



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:04 AM UTC

PDB ID : 1MVT / pdb_00001mvt
Title : Analysis of Two Polymorphic Forms of a Pyrido[2,3-d]pyrimidine N9-C10
Reverse-Bridge Antifolate Binary Complex with Human Dihydrofolate Reduc-
tase
Authors : Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.A.; Gangjee, A.
Deposited on : 2002-09-26
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

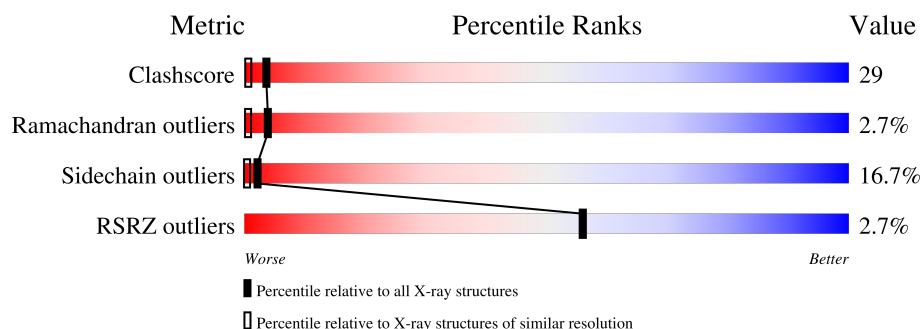
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	187	

2 Entry composition [i](#)

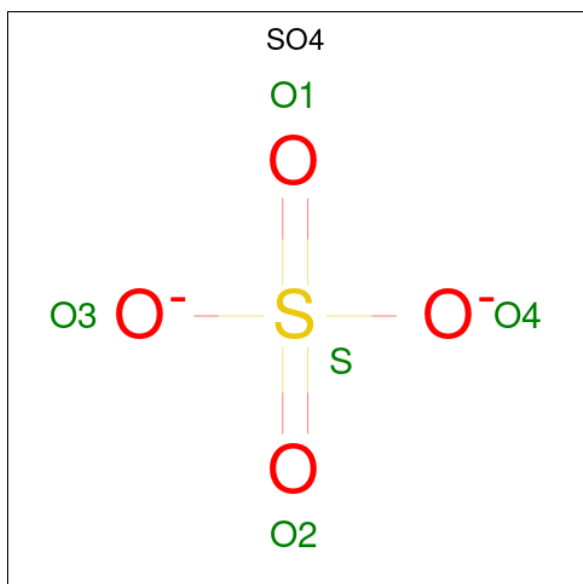
There are 4 unique types of molecules in this entry. The entry contains 1582 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dihydrofolate Reductase.

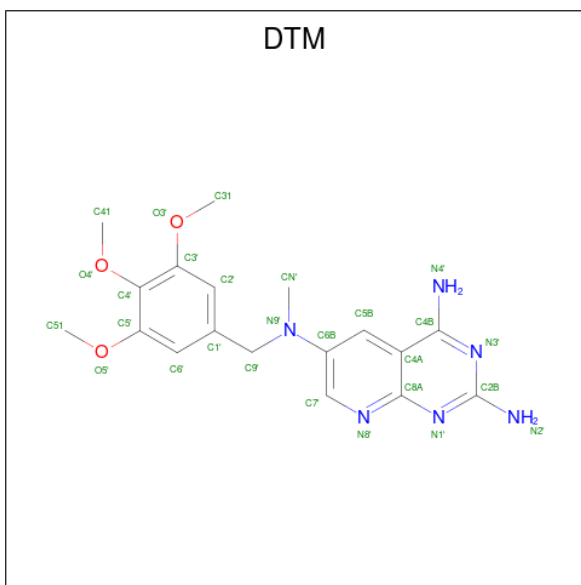
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 2,4-DIAMINO-6-[N-(3',4',5'-TRIMETHOXYBENZYL)-N-METHYLAMINO]PYRIDO[2,3-D]PYRIMIDINE (CCD ID: DTM) (formula: C₁₈H₂₂N₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	18	6	3		

