



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:02 PM UTC

PDB ID : 9EML / pdb_00009eml
Title : SARS-CoV-2 methyltransferase nsp10-16 in complex with SAM and m7GpppA (Cap0-analog)/m7GpppAm (Cap1-analog)
Authors : Kremling, V.; Sprenger, J.; Oberthuer, D.; Kiene, A.
Deposited on : 2024-03-08
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

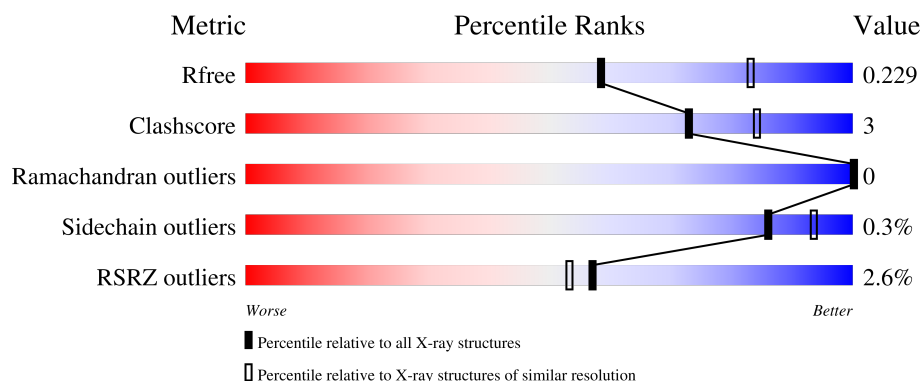
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	304	% 93% 6% .
2	B	140	5% 76% 6% 17%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 7135 atoms, of which 3412 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 nsp16.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	300	Total	C	H	N	O	S	0	6	0
			4806	1532	2404	407	446	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7097	GLU	-	expression tag	UNP P0DTD1
A	7098	ASN	-	expression tag	UNP P0DTD1
A	7099	LEU	-	expression tag	UNP P0DTD1
A	7100	TYR	-	expression tag	UNP P0DTD1
A	7101	PHE	-	expression tag	UNP P0DTD1
A	7102	GLN	-	expression tag	UNP P0DTD1

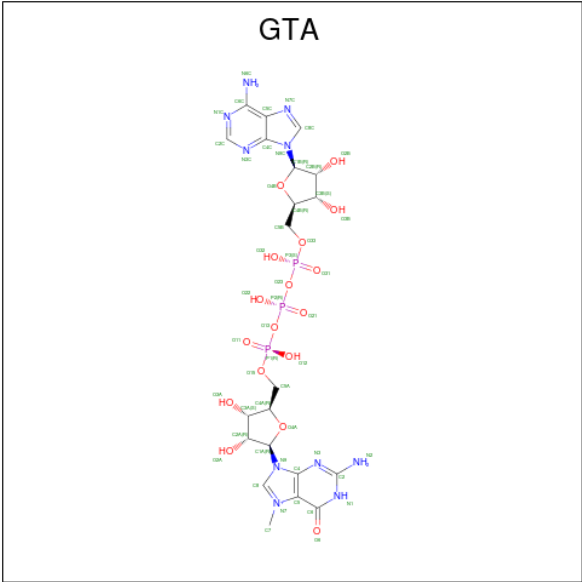
- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	116	Total	C	H	N	O	S	0	4	0
			1697	539	827	147	168	16			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4253	GLY	-	expression tag	UNP P0DTD1

- Molecule 3 is P1-7-METHYLGUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHATE (CCD ID: GTA) (formula: C₂₁H₃₀N₁₀O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	P	0	1
			78	21	27	10	17	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



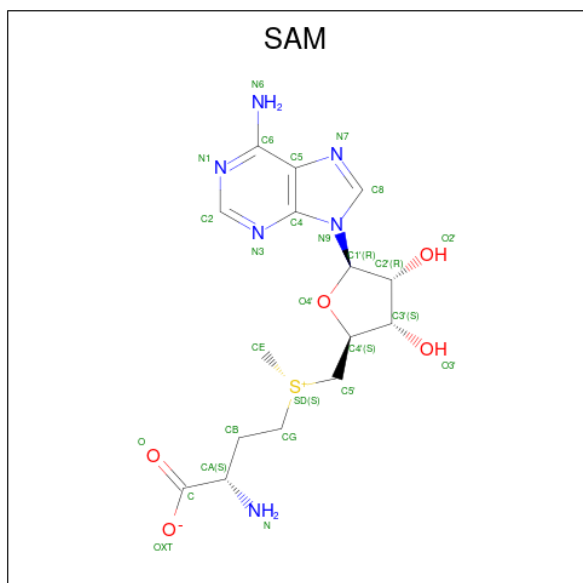
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0
4	A	1	10	2	6	2	0	0

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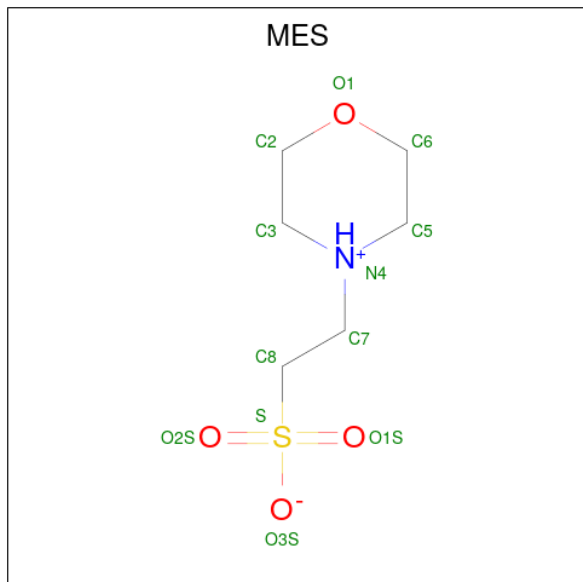
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



