



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:30 PM UTC

PDB ID : 1DLR / pdb_00001dlr
Title : METHOTREXATE-RESISTANT VARIANTS OF HUMAN DIHYDROFOLATE REDUCTASE WITH SUBSTITUTION OF LEUCINE 22: KINETICS, CRYSTALLOGRAPHY AND POTENTIAL AS SELECTABLE MARKERS
Authors : Cody, V.; Galitsky, N.; Luft, J.R.; Pangborn, W.
Deposited on : 1995-01-25
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

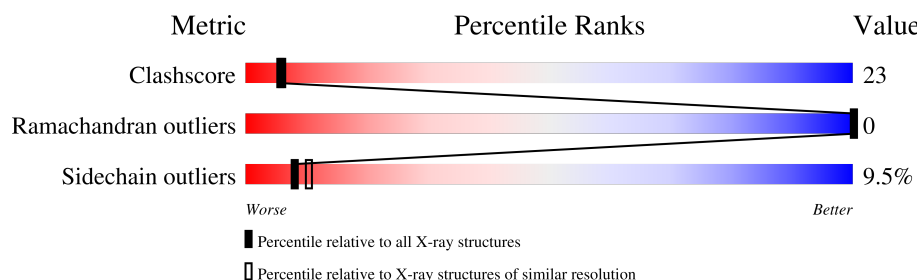
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	186	 31% 46% 21% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1646 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.

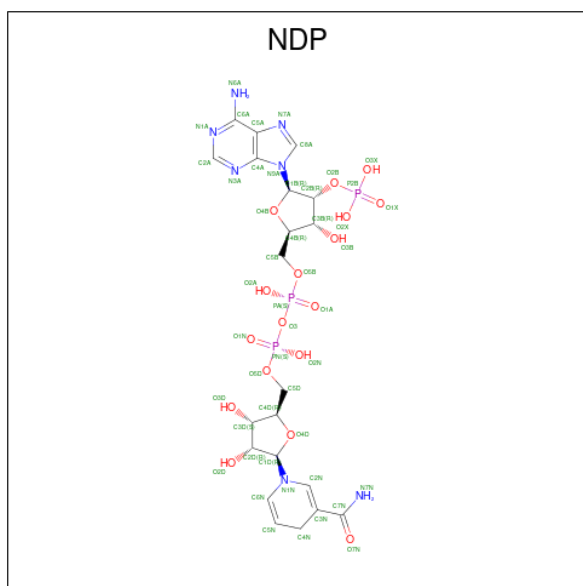
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1505	966	253	279	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

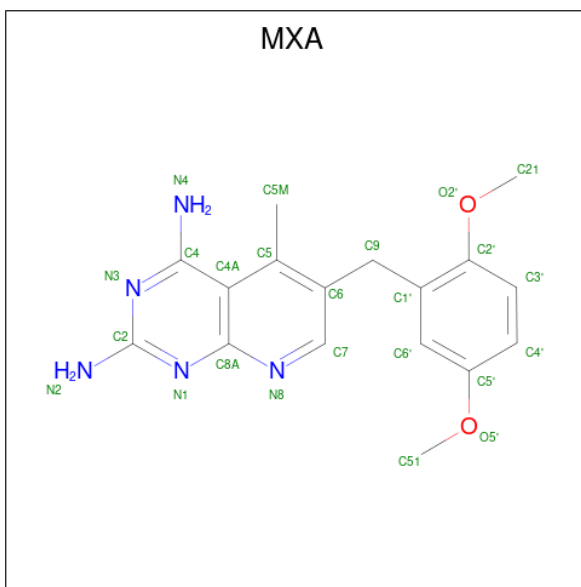
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	PHE	LEU	conflict	UNP P00374

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0

- Molecule 3 is 6-(2,5-DIMETHOXY-BENZYL)-5-METHYL-PYRIDO[2,3-D]PYRIMIDINE-2,4-DIAMINE (CCD ID: MXA) (formula: $C_{17}H_{19}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	17	5	2		

- Molecule 4 is water.