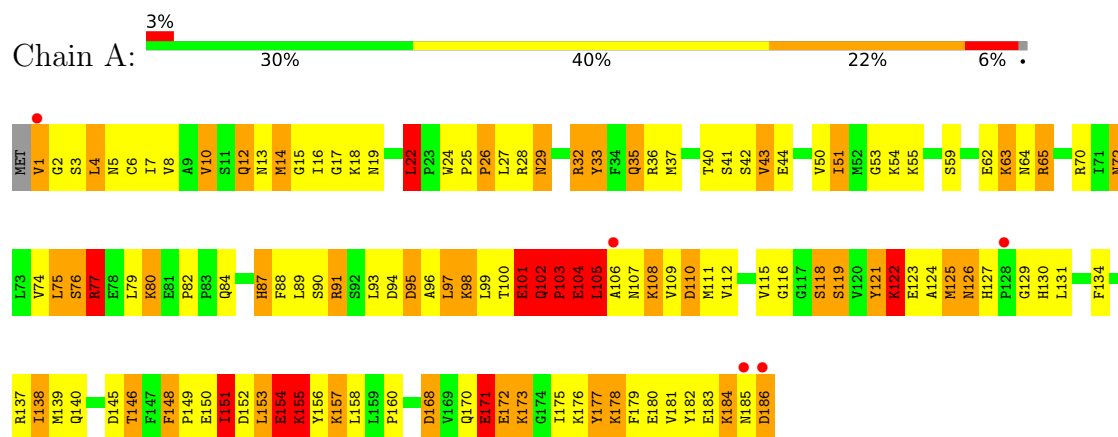
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		

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: Dihydrofolate Reductase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	106.78Å 106.78Å 43.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.80 8.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.3 (8.00-1.80) 86.0 (8.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 1.80Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.194 , (Not available) 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.46 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1582	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, DTM

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	1.40	1/1537 (0.1%)	2.94	175/2073 (8.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLY	N-CA	6.30	1.52	1.45

