



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:08 PM UTC

PDB ID : 1DLS / pdb_00001dls
Title : METHOTREXATE-RESISTANT VARIANTS OF HUMAN DIHYDROFOLATE REDUCTASE WITH SUBSTITUTION OF LEUCINE 22: KINETICS, CRYSTALLOGRAPHY AND POTENTIAL AS SELECTABLE MARKERS
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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

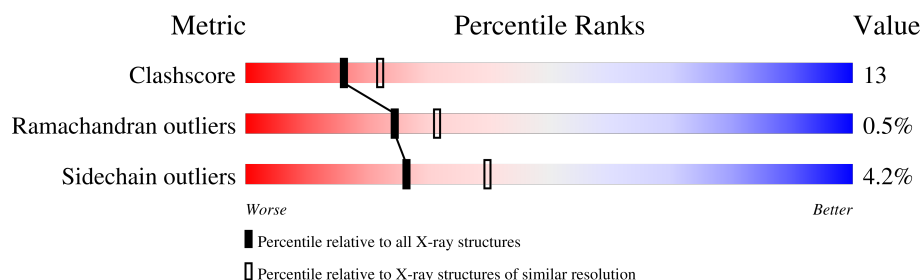
1 Overall quality at a glance

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	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1698 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.

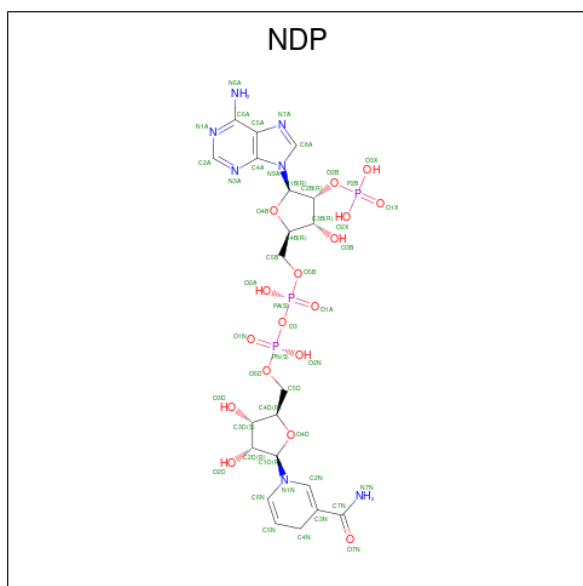
- Molecule 1 is a protein called DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1506	966	253	280	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

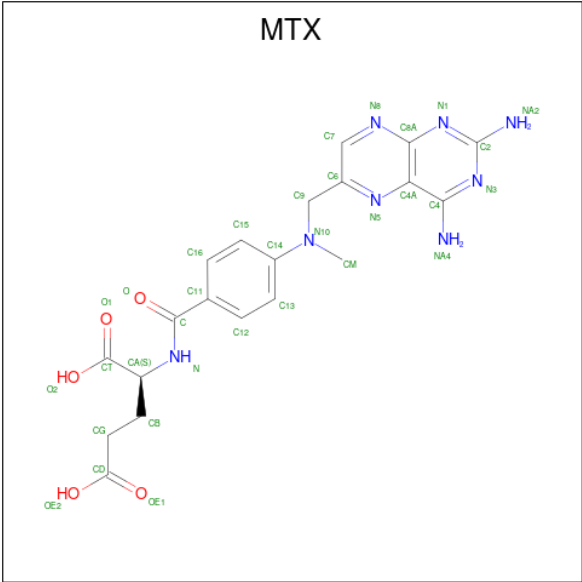
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	TYR	LEU	conflict	UNP P00374

- 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 METHOTREXATE (CCD ID: MTX) (formula: $C_{20}H_{22}N_8O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			33	20	8	5		

- Molecule 4 is water.

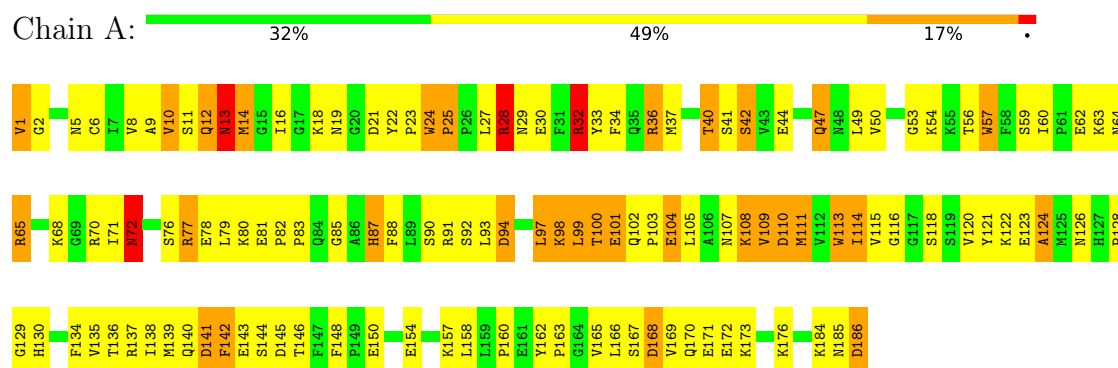
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	111	Total	O	0	0
			111	111		

