



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:31 AM UTC

PDB ID : 9GRP / pdb_00009grp
Title : SARS-CoV-2 methyltransferase nsp10-16 in complex with SAM and beta-chloroethyl theophylline
Authors : Kremling, V.; Sprenger, J.; Oberthuer, D.; Kiene, A.
Deposited on : 2024-09-12
Resolution : 2.10 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

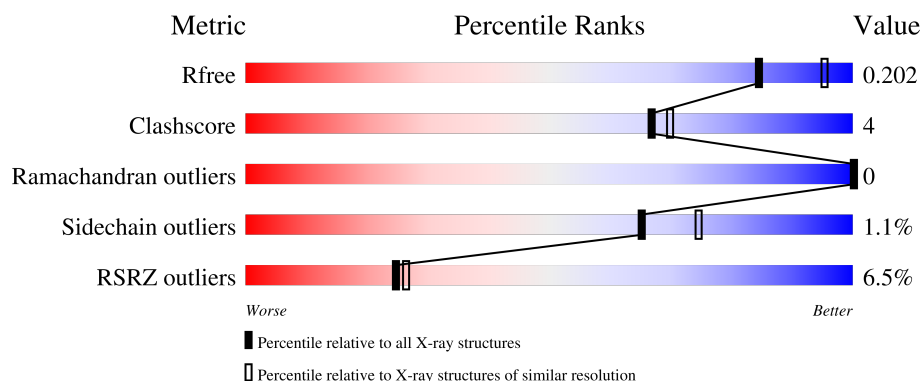
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	6% 89% 9%
2	B	140	7% 77% 5% 18%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3679 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 nsp16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	11	0
			2450	1554	417	462	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

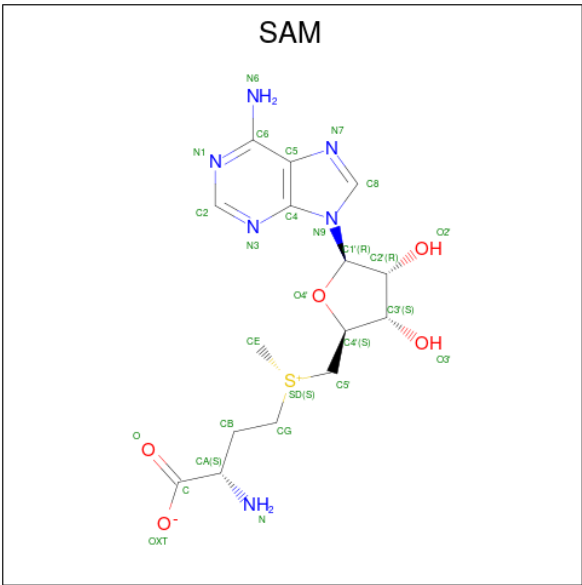
- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	0	0
			848	527	143	163	15			

There is a discrepancy between the modelled and reference sequences:

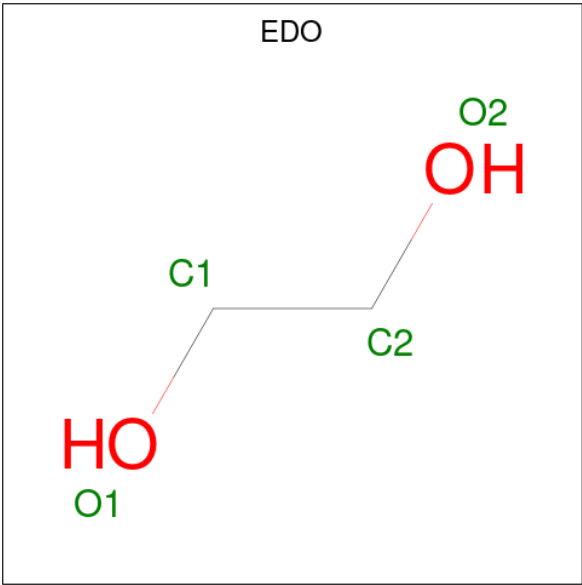
Chain	Residue	Modelled	Actual	Comment	Reference
B	4253	GLY	-	expression tag	UNP P0DTD1

- Molecule 3 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).



