $C_{21}H_{30}N_{10}O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

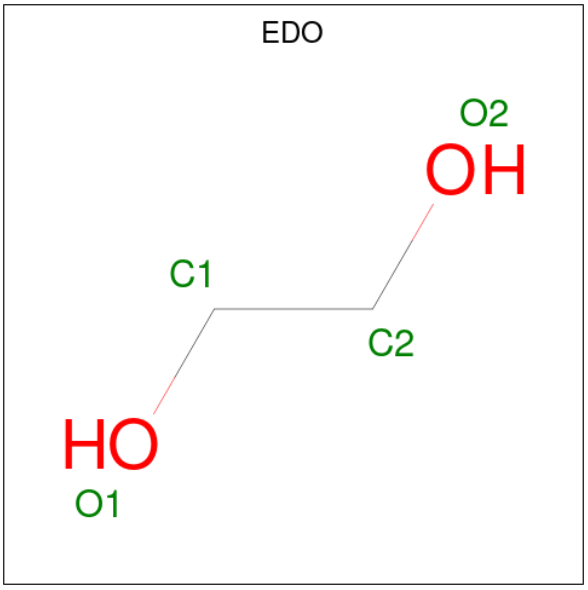


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	AAA	1	51	21	10	17	3	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	BBB	2	2	2	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	BBB	1	4	2	2	0	0

- Molecule 8 is water.

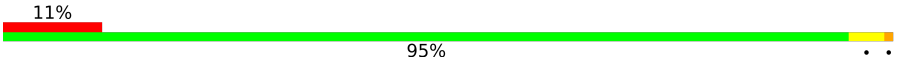
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	AAA	198	198	198	0	0
			Total	O		
8	BBB	52	52	52	0	0

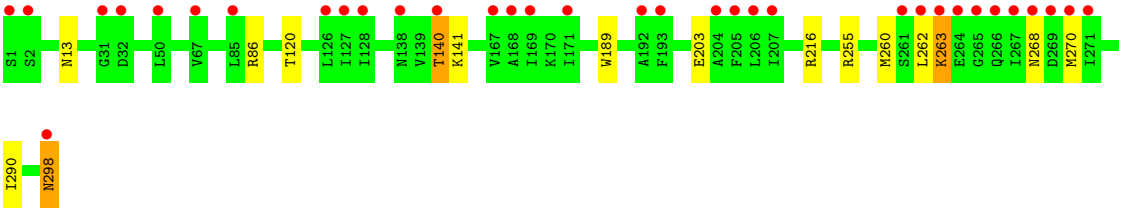
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 2'-O-methyltransferase

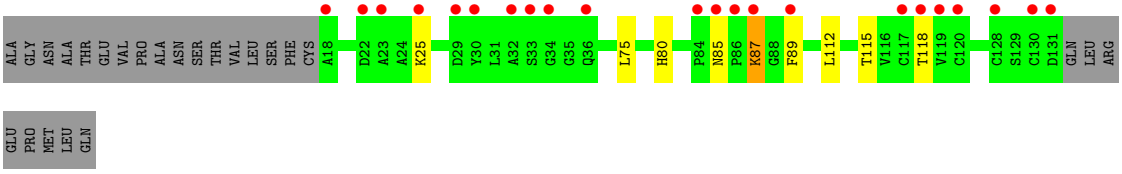
Chain AAA:





- Molecule 2: Non-structural protein 10

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	168.07Å 168.07Å 52.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.87 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.80) 100.0 (29.87-1.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.152 , 0.188 0.152 , 0.188	Depositor DCC
R_{free} test set	3909 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	3516	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SAM, ADN, GTA, EDO

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	AAA	0.75	1/2382 (0.0%)	0.91	4/3234 (0.1%)
2	BBB	0.55	0/851	0.86	0/1155
All	All	0.70	1/3233 (0.0%)	0.90	4/4389 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	203	GLU	CD-OE2	6.79	1.33	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	86	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	AAA	86	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	AAA	255	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	AAA	216	ARG	NE-CZ-NH1	-5.01	117.80	120.30

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	AAA	2331	0	2310	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	BBB	832	0	789	4	0
3	AAA	27	0	22	1	0
4	AAA	19	0	13	7	0
5	AAA	51	0	27	1	0
6	BBB	2	0	0	0	0
7	BBB	4	0	6	1	0
8	AAA	198	0	0	3	0
8	BBB	52	0	0	1	0
All	All	3516	0	3167	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 4.