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	87.50Å 87.50Å 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}	0.156 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1698	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

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: NDP, MTX

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	1.73	15/1542 (1.0%)	3.01	190/2080 (9.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	185	ASN	C-N	8.93	1.45	1.33
1	A	113	TRP	C-N	-8.22	1.25	1.33
1	A	71	ILE	C-O	7.02	1.31	1.24
1	A	53	GLY	N-CA	6.66	1.53	1.45
1	A	56	THR	CA-CB	6.13	1.63	1.53
1	A	54	LYS	CA-CB	6.04	1.62	1.53
1	A	24	TRP	CA-CB	5.96	1.62	1.53
1	A	116	GLY	N-CA	5.83	1.50	1.45
1	A	40	THR	CA-CB	5.52	1.61	1.53
1	A	139	MET	N-CA	5.25	1.53	1.46
1	A	70	ARG	C-O	-5.25	1.17	1.23
1	A	88	PHE	CA-CB	5.19	1.63	1.53
1	A	49	LEU	C-O	5.18	1.30	1.24
1	A	57	TRP	C-N	5.14	1.41	1.33
1	A	37	MET	CG-SD	5.11	1.93	1.80

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ARG	CD-NE-CZ	20.36	152.90	124.40
1	A	65	ARG	NE-CZ-NH2	20.21	137.39	119.20
1	A	25	PRO	O-C-N	-14.37	114.70	121.31
1	A	29	ASN	CA-CB-CG	-13.20	99.40	112.60
1	A	41	SER	CA-C-N	11.19	137.31	120.31
1	A	41	SER	C-N-CA	11.19	137.31	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	91	ARG	CD-NE-CZ	11.05	139.87	124.40
1	A	12	GLN	OE1-CD-NE2	10.69	133.29	122.60
1	A	118	SER	CA-C-O	-10.59	109.33	120.55
1	A	65	ARG	NH1-CZ-NH2	-10.51	105.64	119.30
1	A	28	ARG	NE-CZ-NH1	-10.14	111.36	121.50
1	A	65	ARG	CG-CD-NE	9.79	133.53	112.00
1	A	104	GLU	CA-CB-CG	9.72	133.54	114.10
1	A	19	ASN	CA-CB-CG	-9.63	102.97	112.60
1	A	141	ASP	CA-CB-CG	9.58	122.18	112.60
1	A	27	LEU	CA-C-O	-9.36	110.03	120.70
1	A	141	ASP	CB-CG-OD1	9.35	139.90	118.40
1	A	28	ARG	CD-NE-CZ	-9.23	111.48	124.40
1	A	135	VAL	O-C-N	9.23	132.87	123.18
1	A	79	LEU	O-C-N	9.15	133.66	122.86
1	A	140	GLN	N-CA-CB	9.10	125.70	111.24
1	A	22	TYR	CA-C-O	-9.04	111.11	120.96
1	A	172	GLU	CB-CA-C	8.85	124.84	109.80
1	A	126	ASN	OD1-CG-ND2	-8.75	113.85	122.60
1	A	30	GLU	N-CA-C	-8.72	101.72	111.14
1	A	21	ASP	CA-CB-CG	-8.63	103.97	112.60
1	A	118	SER	O-C-N	8.56	131.19	122.12
1	A	63	LYS	CB-CA-C	-8.50	96.69	110.79
1	A	32	ARG	CA-C-O	8.43	129.49	120.55
1	A	22	TYR	N-CA-C	-8.37	99.15	110.36
1	A	18	LYS	CB-CG-CD	-8.35	92.10	111.30
1	A	72	ASN	OD1-CG-ND2	-8.22	114.38	122.60
1	A	25	PRO	CA-C-O	8.19	126.80	120.90
1	A	92	SER	O-C-N	-8.16	114.69	123.42
1	A	53	GLY	N-CA-C	-8.07	99.85	112.85
1	A	40	THR	CA-C-O	8.00	129.86	120.58
1	A	90	SER	N-CA-CB	7.84	125.63	111.37
1	A	12	GLN	CA-CB-CG	-7.75	98.61	114.10
1	A	137	ARG	NE-CZ-NH1	-7.70	113.80	121.50
1	A	2	GLY	N-CA-C	-7.67	98.66	111.08
1	A	11	SER	N-CA-C	-7.65	100.66	110.53
1	A	118	SER	CB-CA-C	-7.59	98.19	110.79
1	A	56	THR	CA-CB-OG1	-7.56	98.26	109.60
1	A	101	GLU	CB-CG-CD	7.46	125.28	112.60
1	A	110	ASP	CA-CB-CG	-7.39	105.21	112.60
1	A	11	SER	O-C-N	-7.37	113.58	122.65
1	A	98	LYS	O-C-N	-7.34	113.63	122.22
