



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:19 PM UTC

PDB ID : 9GS4 / pdb_00009gs4
Title : SARS-CoV-2 methyltransferase nsp10-16 in complex with SAM and theophylline derivative LAS 54571130
Authors : Kremling, V.; Sprenger, J.; Oberthuer, D.; Kiene, A.
Deposited on : 2024-09-13
Resolution : 2.00 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

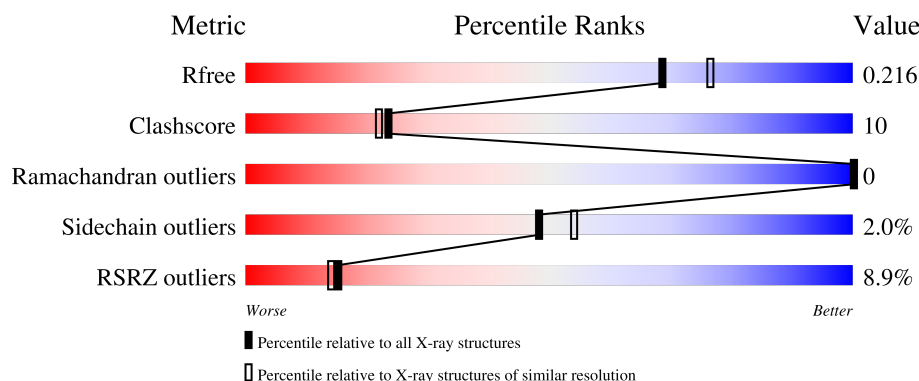
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

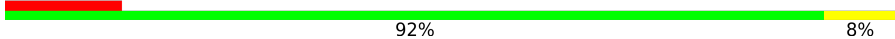
The reported resolution of this entry is 2.00 Å.

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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	301	
2	B	115	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	7101	-	-	X	-
3	EDO	A	7115	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 3630 atoms, of which 35 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	N	O	S			
1	A	301	2364	1508	397	442	17	0	0	0

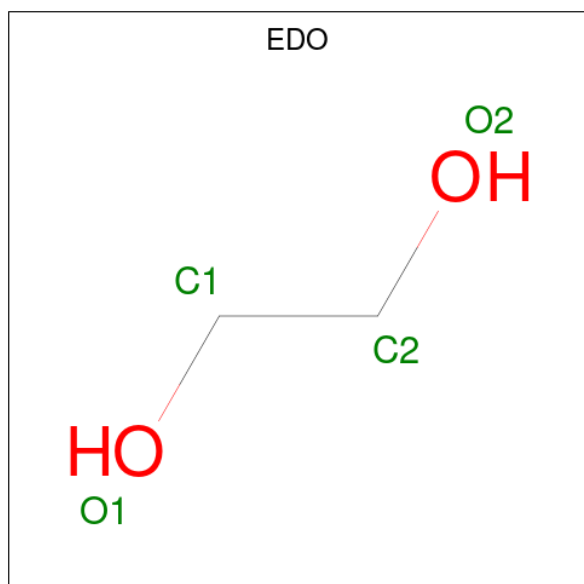
There are 3 discrepancies between the modelled and reference sequences:

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

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

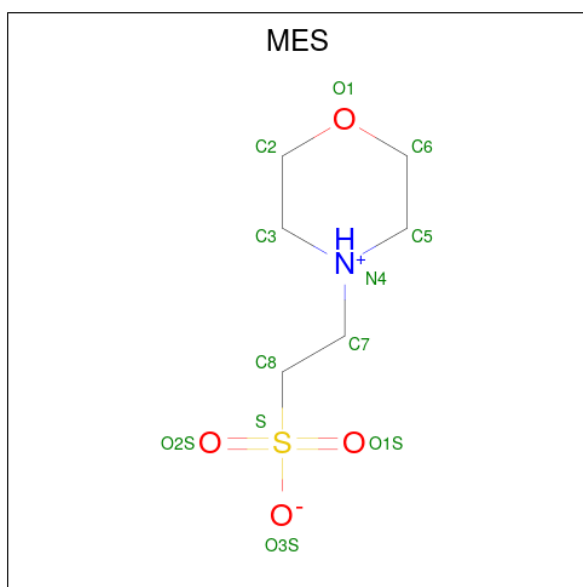
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	115	856	531	145	165	15	0	1	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

