



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:32 AM UTC

PDB ID : 1MVS / pdb_00001mvs
Title : Analysis of Two Polymorphic Forms of a Pyrido[2,3-d]pyrimidine N9-C10 Reverse-Bridge Antifolate Binary Complex with Human Dihydrofolate Reductase
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 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

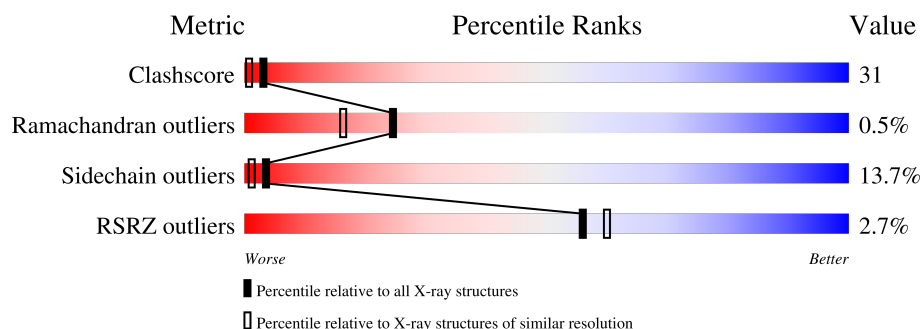
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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](#)

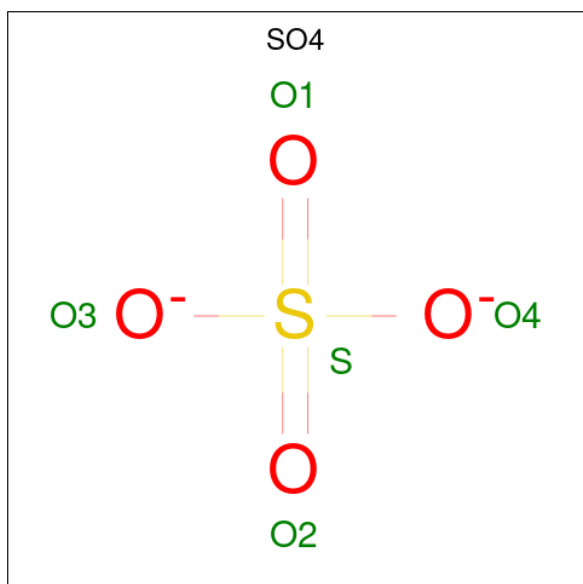
There are 4 unique types of molecules in this entry. The entry contains 1608 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

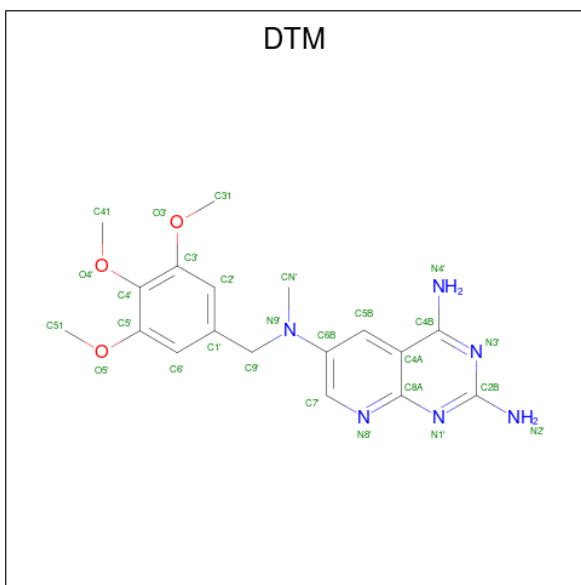
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	0	0	0
			1502	963	253	279	7			

