



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 10:03 PM UTC

PDB ID : 8X41 / pdb_00008x41
Title : Crystal structure of DIMT1 in complex with 5'-methylthioadenosine and adenosine from *Pyrococcus horikoshii*
Authors : Saha, S.; Mandal, S.K.; Dutta, A.; Kanaujia, S.P.
Deposited on : 2023-11-14
Resolution : 2.35 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

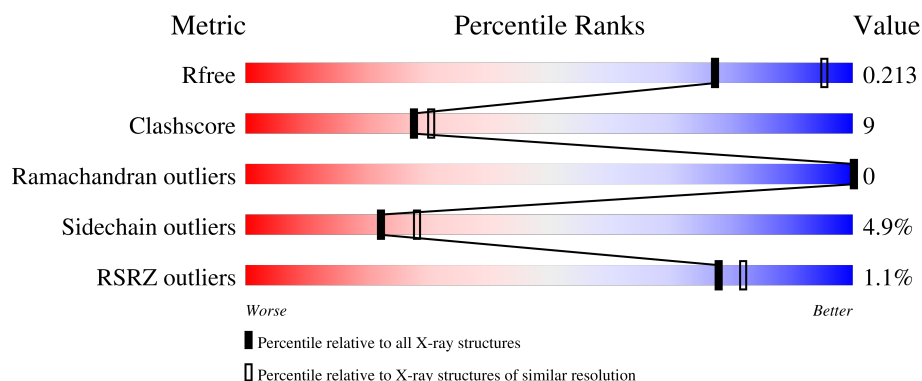
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	
1	B	290	

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
6	SO3	A	313	-	-	X	-
6	SO3	A	314	-	-	X	-
6	SO3	B	307	-	-	X	-
6	SO3	B	308	-	-	X	-
7	GOL	A	317	-	-	X	-
7	GOL	B	312	-	-	X	-
9	ACT	A	325	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 4970 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	269	Total	C	N	O	S	0	0	0
			2189	1416	382	385	6			
1	B	269	Total	C	N	O	S	0	0	0
			2189	1416	382	385	6			

There are 44 discrepancies between the modelled and reference sequences:

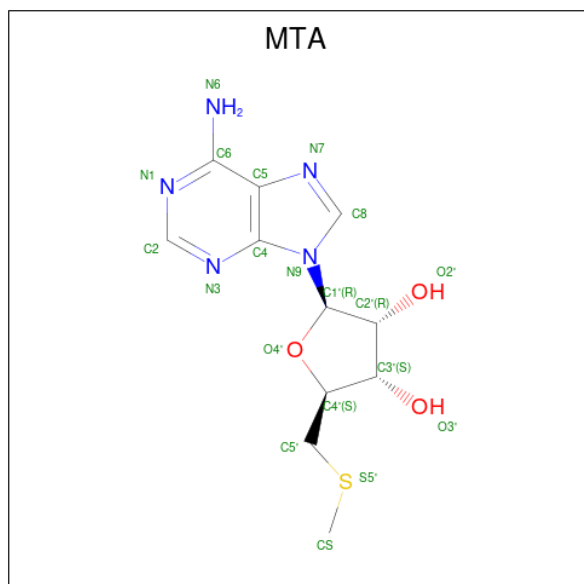
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O59487
A	2	SER	-	expression tag	UNP O59487
A	3	SER	-	expression tag	UNP O59487
A	4	ARG	-	expression tag	UNP O59487
A	5	ILE	-	expression tag	UNP O59487
A	6	ARG	-	expression tag	UNP O59487
A	7	ILE	-	expression tag	UNP O59487
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).



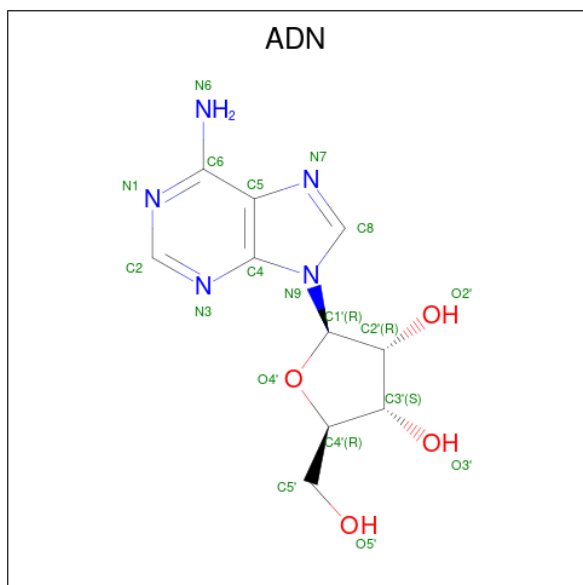
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

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

- Molecule 3 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			19	10	5	4		
3	B	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	Zn	0	0
			7	7		
4	B	3	Total	Zn	0	0
			3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

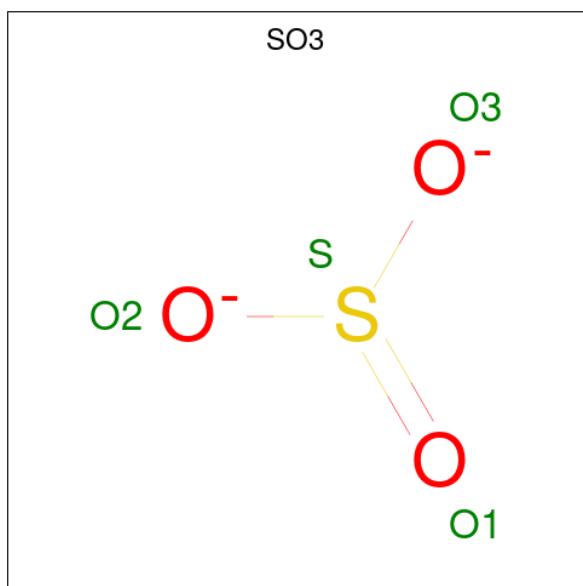
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Cl	0	0
			3	3		

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

- Molecule 6 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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