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

3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	87.00Å 87.00Å 76.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROFFT	Depositor
R, R_{free}	0.167 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1646	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.31	8/1541 (0.5%)	2.77	160/2078 (7.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	LEU	C-N	-9.59	1.20	1.33
1	A	185	ASN	C-N	7.97	1.44	1.33
1	A	23	PRO	C-N	-7.21	1.22	1.32
1	A	121	TYR	CZ-OH	-7.21	1.23	1.38
1	A	176	LYS	C-N	5.90	1.40	1.33
1	A	14	MET	C-N	-5.76	1.27	1.33
1	A	106	ALA	C-N	-5.40	1.26	1.33
1	A	128	PRO	CA-C	-5.12	1.47	1.52

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	CA-C-O	-16.01	105.33	122.14
1	A	5	ASN	OD1-CG-ND2	-13.65	108.95	122.60
1	A	143	GLU	CB-CG-CD	11.30	131.82	112.60
1	A	71	ILE	CB-CA-C	9.56	122.27	111.08
1	A	148	PHE	CA-C-O	-9.49	112.22	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	VAL	N-CA-C	9.27	121.93	108.58
1	A	140	GLN	N-CA-CB	8.54	125.06	111.56
1	A	7	ILE	CA-C-N	8.54	133.40	121.96
1	A	7	ILE	C-N-CA	8.54	133.40	121.96
1	A	129	GLY	O-C-N	8.48	130.90	122.85
1	A	147	PHE	CA-CB-CG	-8.36	105.44	113.80
1	A	23	PRO	O-C-N	-8.34	110.44	122.37
1	A	77	ARG	NE-CZ-NH1	-8.31	113.19	121.50
1	A	146	THR	CB-CA-C	8.27	124.11	109.65
1	A	140	GLN	OE1-CD-NE2	8.23	130.83	122.60
1	A	181	VAL	CB-CA-C	8.20	123.23	110.28
1	A	142	PHE	CA-CB-CG	8.12	121.92	113.80
1	A	123	GLU	O-C-N	-8.05	112.80	122.22
1	A	80	LYS	N-CA-CB	8.03	122.19	110.47
1	A	72	ASN	OD1-CG-ND2	-7.98	114.62	122.60
1	A	132	LYS	CA-C-O	-7.88	111.86	120.36
1	A	116	GLY	O-C-N	7.80	132.76	122.47
1	A	8	VAL	CA-C-N	7.79	133.98	123.00
1	A	8	VAL	C-N-CA	7.79	133.98	123.00
1	A	130	HIS	CA-C-O	7.74	129.47	120.49
1	A	177	TYR	O-C-N	7.70	131.66	123.42
1	A	70	ARG	NE-CZ-NH2	-7.67	112.30	119.20
1	A	9	ALA	CA-C-O	-7.65	112.12	120.30
1	A	154	GLU	N-CA-C	-7.55	102.71	112.23
1	A	78	GLU	CA-C-O	-7.52	110.83	120.00
1	A	177	TYR	CA-C-O	-7.50	113.20	121.23
1	A	32	ARG	CA-C-N	7.47	130.60	120.44
1	A	32	ARG	C-N-CA	7.47	130.60	120.44
1	A	94	ASP	CA-CB-CG	-7.47	105.13	112.60
1	A	182	TYR	CA-C-O	-7.43	112.71	121.11
1	A	80	LYS	N-CA-C	-7.38	104.41	113.41
1	A	118	SER	CB-CA-C	-7.32	98.69	110.84
1	A	21	ASP	CA-C-N	7.28	130.55	120.65
1	A	21	ASP	C-N-CA	7.28	130.55	120.65
1	A	87	HIS	CA-C-O	-7.26	111.31	119.67
1	A	40	THR	CA-C-O	7.24	129.14	120.81
1	A	30	GLU	N-CA-C	-7.12	103.59	111.36