- 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		

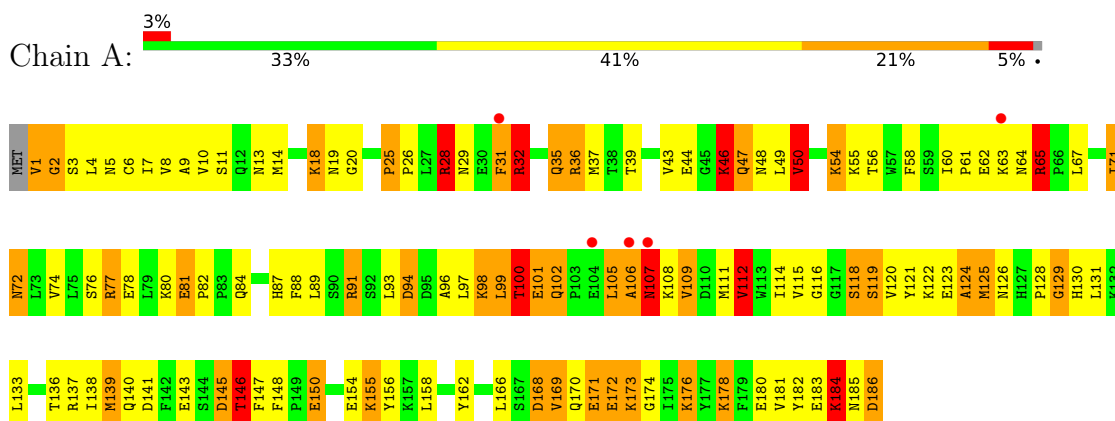
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	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: Dihydrofolate Reductase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	85.49Å 85.49Å 77.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 1.90 8.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.6 (8.00-1.90) 60.2 (8.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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.	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.047 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1608	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: DTM, SO4

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	1.26	2/1537 (0.1%)	2.88	150/2073 (7.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	MET	C-N	-6.54	1.27	1.33
1	A	162	TYR	CA-CB	5.12	1.61	1.53

