

Full wwPDB X-ray Structure Validation Report (i)

Oct 7, 2023 – 01:41 PM EDT

PDB ID : 6DEB

Title: Crystal Structure of Bifunctional Enzyme FolD-Methylenetetrahydrofolat

e Dehydrogenase/Cyclohydrolase in the Complex with Methotrexate from

Campylobacter jejuni

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Deposited on : 2018-05-11

Resolution : 1.70 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 (i) 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 (1)) were used in the production of this report:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

Validation Pipeline (wwPDB-VP) : 2.35.1

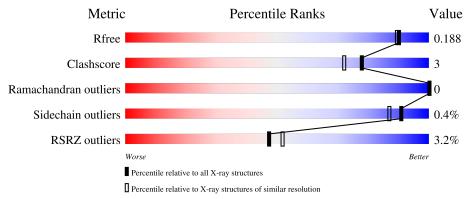


1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\ DIFFRACTION$

The reported resolution of this entry is 1.70 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries},{\rm resolution\ range}({\rm \AA})) \end{array}$
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 <=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	285	96%	•					
1	В	285	95%	5%					



2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5076 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.

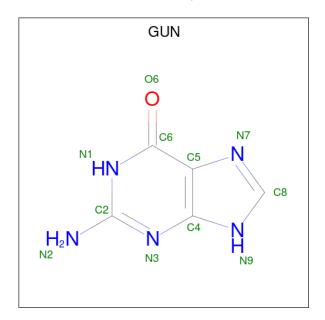
• Molecule 1 is a protein called Bifunctional protein FolD.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
1	A	284	Total 2221	C 1402	N 371	O 434	S 14	0	12	0
1	В	284	Total 2231	C 1408	N 373	O 436	S 14	0	13	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q0PA35
A	-1	ASN	-	expression tag	UNP Q0PA35
Α	0	ALA	-	expression tag	UNP Q0PA35
В	-2	SER	-	expression tag	UNP Q0PA35
В	-1	ASN	-	expression tag	UNP Q0PA35
В	0	ALA	-	expression tag	UNP Q0PA35

• Molecule 2 is GUANINE (three-letter code: GUN) (formula: $C_5H_5N_5O$).



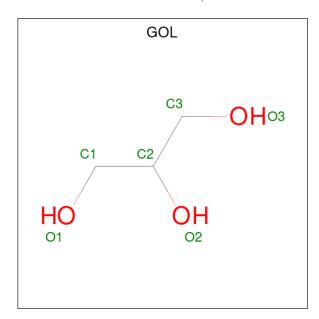


\mathbf{Mol}	Chain	Residues	${f Atoms}$				ZeroOcc	AltConf
2	A	1	Total 11	C 5	N 5	O 1	0	0

• Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



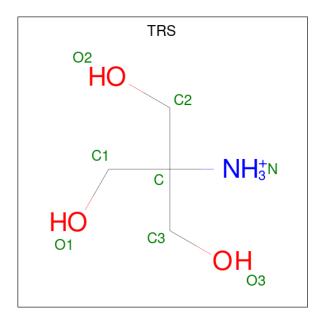
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	В	1	Total C O 6 3 3	0	0
4	В	1	Total C O 6 3 3	0	0

• Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).



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

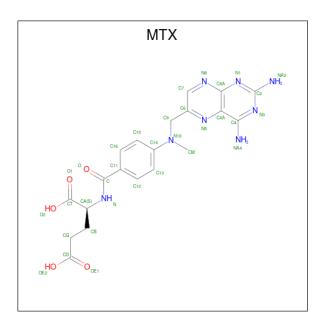
 \bullet Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $\rm C_4H_{12}NO_3).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	В	1	Total 8	C 4	N 1	O 3	0	0

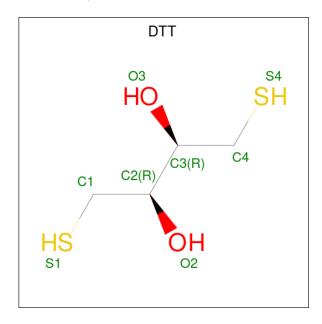
 \bullet Molecule 7 is METHOTREXATE (three-letter code: MTX) (formula: $\mathrm{C}_{20}\mathrm{H}_{22}\mathrm{N}_8\mathrm{O}_5).$





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	В	1	Total 33			0	0
7	В	1	Total 33		N 8	0	0

 \bullet Molecule 8 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2).$



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	В	1	Total 8	C 4	O 2	S 2	0	0



• Molecule 9 is water.

