



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:18 PM GMT

PDB ID : 4L6H
Title : Crystal structure of the Candida albicans Methionine Synthase in complex with Methotrexate and Homocysteine
Authors : Ubhi, D.; Robertus, J.D.
Deposited on : 2013-06-12
Resolution : 1.75 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

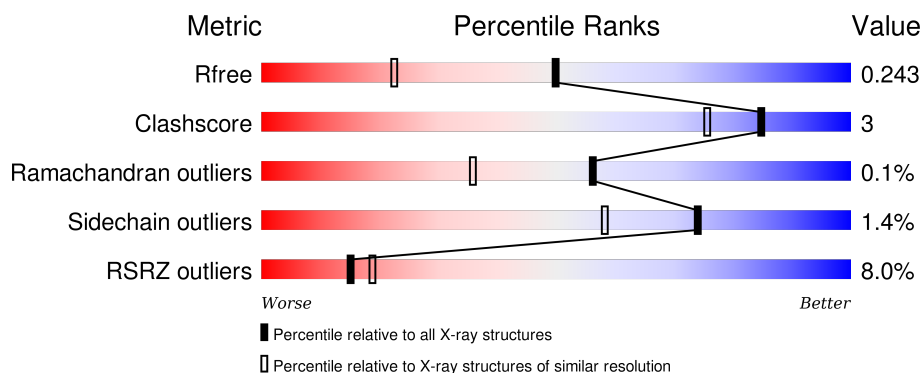
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

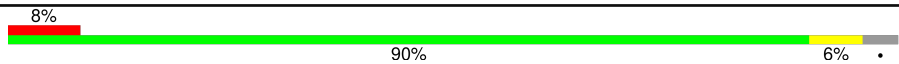
The reported resolution of this entry is 1.75 Å.

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))
R_{free}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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. 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	789	

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
4	MTX	A	803[A]	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MTX	A	803[B]	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6486 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 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	4	0
			5765	3696	958	1100	11			

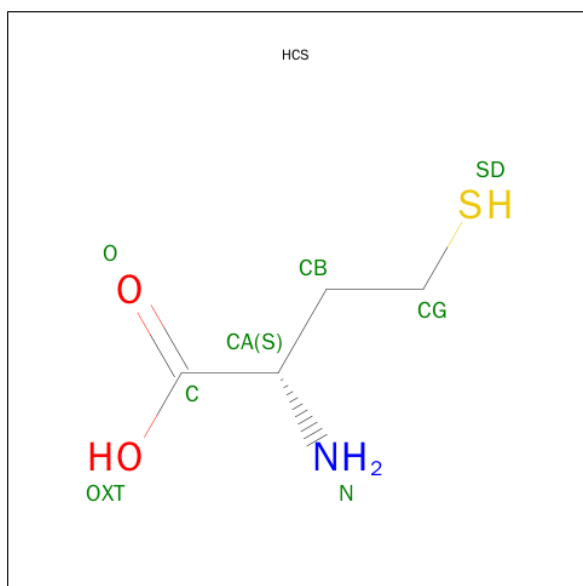
There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP P82610
A	-20	HIS	-	EXPRESSION TAG	UNP P82610
A	-19	HIS	-	EXPRESSION TAG	UNP P82610
A	-18	HIS	-	EXPRESSION TAG	UNP P82610
A	-17	HIS	-	EXPRESSION TAG	UNP P82610
A	-16	HIS	-	EXPRESSION TAG	UNP P82610
A	-15	HIS	-	EXPRESSION TAG	UNP P82610
A	-14	SER	-	EXPRESSION TAG	UNP P82610
A	-13	SER	-	EXPRESSION TAG	UNP P82610
A	-12	GLY	-	EXPRESSION TAG	UNP P82610
A	-11	VAL	-	EXPRESSION TAG	UNP P82610
A	-10	ASP	-	EXPRESSION TAG	UNP P82610
A	-9	LEU	-	EXPRESSION TAG	UNP P82610
A	-8	GLY	-	EXPRESSION TAG	UNP P82610
A	-7	THR	-	EXPRESSION TAG	UNP P82610
A	-6	GLU	-	EXPRESSION TAG	UNP P82610
A	-5	ASN	-	EXPRESSION TAG	UNP P82610
A	-4	LEU	-	EXPRESSION TAG	UNP P82610
A	-3	TYR	-	EXPRESSION TAG	UNP P82610
A	-2	PHE	-	EXPRESSION TAG	UNP P82610
A	-1	GLN	-	EXPRESSION TAG	UNP P82610
A	0	SER	-	EXPRESSION TAG	UNP P82610
A	103	ALA	LYS	engineered mutation	UNP P82610
A	104	ALA	LYS	engineered mutation	UNP P82610
A	107	ALA	GLU	engineered mutation	UNP P82610

