



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:24 AM UTC

PDB ID : 8X45 / pdb_00008x45
Title : Crystal structure of DIMIT1 in complex with 5'-methylthioadenosine from *Pyrococcus horikoshii* (FormII)
Authors : Saha, S.; Kanaujia, S.P.
Deposited on : 2023-11-15
Resolution : 2.50 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

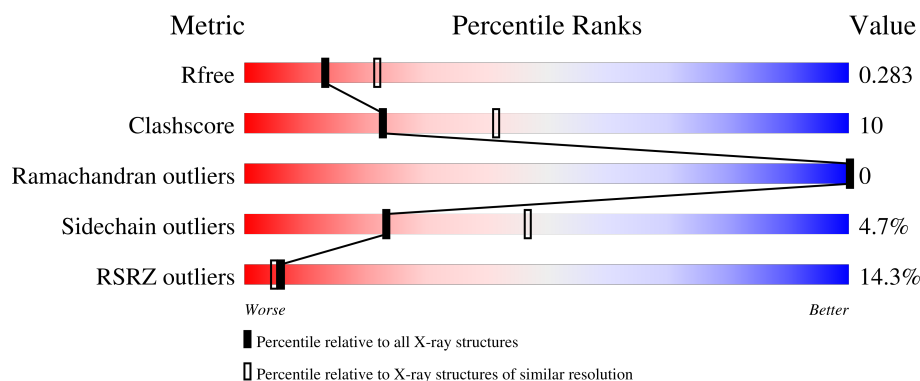
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	13% 72% 19% • 7%
1	B	290	13% 71% 19% • 7%

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	B	303	-	-	X	-
5	GOL	B	304	-	-	X	-
7	PEG	B	308	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 4650 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	270	Total	C	N	O	S	0	1	0
			2200	1422	383	389	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:

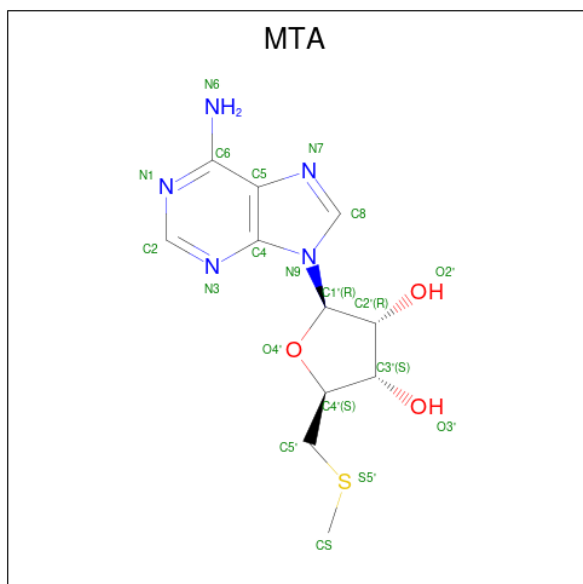
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O59487
A	2	SER	-	expression tag	UNP O59487
A	3	SER	-	expression tag	UNP O59487
A	4	ARG	-	expression tag	UNP O59487
A	5	ILE	-	expression tag	UNP O59487
A	6	ARG	-	expression tag	UNP O59487
A	7	ILE	-	expression tag	UNP O59487
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
			20	11	5	3	1	

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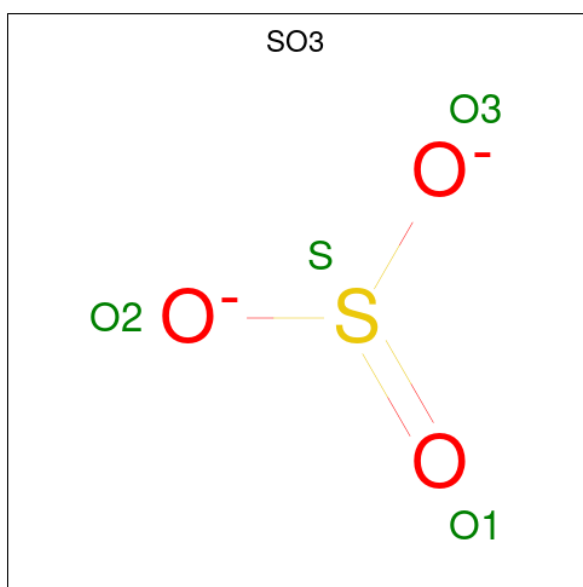
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

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

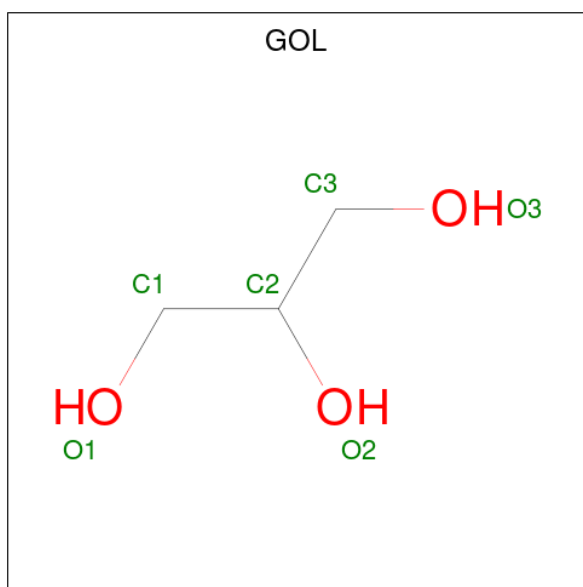
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Zn	0	0
			4	4		
3	B	1	Total	Zn	0	0
			1	1		

