



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:00 PM UTC

PDB ID : 1U72 / pdb_00001u72
Title : Understanding the Role of Leu22 Variants in Methotrexate Resistance: Comparison of Wild-type and Leu22Arg Variant Mouse and Human Dihydrfolate Reductase Ternary Crystal Complexes with Methotrexate and NADPH
Authors : Cody, V.
Deposited on : 2004-08-02
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

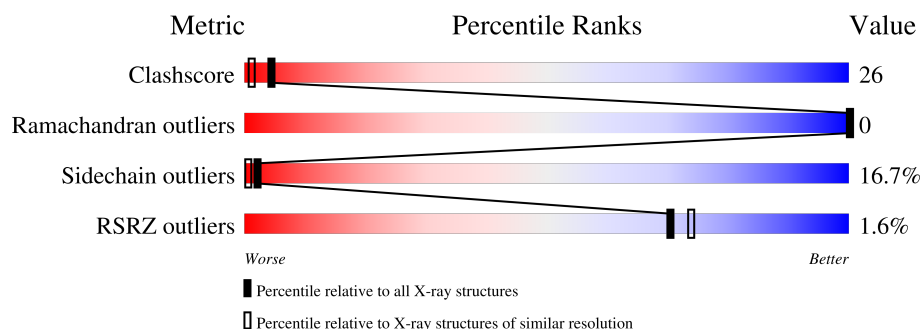
1 Overall quality at a glance

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	186	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1629 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.

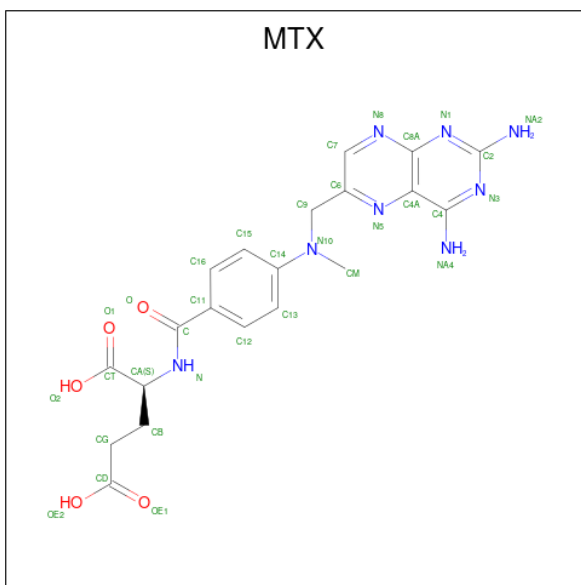
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	186	1502	963	253	279	7	0	0	0

- 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		

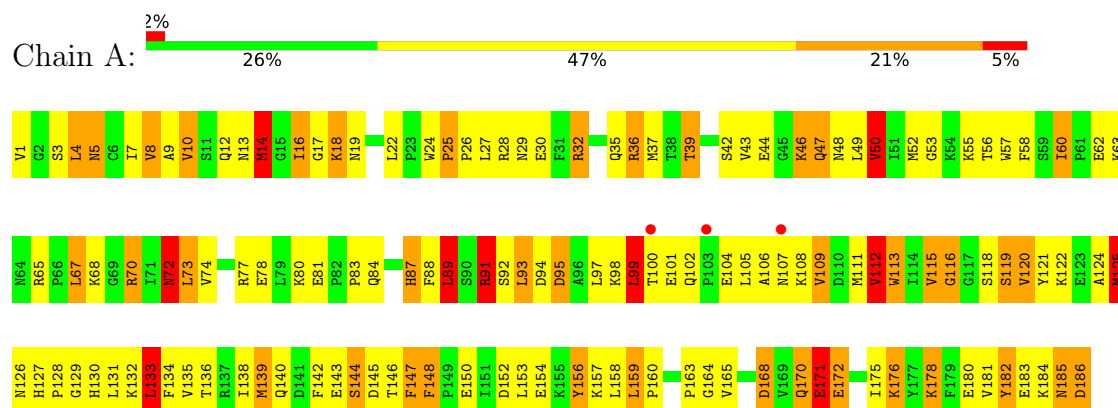
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	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 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	87.38Å 87.38Å 76.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 37.3 (50.00-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 1.90Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, R_{free}	0.159 , 0.213 0.157 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	1629	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.42% 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: MTX, 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	1.18	1/1537 (0.1%)	2.90	176/2073 (8.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	17	GLY	N-CA	5.00	1.50	1.45

