



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2024 – 03:13 pm GMT

PDB ID : 9EMV
Title : SARS-CoV-2 nsp10-16 methyltransferase in complex with Sangivamycin and m7GpppA (Cap0-analog)/m7GpppAm (Cap1-analog)
Authors : Kremling, V.; Sprenger, J.; Oberthuer, D.; Scheer, T.E.S.
Deposited on : 2024-03-11
Resolution : 2.34 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

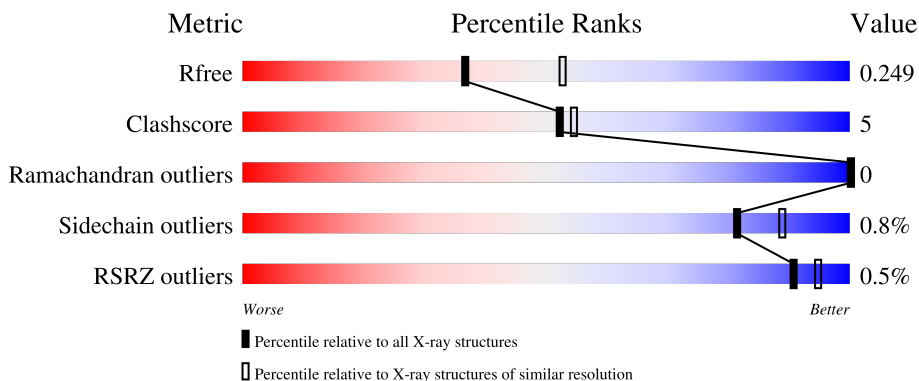
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


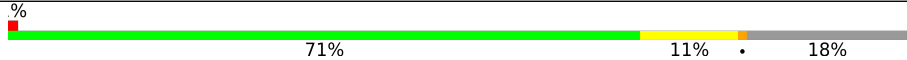
The reported resolution of this entry is 2.34 Å.

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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	
2	B	140	

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6872 atoms, of which 3287 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	
			Total	C	H	N	O				S
1	A	300	4719	1523	2330	406	443	17	0	4	0

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

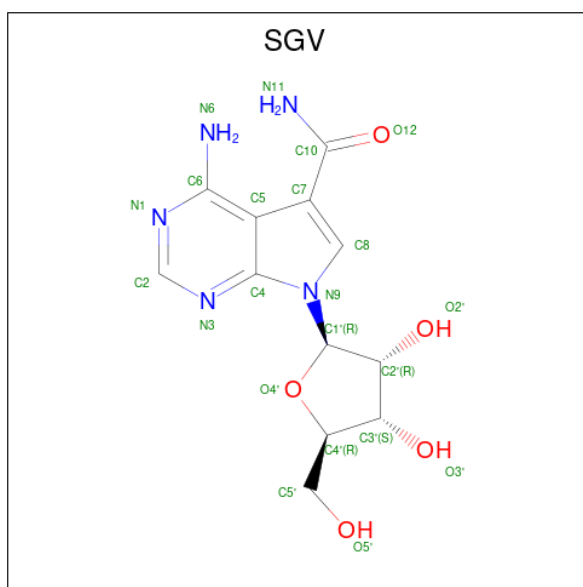
- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	115	1654	527	806	143	163	15	0	1	0

There is a discrepancy between the modelled and reference sequences:

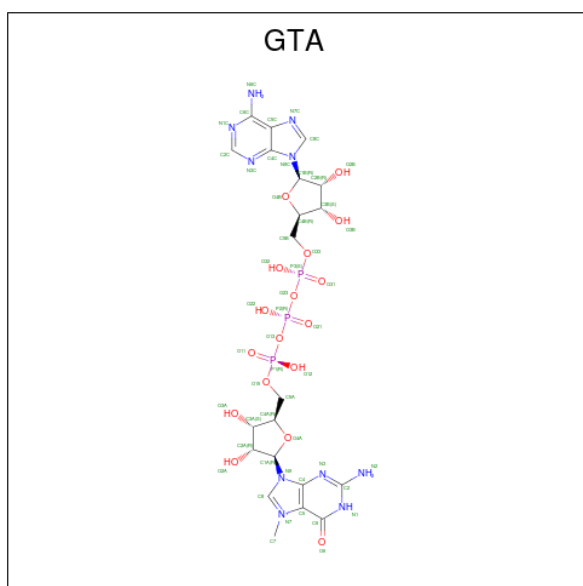
Chain	Residue	Modelled	Actual	Comment	Reference
B	4253	GLY	-	expression tag	UNP P0DTD1

- Molecule 3 is SANGIVAMYCIN (three-letter code: SGV) (formula: C₁₂H₁₅N₅O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
3	A	1	37	12	15	5	5	0	1

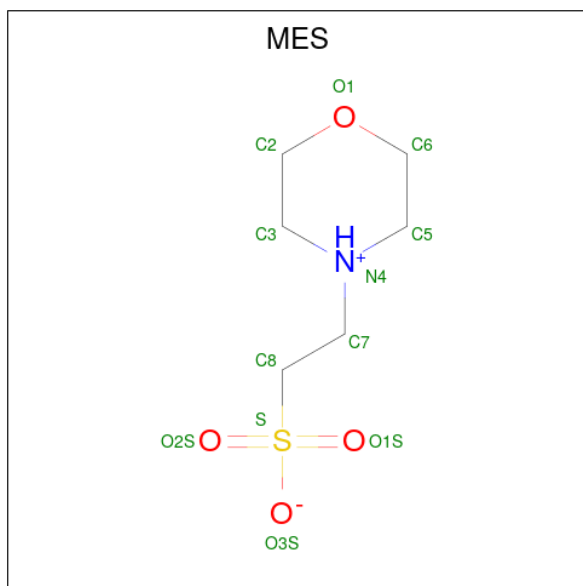
- Molecule 4 is P1-7-METHYLGUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHAT E (three-letter code: GTA) (formula: $C_{21}H_{30}N_{10}O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



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

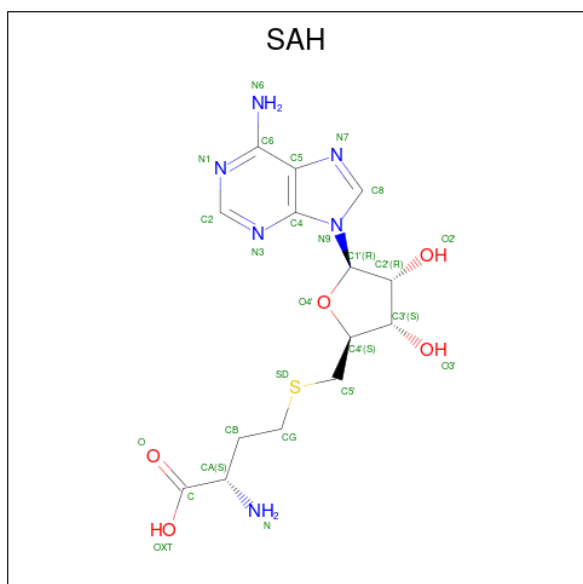
- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES)

(formula: C₆H₁₃NO₄S).



