



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:44 PM UTC

PDB ID : 9GUD / pdb_00009gud
Title : SARS-CoV-2 methyltransferase nsp10-16 in complex with SAM and theophylline derivative LAS 54570922
Authors : Kremling, V.; Sprenger, J.; Oberthuer, D.; Kiene, A.
Deposited on : 2024-09-19
Resolution : 2.05 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

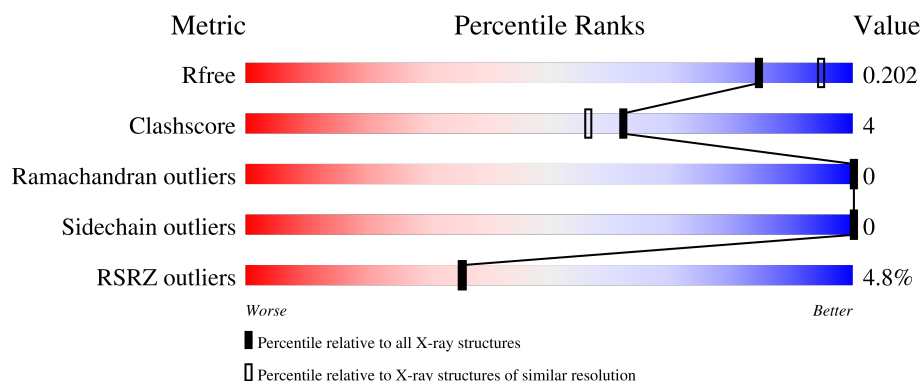
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	5% 88% 11% .
2	B	140	4% 79% . 17%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7237 atoms, of which 3434 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	301	4848	1542	2426	411	452	17	0	14	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	116	1672	533	816	144	164	15	0	0	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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



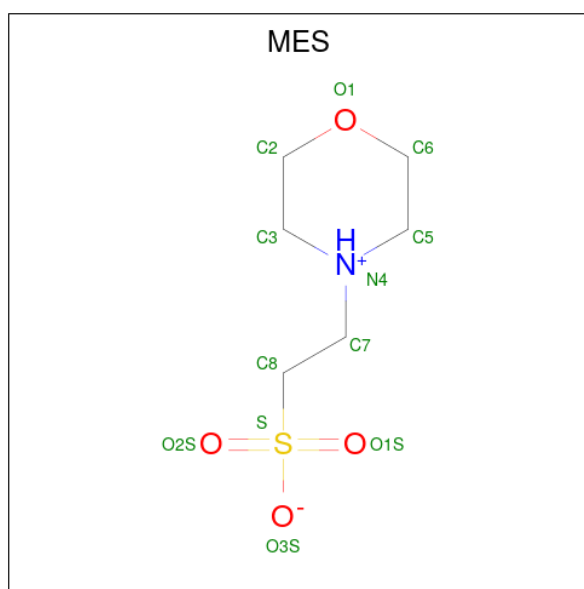
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1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

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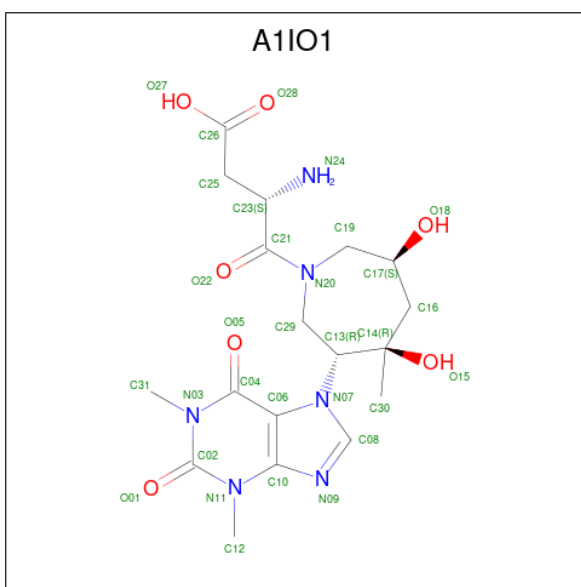
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