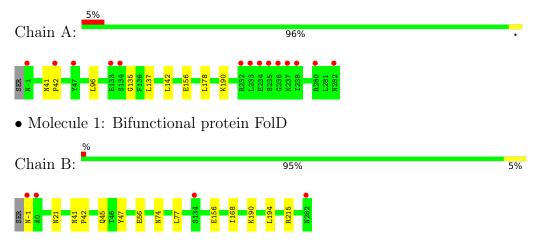
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	235	Total O 235 235	0	0
9	В	262	Total O 262 262	0	0



3 Residue-property plots (i)

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: Bifunctional protein FolD





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	163.87Å 59.09Å 72.99Å	Donositor
a, b, c, α , β , γ	90.00° 100.08° 90.00°	Depositor
Resolution (Å)	38.14 - 1.70	Depositor
rtesolution (A)	38.14 - 1.70	EDS
% Data completeness	95.2 (38.14-1.70)	Depositor
(in resolution range)	95.2 (38.14-1.70)	EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.97 (at 1.70Å)	Xtriage
Refinement program	PHENIX 1.8.1_1161	Depositor
D D.	0.161 , 0.188	Depositor
R, R_{free}	0.162 , 0.188	DCC
R_{free} test set	3640 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	20.0	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 48.0	EDS
L-test for twinning ²	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 7.62% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MTX, DTT, GUN, TRS, K, 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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.43	0/2246	0.57	0/3035	
1	В	0.45	0/2256	0.60	0/3049	
All	All	0.44	0/4502	0.59	0/6084	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2221	0	2304	9	0
1	В	2231	0	2312	17	0
2	A	11	0	5	1	0
3	A	1	0	0	0	0
4	A	18	0	24	0	0
4	В	12	0	16	1	0
5	A	1	0	0	0	0
5	В	2	0	0	0	0
6	В	8	0	12	0	0
7	В	66	0	40	9	0
8	В	8	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	235	0	0	1	0
9	В	262	0	0	2	0
All	All	5076	0	4723	27	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 (27) 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:156[B]:GLU:HG3	1:B:190:LYS:HD3	1.62	0.81
1:A:178:LEU:O	8:B:306:DTT:H3	1.91	0.71
1:B:190:LYS:NZ	8:B:306:DTT:O2	2.26	0.58
1:A:156[B]:GLU:OE2	1:B:190:LYS:HE2	2.05	0.56
1:A:156[B]:GLU:CG	1:B:190:LYS:HD3	2.33	0.56
1:A:190:LYS:HD3	1:B:156:GLU:HG3	1.91	0.52
1:B:168[A]:ILE:HD11	7:B:302:MTX:HG2	1.92	0.51
1:B:168[B]:ILE:HG21	7:B:302:MTX:C11	2.40	0.50
7:B:302:MTX:H91	7:B:303:MTX:HG1	1.94	0.49
1:A:96:LEU:H	2:A:301:GUN:HN1	1.60	0.46
1:B:168[B]:ILE:HG21	7:B:302:MTX:C16	2.45	0.46
1:B:45:GLN:HG2	9:B:444:HOH:O	2.15	0.46
1:B:74:ASN:HD22	1:B:77:LEU:HD12	1.81	0.44
7:B:302:MTX:C16	7:B:303:MTX:H91	2.48	0.44
1:B:168[A]:ILE:CD1	7:B:302:MTX:HG2	2.47	0.44
