



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 08:31 PM GMT

PDB ID : 1MVS  
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 : 1.90 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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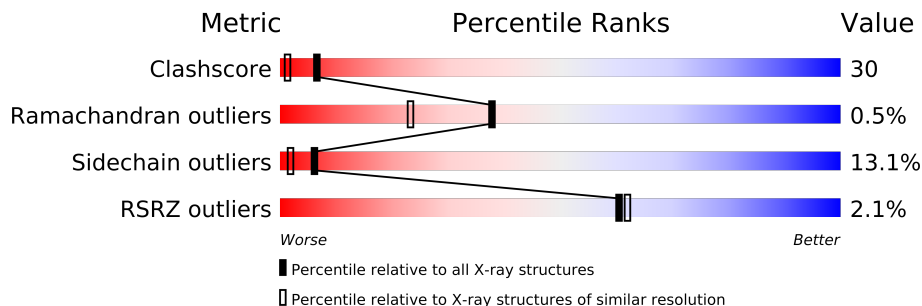
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.90 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	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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 1608 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.

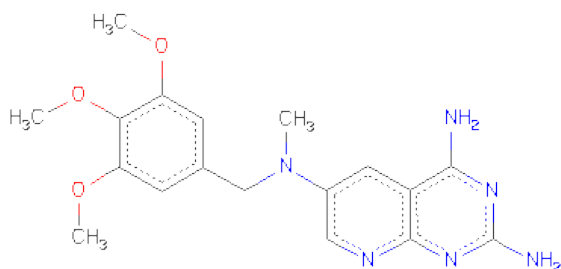
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

- 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
			Total	C	N	O		
3	A	1	27	18	6	3	0	0

- Molecule 4 is water.

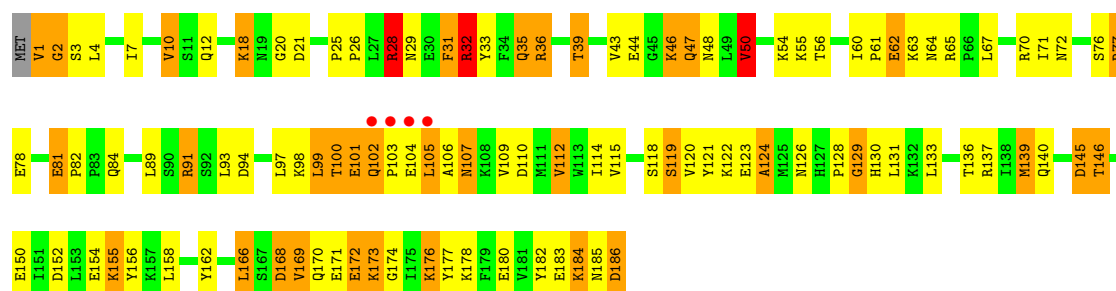
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		

### 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, $\alpha$ , $\beta$ , $\gamma$	85.49Å 85.49Å 77.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.90 53.57 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.6 (8.00-1.90) 61.5 (53.57-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 1.90Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.186 , (Not available) 0.172 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.9	EDS
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 10229 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1608	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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	1.02	1/1537 (0.1%)	2.48	85/2073 (4.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	SER	CB-OG	5.84	1.49	1.42

