



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:14 PM UTC

PDB ID : 8X44 / pdb_00008x44
Title : Crystal structure of DIMIT1 in complex with 5'-methylthioadenosine from *Pyrococcus horikoshii* (FormI)
Authors : Saha, S.; Kanaujia, S.P.
Deposited on : 2023-11-15
Resolution : 2.60 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

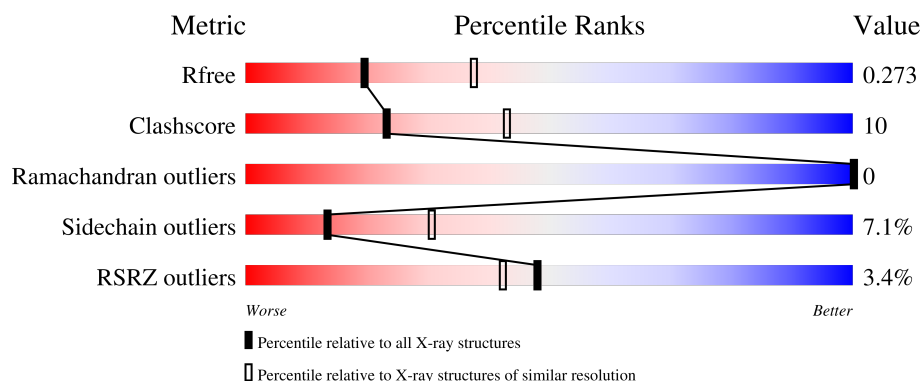
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	290	3% 72% 18% • 8%
1	B	290	3% 70% 19% • 8%

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
4	SO3	A	308	-	-	X	-
4	SO3	A	309	-	-	X	-
4	SO3	B	305	-	-	X	-
4	SO3	B	306	-	-	X	-
5	PEG	B	309	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4680 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 Probable ribosomal RNA small subunit methyltransferase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	3	0
			2195	1420	380	388	7			
1	B	268	Total	C	N	O	S	0	1	0
			2185	1414	380	384	7			

There are 44 discrepancies between the modelled and reference sequences:

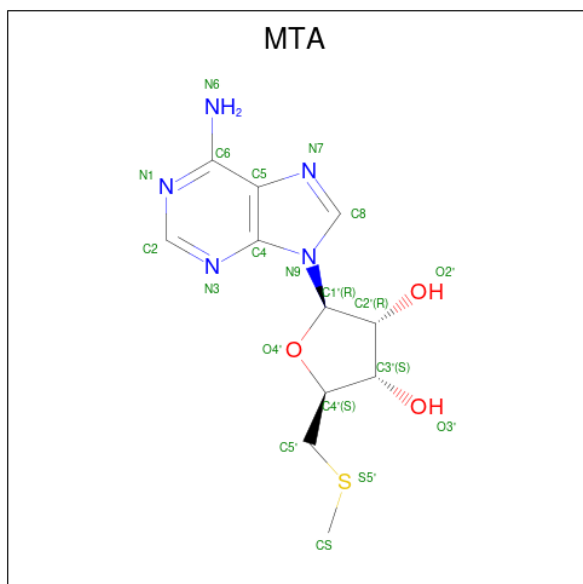
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O59487
A	2	SER	-	expression tag	UNP O59487
A	3	SER	-	expression tag	UNP O59487
A	4	ARG	-	expression tag	UNP O59487
A	5	ILE	-	expression tag	UNP O59487
A	6	ARG	-	expression tag	UNP O59487
A	7	ILE	-	expression tag	UNP O59487
A	8	ASN	-	expression tag	UNP O59487
A	9	THR	-	expression tag	UNP O59487
A	10	LYS	-	expression tag	UNP O59487
A	11	SER	-	expression tag	UNP O59487
A	12	LEU	-	expression tag	UNP O59487
A	13	LEU	-	expression tag	UNP O59487
A	14	VAL	-	expression tag	UNP O59487
A	15	GLN	-	expression tag	UNP O59487
A	16	PRO	-	expression tag	UNP O59487
A	17	GLY	-	expression tag	UNP O59487
A	18	TYR	-	expression tag	UNP O59487
A	19	SER	-	expression tag	UNP O59487
A	20	GLY	-	expression tag	UNP O59487
A	21	SER	-	expression tag	UNP O59487
A	22	LYS	-	expression tag	UNP O59487
B	1	MET	-	initiating methionine	UNP O59487
B	2	SER	-	expression tag	UNP O59487
B	3	SER	-	expression tag	UNP O59487