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	ASN	CA-CB-CG	27.51	140.11	112.60
1	A	51	ILE	CA-C-O	-14.14	105.49	120.48
1	A	126	ASN	CA-CB-CG	14.06	126.66	112.60
1	A	64	ASN	CA-CB-CG	12.11	124.71	112.60
1	A	87	HIS	CA-CB-CG	-11.99	101.81	113.80
1	A	148	PHE	CA-CB-CG	11.76	125.56	113.80
1	A	28	ARG	CD-NE-CZ	11.62	140.66	124.40
1	A	110	ASP	CA-CB-CG	11.35	123.95	112.60
1	A	51	ILE	O-C-N	10.83	134.55	123.18
1	A	107	ASN	OD1-CG-ND2	-10.42	112.18	122.60
1	A	62	GLU	CB-CG-CD	10.04	129.67	112.60
1	A	127	HIS	CA-CB-CG	10.01	123.81	113.80
1	A	36	ARG	NE-CZ-NH2	-9.54	110.61	119.20
1	A	154	GLU	CA-C-N	9.34	139.38	121.54
1	A	154	GLU	C-N-CA	9.34	139.38	121.54
1	A	118	SER	O-C-N	9.17	131.84	122.12
1	A	82	PRO	CB-CA-C	9.14	122.07	110.92
1	A	42	SER	CA-C-N	8.90	134.58	123.10
1	A	42	SER	C-N-CA	8.90	134.58	123.10
1	A	84	GLN	CB-CA-C	8.83	123.08	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	72	ASN	CA-CB-CG	8.65	121.25	112.60
1	A	121	TYR	CA-C-O	-8.37	111.67	120.55
1	A	118	SER	CA-CB-OG	-8.32	94.47	111.10
1	A	65	ARG	NE-CZ-NH1	-8.31	113.19	121.50
1	A	151	ILE	O-C-N	8.16	133.75	122.97
1	A	74	VAL	CA-C-N	8.08	133.52	122.77
1	A	74	VAL	C-N-CA	8.08	133.52	122.77
1	A	122	LYS	N-CA-CB	8.02	121.69	110.07
1	A	138	ILE	CB-CG1-CD1	7.97	130.53	113.80
1	A	152	ASP	CA-CB-CG	-7.94	104.66	112.60
1	A	6	CYS	N-CA-CB	7.78	123.21	110.69
1	A	94	ASP	CA-CB-CG	-7.73	104.87	112.60
1	A	122	LYS	CA-CB-CG	7.67	129.44	114.10
1	A	8	VAL	N-CA-C	7.62	118.41	108.35
1	A	134	PHE	O-C-N	7.58	131.87	123.22
1	A	33	TYR	CB-CG-CD2	-7.56	109.45	120.80
1	A	172	GLU	CB-CG-CD	7.53	125.41	112.60
1	A	19	ASN	CB-CG-ND2	7.45	127.58	116.40
1	A	40	THR	CA-C-O	7.41	129.22	120.70
1	A	168	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	36	ARG	NH1-CZ-NH2	7.32	128.82	119.30
1	A	95	ASP	O-C-N	7.27	130.44	122.15
1	A	13	ASN	N-CA-CB	7.18	120.47	110.56
1	A	134	PHE	CA-C-O	-7.16	112.70	120.36
1	A	155	LYS	CA-C-O	7.06	130.60	120.51
1	A	7	ILE	CA-C-O	6.97	127.75	120.36
1	A	91	ARG	CD-NE-CZ	6.95	134.13	124.40
1	A	84	GLN	CA-CB-CG	6.92	127.93	114.10
1	A	140	GLN	O-C-N	6.90	130.87	123.56
1	A	22	LEU	CA-C-O	-6.84	113.60	120.64
1	A	151	ILE	N-CA-CB	6.80	119.16	111.21
1	A	108	LYS	CA-CB-CG	6.80	127.69	114.10
1	A	28	ARG	CA-C-O	-6.74	113.41	120.55
1	A	33	TYR	CB-CG-CD1	6.73	130.90	120.80
1	A	77	ARG	CA-CB-CG	6.72	127.53	114.10
1	A	121	TYR	O-C-N	6.71	129.23	122.12
1	A	50	VAL	O-C-N	6.68	130.20	123.18
1	A	13	ASN	CA-C-O	-6.68	111.37	119.59