1	A	13	ASN	CA-CB-CG	7.11	119.71	112.60
1	A	13	ASN	CA-C-N	7.11	134.88	123.93
1	A	13	ASN	C-N-CA	7.11	134.88	123.93
1	A	22	PHE	O-C-N	-7.09	114.99	121.30
1	A	95	ASP	CA-CB-CG	7.00	119.60	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	157	LYS	CB-CA-C	-6.96	98.38	109.80
1	A	80	LYS	CA-CB-CG	6.96	128.01	114.10
1	A	102	GLN	N-CA-CB	6.94	119.66	110.29
1	A	80	LYS	O-C-N	6.88	132.13	122.36
1	A	120	VAL	O-C-N	6.75	129.43	121.80
1	A	118	SER	CA-C-N	6.69	129.58	120.54
1	A	118	SER	C-N-CA	6.69	129.58	120.54
1	A	83	PRO	CB-CA-C	-6.67	101.13	111.40
1	A	25	PRO	N-CA-C	-6.66	102.58	110.70
1	A	56	THR	CA-CB-OG1	-6.66	99.61	109.60
1	A	11	SER	N-CA-C	-6.54	102.10	110.53
1	A	90	SER	N-CA-CB	6.52	122.90	111.55
1	A	5	ASN	CB-CG-OD1	6.50	133.79	120.80
1	A	97	LEU	CA-C-O	-6.47	114.03	120.70
1	A	28	ARG	CD-NE-CZ	6.46	133.44	124.40
1	A	150	GLU	CB-CG-CD	6.45	123.56	112.60
1	A	101	GLU	CA-CB-CG	6.41	126.92	114.10
1	A	182	TYR	O-C-N	6.39	131.49	123.19
1	A	145	ASP	CB-CA-C	6.34	121.02	109.99
1	A	165	VAL	N-CA-CB	-6.32	103.94	111.90
1	A	60	ILE	O-C-N	6.29	128.28	121.10
1	A	173	LYS	CA-C-O	-6.24	113.29	121.08
1	A	99	LEU	CA-C-N	6.22	129.24	120.28
1	A	99	LEU	C-N-CA	6.22	129.24	120.28
1	A	127	HIS	O-C-N	6.22	127.50	121.28
1	A	21	ASP	O-C-N	-6.20	114.19	122.74
1	A	127	HIS	CA-C-N	-6.14	113.97	120.66
1	A	127	HIS	C-N-CA	-6.14	113.97	120.66
1	A	35	GLN	O-C-N	-6.07	115.81	122.07
1	A	154	GLU	CA-C-O	-6.06	112.64	119.79
1	A	81	GLU	CG-CD-OE1	6.05	132.32	118.40
1	A	186	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	101	GLU	CB-CG-CD	6.03	122.86	112.60
1	A	74	VAL	CA-C-N	5.98	131.25	123.00
1	A	74	VAL	C-N-CA	5.98	131.25	123.00
1	A	150	GLU	CA-CB-CG	5.97	126.04	114.10
1	A	65	ARG	NE-CZ-NH2	5.96	124.56	119.20
1	A	78	GLU	N-CA-CB	5.95	119.13	110.26
1	A	89	LEU	CA-C-O	-5.94	113.73	120.32
1	A	154	GLU	CB-CG-CD	5.92	122.67	112.60
1	A	98	LYS	CA-C-N	5.89	128.77	120.28
1	A	98	LYS	C-N-CA	5.89	128.77	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	PRO	CB-CA-C	5.89	120.28	111.68
1	A	31	PHE	CA-CB-CG	-5.89	107.91	113.80
1	A	87	HIS	N-CA-CB	5.85	118.88	110.40
1	A	44	GLU	CB-CA-C	-5.81	100.35	109.70
1	A	60	ILE	CA-C-O	-5.81	112.17	119.95
1	A	154	GLU	N-CA-CB	5.80	119.23	110.30
1	A	27	LEU	CA-C-O	-5.78	114.11	120.70
1	A	120	VAL	CA-C-O	-5.78	114.23	120.47
1	A	77	ARG	CA-C-N	5.76	133.91	121.64
1	A	77	ARG	C-N-CA	5.76	133.91	121.64
1	A	102	GLN	N-CA-C	-5.75	102.83	110.07
1	A	91	ARG	CD-NE-CZ	5.72	132.41	124.40