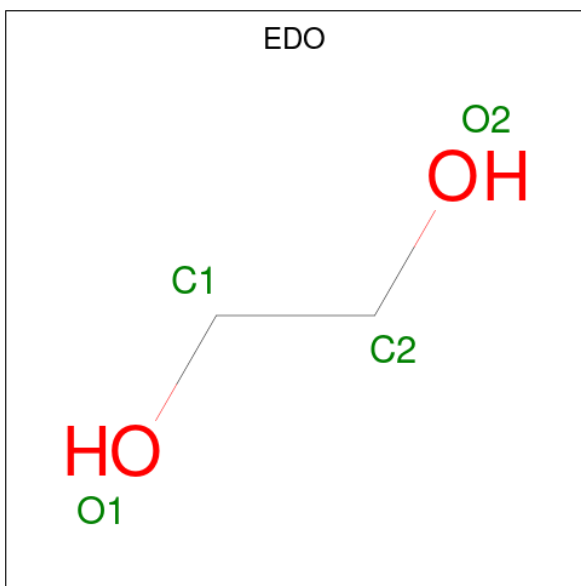
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
5	A	1	25	6	13	1	4	1	0	1

- Molecule 6 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



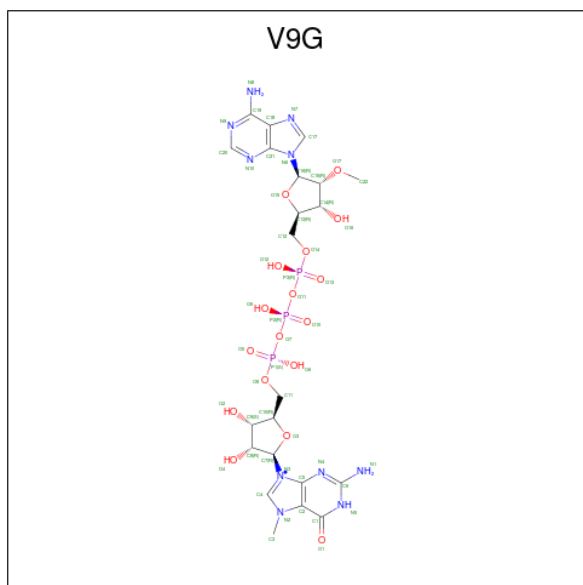
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			S
6	A	1	45	14	19	6	5	1	0	1

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



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

- Molecule 8 is 7-METHYL-GUANOSINE-5'-TRIPHOSPHATE-5'-(2'-O-METHYL)-ADENOSINE (three-letter code: 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	
			Total	C	H	N	O			P
8	A	1	81	22	29	10	17	3	0	1

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

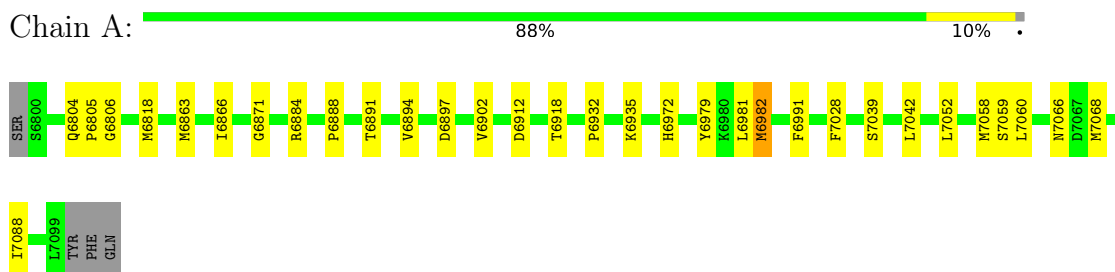
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	121	Total	O	0	0
			121	121		
10	B	30	Total	O	0	0
			30	30		

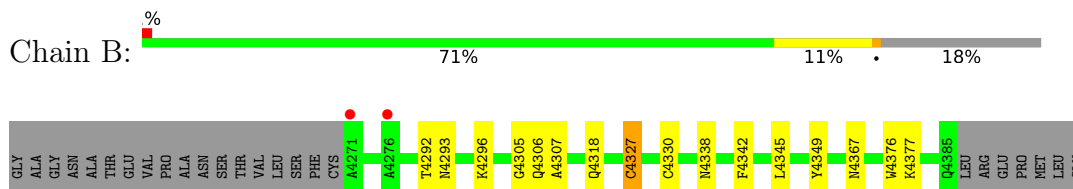
3 Residue-property plots [i](#)

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



- Molecule 2: Non-structural protein 10



4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	169.51Å 169.51Å 52.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.48 – 2.34 49.22 – 2.24	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.48-2.34) 71.5 (49.22-2.24)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.07	Depositor
R, R_{free}	0.203 , 0.256 0.203 , 0.249	Depositor DCC
R_{free} test set	2074 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtrriage
Anisotropy	0.631	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.045 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6872	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: MES, SAH, SGV, V9G, ZN, EDO, GTA

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	0.65	0/2446	0.78	2/3315 (0.1%)
2	B	0.55	0/873	0.68	0/1184
All	All	0.62	0/3319	0.75	2/4499 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6982	MET	CG-SD-CE	10.21	116.54	100.20
1	A	6981	LEU	CB-CG-CD2	-6.41	100.11	111.00

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	2389	2330	2378	25	0
2	B	848	806	801	9	0
3	A	22	15	15	2	0
4	A	51	27	24	5	0
5	A	12	13	13	0	0
6	A	26	19	18	2	0
7	A	24	36	36	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	8	12	12	1	0
8	A	52	29	0	1	0
9	B	2	0	0	0	0
10	A	121	0	0	3	0
10	B	30	0	0	1	0
All	All	3585	3287	3297	37	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 5.