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	126	ASN	CA-CB-CG	16.74	129.34	112.60
1	A	145	ASP	CA-CB-CG	14.69	127.29	112.60
1	A	172	GLU	CA-CB-CG	11.54	137.18	114.10
1	A	113	TRP	CA-C-N	11.20	136.37	122.37
1	A	113	TRP	C-N-CA	11.20	136.37	122.37
1	A	29	ASN	CA-CB-CG	-10.14	102.46	112.60
1	A	115	VAL	O-C-N	10.07	132.63	122.05
1	A	3	SER	N-CA-C	9.71	124.19	110.50
1	A	5	ASN	CA-CB-CG	9.71	122.31	112.60
1	A	120	VAL	O-C-N	9.60	132.65	121.80
1	A	32	ARG	CA-C-N	9.54	132.84	120.44
1	A	32	ARG	C-N-CA	9.54	132.84	120.44
1	A	13	ASN	CA-CB-CG	9.48	122.08	112.60
1	A	119	SER	O-C-N	9.33	132.01	122.12
1	A	67	LEU	O-C-N	9.06	133.94	123.06
1	A	67	LEU	CA-C-O	-8.93	111.22	120.96
1	A	95	ASP	CA-CB-CG	-8.79	103.81	112.60
1	A	120	VAL	CA-C-O	-8.76	111.00	120.47
1	A	163	PRO	CA-C-N	8.58	134.55	121.51
1	A	163	PRO	C-N-CA	8.58	134.55	121.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ASN	OD1-CG-ND2	8.44	131.04	122.60
1	A	168	ASP	CA-CB-CG	-8.33	104.27	112.60
1	A	125	MET	CA-CB-CG	8.28	130.66	114.10
1	A	108	LYS	CA-C-N	8.20	133.26	122.93
1	A	108	LYS	C-N-CA	8.20	133.26	122.93
1	A	147	PHE	CA-CB-CG	-8.17	105.63	113.80
1	A	140	GLN	OE1-CD-NE2	8.12	130.72	122.60
1	A	159	LEU	CA-C-N	8.11	127.75	119.56
1	A	159	LEU	C-N-CA	8.11	127.75	119.56
1	A	9	ALA	CA-C-N	8.06	136.22	122.67
1	A	9	ALA	C-N-CA	8.06	136.22	122.67
1	A	132	LYS	O-C-N	7.94	132.94	123.33
1	A	70	ARG	CA-C-O	-7.90	112.17	120.70
1	A	18	LYS	N-CA-CB	7.88	123.60	110.59
1	A	72	ASN	N-CA-C	7.86	121.46	108.96
1	A	72	ASN	CA-C-O	-7.74	111.76	120.43
1	A	140	GLN	N-CA-CB	7.73	124.11	111.21
1	A	138	ILE	N-CA-C	-7.72	97.11	108.54
1	A	144	SER	CA-C-O	-7.60	112.76	121.58
1	A	87	HIS	CA-C-O	-7.58	110.68	119.24
1	A	115	VAL	CB-CA-C	7.58	121.47	111.85
1	A	26	PRO	CB-CA-C	7.46	120.48	111.46
1	A	50	VAL	CB-CA-C	7.46	121.67	110.63
1	A	133	LEU	CA-CB-CG	7.45	142.36	116.30
1	A	142	PHE	CA-CB-CG	7.42	121.22	113.80
1	A	135	VAL	CA-C-O	-7.38	112.66	120.48
1	A	83	PRO	CA-C-O	-7.22	113.19	121.56
1	A	35	GLN	CB-CG-CD	-7.14	100.45	112.60
1	A	138	ILE	CB-CG1-CD1	7.13	128.78	113.80
1	A	12	GLN	CG-CD-NE2	7.09	127.03	116.40
1	A	3	SER	CA-CB-OG	-7.02	97.06	111.10
1	A	88	PHE	CA-C-O	-6.99	113.50	121.40
1	A	170	GLN	OE1-CD-NE2	-6.99	115.61	122.60
1	A	91	ARG	NE-CZ-NH2	-6.97	112.92	119.20
1	A	10	VAL	CB-CA-C	-6.97	100.08	110.82
1	A	118	SER	N-CA-C	6.93	122.81	111.37
1	A	7	ILE	CB-CA-C	6.91	122.81	110.65
1	A	139	MET	CA-C-O	-6.90	110.64	120.51
1	A	154	GLU	CA-CB-CG	6.88	127.87	114.10
1	A	152	ASP	CA-CB-CG	-6.88	105.72	112.60
1	A	87	HIS	O-C-N	6.88	131.58	122.36
1	A	165	VAL	CB-CA-C	6.85	118.88	110.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	VAL	CA-C-O	6.83	126.69	121.09
1	A	62	GLU	CA-C-N	6.80	130.07	120.28
1	A	62	GLU	C-N-CA	6.80	130.07	120.28
1	A	116	GLY	CA-C-O	-6.78	115.55	122.26
1	A	99	LEU	CA-C-O	6.73	127.55	119.61
1	A	19	ASN	N-CA-CB	-6.72	101.75	111.70
1	A	99	LEU	CA-C-N	6.72	130.53	120.31
1	A	99	LEU	C-N-CA	6.72	130.53	120.31
1	A	19	ASN	OD1-CG-ND2	6.63	129.23	122.60
1	A	78	GLU	CB-CG-CD	6.63	123.87	112.60
1	A	78	GLU	N-CA-C	6.56	119.71	111.24
1	A	181	VAL	CA-C-O	-6.54	113.77	120.25
1	A	156	TYR	N-CA-C	6.48	119.28	108.20
1	A	118	SER	CB-CA-C	-6.47	100.01	110.74
1	A	77	ARG	CB-CA-C	6.41	120.96	109.29
1	A	87	HIS	N-CA-CB	6.34	119.02	110.59
1	A	136	THR	CA-C-O	-6.31	113.36	120.43
1	A	112	VAL	CB-CA-C	6.30	119.96	110.63
1	A	101	GLU	CB-CG-CD	6.30	123.30	112.60
1	A	109	VAL	N-CA-C	6.23	117.27	108.36
1	A	124	ALA	CA-C-N	6.20	129.43	120.38
1	A	124	ALA	C-N-CA	6.20	129.43	120.38
1	A	60	ILE	O-C-N	6.18	128.68	121.57
1	A	165	VAL	N-CA-CB	-6.14	104.24	112.10
1	A	32	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	A	165	VAL	CA-C-N	5.91	129.15	120.82