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



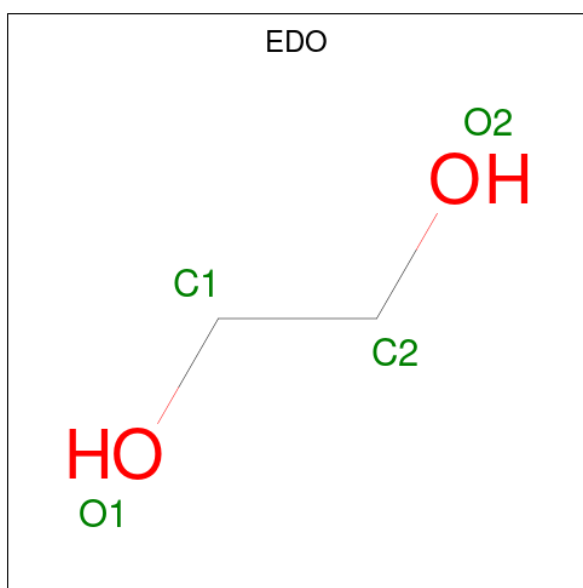
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			4	3	1		
4	B	1	Total	O	S	0	0
			4	3	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



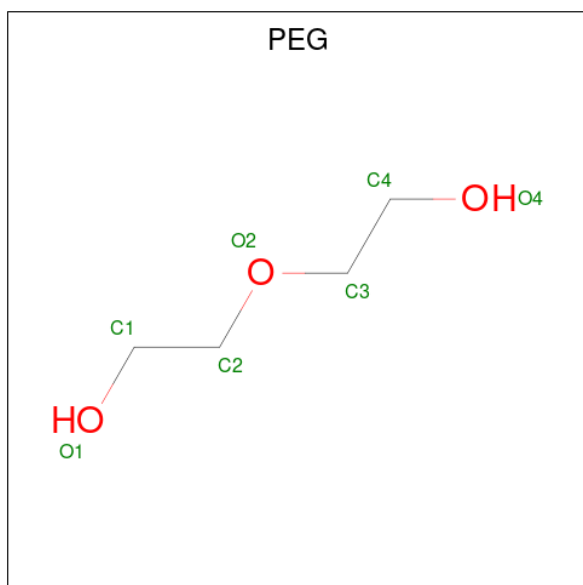
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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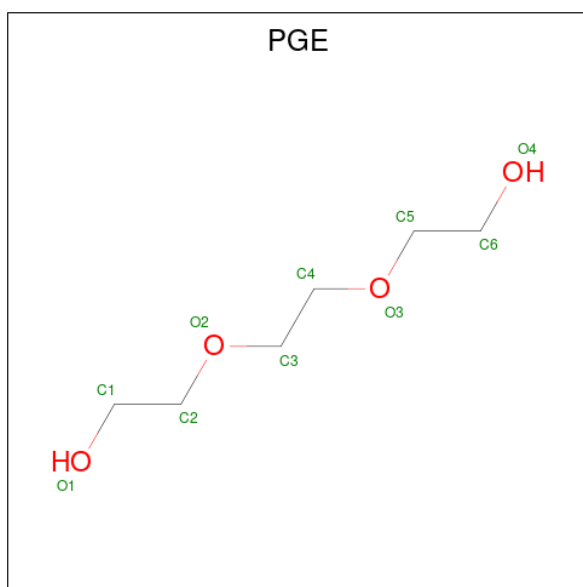
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



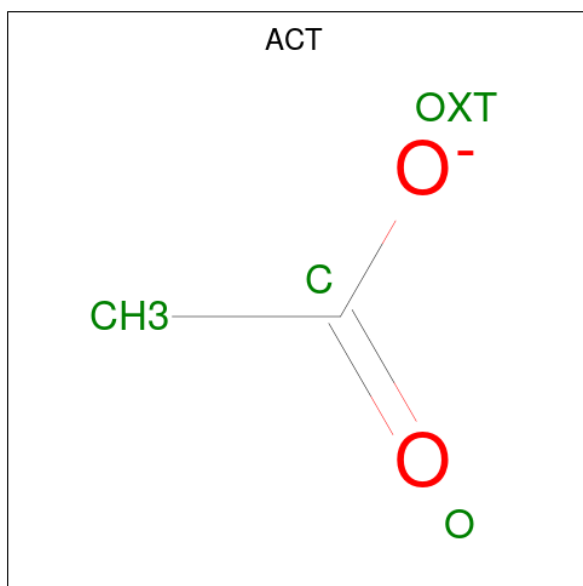
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			10	6	4		