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	CD-NE-CZ	40.27	179.99	123.60
1	A	36	ARG	NE-CZ-NH2	15.43	128.02	120.30
1	A	28	ARG	NE-CZ-NH1	12.71	126.65	120.30
1	A	77	ARG	CD-NE-CZ	12.42	140.99	123.60
1	A	28	ARG	NE-CZ-NH2	-12.11	114.25	120.30
1	A	77	ARG	NE-CZ-NH1	12.04	126.32	120.30
1	A	110	ASP	CB-CG-OD1	11.93	129.04	118.30
1	A	21	ASP	CB-CG-OD2	-11.58	107.88	118.30
1	A	123	GLU	OE1-CD-OE2	10.59	136.01	123.30
1	A	33	TYR	CB-CG-CD1	10.36	127.22	121.00
1	A	47	GLN	CA-CB-CG	9.53	134.37	113.40
1	A	137	ARG	NE-CZ-NH1	-9.22	115.69	120.30
1	A	36	ARG	NE-CZ-NH1	-9.21	115.70	120.30
1	A	33	TYR	CB-CG-CD2	-8.96	115.63	121.00
1	A	32	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	A	180	GLU	CG-CD-OE1	8.03	134.36	118.30
1	A	77	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	70	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	A	162	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	A	152	ASP	CB-CG-OD2	7.51	125.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	CD-NE-CZ	7.47	134.06	123.60
1	A	121	TYR	CB-CG-CD1	-7.21	116.67	121.00
1	A	70	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	177	TYR	CB-CG-CD1	-7.06	116.77	121.00
1	A	169	VAL	CA-CB-CG2	-7.05	100.32	110.90
1	A	128	PRO	CB-CA-C	6.93	129.33	112.00
1	A	44	GLU	OE1-CD-OE2	6.85	131.52	123.30
1	A	115	VAL	CA-CB-CG2	6.80	121.10	110.90
1	A	50	VAL	CA-CB-CG2	6.78	121.08	110.90
1	A	121	TYR	CB-CG-CD2	6.74	125.04	121.00
1	A	177	TYR	CB-CG-CD2	6.68	125.01	121.00
1	A	150	GLU	CB-CG-CD	6.67	132.20	114.20
1	A	129	GLY	O-C-N	6.64	133.32	122.70
1	A	3	SER	N-CA-CB	-6.52	100.73	110.50
1	A	145	ASP	CB-CG-OD1	6.49	124.14	118.30
1	A	104	GLU	OE1-CD-OE2	6.37	130.94	123.30
1	A	172	GLU	N-CA-CB	6.35	122.02	110.60
1	A	78	GLU	OE1-CD-OE2	-6.28	115.76	123.30
1	A	78	GLU	CG-CD-OE1	6.26	130.82	118.30
1	A	152	ASP	CB-CG-OD1	-6.18	112.74	118.30
1	A	180	GLU	CG-CD-OE2	-6.12	106.06	118.30
1	A	99	LEU	CA-CB-CG	6.11	129.35	115.30
1	A	81	GLU	CG-CD-OE2	-6.04	106.22	118.30
1	A	7	ILE	C-N-CA	6.03	136.78	121.70
1	A	102	GLN	N-CA-CB	5.95	121.32	110.60
1	A	112	VAL	CB-CA-C	5.94	122.68	111.40
1	A	21	ASP	OD1-CG-OD2	5.93	134.56	123.30
1	A	120	VAL	O-C-N	5.81	132.00	122.70
1	A	105	LEU	N-CA-CB	-5.80	98.80	110.40
1	A	126	ASN	CA-CB-CG	5.80	126.16	113.40
1	A	18	LYS	N-CA-CB	5.79	121.02	110.60
1	A	121	TYR	CA-CB-CG	5.79	124.40	113.40
1	A	35	GLN	CG-CD-NE2	-5.69	103.05	116.70
1	A	77	ARG	CA-C-O	-5.62	108.29	120.10
1	A	169	VAL	CA-CB-CG1	5.62	119.33	110.90
1	A	101	GLU	OE1-CD-OE2	-5.59	116.59	123.30
1	A	150	GLU	CG-CD-OE2	-5.54	107.22	118.30
1	A	47	GLN	N-CA-CB	5.53	120.54	110.60
1	A	168	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	140	GLN	CG-CD-OE1	-5.51	110.59	121.60
1	A	46	LYS	O-C-N	5.42	131.38	122.70
1	A	32	ARG	CB-CA-C	5.42	121.23	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	THR	CA-CB-OG1	-5.40	97.66	109.00
1	A	2	GLY	N-CA-C	-5.32	99.81	113.10
1	A	136	THR	N-CA-CB	5.30	120.38	110.30
1	A	172	GLU	CA-CB-CG	5.30	125.07	113.40
1	A	168	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	77	ARG	CG-CD-NE	5.23	122.78	111.80
1	A	162	TYR	CB-CG-CD2	5.20	124.12	121.00
1	A	126	ASN	CB-CG-OD1	5.15	131.91	121.60
1	A	81	GLU	CG-CD-OE1	5.12	128.53	118.30
1	A	176	LYS	CB-CA-C	-5.10	100.20	110.40
1	A	166	LEU	CB-CG-CD2	-5.09	102.35	111.00
1	A	158	LEU	O-C-N	-5.07	114.58	122.70
1	A	48	ASN	CB-CG-OD1	-5.06	111.47	121.60
1	A	50	VAL	CG1-CB-CG2	-5.05	102.82	110.90
1	A	31	PHE	N-CA-CB	5.05	119.68	110.60
1	A	62	GLU	OE1-CD-OE2	5.04	129.35	123.30
1	A	101	GLU	O-C-N	5.04	130.77	122.70
1	A	123	GLU	CA-CB-CG	-5.04	102.32	113.40
1	A	10	VAL	CA-CB-CG1	5.03	118.45	110.90
1	A	154	GLU	OE1-CD-OE2	5.02	129.33	123.30
1	A	101	GLU	CB-CA-C	-5.02	100.36	110.40
1	A	124	ALA	N-CA-CB	5.00	117.11	110.10
1	A	173	LYS	N-CA-CB	5.00	119.61	110.60