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

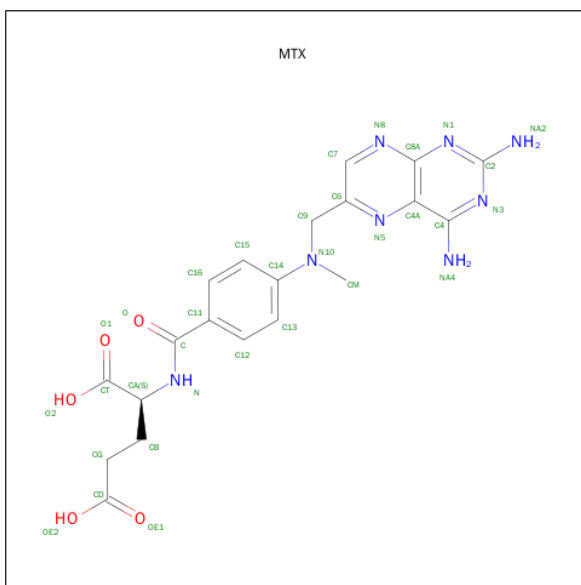
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula: C₄H₉NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			8	4	1	2	1		

- Molecule 4 is METHOTREXATE (three-letter code: MTX) (formula: C₂₀H₂₂N₈O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			66	40	16	10		

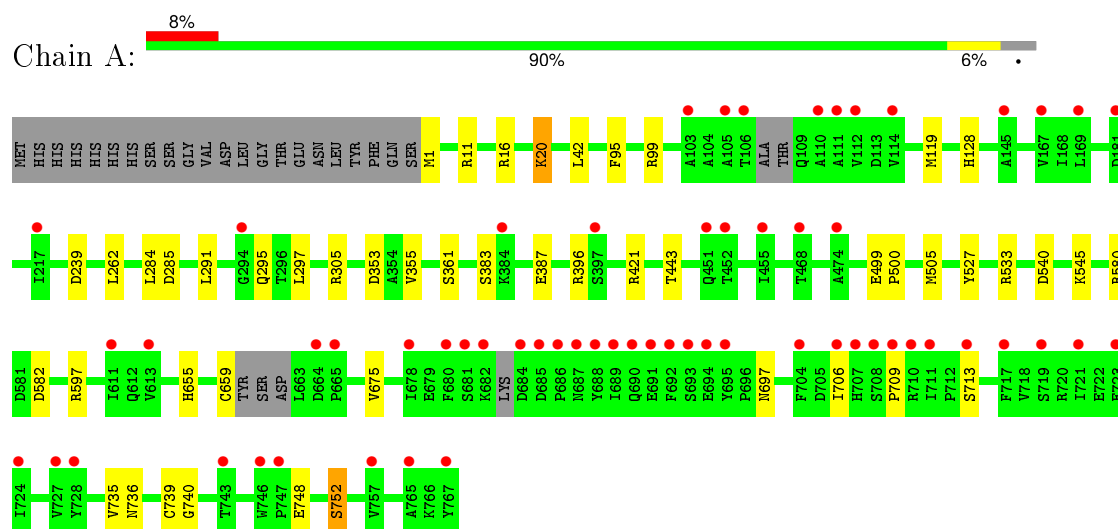
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	646	Total O 646 646	0	0

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 errors 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: 5-methyltetrahydropteroyltriglutamate--homocysteine methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	77.07Å 98.98Å 101.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.89 – 1.75 33.87 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.89-1.75) 99.7 (33.87-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.189 , 0.235 0.199 , 0.243	Depositor DCC
R_{free} test set	3963 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.3	EDS
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 78865 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6486	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: HCS, MTX, ZN

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	0.92	1/5885 (0.0%)	0.93	12/8018 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	SER	CA-CB	5.13	1.60	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	597	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	A	305	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	A	285	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	533	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	505	MET	CB-CG-SD	-5.78	95.07	112.40
1	A	505	MET	CG-SD-CE	-5.54	91.33	100.20
1	A	291	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	540	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	239	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	421	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	A	42	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	A	285	ASP	CB-CG-OD2	-5.07	113.74	118.30

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	5765	0	5529	33	0
2	A	1	0	0	0	0
3	A	8	0	7	0	0
4	A	66	0	40	0	0
5	A	646	0	0	4	0
All	All	6486	0	5576	33	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 3.

