



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:24 am BST

PDB ID : 1TDR
Title : EXPRESSION, CHARACTERIZATION, AND CRYSTALLOGRAPHIC ANALYSIS OF TELLUROMETHIONYL DIHYDROFOLATE REDUCTASE
Authors : Lewinski, K.; Lebioda, L.
Deposited on : 1995-04-13
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

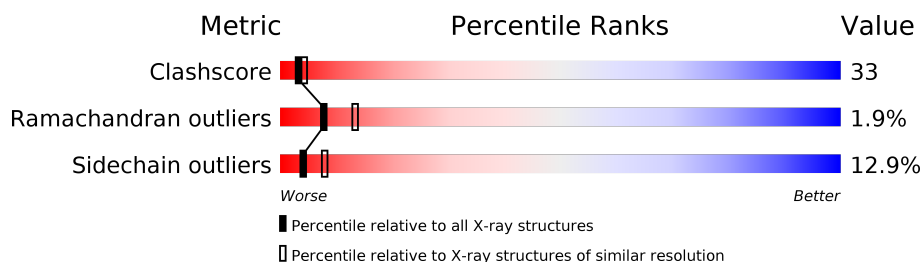
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	159	
1	B	159	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MTX	A	170	-	X	-	-
3	MTX	B	170	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 2944 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 TELLUROMETHIONYL DIHYDROFOLATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	159	Total	C	N	O	S	0	0	0
			1263	804	214	238	7			
1	B	159	Total	C	N	O	S	0	0	0
			1268	806	217	238	7			

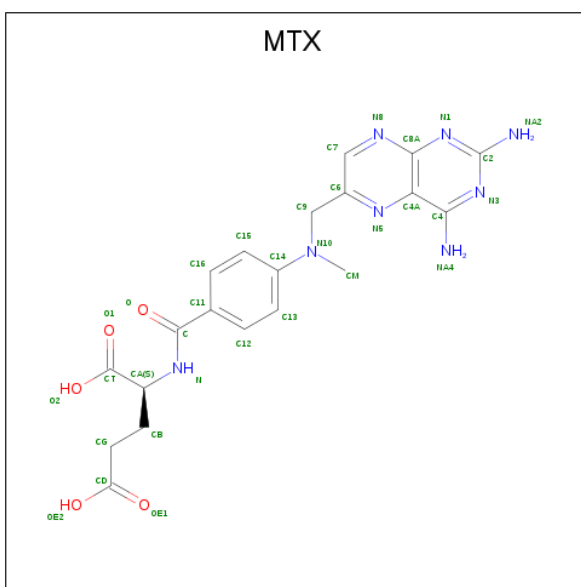
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	ASN	CONFLICT	UNP P00379
A	154	LYS	GLU	CONFLICT	UNP P00379
B	37	ASP	ASN	CONFLICT	UNP P00379
B	154	LYS	GLU	CONFLICT	UNP P00379

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is METHOTREXATE (three-letter code: MTX) (formula: C₂₀H₂₂N₈O₅).



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

- Molecule 4 is TELLURIUM (three-letter code: TE) (formula: Te).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Te	0	0
			2	2		
4	A	2	Total	Te	0	0
			2	2		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

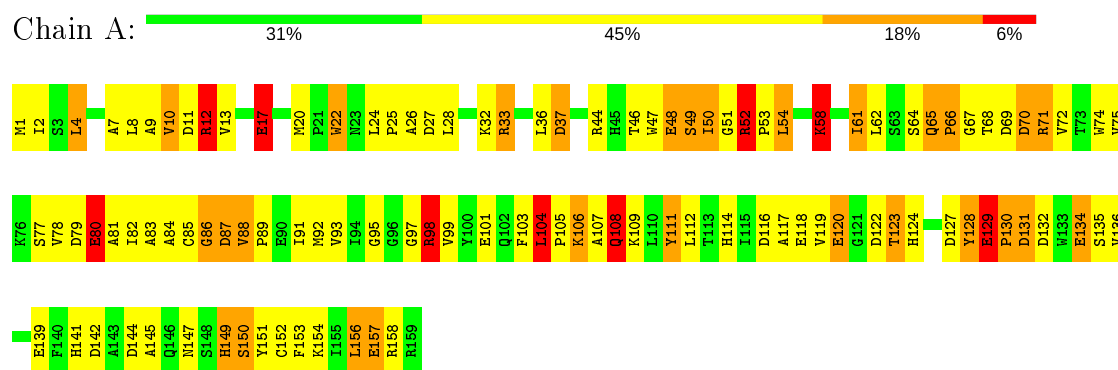
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	176	Total	O	0	0
			176	176		
6	B	164	Total	O	0	0
			164	164		

3 Residue-property plots [i](#)

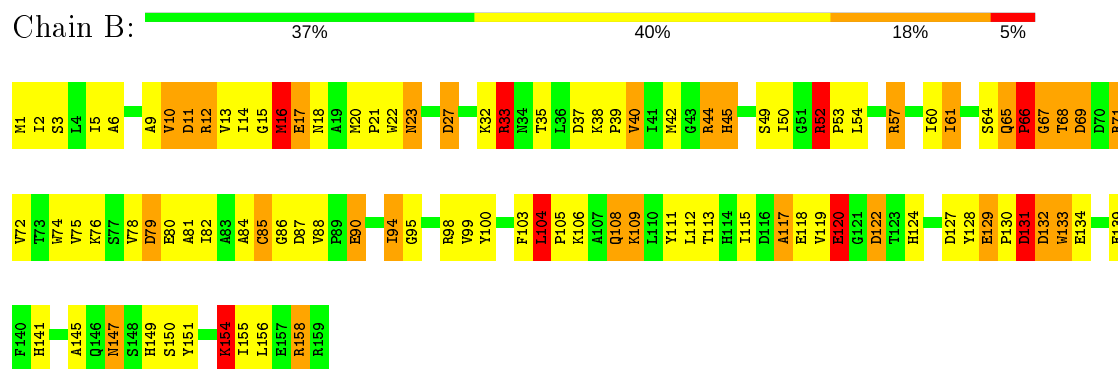
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: TELLUROMETHIONYL DIHYDROFOLATE REDUCTASE



• Molecule 1: TELLUROMETHIONYL DIHYDROFOLATE REDUCTASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	93.00 Å 93.00 Å 74.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (16.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.124 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2944	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: MTX, TE, CA, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	0/1297	2.56	101/1763 (5.7%)
1	B	1.09	0/1302	2.78	96/1769 (5.4%)
All	All	1.06	0/2599	2.67	197/3532 (5.6%)

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

There are no bond length outliers.