1	A	165	VAL	C-N-CA	5.91	129.15	120.82
1	A	60	ILE	N-CA-CB	5.86	116.50	110.23
1	A	36	ARG	NE-CZ-NH2	5.81	124.43	119.20
1	A	144	SER	O-C-N	5.79	130.87	122.94
1	A	77	ARG	N-CA-C	-5.75	106.43	113.50
1	A	170	GLN	CG-CD-OE1	5.71	132.22	120.80
1	A	128	PRO	CA-C-N	-5.68	114.50	122.85
1	A	128	PRO	C-N-CA	-5.68	114.50	122.85
1	A	116	GLY	O-C-N	5.66	130.33	123.37
1	A	116	GLY	CA-C-N	5.65	131.87	121.70
1	A	116	GLY	C-N-CA	5.65	131.87	121.70
1	A	91	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	A	180	GLU	CG-CD-OE2	-5.62	105.47	118.40
1	A	91	ARG	CD-NE-CZ	5.60	132.25	124.40
1	A	60	ILE	CB-CA-C	-5.60	105.73	110.94
1	A	72	ASN	CA-CB-CG	-5.59	107.01	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	GLY	N-CA-C	5.59	118.56	111.85
1	A	170	GLN	CB-CG-CD	5.58	122.09	112.60
1	A	156	TYR	CB-CA-C	-5.57	101.87	110.78
1	A	39	THR	CA-C-O	-5.53	113.26	119.79
1	A	160	PRO	CA-C-O	5.53	126.74	119.00
1	A	68	LYS	N-CA-C	5.51	118.91	110.20
1	A	180	GLU	CG-CD-OE1	5.51	131.07	118.40
1	A	127	HIS	CA-C-O	5.50	124.92	119.75
1	A	91	ARG	CB-CG-CD	5.48	123.91	111.30
1	A	47	GLN	N-CA-C	5.47	118.50	109.85
1	A	89	LEU	CD1-CG-CD2	-5.46	98.78	110.80
1	A	172	GLU	CA-C-O	-5.45	114.06	120.60
1	A	53	GLY	CA-C-O	-5.44	114.67	122.62
1	A	115	VAL	CA-C-N	-5.44	113.84	122.65
1	A	115	VAL	C-N-CA	-5.44	113.84	122.65
1	A	126	ASN	CB-CG-OD1	5.43	131.65	120.80
1	A	164	GLY	CA-C-O	5.41	125.79	119.19
1	A	99	LEU	N-CA-CB	-5.41	100.44	110.18
1	A	16	ILE	O-C-N	-5.41	116.22	122.17
1	A	134	PHE	CA-C-O	-5.40	114.92	120.54
1	A	150	GLU	N-CA-CB	5.37	118.45	110.29
1	A	148	PHE	CA-CB-CG	-5.36	108.44	113.80
1	A	136	THR	N-CA-C	-5.35	100.45	108.96
1	A	176	LYS	CB-CA-C	-5.34	100.37	109.51
1	A	56	THR	N-CA-CB	5.34	118.03	110.13
1	A	73	LEU	N-CA-C	5.34	117.60	108.90
1	A	129	GLY	O-C-N	5.33	128.42	123.35
1	A	119	SER	N-CA-C	-5.33	105.47	111.28
1	A	182	TYR	CA-C-N	-5.32	114.33	122.62
1	A	182	TYR	C-N-CA	-5.32	114.33	122.62
1	A	112	VAL	CA-C-O	5.30	125.96	120.39
1	A	25	PRO	N-CA-C	-5.30	104.23	110.70
1	A	171	GLU	CA-C-N	-5.29	113.26	122.37
1	A	171	GLU	C-N-CA	-5.29	113.26	122.37
1	A	132	LYS	CA-C-O	-5.28	114.26	120.60
1	A	145	ASP	OD1-CG-OD2	-5.27	110.24	122.90
1	A	160	PRO	CB-CA-C	-5.26	104.00	111.68
1	A	186	ASP	CA-C-O	-5.25	105.25	121.00
1	A	78	GLU	CG-CD-OE1	5.24	130.46	118.40
1	A	48	ASN	CB-CG-OD1	-5.24	110.33	120.80
1	A	107	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	A	36	ARG	CD-NE-CZ	-5.23	117.07	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	159	LEU	N-CA-CB	-5.23	102.76	110.14
1	A	48	ASN	CB-CG-ND2	5.21	124.21	116.40
1	A	113	TRP	O-C-N	-5.19	117.25	123.27
1	A	27	LEU	N-CA-C	-5.19	99.33	108.20
1	A	157	LYS	CB-CA-C	-5.18	100.98	109.53
1	A	42	SER	CB-CA-C	-5.18	100.27	110.11
1	A	29	ASN	OD1-CG-ND2	5.17	127.78	122.60
1	A	46	LYS	O-C-N	5.16	129.66	123.16
1	A	47	GLN	OE1-CD-NE2	5.16	127.76	122.60
1	A	145	ASP	CB-CG-OD1	5.15	130.25	118.40
1	A	37	MET	N-CA-C	5.15	116.58	111.07
1	A	170	GLN	N-CA-C	-5.15	102.44	110.42
1	A	150	GLU	CB-CG-CD	5.14	121.34	112.60
1	A	143	GLU	CA-C-O	-5.14	115.06	120.92
1	A	135	VAL	N-CA-C	5.13	115.36	108.17
1	A	4	LEU	N-CA-CB	5.10	118.55	110.55
1	A	175	ILE	CA-C-O	5.10	125.69	120.39
1	A	172	GLU	CB-CA-C	5.08	119.70	109.38
1	A	32	ARG	CD-NE-CZ	5.08	131.51	124.40
1	A	7	ILE	CA-C-N	5.06	127.77	122.11
1	A	7	ILE	C-N-CA	5.06	127.77	122.11
1	A	80	LYS	CB-CA-C	-5.05	100.56	110.11
1	A	158	LEU	CA-C-O	-5.04	114.95	120.69
1	A	154	GLU	CB-CG-CD	5.02	121.14	112.60
1	A	58	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	14	MET	CA-C-O	-5.02	115.78	121.65
1	A	95	ASP	O-C-N	5.01	127.86	122.15
1	A	70	ARG	O-C-N	5.01	129.74	123.23
1	A	156	TYR	CA-C-N	5.00	129.49	122.09
1	A	156	TYR	C-N-CA	5.00	129.49	122.09