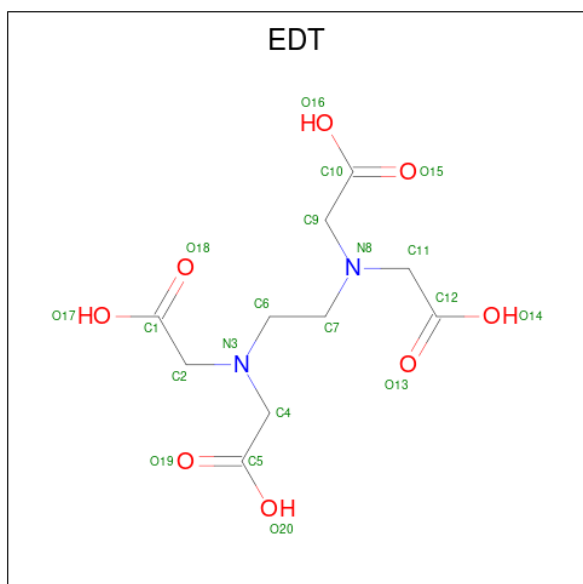
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	S	0	0
			49	15	22	6	5	1		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



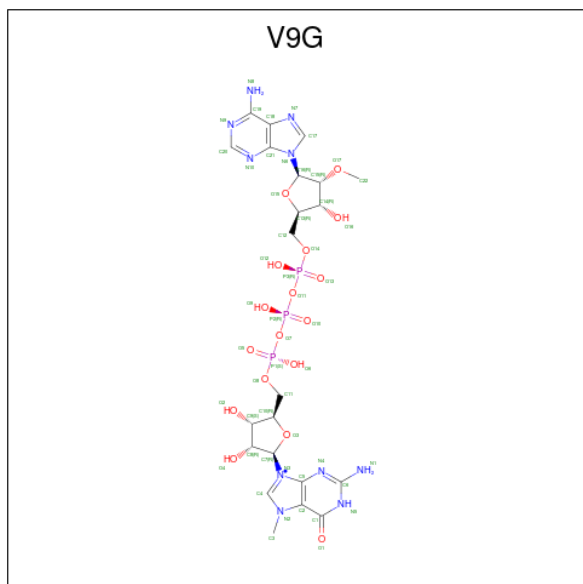
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 7 is {[-(BIS-CARBOXYMETHYL-AMINO)-ETHYL]-CARBOXYMETHYL-AMINO}-ACETIC ACID (CCD ID: EDT) (formula: $C_{10}H_{16}N_2O_8$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	0
			32	10	12	2	8		

- Molecule 8 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-(2'-O-METHYL)-ADENOSINE (CCD ID: V9G) (formula: $C_{22}H_{32}N_{10}O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	H	N	O	P	0	1
			81	22	29	10	17	3		

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	2	Total	Zn	0	0
			2	2		

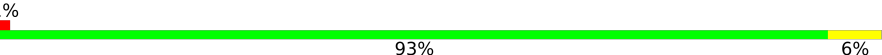
- Molecule 10 is water.

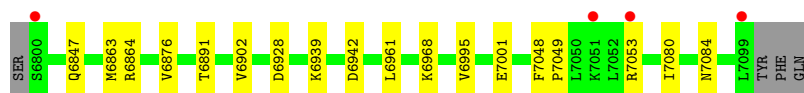
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	181	Total	O	0	0
			181	181		
10	B	54	Total	O	0	0
			54	54		

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 nsp16

Chain A:  93% 6%



- Molecule 2: Non-structural protein 10

Chain B:  5% 76% 6% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.74Å 167.74Å 52.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.07 – 2.40 49.07 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.07-2.40) 86.3 (49.07-2.40)	Depositor EDS
R_{merge}	0.32	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.28 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.178 , 0.240 0.180 , 0.229	Depositor DCC
R_{free} test set	2039 reflections (1.59%)	wwPDB-VP
Wilson B-factor (Å ²)	9.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7135	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: V9G, SAM, EDO, GTA, ZN, EDT, MES

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	0.53	0/2459	0.67	0/3331
2	B	0.48	0/902	0.65	0/1225
All	All	0.52	0/3361	0.66	0/4556

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	A	2402	2404	2394	12	0
2	B	870	827	812	6	0
3	A	51	27	24	2	0
4	A	44	66	66	1	0
4	B	8	12	12	0	0
5	A	27	22	21	1	0
6	A	12	13	12	0	0
7	A	20	12	12	0	0
8	A	52	29	0	1	0
9	B	2	0	0	0	0
10	A	181	0	0	1	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	54	0	0	2	0
All	All	3723	3412	3353	22	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (22) 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)
3:A:7201[A]:GTA:C4B	3:A:7201[A]:GTA:O4B	1.63	1.14
1:A:6968:LYS:NZ	1:A:7001:GLU:OE1	2.00	0.94
1:A:6928:ASP:OD1	1:A:6968:LYS:HE2	1.76	0.84
3:A:7201[A]:GTA:O4B	3:A:7201[A]:GTA:C5B	2.47	0.60
1:A:6847:GLN:OE1	1:A:6995:VAL:HG22	2.09	0.52
2:B:4316:MET:HG3	10:B:4550:HOH:O	2.10	0.51
1:A:6864:ARG:NH2	1:A:7084:ASN:O	2.45	0.49
1:A:6876:VAL:HG12	1:A:6902:VAL:CG2	2.43	0.49
1:A:6876:VAL:HG12	1:A:6902:VAL:HG22	1.97	0.47
2:B:4316:MET:HA	10:B:4550:HOH:O	2.16	0.46
5:A:7203:SAM:HE2	8:A:7216[B]:V9G:C22	2.45	0.46
1:A:7048:PHE:N	1:A:7049:PRO:CD	2.79	0.45
2:B:4309:THR:HG21	2:B:4313:GLU:HG3	1.99	0.45
2:B:4305:GLY:HA2	2:B:4318:GLN:OE1	2.16	0.45
1:A:6863:MET:HB3	1:A:6891:THR:HG23	1.99	0.45
2:B:4307:ALA:HB1	2:B:4376:TRP:CE2	2.53	0.44
1:A:6928:ASP:CG	1:A:6968:LYS:HE2	2.42	0.43
2:B:4327:CYS:HB2	2:B:4345:LEU:HD12	2.02	0.41
1:A:6939:LYS:NZ	1:A:6942:ASP:OD1	2.54	0.41
1:A:7048:PHE:HB3	1:A:7049:PRO:HD3	2.03	0.41
4:A:7211:EDO:C2	10:A:7316:HOH:O	2.68	0.41
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:7400:HOH:O	10:A:7400:HOH:O[5_555]	1.90	0.30
10:A:7447:HOH:O	10:A:7474:HOH:O[5_555]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/304 (100%)	294 (97%)	10 (3%)	0	100	100
2	B	118/140 (84%)	112 (95%)	6 (5%)	0	100	100
All	All	422/444 (95%)	406 (96%)	16 (4%)	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	
1	A	266/264 (101%)	264 (99%)	2 (1%)	73	86
2	B	98/113 (87%)	98 (100%)	0	100	100
All	All	364/377 (97%)	362 (100%)	2 (0%)	86	91