All (37) 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)
4:A:7202[C]:GTA:O4A	4:A:7202[C]:GTA:C1A	1.63	1.24
4:A:7202[C]:GTA:C4B	4:A:7202[C]:GTA:O4B	1.64	1.22
6:A:7204[A]:SAH:C1'	6:A:7204[A]:SAH:O4'	1.63	1.20
1:A:7066:ASN:OD1	1:A:7068:MET:N	2.13	0.81
1:A:7058:MET:HE3	1:A:7060:LEU:HD11	1.80	0.64
4:A:7202[C]:GTA:O4B	4:A:7202[C]:GTA:C5B	2.44	0.62
2:B:4327:CYS:HB2	2:B:4345:LEU:HD12	1.81	0.61
1:A:6804:GLN:HB3	1:A:6805:PRO:HD2	1.87	0.56
1:A:6972:HIS:HD2	10:A:7329:HOH:O	1.89	0.54
3:A:7201[B]:SGV:HN11	3:A:7201[B]:SGV:HN6A	1.54	0.54
1:A:6863:MET:HB3	1:A:6891:THR:HG23	1.90	0.54
1:A:6979:TYR:O	1:A:6982:MET:HB2	2.08	0.53
1:A:6884:ARG:HH11	1:A:6884:ARG:HG3	1.75	0.51
1:A:7058:MET:HE3	1:A:7060:LEU:CD1	2.41	0.51
1:A:6918:THR:HG22	1:A:7088:ILE:HG22	1.94	0.50
1:A:6932:PRO:HB3	8:A:7211[D]:V9G:N8	2.27	0.49
2:B:4338:ASN:ND2	2:B:4342:PHE:O	2.46	0.48
1:A:6871:GLY:H	1:A:6897:ASP:HB2	1.77	0.48
1:A:6888:PRO:HG3	1:A:7052:LEU:CD2	2.43	0.47
1:A:6935:LYS:NZ	4:A:7202[C]:GTA:O21	2.48	0.47
1:A:7059:SER:O	1:A:7060:LEU:HD12	2.14	0.46
2:B:4292:THR:O	2:B:4293:ASN:HB2	2.15	0.46
1:A:6818:MET:CE	10:A:7337:HOH:O	2.64	0.45
2:B:4307:ALA:HB1	2:B:4376:TRP:CE2	2.51	0.45
1:A:6871:GLY:O	6:A:7204[A]:SAH:HA	2.17	0.45
2:B:4367:ASN:O	7:B:4403:EDO:H21	2.19	0.43
1:A:7039:SER:HB2	1:A:7042:LEU:HD12	2.01	0.43
2:B:4305:GLY:HA2	2:B:4318:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6884:ARG:HB3	2:B:4349:TYR:OH	2.20	0.41
1:A:6866:ILE:HA	1:A:6894:VAL:O	2.21	0.41
1:A:6972:HIS:HE1	10:A:7354:HOH:O	2.02	0.41
1:A:6932:PRO:HB3	4:A:7202[C]:GTA:N6C	2.36	0.40
1:A:6912:ASP:OD1	3:A:7201[B]:SGV:N6	2.55	0.40
2:B:4296:LYS:HE3	10:B:4519:HOH:O	2.20	0.40
1:A:6806:GLY:HA3	1:A:6991:PHE:CZ	2.56	0.40
1:A:6818:MET:HG3	1:A:7028:PHE:CG	2.57	0.40
1:A:6902:VAL:HG11	2:B:4330:CYS:O	2.21	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	302/304 (99%)	292 (97%)	10 (3%)	0	100	100
2	B	114/140 (81%)	108 (95%)	6 (5%)	0	100	100
All	All	416/444 (94%)	400 (96%)	16 (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	A	264/264 (100%)	264 (100%)	0	100	100
2	B	94/113 (83%)	91 (97%)	3 (3%)	39	47
All	All	358/377 (95%)	355 (99%)	3 (1%)	81	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	4306	GLN
2	B	4327	CYS
2	B	4377	LYS