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	52	ARG	CD-NE-CZ	31.99	168.39	123.60
1	A	12	ARG	CD-NE-CZ	19.46	150.85	123.60
1	B	12	ARG	CD-NE-CZ	17.77	148.48	123.60
1	B	12	ARG	NE-CZ-NH1	-17.06	111.77	120.30
1	B	12	ARG	NE-CZ-NH2	16.20	128.40	120.30
1	B	57	ARG	NE-CZ-NH2	-15.02	112.79	120.30
1	B	33	ARG	NE-CZ-NH1	14.99	127.79	120.30
1	A	52	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	A	33	ARG	NE-CZ-NH2	-13.83	113.39	120.30
1	B	71	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	B	132	ASP	CB-CG-OD2	-13.80	105.88	118.30
1	A	98	ARG	NE-CZ-NH1	13.71	127.15	120.30
1	A	98	ARG	NE-CZ-NH2	-13.38	113.61	120.30
1	B	52	ARG	NE-CZ-NH1	12.66	126.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	87	ASP	CB-CG-OD1	-12.46	107.08	118.30
1	B	17	GLU	CA-CB-CG	11.46	138.61	113.40
1	A	37	ASP	CB-CG-OD2	-11.19	108.23	118.30
1	B	66	PRO	N-CA-CB	-10.97	90.14	103.30
1	A	12	ARG	NE-CZ-NH2	10.39	125.50	120.30
1	A	101	GLU	OE1-CD-OE2	10.11	135.43	123.30
1	B	16	MET	CA-CB-CG	10.04	130.37	113.30
1	B	33	ARG	NH1-CZ-NH2	-9.71	108.72	119.40
1	A	52	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	B	111	TYR	CB-CG-CD2	9.35	126.61	121.00
1	A	70	ASP	CB-CG-OD1	9.30	126.67	118.30
1	B	27	ASP	CB-CG-OD1	9.24	126.62	118.30
1	B	132	ASP	CB-CG-OD1	9.21	126.59	118.30
1	B	11	ASP	CB-CG-OD1	9.10	126.49	118.30
1	A	134	GLU	CA-CB-CG	9.02	133.23	113.40
1	B	45	HIS	CB-CA-C	8.87	128.15	110.40
1	A	12	ARG	CG-CD-NE	8.86	130.41	111.80
1	B	80	GLU	CA-CB-CG	8.80	132.76	113.40
1	B	66	PRO	C-N-CA	8.78	140.73	122.30
1	A	12	ARG	NH1-CZ-NH2	-8.75	109.77	119.40
1	B	131	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	A	12	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	A	48	GLU	CA-CB-CG	8.66	132.44	113.40
1	A	26	ALA	N-CA-CB	8.48	121.98	110.10
1	A	112	LEU	O-C-N	8.39	136.13	122.70
1	B	158	ARG	NE-CZ-NH2	8.16	124.38	120.30
1	A	129	GLU	CG-CD-OE1	8.09	134.49	118.30
1	B	44	ARG	NE-CZ-NH2	8.06	124.33	120.30
1	B	94	ILE	C-N-CA	7.96	139.01	122.30
1	A	132	ASP	O-C-N	7.85	135.26	122.70
1	B	6	ALA	N-CA-CB	-7.80	99.17	110.10
1	B	131	ASP	N-CA-CB	-7.77	96.62	110.60
1	B	33	ARG	CD-NE-CZ	7.64	134.30	123.60
1	A	108	GLN	CA-CB-CG	7.56	130.04	113.40
1	A	52	ARG	CD-NE-CZ	7.53	134.13	123.60
1	A	116	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	B	23	ASN	CB-CA-C	7.50	125.40	110.40
1	B	139	GLU	CG-CD-OE1	-7.50	103.30	118.30
1	B	85	CYS	CA-CB-SG	7.39	127.30	114.00
1	B	52	ARG	NH1-CZ-NH2	-7.35	111.31	119.40
1	B	154	LYS	CA-CB-CG	7.21	129.25	113.40
1	B	66	PRO	N-CA-C	7.14	130.67	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	A	37	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	144	ASP	CB-CG-OD2	7.12	124.71	118.30
1	B	66	PRO	CA-C-O	7.06	137.15	120.20
1	B	37	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	B	100	TYR	CB-CG-CD2	7.04	125.22	121.00
1	B	11	ASP	CB-CG-OD2	-7.03	111.98	118.30
1	A	101	GLU	CG-CD-OE2	-7.02	104.26	118.30
1	B	133	TRP	CA-CB-CG	-6.93	100.52	113.70
1	A	98	ARG	CD-NE-CZ	6.92	133.29	123.60
1	A	8	LEU	CB-CA-C	-6.89	97.11	110.20
1	B	127	ASP	N-CA-CB	-6.87	98.23	110.60
1	A	139	GLU	CG-CD-OE2	6.86	132.01	118.30
1	A	150	SER	O-C-N	6.82	133.60	122.70
1	B	119	VAL	CB-CA-C	6.80	124.31	111.40
1	B	66	PRO	N-CD-CG	-6.60	93.31	103.20
1	A	33	ARG	NH1-CZ-NH2	6.59	126.65	119.40
1	B	147	ASN	CB-CG-OD1	-6.55	108.50	121.60
1	A	17	GLU	CG-CD-OE1	6.54	131.37	118.30
1	A	87	ASP	CA-CB-CG	-6.53	99.03	113.40
1	A	71	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	90	GLU	CA-CB-CG	6.52	127.75	113.40
1	A	141	HIS	CA-CB-CG	6.51	124.67	113.60
1	B	71	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	50	ILE	C-N-CA	6.47	135.89	122.30
1	B	44	ARG	NE-CZ-NH1	-6.47	117.07	120.30
1	B	57	ARG	CG-CD-NE	6.44	125.32	111.80
1	B	147	ASN	N-CA-CB	-6.42	99.05	110.60
1	A	131	ASP	CB-CA-C	6.41	123.22	110.40
1	A	71	ARG	CD-NE-CZ	6.39	132.55	123.60
1	B	154	LYS	N-CA-CB	6.38	122.09	110.60
1	A	87	ASP	OD1-CG-OD2	6.36	135.39	123.30
1	B	122	ASP	CB-CA-C	6.36	123.13	110.40
1	A	66	PRO	N-CA-C	6.36	128.64	112.10
1	A	10	VAL	CB-CA-C	6.33	123.42	111.40
1	A	52	ARG	N-CA-CB	6.32	121.98	110.60
1	B	52	ARG	CG-CD-NE	6.31	125.05	111.80
1	A	26	ALA	CB-CA-C	-6.27	100.69	110.10
1	B	79	ASP	CB-CA-C	6.27	122.94	110.40
1	A	128	TYR	CB-CG-CD1	-6.24	117.26	121.00
1	A	7	ALA	N-CA-C	-6.22	94.20	111.00
1	B	95	GLY	C-N-CA	6.17	135.27	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	133	TRP	O-C-N	6.17	132.57	122.70