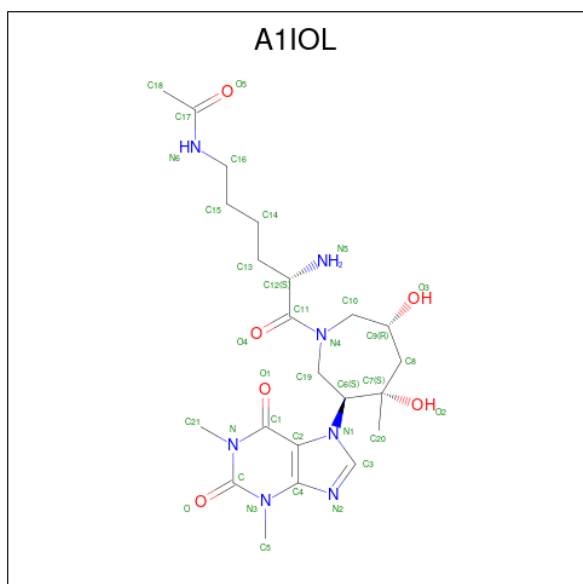


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

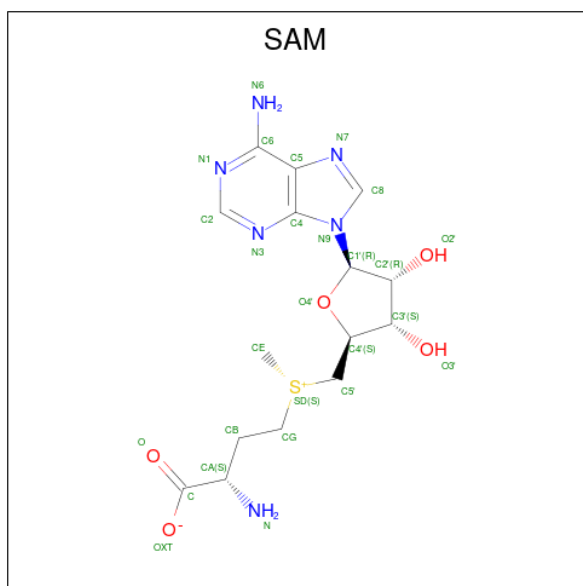
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Na	0	0
			2	2		

- Molecule 6 is {N}-[(5 {S})-5-azanyl-6-[(3 {S},4 {S},6 {R})-3-[1,3-dimethyl-2,6-bis(oxidanyl idene)purin-7-yl]-4-methyl-4,6-bis(oxidanyl)azepan-1-yl]-6-oxidanylidene-hexyl]ethanamide (CCD ID: A1IOL) (formula: C₂₂H₃₅N₇O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			70	22	35	7	6		

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

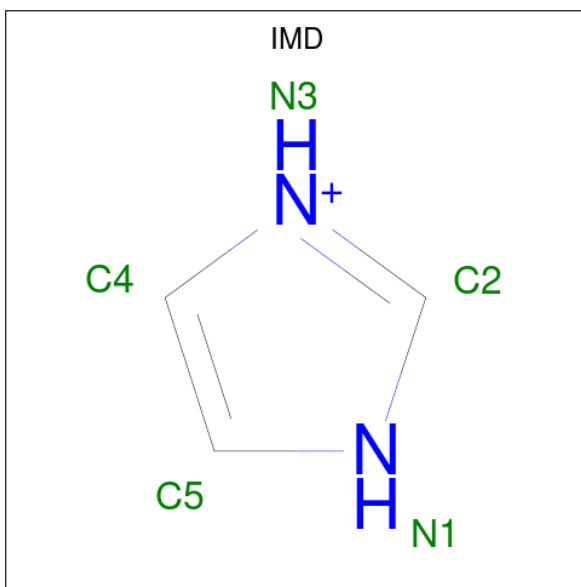


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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

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

- Molecule 9 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



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

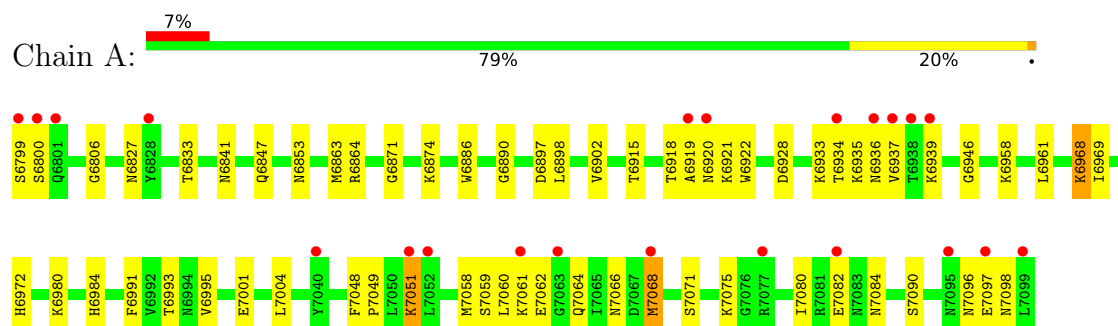
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	165	Total	O	0	0
			165	165		
10	B	63	Total	O	0	0
			63	63		