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



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

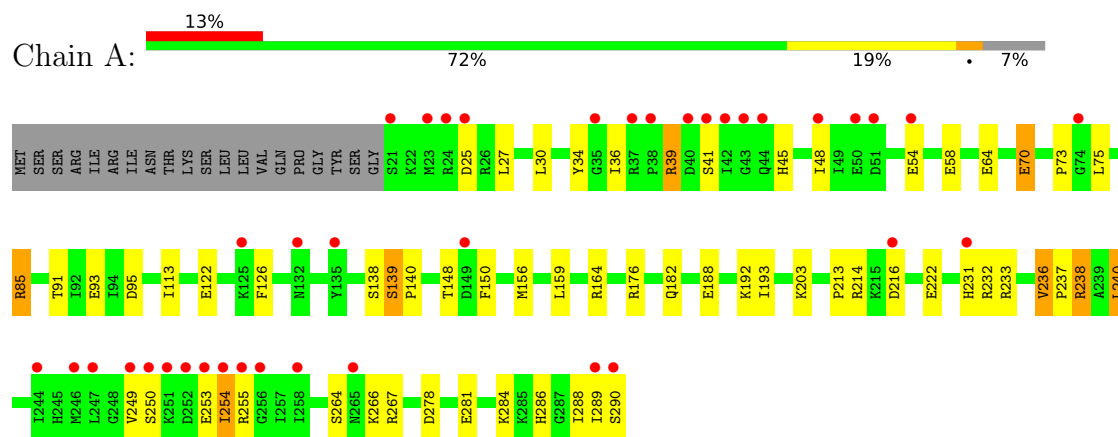
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	79	Total 79	O 79	0	0
10	B	73	Total 73	O 73	0	0

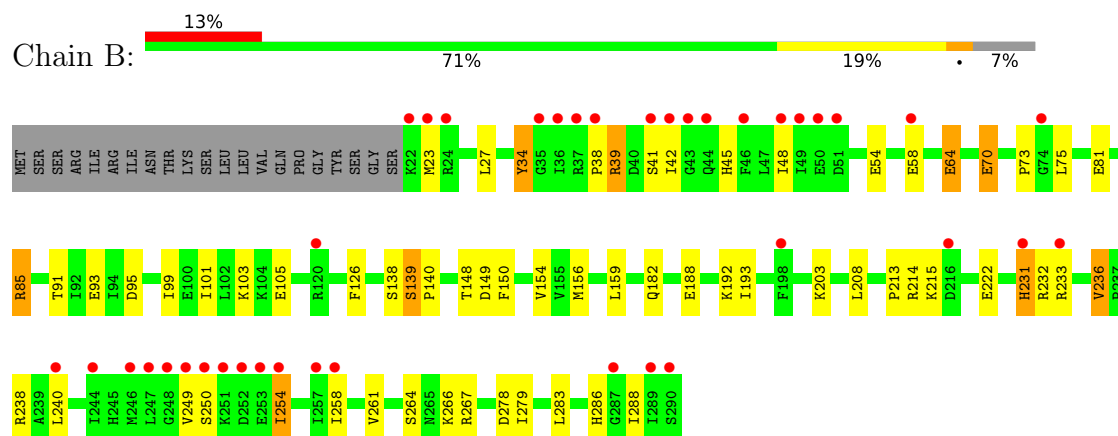
3 Residue-property plots [i](#)

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: 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	120.74Å 80.23Å 85.71Å 90.00° 116.17° 90.00°	Depositor
Resolution (Å)	76.92 – 2.50 76.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (76.92-2.50) 95.0 (76.92-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.231 , 0.282 0.238 , 0.283	Depositor DCC
R_{free} test set	1181 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4650	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.39% 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: PGE, GOL, EDO, ZN, PEG, MTA, ACT, SO3

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	0.60	0/2244	1.16	5/3020 (0.2%)
1	B	0.60	0/2230	1.13	6/3001 (0.2%)
All	All	0.60	0/4474	1.14	11/6021 (0.2%)

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	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	253	GLU	CB-CG-CD	6.55	123.74	112.60
1	A	34	TYR	CB-CA-C	6.31	120.77	109.29
1	A	138	SER	CA-C-N	6.14	126.64	119.83
1	A	138	SER	C-N-CA	6.14	126.64	119.83
1	B	138	SER	CA-C-N	6.00	126.49	119.83
1	B	138	SER	C-N-CA	6.00	126.49	119.83
1	B	231	HIS	CA-CB-CG	-5.75	108.05	113.80
1	B	81	GLU	CB-CG-CD	5.38	121.75	112.60
1	B	34	TYR	CB-CA-C	5.31	118.89	109.65
1	B	70	GLU	CB-CG-CD	5.24	121.50	112.60
1	A	70	GLU	CB-CG-CD	5.17	121.39	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	ARG	Sidechain
1	A	85	ARG	Sidechain
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	2200	0	2309	52	2
1	B	2189	0	2300	48	2
2	A	20	0	15	1	0
2	B	20	0	15	0	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	1	0
4	B	4	0	0	2	0
5	A	6	0	8	2	1
5	B	6	0	8	4	0
6	A	8	0	12	4	0
6	B	8	0	12	0	0
7	A	7	0	10	2	1
7	B	7	0	10	3	1
8	A	10	0	14	1	0
9	B	4	0	3	0	0
10	A	79	0	0	8	0
10	B	73	0	0	6	0
All	All	4650	0	4716	96	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 10.