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	80	0
2	A	48	0	26	5	0
3	A	33	0	20	3	0
4	A	46	0	0	3	0
All	All	1629	0	1557	83	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 26.

All (83) 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:43:VAL:HG11	1:A:46:LYS:HD2	1.21	1.09
1:A:99:LEU:HD22	1:A:105:LEU:HD12	1.33	1.09
1:A:1:VAL:CG2	1:A:100:THR:HG22	1.88	1.01
1:A:43:VAL:CG1	1:A:46:LYS:HD2	1.90	1.01
1:A:1:VAL:HG22	1:A:100:THR:HG22	1.40	1.01
1:A:99:LEU:CD2	1:A:105:LEU:HD12	2.00	0.91
1:A:130:HIS:ND1	1:A:184:LYS:O	2.04	0.91
1:A:168:ASP:O	1:A:170:GLN:NE2	2.06	0.86
1:A:99:LEU:HD22	1:A:105:LEU:CD1	2.05	0.85
1:A:43:VAL:HG11	1:A:46:LYS:CD	2.07	0.85
1:A:72:ASN:H	1:A:87:HIS:HD2	1.26	0.83
1:A:4:LEU:HD23	1:A:131:LEU:CD1	2.09	0.82
1:A:93:LEU:O	1:A:97:LEU:HG	1.79	0.81
1:A:73:LEU:C	1:A:73:LEU:HD23	2.06	0.81
1:A:4:LEU:HD12	1:A:112:VAL:HG22	1.68	0.76
1:A:94:ASP:O	1:A:98:LYS:HG3	1.90	0.72
1:A:159:LEU:O	4:A:212:HOH:O	2.06	0.72
1:A:36:ARG:HG2	1:A:36:ARG:NH1	2.05	0.70
1:A:184:LYS:HG2	1:A:185:ASN:N	2.07	0.68
1:A:99:LEU:HA	1:A:102:GLN:HG2	1.78	0.66
1:A:1:VAL:HG21	1:A:100:THR:HG22	1.75	0.66
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.60	0.65
1:A:91:ARG:HB3	4:A:221:HOH:O	1.97	0.64
1:A:4:LEU:HD23	1:A:131:LEU:HD13	1.80	0.63
1:A:72:ASN:N	1:A:72:ASN:HD22	1.99	0.61
1:A:14:MET:O	1:A:147:PHE:HD2	1.84	0.61
1:A:36:ARG:HH11	1:A:36:ARG:CG	2.15	0.60
1:A:121:TYR:O	1:A:125:MET:HB2	2.02	0.59
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.86	0.58
2:A:187:NDP:H52A	2:A:187:NDP:H8A	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:VAL:HG22	2:A:187:NDP:N7A	2.20	0.56
1:A:73:LEU:HD23	1:A:74:VAL:N	2.21	0.56
1:A:50:VAL:HA	1:A:113:TRP:O	2.06	0.56
1:A:133:LEU:HD22	1:A:156:TYR:CE2	2.40	0.56
1:A:130:HIS:HE1	1:A:183:GLU:CG	2.19	0.56
1:A:50:VAL:HG21	1:A:67:LEU:HD12	1.88	0.55
1:A:72:ASN:H	1:A:87:HIS:CD2	2.16	0.55
1:A:171:GLU:HA	1:A:176:LYS:HA	1.88	0.55
1:A:50:VAL:HG23	1:A:52:MET:CE	2.38	0.54
1:A:47:GLN:O	1:A:109:VAL:HA	2.09	0.53
1:A:182:TYR:CD1	1:A:182:TYR:N	2.76	0.53
1:A:55:LYS:NZ	4:A:194:HOH:O	2.37	0.52
1:A:139:MET:SD	1:A:178:LYS:HD3	2.50	0.52
1:A:168:ASP:OD2	1:A:168:ASP:N	2.42	0.51
1:A:28:ARG:O	1:A:32:ARG:HG3	2.11	0.51
1:A:73:LEU:C	1:A:73:LEU:CD2	2.80	0.51
1:A:130:HIS:CE1	1:A:183:GLU:HG3	2.46	0.51
1:A:39:THR:HG22	1:A:39:THR:O	2.10	0.50
1:A:130:HIS:CE1	1:A:184:LYS:O	2.64	0.49
1:A:139:MET:HB2	1:A:176:LYS:O	2.12	0.49
1:A:57:TRP:O	1:A:65:ARG:HD2	2.13	0.49
1:A:184:LYS:CG	1:A:185:ASN:N	2.76	0.48
1:A:125:MET:HE1	1:A:148:PHE:CE2	2.48	0.48
1:A:16:ILE:O	2:A:187:NDP:H2N	2.14	0.47
1:A:81:GLU:C	1:A:89:LEU:HD23	2.39	0.47
1:A:102:GLN:O	1:A:106:ALA:N	2.44	0.46
1:A:130:HIS:HE1	1:A:183:GLU:CD	2.22	0.46
1:A:60:ILE:O	1:A:65:ARG:HD3	2.16	0.46
1:A:184:LYS:HE2	1:A:186:ASP:CG	2.42	0.45
1:A:130:HIS:HE1	1:A:183:GLU:HG3	1.82	0.45
1:A:133:LEU:HD22	1:A:156:TYR:CD2	2.52	0.45
1:A:52:MET:HA	1:A:116:GLY:O	2.17	0.44
1:A:52:MET:HE2	1:A:52:MET:HB3	1.84	0.44
1:A:91:ARG:HE	1:A:92:SER:HB3	1.83	0.43
1:A:120:VAL:CG2	2:A:187:NDP:N7A	2.81	0.43
1:A:49:LEU:HD23	1:A:112:VAL:HB	2.00	0.43
1:A:50:VAL:HG23	1:A:52:MET:HE1	2.01	0.43
1:A:8:VAL:HG21	1:A:148:PHE:CD1	2.54	0.42
1:A:39:THR:O	1:A:39:THR:CG2	2.68	0.42
1:A:130:HIS:ND1	1:A:185:ASN:HB2	2.34	0.42
1:A:186:ASP:OD1	1:A:186:ASP:C	2.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:NE	1:A:95:ASP:OD2	2.52	0.42
1:A:22:LEU:HD11	3:A:188:MTX:H7	2.01	0.42
3:A:188:MTX:H15	3:A:188:MTX:HM1	1.82	0.42
1:A:24:TRP:HB2	1:A:25:PRO:CD	2.50	0.41
1:A:170:GLN:O	1:A:176:LYS:HA	2.19	0.41
1:A:1:VAL:CG1	1:A:100:THR:HG21	2.50	0.41
1:A:70:ARG:O	1:A:72:ASN:ND2	2.54	0.41
1:A:4:LEU:HD23	1:A:131:LEU:HD11	1.97	0.41
1:A:70:ARG:HH22	3:A:188:MTX:CT	2.34	0.41
1:A:184:LYS:HG2	1:A:185:ASN:H	1.84	0.41
2:A:187:NDP:H6N	2:A:187:NDP:H52N	2.02	0.41
1:A:24:TRP:HA	1:A:25:PRO:HD3	1.76	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%)	176 (96%)	8 (4%)	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%)	140 (83%)	28 (17%)	2 0