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)
7:BBB:203:EDO:H12	8:BBB:316:HOH:O	1.72	0.88
1:AAA:263:LYS:HE3	1:AAA:263:LYS:HA	1.58	0.82
4:AAA:302:ADN:C5'	4:AAA:302:ADN:H8	2.13	0.77
1:AAA:189:TRP:NE1	4:AAA:302:ADN:H5'2	2.01	0.76
2:BBB:75:LEU:HD22	2:BBB:112:LEU:HD11	1.70	0.72
4:AAA:302:ADN:H8	4:AAA:302:ADN:H5'2	1.72	0.71
1:AAA:189:TRP:HE1	4:AAA:302:ADN:H5'2	1.53	0.71
1:AAA:260:MET:CE	1:AAA:262:LEU:HD11	2.34	0.58
2:BBB:87:LYS:O	2:BBB:89:PHE:N	2.37	0.56
2:BBB:85:ASN:OD1	2:BBB:87:LYS:O	2.24	0.56
1:AAA:263:LYS:HE3	1:AAA:263:LYS:CA	2.33	0.54
5:AAA:303:GTA:O3B	8:AAA:401:HOH:O	2.05	0.52
1:AAA:268:ASN:OD1	1:AAA:270:MET:HB3	2.10	0.52
1:AAA:263:LYS:HA	1:AAA:263:LYS:CE	2.36	0.50
4:AAA:302:ADN:H8	4:AAA:302:ADN:O5'	2.15	0.47
1:AAA:13:ASN:OD1	4:AAA:302:ADN:H5'1	2.16	0.45
1:AAA:298:ASN:HD22	1:AAA:298:ASN:C	2.18	0.45
1:AAA:260:MET:HE1	1:AAA:262:LEU:HD11	1.98	0.44
3:AAA:301:SAM:HE1	8:AAA:493:HOH:O	2.17	0.43
1:AAA:189:TRP:HE1	4:AAA:302:ADN:C5'	2.26	0.42
1:AAA:140:THR:OG1	1:AAA:141:LYS:N	2.52	0.41
8:AAA:488:HOH:O	2:BBB:80:HIS:HE1	2.03	0.41
1:AAA:120:THR:HG22	1:AAA:290:ILE:HG22	2.02	0.41

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	AAA	296/298 (99%)	289 (98%)	7 (2%)	0	100	100
2	BBB	112/139 (81%)	104 (93%)	8 (7%)	0	100	100
All	All	408/437 (93%)	393 (96%)	15 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	256/258 (99%)	253 (99%)	3 (1%)	71	65
2	BBB	90/113 (80%)	86 (96%)	4 (4%)	28	14
All	All	346/371 (93%)	339 (98%)	7 (2%)	55	44

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	140	THR
1	AAA	263	LYS
1	AAA	298	ASN
2	BBB	25	LYS
2	BBB	87	LYS
2	BBB	115	THR
2	BBB	118	THR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	GTA	AAA	303	-	46,56,56	0.73	0	46,88,88	0.93	1 (2%)
4	ADN	AAA	302	-	18,21,21	1.00	1 (5%)	18,31,31	2.21	6 (33%)
3	SAM	AAA	301	-	24,29,29	0.75	0	23,42,42	1.23	2 (8%)
7	EDO	BBB	203	-	3,3,3	0.85	0	2,2,2	0.49	0