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	6826	GLN
2	B	4338	ASN

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 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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
6	SAH	A	7204[A]	-	24,28,28	4.86	9 (37%)	25,40,40	1.44	3 (12%)
8	V9G	A	7211[D]	-	46,57,57	5.06	17 (36%)	46,89,89	1.66	9 (19%)
7	EDO	A	7205	-	3,3,3	0.70	0	2,2,2	0.28	0
4	GTA	A	7202[C]	-	46,56,56	4.62	19 (41%)	46,88,88	1.57	7 (15%)
7	EDO	A	7206	-	3,3,3	0.63	0	2,2,2	0.23	0
5	MES	A	7203[F]	-	12,12,12	1.94	2 (16%)	14,16,16	1.58	2 (14%)
7	EDO	A	7208	-	3,3,3	0.55	0	2,2,2	0.22	0
7	EDO	A	7209	-	3,3,3	0.69	0	2,2,2	0.40	0
7	EDO	B	4404	-	3,3,3	0.53	0	2,2,2	0.80	0
7	EDO	B	4403	-	3,3,3	0.64	0	2,2,2	0.12	0
3	SGV	A	7201[B]	-	22,24,24	4.37	11 (50%)	23,36,36	2.65	10 (43%)
7	EDO	A	7210	-	3,3,3	0.78	0	2,2,2	0.09	0
7	EDO	A	7207	-	3,3,3	0.52	0	2,2,2	0.19	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
6	SAH	A	7204[A]	-	-	2/11/31/31	0/3/3/3
8	V9G	A	7211[D]	-	-	5/26/94/94	0/6/6/6
7	EDO	A	7205	-	-	1/1/1/1	-
4	GTA	A	7202[C]	-	-	7/24/64/64	0/6/6/6
7	EDO	A	7206	-	-	1/1/1/1	-
5	MES	A	7203[F]	-	-	3/6/14/14	0/1/1/1
7	EDO	A	7208	-	-	1/1/1/1	-
7	EDO	A	7209	-	-	1/1/1/1	-
7	EDO	B	4404	-	-	1/1/1/1	-
7	EDO	B	4403	-	-	1/1/1/1	-
3	SGV	A	7201[B]	-	-	3/3/26/26	0/3/3/3
7	EDO	A	7210	-	-	1/1/1/1	-
7	EDO	A	7207	-	-	0/1/1/1	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	7204[A]	SAH	O4'-C1'	16.25	1.63	1.41
4	A	7202[C]	GTA	O4A-C1A	16.24	1.63	1.41
8	A	7211[D]	V9G	O15-C16	15.92	1.63	1.41
8	A	7211[D]	V9G	C8-C7	-15.60	1.30	1.53
8	A	7211[D]	V9G	O3-C7	15.58	1.62	1.41
4	A	7202[C]	GTA	C2A-C1A	-14.92	1.31	1.53
6	A	7204[A]	SAH	C2'-C1'	-13.55	1.33	1.53
3	A	7201[B]	SGV	O4'-C1'	10.99	1.56	1.41
8	A	7211[D]	V9G	C14-C13	-9.78	1.28	1.53
4	A	7202[C]	GTA	O4B-C1B	-9.70	1.27	1.41
4	A	7202[C]	GTA	C3B-C4B	-9.30	1.29	1.53
3	A	7201[B]	SGV	C3'-C2'	-9.25	1.28	1.53
4	A	7202[C]	GTA	O4B-C4B	8.67	1.64	1.45
8	A	7211[D]	V9G	O3-C10	-7.83	1.27	1.45
4	A	7202[C]	GTA	O4A-C4A	-7.13	1.29	1.45
8	A	7211[D]	V9G	C14-C15	7.13	1.68	1.52
3	A	7201[B]	SGV	C10-N11	6.79	1.45	1.33
6	A	7204[A]	SAH	O4'-C4'	-6.60	1.30	1.45
3	A	7201[B]	SGV	O4'-C4'	-6.48	1.30	1.45
3	A	7201[B]	SGV	C3'-C4'	6.47	1.69	1.53
8	A	7211[D]	V9G	C6-N1	6.22	1.49	1.34
5	A	7203[F]	MES	C8-S	-5.98	1.69	1.77
8	A	7211[D]	V9G	C6-N4	5.86	1.47	1.33
4	A	7202[C]	GTA	C2-N3	5.66	1.47	1.33
8	A	7211[D]	V9G	C5-N4	4.94	1.49	1.37
8	A	7211[D]	V9G	O4-C8	4.77	1.54	1.43
4	A	7202[C]	GTA	C2-N2	4.62	1.45	1.34
4	A	7202[C]	GTA	C4-N3	4.56	1.48	1.37
3	A	7201[B]	SGV	C2'-C1'	4.33	1.60	1.53
4	A	7202[C]	GTA	O2A-C2A	4.18	1.52	1.43
8	A	7211[D]	V9G	O15-C13	4.04	1.54	1.45
8	A	7211[D]	V9G	C1-N5	4.03	1.43	1.37
6	A	7204[A]	SAH	C6-N6	3.98	1.48	1.34
6	A	7204[A]	SAH	O3'-C3'	-3.78	1.34	1.43
3	A	7201[B]	SGV	C7-C10	3.74	1.56	1.50
8	A	7211[D]	V9G	C19-N8	3.64	1.47	1.34
4	A	7202[C]	GTA	O3B-C3B	3.57	1.51	1.43
3	A	7201[B]	SGV	C8-N9	-3.54	1.32	1.38
8	A	7211[D]	V9G	C2-C1	3.51	1.54	1.45
8	A	7211[D]	V9G	C6-N5	3.20	1.45	1.37
4	A	7202[C]	GTA	C5-C6	3.14	1.53	1.45
4	A	7202[C]	GTA	C6-N1	3.11	1.42	1.37
4	A	7202[C]	GTA	C6C-N6C	3.10	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	7201[B]	SGV	C6-N6	3.08	1.45	1.34
4	A	7202[C]	GTA	O3A-C3A	-3.04	1.35	1.43
6	A	7204[A]	SAH	O-C	2.97	1.31	1.22
3	A	7201[B]	SGV	O2'-C2'	2.94	1.49	1.43
4	A	7202[C]	GTA	C2-N1	2.92	1.44	1.37
3	A	7201[B]	SGV	O12-C10	-2.85	1.18	1.24
4	A	7202[C]	GTA	O2B-C2B	-2.84	1.36	1.43
6	A	7204[A]	SAH	C3'-C4'	2.73	1.60	1.53
6	A	7204[A]	SAH	O2'-C2'	2.71	1.49	1.43
6	A	7204[A]	SAH	OXT-C	-2.70	1.21	1.30
4	A	7202[C]	GTA	O6-C6	-2.67	1.17	1.23
8	A	7211[D]	V9G	O17-C15	2.59	1.49	1.42
5	A	7203[F]	MES	O1S-S	2.13	1.51	1.45
4	A	7202[C]	GTA	C2B-C1B	2.12	1.57	1.53
8	A	7211[D]	V9G	C17-N7	-2.04	1.31	1.34

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7201[B]	SGV	O12-C10-N11	-5.62	114.60	122.58
8	A	7211[D]	V9G	N10-C20-N9	-5.20	120.55	128.68
4	A	7202[C]	GTA	N3C-C2C-N1C	-5.08	120.73	128.68
3	A	7201[B]	SGV	C8-N9-C1'	5.07	129.97	125.48
3	A	7201[B]	SGV	C7-C10-N11	4.87	125.71	118.28
3	A	7201[B]	SGV	N3-C2-N1	-4.48	121.67	128.68
6	A	7204[A]	SAH	N3-C2-N1	-4.23	122.07	128.68
4	A	7202[C]	GTA	P3-O23-P2	-4.09	118.79	132.83
3	A	7201[B]	SGV	C1'-N9-C4	-3.52	120.46	126.64
8	A	7211[D]	V9G	C9-C8-C7	3.44	106.16	100.98
3	A	7201[B]	SGV	C3'-C2'-C1'	3.43	106.14	100.98
4	A	7202[C]	GTA	C2-N1-C6	-3.31	119.01	125.10
4	A	7202[C]	GTA	C3A-C2A-C1A	3.30	105.95	100.98
8	A	7211[D]	V9G	P2-O11-P3	-3.24	121.70	132.83
8	A	7211[D]	V9G	C6-N5-C1	-3.24	119.14	125.10
5	A	7203[F]	MES	C5-N4-C3	3.23	116.09	108.83
3	A	7201[B]	SGV	O4'-C1'-C2'	-3.18	102.28	106.93
5	A	7203[F]	MES	O2S-S-C8	3.15	110.71	106.92
8	A	7211[D]	V9G	C15-C14-C13	3.00	108.50	101.99
8	A	7211[D]	V9G	O1-C1-N5	-2.89	117.24	120.65
8	A	7211[D]	V9G	O15-C13-C12	-2.84	100.03	109.37
4	A	7202[C]	GTA	P2-O13-P1	-2.84	123.10	132.83
6	A	7204[A]	SAH	C3'-C2'-C1'	2.78	105.17	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7202[C]	GTA	O6-C6-N1	-2.74	117.41	120.65
8	A	7211[D]	V9G	P1-O7-P2	-2.72	123.49	132.83
8	A	7211[D]	V9G	O15-C16-C15	2.68	111.23	106.59
3	A	7201[B]	SGV	C2'-C3'-C4'	2.57	107.64	102.64
3	A	7201[B]	SGV	C5'-C4'-C3'	-2.57	108.89	115.09
4	A	7202[C]	GTA	O4B-C4B-C5B	-2.47	101.24	109.37
6	A	7204[A]	SAH	C4-C5-N7	-2.46	106.84	109.40
3	A	7201[B]	SGV	C7-C5-C4	-2.24	105.75	107.54

There are no chirality outliers.