1	A	5	ASN	CA-C-O	-5.72	114.42	121.11
1	A	35	GLN	CG-CD-NE2	-5.69	107.86	116.40
1	A	148	PHE	CB-CA-C	5.69	116.89	108.87
1	A	43	VAL	CB-CA-C	-5.68	101.98	111.29
1	A	47	GLN	CB-CG-CD	-5.66	102.99	112.60
1	A	72	ASN	CB-CG-ND2	5.61	124.81	116.40
1	A	145	ASP	CA-C-O	5.58	125.76	119.18
1	A	133	LEU	CA-C-O	-5.57	114.40	120.36
1	A	92	SER	O-C-N	5.57	128.97	123.46
1	A	130	HIS	O-C-N	-5.56	116.18	123.02
1	A	157	LYS	CA-C-O	-5.55	114.27	120.54
1	A	40	THR	N-CA-C	5.54	118.27	109.96
1	A	32	ARG	CD-NE-CZ	-5.49	116.72	124.40
1	A	35	GLN	CA-C-O	5.47	126.57	120.82
1	A	148	PHE	N-CA-C	-5.46	103.19	110.07
1	A	143	GLU	N-CA-C	-5.46	101.83	109.96
1	A	146	THR	OG1-CB-CG2	5.45	120.21	109.30
1	A	71	ILE	N-CA-C	-5.42	100.52	108.54
1	A	43	VAL	CA-C-N	5.41	128.53	120.90
1	A	43	VAL	C-N-CA	5.41	128.53	120.90
1	A	7	ILE	CB-CA-C	5.40	120.16	110.65
1	A	102	GLN	CB-CG-CD	5.39	121.77	112.60
1	A	139	MET	N-CA-C	5.39	122.28	110.80
1	A	3	SER	CB-CA-C	-5.38	99.64	109.54
1	A	32	ARG	CA-C-O	5.38	126.25	120.55
1	A	135	VAL	CA-C-N	5.38	129.58	122.42
1	A	135	VAL	C-N-CA	5.38	129.58	122.42
1	A	2	GLY	CA-C-N	5.38	129.38	120.94
1	A	2	GLY	C-N-CA	5.38	129.38	120.94
1	A	70	ARG	CD-NE-CZ	-5.35	116.91	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	LEU	CA-C-O	-5.33	114.61	120.36
1	A	171	GLU	CB-CG-CD	5.32	121.65	112.60
1	A	71	ILE	CA-C-O	-5.31	114.47	120.74
1	A	7	ILE	CA-CB-CG2	5.28	119.47	110.50
1	A	138	ILE	N-CA-C	-5.21	100.26	108.23
1	A	166	LEU	CA-C-O	-5.20	115.47	121.19
1	A	25	PRO	O-C-N	5.17	127.57	121.46
1	A	143	GLU	CA-CB-CG	5.17	124.44	114.10
1	A	144	SER	CA-C-O	-5.17	115.39	121.44
1	A	167	SER	O-C-N	5.15	129.17	122.42
1	A	139	MET	O-C-N	-5.15	115.74	122.59
1	A	77	ARG	CG-CD-NE	-5.13	100.71	112.00
1	A	114	ILE	CB-CA-C	5.13	117.77	111.25
1	A	126	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	59	SER	CA-C-O	-5.13	112.95	119.31
1	A	118	SER	N-CA-C	5.12	119.78	111.37
1	A	126	ASN	OD1-CG-ND2	-5.10	117.50	122.60
1	A	25	PRO	N-CA-CB	5.10	108.03	103.08
1	A	9	ALA	N-CA-CB	5.09	118.60	110.65
1	A	2	GLY	N-CA-C	-5.08	101.13	113.18
1	A	110	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	3	SER	N-CA-C	5.07	117.64	110.50
1	A	12	GLN	CA-C-O	-5.07	114.15	119.97
1	A	153	LEU	CB-CA-C	5.05	120.47	110.17
1	A	113	TRP	CA-C-O	-5.05	114.88	120.38
1	A	28	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	A	32	ARG	O-C-N	-5.02	116.80	122.12
1	A	128	PRO	O-C-N	5.02	129.28	123.21
1	A	172	GLU	CB-CA-C	5.01	119.59	109.68

