



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 01:34 AM GMT

PDB ID : 1MVT  
Title : Analysis of Two Polymorphic Forms of a Pyrido[2,3-d]pyrimidineN9-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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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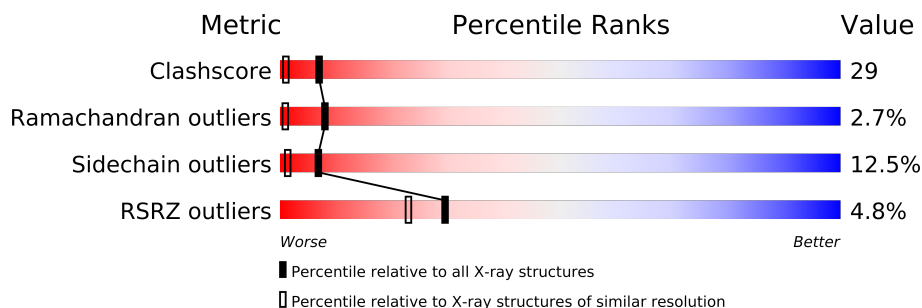
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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	79885	4461 (1.80-1.80)
Ramachandran outliers	78287	4404 (1.80-1.80)
Sidechain outliers	78261	4403 (1.80-1.80)
RSRZ outliers	66119	3515 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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.

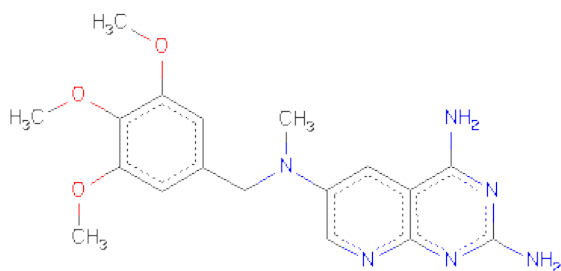
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: DTM) (formula: C<sub>18</sub>H<sub>22</sub>N<sub>6</sub>O<sub>3</sub>).



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

- Molecule 4 is water.

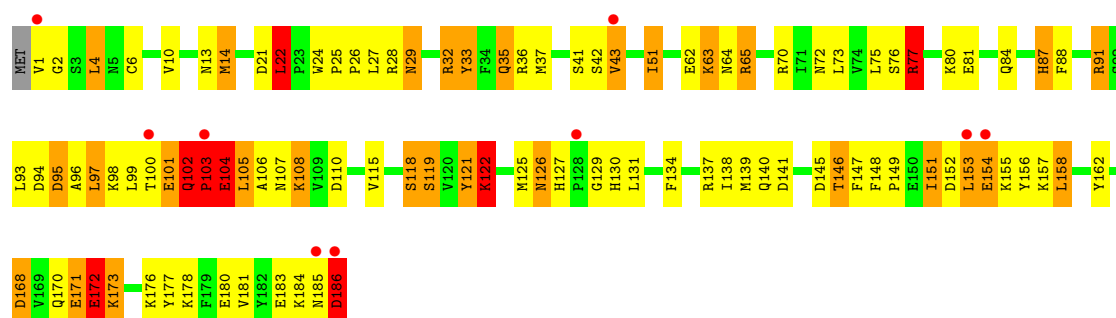
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.78Å 106.78Å 43.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.80 30.82 – 1.80	Depositor EDS
% Data completeness (in resolution range)	85.3 (8.00-1.80) 87.1 (30.82-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.44 (at 1.80Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.194 , (Not available) 0.210 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	22.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 40.3	EDS
Estimated twinning fraction	0.026 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 15377 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	1582	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	1.12	0/1537	2.47	81/2073 (3.9%)

There are no bond length outliers.

