



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:05 AM UTC

PDB ID : 9GRQ / pdb_00009grq
Title : SARS-CoV-2 methyltransferase nsp10-16 in complex with SAM and theophylline
Authors : Kremling, V.; Sprenger, J.; Oberthuer, D.; Kiene, A.
Deposited on : 2024-09-12
Resolution : 1.85 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

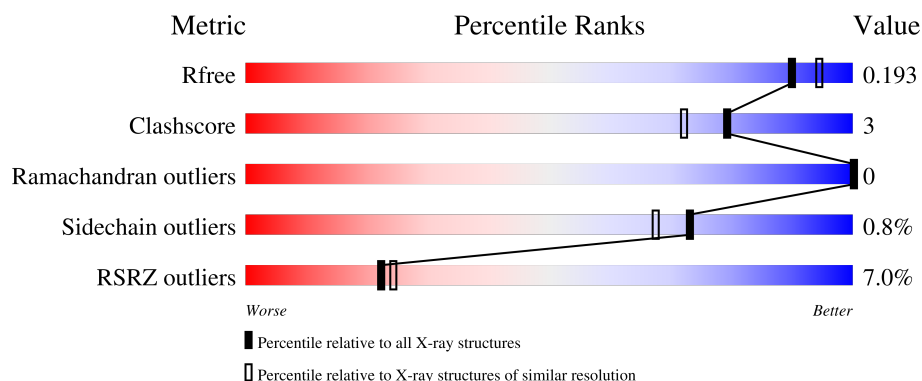
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	7% 93% 5% ..
2	B	140	6% 77% 5% 18%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3832 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	1556	412	465	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

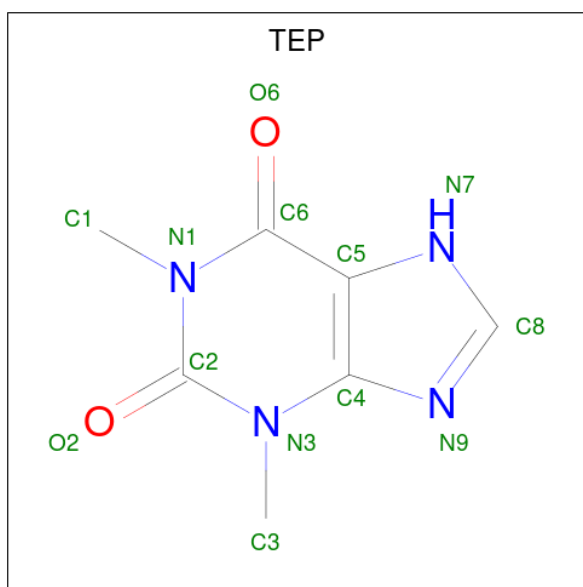
- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	115	Total	C	N	O	S	0	2	0
			867	541	145	165	16			

There is a discrepancy between the modelled and reference sequences:

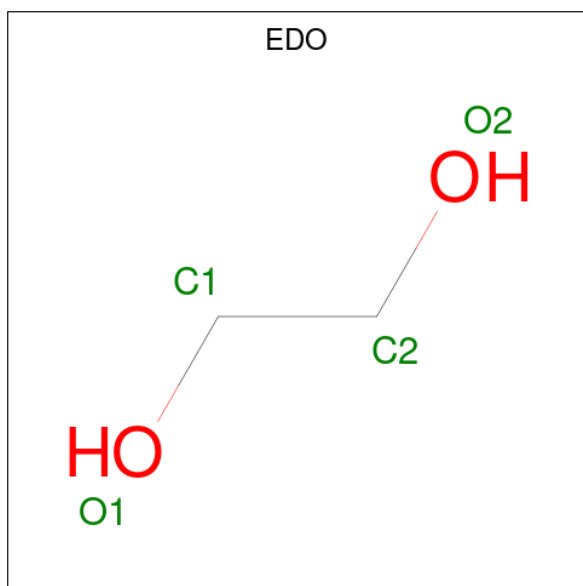
Chain	Residue	Modelled	Actual	Comment	Reference
B	4253	GLY	-	expression tag	UNP P0DTD1

- Molecule 3 is THEOPHYLLINE (CCD ID: TEP) (formula: C₇H₈N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			13	7	4	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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		