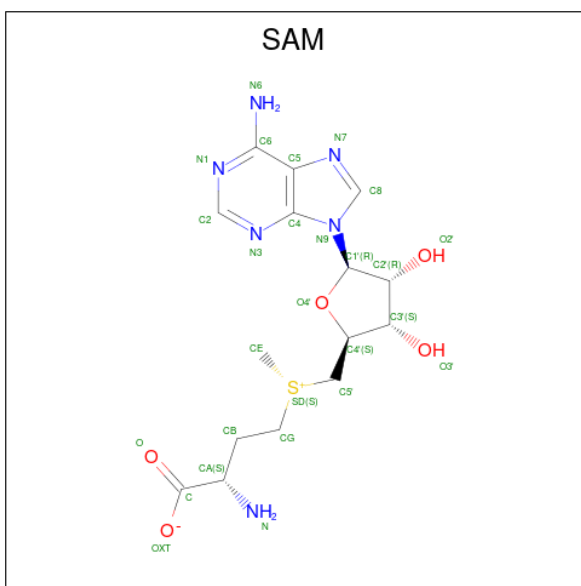
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 5 is (3 {S})-3-azanyl-4-[(3 {R},4 {R},6 {S})-3-[1,3-dimethyl-2,6-bis(oxidanylidene)purin-7-yl]-4-methyl-4,6-bis(oxidanyl)azepan-1-yl]-4-oxidanylidene-butanoic acid (CCD ID: A1IO1) (formula: $C_{18}H_{26}N_6O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	H	N	O	0	0
			56	18	25	6	7		

- Molecule 6 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		
7	B	1	Total	Cl	0	0
			1	1		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

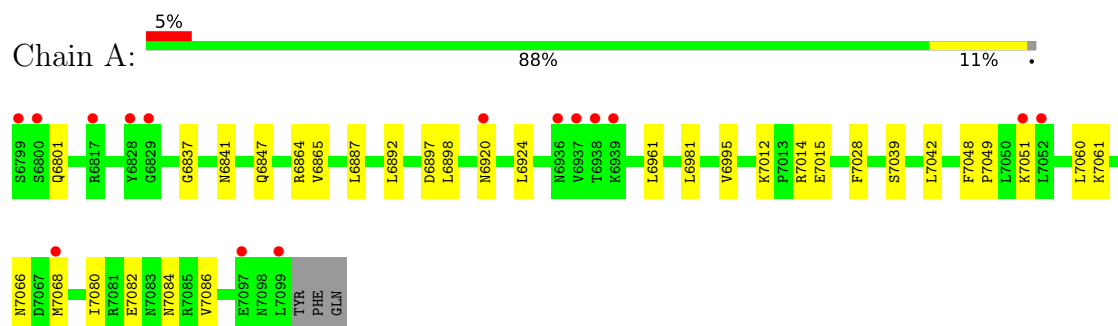
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	264	Total	O	0	0
			264	264		
9	B	98	Total	O	0	0
			98	98		

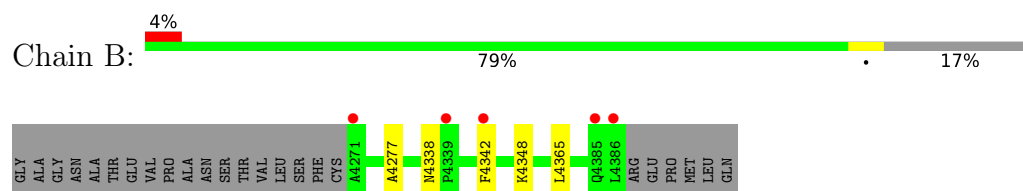
3 Residue-property plots

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.01Å 168.01Å 51.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.75 – 2.05 48.75 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.75-2.05) 100.0 (48.75-2.05)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.69Å)	Xtriage
Refinement program	PHENIX 1.21-5207	Depositor
R, R_{free}	0.187 , 0.200 0.188 , 0.202	Depositor DCC
R_{free} test set	735 reflections (1.02%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7237	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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, ZN, A1IO1, SAM, CL, 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	A	0.11	0/2535	0.30	0/3436
2	B	0.09	0/875	0.28	0/1187
All	All	0.10	0/3410	0.30	0/4623