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

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



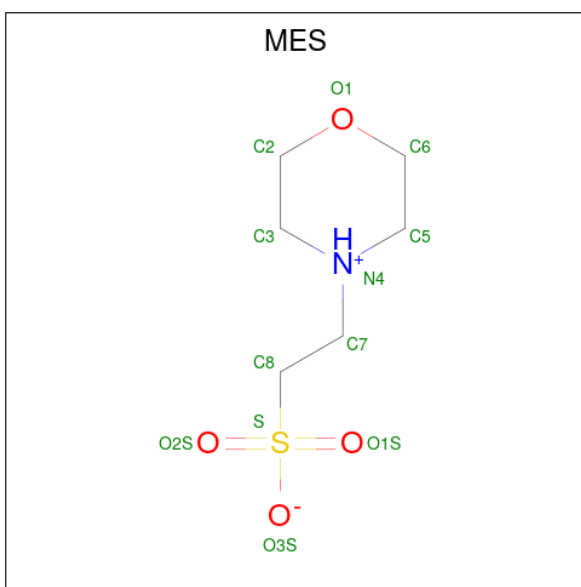
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

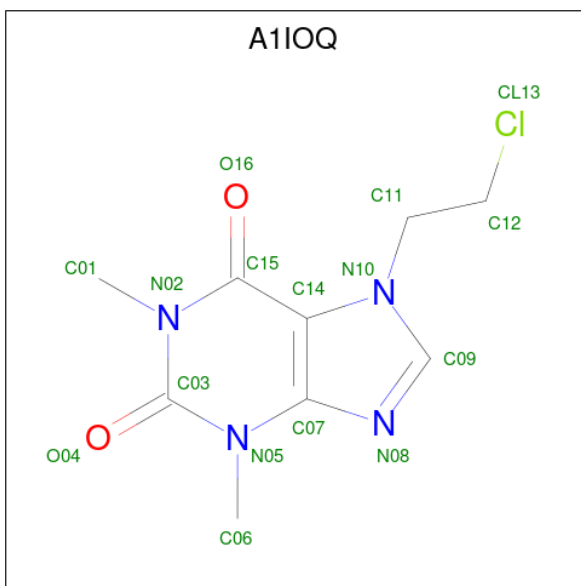
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0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

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is 7-(2-chloroethyl)-1,3-dimethyl-purine-2,6-dione (CCD ID: A1IOQ) (formula: $C_9H_{11}ClN_4O_2$) (labeled as "Ligand of Interest" by depositor).

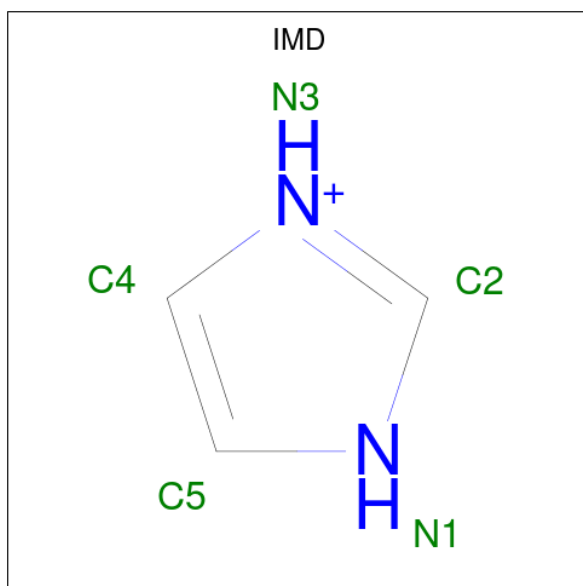


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Cl	N	O	0	0
			16	9	1	4	2		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 8 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).