1	A	11	SER	CA-C-O	7.33	130.36	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	78	GLU	CA-CB-CG	7.31	128.71	114.10
1	A	10	VAL	N-CA-C	7.26	118.28	108.11
1	A	97	LEU	CA-C-O	-7.23	112.22	120.24
1	A	44	GLU	CB-CA-C	-7.23	97.22	109.72
1	A	36	ARG	CD-NE-CZ	-7.20	114.32	124.40
1	A	154	GLU	OE1-CD-OE2	7.15	140.06	122.90
1	A	59	SER	CB-CA-C	7.12	123.39	109.72
1	A	170	GLN	OE1-CD-NE2	-7.11	115.50	122.60
1	A	54	LYS	N-CA-CB	-7.10	99.65	110.16
1	A	91	ARG	O-C-N	7.06	132.43	122.41
1	A	124	ALA	N-CA-C	-7.03	103.66	111.82
1	A	154	GLU	CG-CD-OE2	-6.94	102.44	118.40
1	A	126	ASN	CB-CA-C	6.90	121.66	109.65
1	A	168	ASP	CA-CB-CG	-6.89	105.71	112.60
1	A	166	LEU	CA-C-N	6.84	134.34	122.09
1	A	166	LEU	C-N-CA	6.84	134.34	122.09
1	A	137	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	A	122	LYS	CA-C-O	6.76	127.93	120.63
1	A	120	VAL	O-C-N	6.76	128.53	121.91
1	A	139	MET	N-CA-CB	-6.68	102.38	110.53
1	A	78	GLU	CG-CD-OE1	6.66	133.72	118.40
1	A	185	ASN	N-CA-CB	6.65	120.08	110.37
1	A	77	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	A	140	GLN	O-C-N	6.64	130.59	123.56
1	A	109	VAL	O-C-N	6.58	129.90	122.93
1	A	24	TRP	CA-C-N	6.56	124.45	119.66
1	A	24	TRP	C-N-CA	6.56	124.45	119.66
1	A	22	TYR	O-C-N	6.55	129.86	121.34
1	A	70	ARG	CA-C-O	-6.51	113.49	121.11
1	A	82	PRO	O-C-N	6.49	124.30	121.31
1	A	129	GLY	N-CA-C	-6.49	103.02	111.52
1	A	176	LYS	CB-CG-CD	-6.49	96.37	111.30
1	A	22	TYR	N-CA-CB	6.46	117.23	109.74
1	A	1	VAL	CA-C-O	6.42	131.71	120.80
1	A	2	GLY	O-C-N	6.42	130.83	123.58
1	A	102	GLN	N-CA-C	-6.37	101.63	109.65
1	A	94	ASP	CA-CB-CG	-6.36	106.24	112.60
1	A	28	ARG	CA-C-O	-6.32	112.96	120.10
1	A	163	PRO	CA-C-O	-6.29	114.50	121.23
1	A	36	ARG	CA-CB-CG	6.29	126.68	114.10
1	A	78	GLU	CB-CG-CD	6.29	123.29	112.60
1	A	158	LEU	CA-C-O	-6.29	113.58	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	VAL	N-CA-CB	6.28	118.03	110.31
1	A	122	LYS	CA-CB-CG	-6.27	101.56	114.10
1	A	19	ASN	N-CA-C	6.26	119.81	111.30
1	A	160	PRO	O-C-N	6.21	131.01	122.38
1	A	5	ASN	CB-CG-ND2	6.16	125.64	116.40
1	A	113	TRP	CA-C-N	6.16	130.75	122.01
1	A	113	TRP	C-N-CA	6.16	130.75	122.01
1	A	150	GLU	O-C-N	-6.12	115.71	123.06
1	A	110	ASP	CB-CA-C	6.09	122.54	110.42
1	A	102	GLN	O-C-N	6.06	127.85	121.42
1	A	62	GLU	O-C-N	-6.04	115.72	122.12
1	A	11	SER	CA-C-N	6.03	128.64	120.38
1	A	11	SER	C-N-CA	6.03	128.64	120.38
1	A	109	VAL	N-CA-C	6.01	117.67	108.71
1	A	24	TRP	N-CA-CB	-6.00	102.88	109.72
1	A	41	SER	CA-CB-OG	-5.97	99.16	111.10
1	A	87	HIS	CA-CB-CG	-5.97	107.83	113.80
1	A	116	GLY	CA-C-N	5.96	132.43	121.70
1	A	116	GLY	C-N-CA	5.96	132.43	121.70
1	A	37	MET	CG-SD-CE	-5.94	87.84	100.90
1	A	162	TYR	CA-C-N	5.88	126.18	119.83
1	A	162	TYR	C-N-CA	5.88	126.18	119.83
1	A	6	CYS	N-CA-CB	5.88	120.15	110.69
1	A	64	ASN	O-C-N	-5.88	114.81	122.39
1	A	129	GLY	O-C-N	5.82	128.76	123.00
1	A	142	PHE	CA-C-O	-5.79	113.16	120.28
1	A	99	LEU	N-CA-C	5.78	118.36	111.71
1	A	144	SER	CA-C-O	-5.77	114.69	121.44
1	A	141	ASP	CB-CA-C	5.76	119.26	109.53