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ARG	-	expression tag	UNP O59487
B	5	ILE	-	expression tag	UNP O59487
B	6	ARG	-	expression tag	UNP O59487
B	7	ILE	-	expression tag	UNP O59487
B	8	ASN	-	expression tag	UNP O59487
B	9	THR	-	expression tag	UNP O59487
B	10	LYS	-	expression tag	UNP O59487
B	11	SER	-	expression tag	UNP O59487
B	12	LEU	-	expression tag	UNP O59487
B	13	LEU	-	expression tag	UNP O59487
B	14	VAL	-	expression tag	UNP O59487
B	15	GLN	-	expression tag	UNP O59487
B	16	PRO	-	expression tag	UNP O59487
B	17	GLY	-	expression tag	UNP O59487
B	18	TYR	-	expression tag	UNP O59487
B	19	SER	-	expression tag	UNP O59487
B	20	GLY	-	expression tag	UNP O59487
B	21	SER	-	expression tag	UNP O59487
B	22	LYS	-	expression tag	UNP O59487

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula: $C_{11}H_{15}N_5O_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

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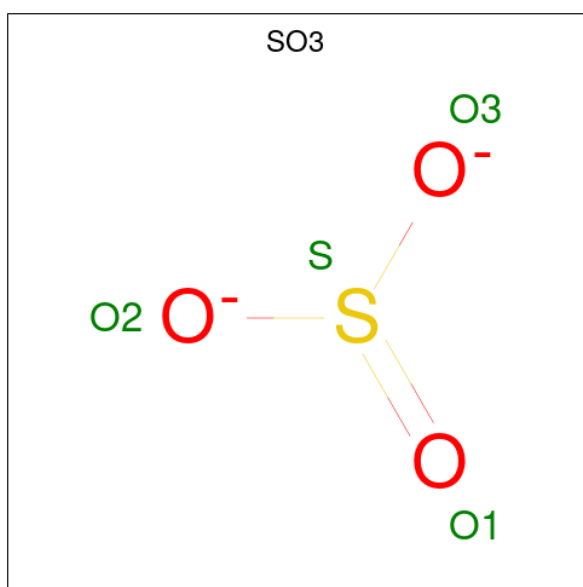
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	Zn	0	0
			6	6		
3	B	2	Total	Zn	0	0
			2	2		

- Molecule 4 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).

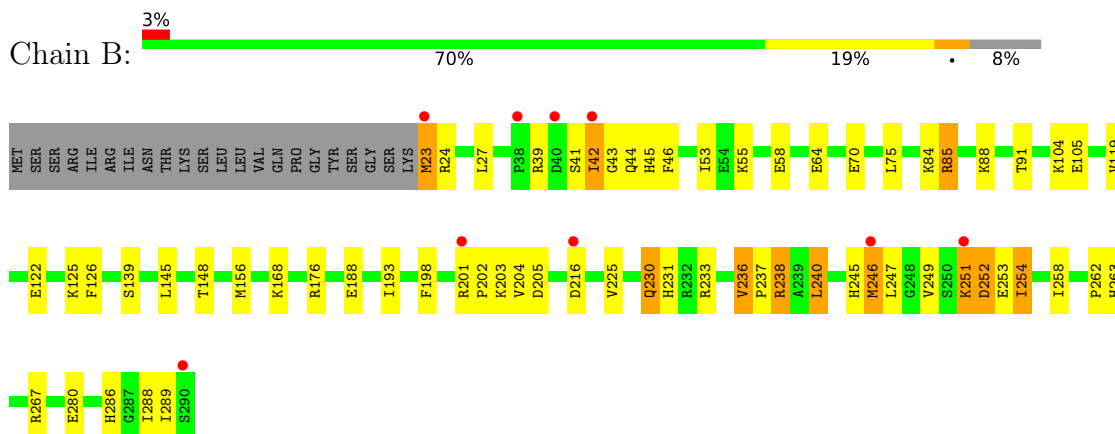


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	95	Total 95	O 95	0	0
9	B	102	Total 102	O 102	0	0