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	NE-CZ-NH2	-19.38	110.61	120.30
1	A	33	TYR	CB-CG-CD2	-19.24	109.45	121.00
1	A	33	TYR	CB-CG-CD1	16.49	130.90	121.00
1	A	91	ARG	NE-CZ-NH1	15.70	128.15	120.30
1	A	65	ARG	NE-CZ-NH1	-14.23	113.19	120.30
1	A	28	ARG	CD-NE-CZ	12.19	140.66	123.60
1	A	107	ASN	CA-CB-CG	12.14	140.11	113.40
1	A	21	ASP	CB-CG-OD1	11.12	128.31	118.30
1	A	145	ASP	CB-CG-OD2	9.94	127.25	118.30
1	A	77	ARG	NE-CZ-NH1	-9.36	115.62	120.30
1	A	104	GLU	OE1-CD-OE2	9.24	134.39	123.30
1	A	32	ARG	NE-CZ-NH1	-9.06	115.77	120.30
1	A	162	TYR	CB-CG-CD1	-8.61	115.84	121.00
1	A	36	ARG	NH1-CZ-NH2	8.56	128.82	119.40
1	A	146	THR	CA-CB-CG2	-8.54	100.44	112.40
1	A	147	PHE	CB-CG-CD1	8.26	126.58	120.80
1	A	91	ARG	NE-CZ-NH2	-8.23	116.19	120.30
1	A	37	MET	CG-SD-CE	-7.96	87.46	100.20
1	A	65	ARG	NH1-CZ-NH2	7.66	127.82	119.40
1	A	91	ARG	CD-NE-CZ	7.53	134.13	123.60
1	A	172	GLU	CG-CD-OE2	-7.47	103.36	118.30
1	A	51	ILE	O-C-N	7.41	134.55	122.70
1	A	122	LYS	CA-CB-CG	7.29	129.44	113.40
1	A	94	ASP	CB-CG-OD2	-7.28	111.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	A	104	GLU	CG-CD-OE2	-7.07	104.15	118.30
1	A	154	GLU	C-N-CA	7.07	139.38	121.70
1	A	6	CYS	N-CA-CB	7.00	123.21	110.60
1	A	121	TYR	CB-CG-CD1	-6.99	116.81	121.00
1	A	51	ILE	CA-C-O	-6.96	105.49	120.10
1	A	87	HIS	CA-CB-CG	-6.94	101.81	113.60
1	A	151	ILE	O-C-N	6.90	133.75	122.70
1	A	162	TYR	CB-CG-CD2	6.71	125.03	121.00
1	A	172	GLU	CG-CD-OE1	6.70	131.70	118.30
1	A	84	GLN	CA-CB-CG	6.61	127.93	113.40
1	A	153	LEU	CB-CA-C	6.57	122.68	110.20
1	A	14	MET	CA-CB-CG	6.56	124.44	113.30
1	A	108	LYS	CA-CB-CG	6.50	127.69	113.40
1	A	168	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	77	ARG	CA-CB-CG	6.42	127.53	113.40
1	A	28	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	A	65	ARG	CA-CB-CG	6.38	127.44	113.40
1	A	95	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	A	84	GLN	CB-CA-C	6.34	123.08	110.40
1	A	33	TYR	OH-CZ-CE2	-6.21	103.34	120.10
1	A	118	SER	CA-CB-OG	-6.20	94.47	111.20
1	A	122	LYS	N-CA-CB	6.16	121.69	110.60
1	A	147	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	A	126	ASN	CA-CB-CG	6.03	126.66	113.40
1	A	127	HIS	CA-CB-CG	6.01	123.81	113.60
1	A	137	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	A	180	GLU	CG-CD-OE1	5.95	130.19	118.30
1	A	138	ILE	CB-CG1-CD1	5.94	130.53	113.90
1	A	126	ASN	N-CA-CB	-5.89	99.99	110.60
1	A	107	ASN	CB-CG-OD1	5.87	133.34	121.60
1	A	81	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	62	GLU	CB-CG-CD	5.73	129.67	114.20
1	A	134	PHE	O-C-N	5.73	131.87	122.70
1	A	118	SER	O-C-N	5.71	131.84	122.70
1	A	63	LYS	CA-CB-CG	5.64	125.81	113.40
1	A	126	ASN	CB-CA-C	5.58	121.55	110.40
1	A	13	ASN	N-CA-CB	5.48	120.47	110.60
1	A	152	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	A	43	VAL	CA-CB-CG1	5.47	119.11	110.90
1	A	32	ARG	CA-CB-CG	5.45	125.38	113.40
1	A	29	ASN	N-CA-CB	5.44	120.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	180	GLU	CG-CD-OE2	-5.42	107.47	118.30
1	A	154	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	A	118	SER	CB-CA-C	-5.26	100.11	110.10
1	A	73	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	A	140	GLN	N-CA-CB	5.19	119.94	110.60
1	A	156	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	A	42	SER	C-N-CA	5.15	134.58	121.70
1	A	64	ASN	CA-CB-CG	5.14	124.71	113.40
1	A	140	GLN	O-C-N	5.11	130.87	122.70
1	A	22	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	A	97	LEU	CB-CA-C	5.10	119.89	110.20
1	A	158	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	A	28	ARG	CG-CD-NE	5.07	122.45	111.80
1	A	115	VAL	CB-CA-C	5.00	120.91	111.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1502	0	1511	86	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	88	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