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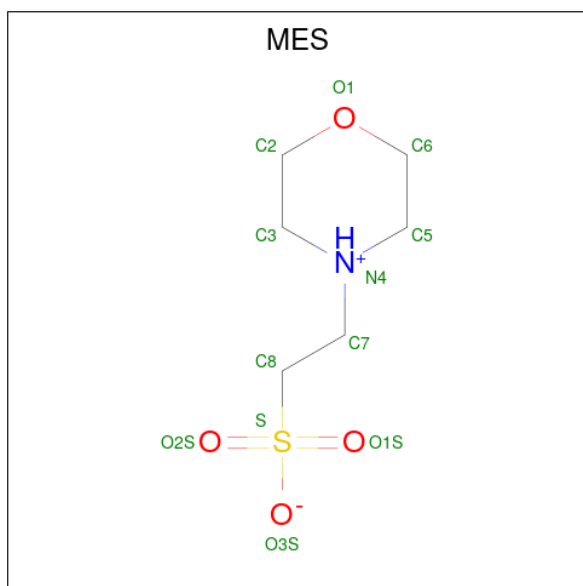
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0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

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

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

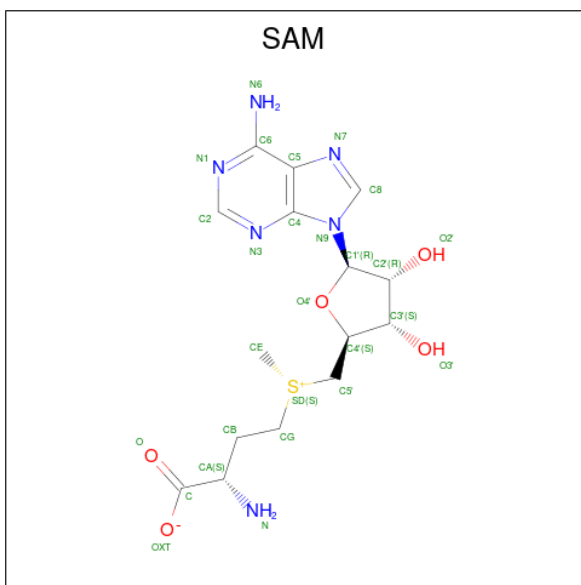


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		

- Molecule 7 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



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

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

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

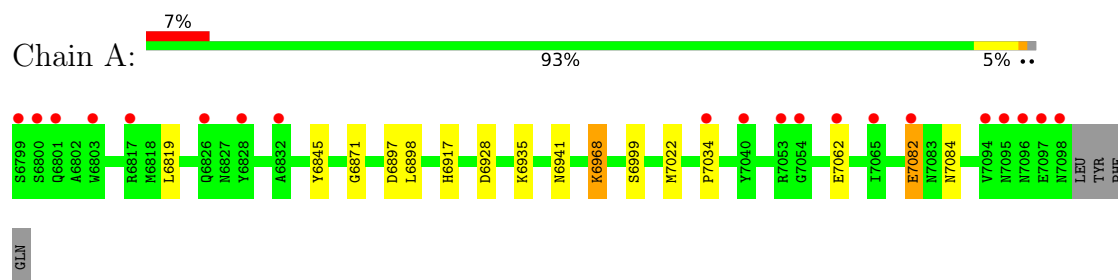
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	232	Total O 232 232	0	0
9	B	103	Total O 103 103	0	0

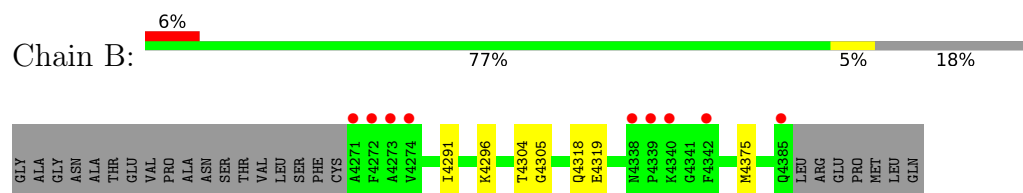
3 Residue-property plots [i](#)

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

- Molecule 1: 2'-O-methyltransferase 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	166.63Å 166.63Å 51.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.10 – 1.85 48.10 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.10-1.85) 100.0 (48.10-1.85)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.185 , 0.191 0.185 , 0.193	Depositor DCC
R_{free} test set	1076 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3832	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: EDO, NA, SAM, ZN, TEP, 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	0.29	0/2502	0.47	0/3394
2	B	0.25	0/887	0.43	0/1202
All	All	0.28	0/3389	0.46	0/4596

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	2450	0	2408	15	0
2	B	867	0	821	4	0
3	A	13	0	8	0	0
4	A	88	0	132	8	0
4	B	24	0	36	1	0
5	A	12	0	12	0	1
5	B	12	0	12	0	0
6	A	2	0	0	0	0
7	A	27	0	22	2	0
8	B	2	0	0	0	0
9	A	232	0	0	1	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	103	0	0	0	2
All	All	3832	0	3451	19	4