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	10	VAL
1	A	14	MET
1	A	18	LYS
1	A	30	GLU
1	A	44	GLU
1	A	50	VAL
1	A	63	LYS
1	A	72	ASN
1	A	84	GLN
1	A	89	LEU
1	A	91	ARG
1	A	93	LEU
1	A	99	LEU
1	A	104	GLU
1	A	111	MET
1	A	112	VAL
1	A	115	VAL
1	A	119	SER
1	A	122	LYS
1	A	125	MET
1	A	133	LEU
1	A	144	SER
1	A	146	THR
1	A	153	LEU
1	A	171	GLU
1	A	172	GLU
1	A	178	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
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	$\# Z > 2$
3	MTX	A	188	-	35,35,35	1.13	2 (5%)	47,49,49	2.23	16 (34%)
2	NDP	A	187	-	51,52,52	2.57	14 (27%)	71,80,80	2.15	26 (36%)

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	-	-	5/25/25/25	0/3/3/3
2	NDP	A	187	-	-	13/34/77/77	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	O4B-C4B	-9.74	1.23	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	187	NDP	P2B-O2B	6.70	1.71	1.59
2	A	187	NDP	C5A-C6A	5.52	1.56	1.41
2	A	187	NDP	C5A-C4A	-5.12	1.29	1.39
2	A	187	NDP	C3B-C4B	4.40	1.64	1.53
2	A	187	NDP	O3B-C3B	3.58	1.51	1.43
2	A	187	NDP	PA-O3	-3.30	1.55	1.59
2	A	187	NDP	C4A-N9A	-3.04	1.31	1.37
3	A	188	MTX	OE1-CD	2.89	1.31	1.22
2	A	187	NDP	C1D-N1N	2.85	1.54	1.46
2	A	187	NDP	PN-O1N	-2.77	1.41	1.50
2	A	187	NDP	O4D-C1D	2.71	1.48	1.42
2	A	187	NDP	P2B-O3X	-2.42	1.45	1.54
2	A	187	NDP	C5A-N7A	2.14	1.43	1.39
2	A	187	NDP	C4N-C3N	2.13	1.54	1.50
3	A	188	MTX	O1-CT	2.11	1.28	1.22

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MTX	CG-CB-CA	-6.34	101.47	113.16
2	A	187	NDP	O3X-P2B-O2X	5.08	126.86	107.80
3	A	188	MTX	C2-N1-C8A	4.64	120.49	115.48
2	A	187	NDP	O7N-C7N-C3N	-4.42	112.57	120.90
2	A	187	NDP	O4D-C4D-C3D	-4.20	96.81	105.15
3	A	188	MTX	CA-N-C	4.08	131.35	121.56
2	A	187	NDP	O3-PA-O1A	-4.01	98.63	110.70
3	A	188	MTX	OE2-CD-OE1	-4.00	113.04	123.33
2	A	187	NDP	C4B-O4B-C1B	3.97	118.23	109.47
2	A	187	NDP	O4B-C1B-C2B	-3.91	99.86	106.59
2	A	187	NDP	C3N-C7N-N7N	3.90	124.59	117.67
3	A	188	MTX	O-C-C11	-3.84	113.30	120.90
2	A	187	NDP	O3B-C3B-C4B	-3.82	100.11	111.08
3	A	188	MTX	O2-CT-O1	3.76	132.61	124.08
3	A	188	MTX	N8-C8A-N1	3.72	119.82	115.77
2	A	187	NDP	C5B-C4B-C3B	-3.68	101.95	115.21
2	A	187	NDP	O3D-C3D-C4D	-3.58	100.80	111.08
2	A	187	NDP	C2D-C1D-N1N	3.51	121.94	113.31
3	A	188	MTX	O-C-N	3.39	128.90	122.47
2	A	187	NDP	PN-O5D-C5D	3.37	140.63	121.35
3	A	188	MTX	C4-C4A-N5	3.22	122.80	120.33
2	A	187	NDP	O4B-C1B-N9A	3.05	113.94	108.09
2	A	187	NDP	C2B-C1B-N9A	3.02	118.72	113.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	188	MTX	N1-C2-N3	-2.87	123.56	127.21
3	A	188	MTX	CT-CA-N	2.79	117.03	110.57
2	A	187	NDP	C1B-N9A-C8A	-2.71	121.08	127.09
2	A	187	NDP	O5D-C5D-C4D	-2.68	99.88	108.99
3	A	188	MTX	OE1-CD-CG	2.65	131.48	123.09
2	A	187	NDP	C2B-C3B-C4B	-2.64	96.32	101.99
2	A	187	NDP	O5D-PN-O1N	2.58	119.18	108.94
2	A	187	NDP	C4A-N9A-C8A	2.50	108.37	105.74
3	A	188	MTX	O1-CT-CA	-2.49	114.23	122.26
2	A	187	NDP	O2A-PA-O3	2.45	113.88	107.27
3	A	188	MTX	C8A-C4A-N5	-2.43	119.63	122.35
3	A	188	MTX	C4A-C8A-N1	-2.42	117.99	121.74
2	A	187	NDP	O2A-PA-O1A	2.39	123.55	112.44
3	A	188	MTX	C4A-C4-NA4	2.34	123.88	120.31
2	A	187	NDP	O2B-C2B-C1B	-2.25	102.16	110.05
2	A	187	NDP	O2X-P2B-O2B	-2.24	97.10	105.85
2	A	187	NDP	C2A-N1A-C6A	-2.21	115.10	118.73
2	A	187	NDP	N3A-C2A-N1A	2.08	131.72	128.58
2	A	187	NDP	C5D-C4D-C3D	2.06	122.61	115.21