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	GLU	Mainchain

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	1505	0	1509	69	0
2	A	48	0	26	6	0
3	A	24	0	19	5	0
4	A	69	0	0	3	0
All	All	1646	0	1554	73	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 23.

All (73) 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:139:MET:HE3	1:A:178:LYS:HE2	1.23	1.16
1:A:105:LEU:HD23	1:A:108:LYS:HD2	1.19	1.08
1:A:139:MET:HE3	1:A:178:LYS:CE	1.89	1.01
1:A:139:MET:CE	1:A:178:LYS:HE2	1.91	1.00
1:A:72:ASN:H	1:A:87:HIS:HD2	1.15	0.93
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.34	0.91
1:A:105:LEU:CD2	1:A:108:LYS:HD2	2.05	0.86
1:A:76:SER:O	1:A:91:ARG:HD3	1.76	0.84
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.59	0.83
1:A:36:ARG:HG2	1:A:36:ARG:NH1	1.91	0.81
3:A:188:MXA:HN42	3:A:188:MXA:H5M3	1.45	0.80
1:A:61:PRO:HG2	1:A:64:ASN:HD22	1.49	0.77
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.16	0.76
1:A:28:ARG:O	1:A:32:ARG:HG3	1.89	0.70
1:A:72:ASN:H	1:A:87:HIS:CD2	2.05	0.70
1:A:105:LEU:HD23	1:A:108:LYS:CD	2.10	0.70
1:A:159:LEU:HD12	1:A:181:VAL:HG22	1.75	0.69
1:A:94:ASP:O	1:A:98:LYS:HG3	1.93	0.68
1:A:94:ASP:HB3	1:A:98:LYS:HZ3	1.60	0.67
1:A:145:ASP:OD1	1:A:146:THR:HG22	1.96	0.65
1:A:99:LEU:O	1:A:99:LEU:HD23	1.96	0.65
1:A:22:PHE:HZ	3:A:188:MXA:C7	2.10	0.65
1:A:94:ASP:HB3	1:A:98:LYS:NZ	2.13	0.64
1:A:156:TYR:CZ	1:A:184:LYS:HD2	2.34	0.62
2:A:187:NDP:H52A	2:A:187:NDP:H8A	1.81	0.62
1:A:139:MET:HE3	1:A:178:LYS:CD	2.30	0.62
1:A:102:GLN:CB	1:A:104:GLU:HG3	2.29	0.61
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PRO:HA	1:A:106:ALA:HB2	1.81	0.60
1:A:102:GLN:HG3	1:A:104:GLU:OE2	2.02	0.59
3:A:188:MXA:HN42	3:A:188:MXA:C5M	2.14	0.59
1:A:155:LYS:HD2	1:A:184:LYS:HE3	1.84	0.58
1:A:37:MET:HA	1:A:37:MET:HE2	1.85	0.58
1:A:102:GLN:HB3	1:A:104:GLU:HG3	1.85	0.58
1:A:57:TRP:O	1:A:65:ARG:HD2	2.04	0.57
1:A:116:GLY:HA3	2:A:187:NDP:H5N	1.88	0.55
1:A:30:GLU:O	1:A:33:TYR:HB3	2.07	0.55
3:A:188:MXA:H5M3	3:A:188:MXA:N4	2.18	0.55
1:A:16:ILE:O	2:A:187:NDP:H2N	2.08	0.54
1:A:61:PRO:HG2	1:A:64:ASN:ND2	2.22	0.53
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.38	0.53
1:A:124:ALA:O	1:A:127:HIS:HB3	2.10	0.52
1:A:121:TYR:OH	2:A:187:NDP:H41N	2.12	0.50
1:A:36:ARG:HH11	1:A:36:ARG:CG	2.16	0.49
1:A:93:LEU:O	1:A:93:LEU:HG	2.13	0.49
1:A:43:VAL:HG11	1:A:46:LYS:HD2	1.95	0.48
1:A:130:HIS:HB2	1:A:185:ASN:ND2	2.29	0.48
1:A:10:VAL:HG22	1:A:14:MET:HA	1.95	0.48
1:A:184:LYS:HE2	1:A:186:ASP:CG	2.39	0.48
1:A:145:ASP:OD1	1:A:145:ASP:C	2.56	0.47
1:A:102:GLN:HB2	1:A:104:GLU:HG3	1.94	0.47
1:A:17:GLY:HA2	1:A:23:PRO:HD3	1.95	0.46
1:A:83:PRO:HD2	1:A:86:ALA:HB3	1.97	0.46
1:A:99:LEU:HD23	1:A:99:LEU:C	2.40	0.46
1:A:17:GLY:HA2	1:A:21:ASP:O	2.17	0.45
1:A:91:ARG:HD2	4:A:234:HOH:O	2.17	0.45
1:A:131:LEU:HD23	1:A:156:TYR:OH	2.18	0.44
1:A:114:ILE:HG23	1:A:120:VAL:HG12	2.00	0.44
1:A:2:GLY:HA3	4:A:189:HOH:O	2.18	0.43
1:A:24:TRP:HD1	1:A:25:PRO:O	2.02	0.43
1:A:24:TRP:HB3	1:A:142:PHE:CE2	2.54	0.43
1:A:22:PHE:CZ	3:A:188:MXA:C7	2.96	0.42
1:A:75:LEU:O	2:A:187:NDP:H1B	2.19	0.42
1:A:155:LYS:HB3	1:A:184:LYS:HE3	2.02	0.42
1:A:36:ARG:NH1	1:A:37:MET:HE3	2.34	0.42
1:A:99:LEU:HA	1:A:102:GLN:HG2	2.02	0.41
1:A:156:TYR:CE1	1:A:184:LYS:HD2	2.56	0.41
1:A:24:TRP:HB2	1:A:25:PRO:HD2	2.03	0.40
1:A:102:GLN:C	1:A:104:GLU:N	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:CE	1:A:178:LYS:CD	2.99	0.40
1:A:17:GLY:HA3	2:A:187:NDP:O3D	2.21	0.40
1:A:93:LEU:O	1:A:97:LEU:HG	2.20	0.40
1:A:28:ARG:CG	4:A:245:HOH:O	2.70	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	184/186 (99%)	175 (95%)	9 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	168/168 (100%)	152 (90%)	16 (10%)	8	10