All (33) 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:1[B]:MET:HA	1:A:1[B]:MET:HE2	1.45	0.95
1:A:659:CYS:HB2	5:A:1145:HOH:O	1.80	0.81
1:A:443:THR:HG22	1:A:735:VAL:CG2	2.13	0.78
1:A:1[B]:MET:CA	1:A:1[B]:MET:HE2	2.14	0.76
1:A:1[B]:MET:CA	1:A:1[B]:MET:CE	2.65	0.73
1:A:1[B]:MET:HA	1:A:1[B]:MET:CE	2.21	0.63
1:A:20[A]:LYS:HD2	5:A:1328:HOH:O	1.99	0.61
1:A:16:ARG:O	1:A:20[A]:LYS:HG3	2.01	0.60
1:A:119:MET:HB3	1:A:527[A]:TYR:CZ	2.40	0.57
1:A:396:ARG:HD3	5:A:1267:HOH:O	2.09	0.53
1:A:119:MET:CB	1:A:527[A]:TYR:CZ	2.93	0.52
1:A:1[B]:MET:HE3	1:A:1[B]:MET:N	2.26	0.51
1:A:748:GLU:O	1:A:752:SER:OG	2.24	0.50
1:A:706:ILE:HG12	1:A:739:CYS:HB3	1.94	0.49
1:A:1[B]:MET:CE	1:A:1[B]:MET:N	2.77	0.47
1:A:295:GLN:N	5:A:1185:HOH:O	2.46	0.47
1:A:16:ARG:O	1:A:20[B]:LYS:HD2	2.15	0.46
1:A:353:ASP:OD2	1:A:355:VAL:HB	2.14	0.46
1:A:580:ARG:HB3	1:A:582:ASP:OD1	2.15	0.46
1:A:383:SER:O	1:A:387:GLU:HG3	2.16	0.46
1:A:739:CYS:SG	1:A:740:GLY:N	2.88	0.45
1:A:119:MET:HB2	1:A:527[A]:TYR:CE1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD23	1:A:297:LEU:C	2.39	0.42
1:A:20[B]:LYS:HD2	1:A:20[B]:LYS:N	2.35	0.41
1:A:655:HIS:HA	1:A:675:VAL:O	2.20	0.41
1:A:20[B]:LYS:HD2	1:A:20[B]:LYS:H	1.86	0.41
1:A:119:MET:HB2	1:A:527[A]:TYR:CZ	2.56	0.41
1:A:284:LEU:C	1:A:284:LEU:HD23	2.41	0.41
1:A:128:HIS:HB2	1:A:527[A]:TYR:CD1	2.56	0.41
1:A:499:GLU:N	1:A:500:PRO:CD	2.84	0.40
1:A:1[B]:MET:CA	1:A:1[B]:MET:HE3	2.50	0.40
1:A:443:THR:HG22	1:A:735:VAL:HG21	1.99	0.40
1:A:95:PHE:O	1:A:99:ARG:HG2	2.21	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	756/789 (96%)	739 (98%)	16 (2%)	1 (0%)	56 36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	709	PRO

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	579/678 (85%)	570 (98%)	9 (2%)	70 52

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	20[A]	LYS
1	A	20[B]	LYS
1	A	262	LEU
1	A	545	LYS
1	A	697	ASN
1	A	713	SER
1	A	736	ASN
1	A	752	SER

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

Mol	Chain	Res	Type
1	A	45	HIS
1	A	667	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	HCS	A	802	2	3,7,7	0.32	0	2,8,8	0.94	0
4	MTX	A	803[A]	-	27,35,35	0.84	0	30,49,49	1.79	9 (30%)
4	MTX	A	803[B]	-	27,35,35	0.93	1 (3%)	30,49,49	2.01	8 (26%)