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	CD-NE-CZ	39.70	179.99	124.40
1	A	128	PRO	CB-CA-C	14.14	129.33	111.23
1	A	126	ASN	CA-CB-CG	13.56	126.16	112.60
1	A	77	ARG	CD-NE-CZ	11.85	140.99	124.40
1	A	150	GLU	CB-CG-CD	11.53	132.20	112.60
1	A	129	GLY	O-C-N	10.43	133.32	123.00
1	A	47	GLN	CA-CB-CG	10.13	134.37	114.10
1	A	7	ILE	CA-C-N	10.10	136.78	122.23
1	A	7	ILE	C-N-CA	10.10	136.78	122.23
1	A	168	ASP	CA-CB-CG	-9.93	102.67	112.60
1	A	120	VAL	O-C-N	9.87	132.00	121.83
1	A	36	ARG	NE-CZ-NH2	9.79	128.02	119.20
1	A	77	ARG	CA-C-O	-9.69	108.29	119.24
1	A	5	ASN	OD1-CG-ND2	-9.26	113.34	122.60
1	A	9	ALA	CA-C-O	-9.25	110.40	120.30
1	A	35	GLN	CG-CD-NE2	-8.90	103.05	116.40
1	A	72	ASN	CA-CB-CG	8.81	121.41	112.60
1	A	140	GLN	OE1-CD-NE2	8.75	131.35	122.60
1	A	136	THR	CA-C-O	-8.57	111.58	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASN	OD1-CG-ND2	-8.49	114.11	122.60
1	A	25	PRO	CB-CA-C	8.39	121.16	110.92
1	A	102	GLN	N-CA-CB	8.35	121.32	110.04
1	A	56	THR	CA-CB-OG1	-7.96	97.66	109.60
1	A	112	VAL	CB-CA-C	7.96	122.68	110.83
1	A	108	LYS	N-CA-C	7.94	123.14	113.38
1	A	105	LEU	N-CA-CB	-7.82	98.80	110.61
1	A	118	SER	O-C-N	7.79	130.38	122.12
1	A	116	GLY	CA-C-O	-7.75	114.01	122.14
1	A	48	ASN	CA-CB-CG	7.63	120.23	112.60
1	A	72	ASN	CA-C-N	7.58	133.69	123.00
1	A	72	ASN	C-N-CA	7.58	133.69	123.00
1	A	77	ARG	N-CA-C	-7.55	104.59	113.88
1	A	3	SER	N-CA-C	7.38	120.38	110.35
1	A	9	ALA	CA-C-N	7.31	133.15	123.06
1	A	9	ALA	C-N-CA	7.31	133.15	123.06
1	A	58	PHE	CA-CB-CG	-7.22	106.58	113.80
1	A	71	ILE	N-CA-CB	7.17	119.17	111.00
1	A	100	THR	N-CA-C	-7.09	103.48	111.14
1	A	106	ALA	N-CA-C	7.06	119.58	111.11
1	A	119	SER	CA-C-O	7.00	128.17	120.82
1	A	180	GLU	CG-CD-OE1	6.94	134.36	118.40
1	A	140	GLN	CB-CG-CD	-6.93	100.81	112.60
1	A	91	ARG	CD-NE-CZ	6.90	134.06	124.40
1	A	47	GLN	CB-CG-CD	-6.88	100.91	112.60
1	A	99	LEU	CA-C-O	6.84	127.79	119.38
1	A	115	VAL	CA-C-O	-6.77	112.51	119.89
1	A	106	ALA	CA-C-N	6.70	133.45	121.66
1	A	106	ALA	C-N-CA	6.70	133.45	121.66
1	A	107	ASN	CA-CB-CG	6.66	119.26	112.60
1	A	158	LEU	O-C-N	-6.65	114.58	122.96
1	A	105	LEU	CA-C-N	6.53	129.35	120.54
1	A	105	LEU	C-N-CA	6.53	129.35	120.54
1	A	141	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	124	ALA	N-CA-C	-6.50	104.27	111.36
1	A	18	LYS	N-CA-CB	6.49	121.02	110.90
1	A	137	ARG	CA-C-N	6.44	130.54	122.43
1	A	137	ARG	C-N-CA	6.44	130.54	122.43
1	A	146	THR	CB-CA-C	6.43	122.43	109.38
1	A	102	GLN	N-CA-C	-6.42	100.87	110.24
1	A	3	SER	N-CA-CB	-6.34	100.73	110.04
1	A	44	GLU	CA-C-O	6.34	128.10	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	VAL	O-C-N	-6.30	116.52	123.20
1	A	115	VAL	CA-CB-CG2	6.29	121.10	110.40
1	A	50	VAL	CA-CB-CG2	6.28	121.08	110.40
1	A	184	LYS	CA-C-O	6.23	128.28	121.06
1	A	101	GLU	O-C-N	6.22	130.77	122.43
1	A	87	HIS	CA-C-O	-6.17	112.26	119.24
1	A	31	PHE	N-CA-CB	6.14	119.68	110.22
1	A	74	VAL	CA-C-O	6.13	127.13	120.57
1	A	32	ARG	CB-CA-C	6.11	121.23	110.85
1	A	172	GLU	N-CA-CB	6.09	122.02	111.13
1	A	74	VAL	CA-C-N	6.07	130.84	122.77
1	A	74	VAL	C-N-CA	6.07	130.84	122.77
1	A	136	THR	N-CA-CB	6.05	120.38	110.39
1	A	46	LYS	O-C-N	6.05	131.38	122.97