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	89	0
2	A	10	0	0	2	0
3	A	27	0	22	3	0
4	A	69	0	0	9	0
All	All	1608	0	1533	91	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 30.

All (91) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:99:LEU:HD22	1:A:105:LEU:HD12	1.22	1.12
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.24	1.09
1:A:139:MET:HE1	1:A:178:LYS:HD3	1.50	0.92
1:A:99:LEU:HD22	1:A:105:LEU:CD1	1.99	0.91
1:A:139:MET:CE	1:A:178:LYS:HD3	2.04	0.87
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.57	0.85
1:A:54:LYS:HD3	4:A:244:HOH:O	1.78	0.84
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.09	0.83
1:A:107:ASN:ND2	1:A:107:ASN:H	1.74	0.82
1:A:60:ILE:HG23	3:A:187:DTM:H312	1.62	0.80
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.82	0.80
1:A:130:HIS:HE1	1:A:183:GLU:OE1	1.65	0.79
1:A:107:ASN:HD22	1:A:107:ASN:H	1.29	0.78
1:A:171:GLU:HG3	1:A:176:LYS:HE2	1.67	0.77
1:A:97:LEU:O	1:A:100:THR:HB	1.88	0.74
1:A:1:VAL:HG11	1:A:100:THR:HG21	1.70	0.73
1:A:1:VAL:CG1	1:A:100:THR:HG21	2.20	0.72
1:A:63:LYS:HG2	4:A:198:HOH:O	1.93	0.69
1:A:28:ARG:H	1:A:28:ARG:HD3	1.59	0.68
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.76	0.66
1:A:54:LYS:CD	4:A:244:HOH:O	2.40	0.65
1:A:1:VAL:CG2	1:A:100:THR:HG21	2.27	0.65
1:A:130:HIS:CE1	1:A:183:GLU:OE1	2.49	0.63
1:A:99:LEU:HA	1:A:102:GLN:CG	2.16	0.61
1:A:94:ASP:O	1:A:98:LYS:HG3	2.01	0.60
1:A:1:VAL:HG21	1:A:100:THR:HG21	1.84	0.60
1:A:55:LYS:HG2	4:A:247:HOH:O	2.01	0.60
1:A:77:ARG:O	1:A:91:ARG:NH2	2.35	0.60
1:A:31:PHE:O	1:A:35:GLN:HG2	2.02	0.59
1:A:139:MET:HE3	1:A:178:LYS:CE	2.31	0.59
1:A:168:ASP:N	1:A:168:ASP:OD2	2.30	0.58
1:A:60:ILE:CG2	3:A:187:DTM:H312	2.33	0.58
1:A:99:LEU:O	1:A:105:LEU:HB2	2.04	0.58
1:A:1:VAL:CG2	1:A:100:THR:CG2	2.81	0.58
1:A:1:VAL:CG1	1:A:100:THR:CG2	2.80	0.58
1:A:156:TYR:CZ	1:A:184:LYS:HD3	2.38	0.57
1:A:1:VAL:O	4:A:190:HOH:O	2.17	0.57
1:A:26:PRO:O	1:A:28:ARG:NH2	2.36	0.57
1:A:77:ARG:N	2:A:188:SO4:O4	2.28	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:29:ASN:OD1	1:A:32:ARG:NH1	2.37	0.56
1:A:4:LEU:CD1	1:A:112:VAL:HG22	2.34	0.56
1:A:171:GLU:CG	1:A:176:LYS:HE2	2.34	0.56
1:A:139:MET:CE	1:A:178:LYS:NZ	2.69	0.56