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 (19) 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:6917:HIS:HA	4:A:7212:EDO:H22	1.70	0.73
1:A:7082:GLU:HG2	1:A:7084:ASN:H	1.55	0.71
1:A:6935:LYS:NZ	4:A:7224:EDO:H12	2.24	0.52
2:B:4291:ILE:HG23	4:B:4409:EDO:H12	1.94	0.49
1:A:7034:PRO:HD3	9:A:7423:HOH:O	2.12	0.48
1:A:6941:ASN:HB3	4:A:7208:EDO:H21	1.96	0.48
1:A:6897[A]:ASP:OD1	1:A:6898:LEU:N	2.45	0.47
1:A:6898:LEU:HD11	4:A:7222:EDO:H21	1.99	0.45
1:A:6897[A]:ASP:OD1	7:A:7216:SAM:H1'	2.17	0.43
1:A:6928:ASP:OD1	1:A:6968:LYS:NZ	2.47	0.43
1:A:7022:MET:HE2	4:A:7223:EDO:H21	2.00	0.43
1:A:6999:SER:OG	4:A:7224:EDO:H22	2.19	0.43
2:B:4304:THR:O	2:B:4375[B]:MET:HE1	2.19	0.42
2:B:4305:GLY:HA2	2:B:4318:GLN:OE1	2.19	0.42
1:A:6871:GLY:O	7:A:7216:SAM:HG2	2.19	0.41
2:B:4296:LYS:HD2	2:B:4319:GLU:CD	2.46	0.41
1:A:6917:HIS:HA	4:A:7212:EDO:C2	2.47	0.41
1:A:6819:LEU:H	4:A:7217:EDO:C2	2.35	0.40
1:A:6845:TYR:OH	1:A:6928:ASP:HB2	2.22	0.40

All (4) 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)
9:A:7521:HOH:O	9:A:7521:HOH:O[5_554]	2.05	0.15
9:A:7436:HOH:O	9:A:7436:HOH:O[5_554]	2.07	0.13
5:A:7204:MES:O2S	9:B:4571:HOH:O[2_545]	2.15	0.05
9:B:4518:HOH:O	9:B:4583:HOH:O[5_554]	2.16	0.04

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%)	299 (97%)	10 (3%)	0	100	100
2	B	115/140 (82%)	113 (98%)	2 (2%)	0	100	100
All	All	424/444 (96%)	412 (97%)	12 (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	271/264 (103%)	268 (99%)	3 (1%)	65	57
2	B	95/113 (84%)	95 (100%)	0	100	100
All	All	366/377 (97%)	363 (99%)	3 (1%)	73	67