1	A	47	GLN	OE1-CD-NE2	6.00	128.60	122.60
1	A	178	LYS	CA-C-N	5.96	130.94	122.72
1	A	178	LYS	C-N-CA	5.96	130.94	122.72
1	A	169	VAL	CA-CB-CG2	-5.93	100.32	110.40
1	A	72	ASN	CA-C-O	-5.91	114.03	120.36
1	A	74	VAL	O-C-N	-5.91	116.47	123.03
1	A	96	ALA	O-C-N	5.90	128.38	122.12
1	A	123	GLU	CA-CB-CG	-5.89	102.32	114.10
1	A	109	VAL	N-CA-C	5.87	117.05	108.53
1	A	126	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	A	6	CYS	N-CA-C	-5.84	100.18	109.59
1	A	145	ASP	CB-CA-C	5.84	119.21	109.80
1	A	121	TYR	CA-CB-CG	5.83	124.40	113.90
1	A	3	SER	CA-C-O	-5.82	115.39	121.55
1	A	171	GLU	N-CA-C	5.82	118.13	108.13
1	A	137	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	A	36	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	A	121	TYR	O-C-N	5.79	128.75	122.15
1	A	19	ASN	N-CA-C	5.75	119.33	111.39
1	A	186	ASP	CA-CB-CG	-5.74	106.86	112.60
1	A	147	PHE	N-CA-C	5.73	117.89	109.24
1	A	35	GLN	CB-CA-C	-5.72	101.29	110.79
1	A	7	ILE	CB-CA-C	5.67	118.60	110.33
1	A	176	LYS	CB-CA-C	-5.65	100.20	109.53
1	A	2	GLY	N-CA-C	-5.64	99.81	113.18
1	A	143	GLU	N-CA-CB	5.64	118.43	109.51
1	A	32	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	108	LYS	CA-C-O	-5.60	112.77	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	LYS	N-CA-CB	5.58	119.61	111.62
1	A	126	ASN	CB-CG-OD1	5.55	131.91	120.80
1	A	80	LYS	CA-C-O	5.52	126.30	119.79
1	A	138	ILE	N-CA-C	-5.51	99.13	107.73
1	A	28	ARG	NE-CZ-NH2	-5.50	114.25	119.20
1	A	88	PHE	O-C-N	5.50	129.52	123.25
1	A	172	GLU	CA-CB-CG	5.49	125.07	114.10
1	A	49	LEU	CA-C-O	-5.48	114.46	120.43
1	A	94	ASP	CA-CB-CG	-5.48	107.12	112.60
1	A	123	GLU	OE1-CD-OE2	5.46	136.01	122.90
1	A	120	VAL	CA-C-O	-5.46	115.06	120.85
1	A	14	MET	CA-C-N	5.44	126.20	120.43
1	A	14	MET	C-N-CA	5.44	126.20	120.43
1	A	50	VAL	N-CA-CB	5.44	118.31	111.46
1	A	98	LYS	CA-C-N	5.42	129.78	120.72
1	A	98	LYS	C-N-CA	5.42	129.78	120.72
1	A	100	THR	O-C-N	5.42	127.94	122.09
1	A	78	GLU	CG-CD-OE1	5.40	130.82	118.40
1	A	154	GLU	N-CA-C	-5.40	106.19	112.89
1	A	65	ARG	CB-CA-C	-5.37	103.14	109.47
1	A	180	GLU	CG-CD-OE2	-5.37	106.06	118.40
1	A	35	GLN	N-CA-C	5.31	117.07	111.28
1	A	54	LYS	N-CA-C	5.30	116.75	111.07
1	A	35	GLN	CG-CD-OE1	5.30	131.40	120.80
1	A	72	ASN	CB-CG-ND2	5.30	124.35	116.40
1	A	81	GLU	CG-CD-OE2	-5.30	106.22	118.40
1	A	148	PHE	CB-CA-C	5.28	117.02	109.26
1	A	169	VAL	CA-CB-CG1	5.25	119.33	110.40
1	A	105	LEU	CA-C-O	5.24	125.56	119.32
1	A	2	GLY	CA-C-N	5.24	128.66	120.75
1	A	2	GLY	C-N-CA	5.24	128.66	120.75
1	A	8	VAL	N-CA-C	5.23	115.90	108.42
1	A	128	PRO	CA-C-N	-5.22	113.47	123.03
1	A	128	PRO	C-N-CA	-5.22	113.47	123.03
1	A	125	MET	O-C-N	5.19	129.50	122.59
1	A	77	ARG	O-C-N	5.19	129.31	122.36
1	A	28	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	A	58	PHE	CA-C-O	-5.13	113.07	119.38
1	A	46	LYS	CB-CA-C	-5.12	101.24	110.36
1	A	140	GLN	CG-CD-OE1	-5.11	110.59	120.80
1	A	47	GLN	N-CA-CB	5.09	120.54	111.69
1	A	162	TYR	CA-CB-CG	-5.07	104.77	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	SER	N-CA-C	-5.07	103.35	110.35
1	A	154	GLU	CA-CB-CG	5.07	124.24	114.10
1	A	176	LYS	O-C-N	5.06	129.03	123.16
1	A	80	LYS	CA-C-N	5.02	132.10	123.11
1	A	80	LYS	C-N-CA	5.02	132.10	123.11