1:B:47:TYR:CD2	7:B:303:MTX:HB1	2.53	0.44
1:B:215[B]:ARG:NH1	9:B:404:HOH:O	2.39	0.44
7:B:302:MTX:H15	7:B:302:MTX:HM1	1.75	0.43
1:B:21:ASN:HD22	1:B:21:ASN:HA	1.75	0.42
1:B:194:LEU:HB2	4:B:308:GOL:H2	2.01	0.42
1:A:135[B]:GLY:N	9:A:401:HOH:O	2.46	0.41
1:A:137:LEU:HD12	1:A:142:LEU:HD13	2.02	0.41
1:B:41:ASN:HA	1:B:42:PRO:HD3	1.95	0.41
1:B:74:ASN:HD22	1:B:74:ASN:HA	1.73	0.41
1:A:41:ASN:HA	1:A:42:PRO:HD3	1.97	0.41
7:B:303:MTX:H15	7:B:303:MTX:HM1	1.92	0.40
8:B:306:DTT:H42	8:B:306:DTT:H12	1.15	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	Perce	Percentiles		
1	A	$294/285\ (103\%)$	289 (98%)	5 (2%)	0	100	100		
1	В	$295/285\ (104\%)$	290 (98%)	5 (2%)	0	100	100		
All	All	589/570 (103%)	579 (98%)	10 (2%)	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 Outlies		Percentiles		
1	A	253/244 (104%)	253 (100%)	0	100	100	
1	В	254/244 (104%)	251 (99%)	3 (1%)	71	59	
All	All	507/488 (104%)	504 (99%)	3 (1%)	91	80	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	-1	ASN
1	В	56[A]	GLU
1	В	56[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	21	ASN
1	В	21	ASN
1	В	22	GLN
1	В	74	ASN
1	В	85	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	Вс	nd leng	ths	Bond angles		
MIOI	Type	Chain	nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MTX	В	302	-	35,35,35	0.87	1 (2%)	46,49,49	1.76	11 (23%)
2	GUN	A	301	-	7,12,12	1.29	0	8,17,17	1.60	2 (25%)
8	DTT	В	306	-	7,7,7	0.79	0	4,8,8	1.59	1 (25%)
4	GOL	A	305	-	5,5,5	0.35	0	5,5,5	0.26	0
4	GOL	A	303	-	5,5,5	0.36	0	5,5,5	0.32	0
7	MTX	В	303	-	35,35,35	0.78	0	46,49,49	1.78	12 (26%)
4	GOL	В	305	-	5,5,5	0.40	0	5,5,5	0.44	0
4	GOL	В	308	-	5,5,5	0.26	0	5,5,5	0.28	0
4	GOL	A	306	-	5,5,5	0.40	0	5,5,5	0.35	0



7	Mol	Type	Chain	Res	Link	Bo	ond leng	$ ag{ths}$	В	ond ang	gles
1	VIOI	Туре	Chain	rtes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
	6	TRS	В	301	-	7,7,7	0.36	0	9,9,9	0.74	0

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
7	MTX	В	302	-	-	12/25/25/25	0/3/3/3
8	DTT	В	306	-	-	6/8/8/8	-
2	GUN	A	301	-	-	-	0/2/2/2
4	GOL	A	305	-	-	4/4/4/4	-
4	GOL	A	303	-	-	2/4/4/4	-
7	MTX	В	303	-	-	3/25/25/25	0/3/3/3
4	GOL	В	305	-	-	0/4/4/4	-
4	GOL	В	308	_	-	2/4/4/4	-
4	GOL	A	306	-	-	2/4/4/4	-
6	TRS	В	301	-	-	9/9/9/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$Ideal(\AA)$
7	В	302	MTX	C6-N5	2.40	1.36	1.32