All (88) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:LEU:HD12	1:A:131:LEU:HD12	1.40	1.04

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	0.86
1:A:72:ASN:H	1:A:87:HIS:CD2	1.96	0.83
3:A:187:DTM:O3'	3:A:187:DTM:H412	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:184:LYS:NZ	1:A:186:ASP:OD2	2.14	0.77
1:A:168:ASP:O	1:A:170:GLN:NE2	2.19	0.75
1:A:35:GLN:HA	1:A:35:GLN:HE21	1.52	0.73
1:A:4:LEU:HD12	1:A:131:LEU:CD1	2.16	0.73
1:A:35:GLN:HE22	1:A:70:ARG:HH12	1.37	0.72
1:A:4:LEU:CD1	1:A:131:LEU:HD12	2.19	0.70
1:A:104:GLU:HB2	1:A:108:LYS:HZ2	1.57	0.69
1:A:139:MET:HE2	1:A:176:LYS:CB	2.23	0.68
1:A:29:ASN:ND2	1:A:32:ARG:HE	1.92	0.68
1:A:77:ARG:HH11	1:A:77:ARG:CG	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
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:139:MET:HE2	1:A:176:LYS:HB2	1.80	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:C41	3:A:187:DTM:O3'	2.47	0.62
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:130:HIS:HE1	1:A:183:GLU:CD	2.08	0.56
1:A:104:GLU:HG2	1:A:104:GLU:O	2.04	0.56
1:A:139:MET:HE2	1:A:176:LYS:HB3	1.87	0.56
1:A:104:GLU:HB2	1:A:108:LYS:HZ1	1.69	0.55
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:91:ARG:HG3	1:A:91:ARG:O	2.08	0.54
1:A:26:PRO:O	1:A:173:LYS:CE	2.57	0.53
1:A:100:THR:C	1:A:101:GLU:HG2	2.27	0.53
1:A:22:LEU:HD11	3:A:187:DTM:HC92	1.91	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:171:GLU:OE2	1:A:176:LYS:HE3	2.11	0.50
1:A:95:ASP:HA	1:A:98:LYS:HE2	1.93	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:171:GLU:CG	1:A:176:LYS:HG2	2.44	0.47
1:A:148:PHE:HE2	1:A:151:ILE:HD11	1.79	0.47
1:A:77:ARG:HG3	1:A:77:ARG:HH11	1.78	0.46
1:A:77:ARG:NH1	1:A:77:ARG:CG	2.77	0.46
1:A:158:LEU:HD12	1:A:181:VAL:O	2.16	0.46
1:A:186:ASP:N	1:A:186:ASP:OD1	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:153:LEU:O	1:A:154:GLU:C	2.57	0.42
1:A:1:VAL:HG12	1:A:2:GLY:N	2.33	0.42
1:A:65:ARG:HD2	1:A:65:ARG:HH11	1.39	0.42
1:A:24:TRP:HB2	1:A:25:PRO:CD	2.49	0.41
1:A:75:LEU:HD12	1:A:75:LEU:HA	1.93	0.41
1:A:4:LEU:HA	1:A:4:LEU:HD22	1.92	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:139:MET:CE	1:A:176:LYS:HB3	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	184/187 (98%)	174 (95%)	5 (3%)	5 (3%)	8 1