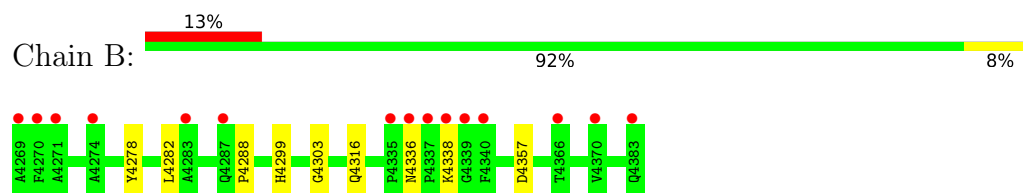
3 Residue-property plots [i](#)

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	168.51Å 168.51Å 51.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.64 – 2.00 48.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.64-2.00) 99.9 (48.64-2.00)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.21.1-5286	Depositor
R, R_{free}	0.201 , 0.222 0.199 , 0.216	Depositor DCC
R_{free} test set	742 reflections (1.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3630	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: IMD, MES, A1IOL, ZN, EDO, NA, SAM

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	0.34	0/2415	0.50	0/3276
2	B	0.31	0/875	0.50	0/1188
All	All	0.33	0/3290	0.50	0/4464

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	2364	0	2352	62	0
2	B	856	0	811	6	0
3	A	52	0	78	25	0
3	B	12	0	18	0	0
4	A	12	0	12	0	0
5	A	2	0	0	0	0
6	A	35	35	0	0	0
7	A	27	0	22	4	0
8	B	2	0	0	0	0
9	B	5	0	5	0	0
10	A	165	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	63	0	0	1	0
All	All	3595	35	3298	68	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 10.