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

Mol	Chain	Res	Type
1	A	6968	LYS
1	A	7062	GLU
1	A	7082	GLU

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

Mol	Chain	Res	Type
2	B	4306	GLN
2	B	4333	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 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	7213	-	3,3,3	0.43	0	2,2,2	0.44	0
4	EDO	A	7225	-	3,3,3	0.39	0	2,2,2	0.60	0
5	MES	A	7204	-	12,12,12	1.94	1 (8%)	15,16,16	1.92	5 (33%)
3	TEP	A	7201	-	14,14,14	1.45	2 (14%)	21,21,21	4.07	11 (52%)
4	EDO	B	4407	-	3,3,3	0.49	0	2,2,2	0.49	0
4	EDO	A	7212	-	3,3,3	0.39	0	2,2,2	0.68	0
4	EDO	A	7208	-	3,3,3	0.49	0	2,2,2	0.13	0
5	MES	B	4406	-	12,12,12	2.10	1 (8%)	15,16,16	2.31	5 (33%)
4	EDO	A	7207	-	3,3,3	0.55	0	2,2,2	0.28	0
4	EDO	A	7215	-	3,3,3	0.43	0	2,2,2	0.47	0
4	EDO	A	7203	-	3,3,3	0.46	0	2,2,2	0.68	0
4	EDO	A	7224	-	3,3,3	0.44	0	2,2,2	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	7220	-	3,3,3	0.42	0	2,2,2	0.48	0
4	EDO	A	7226	-	3,3,3	0.40	0	2,2,2	0.69	0
4	EDO	A	7218	-	3,3,3	0.50	0	2,2,2	0.43	0
4	EDO	A	7206	-	3,3,3	0.43	0	2,2,2	0.49	0
4	EDO	B	4403	-	3,3,3	0.55	0	2,2,2	0.30	0
4	EDO	A	7210	-	3,3,3	0.37	0	2,2,2	0.51	0
4	EDO	A	7205	-	3,3,3	0.33	0	2,2,2	0.77	0
4	EDO	A	7223	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	A	7202	-	3,3,3	0.39	0	2,2,2	0.74	0
4	EDO	B	4404	-	3,3,3	0.50	0	2,2,2	0.33	0
4	EDO	B	4409	-	3,3,3	0.39	0	2,2,2	0.42	0
7	SAM	A	7216	-	27,29,29	3.19	9 (33%)	34,42,42	2.34	11 (32%)
4	EDO	A	7221	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	A	7217	-	3,3,3	0.55	0	2,2,2	0.17	0
4	EDO	A	7209	-	3,3,3	0.46	0	2,2,2	0.52	0
4	EDO	B	4408	-	3,3,3	0.33	0	2,2,2	0.80	0
4	EDO	A	7219	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	A	7214	-	3,3,3	0.42	0	2,2,2	0.38	0
4	EDO	B	4405	-	3,3,3	0.43	0	2,2,2	0.42	0
4	EDO	A	7222	-	3,3,3	0.52	0	2,2,2	0.32	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	7213	-	-	0/1/1/1	-
4	EDO	A	7225	-	-	1/1/1/1	-
5	MES	A	7204	-	-	5/6/14/14	0/1/1/1
3	TEP	A	7201	-	-	-	0/2/2/2
4	EDO	B	4407	-	-	1/1/1/1	-
4	EDO	A	7212	-	-	1/1/1/1	-
4	EDO	A	7208	-	-	0/1/1/1	-
5	MES	B	4406	-	-	1/6/14/14	0/1/1/1
4	EDO	A	7207	-	-	0/1/1/1	-
4	EDO	A	7215	-	-	0/1/1/1	-
4	EDO	A	7203	-	-	0/1/1/1	-
4	EDO	A	7224	-	-	0/1/1/1	-
4	EDO	A	7220	-	-	1/1/1/1	-
4	EDO	A	7226	-	-	1/1/1/1	-
4	EDO	A	7218	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	7206	-	-	0/1/1/1	-
4	EDO	B	4403	-	-	0/1/1/1	-
4	EDO	A	7210	-	-	0/1/1/1	-
4	EDO	A	7205	-	-	1/1/1/1	-
4	EDO	A	7223	-	-	1/1/1/1	-
4	EDO	A	7202	-	-	0/1/1/1	-
4	EDO	B	4404	-	-	1/1/1/1	-
4	EDO	B	4409	-	-	1/1/1/1	-
7	SAM	A	7216	-	-	6/17/33/33	0/3/3/3
4	EDO	A	7221	-	-	1/1/1/1	-
4	EDO	A	7217	-	-	1/1/1/1	-
4	EDO	A	7209	-	-	0/1/1/1	-
4	EDO	B	4408	-	-	0/1/1/1	-
4	EDO	A	7219	-	-	1/1/1/1	-
4	EDO	A	7214	-	-	0/1/1/1	-
4	EDO	B	4405	-	-	0/1/1/1	-
4	EDO	A	7222	-	-	0/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	7216	SAM	C2'-C3'	-9.10	1.28	1.53
5	B	4406	MES	C8-S	-6.75	1.68	1.77
7	A	7216	SAM	O4'-C4'	-6.31	1.31	1.45
5	A	7204	MES	C8-S	-6.17	1.68	1.77
7	A	7216	SAM	C3'-C4'	6.06	1.68	1.53
7	A	7216	SAM	O4'-C1'	5.70	1.55	1.42
7	A	7216	SAM	C6-N6	4.79	1.46	1.34
7	A	7216	SAM	C1'-N9	-4.49	1.33	1.46
3	A	7201	TEP	C6-N1	-3.24	1.33	1.40
7	A	7216	SAM	O2'-C2'	3.23	1.51	1.43
7	A	7216	SAM	C2'-C1'	2.48	1.61	1.53
3	A	7201	TEP	C2-N3	-2.32	1.34	1.39
7	A	7216	SAM	C8-N9	-2.27	1.33	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7201	TEP	C8-N9-C4	8.56	109.18	103.45
3	A	7201	TEP	C5-C4-N9	-8.37	105.76	111.63
7	A	7216	SAM	C5-C4-N3	-6.45	117.84	126.72
3	A	7201	TEP	C5-C6-N1	6.04	120.17	112.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	7201	TEP	C6-C5-C4	-6.01	118.39	123.13
3	A	7201	TEP	N3-C4-N9	5.63	135.12	126.27
3	A	7201	TEP	C4-C5-N7	5.26	107.88	105.29
5	B	4406	MES	C5-N4-C3	5.25	120.16	108.84
7	A	7216	SAM	O4'-C1'-N9	4.75	117.22	108.09
3	A	7201	TEP	C5-C4-N3	-4.64	119.11	121.73
7	A	7216	SAM	C4-C5-N7	-4.25	105.72	110.58
5	A	7204	MES	C5-N4-C3	4.21	117.92	108.84
5	B	4406	MES	C7-N4-C5	3.94	121.75	111.24
7	A	7216	SAM	N3-C4-N9	3.87	133.75	127.17
7	A	7216	SAM	C2-N3-C4	3.73	120.95	111.83
3	A	7201	TEP	O6-C6-C5	-3.67	119.14	126.64
5	B	4406	MES	O1S-S-C8	3.48	111.99	106.73
7	A	7216	SAM	C5-N7-C8	3.46	108.89	103.45
7	A	7216	SAM	N3-C2-N1	-3.42	123.41	128.58
3	A	7201	TEP	N7-C8-N9	-3.39	109.04	112.98
7	A	7216	SAM	O4'-C1'-C2'	-2.90	100.41	106.62
3	A	7201	TEP	C6-N1-C2	-2.86	121.01	125.66
5	A	7204	MES	O1S-S-C8	2.56	110.60	106.73
7	A	7216	SAM	C3'-C2'-C1'	2.50	106.19	101.46
5	B	4406	MES	C7-N4-C3	2.47	117.82	111.24
7	A	7216	SAM	N9-C8-N7	-2.41	110.52	113.94
7	A	7216	SAM	C5-C4-N9	2.39	108.42	105.81
5	A	7204	MES	C2-C3-N4	-2.33	106.58	110.12
5	B	4406	MES	C6-C5-N4	-2.21	106.76	110.12
5	A	7204	MES	C7-N4-C3	2.21	117.12	111.24
3	A	7201	TEP	N3-C2-N1	2.15	119.82	117.14
5	A	7204	MES	O2S-S-O1S	-2.07	107.08	113.82