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
5	GTA	AAA	303	-	-	2/24/64/64	0/6/6/6
4	ADN	AAA	302	-	-	2/2/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAM	AAA	301	-	-	2/12/33/33	0/3/3/3
7	EDO	BBB	203	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	AAA	302	ADN	C5'-C4'	-2.93	1.42	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AAA	302	ADN	C1'-N9-C4	5.21	135.79	126.64
4	AAA	302	ADN	O5'-C5'-C4'	-4.28	96.61	111.29
5	AAA	303	GTA	O2B-C2B-C1B	-3.27	98.78	110.85
4	AAA	302	ADN	O3'-C3'-C2'	3.26	122.36	111.82
4	AAA	302	ADN	O4'-C1'-C2'	-3.12	102.37	106.93
3	AAA	301	SAM	C5-C6-N6	2.58	124.28	120.35
3	AAA	301	SAM	O-C-CA	-2.30	114.03	122.14
4	AAA	302	ADN	C5-C6-N6	2.07	123.50	120.35
4	AAA	302	ADN	C2'-C3'-C4'	-2.05	98.66	102.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	303	GTA	C5A-O15-P1-O11
5	AAA	303	GTA	C5A-O15-P1-O13
7	BBB	203	EDO	O1-C1-C2-O2
4	AAA	302	ADN	O4'-C4'-C5'-O5'
3	AAA	301	SAM	OXT-C-CA-CB
3	AAA	301	SAM	O-C-CA-CB
4	AAA	302	ADN	C3'-C4'-C5'-O5'

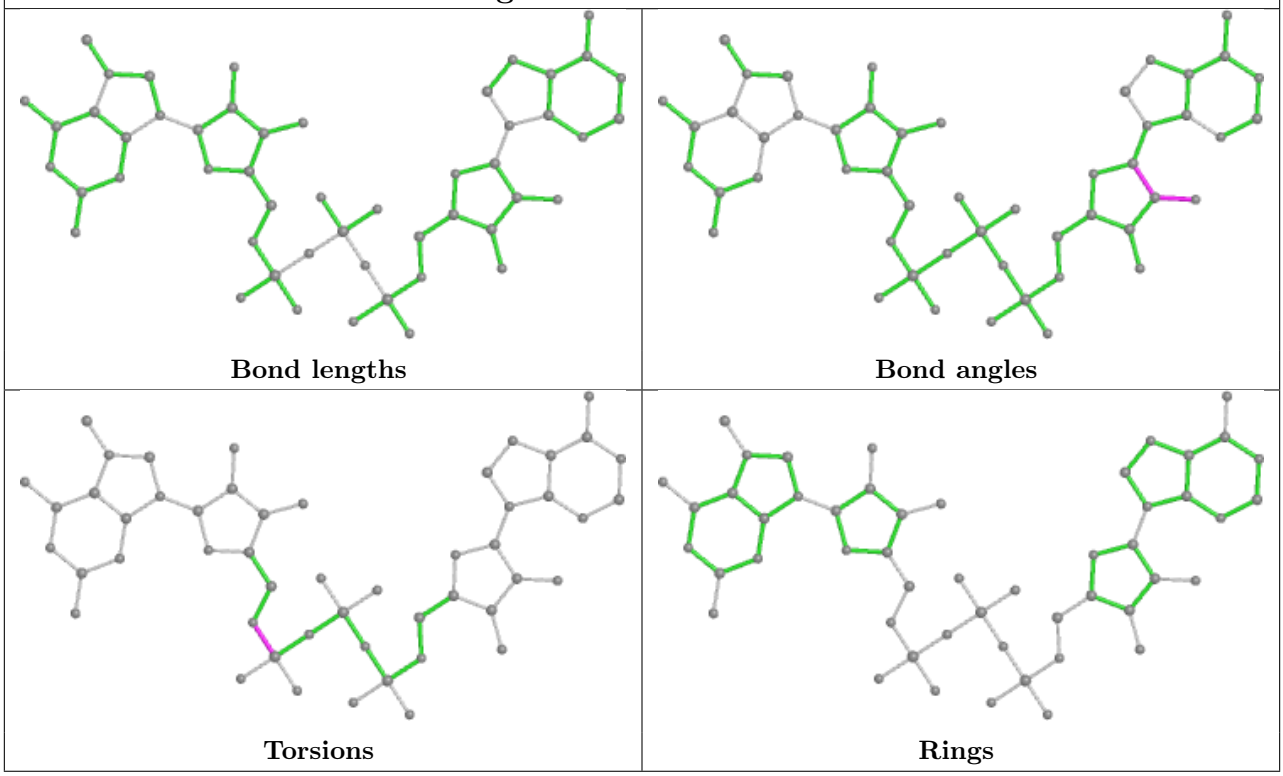
There are no ring outliers.