All (96) 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:B:188:GLU:OE2	7:B:308:PEG:H21	1.08	1.24
1:B:278:ASP:OD2	5:B:304:GOL:H2	1.43	1.18
1:B:188:GLU:OE2	7:B:308:PEG:C2	1.92	1.16
1:A:231:HIS:CE1	1:B:231:HIS:CE1	2.46	1.03
1:A:278:ASP:OD2	5:A:307:GOL:H2	1.58	1.03
1:A:188:GLU:OE1	7:A:310:PEG:O2	1.78	1.01
1:A:45:HIS:NE2	4:A:306:SO3:S	2.36	0.96
1:B:278:ASP:OD2	5:B:304:GOL:C2	2.15	0.95
1:B:45:HIS:NE2	4:B:303:SO3:S	2.39	0.95
1:B:105:GLU:OE1	10:B:401:HOH:O	1.90	0.88
1:A:231:HIS:CE1	1:B:231:HIS:NE2	2.43	0.87
1:A:231:HIS:NE2	1:B:231:HIS:CE1	2.44	0.86
1:A:231:HIS:NE2	1:B:231:HIS:NE2	2.26	0.83
1:B:27:LEU:HD12	1:B:75:LEU:HD12	1.65	0.79
1:A:27:LEU:HD12	1:A:75:LEU:HD12	1.66	0.78
1:B:278:ASP:OD2	5:B:304:GOL:C1	2.41	0.68
1:A:139:SER:HB3	1:A:140:PRO:HD3	1.75	0.67
1:B:139:SER:HB3	1:B:140:PRO:HD3	1.76	0.66
1:A:233:ARG:O	1:A:267:ARG:NH1	2.30	0.65
1:A:281:GLU:HG2	10:A:465:HOH:O	1.97	0.64
1:B:233:ARG:O	1:B:267:ARG:NH1	2.30	0.64
1:B:95:ASP:OD2	10:B:402:HOH:O	2.15	0.64
1:B:39:ARG:NH2	1:B:45:HIS:CE1	2.67	0.63
1:A:39:ARG:NH2	1:A:45:HIS:CE1	2.68	0.62
1:A:289:ILE:O	1:A:290:SER:OG	2.19	0.60
1:B:99:ILE:O	1:B:103:LYS:HG3	2.03	0.59
1:A:39:ARG:HB2	1:A:41:SER:O	2.02	0.58
1:B:39:ARG:HB2	1:B:41:SER:O	2.02	0.58
1:A:249:VAL:HG11	1:A:254:ILE:HD13	1.86	0.57
1:B:249:VAL:HG11	1:B:254:ILE:HD13	1.86	0.57
1:A:54:GLU:O	1:A:58:GLU:HG2	2.04	0.57
1:A:95:ASP:OD2	10:A:401:HOH:O	2.18	0.56
1:A:27:LEU:CD1	1:A:75:LEU:HD12	2.34	0.56
1:B:54:GLU:O	1:B:58:GLU:HG2	2.05	0.56
1:B:27:LEU:HD22	1:B:48:ILE:HG21	1.87	0.56
1:A:278:ASP:OD2	5:A:307:GOL:C2	2.45	0.56
1:A:126:PHE:CZ	1:A:148:THR:HG21	2.41	0.55
1:A:249:VAL:HG12	1:A:250:SER:O	2.07	0.55
1:B:249:VAL:HG12	1:B:250:SER:O	2.08	0.54
1:A:122:GLU:OE1	10:A:402:HOH:O	2.18	0.53
1:B:278:ASP:OD2	5:B:304:GOL:H12	2.09	0.51
1:B:236:VAL:HG13	1:B:266:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ARG:HG3	10:A:428:HOH:O	2.11	0.50
1:B:126:PHE:CZ	1:B:148:THR:HG21	2.47	0.50
1:A:231:HIS:CE1	1:B:231:HIS:HE1	2.22	0.49
1:A:27:LEU:HD12	1:A:75:LEU:CD1	2.40	0.49
1:A:164:ARG:HH21	1:A:164:ARG:HG3	1.75	0.49
1:B:38:PRO:HG2	10:B:468:HOH:O	2.12	0.48
1:B:27:LEU:CD1	1:B:75:LEU:HD12	2.39	0.48
1:A:93:GLU:OE1	2:A:301:MTA:O2'	2.26	0.48
1:A:113:ILE:HD12	6:A:309:EDO:H11	1.95	0.48
1:B:27:LEU:HD12	1:B:75:LEU:CD1	2.42	0.48
1:A:176:ARG:HB2	6:A:308:EDO:H22	1.95	0.48
1:A:236:VAL:HG13	1:A:266:LYS:O	2.13	0.48
1:A:236:VAL:HG22	1:A:264:SER:HA	1.94	0.47
1:B:156:MET:HG2	1:B:193:ILE:CD1	2.45	0.47
1:A:159:LEU:HD22	1:A:192:LYS:HE3	1.97	0.47
1:A:54:GLU:HG2	1:A:85:ARG:HH22	1.80	0.46