1	A	60	ILE	CA-CB-CG2	5.73	120.25	110.50
1	A	114	ILE	CB-CA-C	5.72	117.41	111.23
1	A	123	GLU	N-CA-C	5.69	119.40	112.23
1	A	121	TYR	O-C-N	5.68	128.62	122.15
1	A	34	PHE	CA-CB-CG	-5.62	108.18	113.80
1	A	50	VAL	N-CA-CB	5.61	118.88	111.25
1	A	33	TYR	CB-CG-CD1	-5.59	112.41	120.80
1	A	143	GLU	CB-CG-CD	5.59	122.10	112.60
1	A	77	ARG	CA-CB-CG	-5.58	102.95	114.10
1	A	138	ILE	N-CA-CB	5.57	118.17	111.31
1	A	28	ARG	NH1-CZ-NH2	5.57	126.54	119.30
1	A	13	ASN	OD1-CG-ND2	-5.53	117.07	122.60
1	A	81	GLU	CG-CD-OE1	5.53	131.11	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	GLU	CB-CG-CD	5.51	121.97	112.60
1	A	157	LYS	CB-CA-C	-5.47	100.25	109.72
1	A	103	PRO	O-C-N	5.47	130.02	122.64
1	A	100	THR	O-C-N	5.44	129.72	122.43
1	A	111	MET	CG-SD-CE	5.43	112.85	100.90
1	A	18	LYS	CA-CB-CG	-5.42	103.26	114.10
1	A	13	ASN	CA-C-N	5.40	130.52	122.74
1	A	13	ASN	C-N-CA	5.40	130.52	122.74
1	A	29	ASN	OD1-CG-ND2	5.40	128.00	122.60
1	A	165	VAL	CA-C-O	-5.40	114.75	120.53
1	A	63	LYS	N-CA-CB	5.39	118.05	110.12
1	A	134	PHE	N-CA-C	-5.39	98.44	107.99
1	A	13	ASN	CB-CG-ND2	5.39	124.48	116.40
1	A	154	GLU	CA-C-O	-5.38	112.63	119.31
1	A	14	MET	CA-C-O	-5.38	114.11	120.57
1	A	108	LYS	CB-CA-C	-5.33	99.91	109.24
1	A	115	VAL	CA-C-O	-5.32	114.64	119.91
1	A	79	LEU	CA-C-O	-5.31	115.77	121.56
1	A	32	ARG	O-C-N	-5.31	116.49	122.12
1	A	83	PRO	O-C-N	-5.30	116.35	122.71
1	A	19	ASN	OD1-CG-ND2	-5.29	117.31	122.60
1	A	130	HIS	CA-CB-CG	-5.28	108.52	113.80
1	A	102	GLN	N-CA-CB	5.23	118.54	110.01
1	A	68	LYS	N-CA-C	5.22	117.80	110.23
1	A	165	VAL	CA-C-N	5.22	128.12	120.71
1	A	165	VAL	C-N-CA	5.22	128.12	120.71
1	A	19	ASN	N-CA-CB	-5.20	104.18	111.62
1	A	76	SER	CA-C-N	-5.20	113.27	122.26
1	A	76	SER	C-N-CA	-5.20	113.27	122.26
1	A	57	TRP	N-CA-C	-5.19	105.51	111.07
1	A	171	GLU	O-C-N	5.16	129.45	123.41
1	A	185	ASN	OD1-CG-ND2	5.16	127.76	122.60
1	A	99	LEU	CA-C-N	5.16	129.34	120.72
1	A	99	LEU	C-N-CA	5.16	129.34	120.72
1	A	8	VAL	CA-C-O	-5.16	116.29	121.45
1	A	136	THR	N-CA-CB	5.15	118.87	110.37
1	A	85	GLY	CA-C-N	5.14	128.78	121.42
1	A	85	GLY	C-N-CA	5.14	128.78	121.42
1	A	130	HIS	N-CA-CB	-5.14	101.98	109.95
1	A	148	PHE	CA-C-N	5.14	125.04	119.85
1	A	148	PHE	C-N-CA	5.14	125.04	119.85
1	A	25	PRO	CA-C-N	5.12	125.41	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	PRO	C-N-CA	5.12	125.41	119.93
1	A	143	GLU	CA-C-O	-5.11	114.82	120.70
1	A	128	PRO	CA-C-N	-5.11	113.69	123.03
1	A	128	PRO	C-N-CA	-5.11	113.69	123.03
1	A	28	ARG	N-CA-C	5.08	117.56	111.71
1	A	186	ASP	CB-CA-C	5.08	119.76	110.10
1	A	87	HIS	CB-CG-CD2	-5.06	124.62	131.20
1	A	101	GLU	CA-C-O	5.06	125.40	119.28
1	A	142	PHE	O-C-N	5.06	129.53	123.36
1	A	5	ASN	CA-C-O	-5.05	115.20	121.06
1	A	158	LEU	CD1-CG-CD2	-5.04	99.72	110.80
1	A	9	ALA	CA-C-N	5.02	129.71	123.14
1	A	9	ALA	C-N-CA	5.02	129.71	123.14
1	A	21	ASP	CA-C-O	-5.02	115.83	121.40
1	A	36	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	A	173	LYS	CB-CA-C	-5.01	103.80	111.66