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7053[A]	ARG
1	A	7053[B]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7036	GLN

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Mol	Chain	Res	Type
2	B	4301	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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$
8	V9G	A	7216[B]	-	55,57,57	4.59	26 (47%)	78,89,89	2.11	23 (29%)
3	GTA	A	7201[A]	-	56,56,56	3.49	24 (42%)	83,88,88	1.71	16 (19%)
4	EDO	A	7209	-	3,3,3	0.66	0	2,2,2	0.26	0
4	EDO	A	7205	-	3,3,3	0.49	0	2,2,2	0.39	0
4	EDO	A	7207	-	3,3,3	0.51	0	2,2,2	0.60	0
4	EDO	A	7212	-	3,3,3	0.54	0	2,2,2	0.41	0
6	MES	A	7204	-	12,12,12	2.01	2 (16%)	15,16,16	2.19	5 (33%)
4	EDO	B	4403	-	3,3,3	0.50	0	2,2,2	0.84	0
7	EDT	A	7213	-	19,19,19	1.56	4 (21%)	24,24,24	1.05	0
4	EDO	A	7208	-	3,3,3	0.53	0	2,2,2	0.08	0
4	EDO	A	7210	-	3,3,3	0.53	0	2,2,2	0.32	0
4	EDO	A	7202	-	3,3,3	0.36	0	2,2,2	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	7206	-	3,3,3	0.46	0	2,2,2	0.24	0
4	EDO	A	7211	-	3,3,3	0.62	0	2,2,2	0.32	0
4	EDO	A	7214	-	3,3,3	0.42	0	2,2,2	0.26	0
4	EDO	B	4404	-	3,3,3	0.44	0	2,2,2	0.55	0
5	SAM	A	7203	-	27,29,29	3.79	13 (48%)	34,42,42	2.19	15 (44%)
4	EDO	A	7215	-	3,3,3	0.53	0	2,2,2	0.72	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
8	V9G	A	7216[B]	-	-	7/32/94/94	0/6/6/6
3	GTA	A	7201[A]	-	-	6/32/64/64	0/6/6/6
4	EDO	A	7209	-	-	1/1/1/1	-
4	EDO	A	7205	-	-	1/1/1/1	-
4	EDO	A	7207	-	-	1/1/1/1	-
4	EDO	A	7212	-	-	1/1/1/1	-
6	MES	A	7204	-	-	0/6/14/14	0/1/1/1
4	EDO	B	4403	-	-	1/1/1/1	-
7	EDT	A	7213	-	-	9/21/21/21	-
4	EDO	A	7208	-	-	1/1/1/1	-
4	EDO	A	7210	-	-	1/1/1/1	-
4	EDO	A	7202	-	-	1/1/1/1	-
4	EDO	A	7206	-	-	1/1/1/1	-
4	EDO	A	7211	-	-	0/1/1/1	-
4	EDO	A	7214	-	-	1/1/1/1	-
4	EDO	B	4404	-	-	0/1/1/1	-
5	SAM	A	7203	-	-	2/17/33/33	0/3/3/3
4	EDO	A	7215	-	-	1/1/1/1	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	7216[B]	V9G	C8-C7	-17.14	1.30	1.53
8	A	7216[B]	V9G	C15-C16	-11.78	1.24	1.53
8	A	7216[B]	V9G	C14-C13	-9.71	1.28	1.53
5	A	7203	SAM	C2'-C3'	-9.70	1.27	1.53
3	A	7201[A]	GTA	C3B-C4B	-9.51	1.28	1.53
3	A	7201[A]	GTA	O4A-C1A	8.82	1.62	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	7216[B]	V9G	P3-O11	8.63	1.68	1.59
5	A	7203	SAM	O4'-C4'	-8.42	1.26	1.45
3	A	7201[A]	GTA	O4B-C4B	8.34	1.63	1.45
8	A	7216[B]	V9G	O15-C16	8.20	1.61	1.42
8	A	7216[B]	V9G	C14-C15	7.91	1.70	1.53
8	A	7216[B]	V9G	O3-C10	-7.75	1.27	1.45
8	A	7216[B]	V9G	C5-N4	7.55	1.48	1.33
3	A	7201[A]	GTA	O4A-C4A	-7.41	1.28	1.45
3	A	7201[A]	GTA	C2A-C1A	-6.98	1.31	1.53
5	A	7203	SAM	C3'-C4'	6.79	1.70	1.53
5	A	7203	SAM	O4'-C1'	6.64	1.57	1.42
5	A	7203	SAM	C6-N6	6.30	1.50	1.34
3	A	7201[A]	GTA	O4B-C1B	-6.29	1.27	1.42
8	A	7216[B]	V9G	P1-O7	6.17	1.66	1.59
6	A	7204	MES	C8-S	-6.09	1.69	1.77
8	A	7216[B]	V9G	C6-N1	5.92	1.48	1.34
3	A	7201[A]	GTA	C4-N3	5.87	1.47	1.34
8	A	7216[B]	V9G	C19-N8	5.58	1.48	1.34
8	A	7216[B]	V9G	C6-N4	5.36	1.46	1.33
3	A	7201[A]	GTA	P3-O23	5.29	1.65	1.59
8	A	7216[B]	V9G	P2-O11	5.19	1.65	1.59
3	A	7201[A]	GTA	C2-N3	5.07	1.45	1.33
3	A	7201[A]	GTA	P2-O23	4.94	1.64	1.59
8	A	7216[B]	V9G	O4-C8	4.76	1.54	1.43
3	A	7201[A]	GTA	C6C-N6C	4.76	1.46	1.34
5	A	7203	SAM	C1'-N9	-4.73	1.33	1.46
3	A	7201[A]	GTA	C5-N7	-4.31	1.34	1.39
3	A	7201[A]	GTA	C2-N2	4.30	1.44	1.34
3	A	7201[A]	GTA	O2A-C2A	4.09	1.53	1.43
8	A	7216[B]	V9G	C2-C1	3.91	1.53	1.43
3	A	7201[A]	GTA	P1-O13	3.58	1.63	1.59
8	A	7216[B]	V9G	O15-C13	3.51	1.52	1.45
8	A	7216[B]	V9G	P2-O7	3.46	1.63	1.59
5	A	7203	SAM	O3'-C3'	3.45	1.51	1.43
5	A	7203	SAM	C8-N9	-3.43	1.31	1.37
3	A	7201[A]	GTA	O3B-C3B	3.41	1.51	1.43
5	A	7203	SAM	C4-N3	3.40	1.40	1.34
3	A	7201[A]	GTA	C5-C6	3.32	1.52	1.43
8	A	7216[B]	V9G	C1-N5	3.08	1.44	1.38
3	A	7201[A]	GTA	O3A-C3A	-3.00	1.35	1.43
7	A	7213	EDT	C9-C10	2.90	1.57	1.51
8	A	7216[B]	V9G	C17-N6	-2.90	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	7216[B]	V9G	C6-N5	2.89	1.44	1.37
5	A	7203	SAM	O-C	2.79	1.30	1.22
3	A	7201[A]	GTA	C2-N1	2.70	1.44	1.37
3	A	7201[A]	GTA	P2-O13	2.69	1.62	1.59
3	A	7201[A]	GTA	C8C-N9C	-2.64	1.33	1.37
3	A	7201[A]	GTA	O2B-C2B	-2.63	1.36	1.43
8	A	7216[B]	V9G	O17-C15	2.46	1.48	1.42
7	A	7213	EDT	O15-C10	2.44	1.30	1.22
3	A	7201[A]	GTA	O6-C6	-2.39	1.19	1.23
5	A	7203	SAM	CG-CB	2.37	1.59	1.51
8	A	7216[B]	V9G	C18-N7	-2.36	1.34	1.39
6	A	7204	MES	O2S-S	2.35	1.51	1.45
8	A	7216[B]	V9G	C16-N6	2.35	1.52	1.46
3	A	7201[A]	GTA	C6-N1	2.33	1.43	1.38
7	A	7213	EDT	C2-C1	2.31	1.56	1.51
7	A	7213	EDT	O18-C1	2.27	1.29	1.22
5	A	7203	SAM	C5-C6	2.20	1.47	1.41
8	A	7216[B]	V9G	C21-N6	-2.19	1.33	1.37
8	A	7216[B]	V9G	C5-N3	-2.17	1.33	1.37
5	A	7203	SAM	O2'-C2'	2.11	1.48	1.43
8	A	7216[B]	V9G	O2-C9	-2.09	1.37	1.43