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	94	0
2	A	10	0	0	2	0
3	A	27	0	22	3	0
4	A	69	0	0	10	0
All	All	1608	0	1533	96	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 31.

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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASN:H	1:A:107:ASN:HD22	1.29	0.78
1:A:139:MET:HE3	1:A:178:LYS:HD3	1.64	0.77
1:A:171:GLU:HG3	1:A:176:LYS:HE2	1.67	0.77
1:A:139:MET:HE3	1:A:178:LYS:CE	2.17	0.75
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:139:MET:HE3	1:A:178:LYS:CD	2.24	0.67
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.76	0.66
1:A:1:VAL:CG2	1:A:100:THR:HG21	2.27	0.65
1:A:54:LYS:CD	4:A:244:HOH:O	2.40	0.65
1:A:139:MET:HE1	1:A:178:LYS:HD3	1.80	0.63
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:NZ	2.18	0.59
1:A:60:ILE:CG2	3:A:187:DTM:H312	2.33	0.58
1:A:1:VAL:CG2	1:A:100:THR:CG2	2.81	0.58
1:A:99:LEU:O	1:A:105:LEU:HB2	2.04	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
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:168:ASP:CG	4:A:240:HOH:O	2.49	0.55
1:A:125:MET:HE3	1:A:133:LEU:HD21	1.86	0.55
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:HE1	4:A:196:HOH:O	2.09	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:O5'	3:A:187:DTM:H413	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:HD3	1:A:28:ARG:N	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:N	1:A:28:ARG:CD	2.78	0.47
1:A:2:GLY:HA3	4:A:191:HOH:O	2.14	0.47
1:A:4:LEU:O	1:A:131:LEU:HD12	2.13	0.47
1:A:99:LEU:CA	1:A:102:GLN:HG2	2.17	0.47
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.44	0.47
1:A:20:GLY:HA2	1:A:55:LYS:HE2	1.96	0.46
1:A:184:LYS:HG3	1:A:185:ASN:N	2.30	0.46
1:A:37:MET:HE3	1:A:37:MET:HB3	1.83	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:71:ILE:HD12	1:A:109:VAL:HG22	1.98	0.45
1:A:139:MET:HB2	1:A:176:LYS:O	2.17	0.45
1:A:168:ASP:OD2	1:A:168:ASP:N	2.30	0.45
1:A:50:VAL:HG21	1:A:67:LEU:HD12	1.99	0.44
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.77	0.44
1:A:122:LYS:O	1:A:122:LYS:CG	2.66	0.44
1:A:107:ASN:ND2	1:A:107:ASN:N	2.55	0.43
1:A:25:PRO:HA	1:A:26:PRO:HD3	1.87	0.42
1:A:100:THR:O	1:A:106:ALA:HA	2.19	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:186:ASP:OD1	1:A:186:ASP:C	2.58	0.41
1:A:129:GLY:O	1:A:184:LYS:NZ	2.53	0.41
1:A:171:GLU:CD	1:A:176:LYS:CE	2.93	0.41
1:A:139:MET:CE	1:A:178:LYS:CD	2.86	0.41
1:A:172:GLU:O	1:A:173:LYS:C	2.64	0.41
1:A:47:GLN:O	1:A:109:VAL:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ARG:NH2	1:A:173:LYS:HE3	2.36	0.40
1:A:65:ARG:HH21	1:A:65:ARG:HD3	1.70	0.40
1:A:76:SER:HB3	1:A:89:LEU:HD11	2.02	0.40

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%)	175 (95%)	8 (4%)	1 (0%)	24 16

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	MET

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	168/169 (99%)	145 (86%)	23 (14%)	3 1

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

Mol	Chain	Res	Type
1	A	1	VAL
1	A	10	VAL
1	A	18	LYS
1	A	28	ARG
1	A	32	ARG
1	A	36	ARG
1	A	39	THR
1	A	46	LYS
1	A	50	VAL
1	A	65	ARG
1	A	72	ASN
1	A	84	GLN
1	A	100	THR
1	A	101	GLU
1	A	107	ASN
1	A	112	VAL
1	A	118	SER
1	A	119	SER
1	A	146	THR
1	A	150	GLU
1	A	155	LYS
1	A	166	LEU
1	A	184	LYS