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	1506	0	1509	40	0
2	A	48	0	26	3	0
3	A	33	0	20	0	0
4	A	111	0	0	3	0
All	All	1698	0	1555	41	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 13.

All (41) 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:98:LYS:O	1:A:101:GLU:HG2	1.73	0.87
1:A:13:ASN:H	1:A:13:ASN:HD22	1.24	0.83
1:A:72:ASN:H	1:A:87:HIS:HD2	1.31	0.76
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.15	0.76
1:A:10:VAL:HG22	1:A:14:MET:HA	1.70	0.74
1:A:99:LEU:HD23	1:A:105:LEU:HD12	1.70	0.73
1:A:94:ASP:OD1	4:A:293:HOH:O	2.11	0.68
1:A:111:MET:HE3	1:A:113:TRP:HE1	1.60	0.66
2:A:187:NDP:H52A	2:A:187:NDP:H8A	1.79	0.63
1:A:146:THR:HG21	2:A:187:NDP:H4D	1.79	0.63
1:A:72:ASN:H	1:A:87:HIS:CD2	2.15	0.62
1:A:114:ILE:HD13	1:A:124:ALA:HB2	1.81	0.62
1:A:28:ARG:O	1:A:32:ARG:HG3	2.02	0.60
1:A:13:ASN:H	1:A:13:ASN:ND2	1.93	0.59
1:A:184:LYS:NZ	1:A:186:ASP:OD1	2.36	0.59
1:A:40:THR:O	1:A:111:MET:HE2	2.02	0.58
1:A:13:ASN:HD21	1:A:142:PHE:H	1.53	0.57
1:A:93:LEU:O	1:A:97:LEU:HG	2.07	0.55
1:A:10:VAL:CG2	1:A:14:MET:HA	2.36	0.53
1:A:12:GLN:HB3	1:A:141:ASP:OD1	2.10	0.52
1:A:32:ARG:O	1:A:36:ARG:HG2	2.12	0.50
1:A:47:GLN:O	1:A:109:VAL:HA	2.12	0.49
1:A:23:PRO:HD2	1:A:24:TRP:CZ3	2.47	0.49
1:A:107:ASN:OD1	1:A:108:LYS:HG2	2.13	0.49
1:A:99:LEU:HD21	1:A:105:LEU:HD12	1.93	0.48
1:A:1:VAL:N	1:A:100:THR:CG2	2.78	0.46
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.98	0.46
1:A:145:ASP:OD1	1:A:146:THR:HG22	2.16	0.45
1:A:1:VAL:H1	1:A:100:THR:HG21	1.82	0.45
1:A:57:TRP:CE2	1:A:65:ARG:HD2	2.53	0.44
1:A:16:ILE:O	2:A:187:NDP:H2N	2.16	0.44
1:A:99:LEU:HD21	1:A:105:LEU:CD1	2.48	0.44
1:A:80:LYS:HD3	1:A:80:LYS:HA	1.58	0.43
1:A:98:LYS:HG3	4:A:292:HOH:O	2.17	0.43
1:A:1:VAL:H1	1:A:100:THR:CG2	2.32	0.42
1:A:42:SER:HB2	1:A:110:ASP:OD2	2.21	0.41
1:A:114:ILE:HD13	1:A:124:ALA:CB	2.49	0.41
1:A:28:ARG:HA	1:A:28:ARG:HD3	1.62	0.41
1:A:168:ASP:OD1	1:A:168:ASP:N	2.48	0.41
1:A:13:ASN:ND2	1:A:141:ASP:HA	2.36	0.40
1:A:77:ARG:NH2	4:A:206:HOH:O	2.54	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%)	179 (97%)	4 (2%)	1 (0%)	24	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	GLU

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%)	161 (96%)	7 (4%)	26	40

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	28	ARG
1	A	32	ARG
1	A	42	SER
1	A	47	GLN
1	A	72	ASN
1	A	167	SER

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	13	ASN
1	A	47	GLN
1	A	87	HIS
1	A	185	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	MTX	A	188	-	35,35,35	1.37	5 (14%)	47,49,49	2.40	16 (34%)
2	NDP	A	187	-	51,52,52	2.38	20 (39%)	71,80,80	2.43	32 (45%)