1:B:150:PHE:O	1:B:213:PRO:HG3	2.15	0.46
1:A:39:ARG:CD	10:A:455:HOH:O	2.64	0.46
1:A:176:ARG:H	6:A:308:EDO:H22	1.81	0.46
1:A:73:PRO:HD2	1:A:93:GLU:HB2	1.97	0.46
1:A:27:LEU:HD22	1:A:48:ILE:HG21	1.97	0.45
1:B:159:LEU:HD22	1:B:192:LYS:HD2	1.99	0.45
1:B:236:VAL:HG22	1:B:264:SER:HA	1.97	0.45
1:A:150:PHE:O	1:A:213:PRO:HG3	2.17	0.45
1:A:70:GLU:O	1:A:91:THR:HA	2.16	0.44
1:B:182:GLN:O	1:B:214:ARG:NH1	2.47	0.44
1:A:182:GLN:O	1:A:214:ARG:NH1	2.45	0.44
1:A:232:ARG:NH1	10:A:408:HOH:O	2.50	0.44
1:B:85:ARG:NE	10:B:403:HOH:O	2.36	0.44
1:A:156:MET:HG2	1:A:193:ILE:CD1	2.48	0.44
1:B:279:ILE:O	1:B:283:LEU:HG	2.18	0.43
1:A:188:GLU:OE2	7:A:310:PEG:H31	2.18	0.43
1:B:149:ASP:HB3	10:B:462:HOH:O	2.18	0.43
1:B:188:GLU:OE2	7:B:308:PEG:O2	2.33	0.43
1:B:70:GLU:O	1:B:91:THR:HA	2.18	0.43
1:A:216:ASP:OD1	1:A:216:ASP:N	2.52	0.43
8:A:311:PGE:H5	10:A:450:HOH:O	2.18	0.42
1:B:233:ARG:HH11	1:B:233:ARG:HG3	1.84	0.42
1:B:34:TYR:CE2	1:B:101:ILE:HG23	2.54	0.42
1:B:154:VAL:CG1	1:B:208:LEU:HD11	2.50	0.42
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:HD3	10:A:431:HOH:O	2.20	0.42
1:B:232:ARG:NH1	10:B:406:HOH:O	2.52	0.42
1:B:73:PRO:HD2	1:B:93:GLU:HB2	2.02	0.42
1:B:39:ARG:NH2	1:B:42:ILE:O	2.53	0.42
1:A:176:ARG:H	6:A:308:EDO:C2	2.33	0.41
1:B:258:ILE:O	1:B:261:VAL:HG12	2.20	0.41
1:A:139:SER:CB	1:A:140:PRO:HD3	2.48	0.41
1:A:236:VAL:O	1:A:240:LEU:HD23	2.21	0.41
1:B:39:ARG:NH2	4:B:303:SO3:O3	2.48	0.41
1:A:236:VAL:N	1:A:237:PRO:CD	2.84	0.41
1:B:139:SER:CB	1:B:140:PRO:HD3	2.48	0.41
1:A:164:ARG:HG3	1:A:164:ARG:NH2	2.35	0.40
1:A:284:LYS:HG3	1:A:290:SER:C	2.47	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)
1:B:286:HIS:NE2	7:A:310:PEG:O2[4_556]	2.09	0.11
1:B:64:GLU:OE2	1:B:64:GLU:OE2[2_655]	2.12	0.08
1:A:25:ASP:OD1	5:A:307:GOL:O2[4_556]	2.16	0.04
1:A:286:HIS:NE2	7:B:308:PEG:C2[4_545]	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	269/290 (93%)	264 (98%)	5 (2%)	0	100	100
1	B	267/290 (92%)	261 (98%)	6 (2%)	0	100	100
All	All	536/580 (92%)	525 (98%)	11 (2%)	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%)	233 (96%)	11 (4%)	24	49
1	B	242/261 (93%)	230 (95%)	12 (5%)	22	44
All	All	486/522 (93%)	463 (95%)	23 (5%)	23	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ILE
1	A	39	ARG
1	A	64	GLU
1	A	139	SER
1	A	203	LYS
1	A	222	GLU
1	A	236	VAL
1	A	238	ARG
1	A	240	LEU
1	A	254	ILE
1	A	288	ILE
1	B	23	MET
1	B	39	ARG
1	B	64	GLU
1	B	139	SER
1	B	203	LYS
1	B	215	LYS
1	B	222	GLU
1	B	236	VAL
1	B	238	ARG
1	B	240	LEU
1	B	254	ILE
1	B	288	ILE