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	62	GLU

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Mol	Chain	Res	Type
1	A	63	LYS
1	A	72	ASN
1	A	77	ARG
1	A	84	GLN
1	A	99	LEU
1	A	100	THR
1	A	103	PRO
1	A	104	GLU
1	A	112	VAL
1	A	119	SER
1	A	123	GLU
1	A	131	LEU
1	A	140	GLN
1	A	181	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	12	GLN
1	A	29	ASN
1	A	64	ASN
1	A	87	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	NDP	A	187	-	51,52,52	2.64	18 (35%)	71,80,80	2.40	21 (29%)
3	MXA	A	188	-	25,26,26	1.06	1 (4%)	36,37,37	1.59	6 (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
2	NDP	A	187	-	-	4/34/77/77	0/5/5/5
3	MXA	A	188	-	-	1/8/8/8	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-9.69	1.23	1.45
2	A	187	NDP	P2B-O2B	7.85	1.73	1.59
2	A	187	NDP	C5A-C6A	5.54	1.56	1.41
2	A	187	NDP	C3B-C4B	4.35	1.64	1.53
2	A	187	NDP	C5A-C4A	-3.96	1.32	1.39
2	A	187	NDP	O3B-C3B	3.45	1.51	1.43
2	A	187	NDP	C4N-C3N	3.33	1.56	1.50
2	A	187	NDP	PA-O3	-3.18	1.56	1.59
2	A	187	NDP	C1D-N1N	3.12	1.54	1.46
2	A	187	NDP	O4D-C1D	3.09	1.49	1.42
2	A	187	NDP	C4A-N9A	-2.90	1.31	1.37
2	A	187	NDP	C5A-N7A	2.86	1.44	1.39
2	A	187	NDP	P2B-O2X	-2.64	1.45	1.54
3	A	188	MXA	O5'-C5'	2.53	1.42	1.37
2	A	187	NDP	C4A-N3A	2.44	1.39	1.34
2	A	187	NDP	PN-O2N	-2.37	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O2B-C2B	-2.26	1.36	1.44
2	A	187	NDP	PA-O5B	2.24	1.68	1.59
2	A	187	NDP	O7N-C7N	-2.13	1.19	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NDP	O7N-C7N-C3N	-8.00	105.83	120.90
2	A	187	NDP	O3X-P2B-O2X	6.08	130.61	107.80
2	A	187	NDP	C3N-C7N-N7N	5.76	127.89	117.67
3	A	188	MXA	C51-O5'-C5'	-5.45	105.80	117.50
2	A	187	NDP	O2A-PA-O3	5.08	120.99	107.27
2	A	187	NDP	O3B-C3B-C4B	-5.01	96.69	111.08
2	A	187	NDP	O5D-C5D-C4D	-4.32	94.29	108.99
2	A	187	NDP	O3D-C3D-C4D	-4.19	99.06	111.08
2	A	187	NDP	C4B-O4B-C1B	3.88	118.03	109.47
2	A	187	NDP	C5B-C4B-C3B	-3.85	101.37	115.21
2	A	187	NDP	C1D-N1N-C2N	-3.57	115.26	121.14
2	A	187	NDP	C3N-C2N-N1N	-3.46	118.12	123.20
2	A	187	NDP	C4A-N9A-C8A	3.27	109.17	105.74
3	A	188	MXA	C6'-C1'-C2'	2.97	121.52	118.26
2	A	187	NDP	O3-PA-O1A	-2.78	102.33	110.70
2	A	187	NDP	C2D-C1D-N1N	2.73	120.02	113.31
2	A	187	NDP	N3A-C2A-N1A	2.69	132.65	128.58
2	A	187	NDP	O4B-C1B-C2B	-2.54	102.22	106.59
2	A	187	NDP	O3X-P2B-O2B	-2.50	96.09	105.85
3	A	188	MXA	O2'-C2'-C3'	2.46	128.45	124.30
3	A	188	MXA	N2-C2-N3	-2.44	113.56	117.22
2	A	187	NDP	N6A-C6A-N1A	2.43	123.78	118.38
3	A	188	MXA	C21-O2'-C2'	2.39	121.03	117.51
2	A	187	NDP	O2B-P2B-O1X	-2.37	100.88	109.33
2	A	187	NDP	C2B-C1B-N9A	-2.28	110.00	113.75
2	A	187	NDP	O3B-C3B-C2B	2.07	116.98	111.19
3	A	188	MXA	O5'-C5'-C6'	-2.06	110.20	120.00