4 monomers are involved in 10 short contacts:

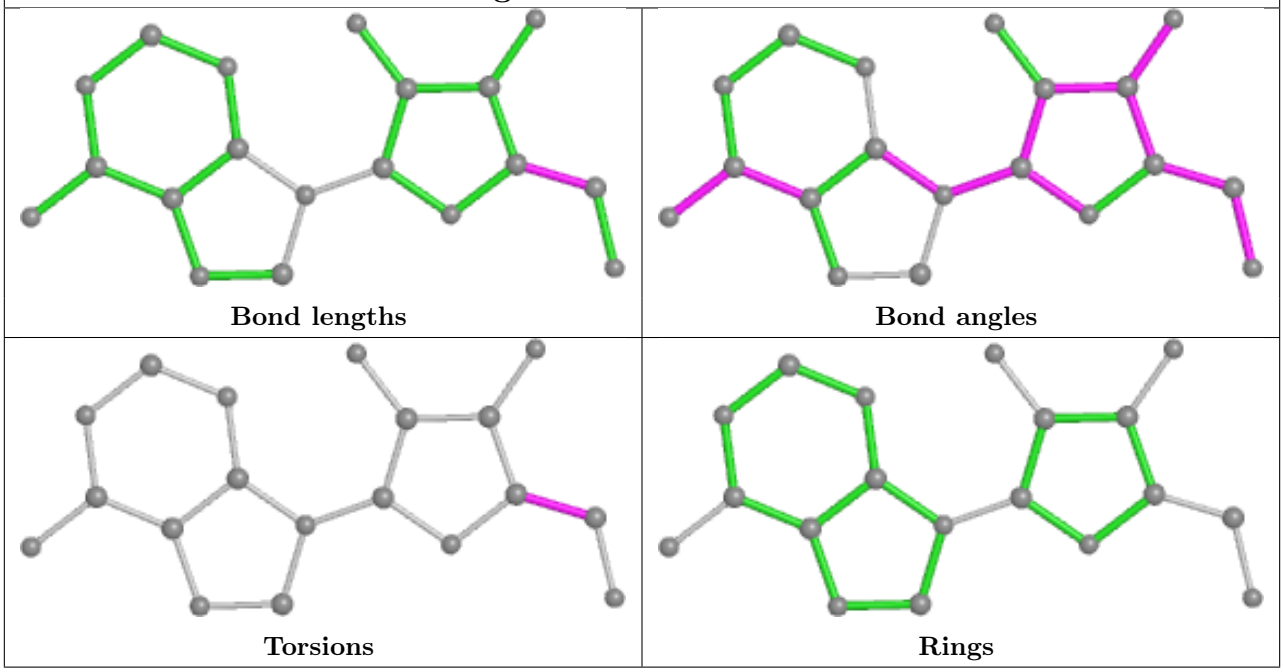
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	AAA	303	GTA	1	0
4	AAA	302	ADN	7	0
3	AAA	301	SAM	1	0
7	BBB	203	EDO	1	0

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 then 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.