There are no chirality outliers.

All (18) torsion outliers are listed below:

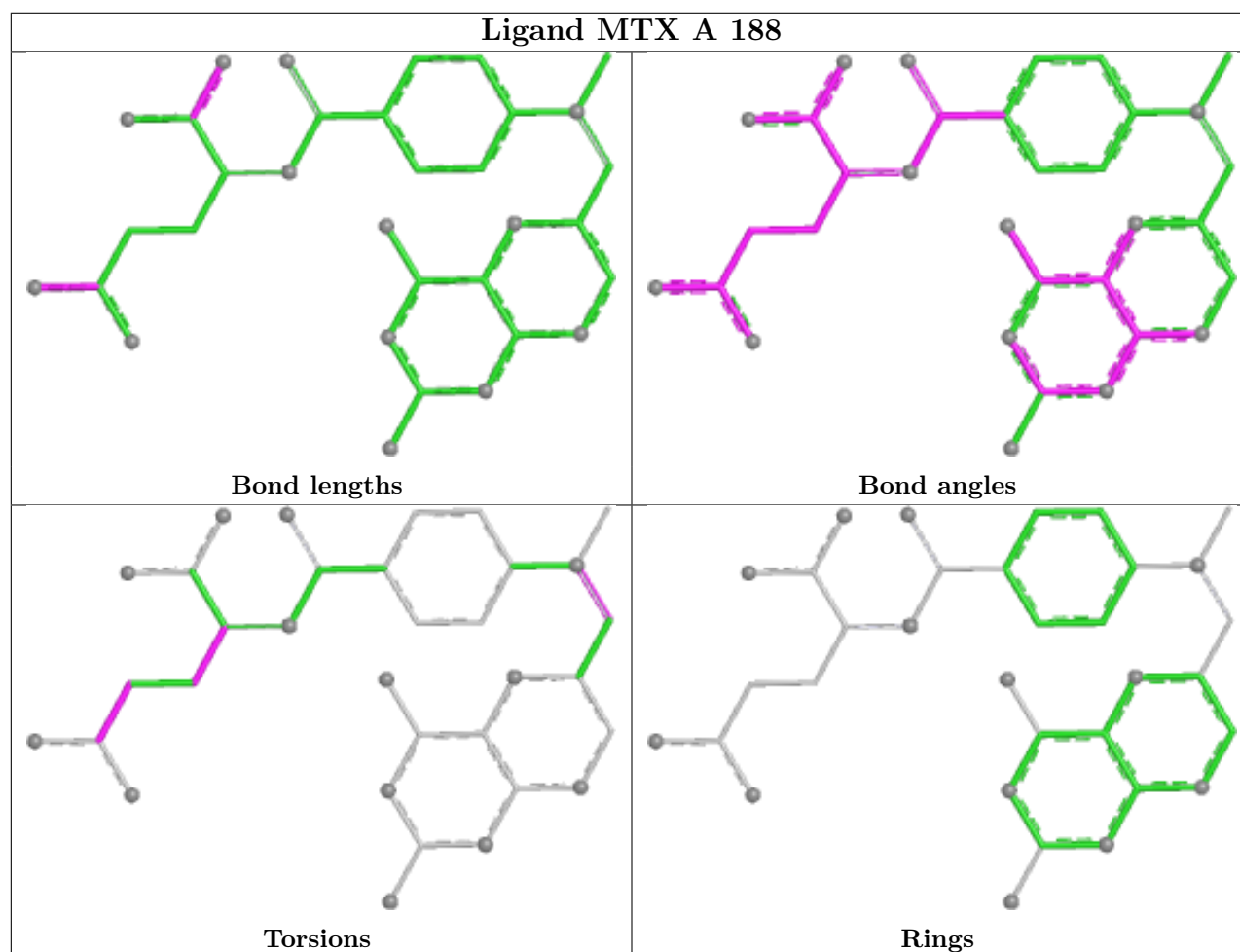
Mol	Chain	Res	Type	Atoms
3	A	188	MTX	N-CA-CB-CG
2	A	187	NDP	C3D-C4D-C5D-O5D
3	A	188	MTX	CT-CA-CB-CG
2	A	187	NDP	O4D-C4D-C5D-O5D
2	A	187	NDP	C5D-O5D-PN-O3
2	A	187	NDP	C5D-O5D-PN-O1N
2	A	187	NDP	C5D-O5D-PN-O2N
2	A	187	NDP	C2D-C1D-N1N-C2N
2	A	187	NDP	O4D-C1D-N1N-C2N
3	A	188	MTX	OE1-CD-CG-CB
2	A	187	NDP	C2N-C3N-C7N-N7N
3	A	188	MTX	OE2-CD-CG-CB
3	A	188	MTX	C6-C9-N10-CM
2	A	187	NDP	PN-O3-PA-O1A
2	A	187	NDP	PA-O3-PN-O2N
2	A	187	NDP	O4D-C1D-N1N-C6N
2	A	187	NDP	C2D-C1D-N1N-C6N
2	A	187	NDP	PN-O3-PA-O2A