1	B	129	GLU	N-CA-CB	6.16	121.68	110.60
1	A	111	TYR	CG-CD1-CE1	6.14	126.22	121.30
1	A	116	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	104	LEU	CA-CB-CG	6.12	129.36	115.30
1	B	33	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	A	2	ILE	O-C-N	6.09	132.45	122.70
1	B	69	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	64	SER	O-C-N	6.07	132.42	122.70
1	A	20	MET	CB-CA-C	6.07	122.53	110.40
1	B	15	GLY	C-N-CA	6.05	136.84	121.70
1	A	156	LEU	CA-CB-CG	6.02	129.15	115.30
1	B	113	THR	N-CA-CB	6.00	121.71	110.30
1	B	69	ASP	CB-CA-C	5.98	122.37	110.40
1	A	131	ASP	CB-CG-OD1	-5.97	112.92	118.30
1	B	120	GLU	CB-CG-CD	5.97	130.32	114.20
1	A	33	ARG	N-CA-CB	-5.93	99.92	110.60
1	A	134	GLU	CG-CD-OE1	5.92	130.14	118.30
1	B	3	SER	O-C-N	-5.85	113.34	122.70
1	A	153	PHE	N-CA-CB	5.83	121.10	110.60
1	B	37	ASP	CA-CB-CG	-5.82	100.59	113.40
1	A	54	LEU	CB-CA-C	5.82	121.26	110.20
1	A	80	GLU	OE1-CD-OE2	5.81	130.27	123.30
1	A	129	GLU	CB-CG-CD	5.78	129.81	114.20
1	B	120	GLU	C-N-CA	-5.77	110.18	122.30
1	A	95	GLY	C-N-CA	5.74	134.35	122.30
1	B	54	LEU	CB-CA-C	5.73	121.09	110.20
1	A	111	TYR	CB-CG-CD1	5.71	124.43	121.00
1	B	3	SER	N-CA-CB	-5.70	101.95	110.50
1	A	88	VAL	CA-CB-CG2	5.69	119.43	110.90
1	A	8	LEU	CA-CB-CG	5.69	128.38	115.30
1	B	40	VAL	CA-CB-CG1	5.67	119.41	110.90
1	B	52	ARG	N-CA-CB	-5.67	100.40	110.60
1	A	120	GLU	CB-CG-CD	5.66	129.47	114.20
1	A	111	TYR	CA-CB-CG	5.64	124.11	113.40
1	A	33	ARG	CG-CD-NE	5.63	123.63	111.80
1	A	99	VAL	CA-CB-CG2	-5.62	102.47	110.90
1	A	111	TYR	CZ-CE2-CD2	5.61	124.85	119.80
1	A	129	GLU	CA-CB-CG	5.59	125.70	113.40
1	A	49	SER	N-CA-CB	5.58	118.88	110.50
1	B	33	ARG	CB-CG-CD	5.58	126.12	111.60
1	A	53	PRO	N-CD-CG	-5.58	94.83	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TYR	CG-CD2-CE2	-5.58	116.84	121.30
1	B	108	GLN	CB-CA-C	5.58	121.55	110.40
1	B	119	VAL	CA-CB-CG2	5.56	119.24	110.90
1	A	128	TYR	CB-CG-CD2	5.56	124.34	121.00
1	B	103	PHE	CD1-CE1-CZ	-5.53	113.47	120.10
1	A	48	GLU	N-CA-CB	5.51	120.53	110.60
1	A	4	LEU	CB-CG-CD1	5.51	120.36	111.00
1	B	139	GLU	CA-C-O	5.51	131.66	120.10
1	B	120	GLU	CA-C-O	-5.49	108.57	120.10
1	A	157	GLU	CB-CA-C	-5.48	99.44	110.40
1	B	85	CYS	N-CA-CB	5.47	120.44	110.60
1	B	14	ILE	CB-CG1-CD1	5.46	129.18	113.90
1	B	139	GLU	OE1-CD-OE2	5.43	129.81	123.30
1	A	86	GLY	N-CA-C	-5.40	99.59	113.10
1	A	28	LEU	CB-CG-CD2	-5.40	101.83	111.00
1	A	79	ASP	CB-CA-C	5.38	121.16	110.40
1	B	49	SER	CB-CA-C	-5.37	99.90	110.10
1	A	58	LYS	CB-CA-C	5.37	121.13	110.40
1	B	115	ILE	CB-CG1-CD1	5.36	128.92	113.90
1	A	11	ASP	CB-CG-OD1	5.35	123.11	118.30
1	A	129	GLU	CG-CD-OE2	-5.34	107.61	118.30
1	B	80	GLU	CG-CD-OE2	-5.32	107.65	118.30
1	B	113	THR	CA-CB-OG1	-5.32	97.82	109.00
1	A	149	HIS	C-N-CA	5.31	134.97	121.70
1	B	124	HIS	N-CA-CB	5.31	120.16	110.60
1	B	50	ILE	O-C-N	5.30	132.22	123.20
1	B	10	VAL	N-CA-CB	-5.30	99.85	111.50
1	A	157	GLU	OE1-CD-OE2	5.22	129.57	123.30
1	B	103	PHE	CB-CA-C	5.22	120.84	110.40
1	A	142	ASP	CA-CB-CG	5.22	124.88	113.40
1	B	13	VAL	O-C-N	5.21	131.04	122.70
1	A	27	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	B	98	ARG	CD-NE-CZ	-5.17	116.36	123.60
1	A	157	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	A	17	GLU	CG-CD-OE2	-5.17	107.96	118.30
1	B	104	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	A	51	GLY	CA-C-N	5.15	128.53	117.20
1	B	66	PRO	O-C-N	-5.15	114.45	123.20
1	A	51	GLY	CA-C-O	-5.14	111.34	120.60
1	B	90	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	A	70	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	50	ILE	CA-C-O	5.13	130.87	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	LYS	C-N-CA	5.11	134.48	121.70
1	B	54	LEU	CA-CB-CG	5.10	127.03	115.30
1	A	132	ASP	CA-C-O	-5.09	109.41	120.10
1	B	117	ALA	N-CA-CB	5.09	117.23	110.10
1	A	111	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	145	ALA	O-C-N	5.08	130.83	122.70
1	A	131	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	26	ALA	O-C-N	5.08	130.82	122.70
1	A	87	ASP	N-CA-C	5.07	124.70	111.00
1	B	112	LEU	O-C-N	5.06	130.80	122.70
1	A	97	GLY	C-N-CA	5.04	134.30	121.70
1	A	111	TYR	CD1-CE1-CZ	-5.02	115.29	119.80
1	A	92	MET	CG-SD-CE	5.01	108.22	100.20
1	B	86	GLY	N-CA-C	5.01	125.63	113.10
1	B	82	ILE	N-CA-CB	-5.01	99.28	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	33	ARG	Sidechain