- Molecule 1: Probable ribosomal RNA small subunit methyltransferase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	79.78Å 85.34Å 106.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.76 – 2.60 66.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (66.76-2.60) 100.0 (66.76-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.62Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.205 , 0.273 0.212 , 0.273	Depositor DCC
R_{free} test set	1163 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtrriage
Anisotropy	0.673	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4680	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3831e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MTA, GOL, CL, SO3, PEG, EDO, ZN

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	0.64	0/2245	1.13	1/3022 (0.0%)
1	B	0.63	0/2229	1.14	2/3000 (0.1%)
All	All	0.64	0/4474	1.14	3/6022 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	247	LEU	CB-CA-C	-5.11	99.75	110.17
1	A	247	LEU	CB-CA-C	-5.03	99.92	110.17
1	B	252	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	267	ARG	Sidechain
1	B	238	ARG	Sidechain
1	B	24	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	85	ARG	Sidechain

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	2195	0	2304	49	0
1	B	2185	0	2296	50	2
2	A	20	0	15	1	0
2	B	20	0	15	0	0
3	A	6	0	0	0	0
3	B	2	0	0	0	0
4	A	8	0	0	7	0
4	B	8	0	0	8	0
5	A	14	0	19	3	0
5	B	14	0	20	10	1
6	B	1	0	0	0	0
7	B	6	0	8	0	0
8	B	4	0	6	0	0
9	A	95	0	0	3	0
9	B	102	0	0	6	0
All	All	4680	0	4683	94	2