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

sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	B	115	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 19 ligands modelled in this entry, 5 are monoatomic - leaving 14 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	$\# Z > 2$
5	GOL	A	307	-	5,5,5	0.11	0	5,5,5	0.68	0
2	MTA	B	301	-	22,22,22	0.35	0	32,32,32	0.70	0
4	SO3	A	306	-	1,3,3	1.80	0	0,3,3	-	-
4	SO3	B	303	-	1,3,3	1.95	0	0,3,3	-	-
5	GOL	B	304	-	5,5,5	0.10	0	5,5,5	0.30	0
6	EDO	B	306	-	3,3,3	0.07	0	2,2,2	0.06	0
8	PGE	A	311	-	9,9,9	0.48	0	8,8,8	0.24	0
7	PEG	A	310	-	6,6,6	0.57	0	5,5,5	0.42	0
2	MTA	A	301	-	22,22,22	0.33	0	32,32,32	1.14	2 (6%)
6	EDO	A	309	-	3,3,3	0.31	0	2,2,2	0.32	0
9	ACT	B	307	-	3,3,3	1.03	0	3,3,3	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	B	305	-	3,3,3	0.14	0	2,2,2	0.27	0
7	PEG	B	308	-	6,6,6	0.33	0	5,5,5	0.58	0
6	EDO	A	308	-	3,3,3	0.15	0	2,2,2	0.17	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
5	GOL	A	307	-	-	0/4/4/4	-
2	MTA	B	301	-	-	2/7/23/23	0/3/3/3
5	GOL	B	304	-	-	2/4/4/4	-
6	EDO	B	306	-	-	1/1/1/1	-
8	PGE	A	311	-	-	6/7/7/7	-
7	PEG	A	310	-	-	2/4/4/4	-
2	MTA	A	301	-	-	1/7/23/23	0/3/3/3
6	EDO	A	309	-	-	1/1/1/1	-
6	EDO	B	305	-	-	0/1/1/1	-
7	PEG	B	308	-	-	2/4/4/4	-
6	EDO	A	308	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	MTA	C4'-C5'-S5'	3.91	126.91	113.89
2	A	301	MTA	O4'-C4'-C5'	2.69	115.77	108.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MTA	C4'-C5'-S5'-CS
2	B	301	MTA	O4'-C4'-C5'-S5'
2	B	301	MTA	C3'-C4'-C5'-S5'
5	B	304	GOL	C1-C2-C3-O3
7	A	310	PEG	C4-C3-O2-C2
7	B	308	PEG	C1-C2-O2-C3
5	B	304	GOL	O2-C2-C3-O3

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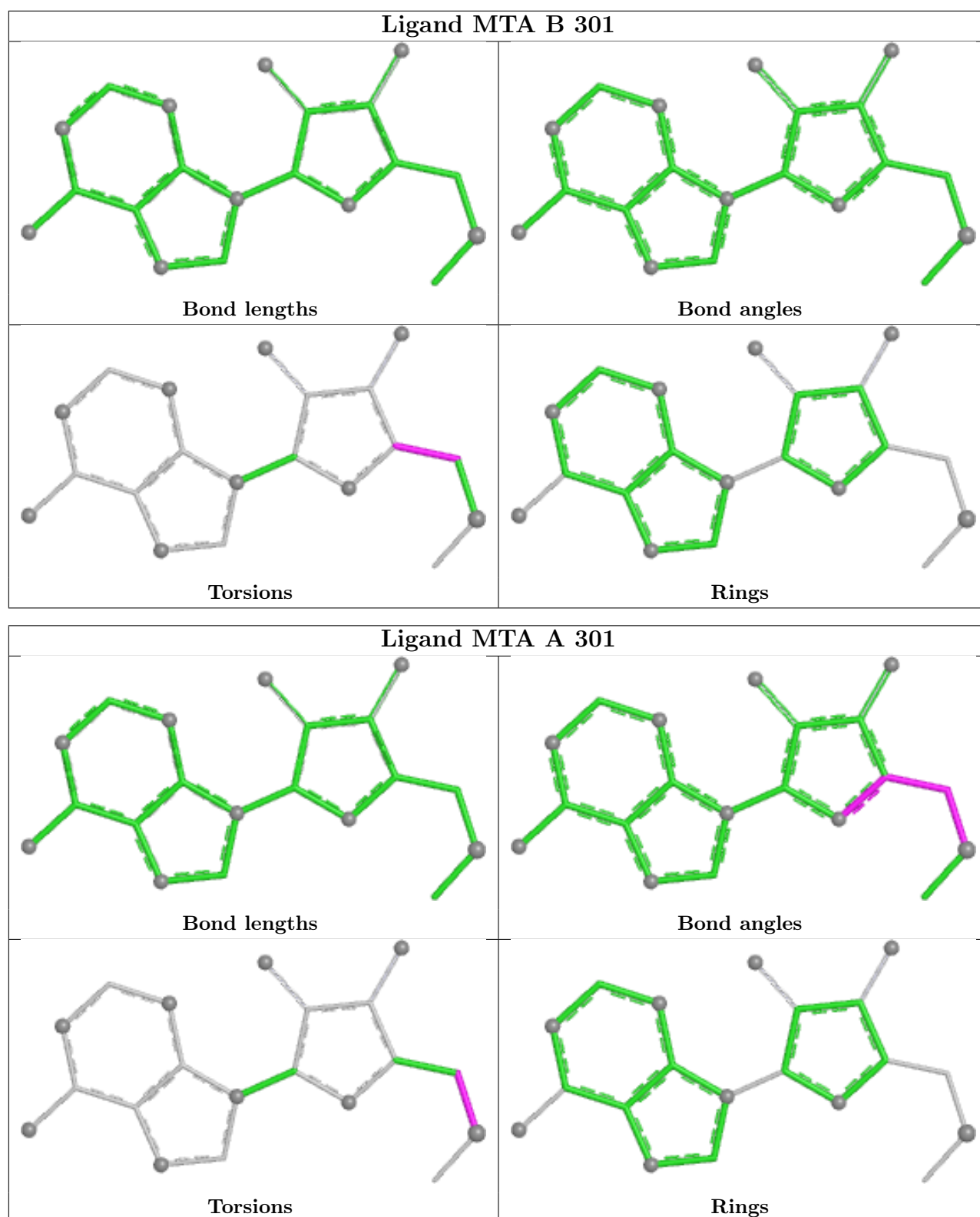
Mol	Chain	Res	Type	Atoms
8	A	311	PGE	O1-C1-C2-O2
7	A	310	PEG	O1-C1-C2-O2
8	A	311	PGE	O3-C5-C6-O4
8	A	311	PGE	C1-C2-O2-C3
6	A	309	EDO	O1-C1-C2-O2
8	A	311	PGE	C6-C5-O3-C4
8	A	311	PGE	O2-C3-C4-O3
8	A	311	PGE	C3-C4-O3-C5
6	B	306	EDO	O1-C1-C2-O2
7	B	308	PEG	C4-C3-O2-C2