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



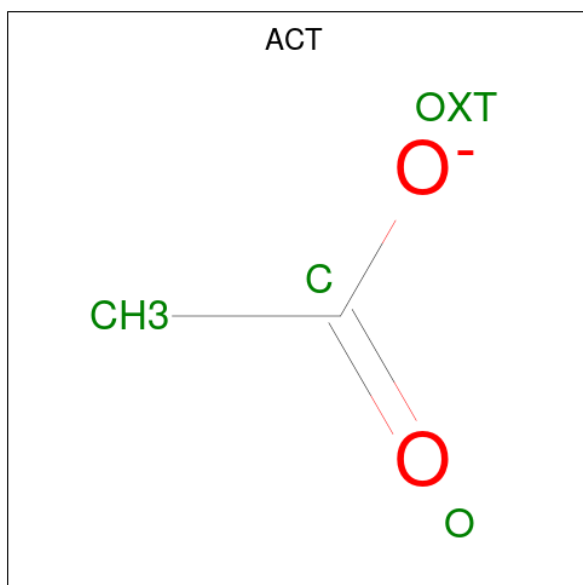
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



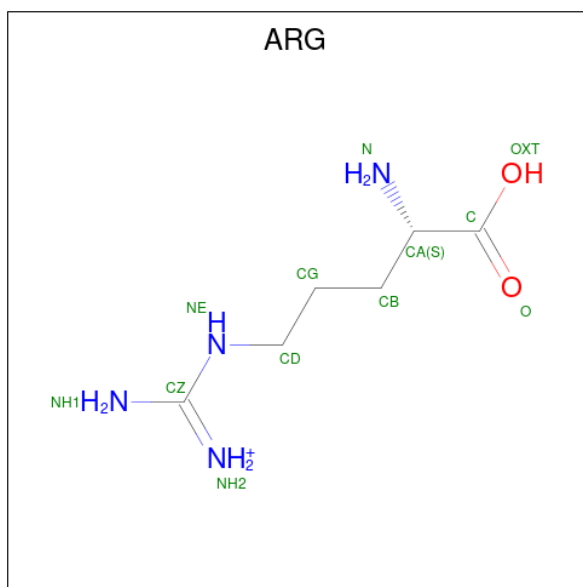
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).



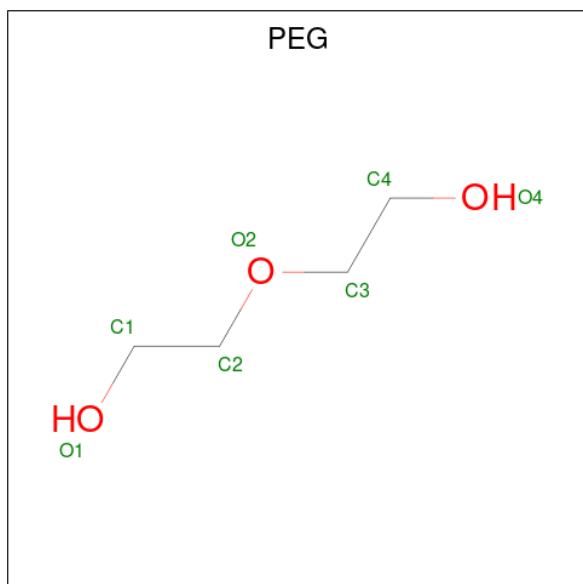
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

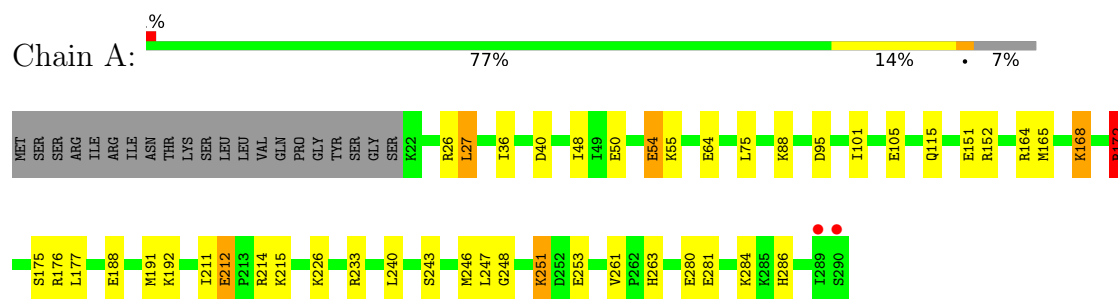
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	190	Total	O	0	0
			190	190		
12	B	191	Total	O	0	0
			191	191		

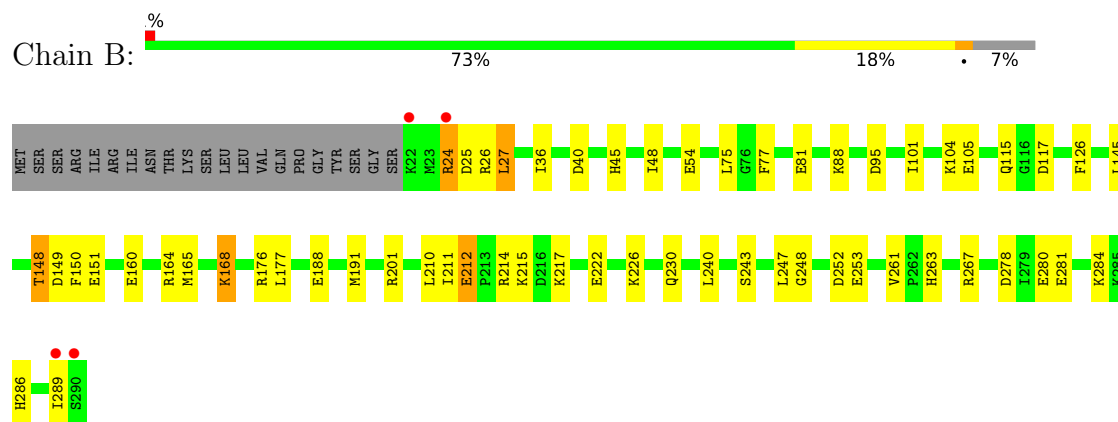
3 Residue-property plots

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: Probable ribosomal RNA small subunit methyltransferase A