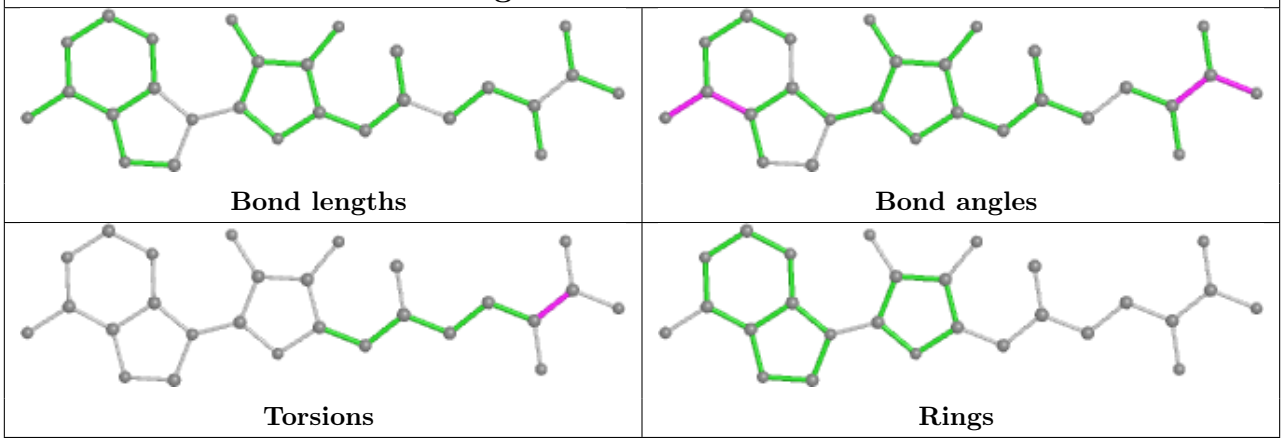
Ligand GTA AAA 303



Ligand ADN AAA 302



Ligand SAM AAA 301



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	AAA	298/298 (100%)	0.40	34 (11%)	5	3	24, 34, 68, 109	0
2	BBB	114/139 (82%)	0.85	22 (19%)	1	0	29, 49, 97, 129	0
All	All	412/437 (94%)	0.53	56 (13%)	3	2	24, 37, 81, 129	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	86	PRO	8.4
2	BBB	130	CYS	7.1
2	BBB	18	ALA	6.4
1	AAA	264	GLU	5.1
2	BBB	119	VAL	5.0
2	BBB	32	ALA	4.9
2	BBB	117	CYS	4.7
2	BBB	87	LYS	4.5
1	AAA	207	ILE	4.3
1	AAA	265	GLY	4.2
2	BBB	33	SER	4.1
2	BBB	34	GLY	4.0
2	BBB	120	CYS	4.0
1	AAA	205	PHE	3.9
2	BBB	22	ASP	3.9
2	BBB	85	ASN	3.8
1	AAA	206	LEU	3.8
1	AAA	169	ILE	3.7
1	AAA	31	GLY	3.6
1	AAA	267	ILE	3.6
2	BBB	118	THR	3.5
1	AAA	298	ASN	3.5
2	BBB	131	ASP	3.4
1	AAA	270	MET	3.4

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Mol	Chain	Res	Type	RSRZ
2	BBB	84	PRO	3.3
2	BBB	128	CYS	3.3
1	AAA	171	ILE	3.2
1	AAA	128	ILE	3.1
2	BBB	25	LYS	3.0
1	AAA	50	LEU	3.0
1	AAA	1	SER	3.0
1	AAA	85	LEU	3.0
2	BBB	30	TYR	3.0
1	AAA	263	LYS	3.0
2	BBB	23	ALA	3.0
2	BBB	29	ASP	2.9
1	AAA	127	ILE	2.9
1	AAA	140	THR	2.8
1	AAA	268	ASN	2.8
1	AAA	138	ASN	2.8
1	AAA	32	ASP	2.7
1	AAA	168	ALA	2.7
2	BBB	89	PHE	2.7
1	AAA	2	SER	2.6
1	AAA	126	LEU	2.5
1	AAA	193	PHE	2.5
1	AAA	261	SER	2.5
1	AAA	167	VAL	2.5
1	AAA	266	GLN	2.4
1	AAA	67	VAL	2.4
1	AAA	271	ILE	2.1
1	AAA	262	LEU	2.1
1	AAA	204	ALA	2.1
2	BBB	36	GLN	2.1
1	AAA	269	ASP	2.0
1	AAA	192	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