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	307	GOL	2	1
4	A	306	SO3	1	0
4	B	303	SO3	2	0
5	B	304	GOL	4	0
8	A	311	PGE	1	0
7	A	310	PEG	2	1
2	A	301	MTA	1	0
6	A	309	EDO	1	0
7	B	308	PEG	3	1
6	A	308	EDO	3	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

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	270/290 (93%)	0.94	38 (14%) 6 5	25, 43, 85, 105	1 (0%)
1	B	269/290 (92%)	1.06	39 (14%) 6 5	23, 45, 78, 109	0
All	All	539/580 (92%)	1.00	77 (14%) 6 5	23, 44, 84, 109	1 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	42	ILE	7.0
1	A	43	GLY	5.5
1	B	43	GLY	5.4
1	A	290	SER	4.7
1	A	42	ILE	4.6
1	B	290	SER	4.5
1	B	253	GLU	4.4
1	B	38	PRO	4.2
1	B	48	ILE	4.1
1	A	38	PRO	4.0
1	B	250	SER	4.0
1	A	35	GLY	4.0
1	B	258	ILE	4.0
1	A	253	GLU	3.9
1	A	135	TYR	3.7
1	B	247	LEU	3.5
1	B	289	ILE	3.5
1	B	249	VAL	3.4
1	A	21	SER	3.4
1	B	35	GLY	3.4
1	A	252	ASP	3.4
1	A	258	ILE	3.4
1	A	41	SER	3.3
1	A	44	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	51	ASP	3.2
1	A	24	ARG	3.1
1	B	287	GLY	3.1
1	B	254	ILE	3.1
1	B	23	MET	3.1
1	B	248	GLY	3.1
1	B	246	MET	2.9
1	B	41	SER	2.9
1	B	244	ILE	2.9
1	A	250	SER	2.9
1	A	244	ILE	2.9
1	B	252	ASP	2.8
1	B	24	ARG	2.8
1	A	254	ILE	2.8
1	B	251	LYS	2.8
1	A	25	ASP	2.8
1	A	54	GLU	2.8
1	A	23	MET	2.7
1	B	46	PHE	2.7
1	B	74	GLY	2.7
1	A	246	MET	2.6
1	A	289	ILE	2.6
1	B	240	LEU	2.6
1	A	40	ASP	2.5
1	B	36	ILE	2.5
1	A	249	VAL	2.5
1	A	125	LYS	2.5
1	B	231	HIS	2.5
1	B	37	ARG	2.5
1	A	247	LEU	2.5
1	B	22	LYS	2.4
1	A	256	GLY	2.4
1	A	48	ILE	2.4
1	A	251	LYS	2.4
1	B	44	GLN	2.4
1	A	231	HIS	2.4
1	B	51	ASP	2.3
1	B	120	ARG	2.3
1	B	257	ILE	2.3
1	A	132	ASN	2.3
1	B	198	PHE	2.2
1	A	265	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	49	ILE	2.2
1	A	50	GLU	2.2
1	A	149[A]	ASP	2.2
1	B	216	ASP	2.1
1	B	50	GLU	2.0
1	A	37	ARG	2.0
1	A	255	ARG	2.0
1	B	233	ARG	2.0
1	B	58	GLU	2.0
1	A	74	GLY	2.0
1	A	216	ASP	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(Å ²)	Q<0.9
9	ACT	B	307	4/4	0.69	0.17	55,55,59,61	0
8	PGE	A	311	10/10	0.70	0.23	69,95,110,112	0
6	EDO	A	309	4/4	0.80	0.22	63,64,70,71	0
5	GOL	A	307	6/6	0.82	0.17	39,41,42,46	0
6	EDO	B	306	4/4	0.82	0.13	60,62,62,62	0
6	EDO	A	308	4/4	0.83	0.14	42,45,50,55	0
7	PEG	B	308	7/7	0.85	0.15	29,32,41,46	0
5	GOL	B	304	6/6	0.87	0.17	35,38,43,45	0
7	PEG	A	310	7/7	0.88	0.16	25,35,39,40	0
6	EDO	B	305	4/4	0.88	0.15	37,44,49,56	0
2	MTA	A	301	20/20	0.89	0.11	27,32,57,57	0
2	MTA	B	301	20/20	0.89	0.11	24,33,64,70	0