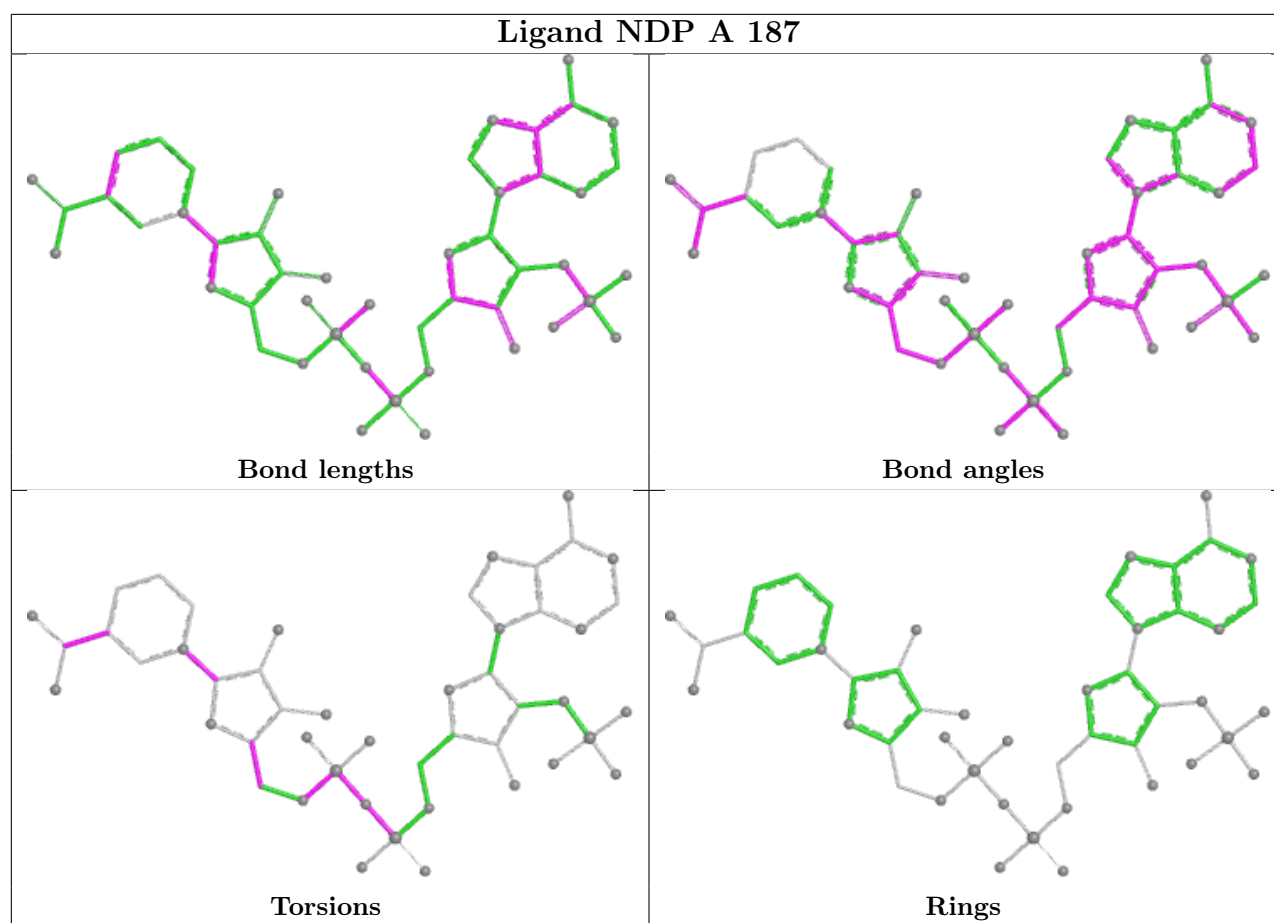
There are no ring outliers.

2 monomers are involved in 8 short contacts:

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

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	186/186 (100%)	-0.29	3 (1%) 70 74	16, 25, 41, 49	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	THR	4.0
1	A	103	PRO	2.6
1	A	107	ASN	2.1

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.