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	7216[B]	V9G	C6-N4-C5	7.43	119.71	112.71
6	A	7204	MES	O2S-S-C8	5.58	115.15	106.73
8	A	7216[B]	V9G	N4-C5-N3	5.08	131.68	125.61
8	A	7216[B]	V9G	C2-C1-N5	4.83	119.44	110.94
8	A	7216[B]	V9G	C15-C16-N6	-4.74	105.95	113.75
5	A	7203	SAM	C5-C4-N3	-4.71	120.23	126.72
3	A	7201[A]	GTA	N3C-C2C-N1C	-4.69	121.48	128.58
8	A	7216[B]	V9G	N10-C20-N9	-4.63	121.57	128.58
3	A	7201[A]	GTA	C5C-C4C-N3C	-4.60	120.38	126.72
8	A	7216[B]	V9G	C18-C21-N10	-4.52	120.49	126.72
3	A	7201[A]	GTA	C2-N3-C4	4.34	119.78	112.30
3	A	7201[A]	GTA	C5-C4-N3	-4.04	120.51	128.15
5	A	7203	SAM	N3-C2-N1	-4.04	122.47	128.58
8	A	7216[B]	V9G	C10-O3-C7	-3.84	105.83	109.74
3	A	7201[A]	GTA	C5-C6-N1	3.76	119.61	111.84
5	A	7203	SAM	C4-C5-N7	-3.67	106.39	110.58
3	A	7201[A]	GTA	N3C-C4C-N9C	3.64	133.36	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	7216[B]	V9G	C20-N10-C21	3.41	120.15	111.83
3	A	7201[A]	GTA	C2C-N3C-C4C	3.41	120.15	111.83
8	A	7216[B]	V9G	C2-C5-N4	-3.41	120.52	126.90
6	A	7204	MES	C5-N4-C3	3.35	116.05	108.84
3	A	7201[A]	GTA	O6-C6-C5	-3.34	120.55	128.01
5	A	7203	SAM	C2-N3-C4	3.23	119.71	111.83
8	A	7216[B]	V9G	N10-C21-N6	3.20	132.62	127.17
5	A	7203	SAM	C5-N7-C8	3.13	108.37	103.45
5	A	7203	SAM	N3-C4-N9	3.12	132.47	127.17
6	A	7204	MES	O1S-S-C8	3.11	111.43	106.73
3	A	7201[A]	GTA	C4C-N9C-C8C	3.11	109.00	105.74
5	A	7203	SAM	N9-C8-N7	-3.10	109.53	113.94
3	A	7201[A]	GTA	N9C-C8C-N7C	-3.07	109.58	113.94
3	A	7201[A]	GTA	C2-N1-C6	-2.99	119.68	125.11
8	A	7216[B]	V9G	C6-N5-C1	-2.97	119.73	125.11
8	A	7216[B]	V9G	C15-C14-C13	2.93	108.30	101.99
8	A	7216[B]	V9G	O9-P2-O11	2.91	115.14	107.27
8	A	7216[B]	V9G	N6-C17-N7	-2.87	109.86	113.94
8	A	7216[B]	V9G	O1-C1-C2	-2.85	120.63	127.62
5	A	7203	SAM	O4'-C1'-N9	2.84	113.54	108.09
3	A	7201[A]	GTA	N9-C4-N3	2.82	131.59	125.95
8	A	7216[B]	V9G	C21-C18-N7	-2.77	107.42	110.58
8	A	7216[B]	V9G	C9-C8-C7	2.74	104.79	100.84
3	A	7201[A]	GTA	O22-P2-O23	2.62	114.34	107.27
3	A	7201[A]	GTA	C5C-N7C-C8C	2.60	107.54	103.45
3	A	7201[A]	GTA	C4C-C5C-N7C	-2.59	107.62	110.58
5	A	7203	SAM	C3'-C2'-C1'	2.57	106.33	101.46
8	A	7216[B]	V9G	C18-N7-C17	2.56	107.47	103.45
5	A	7203	SAM	C4-N9-C8	2.55	108.41	105.74
5	A	7203	SAM	CB-CA-N	2.53	116.72	110.12
6	A	7204	MES	O3S-S-O1S	-2.51	105.12	111.40
8	A	7216[B]	V9G	C21-N6-C17	2.49	108.36	105.74
8	A	7216[B]	V9G	O17-C15-C16	2.48	113.69	108.99
8	A	7216[B]	V9G	O12-P3-O11	2.39	113.74	107.27
5	A	7203	SAM	O4'-C1'-C2'	-2.34	101.61	106.62
5	A	7203	SAM	O3'-C3'-C4'	-2.22	104.71	111.08
8	A	7216[B]	V9G	O16-C14-C15	-2.18	105.09	111.19
8	A	7216[B]	V9G	C13-O15-C16	-2.15	104.72	109.47
5	A	7203	SAM	C4'-O4'-C1'	-2.15	104.73	109.47
5	A	7203	SAM	O3'-C3'-C2'	2.08	118.50	111.82
6	A	7204	MES	O3S-S-C8	-2.04	102.02	106.00
3	A	7201[A]	GTA	C2A-C3A-C4A	-2.02	98.71	102.61