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	1263	0	1219	81	0
1	B	1268	0	1226	85	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	33	0	19	4	0
3	B	33	0	21	2	0
4	A	2	0	0	0	0
4	B	2	0	0	1	0
5	B	1	0	0	0	0
6	A	176	0	0	23	0
6	B	164	0	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2944	0	2485	168	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 33.

All (168) 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:152:CYS:SG	6:A:268:HOH:O	1.90	1.29
1:A:65:GLN:HB3	1:A:66:PRO:CD	1.60	1.28
1:B:45:HIS:HB3	6:B:270:HOH:O	1.10	1.27
1:B:150:SER:HB3	6:B:210:HOH:O	1.27	1.26
1:A:1:MET:HE1	6:A:196:HOH:O	1.19	1.24
1:B:17:GLU:HG3	6:B:193:HOH:O	1.06	1.18
1:A:70:ASP:HA	6:A:324:HOH:O	1.47	1.14
1:A:65:GLN:CB	1:A:66:PRO:HD2	1.82	1.08
1:B:42:MET:SD	4:B:173:TE:TE	0.22	1.05
1:A:32:LYS:HD2	6:A:305:HOH:O	1.56	1.02
1:A:32:LYS:CD	6:A:305:HOH:O	2.11	0.96
1:B:12:ARG:CZ	6:B:332:HOH:O	2.14	0.95
1:B:12:ARG:NH2	6:B:332:HOH:O	2.01	0.94
1:B:104:LEU:HB3	1:B:105:PRO:HD3	1.53	0.91
1:A:32:LYS:NZ	6:A:305:HOH:O	2.04	0.90
1:B:17:GLU:HB3	6:B:311:HOH:O	1.71	0.90
1:A:65:GLN:HB3	1:A:66:PRO:HD2	0.90	0.88
1:A:158:ARG:NH2	6:A:206:HOH:O	2.10	0.84
1:B:17:GLU:CG	6:B:193:HOH:O	1.80	0.82
1:A:119:VAL:O	6:A:192:HOH:O	1.97	0.81
1:B:154:LYS:CE	1:B:156:LEU:HD21	2.09	0.81
1:A:75:VAL:HB	1:A:80:GLU:HB3	1.64	0.80
1:B:108:GLN:HG2	6:B:206:HOH:O	1.81	0.78
1:B:120:GLU:CD	6:B:280:HOH:O	2.21	0.77
1:B:10:VAL:O	1:B:11:ASP:HB2	1.85	0.76
1:A:32:LYS:HD3	6:A:272:HOH:O	1.88	0.73
1:B:22:TRP:CZ2	6:B:263:HOH:O	2.40	0.73
1:B:154:LYS:HE3	1:B:156:LEU:HD21	1.70	0.73
1:A:68:THR:OG1	6:A:326:HOH:O	2.07	0.72
1:B:22:TRP:HZ2	6:B:263:HOH:O	1.70	0.72
1:A:1:MET:CE	6:A:196:HOH:O	1.92	0.71
1:A:69:ASP:O	6:A:324:HOH:O	2.08	0.71
1:A:12:ARG:HH21	1:A:127:ASP:HB2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASP:HB2	6:A:198:HOH:O	1.90	0.70
1:A:98:ARG:HH11	1:A:98:ARG:HB3	1.56	0.70
1:A:1:MET:SD	6:A:196:HOH:O	2.37	0.69
1:B:64:SER:HA	1:B:76:LYS:HE3	1.74	0.69
1:B:149:HIS:NE2	6:B:228:HOH:O	2.26	0.68
1:B:69:ASP:H	1:B:74:TRP:HZ2	1.42	0.68
1:B:33:ARG:HD3	6:B:293:HOH:O	1.93	0.68
1:B:11:ASP:N	6:B:262:HOH:O	1.95	0.67
1:A:154:LYS:HZ2	1:A:156:LEU:HD11	1.61	0.66
1:A:117:ALA:HB2	1:A:149:HIS:CD2	2.31	0.66
1:A:135:SER:HA	1:A:156:LEU:HD12	1.77	0.66
1:B:99:VAL:HG23	6:B:284:HOH:O	1.96	0.66
1:A:127:ASP:CG	6:A:219:HOH:O	2.34	0.65
1:A:10:VAL:HG13	1:A:117:ALA:O	1.97	0.64
1:A:65:GLN:CB	1:A:66:PRO:CD	2.44	0.64
1:B:108:GLN:OE1	1:B:158:ARG:HD2	1.98	0.64
1:B:129:GLU:HG3	1:B:131:ASP:HB2	1.80	0.64
1:B:65:GLN:N	1:B:65:GLN:HE21	1.96	0.64
1:B:9:ALA:HB1	1:B:117:ALA:O	1.97	0.63
1:B:154:LYS:HE2	1:B:156:LEU:HD21	1.78	0.63
1:B:2:ILE:HD12	1:B:106:LYS:HB3	1.82	0.62
1:B:84:ALA:HB2	6:B:289:HOH:O	1.99	0.62
1:B:68:THR:CG2	6:B:290:HOH:O	2.47	0.61
1:A:46:THR:O	1:A:50:ILE:HG13	2.00	0.61
1:B:67:GLY:HA3	6:B:190:HOH:O	2.01	0.61
1:A:47:TRP:CH2	1:A:72:VAL:HG11	2.37	0.59
1:B:129:GLU:O	1:B:133:TRP:HD1	1.84	0.59
1:B:104:LEU:HB3	1:B:105:PRO:CD	2.29	0.59
1:A:98:ARG:NH1	1:A:98:ARG:HB3	2.17	0.58
1:A:36:LEU:O	1:A:37:ASP:HB2	2.02	0.58
1:B:129:GLU:CD	1:B:130:PRO:HD2	2.23	0.58
1:A:114:HIS:O	1:A:151:TYR:HA	2.03	0.58
1:B:45:HIS:CB	6:B:270:HOH:O	1.94	0.58
1:A:134:GLU:O	1:A:156:LEU:HA	2.04	0.57
1:A:54:LEU:HD21	3:A:170:MTX:H16	1.86	0.57
1:B:104:LEU:CB	1:B:105:PRO:HD3	2.28	0.56
1:B:23:ASN:O	1:B:147:ASN:HA	2.05	0.56
1:B:61:ILE:HD12	1:B:61:ILE:N	2.20	0.56
1:A:120:GLU:OE1	6:A:308:HOH:O	2.17	0.56
1:A:4:LEU:HD12	1:A:93:VAL:HB	1.89	0.55
1:A:135:SER:HB2	1:A:154:LYS:NZ	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ILE:HD11	1:B:85:CYS:HB3	1.89	0.54
1:B:149:HIS:CE1	6:B:228:HOH:O	2.61	0.54
1:A:108:GLN:HA	1:A:158:ARG:HB3	1.90	0.53
1:A:61:ILE:HD13	1:A:61:ILE:N	2.23	0.53
1:B:129:GLU:OE2	1:B:130:PRO:HD2	2.09	0.53
1:B:129:GLU:HB3	1:B:132:ASP:CG	2.28	0.53
1:A:89:PRO:HD2	6:A:213:HOH:O	2.08	0.53
1:B:151:TYR:CD1	1:B:151:TYR:N	2.77	0.53
1:B:134:GLU:OE2	6:B:226:HOH:O	2.19	0.53
1:A:12:ARG:NH2	1:A:127:ASP:HB2	2.24	0.52
1:B:128:TYR:O	1:B:130:PRO:HD3	2.09	0.52