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	MTX	A	188	-	-	8/25/25/25	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	187	-	-	12/34/77/77	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-6.77	1.29	1.45
2	A	187	NDP	C5A-C6A	5.73	1.57	1.41
3	A	188	MTX	C8A-N8	-4.52	1.30	1.37
2	A	187	NDP	C5A-C4A	-4.41	1.31	1.39
2	A	187	NDP	C3D-C4D	4.06	1.63	1.53
2	A	187	NDP	O4D-C1D	3.92	1.51	1.42
2	A	187	NDP	C4N-C3N	3.71	1.57	1.50
2	A	187	NDP	O3B-C3B	3.28	1.51	1.43
2	A	187	NDP	P2B-O2B	3.26	1.65	1.59
2	A	187	NDP	C4A-N9A	-3.15	1.31	1.37
2	A	187	NDP	P2B-O3X	-3.07	1.43	1.54
3	A	188	MTX	OE1-CD	3.02	1.32	1.22
2	A	187	NDP	PN-O2N	-2.90	1.41	1.55
2	A	187	NDP	O7N-C7N	-2.78	1.17	1.24
2	A	187	NDP	C5B-C4B	2.73	1.59	1.51
2	A	187	NDP	C3B-C4B	2.72	1.59	1.53
2	A	187	NDP	C1D-N1N	2.57	1.53	1.46
2	A	187	NDP	C5A-N7A	2.50	1.43	1.39
2	A	187	NDP	O4B-C1B	2.37	1.47	1.42
2	A	187	NDP	PA-O1A	-2.34	1.42	1.50
2	A	187	NDP	O5D-C5D	-2.14	1.36	1.44
2	A	187	NDP	C2B-C1B	2.07	1.58	1.53
3	A	188	MTX	O2-CT	-2.06	1.24	1.30
3	A	188	MTX	C2-NA2	-2.05	1.29	1.33
3	A	188	MTX	C12-C11	2.01	1.42	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	187	NDP	O7N-C7N-C3N	-7.43	106.90	120.90
3	A	188	MTX	C2-N1-C8A	5.71	121.64	115.48
3	A	188	MTX	N1-C2-N3	-5.65	120.03	127.21
2	A	187	NDP	O4D-C1D-N1N	-5.16	98.25	108.08
2	A	187	NDP	C3N-C2N-N1N	-5.10	115.71	123.20
3	A	188	MTX	C4-C4A-N5	5.10	124.25	120.33
2	A	187	NDP	O3D-C3D-C4D	-4.71	97.55	111.08
2	A	187	NDP	PN-O5D-C5D	4.61	147.78	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MTX	CA-N-C	4.56	132.50	121.56
2	A	187	NDP	O5B-C5B-C4B	-4.37	94.11	108.99
2	A	187	NDP	C5D-C4D-C3D	-4.27	99.84	115.21
2	A	187	NDP	C4A-N9A-C8A	4.13	110.08	105.74
2	A	187	NDP	C1D-N1N-C2N	-4.11	114.38	121.14
3	A	188	MTX	OE2-CD-OE1	-4.02	113.00	123.33
3	A	188	MTX	C6-C7-N8	-3.98	119.32	123.14
3	A	188	MTX	CB-CA-CT	-3.89	101.12	110.35
2	A	187	NDP	O2A-PA-O1A	3.87	130.45	112.44
3	A	188	MTX	N8-C8A-N1	3.75	119.86	115.77
3	A	188	MTX	C6-C9-N10	3.63	119.16	112.95
2	A	187	NDP	C2A-N1A-C6A	-3.52	112.94	118.73
2	A	187	NDP	O7N-C7N-N7N	3.51	130.76	122.89
2	A	187	NDP	C5B-C4B-C3B	-3.37	103.06	115.21
2	A	187	NDP	C2B-C1B-N9A	-3.28	108.36	113.75
2	A	187	NDP	C2D-C1D-N1N	3.10	120.92	113.31
3	A	188	MTX	C13-C12-C11	-3.05	117.55	120.80
2	A	187	NDP	O3-PA-O1A	-2.75	102.43	110.70
2	A	187	NDP	C5A-C6A-N6A	-2.74	116.51	123.29
3	A	188	MTX	NA2-C2-N3	2.68	121.25	117.22
2	A	187	NDP	O3-PN-O1N	2.61	118.56	110.70
2	A	187	NDP	O2B-C2B-C1B	-2.59	100.95	110.05
2	A	187	NDP	N9A-C8A-N7A	-2.55	110.32	113.94
3	A	188	MTX	O2-CT-O1	2.55	129.86	124.08
2	A	187	NDP	O3D-C3D-C2D	2.48	119.77	111.82
3	A	188	MTX	C11-C-N	2.48	121.63	117.04
3	A	188	MTX	CB-CG-CD	-2.47	105.91	112.49
2	A	187	NDP	N3A-C2A-N1A	2.42	132.25	128.58
2	A	187	NDP	O3B-C3B-C4B	-2.39	104.23	111.08
2	A	187	NDP	N6A-C6A-N1A	2.32	123.55	118.38
2	A	187	NDP	C3B-C2B-C1B	-2.31	98.38	102.81
3	A	188	MTX	C8A-C4A-N5	-2.28	119.80	122.35
2	A	187	NDP	O2X-P2B-O2B	-2.28	96.97	105.85
3	A	188	MTX	C4A-C8A-N1	-2.18	118.36	121.74
2	A	187	NDP	O4B-C4B-C3B	2.17	109.45	105.15
2	A	187	NDP	O4D-C4D-C5D	2.12	116.14	109.33
2	A	187	NDP	C6N-N1N-C2N	2.09	121.56	119.32
2	A	187	NDP	O2A-PA-O3	-2.07	101.69	107.27
2	A	187	NDP	O4B-C1B-N9A	2.04	112.00	108.09
2	A	187	NDP	P2B-O2B-C2B	-2.00	118.08	123.43