1	A	65	ARG	CA-CB-CG	6.67	127.44	114.10
1	A	33	TYR	N-CA-C	-6.67	103.49	111.69
1	A	168	ASP	O-C-N	6.66	130.39	122.94
1	A	91	ARG	NE-CZ-NH1	6.65	128.15	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	PHE	N-CA-C	-6.61	97.96	108.73
1	A	115	VAL	CB-CA-C	6.59	120.91	111.88
1	A	65	ARG	NH1-CZ-NH2	6.56	127.82	119.30
1	A	12	GLN	O-C-N	6.55	129.06	122.12
1	A	172	GLU	CG-CD-OE2	-6.54	103.36	118.40
1	A	90	SER	CA-C-O	-6.53	113.49	121.06
1	A	13	ASN	OD1-CG-ND2	-6.51	116.08	122.60
1	A	89	LEU	CA-C-O	-6.41	113.29	120.66
1	A	44	GLU	CB-CA-C	6.40	120.09	109.53
1	A	153	LEU	CB-CA-C	6.34	122.68	109.68
1	A	79	LEU	CA-C-N	6.30	132.82	121.92
1	A	79	LEU	C-N-CA	6.30	132.82	121.92
1	A	19	ASN	OD1-CG-ND2	-6.30	116.30	122.60
1	A	76	SER	O-C-N	6.30	130.45	123.52
1	A	107	ASN	CB-CG-OD1	6.27	133.34	120.80
1	A	118	SER	CB-CA-C	-6.22	100.11	110.68
1	A	28	ARG	CA-C-N	6.20	131.07	120.72
1	A	28	ARG	C-N-CA	6.20	131.07	120.72
1	A	104	GLU	CG-CD-OE2	-6.19	104.15	118.40
1	A	157	LYS	CA-C-O	-6.16	113.72	120.43
1	A	59	SER	CA-C-O	6.13	126.96	119.11
1	A	151	ILE	CB-CG1-CD1	-6.13	100.92	113.80
1	A	13	ASN	CB-CG-ND2	6.12	125.58	116.40
1	A	26	PRO	CA-C-O	-6.11	114.69	121.23
1	A	37	MET	CG-SD-CE	-6.11	87.46	100.90
1	A	146	THR	CA-CB-OG1	-6.09	100.46	109.60
1	A	29	ASN	N-CA-CB	6.02	120.39	110.39
1	A	29	ASN	CA-C-O	-5.99	112.01	119.38
1	A	171	GLU	CB-CG-CD	5.98	122.77	112.60
1	A	116	GLY	CA-C-N	5.96	132.43	121.70
1	A	116	GLY	C-N-CA	5.96	132.43	121.70
1	A	123	GLU	CB-CG-CD	5.96	122.73	112.60
1	A	175	ILE	CA-C-O	-5.93	114.19	120.48
1	A	146	THR	CA-CB-CG2	-5.92	100.44	110.50
1	A	22	LEU	O-C-N	5.90	129.14	121.64
1	A	74	VAL	O-C-N	-5.90	116.48	123.03
1	A	77	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	A	43	VAL	O-C-N	5.86	129.12	123.14
1	A	63	LYS	CA-CB-CG	5.86	125.81	114.10
1	A	178	LYS	CA-C-N	5.84	130.43	122.19
1	A	178	LYS	C-N-CA	5.84	130.43	122.19
1	A	13	ASN	CA-C-N	5.82	130.84	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASN	C-N-CA	5.82	130.84	122.40
1	A	7	ILE	O-C-N	-5.79	116.95	123.20
1	A	172	GLU	CG-CD-OE1	5.78	131.70	118.40
1	A	90	SER	O-C-N	5.78	129.97	123.27
1	A	32	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	A	160	PRO	CA-C-N	5.70	132.05	121.62
1	A	160	PRO	C-N-CA	5.70	132.05	121.62
1	A	177	TYR	CA-C-O	-5.68	115.19	121.33
1	A	18	LYS	CA-C-N	5.67	130.18	122.07
1	A	18	LYS	C-N-CA	5.67	130.18	122.07
1	A	97	LEU	CB-CA-C	5.67	119.89	110.81