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 (94) 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:84:LYS:NZ	9:A:401:HOH:O	1.56	1.32
1:A:231:HIS:NE2	1:B:231:HIS:NE2	1.98	1.09
1:A:45:HIS:NE2	4:A:308:SO3:S	2.27	1.06
1:A:231:HIS:CE1	1:B:231:HIS:CE1	2.43	1.06
1:B:45:HIS:NE2	4:B:305:SO3:S	2.30	1.04
1:A:231:HIS:CE1	1:B:231:HIS:NE2	2.29	1.00
1:A:231:HIS:NE2	1:B:231:HIS:CE1	2.28	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLU:OE1	9:B:401:HOH:O	1.94	0.84
1:B:286:HIS:NE2	5:B:309:PEG:O4	1.80	0.80
1:B:286:HIS:HE2	5:B:309:PEG:C4	1.96	0.79
1:B:205:ASP:OD2	4:B:306:SO3:S	2.45	0.74
1:A:249:VAL:HG11	1:A:254:ILE:HD13	1.70	0.73
1:B:286:HIS:CE1	5:B:309:PEG:HO4	2.00	0.73
1:A:205:ASP:OD2	4:A:309:SO3:S	2.48	0.72
1:A:253:GLU:OE1	4:B:305:SO3:O1	2.08	0.72
1:B:249:VAL:HG11	1:B:254:ILE:HD13	1.74	0.69
1:B:286:HIS:CE1	5:B:309:PEG:O4	2.46	0.65
1:A:27:LEU:CD1	1:A:75:LEU:HD12	2.27	0.65
5:B:309:PEG:C4	9:B:402:HOH:O	2.45	0.64
1:A:126:PHE:CZ	1:A:148:THR:HG21	2.32	0.64
1:B:27:LEU:HD12	1:B:75:LEU:CD1	2.28	0.64
1:B:126:PHE:CZ	1:B:148:THR:HG21	2.33	0.64
1:A:27:LEU:HD12	1:A:75:LEU:CD1	2.29	0.63
1:A:253:GLU:CD	4:B:305:SO3:O3	2.42	0.62
1:B:39:ARG:HD2	1:B:44:GLN:O	1.99	0.62
4:A:308:SO3:O2	1:B:253:GLU:CD	2.43	0.62
1:B:27:LEU:CD1	1:B:75:LEU:HD12	2.32	0.60
1:B:280:GLU:HG2	1:B:289:ILE:HD11	1.84	0.60
1:A:176:ARG:HH12	5:A:310:PEG:H42	1.67	0.59
1:A:280:GLU:HG2	1:A:289:ILE:HD11	1.85	0.59
1:A:253:GLU:OE1	4:B:305:SO3:O3	2.21	0.57
4:A:308:SO3:O1	1:B:253:GLU:OE1	2.23	0.56
1:A:230:GLN:NE2	1:B:230:GLN:HE21	2.04	0.56
1:B:240:LEU:HB3	1:B:258:ILE:HD13	1.89	0.55
1:B:286:HIS:NE2	5:B:309:PEG:C4	2.62	0.54
1:A:42:ILE:HG12	1:B:288:ILE:HD13	1.89	0.54
1:A:240:LEU:HB3	1:A:258:ILE:HD13	1.88	0.53
1:B:39:ARG:HG2	1:B:41:SER:O	2.09	0.53
1:B:46:PHE:O	1:B:198:PHE:HA	2.08	0.53
1:B:246[A]:MET:HE2	9:B:491:HOH:O	2.08	0.53
5:B:309:PEG:O4	9:B:402:HOH:O	2.17	0.53
1:B:39:ARG:CD	1:B:44:GLN:O	2.56	0.53
1:B:27:LEU:CD1	1:B:75:LEU:CD1	2.87	0.53
1:A:46:PHE:O	1:A:198:PHE:HA	2.09	0.52
1:A:126:PHE:HZ	1:A:148:THR:HG21	1.74	0.51
1:A:230:GLN:HE21	1:B:230:GLN:NE2	2.07	0.51
1:A:105:GLU:OE1	9:A:402:HOH:O	2.19	0.51
1:A:253:GLU:OE1	4:B:305:SO3:S	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:MET:HG2	1:B:193:ILE:CD1	2.41	0.51
1:A:55:LYS:HA	1:A:58:GLU:HG2	1.93	0.50
1:A:198:PHE:HB2	1:A:202:PRO:HD3	1.94	0.50
1:A:156:MET:HG2	1:A:193:ILE:CD1	2.41	0.50
1:A:27:LEU:CD1	1:A:75:LEU:CD1	2.88	0.49
4:A:308:SO3:O2	1:B:253:GLU:OE1	2.31	0.49
1:A:262:PRO:HB2	1:A:263:HIS:CD2	2.48	0.49
1:B:198:PHE:HB2	1:B:202:PRO:HD3	1.95	0.48
1:A:93:GLU:OE1	2:A:301:MTA:O2'	2.27	0.48
1:B:23:MET:HE1	1:B:53:ILE:HD12	1.95	0.48
1:B:85:ARG:HH11	1:B:85:ARG:HG3	1.79	0.48
1:B:42:ILE:HD12	1:B:43:GLY:N	2.29	0.47
1:B:262:PRO:HB2	1:B:263:HIS:CD2	2.49	0.47
1:B:55:LYS:HA	1:B:58:GLU:HG2	1.96	0.47
1:A:42:ILE:HD12	1:A:43:GLY:N	2.30	0.46
1:B:286:HIS:HE2	5:B:309:PEG:C3	2.28	0.46
1:A:23:MET:HE1	1:A:53:ILE:HD12	1.97	0.46
1:A:95:ASP:OD1	1:A:97:LYS:HB3	2.16	0.46
1:B:145:LEU:O	1:B:148:THR:HB	2.14	0.46
1:B:201:ARG:NH2	9:B:414:HOH:O	2.48	0.46
1:A:230:GLN:NE2	1:B:230:GLN:NE2	2.63	0.46
1:A:145:LEU:O	1:A:148:THR:HB	2.16	0.46
1:A:222:GLU:CD	5:A:310:PEG:H41	2.42	0.45
1:A:236:VAL:N	1:A:237:PRO:CD	2.80	0.45
1:A:176:ARG:NH1	5:A:310:PEG:H42	2.30	0.44
1:B:45:HIS:CD2	4:B:305:SO3:S	3.09	0.44
1:B:236:VAL:N	1:B:237:PRO:CD	2.80	0.44
1:B:216:ASP:N	1:B:216:ASP:OD1	2.50	0.44
1:A:205:ASP:CG	4:A:309:SO3:S	3.01	0.44
1:B:205:ASP:CG	4:B:306:SO3:S	3.01	0.44
1:B:70:GLU:O	1:B:91:THR:HA	2.17	0.44
1:A:176:ARG:HG3	1:A:225:VAL:HG12	2.00	0.43
1:A:155:VAL:HG23	1:A:157:TYR:CE2	2.54	0.43
1:A:45:HIS:CD2	4:A:308:SO3:S	3.09	0.43
1:B:176:ARG:HG3	1:B:225:VAL:HG12	2.00	0.42
1:A:70:GLU:O	1:A:91:THR:HA	2.18	0.42
1:B:245:HIS:ND1	1:B:251:LYS:HG2	2.34	0.42
5:B:309:PEG:C1	9:B:412:HOH:O	2.67	0.42
1:A:70:GLU:HG2	1:A:71:VAL:N	2.36	0.41
1:A:95:ASP:OD2	9:A:403:HOH:O	2.21	0.41
1:A:85:ARG:HH11	1:A:85:ARG:HG3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LEU:HD22	1:A:192:LYS:HE3	2.02	0.40
1:B:233:ARG:HH12	1:B:267:ARG:HD3	1.86	0.40
1:A:233:ARG:HH12	1:A:267:ARG:HD3	1.85	0.40
1:B:286:HIS:NE2	5:B:309:PEG:C3	2.84	0.40