There are no chirality outliers.

All (20) torsion outliers are listed below:

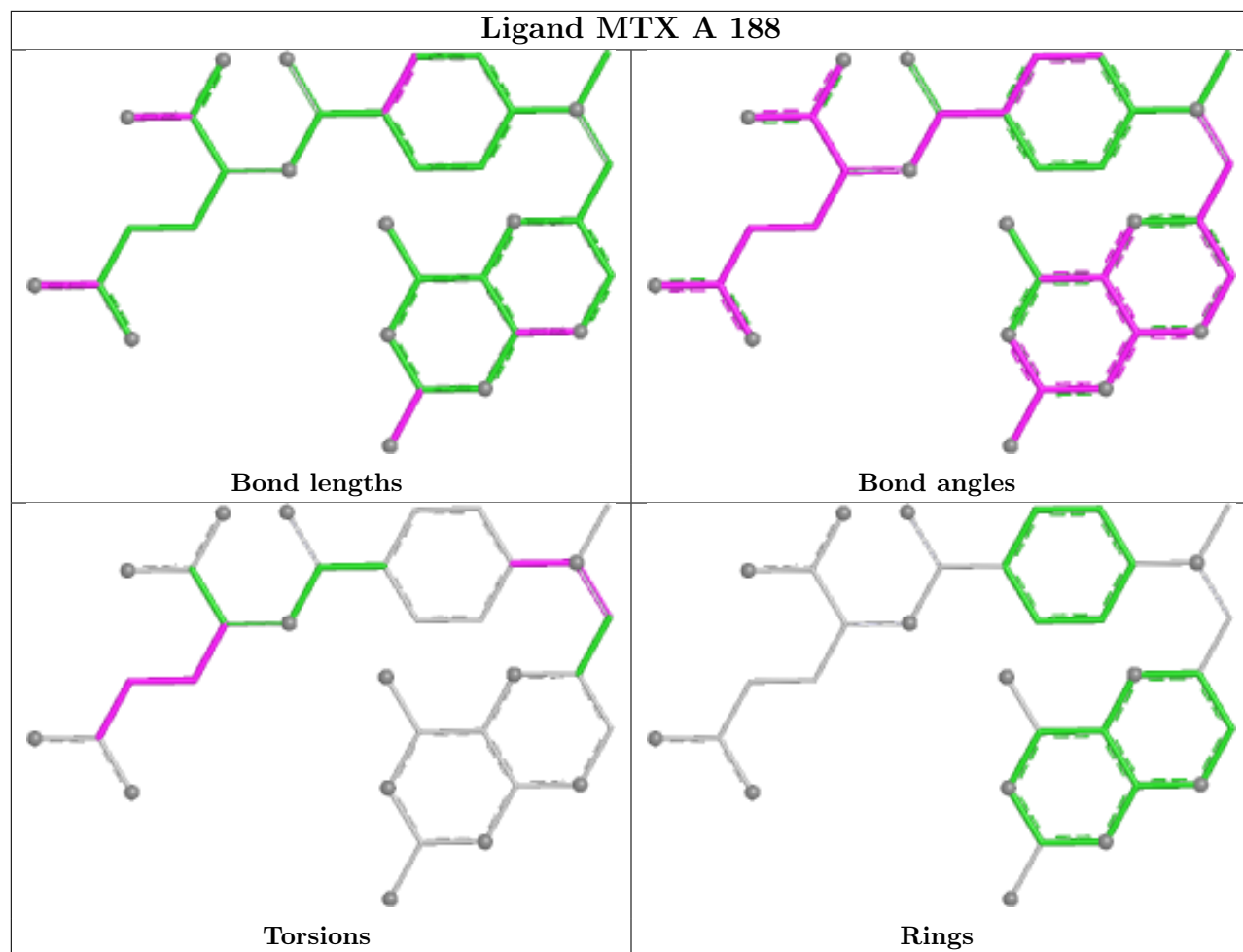
Mol	Chain	Res	Type	Atoms
2	A	187	NDP	C5B-O5B-PA-O2A
2	A	187	NDP	C5D-O5D-PN-O1N
2	A	187	NDP	O4D-C4D-C5D-O5D
2	A	187	NDP	C3D-C4D-C5D-O5D
3	A	188	MTX	N-CA-CB-CG
3	A	188	MTX	CT-CA-CB-CG
3	A	188	MTX	C13-C14-N10-CM
3	A	188	MTX	C6-C9-N10-CM
3	A	188	MTX	C15-C14-N10-CM
2	A	187	NDP	C2D-C1D-N1N-C2N
2	A	187	NDP	C5D-O5D-PN-O3
2	A	187	NDP	C5D-O5D-PN-O2N
2	A	187	NDP	O4D-C1D-N1N-C2N
3	A	188	MTX	OE1-CD-CG-CB
3	A	188	MTX	OE2-CD-CG-CB
3	A	188	MTX	CA-CB-CG-CD
2	A	187	NDP	PN-O3-PA-O2A
2	A	187	NDP	PA-O3-PN-O1N
2	A	187	NDP	PN-O3-PA-O1A
2	A	187	NDP	PA-O3-PN-O2N