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
7	В	302	MTX	C2-N1-C8A	5.23	121.33	115.36
7	В	303	MTX	N1-C2-N3	-5.17	120.33	127.22
7	В	302	MTX	N8-C8A-N1	4.75	121.25	115.82
7	В	302	MTX	N1-C2-N3	-4.23	121.58	127.22
7	В	303	MTX	C2-N1-C8A	3.94	119.86	115.36
7	В	303	MTX	N8-C8A-N1	3.46	119.77	115.82
7	В	303	MTX	CA-N-C	2.91	128.71	121.60
7	В	302	MTX	C4A-C4-N3	-2.66	119.26	121.01
7	В	303	MTX	CB-CA-CT	-2.66	103.94	110.35
7	В	303	MTX	C6-C9-N10	-2.60	109.14	113.60
7	В	302	MTX	C6-C7-N8	-2.55	120.63	123.13
7	В	303	MTX	C13-C14-N10	-2.55	117.95	121.62
7	В	302	MTX	C7-N8-C8A	2.47	119.18	116.69

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Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	A	301	GUN	C8-N7-C5	2.45	107.66	102.99
7	В	303	MTX	C15-C16-C11	-2.43	117.95	120.78
2	A	301	GUN	C5-C6-N1	2.36	118.12	113.95
7	В	302	MTX	CB-CA-N	2.35	115.62	110.88
7	В	303	MTX	C4A-C4-N3	-2.34	119.47	121.01
7	В	302	MTX	C8A-C4A-N5	-2.33	119.60	122.41
7	В	303	MTX	NA2-C2-N1	2.27	121.49	117.79
7	В	302	MTX	CA-N-C	2.23	127.06	121.60
7	В	302	MTX	C4A-C8A-N1	-2.22	118.11	121.71
7	В	303	MTX	CM-N10-C9	2.21	120.72	114.84
7	В	303	MTX	C7-N8-C8A	2.18	118.88	116.69
8	В	306	DTT	C2-C1-S1	-2.17	108.16	114.47
7	В	302	MTX	OE2-CD-CG	2.11	120.81	114.03

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	305	GOL	C1-C2-C3-O3
4	A	306	GOL	O1-C1-C2-C3
4	В	308	GOL	O1-C1-C2-C3
6	В	301	TRS	C1-C-C2-O2
6	В	301	TRS	C3-C-C2-O2
6	В	301	TRS	N-C-C2-O2
6	В	301	TRS	C2-C-C3-O3
8	В	306	DTT	S1-C1-C2-O2
8	В	306	DTT	S1-C1-C2-C3
8	В	306	DTT	C1-C2-C3-C4
8	В	306	DTT	C2-C3-C4-S4
8	В	306	DTT	O3-C3-C4-S4
7	В	302	MTX	CA-CB-CG-CD
7	В	302	MTX	CB-CA-N-C
7	В	302	MTX	CB-CA-CT-O1
7	В	302	MTX	CB-CA-CT-O2
4	A	303	GOL	C1-C2-C3-O3
4	A	305	GOL	O1-C1-C2-C3
7	В	302	MTX	C11-C-N-CA
4	A	305	GOL	O2-C2-C3-O3
4	A	306	GOL	O1-C1-C2-O2
4	В	308	GOL	O1-C1-C2-O2
6	В	301	TRS	C1-C-C3-O3
4	A	303	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	В	302	MTX	O-C-N-CA
7	В	302	MTX	N-CA-CT-O2
8	В	306	DTT	O2-C2-C3-C4
4	A	305	GOL	O1-C1-C2-O2
7	В	302	MTX	N-CA-CT-O1
6	В	301	TRS	C2-C-C1-O1
6	В	301	TRS	N-C-C3-O3
7	В	302	MTX	C6-C9-N10-CM
6	В	301	TRS	C3-C-C1-O1
7	В	302	MTX	CT-CA-CB-CG
7	В	303	MTX	C13-C14-N10-CM
7	В	302	MTX	OE2-CD-CG-CB
7	В	302	MTX	OE1-CD-CG-CB
7	В	303	MTX	C6-C9-N10-C14
6	В	301	TRS	N-C-C1-O1
7	В	303	MTX	OE2-CD-CG-CB