All (2) 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)
1:B:188:GLU:OE1	5:B:309:PEG:O4[3_455]	1.52	0.68
1:B:64:GLU:OE2	1:B:64:GLU:OE2[2_566]	1.77	0.43

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	269/290 (93%)	260 (97%)	9 (3%)	0	100	100
1	B	267/290 (92%)	257 (96%)	10 (4%)	0	100	100
All	All	536/580 (92%)	517 (96%)	19 (4%)	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	244/261 (94%)	230 (94%)	14 (6%)	18	40
1	B	242/261 (93%)	221 (91%)	21 (9%)	9	21
All	All	486/522 (93%)	451 (93%)	35 (7%)	13	30

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	MET
1	A	39	ARG
1	A	122	GLU
1	A	125	LYS
1	A	139	SER
1	A	168	LYS
1	A	204	VAL
1	A	230	GLN
1	A	231	HIS
1	A	236	VAL
1	A	238	ARG
1	A	240	LEU
1	A	254	ILE
1	A	284	LYS
1	B	23	MET
1	B	42	ILE
1	B	84	LYS
1	B	88	LYS
1	B	104	LYS
1	B	119	VAL
1	B	122	GLU
1	B	125	LYS
1	B	139	SER
1	B	168	LYS
1	B	203	LYS
1	B	204	VAL
1	B	230	GLN
1	B	236	VAL
1	B	238	ARG
1	B	240	LEU
1	B	246[A]	MET
1	B	246[B]	MET
1	B	251	LYS
1	B	252	ASP
1	B	254	ILE

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	115	GLN
1	A	230	GLN
1	B	115	GLN
1	B	230	GLN

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 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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	$\# Z > 2$
2	MTA	A	301	-	22,22,22	0.48	0	32,32,32	0.80	1 (3%)
2	MTA	B	301	-	22,22,22	0.30	0	32,32,32	0.81	1 (3%)
4	SO3	A	308	-	1,3,3	2.40	1 (100%)	0,3,3	-	-
5	PEG	A	310	-	6,6,6	0.28	0	5,5,5	0.15	0
4	SO3	B	306	-	1,3,3	1.59	0	0,3,3	-	-
5	PEG	B	310	-	6,6,6	0.32	0	5,5,5	0.20	0
5	PEG	A	311	3	6,6,6	0.55	0	5,5,5	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO3	B	305	-	1,3,3	2.20	1 (100%)	0,3,3	-	-
7	GOL	B	307	-	5,5,5	0.17	0	5,5,5	0.59	0
8	EDO	B	308	-	3,3,3	0.67	0	2,2,2	0.66	0
4	SO3	A	309	-	1,3,3	1.59	0	0,3,3	-	-
5	PEG	B	309	-	6,6,6	0.46	0	5,5,5	0.75	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
2	MTA	A	301	-	-	1/7/23/23	0/3/3/3
2	MTA	B	301	-	-	1/7/23/23	0/3/3/3
5	PEG	A	310	-	-	2/4/4/4	-
5	PEG	B	310	-	-	3/4/4/4	-
5	PEG	A	311	3	-	3/4/4/4	-
7	GOL	B	307	-	-	4/4/4/4	-
5	PEG	B	309	-	-	0/4/4/4	-
8	EDO	B	308	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	308	SO3	O1-S	2.40	1.54	1.44
4	B	305	SO3	O1-S	2.20	1.53	1.44