- Molecule 1: Probable ribosomal RNA small subunit methyltransferase A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.38Å 77.26Å 94.23Å 90.00° 119.95° 90.00°	Depositor
Resolution (Å)	62.16 – 2.35 62.16 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.16-2.35) 99.9 (62.16-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.04 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.165 , 0.205 0.173 , 0.213	Depositor DCC
R_{free} test set	1558 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	27.2	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4970	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MTA, ACT, PEG, ADN, EDO, SO3, GOL, 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	1/2230 (0.0%)	1.02	1/3001 (0.0%)
1	B	0.63	1/2230 (0.0%)	1.02	1/3001 (0.0%)
All	All	0.63	2/4460 (0.0%)	1.02	2/6002 (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	2
1	B	0	4
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	GLU	CD-OE2	7.52	1.39	1.25
1	A	212	GLU	CD-OE2	5.99	1.36	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	54	GLU	CB-CG-CD	6.00	122.81	112.60
1	A	54	GLU	CB-CG-CD	5.14	121.33	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	ARG	Sidechain
1	A	214	ARG	Sidechain
1	B	214	ARG	Sidechain
1	B	24	ARG	Sidechain
1	B	267	ARG	Sidechain
1	B	289	ILE	Peptide

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	2189	0	2300	36	4
1	B	2189	0	2300	43	4
2	A	20	0	15	0	0
2	B	20	0	15	1	0
3	A	19	0	13	1	0
3	B	19	0	13	1	0
4	A	7	0	0	0	0
4	B	3	0	0	0	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	8	0	0	5	0
6	B	8	0	0	5	0
7	A	36	0	48	9	0
7	B	24	0	32	8	1
8	A	16	0	24	2	0
9	A	4	0	3	2	0
9	B	4	0	3	1	0
10	A	12	0	12	0	0
11	B	7	0	10	1	0
12	A	190	0	0	13	4
12	B	191	0	0	15	3
All	All	4970	0	4788	84	9

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 9.

All (84) 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:263:HIS:ND1	6:A:314:SO3:S	1.99	1.34
1:B:263:HIS:ND1	6:B:308:SO3:S	2.00	1.34
1:A:95:ASP:OD2	6:A:313:SO3:S	1.93	1.26
1:B:95:ASP:OD2	6:B:307:SO3:S	1.92	1.26
7:B:312:GOL:O2	12:B:401:HOH:O	1.60	1.15
6:B:308:SO3:O3	12:B:402:HOH:O	1.70	1.10
6:A:314:SO3:O3	12:A:402:HOH:O	1.75	1.04
1:B:24:ARG:NH1	1:B:25:ASP:OD1	2.02	0.91
1:A:188:GLU:OE1	12:A:403:HOH:O	1.87	0.90
1:B:281:GLU:OE2	12:B:403:HOH:O	1.90	0.89
1:A:280:GLU:OE2	12:A:404:HOH:O	1.90	0.89
1:A:281:GLU:OE2	12:A:405:HOH:O	1.94	0.84
1:B:212:GLU:OE2	7:B:312:GOL:O2	1.96	0.81
1:B:188:GLU:OE1	12:B:404:HOH:O	1.98	0.81
1:B:286:HIS:HD2	7:B:311:GOL:H2	1.46	0.79
1:B:280:GLU:OE2	12:B:405:HOH:O	2.01	0.78
1:B:148:THR:HG22	1:B:150:PHE:HD2	1.51	0.74
7:B:311:GOL:O2	12:B:406:HOH:O	2.05	0.74
1:A:248:GLY:HA3	1:B:40:ASP:OD2	1.88	0.73
1:A:40:ASP:OD2	1:B:248:GLY:HA3	1.90	0.72
1:B:286:HIS:CD2	7:B:311:GOL:H2	2.24	0.71
1:A:286:HIS:ND1	7:A:319:GOL:H2	2.06	0.71
1:A:151:GLU:OE1	12:A:406:HOH:O	2.09	0.70
1:B:77:PHE:HB2	11:B:313:PEG:H42	1.77	0.66
1:A:54:GLU:OE2	12:A:407:HOH:O	2.14	0.65
1:A:95:ASP:CG	6:A:313:SO3:S	2.78	0.64
1:B:95:ASP:CG	6:B:307:SO3:S	2.78	0.64
1:B:201:ARG:HD3	12:B:545:HOH:O	1.98	0.63
1:A:176:ARG:HH12	7:A:317:GOL:C1	2.11	0.63
1:A:27:LEU:HD12	1:A:75:LEU:HD12	1.80	0.63
1:A:64:GLU:H	1:A:64:GLU:CD	2.08	0.61
1:B:26:ARG:NH2	1:B:105:GLU:OE2	2.33	0.60
1:A:176:ARG:HH12	7:A:317:GOL:H12	1.68	0.59
1:A:246:MET:SD	1:A:251:LYS:HD3	2.42	0.59
1:B:151:GLU:OE1	12:B:407:HOH:O	2.17	0.57
1:B:45:HIS:O	2:B:301:MTA:HCS1	2.06	0.56
1:A:164:ARG:HH21	8:A:323:EDO:H22	1.71	0.56
1:B:222:GLU:HG2	12:B:468:HOH:O	2.06	0.55
1:A:263:HIS:CE1	6:A:314:SO3:S	2.93	0.55
1:B:27:LEU:HD12	1:B:75:LEU:HD12	1.88	0.54
1:B:263:HIS:CE1	6:B:308:SO3:S	2.95	0.54
1:B:164:ARG:HD2	12:B:552:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ARG:NH1	12:A:410:HOH:O	2.37	0.53
1:B:222:GLU:CG	12:B:468:HOH:O	2.58	0.52
1:A:27:LEU:HD13	1:A:48:ILE:CG2	2.40	0.52
1:B:27:LEU:HD13	1:B:48:ILE:CG2	2.40	0.52
1:B:165:MET:HE1	1:B:211:ILE:HD11	1.93	0.51
1:B:148:THR:HG22	1:B:150:PHE:CD2	2.40	0.50
1:A:50:GLU:HB2	12:A:413:HOH:O	2.11	0.50
1:B:36:ILE:HD11	1:B:101:ILE:HD13	1.93	0.50
1:B:104:LYS:NZ	12:B:411:HOH:O	2.39	0.50
1:B:160:GLU:HB2	9:B:314:ACT:H1	1.94	0.49
1:B:176:ARG:HB3	7:B:310:GOL:H31	1.94	0.49
1:A:36:ILE:HD11	1:A:101:ILE:HD13	1.94	0.48
1:A:26:ARG:NH2	1:A:105:GLU:OE2	2.47	0.48
1:B:210:LEU:CD2	7:B:312:GOL:H2	2.44	0.48
1:A:55:LYS:HG2	1:A:191:MET:HE3	1.95	0.48
1:B:168:LYS:HA	1:B:168:LYS:HE2	1.95	0.47
7:A:315:GOL:H12	12:A:522:HOH:O	2.13	0.47
1:A:165:MET:HG3	1:A:177:LEU:HD21	1.97	0.47
1:B:165:MET:HG3	1:B:177:LEU:HD21	1.96	0.46
1:B:145:LEU:O	1:B:148:THR:HB	2.15	0.46
1:A:168:LYS:HA	1:A:168:LYS:HE2	1.98	0.46
1:A:165:MET:HE1	1:A:211:ILE:HD11	1.98	0.46
1:A:176:ARG:HB3	7:A:315:GOL:H11	1.97	0.46
1:B:252:ASP:OD1	12:B:408:HOH:O	2.21	0.45
1:A:176:ARG:HH12	7:A:317:GOL:H11	1.82	0.45
1:B:243:SER:O	3:B:302:ADN:H8	2.17	0.45
1:B:126:PHE:CZ	1:B:148:THR:HG21	2.52	0.44
1:A:175:SER:HB2	7:A:315:GOL:H2	1.99	0.44
1:B:240:LEU:CD1	1:B:261:VAL:HG21	2.48	0.44
8:A:323:EDO:H21	12:A:472:HOH:O	2.17	0.44
1:B:24:ARG:NH1	12:B:410:HOH:O	2.24	0.43
1:A:248:GLY:CA	1:B:40:ASP:OD2	2.62	0.43
1:A:240:LEU:CD1	1:A:261:VAL:HG21	2.49	0.42
1:B:81:GLU:OE2	7:B:309:GOL:H11	2.21	0.41
1:A:176:ARG:NH1	7:A:317:GOL:C1	2.82	0.41
9:A:325:ACT:H2	12:A:575:HOH:O	2.19	0.41
1:A:26:ARG:HG2	1:A:26:ARG:HH11	1.86	0.41
1:A:152:ARG:HD2	7:A:316:GOL:H31	2.03	0.41
9:A:325:ACT:CH3	12:A:575:HOH:O	2.68	0.40
12:A:414:HOH:O	1:B:230:GLN:NE2	2.54	0.40
1:B:117:ASP:OD2	12:B:409:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:SER:O	3:A:302:ADN:H8	2.22	0.40