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

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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	0.52	0	6,6,6	0.46	0
3	DTM	A	187	-	29,29,29	1.94	5 (17%)	39,41,41	3.06	20 (51%)
2	SO4	A	189	-	4,4,4	0.84	0	6,6,6	0.54	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	-	-	5/14/14/14	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	187	DTM	C4B-C4A	-5.82	1.39	1.45
3	A	187	DTM	C9'-N9'	4.86	1.56	1.46
3	A	187	DTM	C6'-C5'	4.02	1.45	1.38
3	A	187	DTM	C7'-C6B	2.96	1.43	1.38
3	A	187	DTM	C7'-N8'	2.89	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'	8.01	133.75	121.45
3	A	187	DTM	C51-O5'-C5'	-7.34	106.75	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	187	DTM	C1'-C9'-N9'	-5.75	105.57	113.53
3	A	187	DTM	N1'-C2B-N3'	-5.09	120.74	127.21
3	A	187	DTM	C31-O3'-C3'	-4.92	110.29	117.51
3	A	187	DTM	C2B-N1'-C8A	4.38	120.21	115.48
3	A	187	DTM	C6B-C5B-C4A	3.65	124.61	121.19
3	A	187	DTM	C4A-C4B-N3'	-3.53	118.18	121.97
3	A	187	DTM	C5B-C4A-C8A	-3.50	115.10	118.11
3	A	187	DTM	N4'-C4B-N3'	-3.39	108.01	117.11
3	A	187	DTM	C2'-C3'-C4'	3.24	123.83	120.22
3	A	187	DTM	CN'-N9'-C6B	3.12	124.76	119.59
3	A	187	DTM	O3'-C3'-C4'	-3.04	109.92	115.14
3	A	187	DTM	C7'-N8'-C8A	2.75	121.03	117.20
3	A	187	DTM	C41-O4'-C4'	2.63	121.87	114.74
3	A	187	DTM	C9'-C1'-C6'	-2.53	115.51	120.27
3	A	187	DTM	C6'-C1'-C2'	2.34	122.19	119.01
3	A	187	DTM	O5'-C5'-C4'	2.32	119.11	115.14
3	A	187	DTM	C3'-C2'-C1'	-2.12	116.90	120.04
3	A	187	DTM	C5B-C4A-C4B	2.06	126.62	124.75

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	187	DTM	C4'-C3'-O3'-C31
3	A	187	DTM	C2'-C3'-O3'-C31
3	A	187	DTM	C3'-C4'-O4'-C41
3	A	187	DTM	C1'-C9'-N9'-CN'
3	A	187	DTM	C5'-C4'-O4'-C41

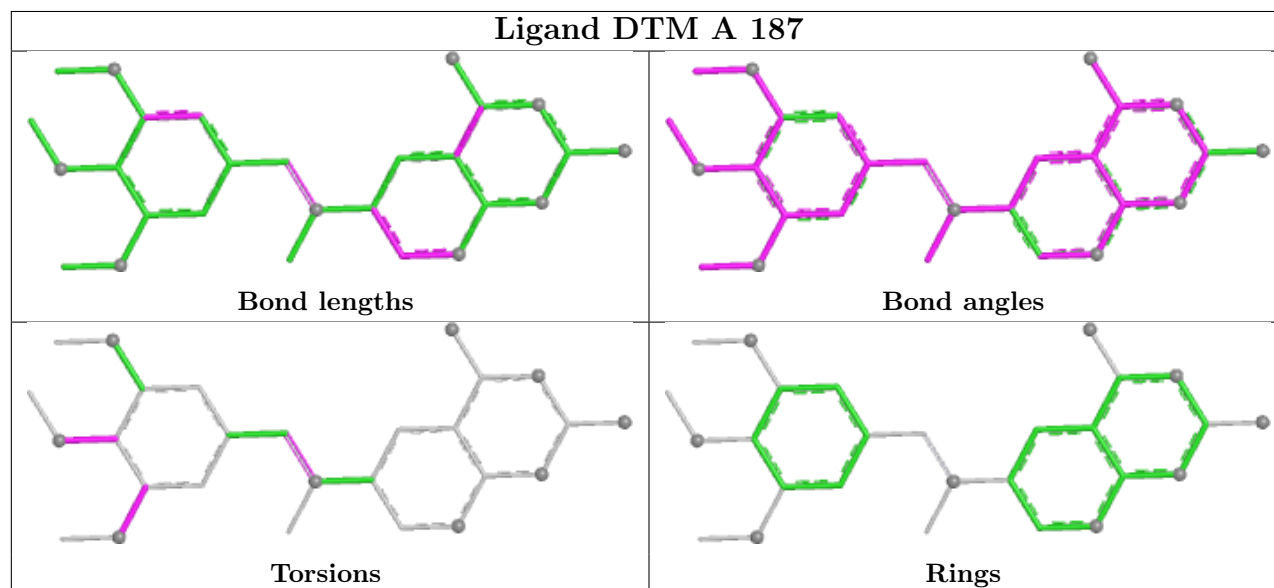
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	188	SO4	1	0
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%)	-0.30	5 (2%) 56 60	16, 26, 47, 56	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	ALA	3.5
1	A	107	ASN	3.1
1	A	104	GLU	2.8
1	A	31	PHE	2.2
1	A	63	LYS	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](#)