All (68) 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:6980:LYS:HE2	3:A:7113:EDO:H22	1.40	1.03
1:A:6921:LYS:H	3:A:7115:EDO:H12	1.36	0.90
1:A:6833:THR:H	3:A:7107:EDO:H22	1.35	0.89
1:A:6864:ARG:HH12	3:A:7115:EDO:H11	1.36	0.89
2:B:4336[A]:ASN:OD1	2:B:4338:LYS:N	2.05	0.88
1:A:6847:GLN:HE22	1:A:6995:VAL:H	1.20	0.83
1:A:7061:LYS:H	1:A:7064:GLN:HE21	1.25	0.83
1:A:6920:ASN:HB3	3:A:7115:EDO:H21	1.67	0.77
1:A:6853:ASN:HD21	1:A:6886:TRP:HE1	1.35	0.74
1:A:6918:THR:HG21	1:A:6922:TRP:HE1	1.55	0.72
1:A:6935:LYS:HE3	3:A:7108:EDO:H21	1.74	0.69
1:A:6864:ARG:HH12	3:A:7115:EDO:C1	2.04	0.68
1:A:6863:MET:H	3:A:7101:EDO:H12	1.60	0.67
1:A:6920:ASN:CB	3:A:7115:EDO:H21	2.25	0.66
1:A:6936:ASN:ND2	1:A:6939:LYS:HG3	2.12	0.65
1:A:6853:ASN:ND2	1:A:6886:TRP:HE1	1.94	0.64
1:A:6928:ASP:OD2	7:A:7117:SAM:HG1	1.96	0.64
1:A:6833:THR:H	3:A:7107:EDO:C2	2.09	0.63
1:A:6864:ARG:NH1	3:A:7115:EDO:H11	2.11	0.63
1:A:7082:GLU:HB2	3:A:7115:EDO:O1	2.00	0.62
1:A:6921:LYS:N	3:A:7115:EDO:H12	2.12	0.59
1:A:7096:ASN:HD21	1:A:7098:ASN:HD22	1.50	0.58
1:A:6847:GLN:HE22	1:A:6995:VAL:N	1.98	0.58
1:A:7066:ASN:OD1	1:A:7068:MET:N	2.37	0.57
2:B:4336[B]:ASN:N	2:B:4336[B]:ASN:OD1	2.38	0.56
2:B:4299:HIS:HE1	10:B:4530:HOH:O	1.89	0.55
1:A:7058:MET:HE1	1:A:7060:LEU:HD11	1.89	0.54
1:A:7058:MET:CE	1:A:7060:LEU:HD11	2.39	0.53
1:A:6968:LYS:HE3	1:A:7001:GLU:OE2	2.08	0.52
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	1.92	0.52
1:A:6827:ASN:HB3	10:A:7334:HOH:O	2.10	0.51
1:A:7096:ASN:C	1:A:7096:ASN:HD22	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6958:LYS:HE3	3:A:7112:EDO:H22	1.94	0.48
1:A:7071:SER:O	1:A:7075:LYS:HG3	2.13	0.48
1:A:6847:GLN:NE2	1:A:6995:VAL:H	2.00	0.48
1:A:6915:THR:HG22	3:A:7114:EDO:H11	1.97	0.47
1:A:7061:LYS:H	1:A:7064:GLN:NE2	2.01	0.47
1:A:6984:HIS:HD2	10:A:7207:HOH:O	1.97	0.47
1:A:6864:ARG:NH2	1:A:7084:ASN:O	2.48	0.47
1:A:6897:ASP:OD1	1:A:6898:LEU:N	2.48	0.47
1:A:7059:SER:OG	1:A:7082:GLU:OE2	2.34	0.46
1:A:6847:GLN:HE21	1:A:6993:THR:HB	1.80	0.46
1:A:6935:LYS:HE3	3:A:7108:EDO:C2	2.45	0.46
1:A:6841:ASN:ND2	7:A:7117:SAM:O	2.49	0.45
1:A:6915:THR:O	1:A:7090:SER:HA	2.17	0.45
1:A:6969:ILE:HD13	1:A:7004:LEU:HG	1.98	0.45
1:A:6874:LYS:HE3	10:A:7296:HOH:O	2.16	0.44
1:A:6863:MET:H	3:A:7101:EDO:C1	2.28	0.44
1:A:7062:GLU:HA	1:A:7062:GLU:OE1	2.17	0.44
2:B:4278:TYR:CE1	2:B:4282:LEU:HD11	2.53	0.44
1:A:7051:LYS:HE3	1:A:7051:LYS:HB2	1.75	0.44
1:A:6972:HIS:CE1	3:A:7106:EDO:H12	2.53	0.43
1:A:7048:PHE:N	1:A:7049:PRO:CD	2.82	0.43
1:A:6871:GLY:O	7:A:7117:SAM:HB1	2.18	0.43
2:B:4303:GLY:HA2	2:B:4316:GLN:OE1	2.18	0.43
1:A:6937:VAL:HG23	3:A:7106:EDO:O1	2.18	0.42
1:A:6980:LYS:HE2	3:A:7113:EDO:C2	2.30	0.42
1:A:7097:GLU:H	1:A:7097:GLU:CD	2.25	0.42
1:A:6946:GLY:HA3	3:A:7102:EDO:O2	2.19	0.42
1:A:6806:GLY:HA3	1:A:6991:PHE:CZ	2.55	0.42
1:A:6919:ALA:N	3:A:7104:EDO:H21	2.35	0.42
1:A:6934:THR:C	1:A:6936:ASN:H	2.28	0.41
2:B:4288:PRO:HB3	2:B:4357:ASP:CG	2.45	0.41
1:A:6890:GLY:C	3:A:7101:EDO:H22	2.45	0.41
1:A:6920:ASN:CB	3:A:7115:EDO:C2	2.98	0.41
1:A:6863:MET:N	3:A:7101:EDO:H12	2.29	0.41
1:A:6928:ASP:O	7:A:7117:SAM:H5'2	2.21	0.41
1:A:7061:LYS:N	1:A:7064:GLN:HE21	2.05	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	299/301 (99%)	289 (97%)	10 (3%)	0	100	100
2	B	114/115 (99%)	111 (97%)	3 (3%)	0	100	100
All	All	413/416 (99%)	400 (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	261/261 (100%)	254 (97%)	7 (3%)	39	42
2	B	94/93 (101%)	94 (100%)	0	100	100
All	All	355/354 (100%)	348 (98%)	7 (2%)	48	54