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	HCS	A	802	2	-	0/3/7/7	0/0/0/0
4	MTX	A	803[A]	-	-	0/19/25/25	0/3/3/3
4	MTX	A	803[B]	-	-	0/19/25/25	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803[B]	MTX	C6-N5	2.21	1.37	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803[B]	MTX	C6-C9-N10	-5.07	104.96	113.78
4	A	803[A]	MTX	C6-C9-N10	-3.68	107.38	113.78
4	A	803[A]	MTX	N1-C2-N3	-3.59	121.98	127.44
4	A	803[B]	MTX	C4A-C8A-N1	-3.53	116.40	122.11
4	A	803[B]	MTX	N1-C2-N3	-2.94	122.96	127.44
4	A	803[B]	MTX	CG-CB-CA	-2.61	107.68	112.99
4	A	803[A]	MTX	O-C-C11	-2.50	116.70	120.97
4	A	803[B]	MTX	CM-N10-C14	-2.29	115.64	119.56
4	A	803[A]	MTX	C4A-C8A-N1	-2.04	118.81	122.11
4	A	803[A]	MTX	C9-C6-N5	2.01	120.40	117.11
4	A	803[A]	MTX	C9-N10-C14	2.07	123.77	119.36
4	A	803[A]	MTX	C7-N8-C8A	2.14	119.45	116.93
4	A	803[A]	MTX	C11-C-N	2.82	121.95	116.93
4	A	803[B]	MTX	C11-C-N	2.92	122.13	116.93
4	A	803[B]	MTX	CM-N10-C9	2.93	122.17	114.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803[A]	MTX	N8-C8A-N1	4.07	121.96	116.14
4	A	803[B]	MTX	N8-C8A-N1	4.64	122.78	116.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	761/789 (96%)	0.42	61 (8%) 15 19	11, 24, 63, 118	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	ILE	6.8
1	A	707	HIS	6.5
1	A	709	PRO	6.1
1	A	111	ALA	5.7
1	A	692	PHE	5.5
1	A	685	ASP	5.3
1	A	112	VAL	5.3
1	A	727	VAL	5.3
1	A	708	SER	5.1
1	A	724	ILE	5.0
1	A	682	LYS	4.6
1	A	717	PHE	4.5
1	A	688	TYR	4.3
1	A	691	GLU	4.3
1	A	687	ASN	4.2
1	A	767	TYR	4.2
1	A	110	ALA	4.2
1	A	695	TYR	4.1
1	A	106	THR	4.0
1	A	721	ILE	4.0
1	A	684	ASP	3.9
1	A	686	PRO	3.9
1	A	114	VAL	3.7
1	A	765	ALA	3.7
1	A	710	ARG	3.6
1	A	747	PRO	3.6
1	A	681	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	167	VAL	3.6
1	A	693	SER	3.5
1	A	711	ILE	3.5
1	A	694	GLU	3.4
1	A	680	PHE	3.2
1	A	728	TYR	3.1
1	A	690	GLN	3.0
1	A	613	VAL	2.9
1	A	743	THR	2.8
1	A	145	ALA	2.8
1	A	217	ILE	2.7
1	A	704	PHE	2.7
1	A	103	ALA	2.7
1	A	746	TRP	2.6
1	A	706	ILE	2.6
1	A	294	GLY	2.6
1	A	451	GLN	2.6
1	A	757	VAL	2.5
1	A	455	ILE	2.5
1	A	723	GLU	2.5
1	A	611	ILE	2.5
1	A	105	ALA	2.5
1	A	468	THR	2.4
1	A	452	THR	2.4
1	A	665	PRO	2.4
1	A	397	SER	2.4
1	A	713	SER	2.4
1	A	719	SER	2.3
1	A	169	LEU	2.3
1	A	664	ASP	2.2
1	A	384	LYS	2.2
1	A	474	ALA	2.1
1	A	181	ASP	2.0
1	A	678	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	MTX	A	803[B]	33/33	0.75	0.25	7.70	23,34,40,44	33
4	MTX	A	803[A]	33/33	0.75	0.25	6.99	27,53,62,67	33
3	HCS	A	802	8/8	0.92	0.10	-0.37	24,29,33,34	0
2	ZN	A	801	1/1	0.98	0.07	-2.93	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.