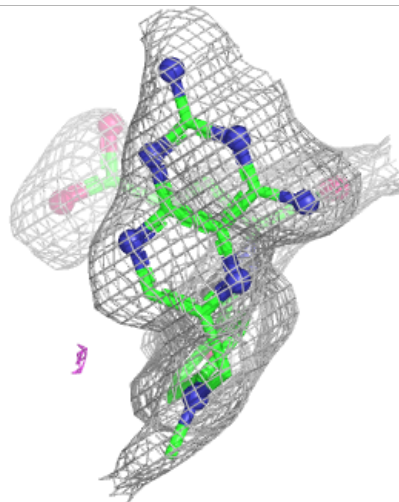
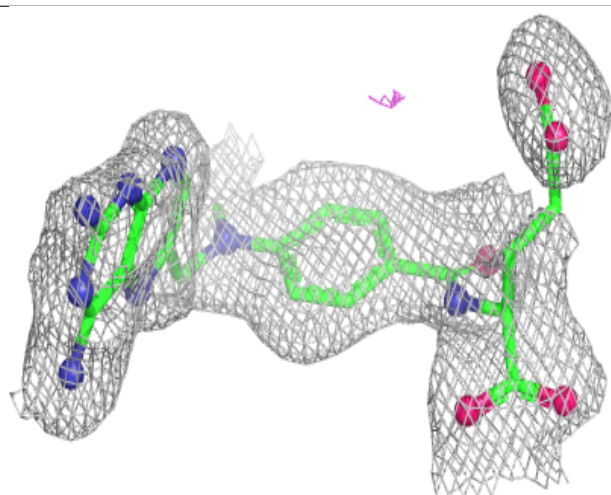
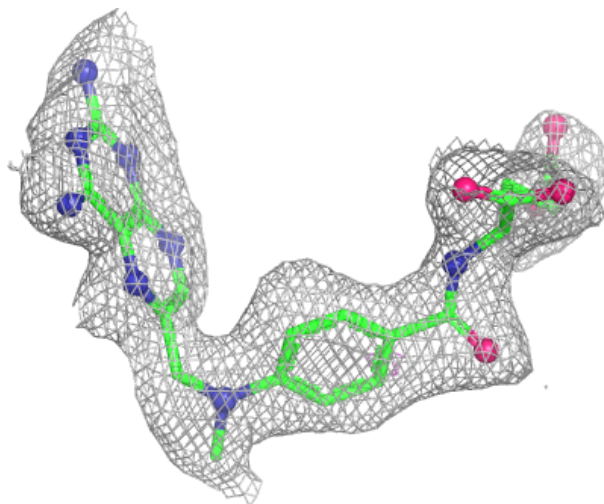
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MTX	A	188	33/33	0.96	0.05	15,19,28,28	0
2	NDP	A	187	48/48	0.98	0.05	16,23,28,28	0

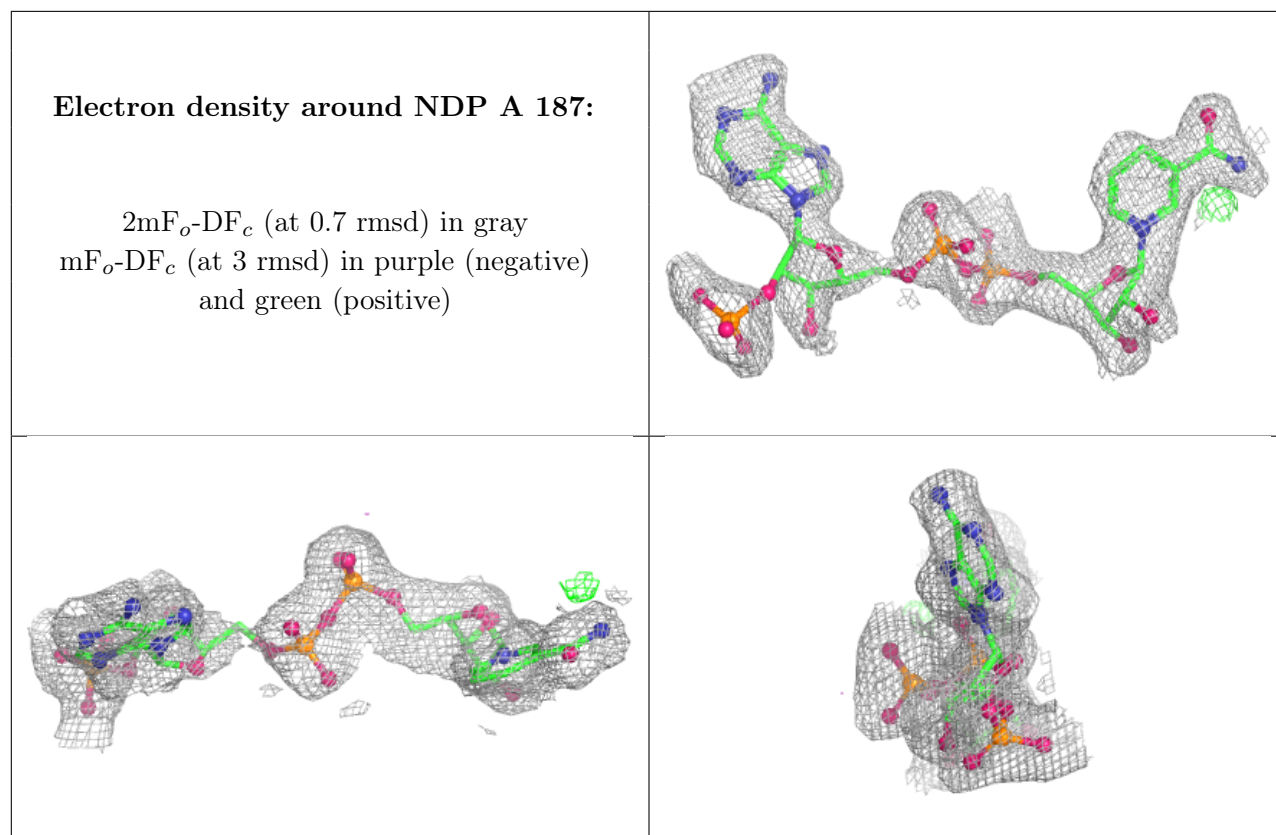
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around MTX A 188:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.