1	A	36	ARG	N-CA-CB	-5.65	101.81	110.12
1	A	32	ARG	CA-CB-CG	5.64	125.38	114.10
1	A	182	TYR	CA-C-O	-5.60	114.55	121.11
1	A	140	GLN	CA-C-O	-5.59	114.48	120.75
1	A	137	ARG	CA-C-O	-5.59	115.11	120.92
1	A	29	ASN	OD1-CG-ND2	-5.58	117.02	122.60
1	A	157	LYS	CB-CA-C	-5.58	100.55	109.75
1	A	12	GLN	OE1-CD-NE2	5.57	128.17	122.60
1	A	76	SER	CA-C-O	-5.57	114.02	120.31
1	A	97	LEU	CA-C-N	5.53	127.95	120.38
1	A	97	LEU	C-N-CA	5.53	127.95	120.38
1	A	179	PHE	O-C-N	-5.53	116.92	123.22
1	A	33	TYR	OH-CZ-CE2	-5.52	103.34	119.90
1	A	112	VAL	O-C-N	5.51	128.96	123.18
1	A	98	LYS	CB-CA-C	-5.49	101.34	110.68
1	A	140	GLN	N-CA-CB	5.47	119.94	111.24
1	A	172	GLU	CA-C-N	-5.47	115.10	123.47
1	A	172	GLU	C-N-CA	-5.47	115.10	123.47
1	A	26	PRO	O-C-N	5.44	129.26	123.01
1	A	29	ASN	CA-CB-CG	-5.43	107.17	112.60
1	A	175	ILE	N-CA-C	-5.42	100.58	108.17
1	A	103	PRO	CA-C-N	-5.40	115.00	122.30
1	A	103	PRO	C-N-CA	-5.40	115.00	122.30
1	A	15	GLY	O-C-N	5.39	128.75	123.35
1	A	72	ASN	CB-CG-ND2	5.38	124.47	116.40
1	A	95	ASP	CA-C-O	-5.37	114.73	120.42
1	A	155	LYS	O-C-N	-5.36	115.46	122.59
1	A	98	LYS	CG-CD-CE	5.35	123.60	111.30
1	A	105	LEU	CA-C-O	-5.35	112.86	120.51
1	A	3	SER	O-C-N	5.30	129.19	123.10
1	A	5	ASN	CA-CB-CG	5.29	117.89	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	GLN	CG-CD-NE2	-5.28	108.48	116.40
1	A	10	VAL	N-CA-CB	-5.28	102.78	111.44
1	A	3	SER	CA-C-O	-5.27	115.81	121.45
1	A	98	LYS	CB-CG-CD	5.27	123.42	111.30
1	A	109	VAL	CA-C-O	5.24	126.92	120.84
1	A	53	GLY	N-CA-C	-5.23	104.43	112.85
1	A	150	GLU	O-C-N	5.23	129.51	122.82
1	A	138	ILE	CA-CB-CG1	-5.21	101.54	110.40
1	A	126	ASN	N-CA-CB	-5.20	99.99	111.69
1	A	127	HIS	CA-C-O	5.19	124.84	119.86
1	A	104	GLU	N-CA-CB	5.19	118.89	110.17
1	A	14	MET	CA-CB-CG	5.17	124.44	114.10
1	A	145	ASP	CB-CA-C	5.16	118.63	109.75
1	A	112	VAL	CA-C-O	-5.14	115.03	120.48
1	A	140	GLN	CG-CD-OE1	5.14	131.08	120.80
1	A	118	SER	CA-C-O	-5.13	115.09	120.63
1	A	180	GLU	CG-CD-OE1	5.13	130.19	118.40
1	A	43	VAL	CA-CB-CG1	5.12	119.11	110.40
1	A	177	TYR	O-C-N	5.12	129.09	123.25
1	A	111	MET	CA-C-N	-5.11	116.86	123.19
1	A	111	MET	C-N-CA	-5.11	116.86	123.19
1	A	75	LEU	O-C-N	-5.10	117.41	123.22
1	A	184	LYS	CG-CD-CE	5.08	122.99	111.30
1	A	124	ALA	N-CA-C	5.08	116.89	111.36
1	A	156	TYR	CA-C-O	-5.06	114.90	120.36
1	A	55	LYS	N-CA-CB	-5.05	102.45	110.28
1	A	125	MET	CA-C-O	5.03	125.44	119.10
1	A	16	ILE	CB-CA-C	5.03	119.54	111.29
1	A	80	LYS	CG-CD-CE	5.03	122.87	111.30