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	MTA	C4'-C5'-S5'	2.82	123.27	113.89
2	B	301	MTA	C4'-C5'-S5'	2.09	120.84	113.89

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MTA	C4'-C5'-S5'-CS
2	B	301	MTA	C4'-C5'-S5'-CS
7	B	307	GOL	O1-C1-C2-C3

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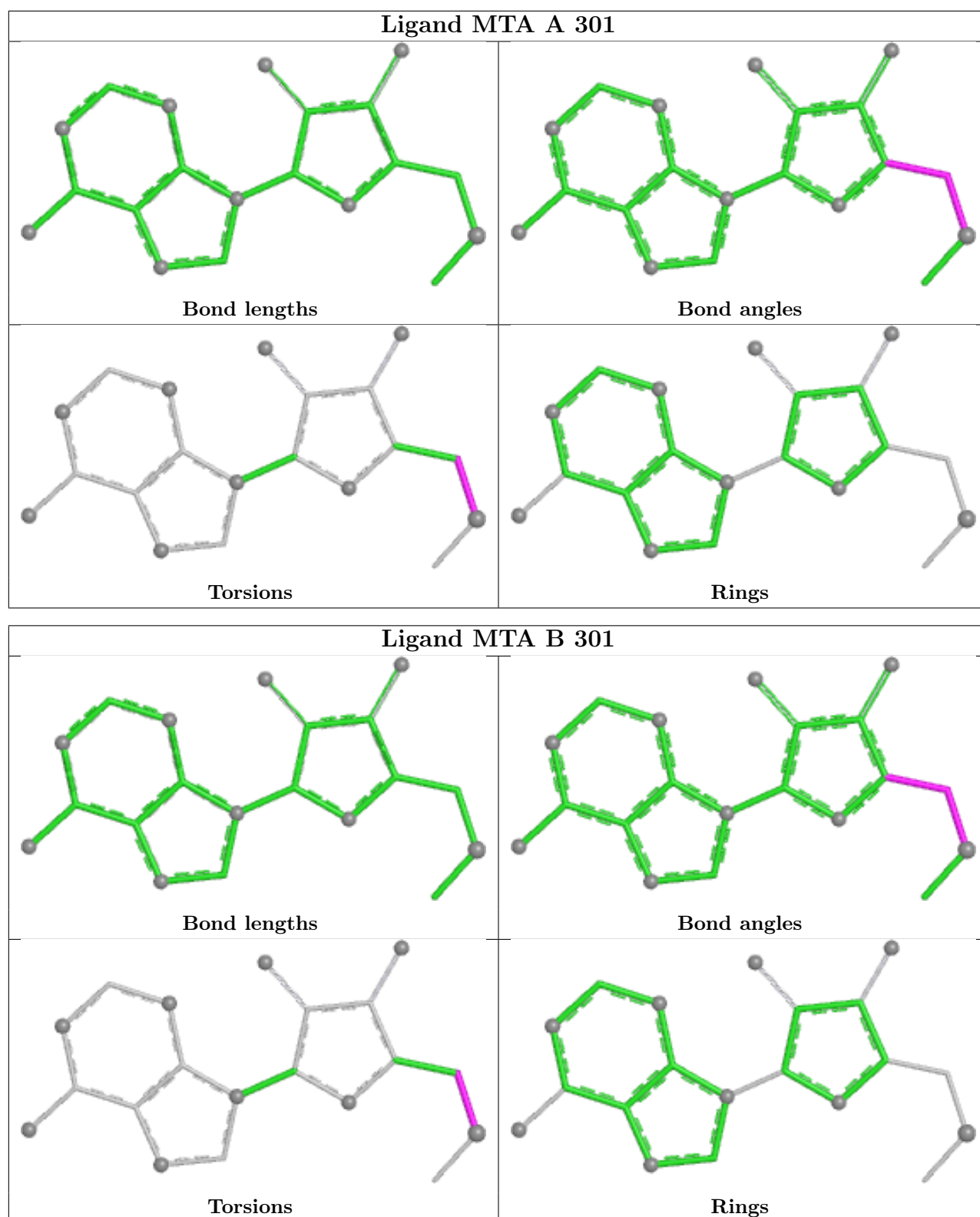
Mol	Chain	Res	Type	Atoms
7	B	307	GOL	C1-C2-C3-O3
7	B	307	GOL	O1-C1-C2-O2
5	A	310	PEG	O2-C3-C4-O4
5	A	311	PEG	O2-C3-C4-O4
5	B	310	PEG	O1-C1-C2-O2
7	B	307	GOL	O2-C2-C3-O3
5	A	310	PEG	O1-C1-C2-O2
5	A	311	PEG	O1-C1-C2-O2
5	A	311	PEG	C1-C2-O2-C3
5	B	310	PEG	C1-C2-O2-C3
8	B	308	EDO	O1-C1-C2-O2
5	B	310	PEG	O2-C3-C4-O4

There are no ring outliers.