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	2422	2426	2344	23	0
2	B	856	816	816	3	0
3	A	80	120	120	6	0
3	B	8	12	12	0	0
4	A	12	13	13	1	0
5	A	31	25	0	0	0
6	A	27	22	22	1	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
8	B	2	0	0	0	0
9	A	264	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	98	0	0	1	0
All	All	3803	3434	3327	28	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 (28) 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:7213[D]:EDO:O1	9:A:7301:HOH:O	1.99	0.79
4:A:7202:MES:O2S	9:A:7302:HOH:O	2.12	0.64
1:A:7012:LYS:NZ	9:A:7308:HOH:O	2.30	0.62
1:A:7061:LYS:N	1:A:7061:LYS:HD2	2.17	0.59
1:A:6887:LEU:O	9:A:7303:HOH:O	2.17	0.58
2:B:4338:ASN:ND2	2:B:4342:PHE:HB3	2.22	0.54
1:A:6892:LEU:HD12	1:A:7086:VAL:HG21	1.91	0.53
1:A:7051:LYS:HD2	1:A:7051:LYS:H	1.78	0.49
2:B:4348:LYS:NZ	9:B:4504:HOH:O	2.47	0.47
1:A:7082:GLU:HB2	3:A:7209:EDO:H21	1.98	0.45
1:A:6865:VAL:HG22	1:A:6924:LEU:HB3	1.99	0.44
1:A:7014:ARG:NH2	1:A:7015:GLU:OE2	2.51	0.44
2:B:4277:ALA:HA	2:B:4365:LEU:HD21	1.98	0.44
1:A:6841:ASN:ND2	6:A:7222:SAM:OXT	2.51	0.44
1:A:6897:ASP:OD1	1:A:6898:LEU:N	2.50	0.43
1:A:7048:PHE:N	1:A:7049:PRO:CD	2.82	0.43
1:A:6981:LEU:HD13	3:A:7207:EDO:H12	2.01	0.42
1:A:6801:GLN:HE21	3:A:7215:EDO:C1	2.31	0.42
1:A:6920:ASN:HA	3:A:7209:EDO:H22	2.02	0.42
1:A:6847:GLN:OE1	1:A:6995:VAL:HG22	2.19	0.42
1:A:7039[B]:SER:HB3	1:A:7042:LEU:HD12	2.02	0.42
1:A:7066:ASN:OD1	1:A:7068:MET:N	2.52	0.42
1:A:7051:LYS:HD2	1:A:7051:LYS:N	2.35	0.41
1:A:6864:ARG:NH2	1:A:7084:ASN:O	2.54	0.41
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	2.03	0.41
1:A:7060:LEU:C	1:A:7061:LYS:HD2	2.46	0.41
1:A:6837:GLY:HA3	3:A:7212:EDO:H22	2.03	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	313/304 (103%)	302 (96%)	11 (4%)	0	100	100
2	B	114/140 (81%)	112 (98%)	2 (2%)	0	100	100
All	All	427/444 (96%)	414 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/264 (104%)	275 (100%)	0	100	100
2	B	94/113 (83%)	94 (100%)	0	100	100
All	All	369/377 (98%)	369 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6804	GLN
1	A	7008	ASN
1	A	7016	GLN
2	B	4306	GLN