There are no chirality outliers.

There are no planarity outliers.

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	1502	0	1511	88	0
2	A	10	0	0	1	0
3	A	27	0	22	3	0
4	A	43	0	0	2	0
All	All	1582	0	1533	90	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (90) 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:4:LEU:HD12	1:A:131:LEU:HD12	1.40	1.04
1:A:80:LYS:HE2	4:A:223:HOH:O	1.63	0.96
1:A:29:ASN:HD21	1:A:32:ARG:HH11	1.13	0.96
1:A:29:ASN:ND2	1:A:32:ARG:HH11	1.64	0.96
1:A:72:ASN:H	1:A:87:HIS:HD2	1.08	0.95
1:A:101:GLU:HA	1:A:106:ALA:HB2	1.50	0.92
1:A:104:GLU:HB2	1:A:108:LYS:NZ	1.86	0.90
1:A:35:GLN:NE2	1:A:70:ARG:HH12	1.71	0.88
1:A:97:LEU:O	1:A:100:THR:HB	1.73	0.87
1:A:100:THR:HG22	1:A:100:THR:O	1.74	0.85
1:A:72:ASN:H	1:A:87:HIS:CD2	1.96	0.83
3:A:187:DTM:H412	3:A:187:DTM:O3'	1.79	0.83
1:A:100:THR:O	1:A:101:GLU:HG2	1.79	0.83
1:A:104:GLU:O	1:A:105:LEU:HG	1.77	0.83
1:A:41:SER:OG	1:A:110:ASP:OD1	1.99	0.79
1:A:29:ASN:HD21	1:A:32:ARG:NH1	1.81	0.79
1:A:168:ASP:O	1:A:170:GLN:NE2	2.19	0.75
1:A:35:GLN:HE21	1:A:35:GLN:HA	1.52	0.73
1:A:184:LYS:NZ	1:A:186:ASP:OD2	2.14	0.73
1:A:4:LEU:HD12	1:A:131:LEU:CD1	2.16	0.73
1:A:139:MET:HE2	1:A:176:LYS:CB	2.19	0.72
1:A:35:GLN:HE22	1:A:70:ARG:HH12	1.37	0.72
1:A:104:GLU:HB2	1:A:108:LYS:HZ2	1.54	0.71
1:A:4:LEU:CD1	1:A:131:LEU:HD12	2.19	0.70
1:A:29:ASN:ND2	1:A:32:ARG:HE	1.92	0.68
1:A:139:MET:HE2	1:A:176:LYS:HB3	1.75	0.67
1:A:77:ARG:CG	1:A:77:ARG:HH11	2.07	0.67
1:A:122:LYS:HD3	1:A:149:PRO:HG3	1.77	0.67
1:A:130:HIS:HE1	1:A:183:GLU:OE1	1.78	0.66
1:A:130:HIS:CE1	1:A:183:GLU:HG3	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:THR:O	1:A:100:THR:CG2	2.42	0.65
1:A:146:THR:HG21	4:A:201:HOH:O	1.96	0.65
1:A:172:GLU:O	1:A:173:LYS:HB2	1.96	0.64
1:A:29:ASN:ND2	1:A:32:ARG:NH1	2.40	0.64
1:A:51:ILE:CG2	1:A:75:LEU:HD22	2.28	0.64
1:A:1:VAL:HG12	1:A:2:GLY:H	1.64	0.63
1:A:99:LEU:HG	1:A:105:LEU:HD12	1.82	0.62
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.81	0.62
3:A:187:DTM:O3'	3:A:187:DTM:C41	2.47	0.62
1:A:130:HIS:HE1	1:A:183:GLU:CD	2.08	0.61
1:A:76:SER:OG	2:A:189:SO4:O1	2.16	0.61
1:A:104:GLU:O	1:A:105:LEU:CB	2.50	0.59
1:A:27:LEU:HD22	1:A:172:GLU:HB3	1.84	0.59
1:A:104:GLU:O	1:A:105:LEU:CG	2.51	0.58
1:A:100:THR:C	1:A:101:GLU:HG2	2.27	0.58
1:A:171:GLU:HG2	1:A:176:LYS:HG2	1.85	0.57
1:A:121:TYR:O	1:A:125:MET:HB2	2.05	0.56
1:A:104:GLU:O	1:A:104:GLU:HG2	2.04	0.56
1:A:139:MET:HE2	1:A:176:LYS:HB2	1.85	0.56
1:A:10:VAL:HG22	1:A:14:MET:HA	1.88	0.55
1:A:72:ASN:N	1:A:87:HIS:HD2	1.91	0.55
1:A:26:PRO:O	1:A:173:LYS:CE	2.57	0.53
1:A:91:ARG:O	1:A:91:ARG:HG3	2.08	0.53
1:A:104:GLU:HB2	1:A:108:LYS:HZ1	1.72	0.53
1:A:22:LEU:HD11	3:A:187:DTM:HC92	1.91	0.52
1:A:125:MET:HE1	1:A:149:PRO:HG2	1.92	0.52
1:A:102:GLN:CB	1:A:103:PRO:CD	2.88	0.52
1:A:183:GLU:HG2	1:A:184:LYS:N	2.25	0.52
1:A:95:ASP:HA	1:A:98:LYS:HE2	1.93	0.50
1:A:171:GLU:OE2	1:A:176:LYS:HE3	2.11	0.50
1:A:1:VAL:O	1:A:110:ASP:O	2.29	0.50
1:A:171:GLU:OE2	1:A:176:LYS:NZ	2.44	0.50
1:A:104:GLU:HB2	1:A:108:LYS:CE	2.42	0.49
1:A:26:PRO:O	1:A:173:LYS:HE2	2.13	0.49
1:A:104:GLU:O	1:A:105:LEU:HB2	2.12	0.49
1:A:121:TYR:O	1:A:125:MET:HE3	2.13	0.48
1:A:171:GLU:CG	1:A:176:LYS:HG2	2.44	0.47
1:A:153:LEU:O	1:A:154:GLU:C	2.57	0.47
1:A:148:PHE:HE2	1:A:151:ILE:HD11	1.79	0.47
1:A:77:ARG:HH11	1:A:77:ARG:HG3	1.78	0.46
1:A:77:ARG:CG	1:A:77:ARG:NH1	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD12	1:A:181:VAL:O	2.16	0.46
1:A:186:ASP:OD1	1:A:186:ASP:N	2.49	0.46
1:A:130:HIS:CE1	1:A:183:GLU:CG	2.99	0.45
1:A:130:HIS:HA	1:A:184:LYS:O	2.17	0.45
1:A:96:ALA:O	1:A:99:LEU:HB3	2.17	0.45
1:A:51:ILE:HG22	1:A:75:LEU:HD22	1.97	0.44
1:A:171:GLU:OE2	1:A:176:LYS:CE	2.66	0.43
1:A:29:ASN:ND2	1:A:32:ARG:NE	2.63	0.43
1:A:119:SER:HA	1:A:122:LYS:HG2	2.00	0.43
1:A:172:GLU:OE1	1:A:177:TYR:OH	2.25	0.43
1:A:129:GLY:O	1:A:185:ASN:HA	2.18	0.43
1:A:1:VAL:HG12	1:A:2:GLY:N	2.33	0.42
1:A:65:ARG:HH11	1:A:65:ARG:HD2	1.39	0.42
1:A:24:TRP:HB2	1:A:25:PRO:CD	2.49	0.41
1:A:130:HIS:CE1	1:A:183:GLU:CD	2.95	0.41
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.93	0.41
1:A:4:LEU:HD22	1:A:4:LEU:HA	1.92	0.41
1:A:87:HIS:HB3	1:A:88:PHE:CE1	2.56	0.41
1:A:99:LEU:HG	1:A:105:LEU:CD1	2.49	0.41

