



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:35 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

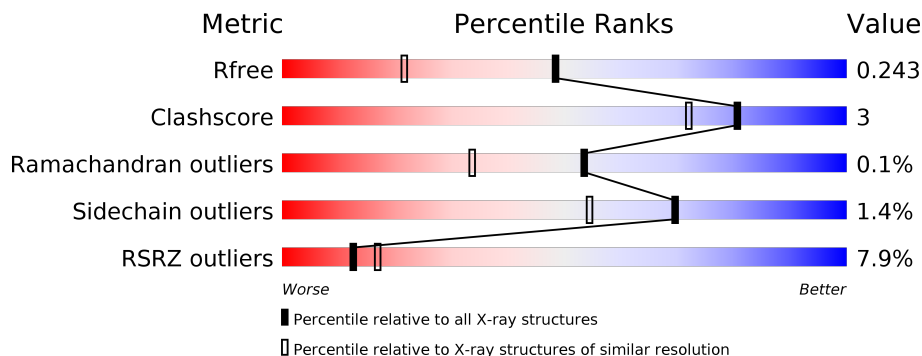
# 1 Overall quality at a glance

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))
$R_{free}$	111664	1952 (1.76-1.76)
Clashscore	122126	2072 (1.76-1.76)
Ramachandran outliers	120053	2050 (1.76-1.76)
Sidechain outliers	120020	2050 (1.76-1.76)
RSRZ outliers	108989	1913 (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  $\geq 3$ , 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	<div> <div>8%</div> <div>90%</div> <div>6%</div> <div>.</div> </div>

## 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			

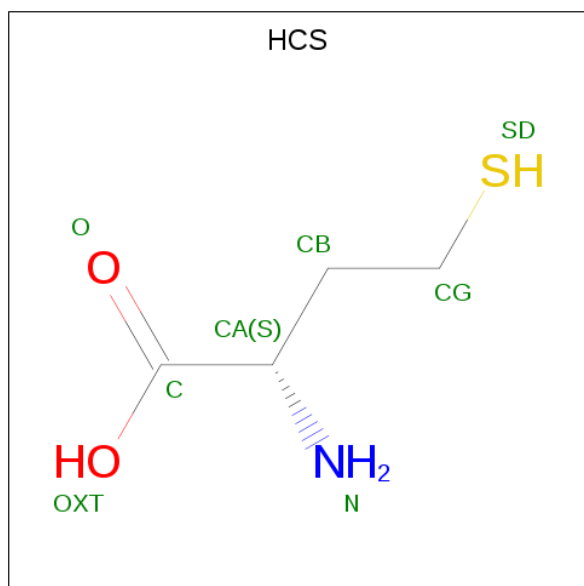
There are 25 discrepancies between the modelled and reference sequences:

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).

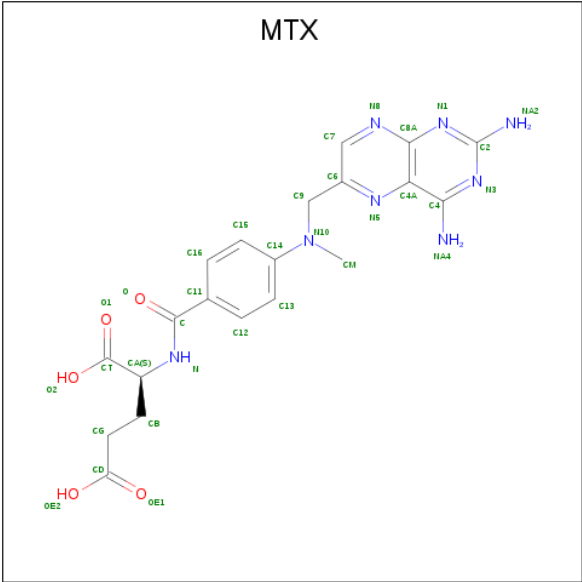
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>2</sub>S).



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: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>).



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

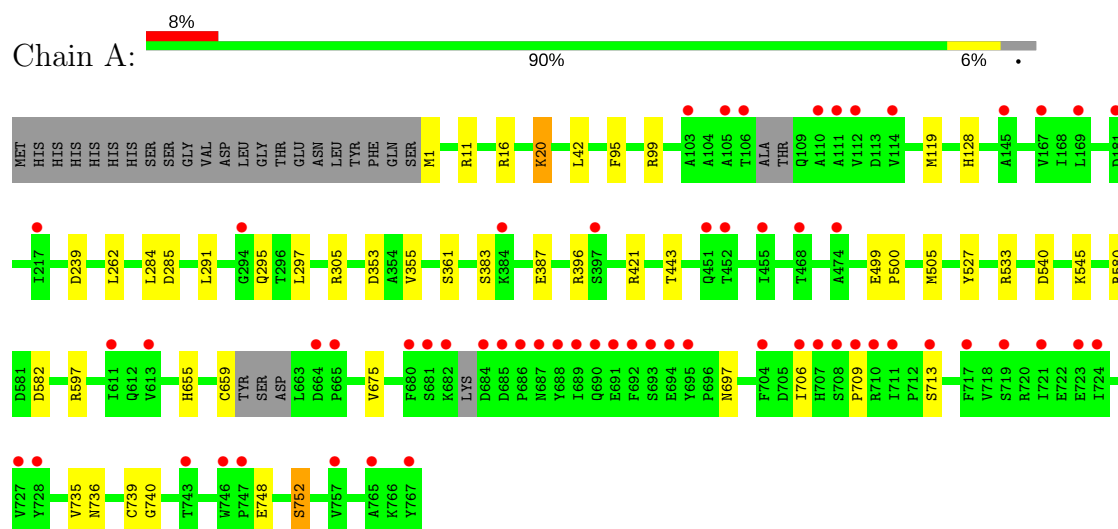
- Molecule 5 is water.