All (27) torsion outliers are listed below:

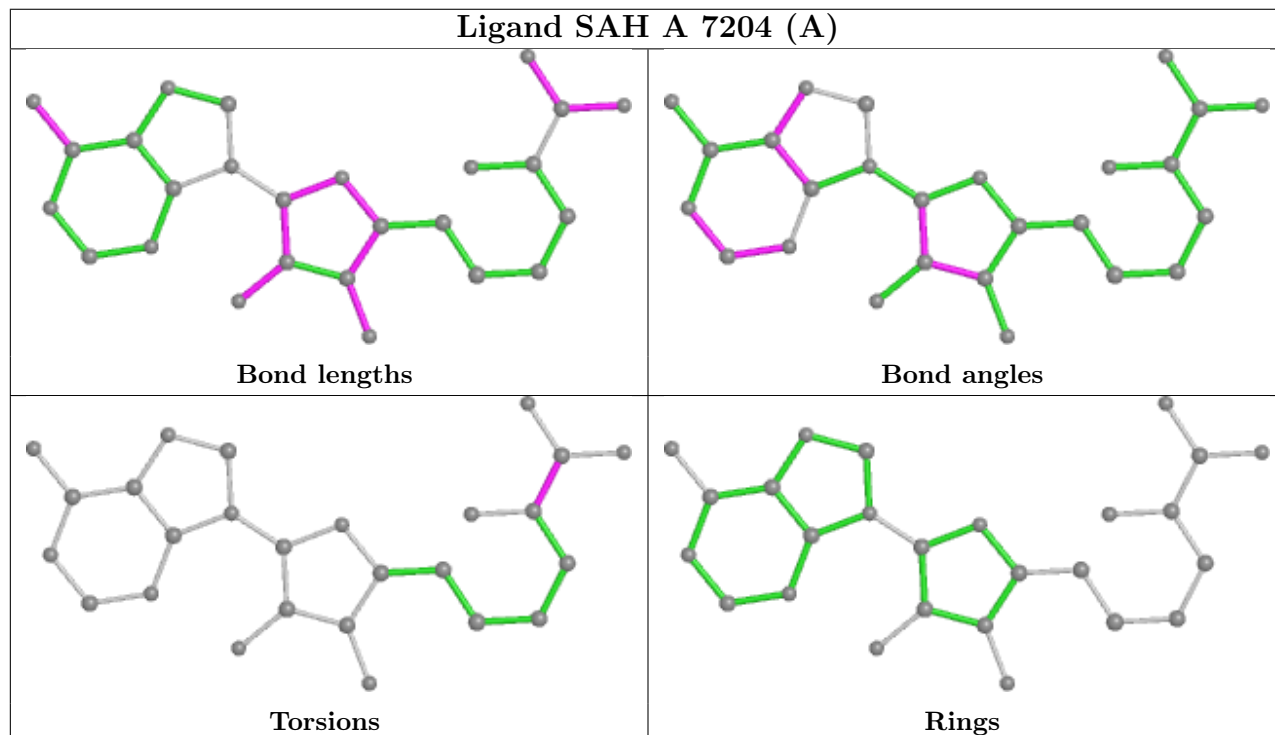
Mol	Chain	Res	Type	Atoms
4	A	7202[C]	GTA	C5A-O15-P1-O11
4	A	7202[C]	GTA	C5B-O33-P3-O23
4	A	7202[C]	GTA	O4B-C4B-C5B-O33
5	A	7203[F]	MES	C7-C8-S-O1S
5	A	7203[F]	MES	C7-C8-S-O3S
8	A	7211[D]	V9G	C12-O14-P3-O11
8	A	7211[D]	V9G	C11-O8-P1-O5
8	A	7211[D]	V9G	O14-C12-C13-O15
4	A	7202[C]	GTA	C3B-C4B-C5B-O33
7	A	7206	EDO	O1-C1-C2-O2
7	A	7208	EDO	O1-C1-C2-O2
7	B	4403	EDO	O1-C1-C2-O2
3	A	7201[B]	SGV	O4'-C4'-C5'-O5'
4	A	7202[C]	GTA	C5B-O33-P3-O32
4	A	7202[C]	GTA	C5B-O33-P3-O31
8	A	7211[D]	V9G	C12-O14-P3-O13
8	A	7211[D]	V9G	C12-O14-P3-O12
5	A	7203[F]	MES	C7-C8-S-O2S
6	A	7204[A]	SAH	O-C-CA-CB
3	A	7201[B]	SGV	C3'-C4'-C5'-O5'
7	A	7209	EDO	O1-C1-C2-O2
7	A	7210	EDO	O1-C1-C2-O2
6	A	7204[A]	SAH	OXT-C-CA-CB
7	B	4404	EDO	O1-C1-C2-O2
4	A	7202[C]	GTA	C5A-O15-P1-O13
3	A	7201[B]	SGV	O12-C10-C7-C8
7	A	7205	EDO	O1-C1-C2-O2