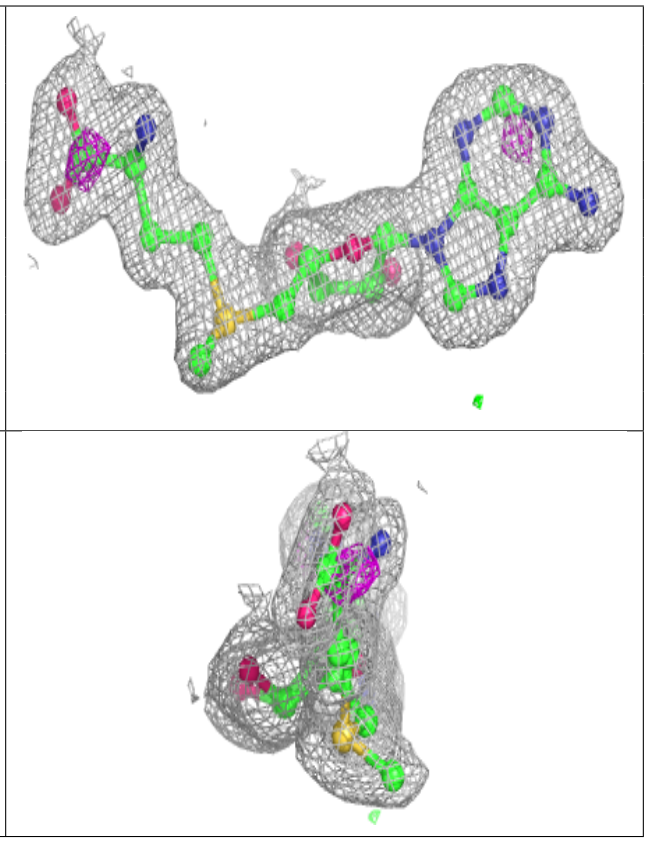
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	BBB	203	4/4	0.85	0.16	55,57,65,71	0
3	SAM	AAA	301	27/27	0.90	0.11	31,38,43,47	2
4	ADN	AAA	302	19/19	0.93	0.17	34,54,95,100	0
5	GTA	AAA	303	51/51	0.95	0.18	35,42,75,84	0
6	ZN	BBB	202	1/1	0.99	0.07	73,73,73,73	0
6	ZN	BBB	201	1/1	1.00	0.04	45,45,45,45	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.

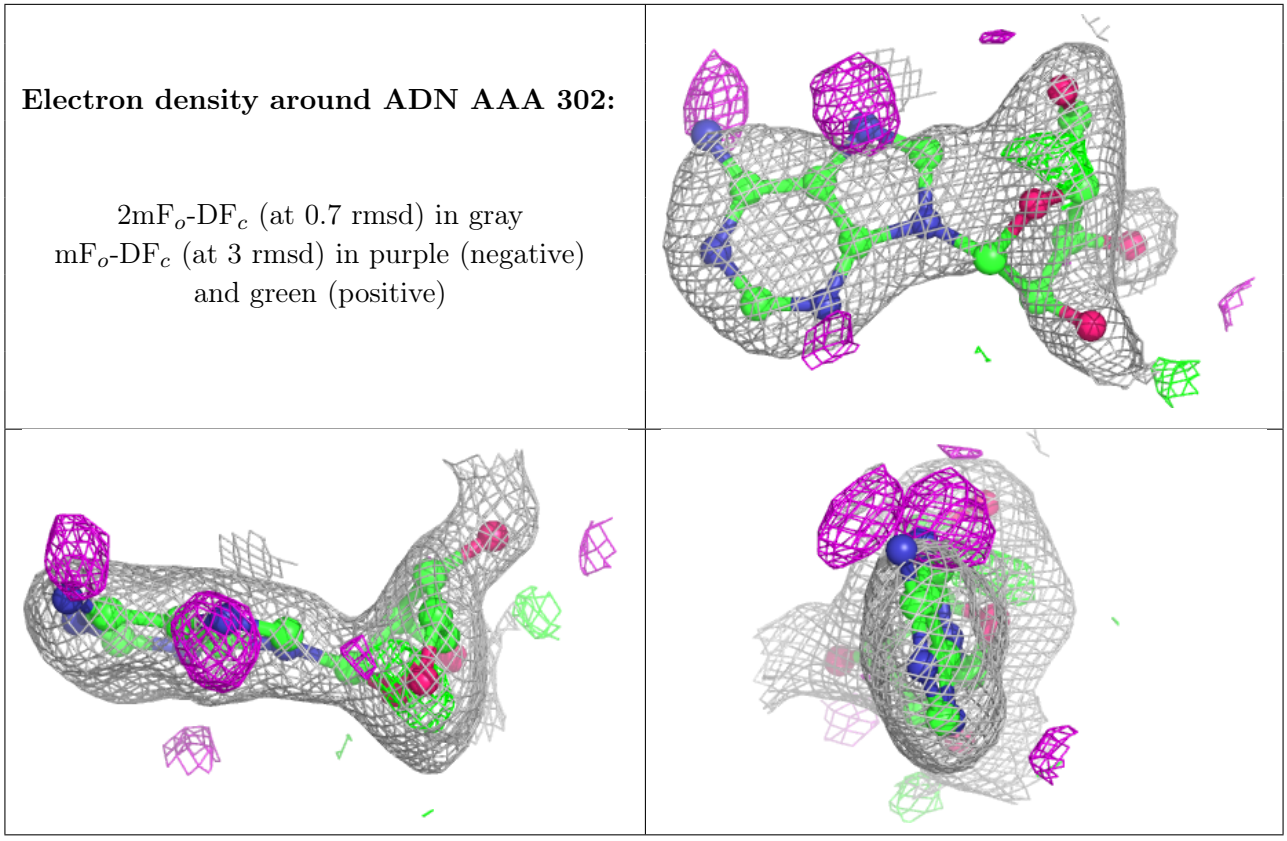
Electron density around SAM AAA 301:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