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 30 ligands modelled in this entry, 5 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
3	EDO	A	7204	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	A	7201	-	3,3,3	0.42	0	2,2,2	0.44	0
3	EDO	A	7206	-	3,3,3	0.43	0	2,2,2	0.50	0
3	EDO	A	7218	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	A	7210	-	3,3,3	0.43	0	2,2,2	0.41	0
3	EDO	A	7214	-	3,3,3	0.43	0	2,2,2	0.39	0
3	EDO	A	7203	-	3,3,3	0.43	0	2,2,2	0.31	0
3	EDO	B	4404	-	3,3,3	0.44	0	2,2,2	0.35	0
4	MES	A	7202	-	12,12,12	2.26	1 (8%)	15,16,16	1.39	3 (20%)
3	EDO	A	7209	-	3,3,3	0.44	0	2,2,2	0.42	0
3	EDO	A	7220	-	3,3,3	0.43	0	2,2,2	0.36	0
3	EDO	A	7213[D]	-	3,3,3	0.42	0	2,2,2	0.39	0
3	EDO	A	7205	-	3,3,3	0.43	0	2,2,2	0.36	0
5	A1IO1	A	7221	-	29,33,33	2.88	10 (34%)	38,51,51	1.94	14 (36%)
3	EDO	A	7208	-	3,3,3	0.36	0	2,2,2	0.60	0
3	EDO	B	4403	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	A	7207	-	3,3,3	0.43	0	2,2,2	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	7211	-	3,3,3	0.43	0	2,2,2	0.35	0
3	EDO	A	7216	-	3,3,3	0.44	0	2,2,2	0.33	0
6	SAM	A	7222	-	27,29,29	3.43	12 (44%)	34,42,42	3.57	17 (50%)
3	EDO	A	7215	-	3,3,3	0.41	0	2,2,2	0.36	0
3	EDO	A	7219	-	3,3,3	0.44	0	2,2,2	0.29	0
3	EDO	A	7225	-	3,3,3	0.43	0	2,2,2	0.37	0
3	EDO	A	7212	-	3,3,3	0.41	0	2,2,2	0.45	0
3	EDO	A	7217	-	3,3,3	0.42	0	2,2,2	0.38	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
3	EDO	A	7204	-	-	1/1/1/1	-
3	EDO	A	7201	-	-	1/1/1/1	-
3	EDO	A	7206	-	-	1/1/1/1	-
3	EDO	A	7218	-	-	0/1/1/1	-
3	EDO	A	7210	-	-	0/1/1/1	-
3	EDO	A	7214	-	-	1/1/1/1	-
3	EDO	A	7203	-	-	1/1/1/1	-
3	EDO	B	4404	-	-	1/1/1/1	-
4	MES	A	7202	-	-	3/6/14/14	0/1/1/1
3	EDO	A	7209	-	-	1/1/1/1	-
3	EDO	A	7220	-	-	0/1/1/1	-
3	EDO	A	7213[D]	-	-	1/1/1/1	-
3	EDO	A	7205	-	-	1/1/1/1	-
5	A1IO1	A	7221	-	-	4/12/35/35	1/3/3/3
3	EDO	A	7208	-	-	0/1/1/1	-
3	EDO	B	4403	-	-	1/1/1/1	-
3	EDO	A	7207	-	-	1/1/1/1	-
3	EDO	A	7211	-	-	1/1/1/1	-
3	EDO	A	7216	-	-	1/1/1/1	-
6	SAM	A	7222	-	-	0/17/33/33	0/3/3/3
3	EDO	A	7215	-	-	0/1/1/1	-
3	EDO	A	7219	-	-	0/1/1/1	-
3	EDO	A	7225	-	-	0/1/1/1	-
3	EDO	A	7212	-	-	1/1/1/1	-
3	EDO	A	7217	-	-	1/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	7222	SAM	C2'-C3'	-10.43	1.25	1.53
5	A	7221	A1IO1	C21-N20	8.53	1.47	1.35
4	A	7202	MES	C8-S	-7.56	1.67	1.77
6	A	7222	SAM	O4'-C4'	-6.86	1.29	1.45