There are no symmetry-related clashes.

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	184/187 (98%)	174 (95%)	5 (3%)	5 (3%)	4 0

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
1	A	101	GLU

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Mol	Chain	Res	Type
1	A	105	LEU
1	A	103	PRO
1	A	102	GLN

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	168/169 (99%)	140 (83%)	28 (17%)	2 0

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	4	LEU
1	A	12	GLN
1	A	22	LEU
1	A	33	TYR
1	A	35	GLN
1	A	43	VAL
1	A	54	LYS
1	A	63	LYS
1	A	77	ARG
1	A	93	LEU
1	A	101	GLU
1	A	102	GLN
1	A	103	PRO
1	A	104	GLU
1	A	118	SER
1	A	119	SER
1	A	122	LYS
1	A	126	ASN
1	A	138	ILE
1	A	151	ILE
1	A	154	GLU
1	A	155	LYS

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Mol	Chain	Res	Type
1	A	157	LYS
1	A	171	GLU
1	A	173	LYS
1	A	178	LYS
1	A	186	ASP

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	29	ASN
1	A	35	GLN
1	A	87	HIS
1	A	130	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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	SO4	A	188	-	4,4,4	0.94	0	6,6,6	0.82	0
3	DTM	A	187	-	29,29,29	1.94	6 (20%)	39,41,41	2.52	17 (43%)
2	SO4	A	189	-	4,4,4	0.66	0	6,6,6	1.21	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTM	A	187	-	-	1/14/14/14	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	187	DTM	C4B-C4A	-7.04	1.38	1.45
3	A	187	DTM	C9'-N9'	2.96	1.52	1.46
3	A	187	DTM	C7'-C6B	2.83	1.43	1.38
3	A	187	DTM	C7'-N8'	2.62	1.36	1.31
3	A	187	DTM	C8A-N8'	-2.49	1.33	1.37
3	A	187	DTM	C2'-C1'	2.14	1.42	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	187	DTM	N1'-C2B-N3'	-5.72	119.94	127.21
3	A	187	DTM	C2B-N1'-C8A	4.99	120.87	115.48
3	A	187	DTM	C7'-N8'-C8A	4.54	123.52	117.20
3	A	187	DTM	C4A-C4B-N4'	4.09	127.72	121.45
3	A	187	DTM	C1'-C9'-N9'	-4.07	107.90	113.53
3	A	187	DTM	C6B-C7'-N8'	-3.99	117.77	124.16
3	A	187	DTM	C51-O5'-C5'	-3.46	112.43	117.51
3	A	187	DTM	O3'-C3'-C4'	-3.26	109.54	115.14
3	A	187	DTM	O5'-C5'-C4'	3.23	120.68	115.14
3	A	187	DTM	C9'-C1'-C6'	-3.12	114.40	120.27
3	A	187	DTM	O5'-C5'-C6'	-3.05	118.83	124.08
3	A	187	DTM	O3'-C3'-C2'	2.87	129.02	124.08
3	A	187	DTM	CN'-N9'-C6B	2.70	124.07	119.59
3	A	187	DTM	C31-O3'-C3'	-2.55	113.78	117.51
3	A	187	DTM	C9'-C1'-C2'	2.47	124.93	120.27
2	A	189	SO4	O4-S-O3	-2.33	95.66	108.54
3	A	187	DTM	O4'-C4'-C3'	-2.28	116.86	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	187	DTM	N8'-C8A-N1'	2.12	118.08	115.77

There are no chirality outliers.

All (1) torsion outliers are listed below:

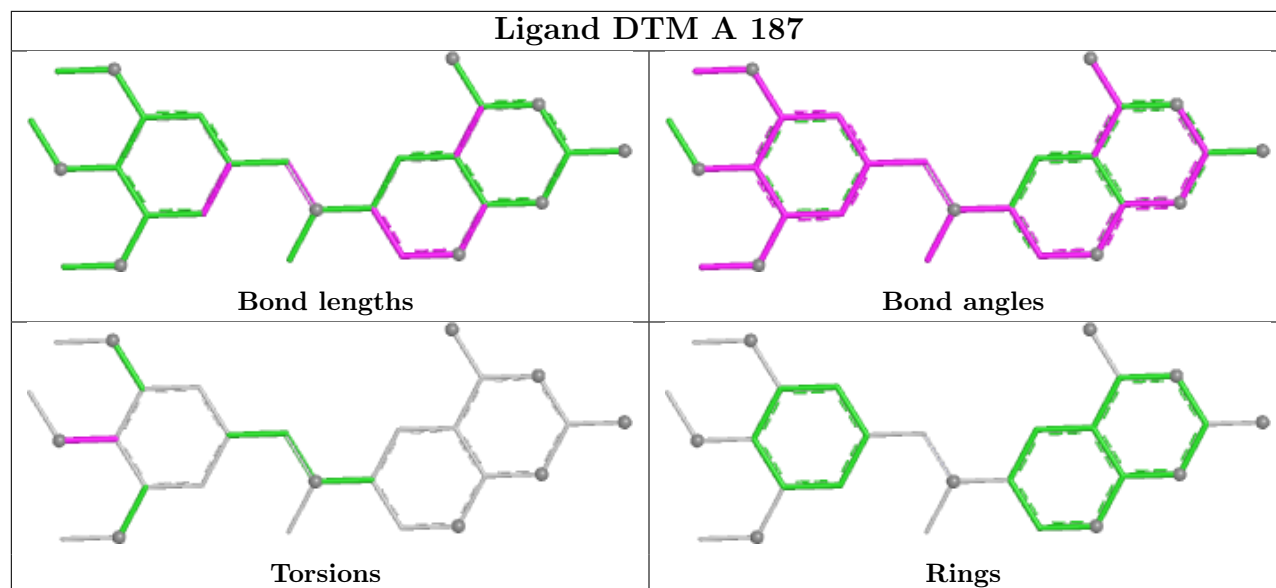
Mol	Chain	Res	Type	Atoms
3	A	187	DTM	C3'-C4'-O4'-C41