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6799	SER
1	A	6800	SER
1	A	6902	VAL
1	A	6933	LYS
1	A	6968	LYS
1	A	7051	LYS
1	A	7068	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6804	GLN
1	A	6847	GLN
1	A	6853	ASN
1	A	6917	HIS
1	A	6920	ASN
1	A	6972	HIS
1	A	6996	ASN
1	A	7016	GLN
1	A	7064	GLN
1	A	7084	ASN
1	A	7096	ASN
2	B	4299	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	7104	-	3,3,3	0.42	0	2,2,2	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	7113	-	3,3,3	0.57	0	2,2,2	0.27	0
3	EDO	A	7108	-	3,3,3	0.62	0	2,2,2	0.19	0
7	SAM	A	7117	-	27,29,29	1.28	4 (14%)	34,42,42	2.10	10 (29%)
3	EDO	A	7105	-	3,3,3	0.54	0	2,2,2	0.37	0
3	EDO	A	7106	-	3,3,3	0.57	0	2,2,2	0.14	0
3	EDO	A	7109	-	3,3,3	0.59	0	2,2,2	0.20	0
3	EDO	A	7112	-	3,3,3	0.48	0	2,2,2	0.42	0
3	EDO	B	4403	-	3,3,3	0.52	0	2,2,2	0.26	0
6	A1IOL	A	7116	-	33,37,37	0.34	0	42,55,55	0.92	1 (2%)
3	EDO	A	7107	-	3,3,3	0.48	0	2,2,2	0.47	0
9	IMD	B	4406	-	5,5,5	0.66	0	5,5,5	0.41	0
3	EDO	A	7115	-	3,3,3	0.46	0	2,2,2	0.49	0
3	EDO	B	4405	-	3,3,3	0.43	0	2,2,2	0.70	0
3	EDO	A	7101	-	3,3,3	0.59	0	2,2,2	0.08	0
4	MES	A	7103	-	12,12,12	1.94	1 (8%)	15,16,16	1.77	3 (20%)
3	EDO	A	7111	-	3,3,3	0.51	0	2,2,2	0.27	0
3	EDO	B	4404	-	3,3,3	0.57	0	2,2,2	0.13	0
3	EDO	A	7114	-	3,3,3	0.52	0	2,2,2	0.28	0
3	EDO	A	7102	-	3,3,3	0.41	0	2,2,2	0.60	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	7104	-	-	1/1/1/1	-
3	EDO	A	7113	-	-	1/1/1/1	-
3	EDO	A	7108	-	-	0/1/1/1	-
7	SAM	A	7117	-	-	8/17/33/33	0/3/3/3
3	EDO	A	7105	-	-	0/1/1/1	-
3	EDO	A	7106	-	-	1/1/1/1	-
3	EDO	A	7109	-	-	0/1/1/1	-
3	EDO	A	7112	-	-	0/1/1/1	-
3	EDO	B	4403	-	-	1/1/1/1	-
6	A1IOL	A	7116	-	-	8/16/39/39	0/3/3/3
3	EDO	A	7107	-	-	0/1/1/1	-
9	IMD	B	4406	-	-	-	0/1/1/1
3	EDO	A	7115	-	-	0/1/1/1	-
3	EDO	B	4405	-	-	1/1/1/1	-
3	EDO	A	7101	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	A	7103	-	-	3/6/14/14	0/1/1/1
3	EDO	A	7111	-	-	1/1/1/1	-
3	EDO	B	4404	-	-	1/1/1/1	-
3	EDO	A	7114	-	-	1/1/1/1	-
3	EDO	A	7102	-	-	0/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	7103	MES	C8-S	-6.23	1.68	1.77
7	A	7117	SAM	C2-N3	3.43	1.40	1.33
7	A	7117	SAM	C2-N1	3.09	1.39	1.33
7	A	7117	SAM	C8-N7	2.63	1.36	1.31
7	A	7117	SAM	OXT-C	-2.39	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	7117	SAM	C5-C4-N3	-5.19	119.57	126.72
4	A	7103	MES	C5-N4-C3	4.87	119.34	108.84
7	A	7117	SAM	N3-C2-N1	-4.25	122.15	128.58
6	A	7116	A1IOL	C8-C7-C6	-4.18	101.78	113.35
7	A	7117	SAM	C5-N7-C8	4.16	109.99	103.45
7	A	7117	SAM	N9-C8-N7	-4.02	108.24	113.94
7	A	7117	SAM	C4-C5-N7	-3.72	106.33	110.58
7	A	7117	SAM	C2-N3-C4	3.27	119.83	111.83
7	A	7117	SAM	N3-C4-N9	3.00	132.28	127.17
7	A	7117	SAM	O4'-C1'-N9	2.90	113.66	108.09
4	A	7103	MES	C7-N4-C3	2.49	117.87	111.24
7	A	7117	SAM	C6-C5-C4	2.45	120.53	117.18
4	A	7103	MES	O1S-S-C8	2.28	110.17	106.73
7	A	7117	SAM	C5-C4-N9	2.14	108.15	105.81

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	7103	MES	C7-C8-S-O2S
4	A	7103	MES	C7-C8-S-O3S
6	A	7116	A1IOL	C19-C6-N1-C3
6	A	7116	A1IOL	O4-C11-N4-C10