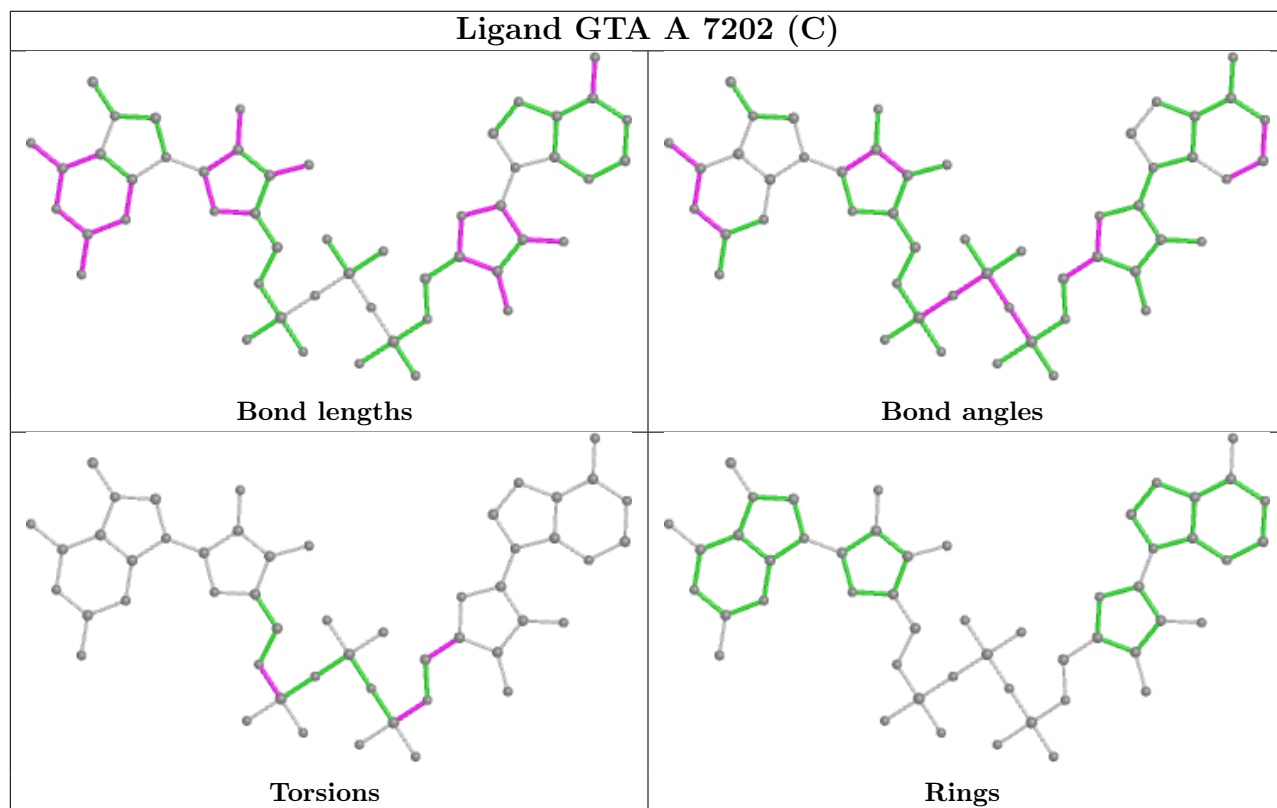
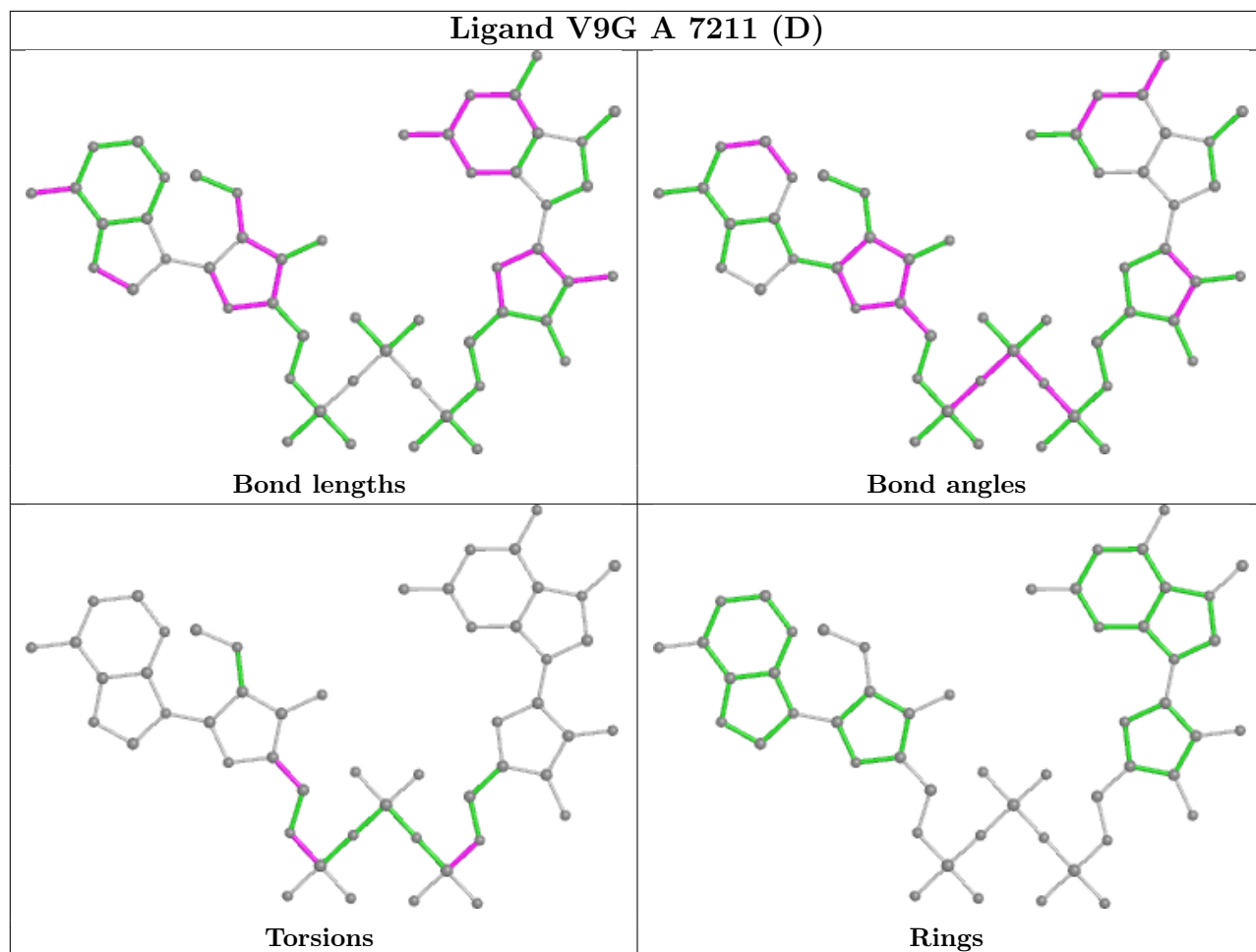
There are no ring outliers.