5	A	7221	A1IO1	C10-N11	6.83	1.49	1.38
5	A	7221	A1IO1	C02-N11	6.19	1.51	1.39
6	A	7222	SAM	C3'-C4'	5.73	1.67	1.53
5	A	7221	A1IO1	C02-N03	5.70	1.50	1.39
6	A	7222	SAM	C6-N6	5.39	1.48	1.34
6	A	7222	SAM	C1'-N9	-4.64	1.33	1.46
6	A	7222	SAM	O4'-C1'	4.24	1.51	1.42
6	A	7222	SAM	O2'-C2'	3.00	1.50	1.43
6	A	7222	SAM	C5-C4	-2.75	1.34	1.39
5	A	7221	A1IO1	O15-C14	-2.63	1.40	1.44
6	A	7222	SAM	C8-N9	-2.61	1.33	1.37
6	A	7222	SAM	C5-N7	-2.45	1.34	1.39
5	A	7221	A1IO1	O22-C21	2.35	1.26	1.22
5	A	7221	A1IO1	C25-C26	2.34	1.57	1.51
6	A	7222	SAM	O3'-C3'	2.32	1.48	1.43
5	A	7221	A1IO1	C06-C04	2.27	1.48	1.43
5	A	7221	A1IO1	C04-N03	2.16	1.44	1.40
6	A	7222	SAM	C2'-C1'	2.15	1.60	1.53
5	A	7221	A1IO1	C08-N07	-2.06	1.32	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	7222	SAM	C1'-N9-C8	-9.89	105.15	127.09
6	A	7222	SAM	C4-N9-C1'	8.56	146.66	126.63
6	A	7222	SAM	N6-C6-N1	-6.53	103.84	118.38
6	A	7222	SAM	N3-C2-N1	-5.82	119.77	128.58
6	A	7222	SAM	C5-C6-N6	5.22	136.21	123.29
6	A	7222	SAM	C4'-O4'-C1'	-4.94	98.55	109.47
5	A	7221	A1IO1	C06-C04-N03	4.75	120.76	112.06
6	A	7222	SAM	C5-C4-N3	-4.65	120.31	126.72
6	A	7222	SAM	N9-C8-N7	-4.31	107.82	113.94
6	A	7222	SAM	O4'-C1'-N9	4.12	116.00	108.09
5	A	7221	A1IO1	C08-N07-C06	3.65	107.93	105.53
5	A	7221	A1IO1	N11-C10-N09	3.42	131.65	126.27
6	A	7222	SAM	O4'-C1'-C2'	-3.39	99.36	106.62
6	A	7222	SAM	C2-N3-C4	3.38	120.09	111.83
5	A	7221	A1IO1	O05-C04-C06	-3.27	119.68	126.38
5	A	7221	A1IO1	C29-C13-N07	-3.25	105.62	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	7222	SAM	C5-N7-C8	3.07	108.28	103.45
5	A	7221	A1IO1	C06-C10-N09	-2.76	106.62	112.10
4	A	7202	MES	C5-N4-C3	2.74	114.74	108.84
6	A	7222	SAM	C4-C5-N7	-2.70	107.50	110.58
5	A	7221	A1IO1	N11-C02-N03	-2.59	113.89	117.14
5	A	7221	A1IO1	C04-C06-C10	-2.58	119.67	122.92
6	A	7222	SAM	N3-C4-N9	2.53	131.47	127.17
5	A	7221	A1IO1	O22-C21-N20	-2.48	118.65	121.61
5	A	7221	A1IO1	C08-N09-C10	2.47	108.89	102.98
6	A	7222	SAM	C4-N9-C8	2.33	108.18	105.74
4	A	7202	MES	O3S-S-C8	2.28	110.46	106.00
6	A	7222	SAM	CG-SD-C5'	2.24	108.92	103.43
6	A	7222	SAM	C5-C4-N9	2.21	108.22	105.81
5	A	7221	A1IO1	C23-C21-N20	2.20	122.16	118.85
5	A	7221	A1IO1	N07-C08-N09	-2.13	109.44	113.40
5	A	7221	A1IO1	C04-N03-C02	-2.11	122.24	125.66
4	A	7202	MES	O2S-S-C8	2.03	109.79	106.73
5	A	7221	A1IO1	O27-C26-C25	2.00	120.22	114.00