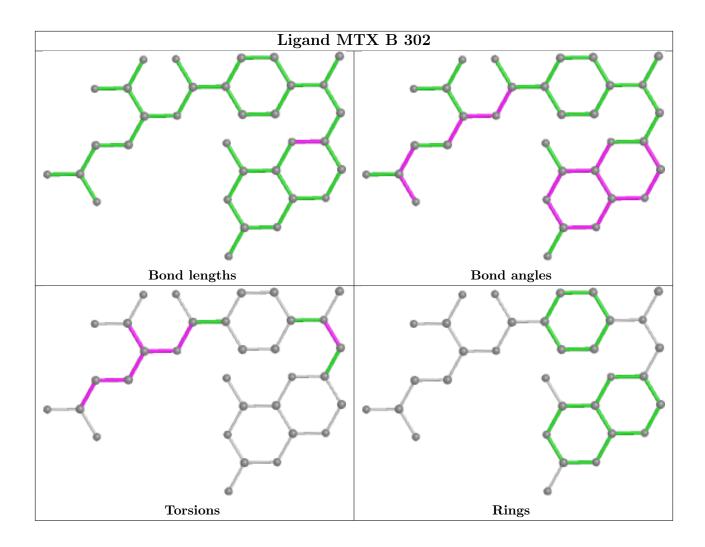
There are no ring outliers.

5 monomers are involved in 14 short contacts:

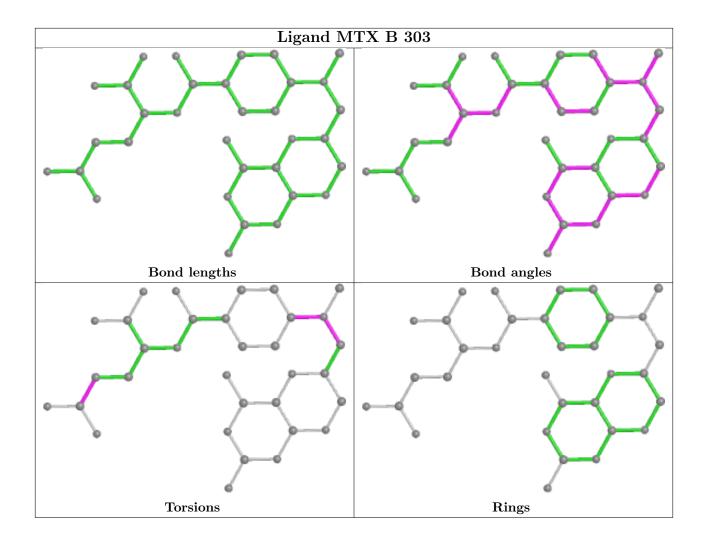
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	В	302	MTX	7	0
2	A	301	GUN	1	0
8	В	306	DTT	3	0
7	В	303	MTX	4	0
4	В	308	GOL	1	0

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 then 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, 95^{th} 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 $>$	$\# \mathrm{RSRZ}{>}2$	$OWAB(Å^2)$	Q < 0.9
1	A	$284/285 \ (99\%)$	0.10	14 (4%) 29 33	13, 20, 42, 79	0
1	В	$284/285 \ (99\%)$	-0.05	4 (1%) 75 79	12, 19, 34, 74	0
All	All	568/570 (99%)	0.03	18 (3%) 47 52	12, 19, 37, 79	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	0	ALA	5.8
1	A	234	GLU	5.2
1	A	235	SER	5.0
1	A	233	LEU	4.6
1	A	236	GLY	4.2
1	В	282	ASN	4.0
1	В	-1	ASN	3.8
1	A	282	ASN	3.5
1	A	232	ARG	3.4
1	В	134[A]	SER	3.2
1	A	42	PRO	3.1
1	A	280	ARG	3.0
1	A	47	TYR	2.8
1	A	-1	ASN	2.7
1	A	238	ILE	2.6
1	A	134[A]	SER	2.5
1	A	237	LYS	2.4
1	A	133[A]	GLU	2.3

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 monosaccharides in this entry.