All (9) 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:A:253:GLU:OE2	12:B:401:HOH:O[4_545]	1.61	0.59
1:B:253:GLU:OE1	12:A:401:HOH:O[4_556]	1.64	0.56
1:A:253:GLU:OE2	1:B:212:GLU:OE2[4_545]	1.78	0.42
1:A:212:GLU:OE2	1:B:253:GLU:OE1[4_546]	1.92	0.28
1:B:24:ARG:NH1	1:B:278:ASP:OD2[4_545]	1.98	0.22
1:A:253:GLU:OE2	7:B:312:GOL:O2[4_545]	2.00	0.20
12:A:553:HOH:O	12:B:544:HOH:O[4_545]	2.12	0.08
12:A:466:HOH:O	12:A:497:HOH:O[4_556]	2.17	0.03
12:A:571:HOH:O	12:B:558:HOH:O[2_656]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	267/290 (92%)	266 (100%)	1 (0%)	0	100	100
1	B	267/290 (92%)	265 (99%)	2 (1%)	0	100	100
All	All	534/580 (92%)	531 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	242/261 (93%)	230 (95%)	12 (5%)	22	27
1	B	242/261 (93%)	230 (95%)	12 (5%)	22	27
All	All	484/522 (93%)	460 (95%)	24 (5%)	22	27

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	88	LYS
1	A	115	GLN
1	A	168	LYS
1	A	172	ARG
1	A	192	LYS
1	A	215	LYS
1	A	226	LYS
1	A	233	ARG
1	A	247	LEU
1	A	251	LYS
1	A	284	LYS
1	B	27	LEU
1	B	88	LYS
1	B	115	GLN
1	B	148	THR
1	B	149	ASP
1	B	168	LYS
1	B	191	MET
1	B	215	LYS
1	B	217	LYS
1	B	226	LYS
1	B	247	LEU
1	B	284	LYS

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	61	ASN
1	A	115	GLN
1	B	115	GLN
1	B	223	ASN

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 40 ligands modelled in this entry, 14 are monoatomic - leaving 26 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
7	GOL	A	318	-	5,5,5	0.21	0	5,5,5	0.48	0
7	GOL	A	319	-	5,5,5	0.21	0	5,5,5	0.56	0
9	ACT	A	325	-	3,3,3	0.86	0	3,3,3	0.71	0
7	GOL	B	309	-	5,5,5	0.25	0	5,5,5	0.49	0
2	MTA	A	301	-	22,22,22	0.97	1 (4%)	32,32,32	0.93	1 (3%)
8	EDO	A	323	-	3,3,3	0.36	0	2,2,2	0.63	0
3	ADN	B	302	-	21,21,21	0.40	0	31,31,31	0.64	0
7	GOL	B	311	-	5,5,5	0.22	0	5,5,5	0.53	0
2	MTA	B	301	-	22,22,22	0.93	1 (4%)	32,32,32	1.01	1 (3%)
7	GOL	B	310	-	5,5,5	0.27	0	5,5,5	0.76	0
8	EDO	A	324	-	3,3,3	0.29	0	2,2,2	0.28	0
7	GOL	A	317	-	5,5,5	0.19	0	5,5,5	0.44	0
7	GOL	A	315	-	5,5,5	0.10	0	5,5,5	0.37	0
6	SO3	A	313	-	1,3,3	1.95	0	0,3,3	-	-
9	ACT	B	314	-	3,3,3	0.92	0	3,3,3	1.00	0
3	ADN	A	302	-	21,21,21	0.42	0	31,31,31	0.80	1 (3%)
10	ARG	A	326	-	10,11,11	0.82	0	9,13,13	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	A	322	-	3,3,3	0.27	0	2,2,2	0.43	0
7	GOL	A	320	-	5,5,5	0.19	0	5,5,5	0.39	0
7	GOL	B	312	-	5,5,5	0.38	0	5,5,5	0.62	0
11	PEG	B	313	-	6,6,6	0.30	0	5,5,5	0.40	0
7	GOL	A	316	-	5,5,5	0.36	0	5,5,5	0.77	0
6	SO3	A	314	-	1,3,3	2.82	1 (100%)	0,3,3	-	-
6	SO3	B	308	-	1,3,3	2.77	1 (100%)	0,3,3	-	-
6	SO3	B	307	-	1,3,3	2.11	1 (100%)	0,3,3	-	-
8	EDO	A	321	-	3,3,3	0.24	0	2,2,2	0.13	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
7	GOL	A	318	-	-	4/4/4/4	-
7	GOL	A	319	-	-	2/4/4/4	-
7	GOL	B	309	-	-	0/4/4/4	-
2	MTA	A	301	-	-	1/7/23/23	0/3/3/3
8	EDO	A	323	-	-	1/1/1/1	-
3	ADN	B	302	-	-	1/6/22/22	0/3/3/3
7	GOL	B	311	-	-	3/4/4/4	-
2	MTA	B	301	-	-	2/7/23/23	0/3/3/3
7	GOL	B	310	-	-	4/4/4/4	-
8	EDO	A	324	-	-	1/1/1/1	-
7	GOL	A	317	-	-	2/4/4/4	-
7	GOL	A	315	-	-	4/4/4/4	-
3	ADN	A	302	-	-	2/6/22/22	0/3/3/3
10	ARG	A	326	-	-	0/11/11/11	-
8	EDO	A	322	-	-	1/1/1/1	-
7	GOL	A	320	-	-	0/4/4/4	-
7	GOL	B	312	-	-	1/4/4/4	-
11	PEG	B	313	-	-	3/4/4/4	-
7	GOL	A	316	-	-	2/4/4/4	-
8	EDO	A	321	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	MTA	C5'-S5'	-3.93	1.71	1.81
2	B	301	MTA	C5'-S5'	-3.74	1.72	1.81
6	A	314	SO3	O1-S	2.82	1.56	1.44
6	B	308	SO3	O1-S	2.77	1.56	1.44
6	B	307	SO3	O1-S	2.11	1.53	1.44