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	188	MXA	C7-C6-C9-C1'
2	A	187	NDP	C5D-O5D-PN-O3
2	A	187	NDP	O4D-C1D-N1N-C2N

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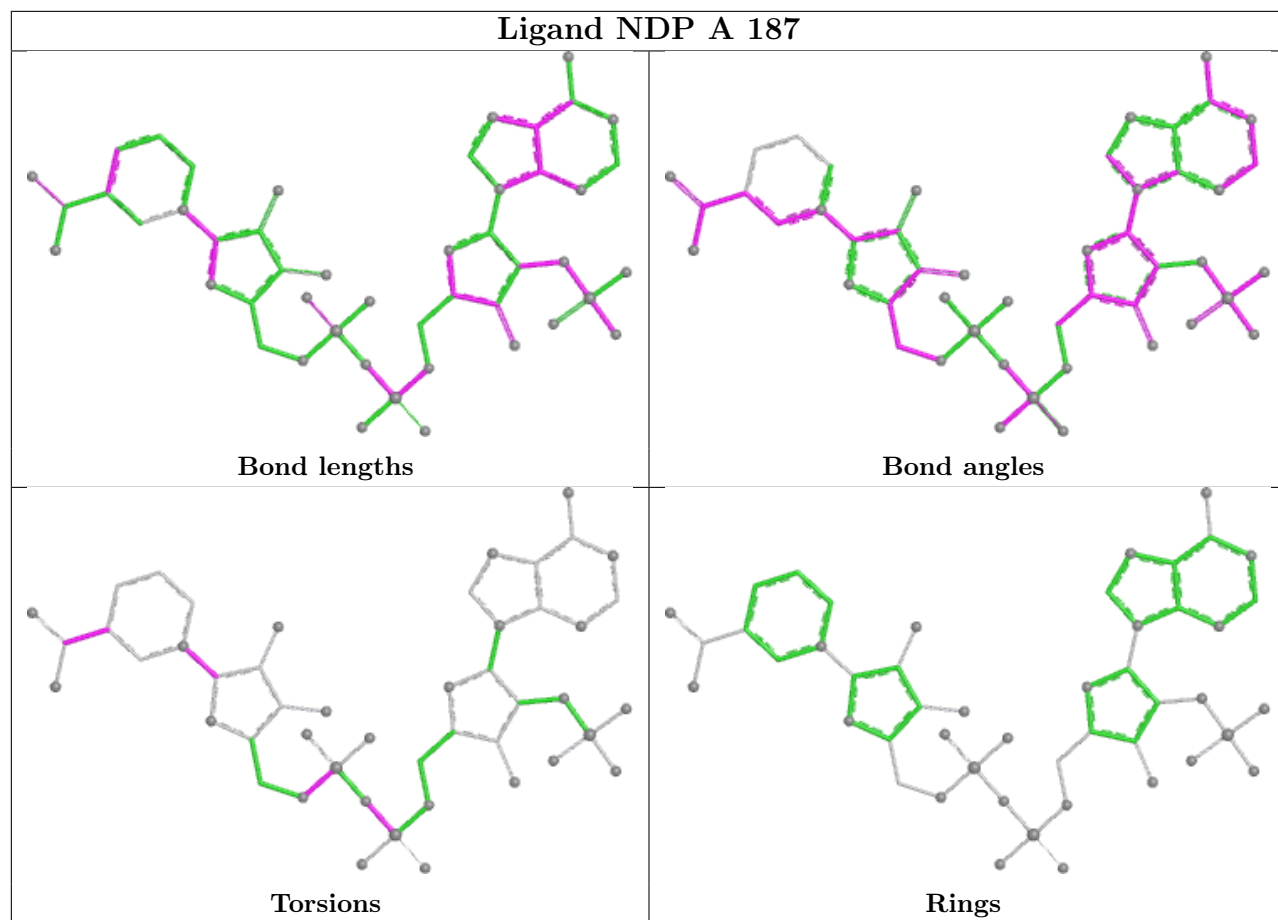
Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C2N-C3N-C7N-N7N
2	A	187	NDP	PN-O3-PA-O1A