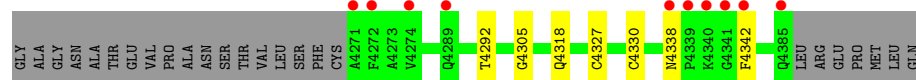
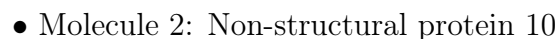


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	N	0	0
			5	3	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	169	Total	O	0	0
			169	169		
9	B	66	Total	O	0	0
			66	66		

- Molecule 1: 2'-O-methyltransferase nsp16



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 51.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.42 – 2.10 48.42 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.42-2.10) 99.9 (48.42-2.10)	Depositor EDS
R_{merge}	0.39	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.65Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.184 , 0.204 0.185 , 0.202	Depositor DCC
R_{free} test set	773 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	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	0.96	EDS
Total number of atoms	3679	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, IMD, SAM, MES, A1IOQ

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	0.31	0/2501	0.48	0/3391
2	B	0.28	0/867	0.45	0/1176
All	All	0.30	0/3368	0.47	0/4567

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

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	2450	0	2417	21	0
2	B	848	0	805	4	0
3	A	27	0	22	1	0
4	A	72	0	108	6	0
4	B	12	0	18	1	0
5	A	12	0	12	1	0
6	A	16	0	0	0	0
7	B	2	0	0	0	0
8	B	5	0	5	0	0
9	A	169	0	0	0	0
9	B	66	0	0	0	0
All	All	3679	0	3387	25	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 (25) 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)
1:A:6918[A]:THR:HG21	1:A:6922:TRP:HE1	1.47	0.79
1:A:6928:ASP:OD1	1:A:6968:LYS:NZ	2.31	0.59
1:A:6917:HIS:HA	4:A:7213:EDO:H21	1.85	0.58
1:A:6936:ASN:ND2	1:A:6939:LYS:HD2	2.22	0.55
1:A:6833:THR:H	4:A:7209:EDO:H22	1.73	0.54
1:A:6872:SER:O	4:A:7219:EDO:H12	2.08	0.53
1:A:6862[B]:ASN:O	1:A:6862[B]:ASN:ND2	2.44	0.51
1:A:6833:THR:H	4:A:7209:EDO:C2	2.26	0.48
2:B:4292:THR:H	4:B:4406:EDO:H11	1.79	0.47
2:B:4305:GLY:HA2	2:B:4318:GLN:OE1	2.15	0.46
2:B:4338:ASN:ND2	2:B:4342:PHE:HB3	2.30	0.46
2:B:4327:CYS:HB3	2:B:4330:CYS:HB2	1.98	0.46
1:A:6852:LEU:HB3	1:A:6857:LEU:HD11	1.99	0.45
1:A:6987:TRP:CD2	5:A:7204:MES:H32	2.52	0.44
1:A:6928:ASP:OD2	3:A:7201:SAM:HG1	2.18	0.43
1:A:7058:MET:O	1:A:7080:ILE:HA	2.18	0.43
1:A:6861:TYR:HA	4:A:7202:EDO:H11	2.00	0.41
1:A:6864:ARG:NH1	1:A:6920[B]:ASN:HB3	2.34	0.41
1:A:6864:ARG:NH2	1:A:7084:ASN:O	2.53	0.41
1:A:7085:ARG:H	1:A:7085:ARG:HG2	1.67	0.41
1:A:6846:THR:O	1:A:6850:GLN:HG3	2.20	0.41
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	2.02	0.41
1:A:6857:LEU:O	1:A:7053[A]:ARG:NH2	2.39	0.41
1:A:6981:LEU:HD13	4:A:7214:EDO:H12	2.01	0.41
1:A:6864:ARG:NH1	1:A:6920[A]:ASN:HB2	2.36	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	
1	A	309/304 (102%)	301 (97%)	8 (3%)	0	100	100
2	B	113/140 (81%)	112 (99%)	1 (1%)	0	100	100
All	All	422/444 (95%)	413 (98%)	9 (2%)	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	271/264 (103%)	267 (98%)	4 (2%)	57	65
2	B	93/113 (82%)	93 (100%)	0	100	100
All	All	364/377 (97%)	360 (99%)	4 (1%)	65	74