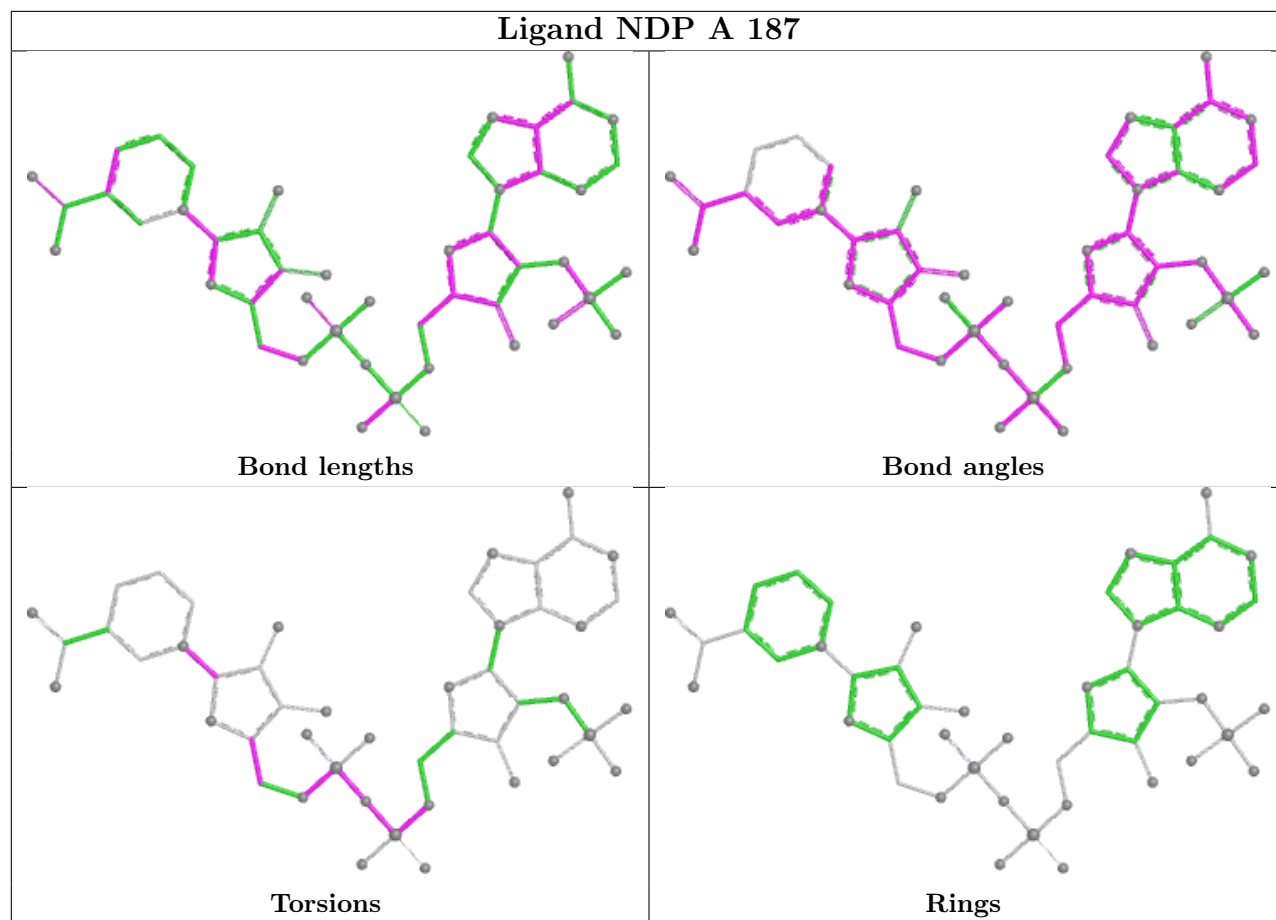
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	187	NDP	3	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

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.