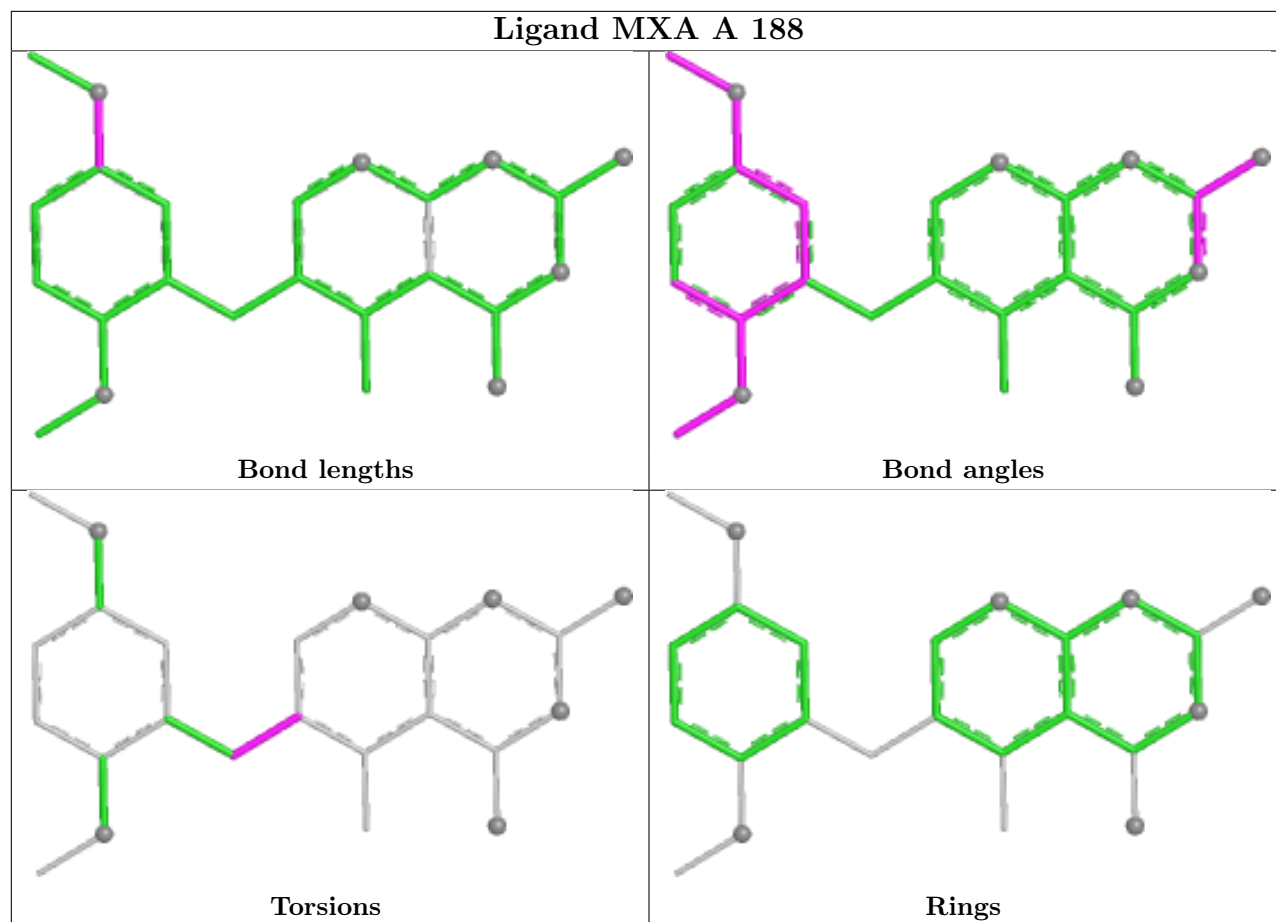
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	6	0
3	A	188	MXA	5	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	105:LEU	C	106:ALA	N	1.20

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.