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	7204	MES	C8-C7-N4-C3
5	A	7204	MES	C7-C8-S-O1S
5	A	7204	MES	C7-C8-S-O2S
5	A	7204	MES	C7-C8-S-O3S
5	B	4406	MES	C8-C7-N4-C5
7	A	7216	SAM	C4'-C5'-SD-CG
4	A	7212	EDO	O1-C1-C2-O2
4	A	7217	EDO	O1-C1-C2-O2
4	A	7219	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	7204	MES	C8-C7-N4-C5
4	A	7225	EDO	O1-C1-C2-O2
7	A	7216	SAM	O4'-C4'-C5'-SD
7	A	7216	SAM	C3'-C4'-C5'-SD
7	A	7216	SAM	O-C-CA-CB
7	A	7216	SAM	OXT-C-CA-CB
4	A	7221	EDO	O1-C1-C2-O2
4	A	7205	EDO	O1-C1-C2-O2
4	B	4404	EDO	O1-C1-C2-O2
4	B	4409	EDO	O1-C1-C2-O2
4	A	7223	EDO	O1-C1-C2-O2
4	A	7226	EDO	O1-C1-C2-O2
4	A	7218	EDO	O1-C1-C2-O2
4	B	4407	EDO	O1-C1-C2-O2
4	A	7220	EDO	O1-C1-C2-O2
7	A	7216	SAM	OXT-C-CA-N

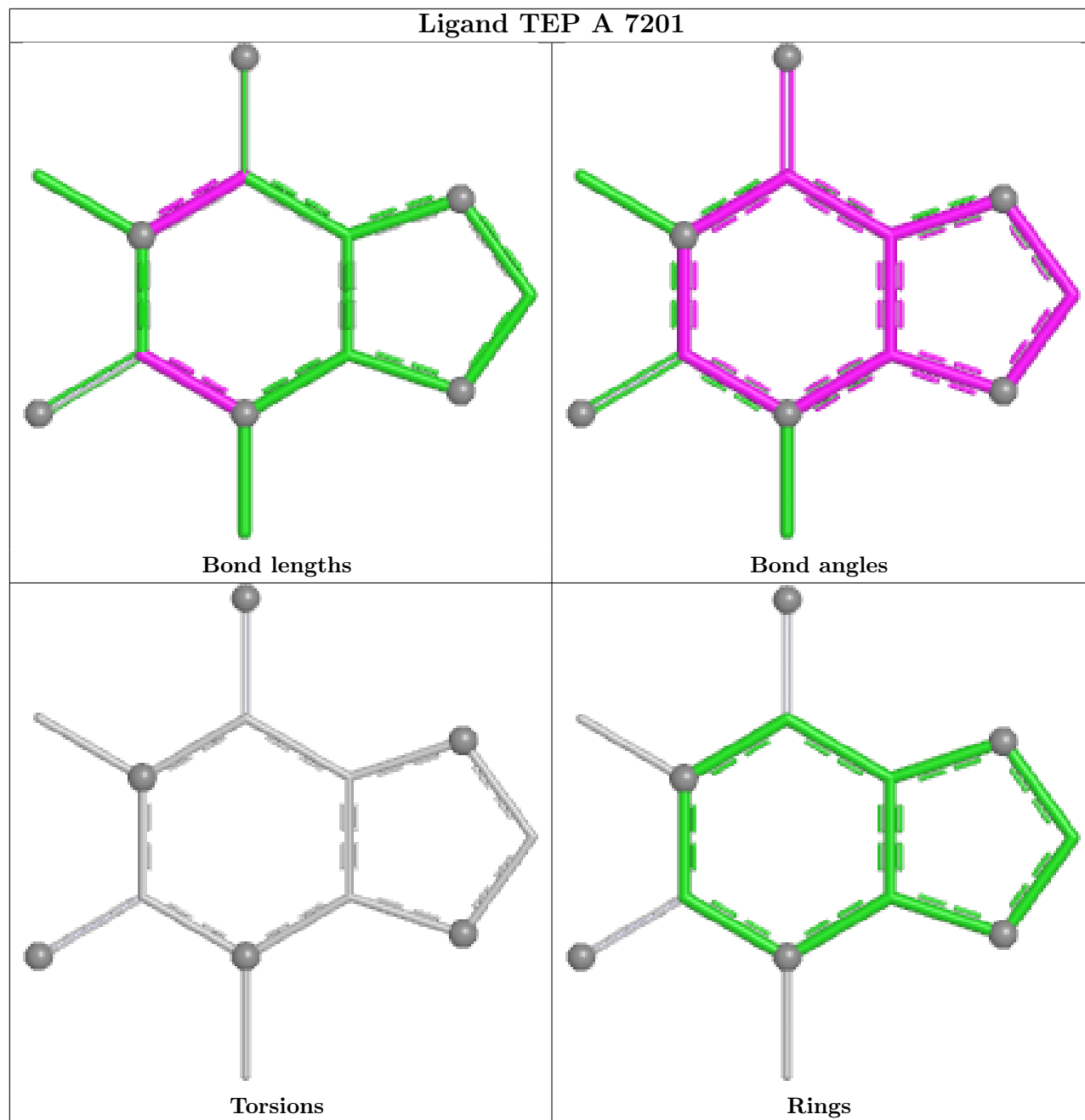
There are no ring outliers.