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6874	LYS
1	A	6900	ASP
1	A	6968	LYS
1	A	7061	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	6804	GLN
1	A	7008	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 2 are monoatomic - leaving 25 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	EDO	A	7214	-	3,3,3	0.47	0	2,2,2	0.26	0
5	MES	A	7204	-	12,12,12	1.93	1 (8%)	15,16,16	2.11	4 (26%)
4	EDO	A	7207	-	3,3,3	0.59	0	2,2,2	0.19	0
4	EDO	A	7212	-	3,3,3	0.49	0	2,2,2	0.41	0
4	EDO	A	7208	-	3,3,3	0.50	0	2,2,2	0.32	0
4	EDO	A	7217	-	3,3,3	0.34	0	2,2,2	0.77	0
6	A1IOQ	A	7218	-	17,17,17	2.55	4 (23%)	25,25,25	2.19	12 (48%)
4	EDO	A	7220	-	3,3,3	0.51	0	2,2,2	0.23	0
4	EDO	B	4404	-	3,3,3	0.31	0	2,2,2	0.71	0
4	EDO	A	7203	-	3,3,3	0.46	0	2,2,2	0.46	0
4	EDO	A	7209	-	3,3,3	0.43	0	2,2,2	0.66	0
4	EDO	A	7213	-	3,3,3	0.43	0	2,2,2	0.51	0
4	EDO	A	7219	-	3,3,3	0.50	0	2,2,2	0.39	0
4	EDO	A	7216	-	3,3,3	0.48	0	2,2,2	0.27	0
4	EDO	A	7215	-	3,3,3	0.60	0	2,2,2	0.10	0
4	EDO	B	4403	-	3,3,3	0.54	0	2,2,2	0.19	0
4	EDO	A	7211	-	3,3,3	0.51	0	2,2,2	0.23	0
4	EDO	B	4406	-	3,3,3	0.55	0	2,2,2	0.26	0
4	EDO	A	7206	-	3,3,3	0.59	0	2,2,2	0.06	0
4	EDO	A	7205	-	3,3,3	0.38	0	2,2,2	0.82	0
4	EDO	A	7221	-	3,3,3	0.47	0	2,2,2	0.21	0
8	IMD	B	4405	-	5,5,5	0.68	0	5,5,5	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	7210	-	3,3,3	0.50	0	2,2,2	0.35	0
3	SAM	A	7201	-	27,29,29	1.33	3 (11%)	34,42,42	2.14	11 (32%)
4	EDO	A	7202	-	3,3,3	0.44	0	2,2,2	0.45	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
4	EDO	A	7214	-	-	0/1/1/1	-
5	MES	A	7204	-	-	4/6/14/14	0/1/1/1
4	EDO	A	7207	-	-	0/1/1/1	-
4	EDO	A	7212	-	-	0/1/1/1	-
4	EDO	A	7208	-	-	1/1/1/1	-
4	EDO	A	7217	-	-	1/1/1/1	-
6	A1IOQ	A	7218	-	-	0/3/3/3	0/2/2/2
4	EDO	A	7220	-	-	0/1/1/1	-
4	EDO	B	4404	-	-	0/1/1/1	-
4	EDO	A	7203	-	-	0/1/1/1	-
4	EDO	A	7209	-	-	0/1/1/1	-
4	EDO	A	7213	-	-	0/1/1/1	-
4	EDO	A	7219	-	-	0/1/1/1	-
4	EDO	A	7216	-	-	0/1/1/1	-
4	EDO	A	7215	-	-	0/1/1/1	-
4	EDO	B	4403	-	-	0/1/1/1	-
4	EDO	A	7211	-	-	0/1/1/1	-
4	EDO	B	4406	-	-	1/1/1/1	-
4	EDO	A	7206	-	-	0/1/1/1	-
4	EDO	A	7205	-	-	1/1/1/1	-
4	EDO	A	7221	-	-	1/1/1/1	-
8	IMD	B	4405	-	-	-	0/1/1/1
4	EDO	A	7210	-	-	1/1/1/1	-
3	SAM	A	7201	-	-	4/17/33/33	0/3/3/3
4	EDO	A	7202	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	7218	A1IOQ	C07-N05	6.54	1.48	1.38
5	A	7204	MES	C8-S	-6.19	1.68	1.77
6	A	7218	A1IOQ	C03-N05	4.39	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	7218	A1IOQ	C14-C15	4.27	1.53	1.43
6	A	7218	A1IOQ	C03-N02	3.69	1.46	1.39
3	A	7201	SAM	C2-N3	3.38	1.39	1.33
3	A	7201	SAM	C2-N1	3.20	1.39	1.33
3	A	7201	SAM	C8-N7	2.97	1.37	1.31