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	MTA	O4'-C4'-C5'	-4.16	98.13	108.83
2	A	301	MTA	O4'-C4'-C5'	-3.47	99.91	108.83
3	A	302	ADN	O3'-C3'-C4'	2.93	119.49	111.08

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	315	GOL	O1-C1-C2-C3
7	A	315	GOL	C1-C2-C3-O3
7	A	316	GOL	C1-C2-C3-O3
7	A	318	GOL	O1-C1-C2-O2
7	A	318	GOL	O1-C1-C2-C3
7	A	318	GOL	C1-C2-C3-O3
7	A	318	GOL	O2-C2-C3-O3
7	A	319	GOL	C1-C2-C3-O3
7	A	315	GOL	O1-C1-C2-O2
7	A	315	GOL	O2-C2-C3-O3
7	B	310	GOL	O2-C2-C3-O3
7	A	317	GOL	C1-C2-C3-O3
7	B	310	GOL	O1-C1-C2-C3
7	B	310	GOL	C1-C2-C3-O3
7	B	311	GOL	O1-C1-C2-C3
7	A	316	GOL	O2-C2-C3-O3
7	A	319	GOL	O2-C2-C3-O3
8	A	321	EDO	O1-C1-C2-O2
8	A	324	EDO	O1-C1-C2-O2
11	B	313	PEG	C4-C3-O2-C2
7	A	317	GOL	O2-C2-C3-O3
7	B	310	GOL	O1-C1-C2-O2
7	B	311	GOL	O1-C1-C2-O2
7	B	311	GOL	O2-C2-C3-O3
7	B	312	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	302	ADN	C2'-C1'-N9-C8
11	B	313	PEG	C1-C2-O2-C3
11	B	313	PEG	O2-C3-C4-O4
2	B	301	MTA	C4'-C5'-S5'-CS
8	A	322	EDO	O1-C1-C2-O2
8	A	323	EDO	O1-C1-C2-O2
3	B	302	ADN	C2'-C1'-N9-C8
2	A	301	MTA	C2'-C1'-N9-C8
2	B	301	MTA	C2'-C1'-N9-C8
3	A	302	ADN	O4'-C1'-N9-C8

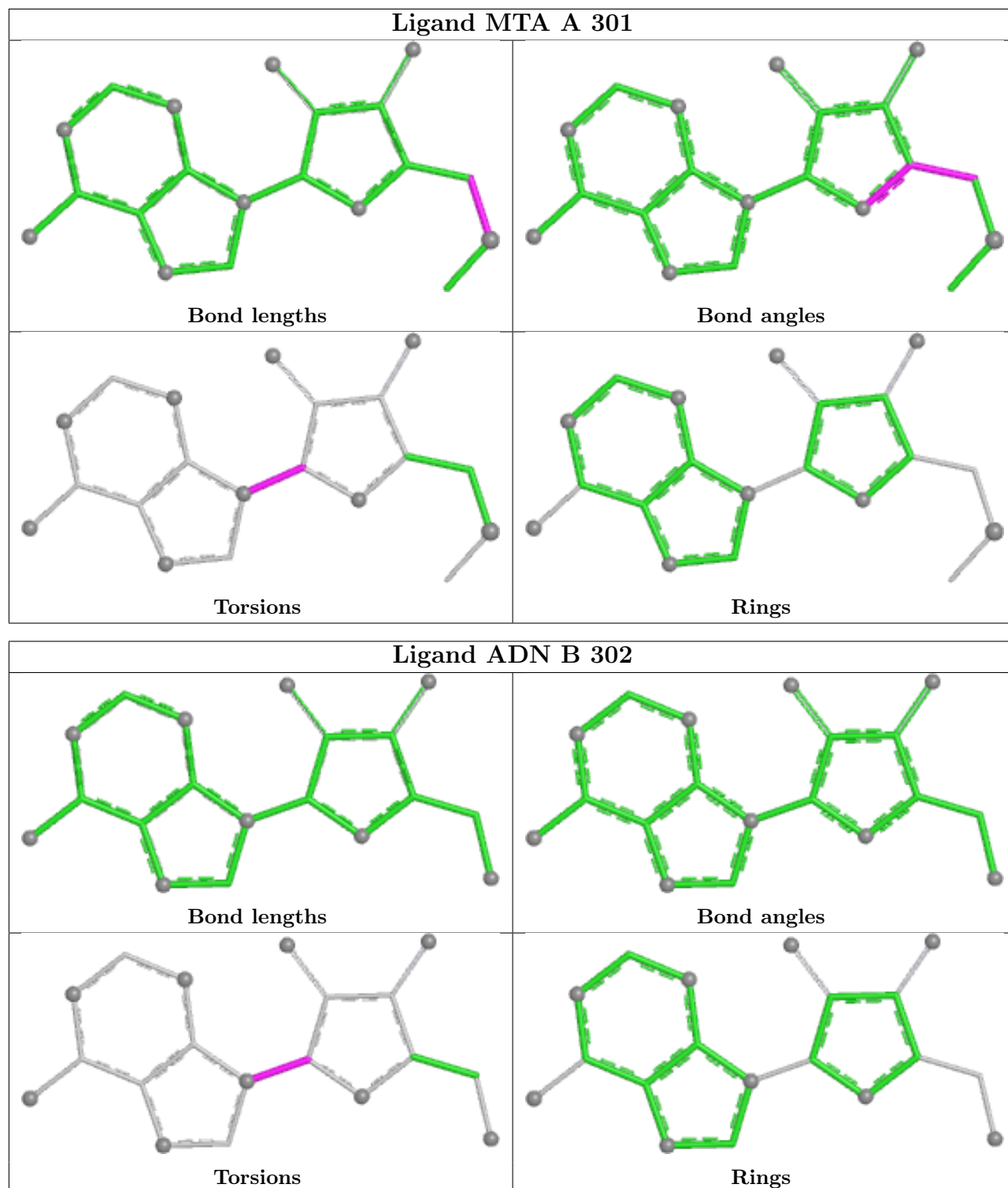
There are no ring outliers.