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	7221	A1IO1	C21-C23-C25-C26
4	A	7202	MES	C7-C8-S-O3S
3	A	7204	EDO	O1-C1-C2-O2
3	A	7207	EDO	O1-C1-C2-O2
3	A	7211	EDO	O1-C1-C2-O2
5	A	7221	A1IO1	N24-C23-C25-C26
3	A	7212	EDO	O1-C1-C2-O2
3	A	7213[D]	EDO	O1-C1-C2-O2
3	A	7214	EDO	O1-C1-C2-O2
3	B	4404	EDO	O1-C1-C2-O2
5	A	7221	A1IO1	C23-C25-C26-O27
3	A	7216	EDO	O1-C1-C2-O2
4	A	7202	MES	C7-C8-S-O1S
4	A	7202	MES	C7-C8-S-O2S
5	A	7221	A1IO1	C23-C25-C26-O28
3	A	7217	EDO	O1-C1-C2-O2
3	A	7203	EDO	O1-C1-C2-O2
3	A	7206	EDO	O1-C1-C2-O2
3	A	7201	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	A	7205	EDO	O1-C1-C2-O2
3	A	7209	EDO	O1-C1-C2-O2
3	B	4403	EDO	O1-C1-C2-O2

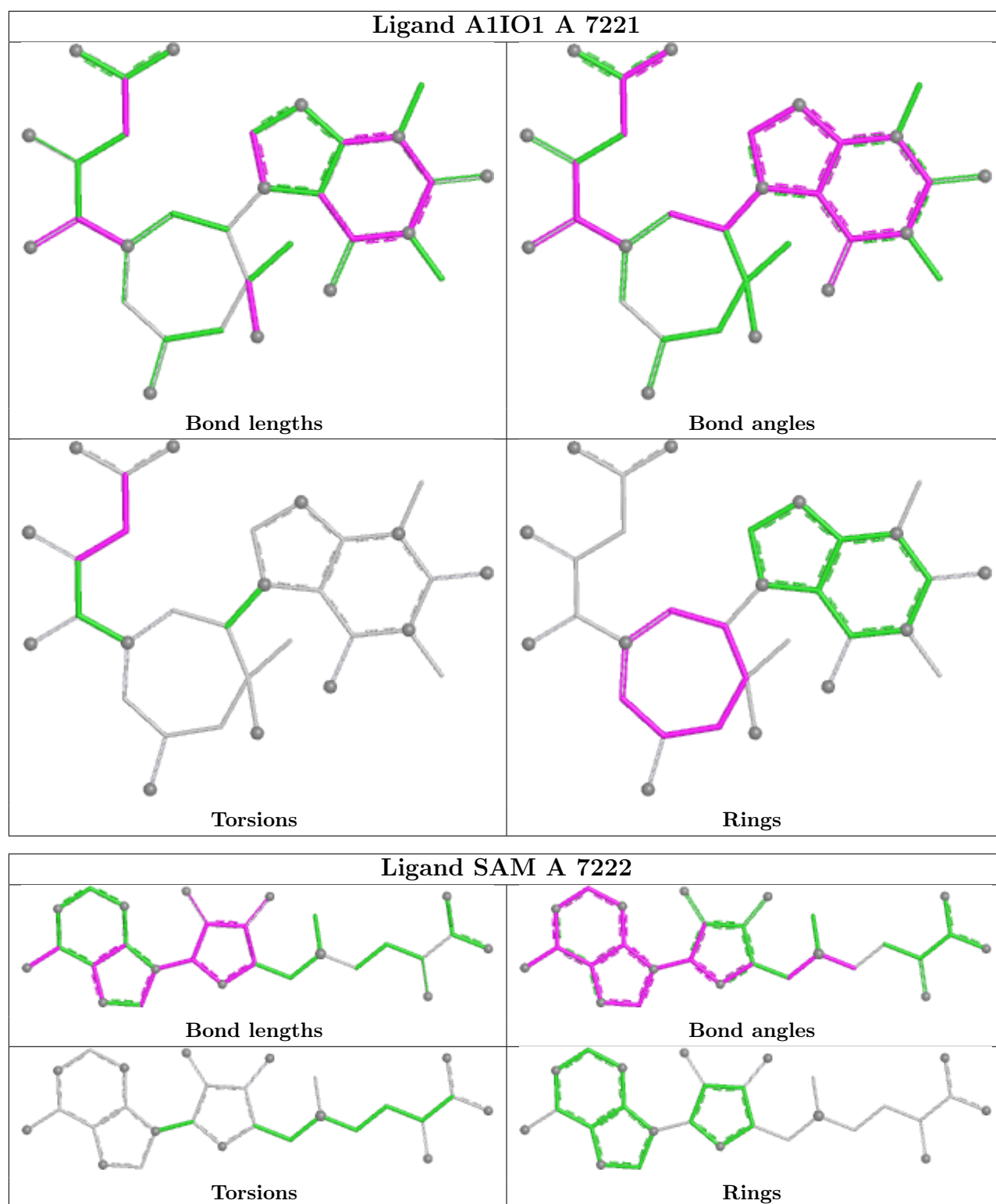
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	7221	A1IO1	C13-C14-C16-C17-C19-C29-N20