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	7204	MES	C5-N4-C3	5.72	121.15	108.84
3	A	7201	SAM	C5-C4-N3	-5.10	119.70	126.72
3	A	7201	SAM	O4'-C1'-N9	4.66	117.03	108.09
3	A	7201	SAM	N3-C2-N1	-4.31	122.06	128.58
6	A	7218	A1IOQ	C14-C15-N02	4.20	119.75	112.06
3	A	7201	SAM	C5-N7-C8	4.07	109.85	103.45
3	A	7201	SAM	C4-C5-N7	-3.84	106.19	110.58
6	A	7218	A1IOQ	C15-N02-C03	-3.66	119.72	125.66
3	A	7201	SAM	N9-C8-N7	-3.63	108.78	113.94
6	A	7218	A1IOQ	N05-C07-N08	3.56	131.86	126.27
5	A	7204	MES	O1S-S-C8	3.25	111.64	106.73
3	A	7201	SAM	C2-N3-C4	3.23	119.72	111.83
6	A	7218	A1IOQ	N10-C09-N08	-3.17	110.21	113.52
6	A	7218	A1IOQ	O16-C15-C14	-3.07	120.10	126.38
3	A	7201	SAM	N3-C4-N9	2.77	131.87	127.17
6	A	7218	A1IOQ	C09-N10-C14	2.68	107.54	105.86
6	A	7218	A1IOQ	N05-C03-N02	2.68	120.48	117.14
3	A	7201	SAM	C5-C4-N9	2.40	108.42	105.81
6	A	7218	A1IOQ	C06-N05-C03	2.40	121.51	117.33
6	A	7218	A1IOQ	C14-C07-N08	-2.35	107.44	112.10
3	A	7201	SAM	C6-C5-C4	2.33	120.36	117.18
6	A	7218	A1IOQ	C15-C14-C07	-2.33	119.98	122.92
6	A	7218	A1IOQ	C01-N02-C03	2.29	121.32	117.33
3	A	7201	SAM	OXT-C-O	-2.24	119.00	124.08
6	A	7218	A1IOQ	C07-C14-N10	2.22	107.05	104.96
5	A	7204	MES	O3S-S-C8	2.11	110.14	106.00
5	A	7204	MES	C2-C3-N4	2.03	113.20	110.12

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	7201	SAM	N-CA-CB-CG

Continued on next page...

Continued from previous page...