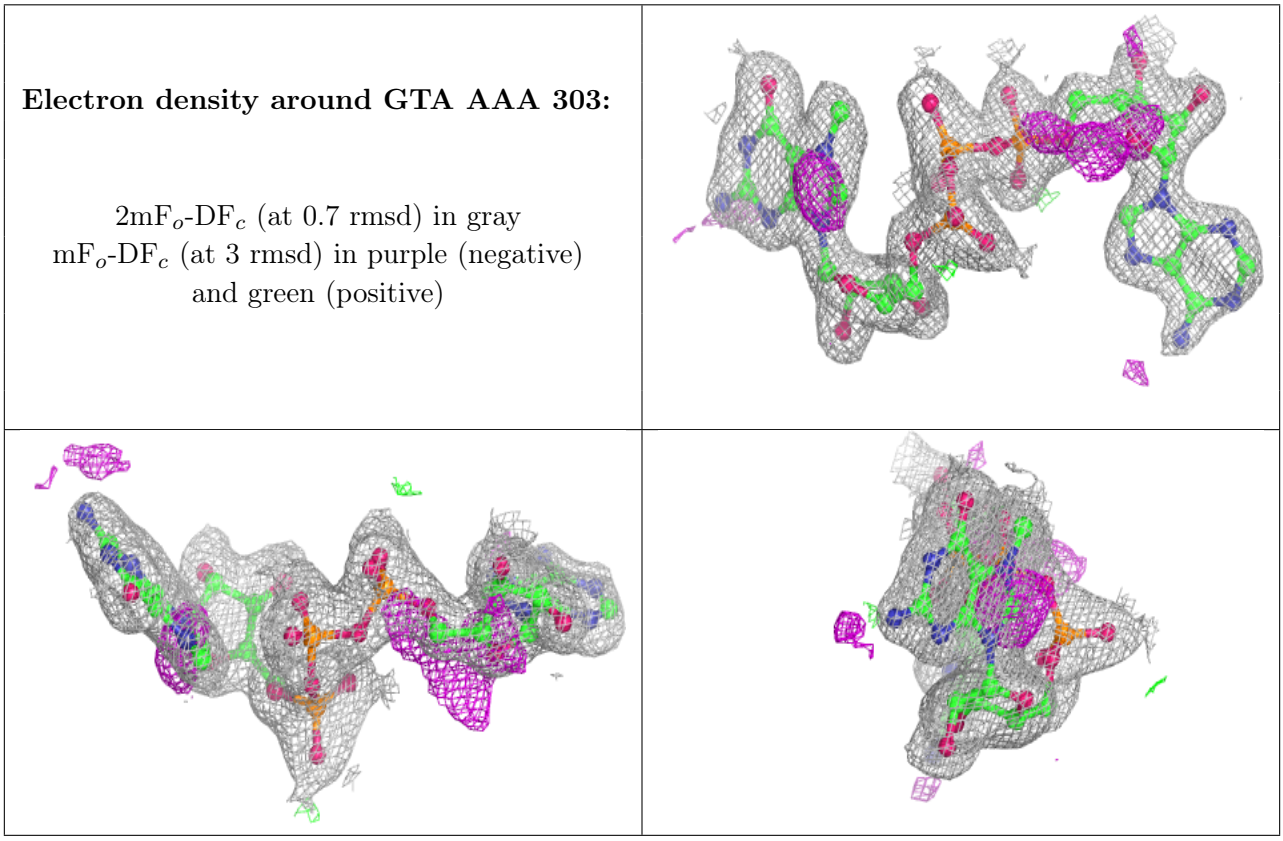
Electron density around ADN AAA 302:

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



Electron density around GTA AAA 303:

$2mF_o$-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.