1:A:156:TYR:CE2	1:A:184:LYS:HB3	2.41	0.55
1:A:171:GLU:OE2	1:A:174:GLY:HA2	2.06	0.55
1:A:139:MET:HE3	1:A:178:LYS:NZ	2.22	0.55
1:A:93:LEU:O	1:A:97:LEU:HG	2.06	0.54
1:A:26:PRO:O	1:A:173:LYS:HE3	2.07	0.54
1:A:168:ASP:O	1:A:170:GLN:NE2	2.41	0.51
1:A:168:ASP:CG	4:A:240:HOH:O	2.49	0.51
1:A:29:ASN:N	1:A:172:GLU:OE1	2.36	0.50
1:A:43:VAL:HG13	1:A:46:LYS:HG3	1.93	0.50
3:A:187:DTM:H413	3:A:187:DTM:O5'	2.11	0.50
1:A:62:GLU:HG3	1:A:65:ARG:NH1	2.27	0.50
2:A:189:SO4:O4	4:A:228:HOH:O	2.19	0.50
1:A:76:SER:O	1:A:91:ARG:HA	2.11	0.50
1:A:1:VAL:HG22	1:A:100:THR:CG2	2.42	0.50
1:A:28:ARG:N	1:A:28:ARG:HD3	2.25	0.50
1:A:31:PHE:HE1	4:A:258:HOH:O	1.94	0.49
1:A:184:LYS:NZ	1:A:186:ASP:OD1	2.46	0.49
1:A:1:VAL:HG13	1:A:100:THR:HG23	1.95	0.48
1:A:61:PRO:HG2	1:A:64:ASN:HD22	1.78	0.48
1:A:81:GLU:HB2	1:A:82:PRO:HD2	1.97	0.47
1:A:28:ARG:CD	1:A:28:ARG:N	2.78	0.47
1:A:99:LEU:CA	1:A:102:GLN:HG2	2.17	0.47
1:A:4:LEU:O	1:A:131:LEU:HD12	2.13	0.47
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.44	0.47
1:A:2:GLY:HA3	4:A:191:HOH:O	2.14	0.47
1:A:20:GLY:HA2	1:A:55:LYS:HE2	1.96	0.46
1:A:139:MET:CE	1:A:178:LYS:CD	2.86	0.46
1:A:184:LYS:HG3	1:A:185:ASN:N	2.30	0.46
1:A:155:LYS:HB2	1:A:155:LYS:HE2	1.71	0.45
1:A:1:VAL:HG13	1:A:100:THR:CG2	2.47	0.45
1:A:139:MET:HB2	1:A:176:LYS:O	2.17	0.45
1:A:139:MET:HE3	1:A:178:LYS:HD3	1.94	0.45
1:A:71:ILE:HD12	1:A:109:VAL:HG22	1.98	0.45
1:A:50:VAL:HG21	1:A:67:LEU:HD12	1.99	0.44
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.77	0.44
1:A:122:LYS:CG	1:A:122:LYS:O	2.66	0.44
1:A:107:ASN:N	1:A:107:ASN:ND2	2.55	0.43
1:A:100:THR:O	1:A:106:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.87	0.42
1:A:133:LEU:HB2	1:A:182:TYR:HB2	2.01	0.42
1:A:169:VAL:H	1:A:169:VAL:HG23	1.68	0.42
1:A:139:MET:HE3	1:A:178:LYS:HZ3	1.85	0.42
1:A:129:GLY:O	1:A:184:LYS:NZ	2.53	0.41
1:A:35:GLN:O	1:A:39:THR:OG1	2.15	0.41
1:A:47:GLN:O	1:A:109:VAL:HA	2.21	0.40
1:A:28:ARG:NH2	1:A:173:LYS:HE3	2.36	0.40
1:A:76:SER:HB3	1:A:89:LEU:HD11	2.02	0.40
1:A:65:ARG:HD3	1:A:65:ARG:HH21	1.70	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%)	175 (95%)	8 (4%)	1 (0%)	38 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	MET