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	LYS
1	A	101	GLU
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%)	147 (88%)	21 (12%)	7 1

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	22	LEU
1	A	33	TYR
1	A	35	GLN
1	A	43	VAL
1	A	63	LYS
1	A	77	ARG
1	A	93	LEU
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	157	LYS
1	A	171	GLU
1	A	172	GLU
1	A	173	LYS
1	A	178	LYS
1	A	186	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	35	GLN
1	A	84	GLN
1	A	87	HIS
1	A	130	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry

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$
3	DTM	A	187	-	29,29,29	2.17	5 (17%)	41,41,41	2.43	17 (41%)
2	SO4	A	188	-	4,4,4	1.64	2 (50%)	6,6,6	0.49	0
2	SO4	A	189	-	4,4,4	1.40	1 (25%)	6,6,6	1.44	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	-	-	0/14/14/14	0/1/3/3
2	SO4	A	188	-	-	0/0/0/0	0/0/0/0
2	SO4	A	189	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	187	DTM	C4B-C4A	-8.92	1.38	1.45
3	A	187	DTM	C7'-C6B	3.24	1.43	1.38
3	A	187	DTM	C9'-N9'	3.17	1.52	1.46
3	A	187	DTM	C7'-N8'	2.49	1.36	1.31
2	A	188	SO4	O3-S	2.41	1.55	1.47
2	A	189	SO4	O3-S	2.28	1.55	1.47
2	A	188	SO4	O2-S	2.19	1.54	1.47
3	A	187	DTM	C8A-N8'	-2.17	1.33	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	187	DTM	C7'-N8'-C8A	5.94	123.52	116.85
3	A	187	DTM	C4A-C4B-N4'	4.88	127.72	121.11
3	A	187	DTM	N1'-C2B-N3'	-4.81	119.94	127.54
3	A	187	DTM	C1'-C9'-N9'	-4.76	107.90	113.44
3	A	187	DTM	C2B-N1'-C8A	4.20	120.87	115.30
3	A	187	DTM	C51-O5'-C5'	-3.48	112.43	117.59
3	A	187	DTM	O3'-C3'-C4'	-3.32	109.54	115.31
3	A	187	DTM	C6B-C7'-N8'	-3.21	117.77	123.08
2	A	189	SO4	O4-S-O3	-3.17	95.66	109.08
3	A	187	DTM	O5'-C5'-C6'	-3.10	118.83	124.23
3	A	187	DTM	O5'-C5'-C4'	3.08	120.68	115.31
3	A	187	DTM	C9'-C1'-C6'	-2.85	114.40	120.20
3	A	187	DTM	O3'-C3'-C2'	2.75	129.02	124.23
3	A	187	DTM	C31-O3'-C3'	-2.58	113.78	117.59
3	A	187	DTM	CN'-N9'-C6B	2.42	124.07	119.58
3	A	187	DTM	C9'-C1'-C2'	2.32	124.93	120.20
3	A	187	DTM	O4'-C4'-C3'	-2.28	116.86	120.13
3	A	187	DTM	C3'-C2'-C1'	-2.01	117.14	120.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	186/187 (99%)	0.18	9 (4%) 29 23	7, 19, 45, 53	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	186	ASP	5.6
1	A	1	VAL	5.3
1	A	185	ASN	3.5
1	A	154	GLU	3.4
1	A	128	PRO	3.2
1	A	100	THR	2.7
1	A	103	PRO	2.6
1	A	43	VAL	2.6
1	A	153	LEU	2.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DTM	A	187	27/27	0.11	-0.00	4,16,21,22	0
2	SO4	A	189	5/5	0.10	-0.47	36,37,38,39	0
2	SO4	A	188	5/5	0.06	-1.98	21,22,23,24	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.