1:A:78:VAL:HG13	1:A:103:PHE:CE1	2.45	0.52
1:A:10:VAL:O	1:A:13:VAL:HG23	2.09	0.52
1:B:133:TRP:HB3	1:B:156:LEU:HB3	1.91	0.52
1:A:75:VAL:HG21	1:A:81:ALA:HB2	1.90	0.52
1:A:128:TYR:O	1:A:130:PRO:HD3	2.09	0.51
1:B:141:HIS:HB3	6:B:231:HOH:O	2.11	0.51
1:A:107:ALA:O	1:A:158:ARG:NH1	2.43	0.51
1:A:52:ARG:NH2	3:A:170:MTX:O	2.42	0.51
1:A:75:VAL:HG11	1:A:81:ALA:HA	1.92	0.51
1:A:82:ILE:O	1:A:83:ALA:C	2.49	0.51
1:B:69:ASP:CG	1:B:71:ARG:HE	2.14	0.51
1:A:135:SER:CB	1:A:154:LYS:HZ3	2.24	0.50
1:B:1:MET:HE3	1:B:90:GLU:HB2	1.93	0.50
1:B:66:PRO:O	1:B:68:THR:HG22	2.11	0.50
1:A:123:THR:HG22	1:A:124:HIS:N	2.26	0.50
1:B:134:GLU:O	1:B:156:LEU:HA	2.12	0.50
1:A:91:ILE:HD12	6:A:235:HOH:O	2.12	0.50
1:B:129:GLU:C	1:B:131:ASP:H	2.15	0.50
1:B:16:MET:HB3	1:B:18:ASN:O	2.12	0.49
1:A:12:ARG:HH21	1:A:127:ASP:CB	2.23	0.49
1:B:61:ILE:CD1	1:B:61:ILE:N	2.75	0.49
1:A:69:ASP:OD1	1:A:71:ARG:HG3	2.12	0.48
1:A:9:ALA:HB2	1:A:22:TRP:HZ3	1.77	0.48
1:A:119:VAL:HG12	1:A:120:GLU:N	2.28	0.48
1:B:155:ILE:C	1:B:156:LEU:HD23	2.33	0.48
1:B:39:PRO:HG2	1:B:88:VAL:HG21	1.95	0.48
1:A:123:THR:HG22	1:A:124:HIS:H	1.79	0.48
1:B:154:LYS:HG2	6:B:185:HOH:O	2.12	0.48
1:B:52:ARG:HG2	1:B:53:PRO:O	2.14	0.48
1:A:77:SER:OG	1:A:80:GLU:OE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ALA:C	1:A:85:CYS:H	2.18	0.47
3:B:170:MTX:HM1	3:B:170:MTX:H13	1.75	0.46
1:B:38:LYS:HG3	6:B:336:HOH:O	2.16	0.46
1:B:129:GLU:HB3	1:B:132:ASP:OD1	2.16	0.46
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.97	0.46
1:A:83:ALA:O	1:A:85:CYS:N	2.49	0.46
1:A:49:SER:HA	1:B:145:ALA:HB1	1.98	0.45
1:B:61:ILE:HD13	1:B:72:VAL:CG2	2.46	0.45
1:B:11:ASP:O	1:B:12:ARG:HB2	2.16	0.45
1:B:1:MET:CE	1:B:90:GLU:HB2	2.46	0.45
1:B:129:GLU:HG3	1:B:131:ASP:CB	2.45	0.45
1:A:83:ALA:O	1:A:86:GLY:N	2.47	0.45
1:A:135:SER:CB	1:A:154:LYS:NZ	2.80	0.45
1:A:157:GLU:HB2	6:A:327:HOH:O	2.16	0.44
1:A:65:GLN:HB3	1:A:66:PRO:HD3	1.80	0.44
1:A:129:GLU:O	1:A:131:ASP:N	2.50	0.44
1:A:154:LYS:HG2	1:A:156:LEU:HD13	1.99	0.44
1:A:98:ARG:HD2	1:A:98:ARG:HA	1.79	0.44
1:B:44:ARG:HH12	1:B:68:THR:HG21	1.83	0.44
1:B:68:THR:HG21	6:B:290:HOH:O	2.11	0.44
3:A:170:MTX:HA	3:A:170:MTX:OE2	2.17	0.44
1:A:78:VAL:HG13	1:A:103:PHE:CZ	2.52	0.44
1:B:5:ILE:CG2	1:B:94:ILE:HG22	2.48	0.44
1:A:154:LYS:NZ	1:A:156:LEU:HD11	2.30	0.44
1:B:156:LEU:HD23	1:B:156:LEU:N	2.32	0.44
1:B:75:VAL:HG21	1:B:81:ALA:HA	1.99	0.44
1:A:122:ASP:N	6:A:198:HOH:O	2.11	0.43
1:B:129:GLU:HA	1:B:130:PRO:HD2	1.72	0.43
1:B:68:THR:HG23	1:B:74:TRP:CH2	2.53	0.43
1:B:109:LYS:HE2	1:B:155:ILE:HG21	2.00	0.43
1:B:66:PRO:HB2	6:B:328:HOH:O	2.18	0.43
1:A:67:GLY:HA2	1:A:74:TRP:CD2	2.54	0.42
1:B:27:ASP:OD2	3:B:170:MTX:N1	2.52	0.42
1:B:78:VAL:O	1:B:81:ALA:HB3	2.19	0.42
1:B:35:THR:OG1	1:B:57:ARG:NH1	2.52	0.42
1:A:25:PRO:HD2	1:A:147:ASN:OD1	2.19	0.42
1:B:104:LEU:O	1:B:158:ARG:NH2	2.51	0.42
1:B:133:TRP:N	1:B:133:TRP:CD1	2.87	0.42
1:A:109:LYS:NZ	6:A:274:HOH:O	2.53	0.41
1:A:135:SER:HB2	1:A:154:LYS:HZ1	1.83	0.41
1:A:156:LEU:HD11	6:A:323:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:VAL:O	1:B:40:VAL:HG23	2.20	0.41
1:B:60:ILE:CD1	1:B:85:CYS:HB3	2.49	0.41
3:A:170:MTX:H13	3:A:170:MTX:HM1	1.88	0.41
1:B:129:GLU:O	1:B:133:TRP:CD1	2.70	0.41
1:A:24:LEU:HD23	1:A:147:ASN:HB3	2.02	0.41
1:B:32:LYS:O	1:B:33:ARG:C	2.58	0.41
1:A:44:ARG:HG2	1:A:48:GLU:OE2	2.21	0.41
1:A:66:PRO:O	1:A:68:THR:HG23	2.21	0.40
1:A:78:VAL:HG12	1:A:106:LYS:NZ	2.36	0.40
1:A:58:LYS:NZ	6:A:289:HOH:O	2.54	0.40
1:B:20:MET:HE2	1:B:22:TRP:CH2	2.57	0.40
1:B:64:SER:C	1:B:65:GLN:HE21	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	157/159 (99%)	142 (90%)	11 (7%)	4 (2%)	5	8
1	B	157/159 (99%)	145 (92%)	10 (6%)	2 (1%)	12	21
All	All	314/318 (99%)	287 (91%)	21 (7%)	6 (2%)	8	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	84	ALA
1	B	66	PRO
1	B	67	GLY
1	A	17	GLU
1	A	65	GLN
1	A	130	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	135/136 (99%)	115 (85%)	20 (15%)	3	5
1	B	136/136 (100%)	121 (89%)	15 (11%)	6	12
All	All	271/272 (100%)	236 (87%)	35 (13%)	4	8