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	7202	MES	1	0
3	A	7209	EDO	2	0
3	A	7213[D]	EDO	1	0
3	A	7207	EDO	1	0
6	A	7222	SAM	1	0
3	A	7215	EDO	1	0
3	A	7212	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

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	301/304 (99%)	-0.01	15 (4%) 34 34	17, 41, 78, 108	7 (2%)
2	B	116/140 (82%)	0.31	5 (4%) 40 40	33, 53, 93, 118	0
All	All	417/444 (93%)	0.08	20 (4%) 35 36	17, 44, 85, 118	7 (1%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4386	LEU	8.3
1	A	7099	LEU	5.7
1	A	6937	VAL	4.2
1	A	6817[A]	ARG	3.7
1	A	6799	SER	3.4
2	B	4271	ALA	3.4
1	A	7052	LEU	3.4
2	B	4342	PHE	3.4
2	B	4339	PRO	3.2
1	A	6938	THR	3.0
1	A	7051	LYS	3.0
1	A	6829	GLY	2.9
1	A	6800	SER	2.8
1	A	6936	ASN	2.7
1	A	6939	LYS	2.6
1	A	6828	TYR	2.3
1	A	7068	MET	2.2
2	B	4385	GLN	2.1
1	A	6920	ASN	2.1
1	A	7097	GLU	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($\text{\AA}^2$)	Q<0.9
3	EDO	A	7218	4/4	0.66	0.19	73,97,109,117	0
3	EDO	A	7225	4/4	0.69	0.24	79,94,108,108	0
3	EDO	A	7211	4/4	0.77	0.23	73,88,100,100	0
6	SAM	A	7222	27/27	0.78	0.20	50,72,111,113	0
3	EDO	A	7215	4/4	0.81	0.19	61,74,81,87	0
3	EDO	A	7208	4/4	0.82	0.24	54,65,85,103	0
3	EDO	A	7220	4/4	0.83	0.23	71,86,109,109	0
3	EDO	A	7216	4/4	0.83	0.17	60,78,99,99	0
5	A1IO1	A	7221	31/31	0.83	0.20	47,83,101,105	56
3	EDO	A	7210	4/4	0.83	0.23	58,83,100,100	0
3	EDO	A	7214	4/4	0.85	0.17	61,74,86,96	0
3	EDO	A	7207	4/4	0.85	0.20	64,76,91,91	0
3	EDO	A	7217	4/4	0.87	0.17	57,68,81,83	0
3	EDO	B	4403	4/4	0.87	0.20	66,80,93,93	0
3	EDO	A	7212	4/4	0.87	0.18	61,73,81,89	0
3	EDO	A	7204	4/4	0.87	0.22	49,82,99,99	0
3	EDO	A	7205	4/4	0.88	0.19	43,66,79,79	0
3	EDO	A	7219	4/4	0.89	0.16	64,77,92,92	0
3	EDO	A	7213[D]	4/4	0.90	0.17	40,50,63,76	10
3	EDO	A	7209	4/4	0.90	0.14	42,64,77,77	0
3	EDO	A	7206	4/4	0.91	0.18	46,73,97,97	0
3	EDO	B	4404	4/4	0.91	0.14	64,77,100,100	0
3	EDO	A	7203	4/4	0.92	0.14	52,64,77,77	0
7	CL	A	7224	1/1	0.93	0.18	84,84,84,84	0
4	MES	A	7202	12/12	0.94	0.11	37,56,87,90	0
3	EDO	A	7201	4/4	0.95	0.10	44,53,66,79	0
7	CL	A	7223	1/1	0.97	0.15	66,66,66,66	0