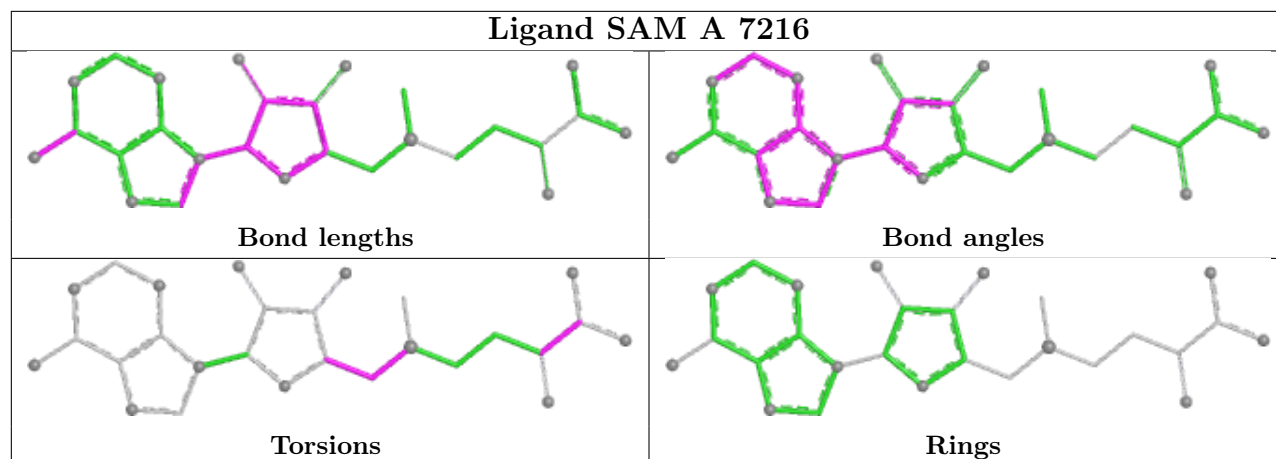
9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	7204	MES	0	1
4	A	7212	EDO	2	0
4	A	7208	EDO	1	0
4	A	7224	EDO	2	0
4	A	7223	EDO	1	0
4	B	4409	EDO	1	0
7	A	7216	SAM	2	0
4	A	7217	EDO	1	0
4	A	7222	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%)	0.06	20 (6%) 24 26	11, 30, 58, 73	11 (3%)
2	B	115/140 (82%)	0.29	9 (7%) 19 20	21, 37, 64, 77	2 (1%)
All	All	415/444 (93%)	0.12	29 (6%) 22 24	11, 32, 61, 77	13 (3%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4342[A]	PHE	9.1
1	A	6803	TRP	9.1
2	B	4271	ALA	7.6
1	A	6799	SER	5.1
1	A	6800	SER	4.4
2	B	4339	PRO	4.2
1	A	7098	ASN	3.9
2	B	4272	PHE	3.4
2	B	4273	ALA	3.3
1	A	7040[A]	TYR	3.2
1	A	6801[A]	GLN	3.2
2	B	4338	ASN	3.1
1	A	7094	VAL	3.0
1	A	7097[A]	GLU	3.0
1	A	7095	ASN	3.0
2	B	4385	GLN	2.9
1	A	7065	ILE	2.9
1	A	7096	ASN	2.6
2	B	4274	VAL	2.5
1	A	6832	ALA	2.5
2	B	4340	LYS	2.5
1	A	7053	ARG	2.4
1	A	7054	GLY	2.4
1	A	6817[A]	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	7082	GLU	2.2
1	A	6826	GLN	2.1
1	A	6828	TYR	2.1
1	A	7062	GLU	2.0
1	A	7034	PRO	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
4	EDO	A	7222	4/4	0.69	0.23	69,71,74,75	0
4	EDO	B	4404	4/4	0.80	0.20	52,55,68,70	0
5	MES	A	7204	12/12	0.81	0.20	35,50,67,96	0
5	MES	B	4406	12/12	0.83	0.17	38,49,61,67	0
4	EDO	B	4408	4/4	0.84	0.21	46,50,60,64	0
4	EDO	B	4407	4/4	0.86	0.19	52,62,67,69	0
4	EDO	B	4403	4/4	0.86	0.16	46,46,49,62	0
4	EDO	A	7219	4/4	0.87	0.17	33,35,47,49	0
4	EDO	A	7224	4/4	0.87	0.18	39,48,49,50	0
4	EDO	A	7225	4/4	0.87	0.22	59,62,67,72	0
4	EDO	A	7206	4/4	0.89	0.16	44,51,52,57	0
4	EDO	A	7217	4/4	0.89	0.16	48,56,57,59	0
3	TEP	A	7201	13/13	0.89	0.12	43,48,57,57	0
4	EDO	B	4409	4/4	0.89	0.18	49,51,59,59	0
4	EDO	A	7226	4/4	0.89	0.12	40,43,59,65	0
4	EDO	A	7220	4/4	0.89	0.14	45,52,55,62	0
7	SAM	A	7216	27/27	0.89	0.13	30,42,47,48	0
4	EDO	A	7213	4/4	0.90	0.14	45,46,60,64	0