### 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%)	146 (87%)	22 (13%)	6 2

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	VAL
1	A	10	VAL
1	A	12	GLN
1	A	18	LYS
1	A	28	ARG
1	A	32	ARG
1	A	36	ARG
1	A	39	THR
1	A	50	VAL
1	A	72	ASN
1	A	84	GLN
1	A	100	THR
1	A	101	GLU
1	A	103	PRO
1	A	107	ASN
1	A	118	SER
1	A	119	SER
1	A	146	THR
1	A	155	LYS
1	A	166	LEU
1	A	184	LYS
1	A	186	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	107	ASN
1	A	130	HIS
1	A	185	ASN

### 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	2.12	5 (17%)	41,41,41	3.07	20 (48%)
2	SO4	A	188	-	4,4,4	0.94	0	6,6,6	0.40	0
2	SO4	A	189	-	4,4,4	1.19	0	6,6,6	0.63	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
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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	187	DTM	C4B-C4A	-7.34	1.39	1.45
3	A	187	DTM	C9'-N9'	5.39	1.56	1.46
3	A	187	DTM	C6'-C5'	3.59	1.45	1.38
3	A	187	DTM	C7'-C6B	3.38	1.43	1.38
3	A	187	DTM	C7'-N8'	2.74	1.36	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	187	DTM	C4A-C4B-N4'	9.33	133.75	121.11
3	A	187	DTM	C51-O5'-C5'	-7.33	106.75	117.59
3	A	187	DTM	C1'-C9'-N9'	-6.76	105.57	113.44
3	A	187	DTM	C31-O3'-C3'	-4.93	110.29	117.59
3	A	187	DTM	N1'-C2B-N3'	-4.30	120.74	127.54
3	A	187	DTM	C6B-C5B-C4A	4.01	124.61	120.96
3	A	187	DTM	C7'-N8'-C8A	3.72	121.03	116.85
3	A	187	DTM	C2B-N1'-C8A	3.70	120.21	115.30
3	A	187	DTM	C5B-C4A-C8A	-3.49	115.10	117.90
3	A	187	DTM	C4A-C4B-N3'	-3.30	118.18	121.95
3	A	187	DTM	C5B-C6B-C7'	-3.28	115.37	119.70
3	A	187	DTM	O3'-C3'-C4'	-3.10	109.92	115.31
3	A	187	DTM	C2'-C3'-C4'	2.98	123.83	120.22
3	A	187	DTM	CN'-N9'-C6B	2.79	124.76	119.58
3	A	187	DTM	C41-O4'-C4'	2.55	121.87	114.90
3	A	187	DTM	N4'-C4B-N3'	-2.34	108.01	116.23
3	A	187	DTM	C9'-C1'-C6'	-2.30	115.51	120.20
3	A	187	DTM	O5'-C5'-C4'	2.18	119.11	115.31
3	A	187	DTM	C3'-C2'-C1'	-2.17	116.90	120.09
3	A	187	DTM	C6'-C1'-C2'	2.15	122.19	118.95

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%)	-0.08	4 (2%) 59 60	16, 26, 47, 56	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	4.2
1	A	104	GLU	2.2
1	A	103	PRO	2.0
1	A	102	GLN	2.0

### 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(Å <sup>2</sup> )	Q<0.9
2	SO4	A	188	5/5	0.12	-0.18	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DTM	A	187	27/27	0.09	-0.43	22,26,29,30	0
2	SO4	A	189	5/5	0.08	-0.66	25,25,26,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.