7 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	MTA	1	0
4	A	308	SO3	5	0
5	A	310	PEG	3	0
4	B	306	SO3	2	0
4	B	305	SO3	6	0
4	A	309	SO3	2	0
5	B	309	PEG	10	1

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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	268/290 (92%)	-0.09	9 (3%)	48	42	20, 37, 71, 90	3 (1%)
1	B	268/290 (92%)	-0.05	9 (3%)	48	42	20, 38, 71, 95	1 (0%)
All	All	536/580 (92%)	-0.07	18 (3%)	48	42	20, 37, 71, 95	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	MET	3.1
1	A	258	ILE	2.9
1	B	246[A]	MET	2.8
1	A	253	GLU	2.8
1	A	38	PRO	2.8
1	B	38	PRO	2.7
1	A	290	SER	2.7
1	B	40	ASP	2.5
1	A	252	ASP	2.5
1	B	42	ILE	2.4
1	A	42	ILE	2.4
1	B	216	ASP	2.3
1	B	251	LYS	2.2
1	A	287	GLY	2.2
1	A	289	ILE	2.1
1	B	290	SER	2.1
1	B	201	ARG	2.0
1	A	246[A]	MET	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

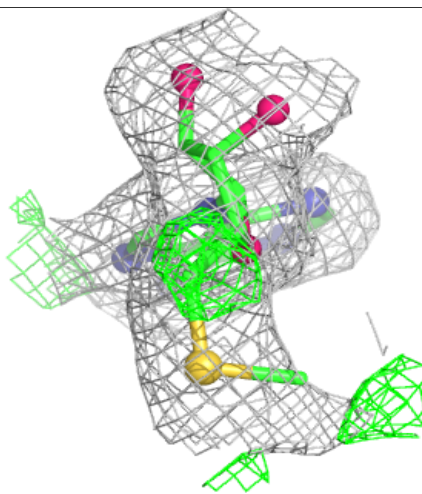
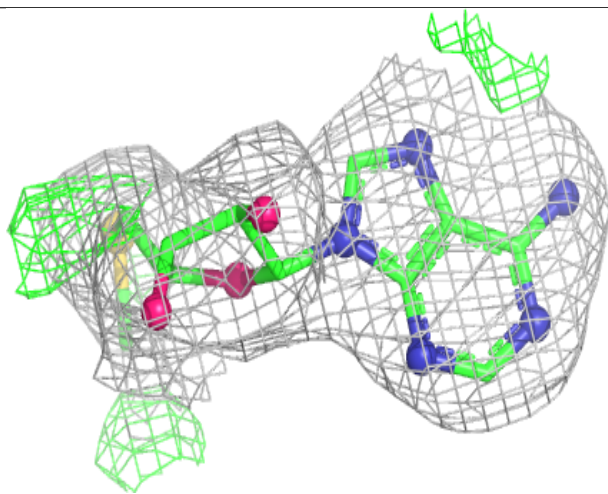
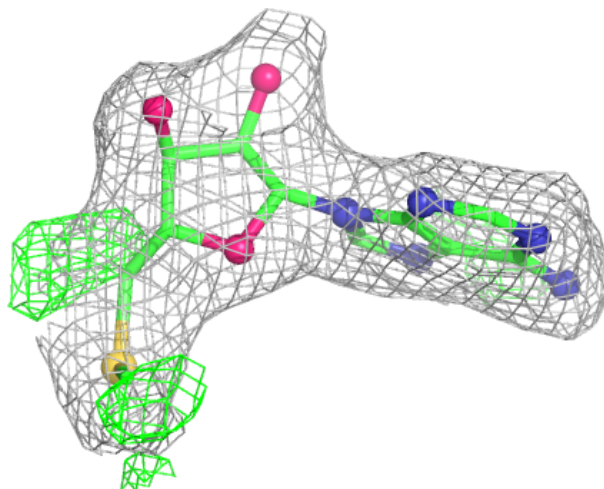
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO3	A	309	4/4	0.57	0.14	73,78,80,92	0
7	GOL	B	307	6/6	0.58	0.18	63,72,75,75	0
4	SO3	B	306	4/4	0.63	0.13	70,72,79,88	0
5	PEG	A	311	7/7	0.77	0.19	44,49,57,58	0
5	PEG	A	310	7/7	0.83	0.18	65,73,79,79	0
8	EDO	B	308	4/4	0.90	0.14	45,53,55,55	0
5	PEG	B	310	7/7	0.91	0.15	56,74,82,82	0
2	MTA	A	301	20/20	0.92	0.10	22,28,60,66	0
6	CL	B	304	1/1	0.93	0.08	63,63,63,63	0
5	PEG	B	309	7/7	0.93	0.15	18,36,48,52	0
2	MTA	B	301	20/20	0.93	0.10	24,34,76,81	0
4	SO3	B	305	4/4	0.96	0.06	27,28,29,35	0
3	ZN	B	303	1/1	0.96	0.05	66,66,66,66	0
3	ZN	A	307	1/1	0.96	0.04	55,55,55,55	0
3	ZN	A	306	1/1	0.97	0.05	65,65,65,65	0
4	SO3	A	308	4/4	0.97	0.08	27,29,30,33	0
3	ZN	A	303	1/1	0.98	0.03	51,51,51,51	0
3	ZN	A	304	1/1	0.98	0.03	52,52,52,52	0
3	ZN	A	302	1/1	0.99	0.02	41,41,41,41	0
3	ZN	A	305	1/1	0.99	0.04	61,61,61,61	0
3	ZN	B	302	1/1	0.99	0.03	43,43,43,43	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.