There are no chirality outliers.

All (35) torsion outliers are listed below:

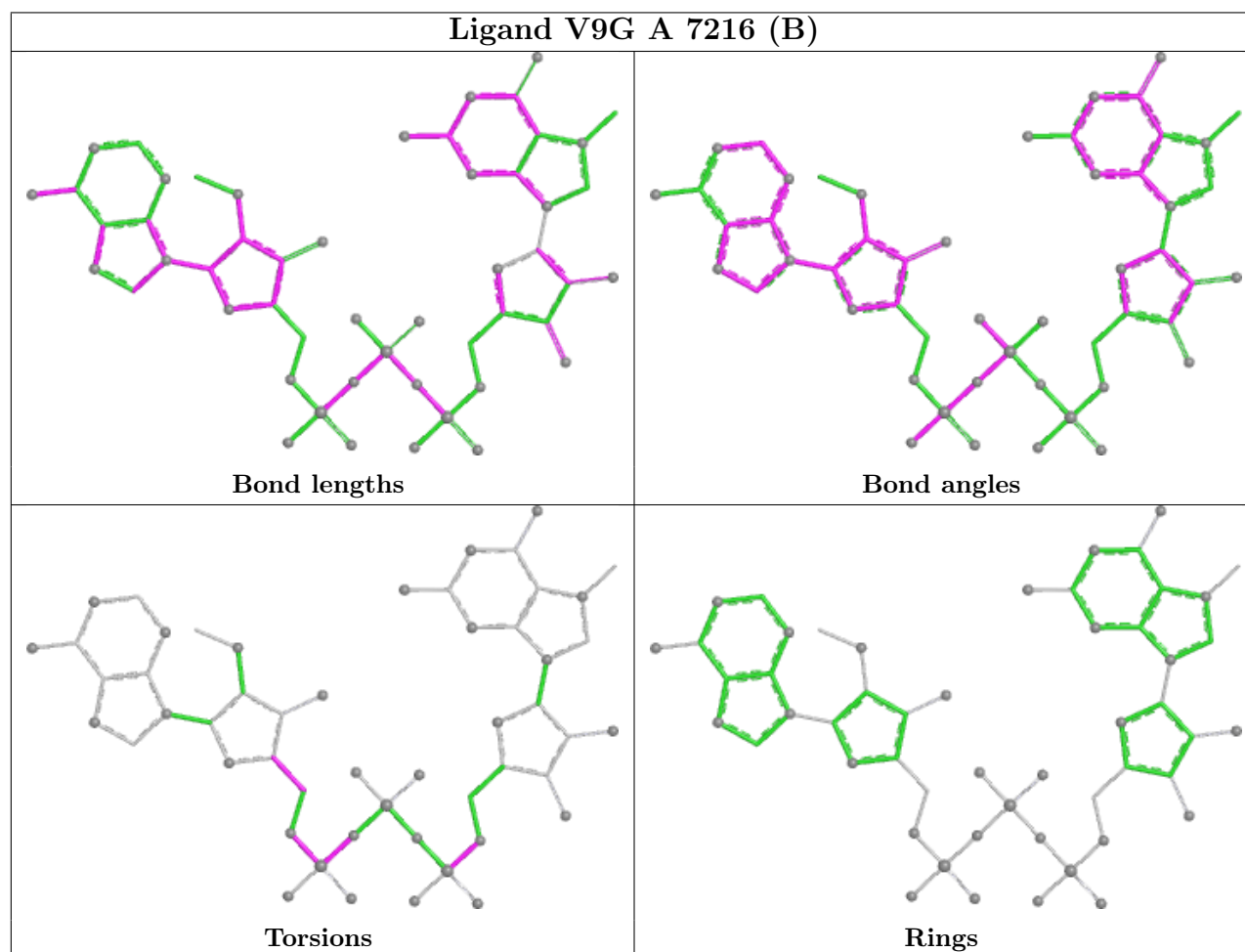
Mol	Chain	Res	Type	Atoms
3	A	7201[A]	GTA	C5A-O15-P1-O11
3	A	7201[A]	GTA	C5A-O15-P1-O13
3	A	7201[A]	GTA	C5B-O33-P3-O32
7	A	7213	EDT	O15-C10-C9-N8
8	A	7216[B]	V9G	C12-O14-P3-O13
8	A	7216[B]	V9G	C11-O8-P1-O7
8	A	7216[B]	V9G	C11-O8-P1-O6
7	A	7213	EDT	O16-C10-C9-N8
3	A	7201[A]	GTA	O4B-C4B-C5B-O33
7	A	7213	EDT	N3-C6-C7-N8
8	A	7216[B]	V9G	O14-C12-C13-O15
4	A	7202	EDO	O1-C1-C2-O2
4	A	7205	EDO	O1-C1-C2-O2
4	A	7210	EDO	O1-C1-C2-O2
3	A	7201[A]	GTA	C3B-C4B-C5B-O33
7	A	7213	EDT	C6-C7-N8-C11
5	A	7203	SAM	OXT-C-CA-CB
5	A	7203	SAM	O-C-CA-CB
7	A	7213	EDT	C1-C2-N3-C4
7	A	7213	EDT	C1-C2-N3-C6
3	A	7201[A]	GTA	C5B-O33-P3-O23
8	A	7216[B]	V9G	C12-O14-P3-O11
7	A	7213	EDT	C6-C7-N8-C9
8	A	7216[B]	V9G	P2-O11-P3-O12
4	A	7208	EDO	O1-C1-C2-O2
4	A	7209	EDO	O1-C1-C2-O2
4	A	7214	EDO	O1-C1-C2-O2
4	A	7212	EDO	O1-C1-C2-O2
4	A	7215	EDO	O1-C1-C2-O2
4	B	4403	EDO	O1-C1-C2-O2
4	A	7206	EDO	O1-C1-C2-O2
4	A	7207	EDO	O1-C1-C2-O2
8	A	7216[B]	V9G	P2-O11-P3-O13
7	A	7213	EDT	C12-C11-N8-C7
7	A	7213	EDT	C5-C4-N3-C2

There are no ring outliers.