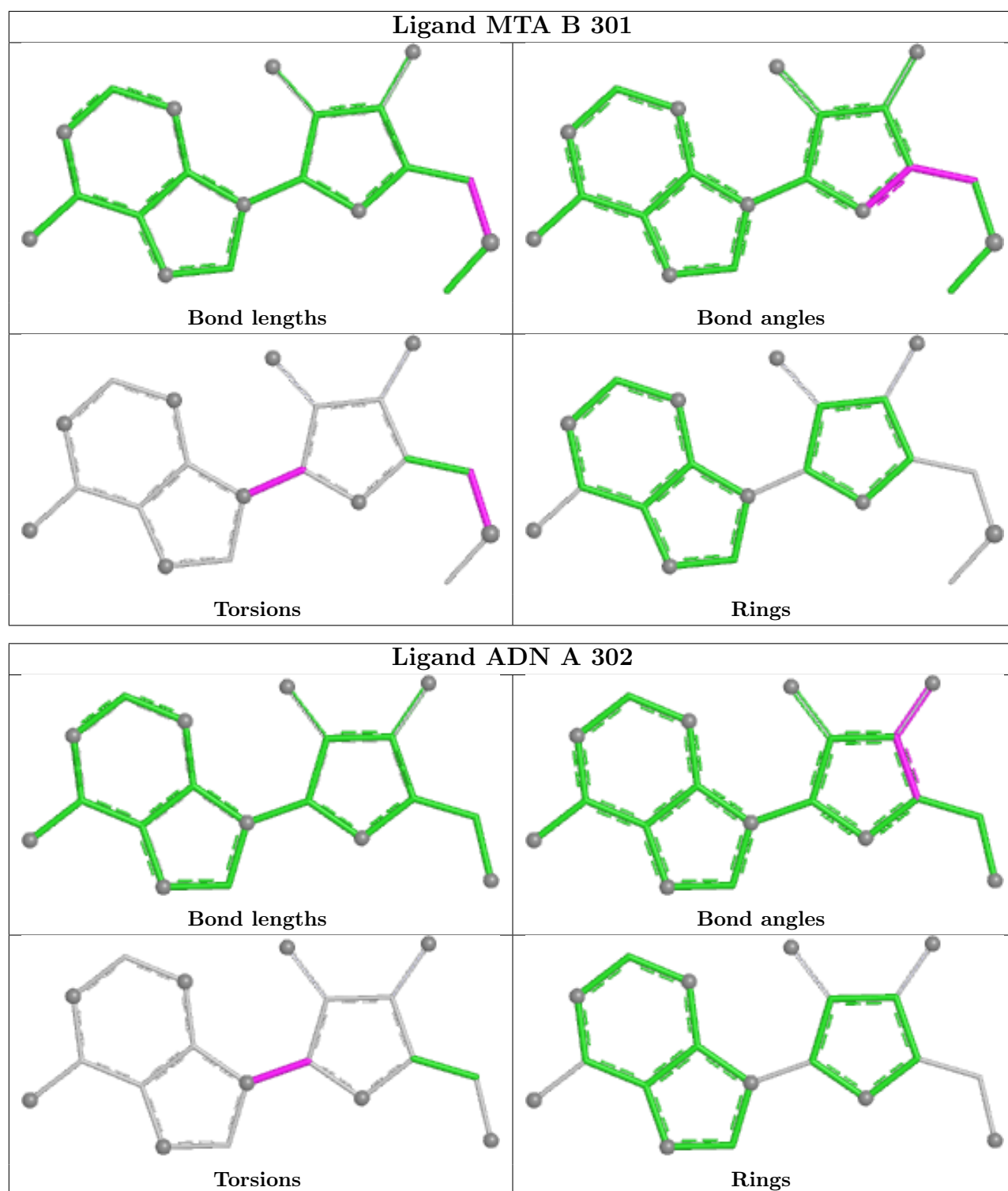
19 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	319	GOL	1	0
9	A	325	ACT	2	0
7	B	309	GOL	1	0
8	A	323	EDO	2	0
3	B	302	ADN	1	0
7	B	311	GOL	3	0
2	B	301	MTA	1	0
7	B	310	GOL	1	0
7	A	317	GOL	4	0
7	A	315	GOL	3	0
6	A	313	SO3	2	0
9	B	314	ACT	1	0
3	A	302	ADN	1	0
7	B	312	GOL	3	1
11	B	313	PEG	1	0
7	A	316	GOL	1	0
6	A	314	SO3	3	0
6	B	308	SO3	3	0
6	B	307	SO3	2	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 ⓘ

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	269/290 (92%)	-0.16	2 (0%) 84 87	18, 28, 51, 87	0
1	B	269/290 (92%)	-0.11	4 (1%) 72 77	17, 28, 51, 83	0
All	All	538/580 (92%)	-0.13	6 (1%) 78 82	17, 28, 51, 87	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	SER	4.4
1	B	290	SER	4.0
1	B	289	ILE	3.3
1	A	289	ILE	3.2
1	B	22	LYS	2.5
1	B	24	ARG	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.