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Mol	Chain	Res	Type	Atoms
6	A	7116	A1IOL	O4-C11-N4-C19
7	A	7117	SAM	N-CA-CB-CG
7	A	7117	SAM	CB-CG-SD-CE
3	A	7106	EDO	O1-C1-C2-O2
3	A	7113	EDO	O1-C1-C2-O2
6	A	7116	A1IOL	C18-C17-N6-C16
3	A	7114	EDO	O1-C1-C2-O2
3	B	4403	EDO	O1-C1-C2-O2
4	A	7103	MES	C7-C8-S-O1S
6	A	7116	A1IOL	O5-C17-N6-C16
7	A	7117	SAM	OXT-C-CA-CB
3	B	4404	EDO	O1-C1-C2-O2
3	B	4405	EDO	O1-C1-C2-O2
6	A	7116	A1IOL	N4-C11-C12-N5
7	A	7117	SAM	C-CA-CB-CG
6	A	7116	A1IOL	C11-C12-C13-C14
6	A	7116	A1IOL	O4-C11-C12-N5
3	A	7111	EDO	O1-C1-C2-O2
7	A	7117	SAM	O-C-CA-CB
3	A	7104	EDO	O1-C1-C2-O2
7	A	7117	SAM	CB-CG-SD-C5'
7	A	7117	SAM	O-C-CA-N
7	A	7117	SAM	OXT-C-CA-N

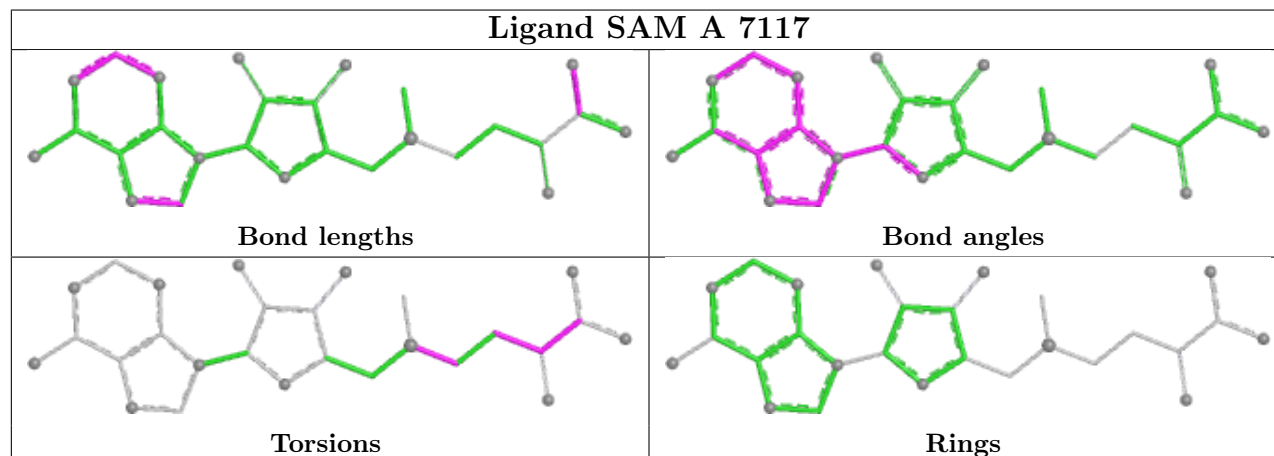
There are no ring outliers.