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	17	GLU
1	A	22	TRP
1	A	52	ARG
1	A	58	LYS
1	A	61	ILE
1	A	62	LEU
1	A	80	GLU
1	A	87	ASP
1	A	88	VAL
1	A	98	ARG
1	A	104	LEU
1	A	106	LYS
1	A	108	GLN
1	A	111	TYR
1	A	118	GLU
1	A	123	THR
1	A	129	GLU
1	A	136	VAL
1	A	150	SER
1	B	16	MET
1	B	21	PRO
1	B	33	ARG
1	B	52	ARG
1	B	61	ILE
1	B	65	GLN
1	B	68	THR

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Mol	Chain	Res	Type
1	B	79	ASP
1	B	87	ASP
1	B	104	LEU
1	B	118	GLU
1	B	120	GLU
1	B	122	ASP
1	B	131	ASP
1	B	154	LYS

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

Mol	Chain	Res	Type
1	A	65	GLN
1	A	108	GLN
1	B	65	GLN
1	B	124	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 for Mogul analysis.

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	170	-	29,35,35	3.59	14 (48%)	38,49,49	6.24	27 (71%)
3	MTX	B	170	-	29,35,35	3.06	15 (51%)	38,49,49	5.88	29 (76%)

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	170	-	-	5/19/25/25	0/3/3/3
3	MTX	B	170	-	-	3/19/25/25	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	170	MTX	O-C	7.77	1.39	1.23
3	A	170	MTX	CA-N	7.36	1.56	1.46
3	A	170	MTX	C4A-C8A	-6.99	1.28	1.40
3	A	170	MTX	C7-C6	6.92	1.51	1.39
3	B	170	MTX	C4A-C8A	-6.45	1.29	1.40
3	B	170	MTX	CA-N	5.94	1.54	1.46
3	B	170	MTX	O-C	5.88	1.35	1.23
3	A	170	MTX	C14-N10	5.40	1.54	1.39
3	B	170	MTX	C14-N10	4.98	1.53	1.39
3	A	170	MTX	CM-N10	4.97	1.54	1.46
3	A	170	MTX	C9-N10	4.92	1.56	1.46
3	B	170	MTX	C7-C6	4.32	1.47	1.39
3	B	170	MTX	CM-N10	4.22	1.53	1.46
3	A	170	MTX	C8A-N8	4.11	1.42	1.37
3	B	170	MTX	C9-N10	3.91	1.54	1.46
3	B	170	MTX	C15-C14	3.70	1.46	1.39
3	A	170	MTX	C15-C14	3.62	1.46	1.39
3	A	170	MTX	C4-NA4	-3.43	1.21	1.34
3	A	170	MTX	C16-C11	-3.06	1.34	1.39
3	B	170	MTX	C2-N3	-2.83	1.30	1.35
3	A	170	MTX	C11-C	2.56	1.55	1.50
3	B	170	MTX	C11-C	2.55	1.55	1.50
3	B	170	MTX	C6-N5	-2.51	1.27	1.32
3	B	170	MTX	C12-C11	2.36	1.43	1.39
3	B	170	MTX	C-N	2.27	1.39	1.34
3	B	170	MTX	C4-NA4	-2.25	1.25	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	170	MTX	C2-NA2	-2.11	1.29	1.33
3	A	170	MTX	C7-N8	2.08	1.35	1.31
3	A	170	MTX	C2-N3	-2.02	1.31	1.35