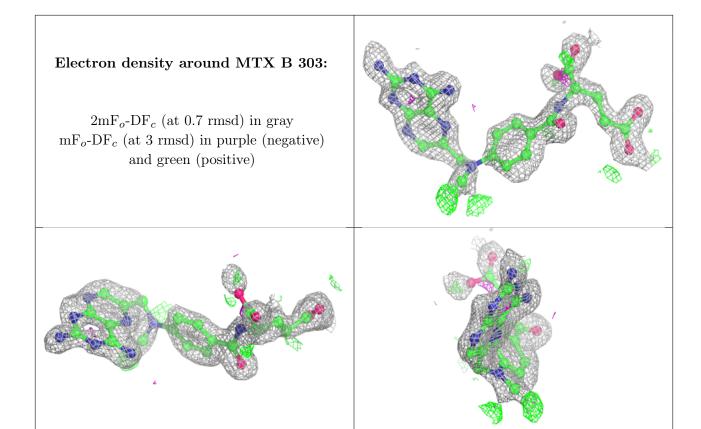
6.4 Ligands (i)

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, 95^{th} 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.

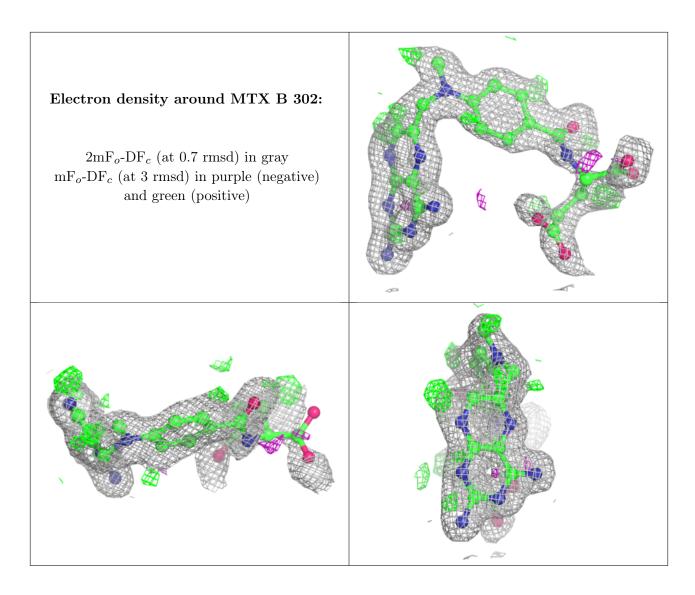
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}({ m \AA}^2)$	Q < 0.9
4	GOL	A	305	6/6	0.66	0.19	56,58,60,62	0
4	GOL	В	308	6/6	0.69	0.26	41,46,48,53	0
7	MTX	В	303	33/33	0.69	0.19	21,32,41,48	33
6	TRS	В	301	8/8	0.72	0.19	31,37,44,44	0
8	DTT	В	306	8/8	0.74	0.20	42,46,48,49	8
2	GUN	A	301	11/11	0.75	0.17	23,32,36,39	11
4	GOL	В	305	6/6	0.76	0.18	39,51,53,55	0
7	MTX	В	302	33/33	0.81	0.17	18,31,58,60	33
4	GOL	A	303	6/6	0.83	0.20	37,49,55,58	0
4	GOL	A	306	6/6	0.85	0.21	36,47,48,50	0
5	CL	В	307	1/1	0.96	0.10	25,25,25,25	0
5	CL	A	304	1/1	0.97	0.08	32,32,32,32	0
5	CL	В	304	1/1	0.98	0.06	28,28,28,28	0
3	K	A	302	1/1	1.00	0.06	21,21,21,21	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.









6.5 Other polymers (i)

There are no such residues in this entry.