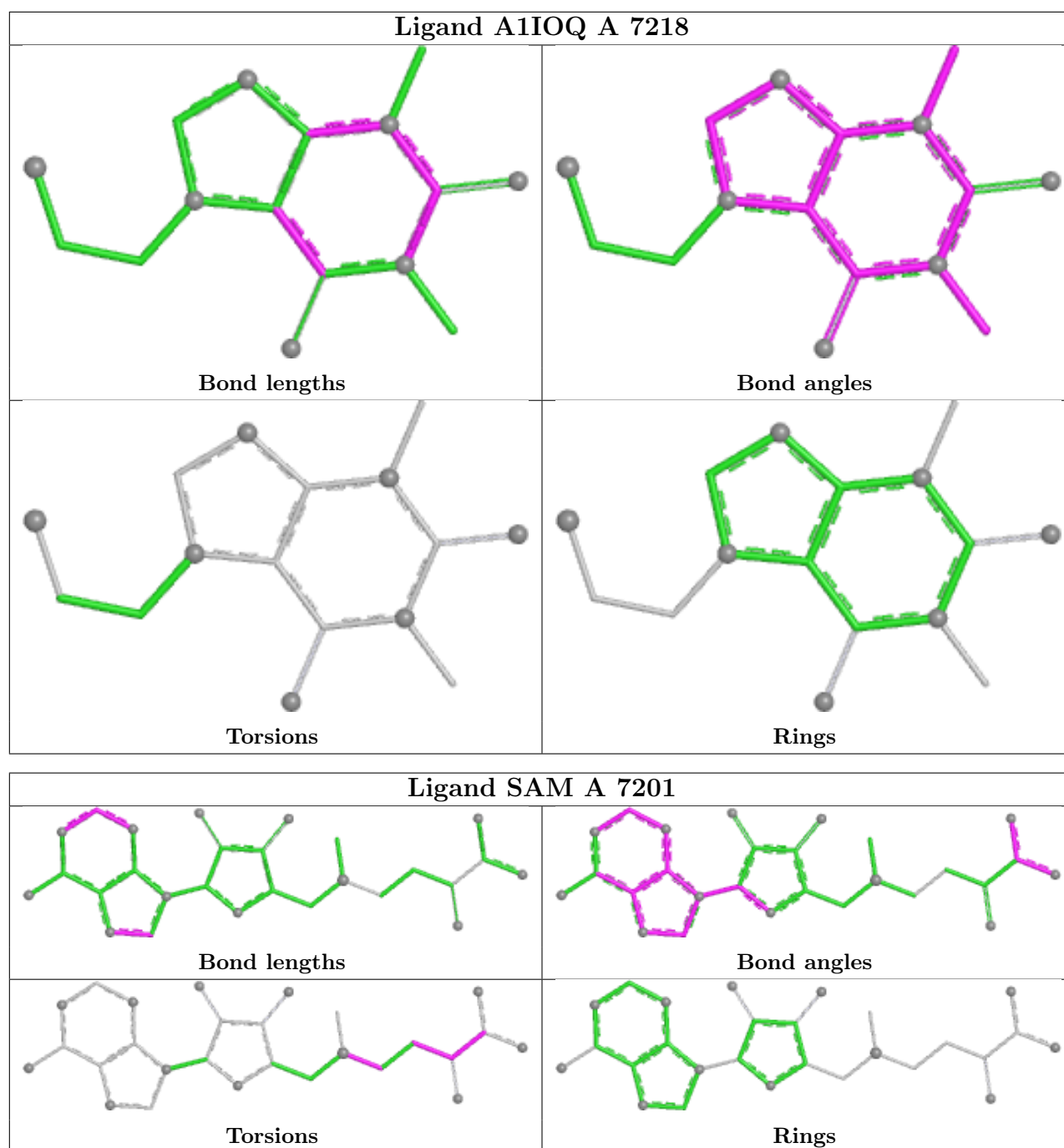
Mol	Chain	Res	Type	Atoms
5	A	7204	MES	C7-C8-S-O1S
5	A	7204	MES	C7-C8-S-O2S
5	A	7204	MES	C7-C8-S-O3S
4	A	7208	EDO	O1-C1-C2-O2
3	A	7201	SAM	CB-CG-SD-CE
3	A	7201	SAM	OXT-C-CA-CB
3	A	7201	SAM	O-C-CA-CB
4	A	7210	EDO	O1-C1-C2-O2
4	A	7202	EDO	O1-C1-C2-O2
5	A	7204	MES	C8-C7-N4-C5
4	A	7217	EDO	O1-C1-C2-O2
4	B	4406	EDO	O1-C1-C2-O2
4	A	7205	EDO	O1-C1-C2-O2
4	A	7221	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	7214	EDO	1	0
5	A	7204	MES	1	0
4	A	7209	EDO	2	0
4	A	7213	EDO	1	0
4	A	7219	EDO	1	0
4	B	4406	EDO	1	0
3	A	7201	SAM	1	0
4	A	7202	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 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, 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%)	0.17	17 (5%)	29 31	16, 41, 76, 95	11 (3%)
2	B	115/140 (82%)	0.37	10 (8%)	16 16	35, 52, 84, 98	0
All	All	415/444 (93%)	0.23	27 (6%)	25 26	16, 43, 79, 98	11 (2%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6799	SER	5.0
2	B	4271	ALA	4.8
1	A	6938	THR	4.3
2	B	4342	PHE	4.2
1	A	6937	VAL	3.8
1	A	6800	SER	3.6
1	A	7053[A]	ARG	3.6
1	A	7095	ASN	3.6
1	A	6873	ASP	3.4
2	B	4339	PRO	3.4
1	A	7098	ASN	3.3
1	A	6936	ASN	3.2
1	A	7097[A]	GLU	3.2
2	B	4274	VAL	2.7