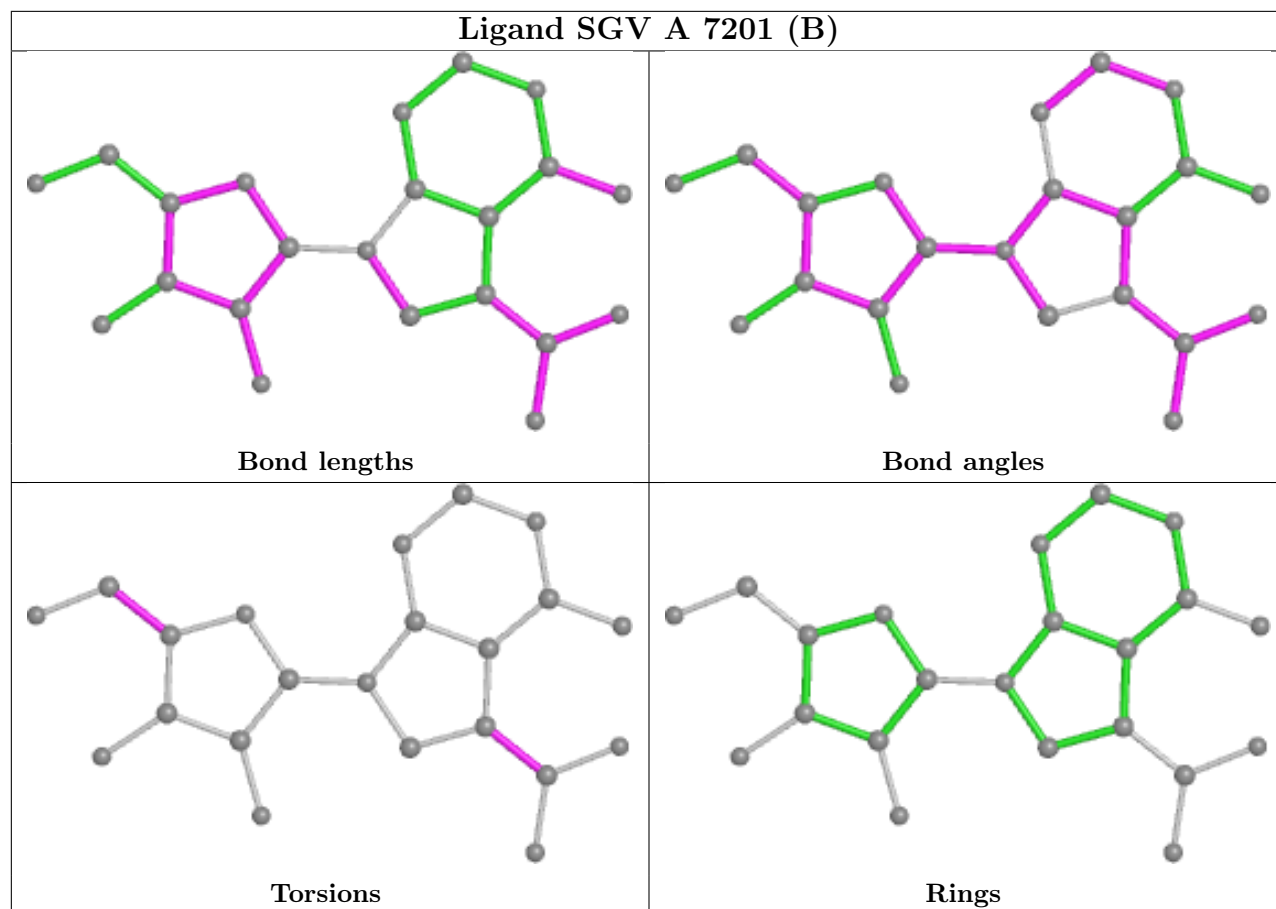
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	7204[A]	SAH	2	0
8	A	7211[D]	V9G	1	0
4	A	7202[C]	GTA	5	0
7	B	4403	EDO	1	0
3	A	7201[B]	SGV	2	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 [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%)	-0.27	0 100 100	36, 51, 75, 120	0
2	B	115/140 (82%)	-0.07	2 (1%) 70 78	43, 66, 102, 123	0
All	All	415/444 (93%)	-0.21	2 (0%) 91 95	36, 54, 91, 123	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4271	ALA	4.4
2	B	4276	ALA	2.3

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.

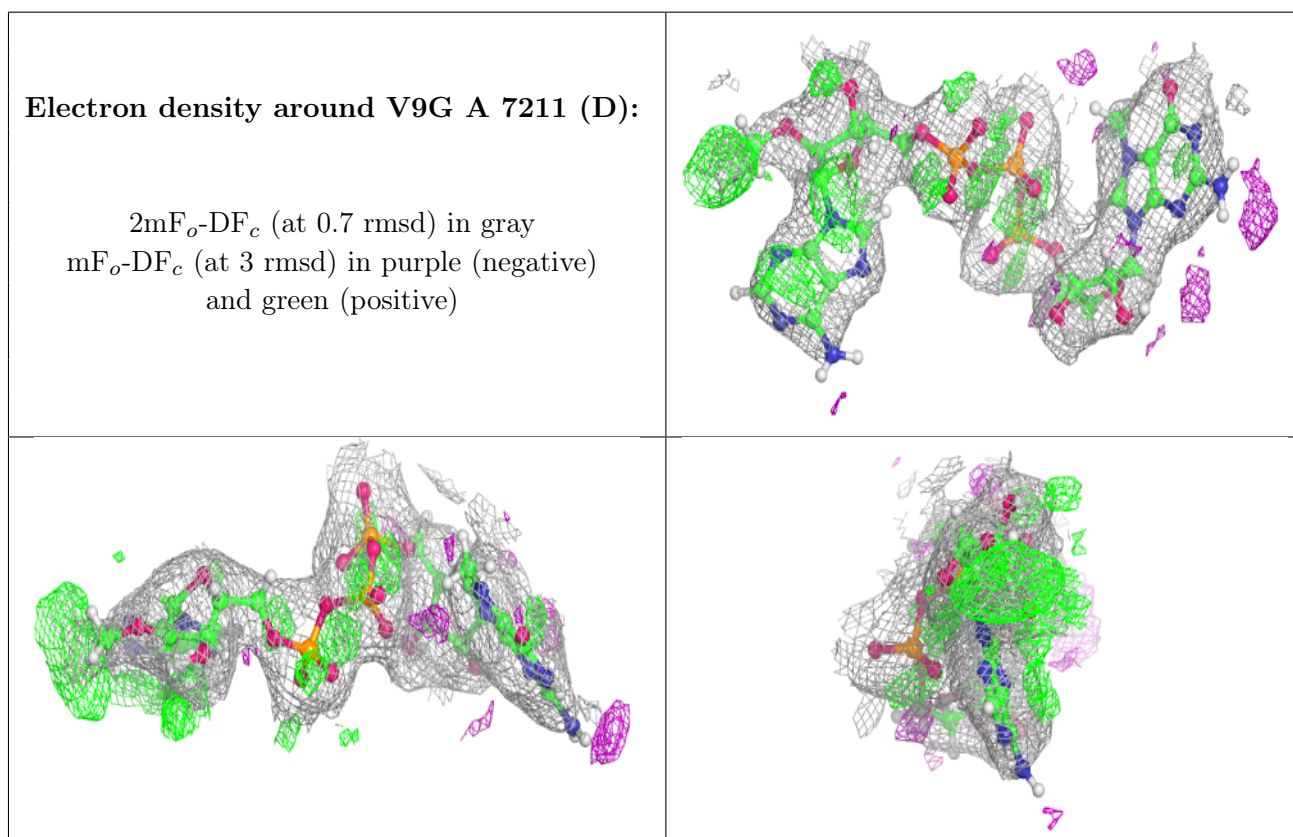
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	A	7209	4/4	0.65	0.31	60,73,87,87	0
7	EDO	A	7206	4/4	0.75	0.25	70,84,99,99	0
7	EDO	B	4403	4/4	0.75	0.15	80,96,110,111	0