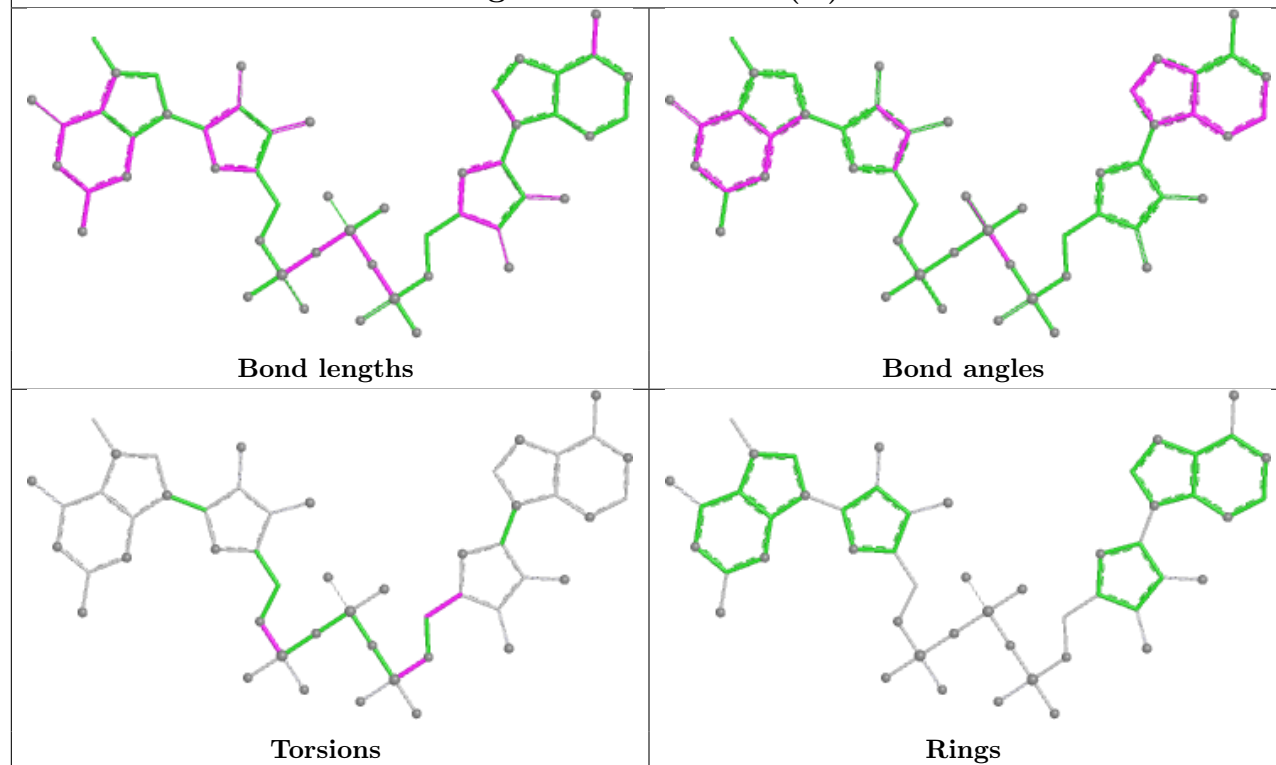
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	7216[B]	V9G	1	0
3	A	7201[A]	GTA	2	0
4	A	7211	EDO	1	0
5	A	7203	SAM	1	0

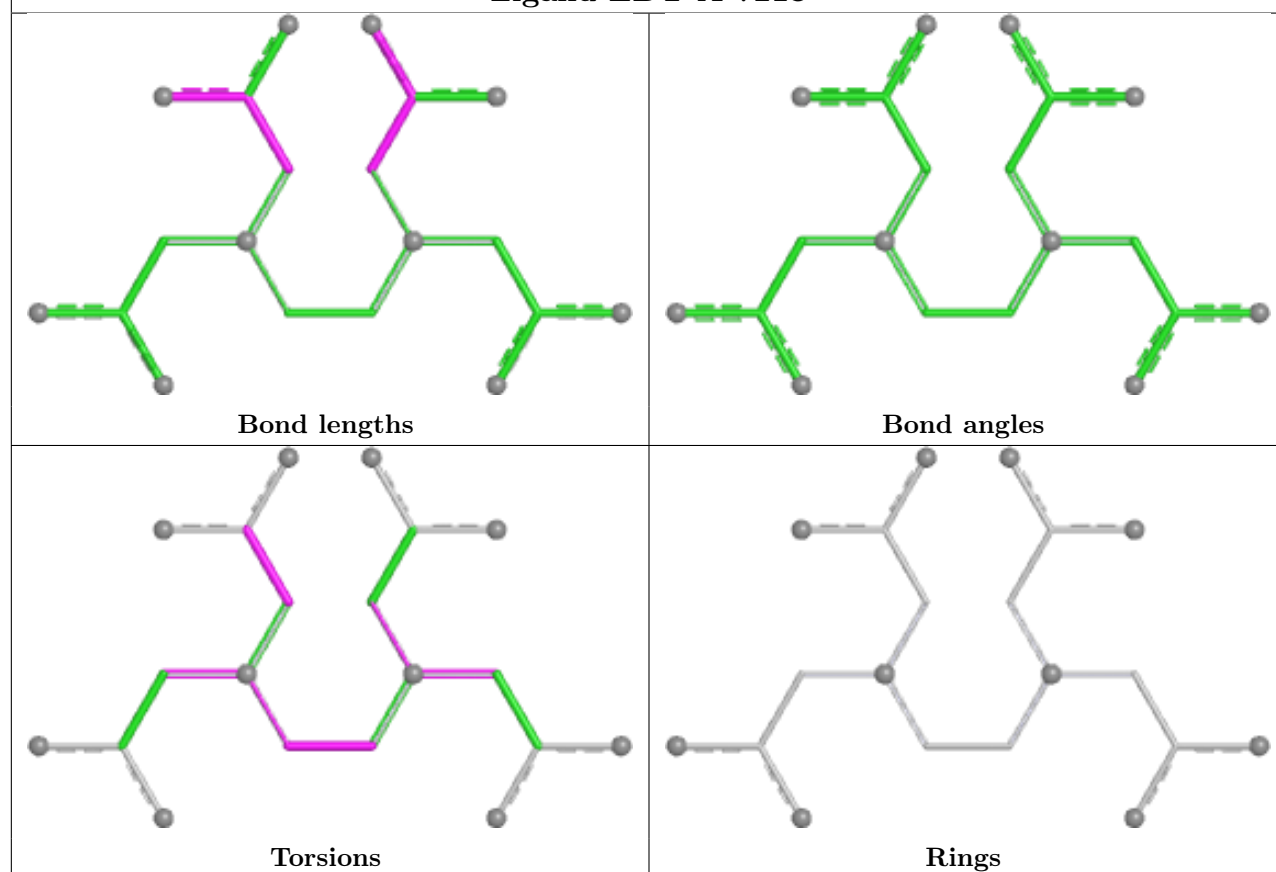
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