1	A	7052	LEU	2.6
2	B	4338	ASN	2.6
1	A	6939	LYS	2.5
2	B	4341	GLY	2.2
2	B	4385	GLN	2.2
1	A	7051	LYS	2.2
2	B	4272	PHE	2.2
1	A	6829	GLY	2.2
1	A	6919	ALA	2.1
2	B	4289	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	4340	LYS	2.0
1	A	7094	VAL	2.0
1	A	6832	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 oligosaccharides 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
4	EDO	A	7220	4/4	0.78	0.23	77,81,83,86	0
4	EDO	A	7219	4/4	0.82	0.22	55,63,69,70	0
4	EDO	B	4404	4/4	0.82	0.23	54,56,60,76	0
4	EDO	A	7217	4/4	0.84	0.18	53,63,63,64	0
4	EDO	A	7208	4/4	0.84	0.21	70,78,80,87	0
4	EDO	A	7210	4/4	0.85	0.19	50,64,69,69	0
6	A1IOQ	A	7218	16/16	0.85	0.15	59,72,88,107	0
3	SAM	A	7201	27/27	0.86	0.15	46,61,73,77	0
4	EDO	A	7212	4/4	0.87	0.20	60,65,68,76	0
4	EDO	A	7221	4/4	0.87	0.23	84,85,86,93	0
4	EDO	B	4403	4/4	0.87	0.17	58,60,68,71	0
4	EDO	A	7209	4/4	0.87	0.18	56,59,60,76	0
4	EDO	A	7206	4/4	0.87	0.18	54,59,67,68	0
8	IMD	B	4405	5/5	0.87	0.19	68,69,71,77	0
4	EDO	A	7202	4/4	0.89	0.16	57,59,63,66	0
4	EDO	A	7214	4/4	0.89	0.16	61,62,65,73	0
4	EDO	A	7207	4/4	0.90	0.19	59,66,66,66	0
4	EDO	A	7216	4/4	0.91	0.16	62,67,67,81	0
4	EDO	A	7213	4/4	0.91	0.20	59,59,68,71	0
4	EDO	A	7215	4/4	0.91	0.24	49,52,61,67	0