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	170	MTX	C4A-C4-N3	-26.37	103.69	121.01
3	B	170	MTX	C4A-C4-N3	-25.53	104.25	121.01
3	A	170	MTX	N8-C8A-N1	-11.04	103.22	115.82
3	A	170	MTX	C11-C-N	-8.29	101.17	117.06
3	A	170	MTX	C2-N1-C8A	-8.05	106.16	115.36
3	B	170	MTX	C7-C6-N5	-7.82	115.74	120.85
3	A	170	MTX	C6-C7-N8	-7.17	116.10	123.13
3	A	170	MTX	C4A-C8A-N1	7.04	133.12	121.71
3	A	170	MTX	NA2-C2-N3	6.75	127.74	117.25
3	B	170	MTX	N1-C2-N3	-6.51	118.54	127.22
3	A	170	MTX	C15-C16-C11	-6.45	113.27	120.78
3	B	170	MTX	C6-C9-N10	-6.42	102.59	113.60
3	A	170	MTX	C9-C6-N5	6.39	127.20	116.96
3	B	170	MTX	CG-CB-CA	-6.31	100.29	113.04
3	B	170	MTX	CB-CG-CD	6.28	127.09	113.59
3	B	170	MTX	N8-C8A-N1	-6.27	108.66	115.82
3	B	170	MTX	O-C-C11	-6.00	110.24	120.94
3	B	170	MTX	O-C-N	5.79	133.10	122.45
3	B	170	MTX	C2-N1-C8A	-5.77	108.77	115.36
3	B	170	MTX	C11-C-N	-5.55	106.42	117.06
3	B	170	MTX	C2-N3-C4	5.45	132.28	116.72
3	A	170	MTX	O-C-C11	-5.44	111.23	120.94
3	A	170	MTX	CB-CG-CD	5.43	125.26	113.59
3	B	170	MTX	C4A-C8A-N1	5.34	130.35	121.71
3	B	170	MTX	C12-C13-C14	-5.24	113.43	120.32
3	A	170	MTX	C2-N3-C4	5.09	131.24	116.72
3	B	170	MTX	C9-C6-N5	4.93	124.87	116.96
3	A	170	MTX	C7-C6-N5	-4.92	117.64	120.85
3	A	170	MTX	N1-C2-N3	-4.51	121.20	127.22
3	A	170	MTX	C13-C12-C11	-4.34	115.72	120.78
3	A	170	MTX	NA2-C2-N1	-4.28	110.81	117.79
3	A	170	MTX	CB-CA-N	4.28	116.42	110.19
3	A	170	MTX	C9-C6-C7	-4.23	114.22	121.60
3	B	170	MTX	C6-C7-N8	-4.08	119.13	123.13
3	B	170	MTX	C4-C4A-N5	-4.04	117.22	120.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	170	MTX	NA4-C4-N3	3.79	127.38	117.07
3	B	170	MTX	C7-N8-C8A	3.76	120.47	116.69
3	A	170	MTX	C16-C15-C14	-3.72	115.43	120.32
3	B	170	MTX	C6-N5-C4A	3.63	123.91	118.04
3	A	170	MTX	CG-CB-CA	-3.52	105.93	113.04
3	A	170	MTX	O-C-N	3.49	128.87	122.45
3	B	170	MTX	C13-C14-N10	-3.35	116.80	121.62
3	B	170	MTX	C15-C14-C13	3.31	125.90	119.16
3	A	170	MTX	C16-C11-C12	3.29	123.28	118.59
3	B	170	MTX	C12-C11-C	-3.18	110.32	120.62
3	B	170	MTX	C16-C15-C14	-3.15	116.17	120.32
3	A	170	MTX	C12-C11-C	-3.05	110.75	120.62
3	B	170	MTX	C15-C14-N10	-3.02	117.28	121.62
3	B	170	MTX	CA-N-C	-2.77	118.76	122.34
3	A	170	MTX	C13-C14-N10	-2.67	117.78	121.62
3	B	170	MTX	C8A-C4A-N5	-2.56	119.32	122.41
3	B	170	MTX	CM-N10-C14	-2.40	115.43	119.57
3	A	170	MTX	CA-N-C	-2.20	119.51	122.34
3	A	170	MTX	C6-C9-N10	-2.19	109.84	113.60
3	B	170	MTX	CB-CA-N	2.18	113.37	110.19
3	B	170	MTX	NA2-C2-N3	2.08	120.49	117.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