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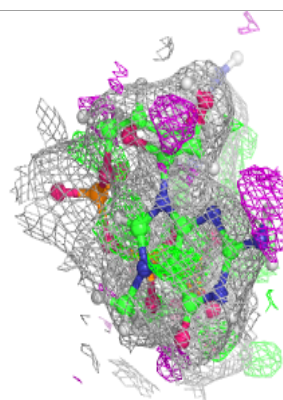
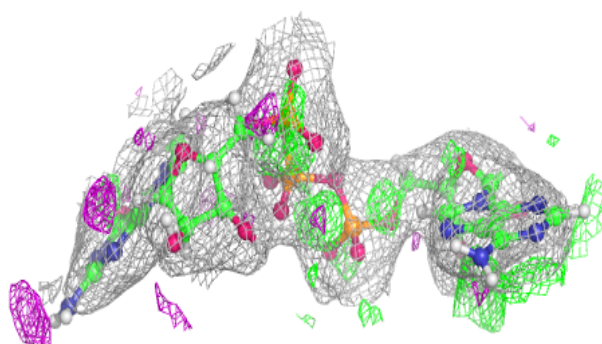
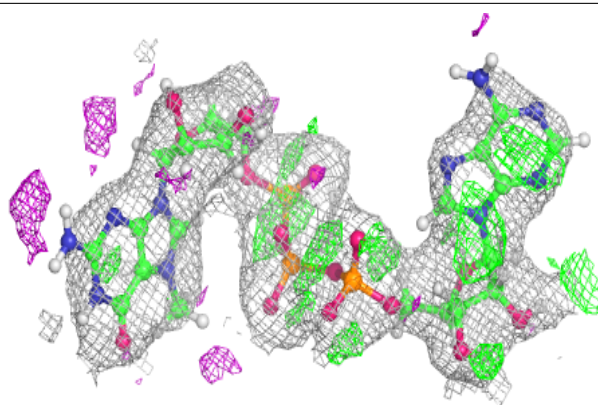
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	EDO	A	7210	4/4	0.86	0.21	68,82,84,90	0
5	MES	A	7203[F]	12/12	0.86	0.11	56,88,116,130	0
7	EDO	A	7207	4/4	0.89	0.21	76,100,123,125	0
7	EDO	A	7205	4/4	0.89	0.18	72,92,112,112	0
7	EDO	B	4404	4/4	0.90	0.18	63,79,94,94	0
7	EDO	A	7208	4/4	0.92	0.16	70,86,103,103	0
8	V9G	A	7211[D]	52/52	0.96	0.15	37,58,80,96	81
4	GTA	A	7202[C]	51/51	0.97	0.16	37,59,81,96	78
3	SGV	A	7201[B]	22/22	0.97	0.10	34,52,65,67	37
6	SAH	A	7204[A]	26/26	0.97	0.12	40,53,67,68	45
9	ZN	B	4401	1/1	0.99	0.14	53,53,53,53	0
9	ZN	B	4402	1/1	1.00	0.13	73,73,73,73	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.

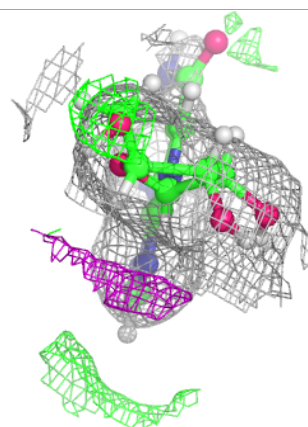
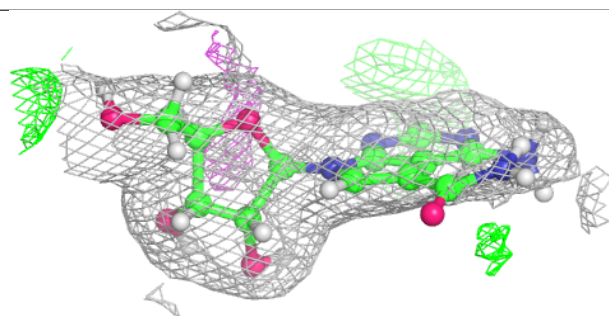
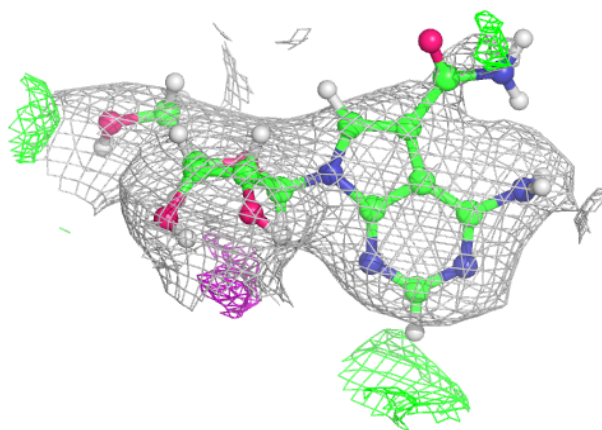


Electron density around GTA A 7202 (C):

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

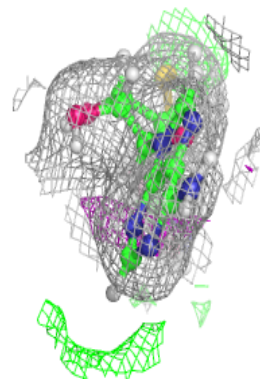
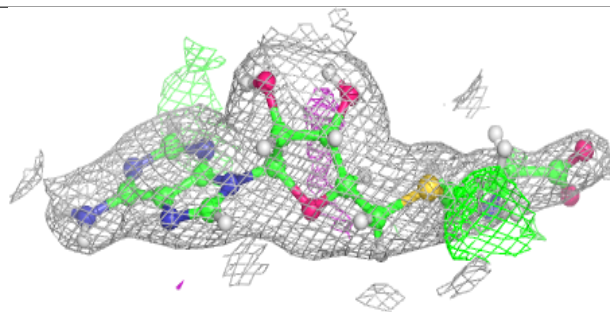
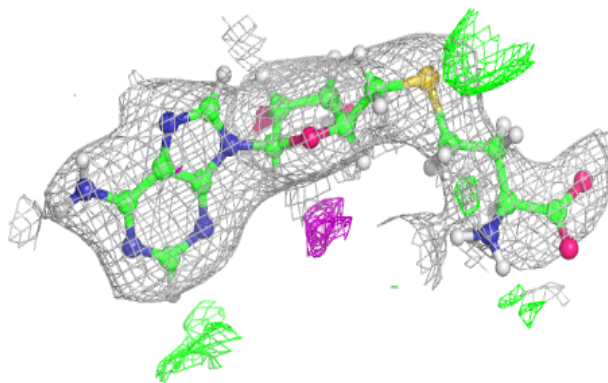
**Electron density around SGV A 7201 (B):**

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



Electron density around SAH A 7204 (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.