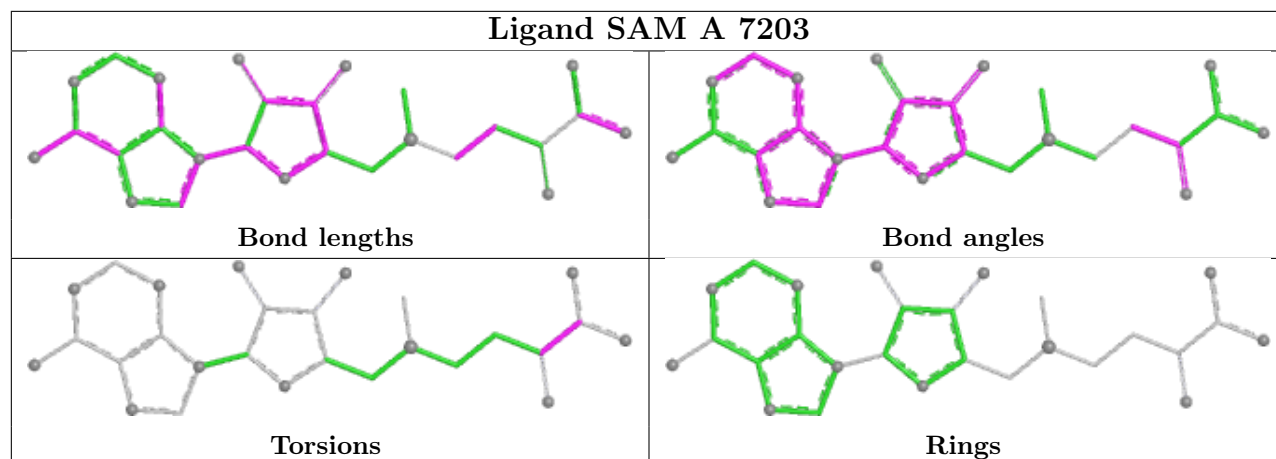


Ligand GTA A 7201 (A)



Ligand EDT A 7213





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	A	300/304 (98%)	-0.32	4 (1%) 75 71	25, 50, 81, 118	5 (1%)
2	B	116/140 (82%)	0.05	7 (6%) 27 24	34, 61, 100, 116	2 (1%)
All	All	416/444 (93%)	-0.22	11 (2%) 57 53	25, 53, 90, 118	7 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4289[A]	GLN	6.1
1	A	7051[A]	LYS	6.1
1	A	7099	LEU	5.4
2	B	4270	CYS	3.5
1	A	7053[A]	ARG	3.2
1	A	6800	SER	3.0
2	B	4385	GLN	3.0
2	B	4271	ALA	2.9
2	B	4342	PHE	2.5
2	B	4339	PRO	2.4
2	B	4368[A]	THR	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

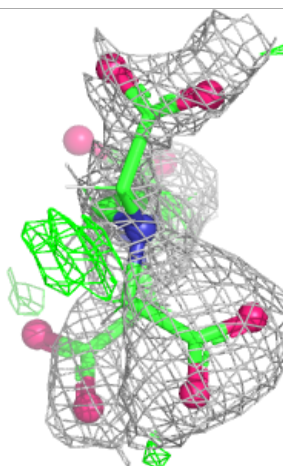
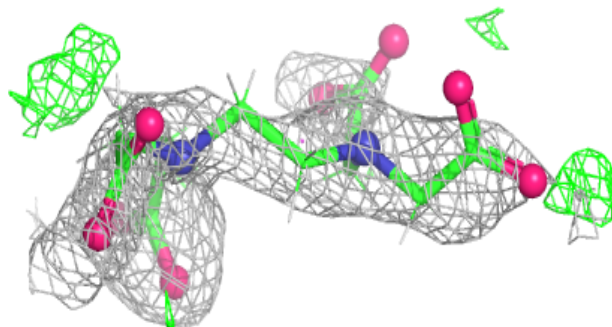
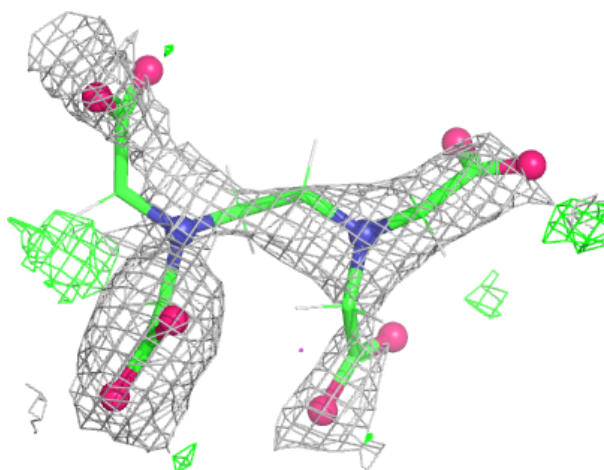
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	A	7208	4/4	0.81	0.28	75,89,100,120	0
4	EDO	A	7215	4/4	0.83	0.24	68,83,99,99	0
4	EDO	B	4404	4/4	0.83	0.19	70,84,95,114	0
7	EDT	A	7213	20/20	0.84	0.24	62,90,111,113	32
4	EDO	A	7205	4/4	0.85	0.20	69,82,98,98	0
6	MES	A	7204	12/12	0.87	0.16	60,88,134,152	0
4	EDO	A	7207	4/4	0.89	0.18	76,92,106,106	0
4	EDO	A	7212	4/4	0.89	0.20	72,88,112,112	0
4	EDO	A	7202	4/4	0.90	0.18	53,77,94,110	0
4	EDO	A	7209	4/4	0.90	0.20	61,89,109,109	0
4	EDO	B	4403	4/4	0.90	0.16	57,79,100,100	0
4	EDO	A	7206	4/4	0.91	0.16	58,74,90,108	0
4	EDO	A	7214	4/4	0.94	0.14	51,74,89,95	0
4	EDO	A	7211	4/4	0.95	0.13	48,62,95,102	0
5	SAM	A	7203	27/27	0.96	0.09	43,62,88,92	0
8	V9G	A	7216[B]	52/52	0.96	0.08	36,56,77,95	81
3	GTA	A	7201[A]	51/51	0.97	0.08	36,55,79,95	78
4	EDO	A	7210	4/4	0.97	0.10	50,72,86,86	0
9	ZN	B	4402	1/1	0.99	0.03	75,75,75,75	0
9	ZN	B	4401	1/1	1.00	0.02	47,47,47,47	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.