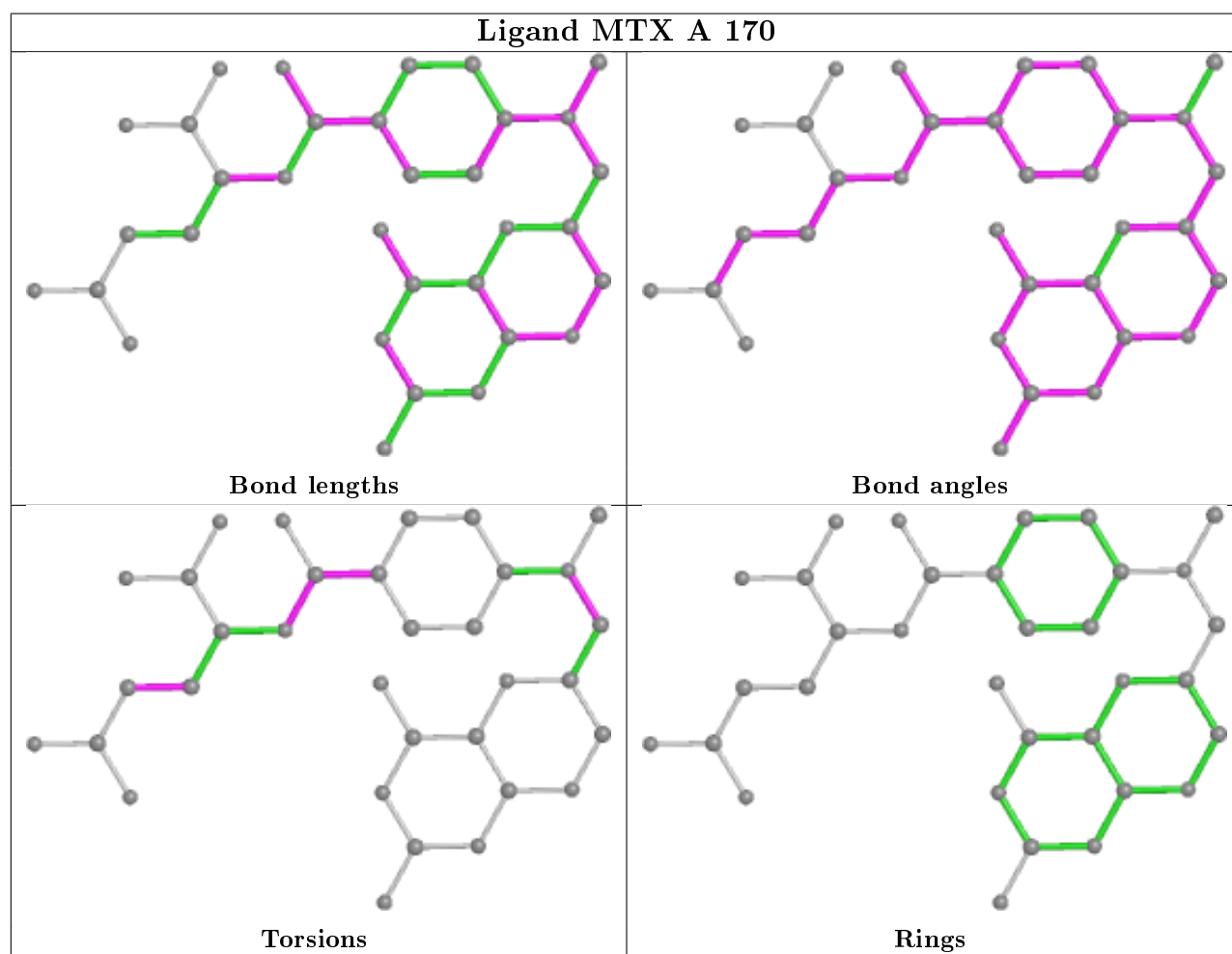
Mol	Chain	Res	Type	Atoms
3	A	170	MTX	C6-C9-N10-C14
3	B	170	MTX	N-C-C11-C16
3	B	170	MTX	O-C-N-CA
3	A	170	MTX	O-C-N-CA
3	A	170	MTX	N-C-C11-C16
3	B	170	MTX	C6-C9-N10-CM
3	A	170	MTX	C6-C9-N10-CM
3	A	170	MTX	CA-CB-CG-CD

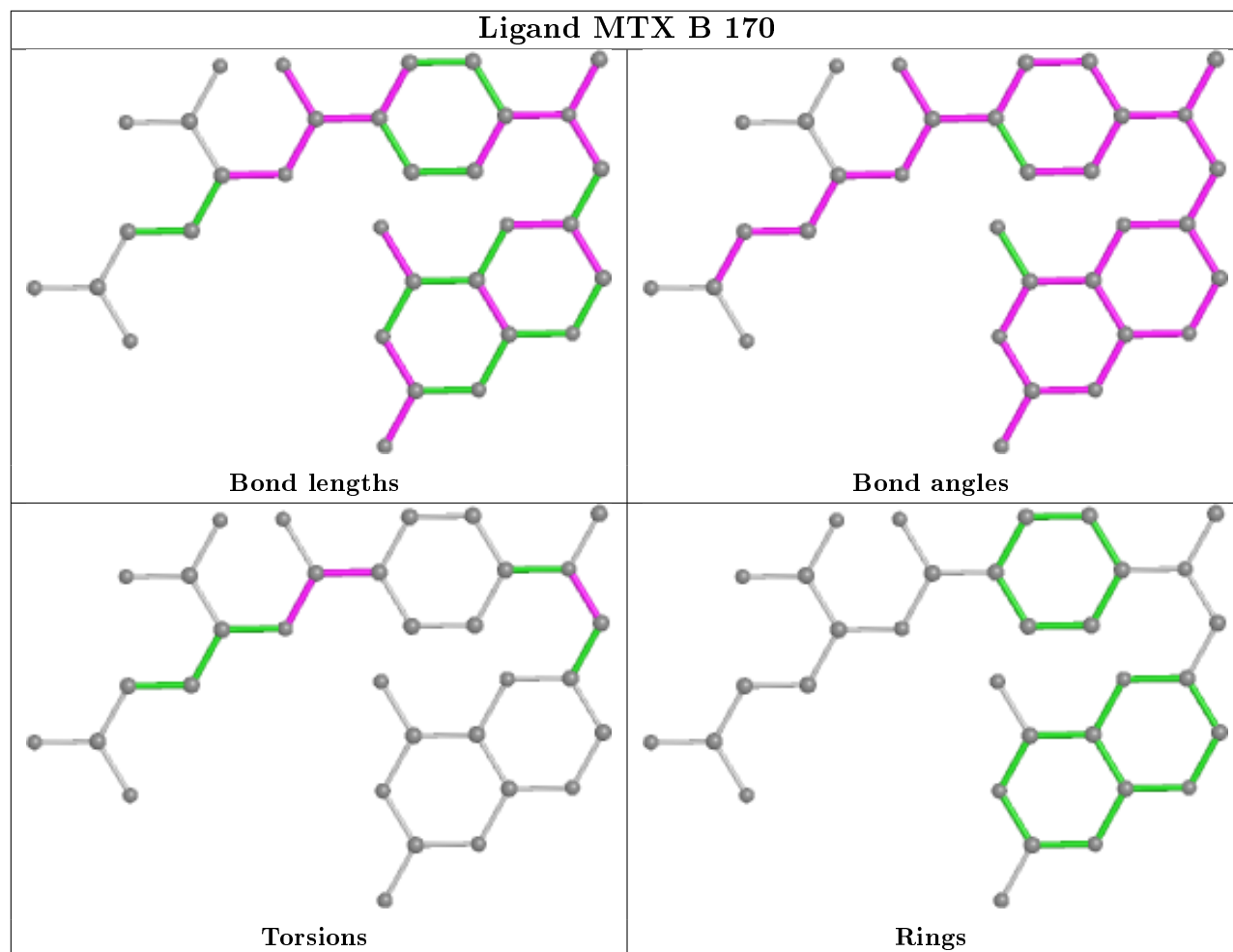
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	170	MTX	4	0
3	B	170	MTX	2	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.