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	187	DTM	3	0
2	A	189	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	186/187 (99%)	-0.20	5 (2%) 56 56	7, 19, 45, 53	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	3.5
1	A	186	ASP	2.6
1	A	185	ASN	2.3
1	A	128	PRO	2.2
1	A	106	ALA	2.2

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](#)

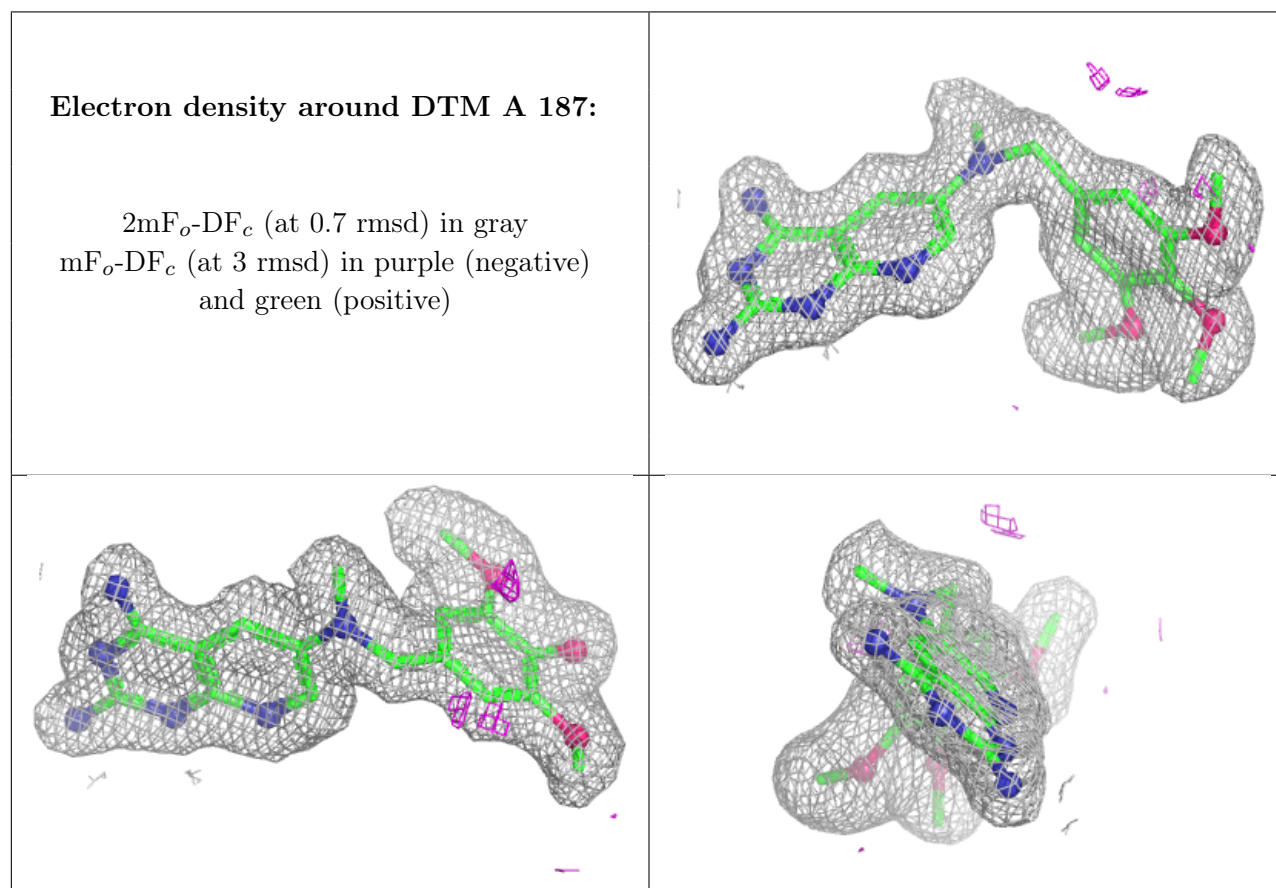
There are no oligosaccharides in this entry.

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
3	DTM	A	187	27/27	0.94	0.05	4,16,21,22	0
2	SO4	A	189	5/5	0.95	0.09	36,37,38,39	0
2	SO4	A	188	5/5	0.99	0.06	21,22,23,24	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.