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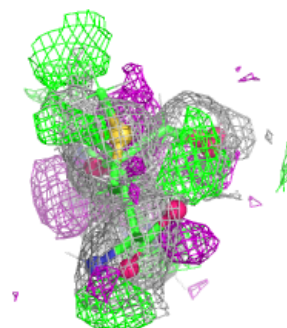
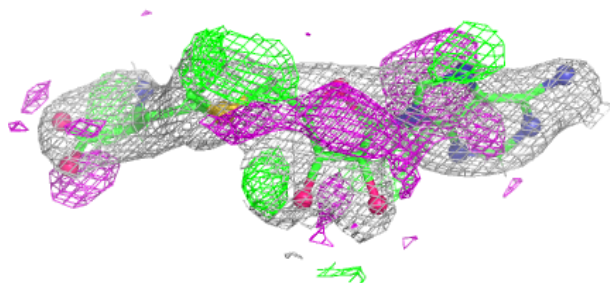
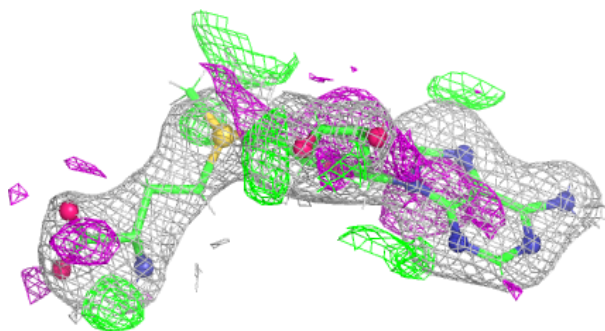
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	CL	B	4405	1/1	0.97	0.19	73,73,73,73	0
8	ZN	B	4401	1/1	0.98	0.04	43,43,43,43	0
8	ZN	B	4402	1/1	0.98	0.05	71,71,71,71	0

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.

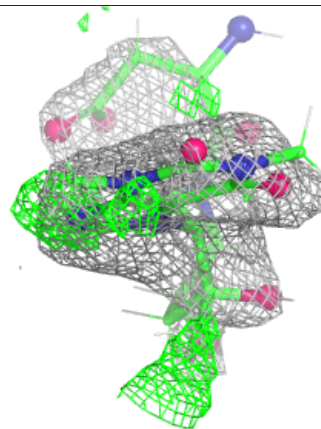
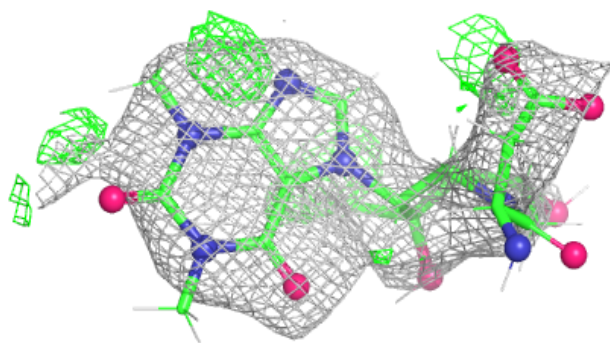
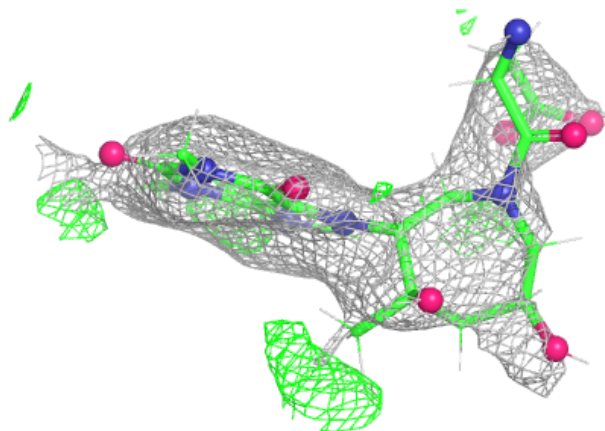
Electron density around SAM A 7222:

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 A1IO1 A 7221:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.