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

### 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 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6486	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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:N	1:A:20[B]:LYS:HD2	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%)	53 34

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%)	65 48

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 ⓘ

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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	2,7,7	0.97	0	2,8,8	2.34	1 (50%)
4	MTX	A	803[A]	-	28,35,35	0.89	1 (3%)	36,49,49	2.05	10 (27%)
4	MTX	A	803[B]	-	28,35,35	1.00	1 (3%)	36,49,49	2.53	14 (38%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803[A]	MTX	C6-N5	2.05	1.36	1.32
4	A	803[B]	MTX	C6-N5	2.50	1.37	1.32

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803[B]	MTX	C6-C9-N10	-5.02	104.96	113.66
4	A	803[B]	MTX	CA-N-C	-4.71	115.96	122.25
4	A	803[A]	MTX	N1-C2-N3	-3.70	121.98	127.41
4	A	803[A]	MTX	C6-C9-N10	-3.62	107.38	113.66
4	A	803[B]	MTX	C4A-C8A-N1	-3.53	116.40	122.18
4	A	803[B]	MTX	CT-CA-N	-3.47	104.87	112.39
3	A	802	HCS	CB-CG-SD	-3.29	110.31	113.74
4	A	803[B]	MTX	N1-C2-N3	-3.03	122.96	127.41
4	A	803[B]	MTX	CG-CB-CA	-2.76	107.68	113.19
4	A	803[B]	MTX	C6-C7-N8	-2.66	120.52	123.13
4	A	803[A]	MTX	O-C-C11	-2.42	116.70	120.93
4	A	803[B]	MTX	CM-N10-C14	-2.24	115.64	119.60
4	A	803[A]	MTX	C9-C6-C7	-2.20	117.77	121.60
4	A	803[A]	MTX	C4A-C8A-N1	-2.06	118.81	122.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803[A]	MTX	C9-C6-N5	2.03	120.40	117.06
4	A	803[A]	MTX	C9-N10-C14	2.16	123.77	119.50
4	A	803[B]	MTX	C7-C6-N5	2.45	122.44	120.85
4	A	803[B]	MTX	CB-CA-CT	2.65	116.05	112.11
4	A	803[A]	MTX	C11-C-N	2.74	121.95	116.98
4	A	803[B]	MTX	C11-C-N	2.84	122.13	116.98
4	A	803[B]	MTX	CM-N10-C9	2.85	122.17	114.43
4	A	803[A]	MTX	N8-C8A-N1	4.96	121.96	115.97
4	A	803[B]	MTX	N8-C8A-N1	5.64	122.78	115.97
4	A	803[A]	MTX	C2-N1-C8A	6.17	122.36	115.16
4	A	803[B]	MTX	C2-N1-C8A	6.67	122.95	115.16

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	761/789 (96%)	0.39	60 (7%) 12 17	11, 24, 63, 118	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	689	ILE	6.7
1	A	707	HIS	6.4
1	A	709	PRO	6.0
1	A	111	ALA	5.6
1	A	692	PHE	5.4
1	A	685	ASP	5.4
1	A	112	VAL	5.2
1	A	727	VAL	5.2
1	A	724	ILE	5.0
1	A	708	SER	4.9
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	4.1
1	A	767	TYR	4.1
1	A	110	ALA	4.1
1	A	106	THR	4.1
1	A	695	TYR	4.0
1	A	721	ILE	4.0
1	A	684	ASP	4.0
1	A	686	PRO	3.9
1	A	710	ARG	3.6
1	A	114	VAL	3.6
1	A	765	ALA	3.6
1	A	681	SER	3.6
1	A	747	PRO	3.6

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

## 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 carbohydrates in this entry.

## 6.4 Ligands

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MTX	A	803[A]	33/33	0.76	0.25	27,53,62,67	33
4	MTX	A	803[B]	33/33	0.76	0.25	23,34,40,44	33
3	HCS	A	802	8/8	0.92	0.10	24,29,33,34	0
2	ZN	A	801	1/1	0.98	0.06	35,35,35,35	0

## 6.5 Other polymers

There are no such residues in this entry.