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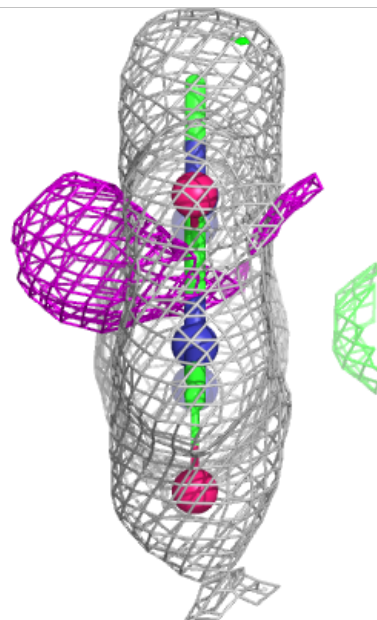
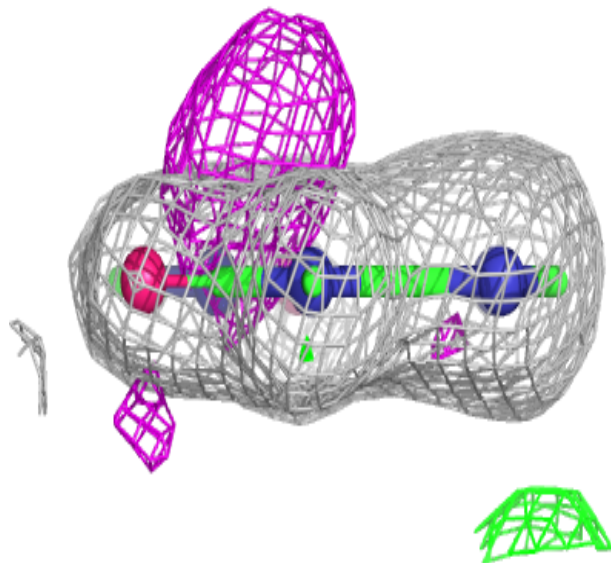
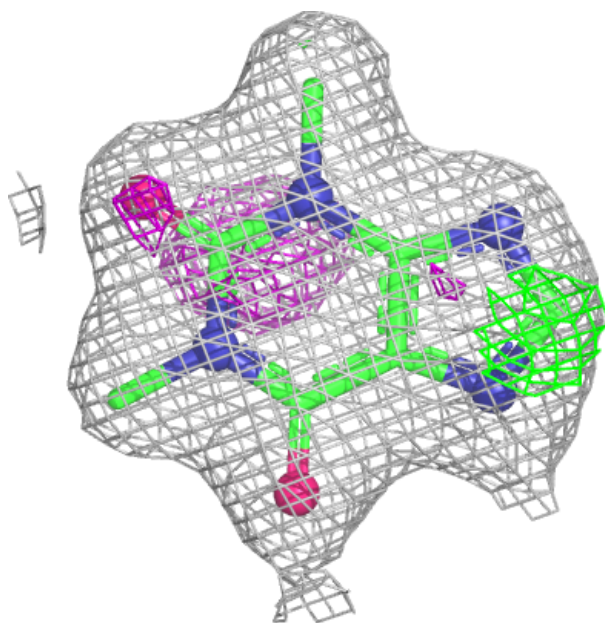
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	7218	4/4	0.90	0.16	47,56,62,65	0
4	EDO	A	7209	4/4	0.91	0.15	42,46,49,54	0
4	EDO	A	7203	4/4	0.91	0.13	40,41,43,45	0
4	EDO	A	7221	4/4	0.91	0.13	41,47,57,57	0
4	EDO	A	7215	4/4	0.92	0.14	53,56,57,71	0
4	EDO	A	7205	4/4	0.92	0.17	45,52,56,59	0
4	EDO	A	7207	4/4	0.92	0.14	38,40,48,49	0
4	EDO	A	7212	4/4	0.93	0.14	37,49,55,63	0
4	EDO	A	7223	4/4	0.94	0.14	37,41,58,65	0
4	EDO	A	7210	4/4	0.94	0.13	37,42,44,46	0
4	EDO	B	4405	4/4	0.94	0.10	40,42,45,51	0
4	EDO	A	7202	4/4	0.95	0.11	38,42,43,53	0
4	EDO	A	7208	4/4	0.95	0.11	42,43,46,53	0
4	EDO	A	7214	4/4	0.96	0.10	30,36,37,43	0
6	NA	A	7227	1/1	0.98	0.12	42,42,42,42	0
6	NA	A	7211	1/1	0.99	0.08	36,36,36,36	0
8	ZN	B	4402	1/1	0.99	0.04	52,52,52,52	0
8	ZN	B	4401	1/1	1.00	0.01	35,35,35,35	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.