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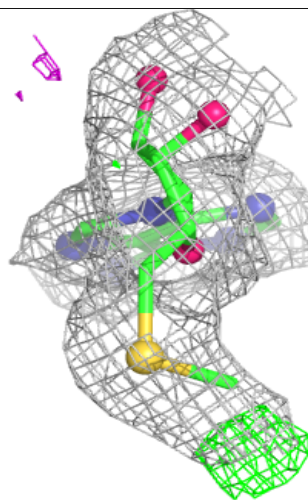
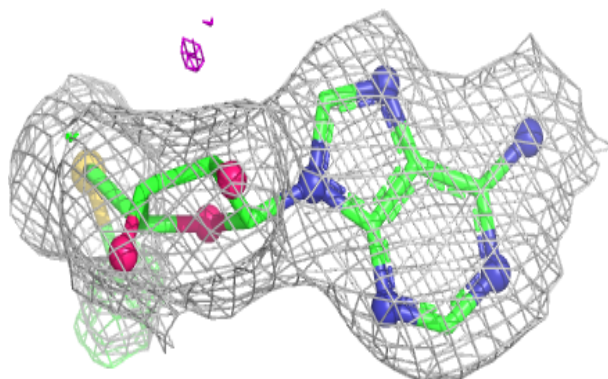
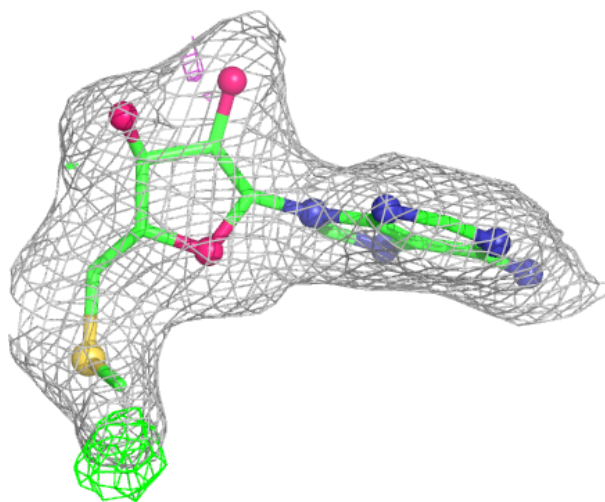
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO3	B	303	4/4	0.90	0.12	41,43,50,51	0
4	SO3	A	306	4/4	0.94	0.10	37,42,44,45	0
3	ZN	A	305	1/1	0.95	0.08	72,72,72,72	0
3	ZN	A	304	1/1	0.97	0.04	67,67,67,67	0
3	ZN	A	302	1/1	0.99	0.04	53,53,53,53	0
3	ZN	A	303	1/1	0.99	0.03	67,67,67,67	0
3	ZN	B	302	1/1	0.99	0.02	48,48,48,48	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.

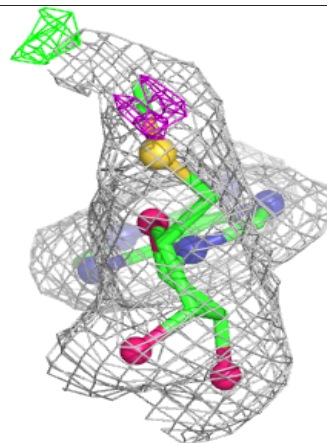
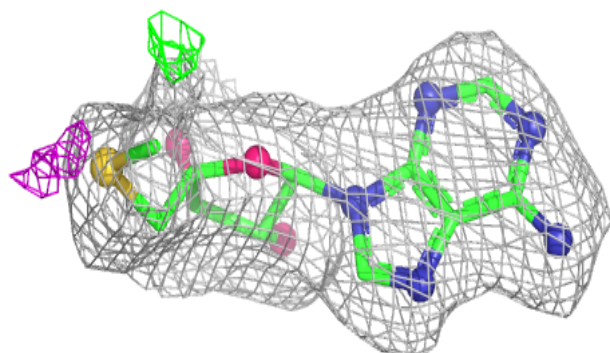
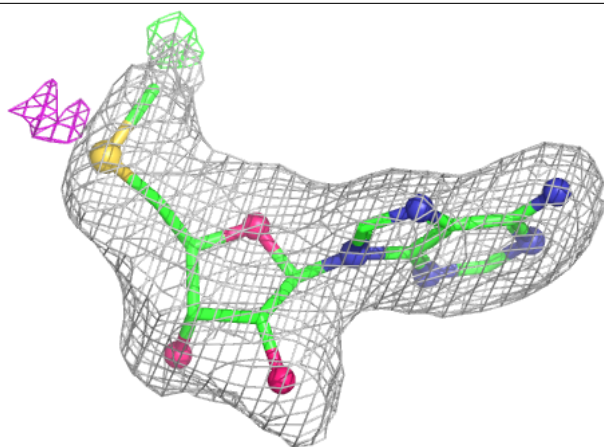
Electron density around MTA A 301:

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.