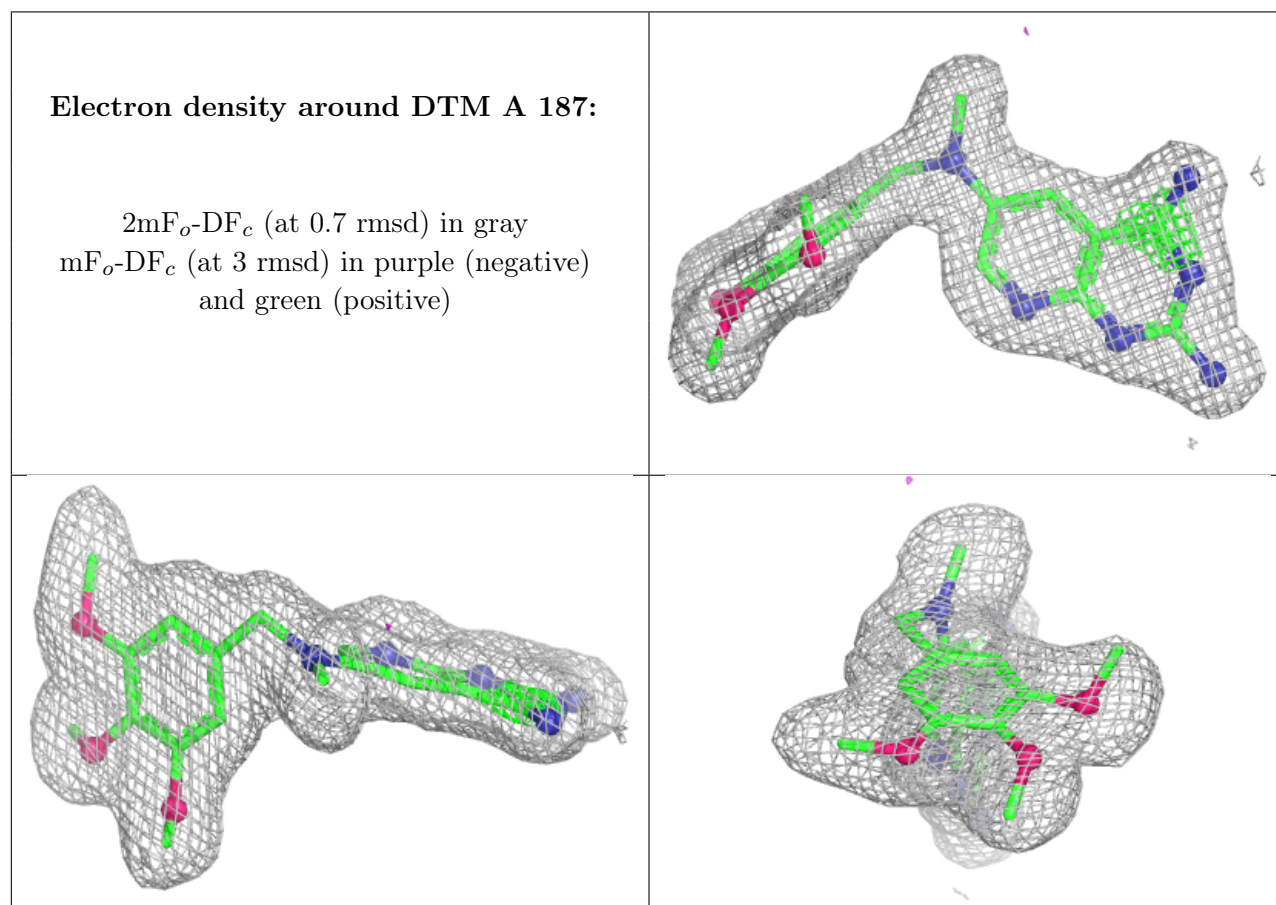
There are no oligosaccharides in this entry.

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	0.91	0.06	22,26,29,30	0
2	SO4	A	188	5/5	0.96	0.08	45,45,45,45	0
2	SO4	A	189	5/5	0.99	0.05	25,25,26,27	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.