Continued on next page...

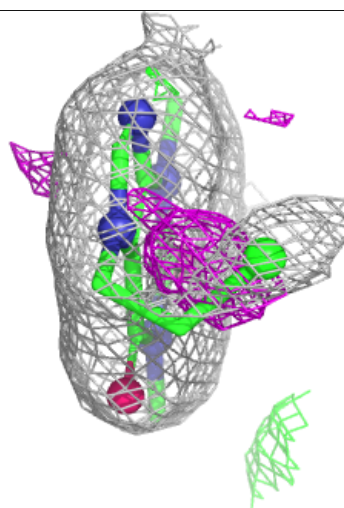
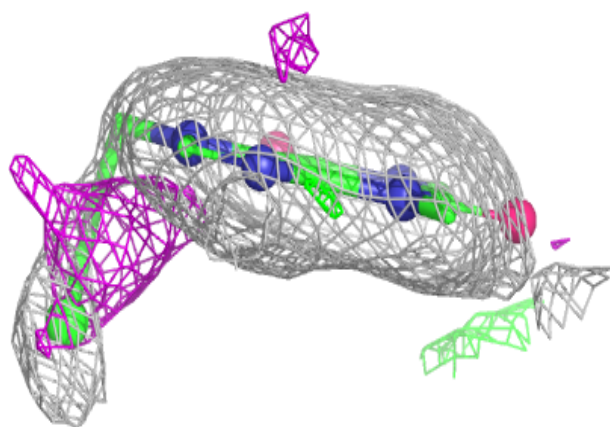
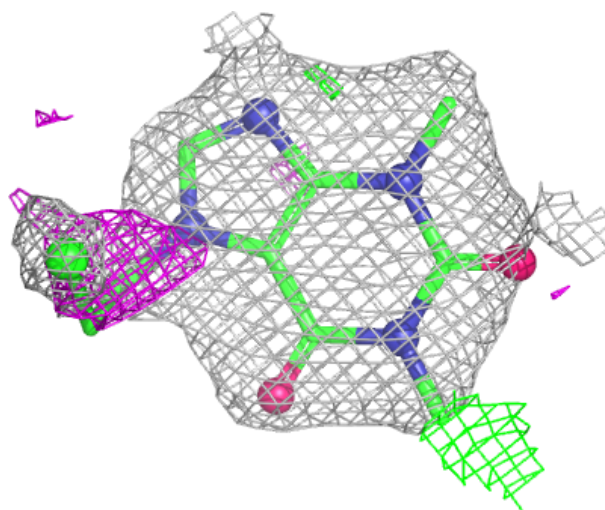
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MES	A	7204	12/12	0.92	0.13	44,54,75,75	0
4	EDO	A	7203	4/4	0.93	0.14	50,50,57,61	0
4	EDO	A	7205	4/4	0.93	0.17	58,64,65,81	0
4	EDO	B	4406	4/4	0.93	0.14	59,63,64,74	0
4	EDO	A	7211	4/4	0.96	0.12	50,56,58,69	0
7	ZN	B	4402	1/1	0.99	0.03	78,78,78,78	0
7	ZN	B	4401	1/1	1.00	0.02	49,49,49,49	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.

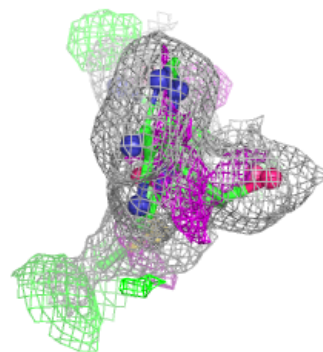
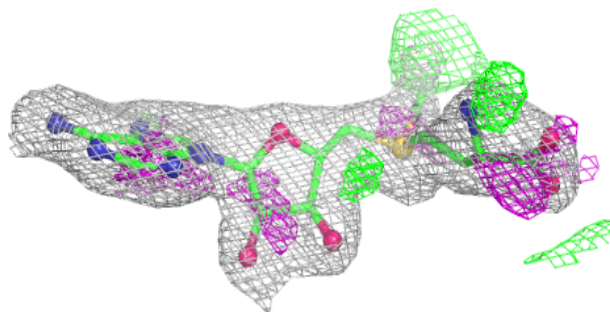
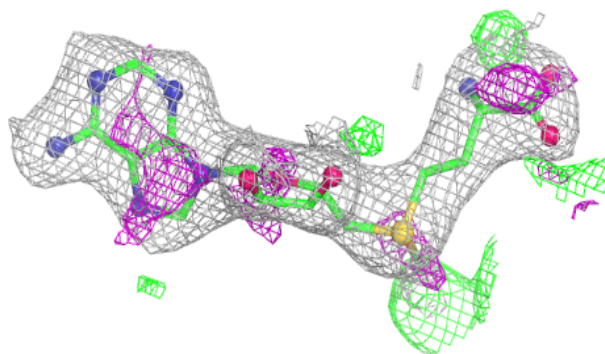
Electron density around A1IOQ A 7218:

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 7201:

$2mF_o-DF_c$ (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.