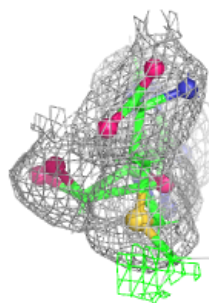
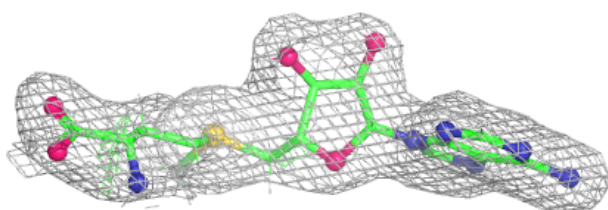
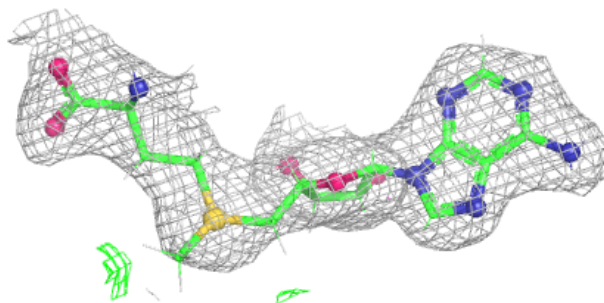
Electron density around EDT A 7213:

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

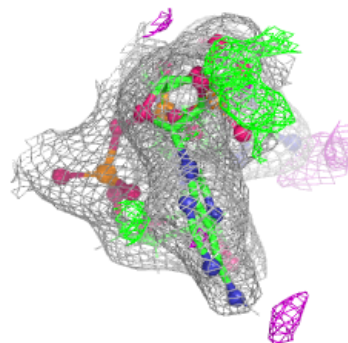
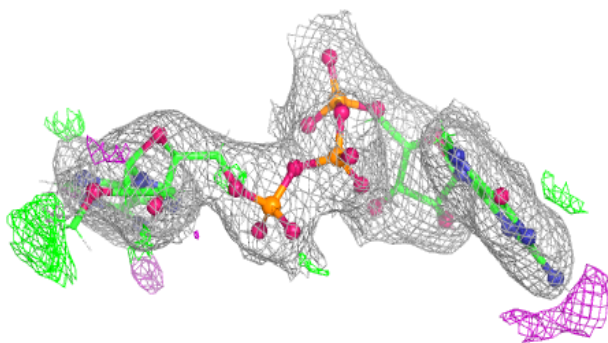
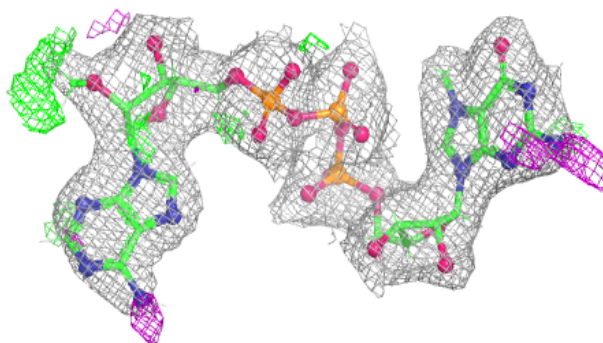


Electron density around SAM A 7203:

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

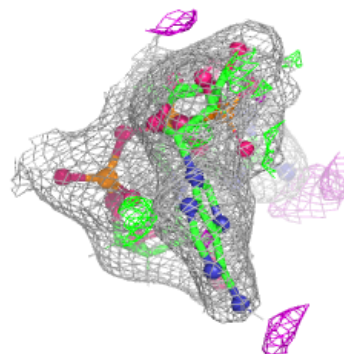
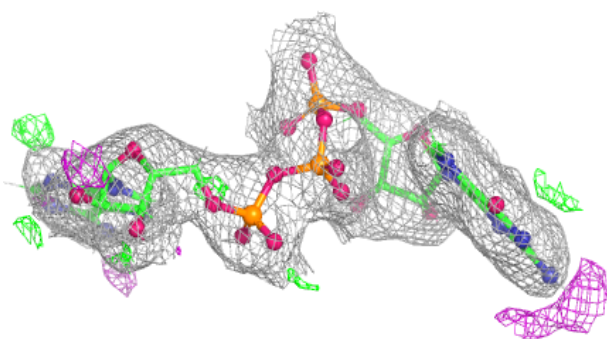
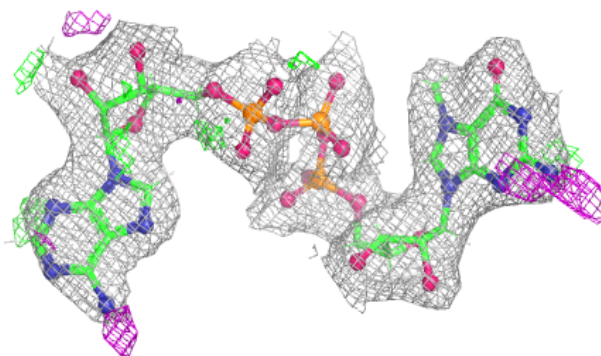
**Electron density around V9G A 7216 (B):**

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



Electron density around GTA A 7201 (A):

$2mF_o-DF_c$ (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.