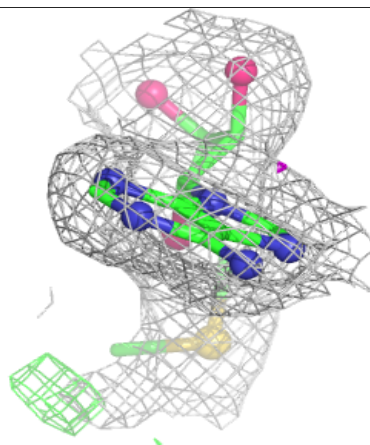
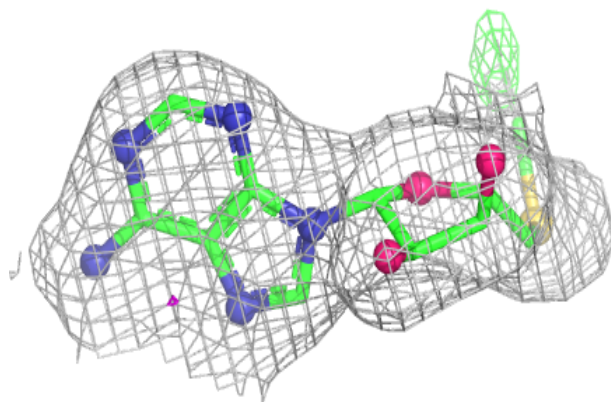
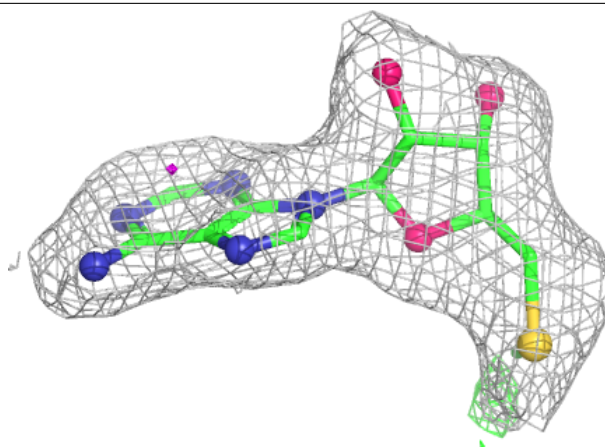
Electron density around MTA A 301:

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



Electron density around MTA B 301:

$2mF_o-DF_c$ (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.