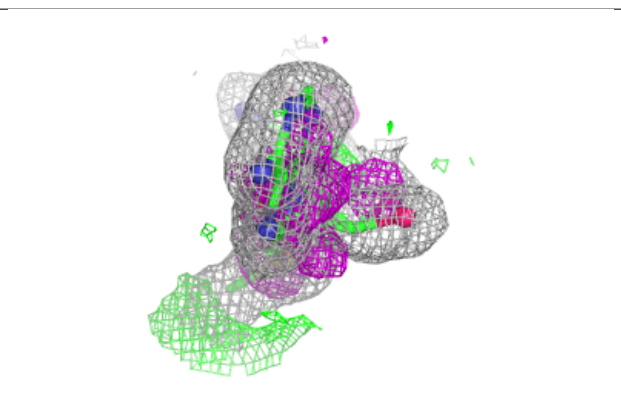
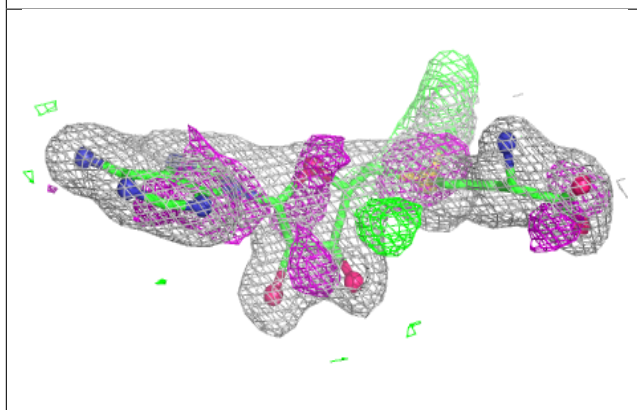
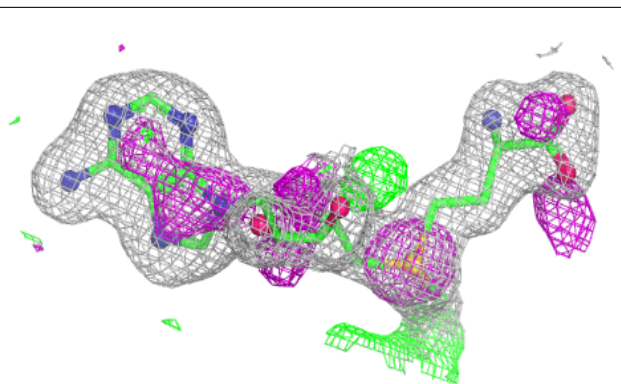
Electron density around TEP A 7201:

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



Electron density around SAM A 7216:

$2mF_o-DF_c$ (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.