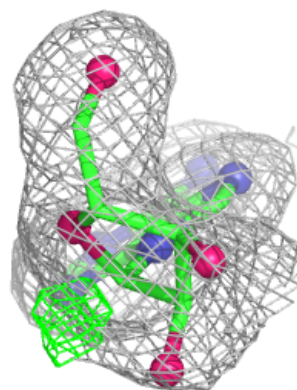
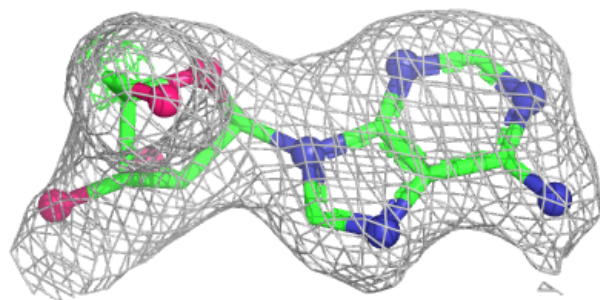
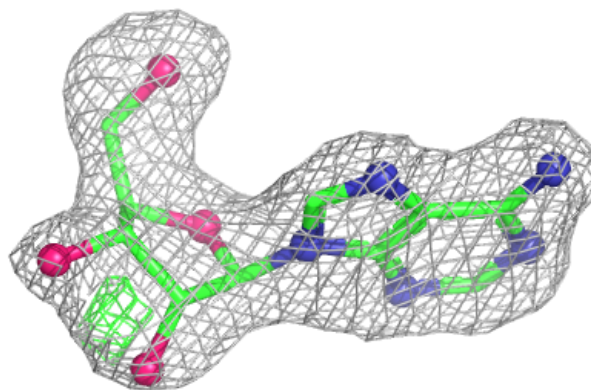
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	GOL	A	320	6/6	0.57	0.23	53,56,59,61	0
8	EDO	A	321	4/4	0.58	0.26	56,60,64,65	0
7	GOL	B	309	6/6	0.69	0.20	55,59,63,64	0
8	EDO	A	323	4/4	0.77	0.21	46,48,53,54	0
7	GOL	A	316	6/6	0.79	0.16	35,44,50,51	0
10	ARG	A	326	12/12	0.79	0.18	58,69,85,85	0
11	PEG	B	313	7/7	0.80	0.27	63,69,72,75	0
8	EDO	A	324	4/4	0.83	0.18	48,52,56,56	0
7	GOL	B	311	6/6	0.86	0.14	34,40,45,45	0
4	ZN	B	305	1/1	0.86	0.11	104,104,104,104	0
7	GOL	A	317	6/6	0.86	0.14	41,49,51,54	0
4	ZN	A	308	1/1	0.87	0.10	108,108,108,108	0
7	GOL	A	319	6/6	0.88	0.12	37,44,48,55	0
7	GOL	B	310	6/6	0.89	0.14	28,38,44,52	0
3	ADN	B	302	19/19	0.90	0.11	29,38,57,58	0
3	ADN	A	302	19/19	0.91	0.10	30,38,54,61	0
7	GOL	B	312	6/6	0.91	0.14	22,34,38,42	0
7	GOL	A	315	6/6	0.91	0.12	29,36,38,44	0
8	EDO	A	322	4/4	0.91	0.18	47,52,52,55	0
4	ZN	A	309	1/1	0.93	0.08	95,95,95,95	0
4	ZN	B	304	1/1	0.94	0.14	95,95,95,95	0
7	GOL	A	318	6/6	0.94	0.12	38,51,53,56	0
9	ACT	A	325	4/4	0.95	0.09	24,31,35,37	0
2	MTA	B	301	20/20	0.95	0.07	16,19,35,39	0
5	CL	A	311	1/1	0.95	0.18	47,47,47,47	0
6	SO3	B	307	4/4	0.96	0.08	20,22,27,28	0
9	ACT	B	314	4/4	0.96	0.09	24,30,35,36	0
5	CL	B	306	1/1	0.96	0.19	50,50,50,50	0
6	SO3	A	313	4/4	0.96	0.07	21,25,27,29	0
5	CL	A	312	1/1	0.97	0.11	47,47,47,47	0
6	SO3	A	314	4/4	0.97	0.06	6,8,10,10	0
2	MTA	A	301	20/20	0.97	0.07	19,23,43,49	0
4	ZN	A	307	1/1	0.98	0.06	57,57,57,57	0
6	SO3	B	308	4/4	0.98	0.06	7,10,12,14	0
4	ZN	A	305	1/1	0.99	0.03	41,41,41,41	0
4	ZN	B	303	1/1	0.99	0.02	27,27,27,27	0
4	ZN	A	306	1/1	0.99	0.02	42,42,42,42	0
4	ZN	A	303	1/1	0.99	0.03	29,29,29,29	0
5	CL	A	310	1/1	0.99	0.03	29,29,29,29	0
4	ZN	A	304	1/1	0.99	0.03	42,42,42,42	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.

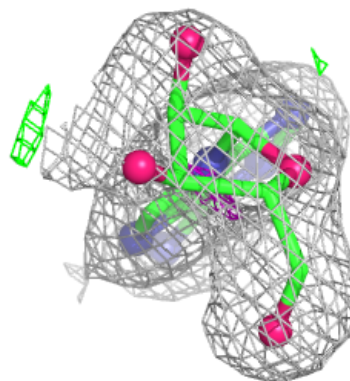
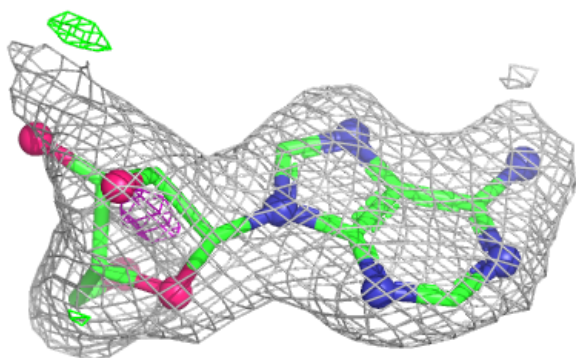
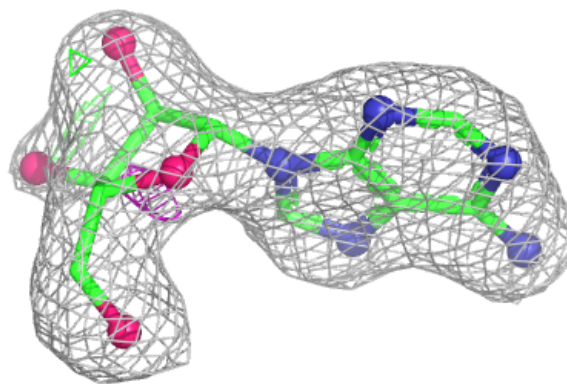
Electron density around ADN B 302:

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

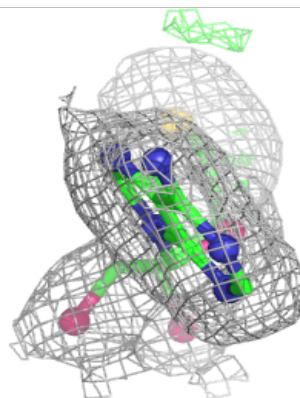
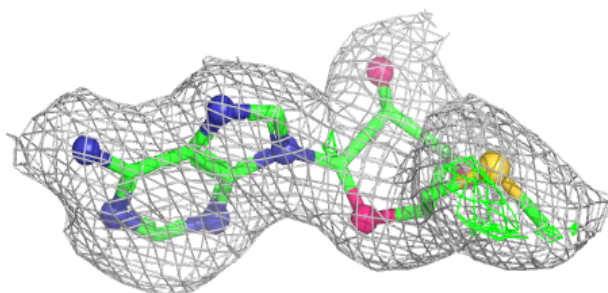
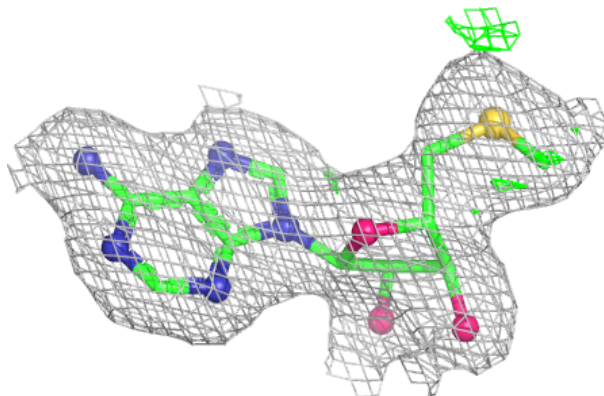


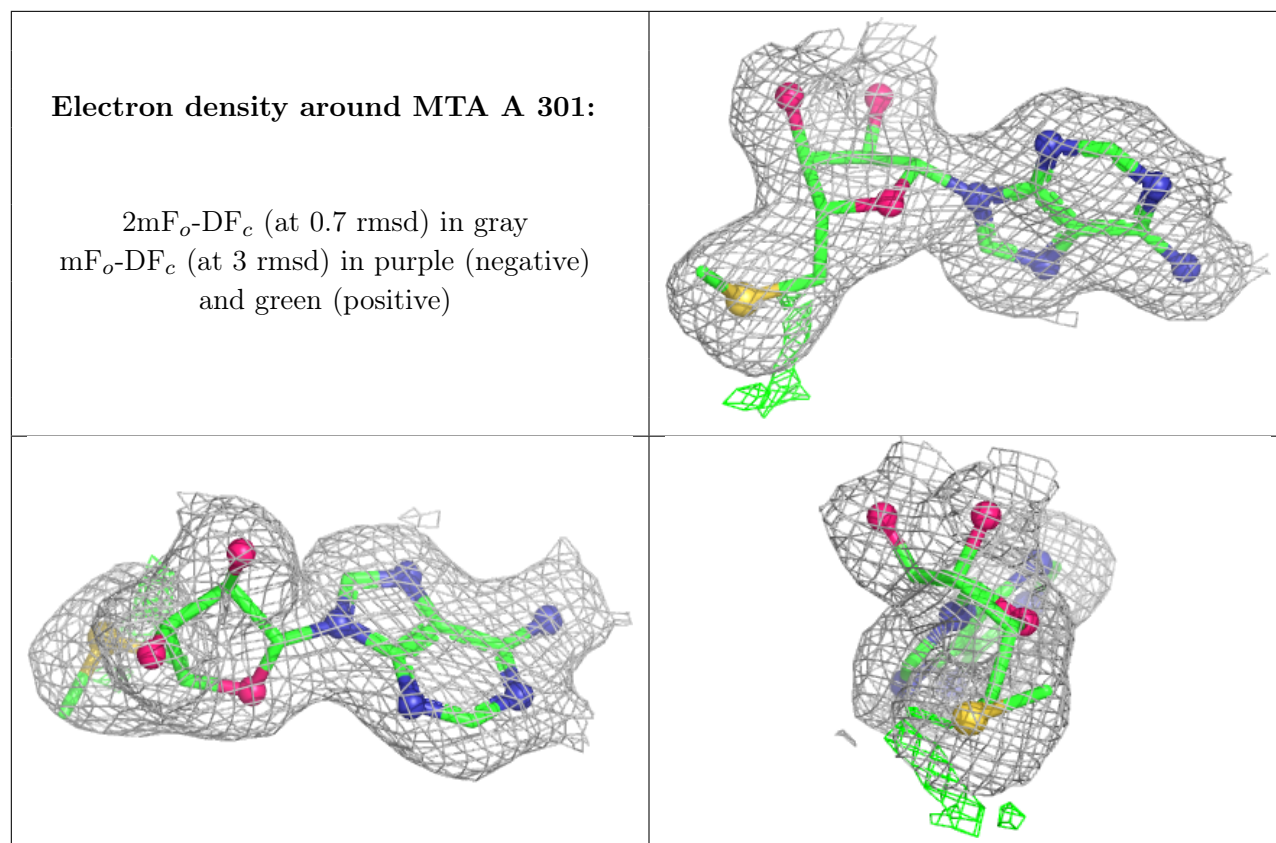
Electron density around ADN A 302:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.