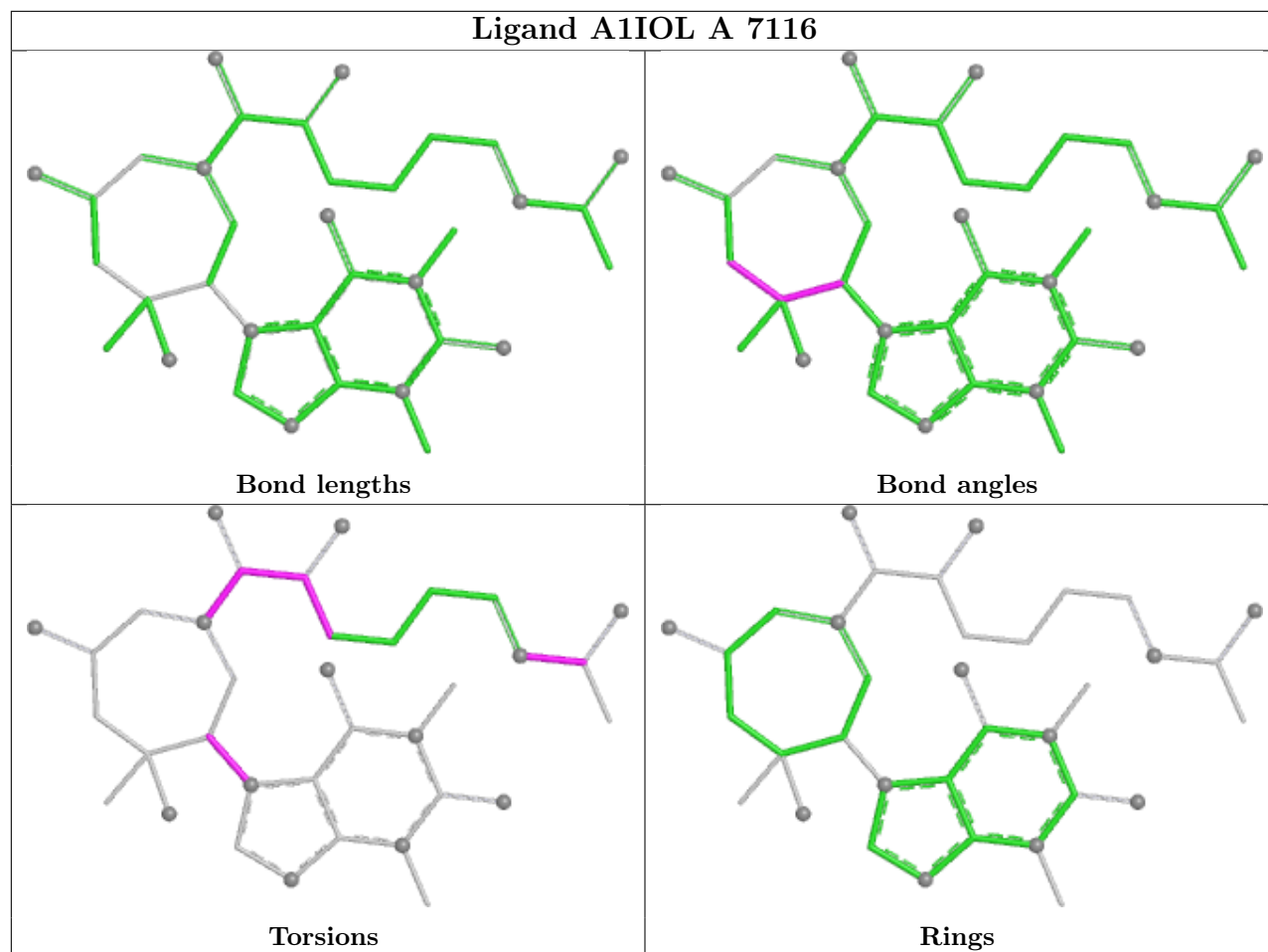
11 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7104	EDO	1	0
3	A	7113	EDO	2	0
3	A	7108	EDO	2	0
7	A	7117	SAM	4	0
3	A	7106	EDO	2	0
3	A	7112	EDO	1	0
3	A	7107	EDO	2	0
3	A	7115	EDO	9	0
3	A	7101	EDO	4	0
3	A	7114	EDO	1	0
3	A	7102	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	301/301 (100%)	0.23	22 (7%) 21 19	31, 40, 66, 96	0
2	B	115/115 (100%)	0.77	15 (13%) 7 6	34, 47, 76, 99	1 (0%)
All	All	416/416 (100%)	0.37	37 (8%) 15 14	31, 42, 71, 99	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6937	VAL	6.8
1	A	6799	SER	5.5
1	A	6938	THR	5.4
1	A	7099	LEU	5.4
2	B	4269	ALA	5.2
2	B	4337	PRO	5.0
1	A	6800	SER	4.4
2	B	4336[A]	ASN	4.1
2	B	4339	GLY	3.9
1	A	7052	LEU	3.7
1	A	6939	LYS	3.4
2	B	4340	PHE	3.4
1	A	6936	ASN	3.3
2	B	4338	LYS	3.1
2	B	4370	VAL	2.8
1	A	6919	ALA	2.6
1	A	7051	LYS	2.6
1	A	6828	TYR	2.5
2	B	4335	PRO	2.5
2	B	4383	GLN	2.5
2	B	4271	ALA	2.4
2	B	4283	ALA	2.4
1	A	7097	GLU	2.4
2	B	4270	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	7063	GLY	2.3
1	A	7082	GLU	2.3
2	B	4274	ALA	2.2
1	A	7040	TYR	2.2
2	B	4287	GLN	2.2
1	A	6920	ASN	2.2
1	A	7061	LYS	2.2
1	A	7068	MET	2.2
1	A	7095	ASN	2.1
1	A	6934	THR	2.1
1	A	7077	ARG	2.1
1	A	6801	GLN	2.1
2	B	4366	THR	2.1

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	7101	4/4	0.78	0.25	48,53,56,61	0
3	EDO	A	7113	4/4	0.79	0.26	58,59,64,65	0
6	A1IOL	A	7116	35/35	0.80	0.26	48,73,107,114	70
3	EDO	A	7115	4/4	0.81	0.19	50,56,58,61	0
3	EDO	A	7107	4/4	0.81	0.21	49,52,53,65	0
3	EDO	B	4404	4/4	0.83	0.25	64,64,69,70	0
3	EDO	A	7108	4/4	0.84	0.20	48,57,58,62	0
3	EDO	A	7109	4/4	0.84	0.22	45,51,58,58	0
3	EDO	A	7106	4/4	0.84	0.20	57,58,64,67	0
3	EDO	A	7105	4/4	0.86	0.18	45,45,53,60	0

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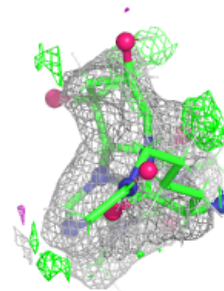
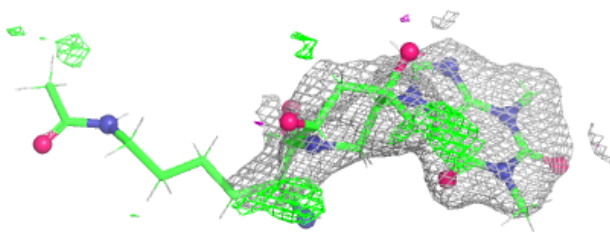
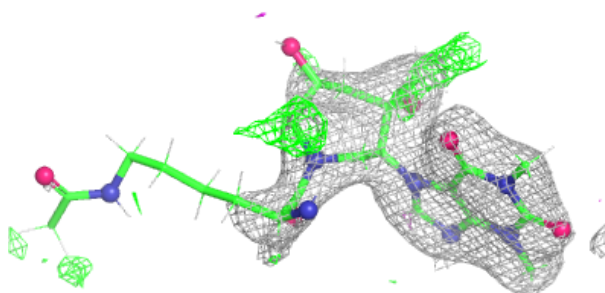
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	7112	4/4	0.86	0.21	52,56,59,61	0
7	SAM	A	7117	27/27	0.86	0.17	35,43,46,52	27
3	EDO	A	7111	4/4	0.88	0.20	55,58,58,63	0
3	EDO	A	7104	4/4	0.89	0.17	50,55,56,57	0
3	EDO	B	4403	4/4	0.90	0.17	62,64,64,68	0
3	EDO	A	7114	4/4	0.90	0.16	55,59,61,61	0
3	EDO	A	7102	4/4	0.91	0.15	43,44,52,53	0
4	MES	A	7103	12/12	0.91	0.14	37,43,57,65	12
9	IMD	B	4406	5/5	0.91	0.17	61,62,62,63	0
3	EDO	B	4405	4/4	0.93	0.15	50,51,51,57	0
5	NA	A	7118	1/1	0.96	0.10	56,56,56,56	0
8	ZN	B	4402	1/1	0.97	0.06	67,67,67,67	0
5	NA	A	7110	1/1	0.99	0.09	42,42,42,42	0
8	ZN	B	4401	1/1	0.99	0.03	45,45,45,45	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.

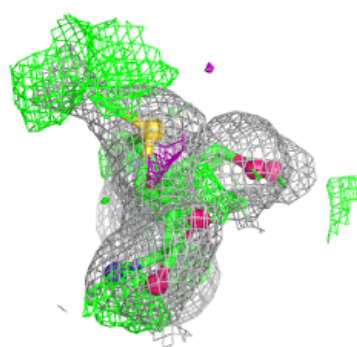
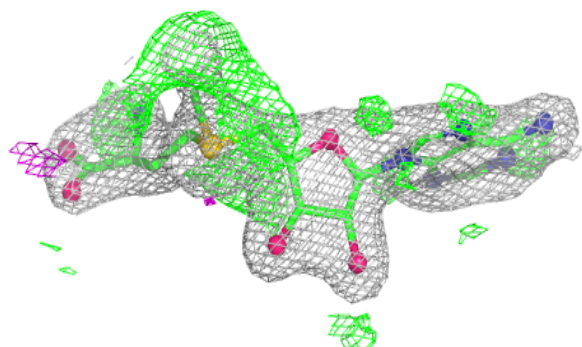
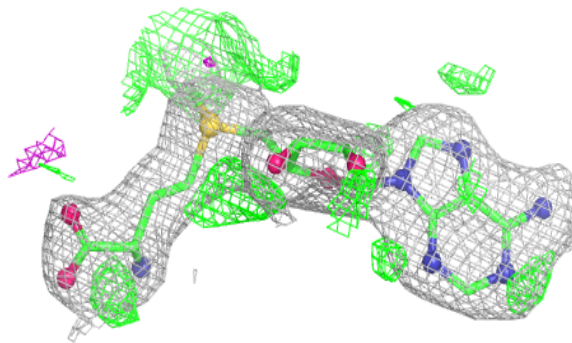
Electron density around A1IOL A 7116:

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 7117:

$2mF_o-DF_c$ (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.