



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:34 AM GMT

PDB ID : 2XKK  
Title : CRYSTAL STRUCTURE OF MOXIFLOXACIN, DNA, AND A. BAUMANNII TOPO IV (PARE-PARC FUSION TRUNCATE)  
Authors : Wohlkonig, A.; Chan, P.F.; Fosberry, A.P.; Homes, P.; Huang, J.; Kranz, M.; Leydon, V.R.; Miles, T.J.; Pearson, N.D.; Perera, R.L.; Shillings, A.J.; Gwynn, M.N.; Bax, B.D.  
Deposited on : 2010-07-08  
Resolution : 3.25 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

<http://wwpdb.org/validation/2016/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 (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

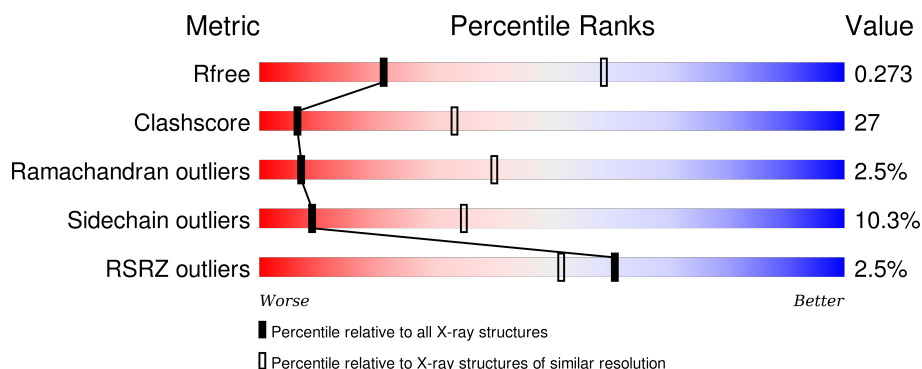
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	767	<div> <div>3%</div> <div>46%</div> <div>40%</div> <div>•</div> <div>10%</div> </div>
1	C	767	<div> <div>%</div> <div>47%</div> <div>40%</div> <div>6%</div> <div>7%</div> </div>
2	E	34	<div> <div>3%</div> <div>38%</div> <div>35%</div> <div>24%</div> </div>
3	F	34	<div> <div>3%</div> <div>41%</div> <div>32%</div> <div>24%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MX	E	1100	-	-	X	-
5	MX	F	1100	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11873 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 TOPOISOMERASE IV.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	692	Total	C	N	O	P	S	0	1	0
			5249	3313	905	1011	1	19			
1	C	711	Total	C	N	O	P	S	0	1	0
			5464	3441	951	1051	1	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	346	MET	-	EXPRESSION TAG	UNP B0V9T6
C	346	MET	-	EXPRESSION TAG	UNP B0V9T6

- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	26	Total	C	N	O	P	0	0	0
			534	256	104	149	25			

- Molecule 3 is a DNA chain called DNA.

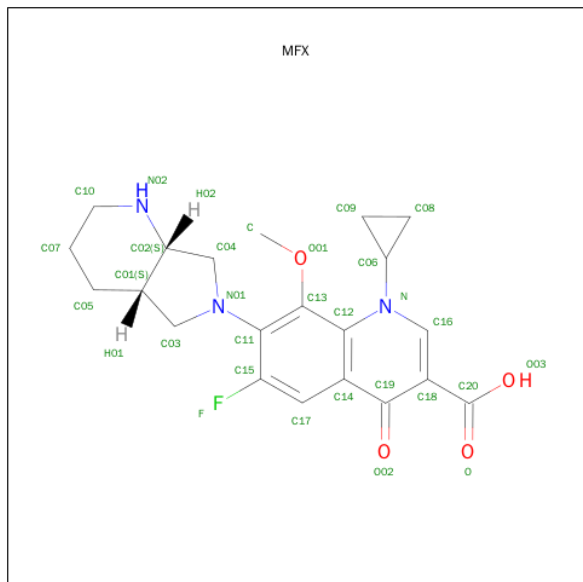
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	26	Total	C	N	O	P	0	0	0
			524	254	88	157	25			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	C	2	Total	Mg	0	0
			2	2		

- Molecule 5 is 1-CYCLOPROPYL-6-FLUORO-8-METHOXY-7-[(4AS,7AS)-OCTAHYDRO

-6H-PYRROLO[3,4-B]PYRIDIN-6-YL]-4-OXO-1,4-DIHYDROQUINOLINE-3-CARBOXYLIC ACID (three-letter code: MFX) (formula: C<sub>21</sub>H<sub>24</sub>FN<sub>3</sub>O<sub>4</sub>).

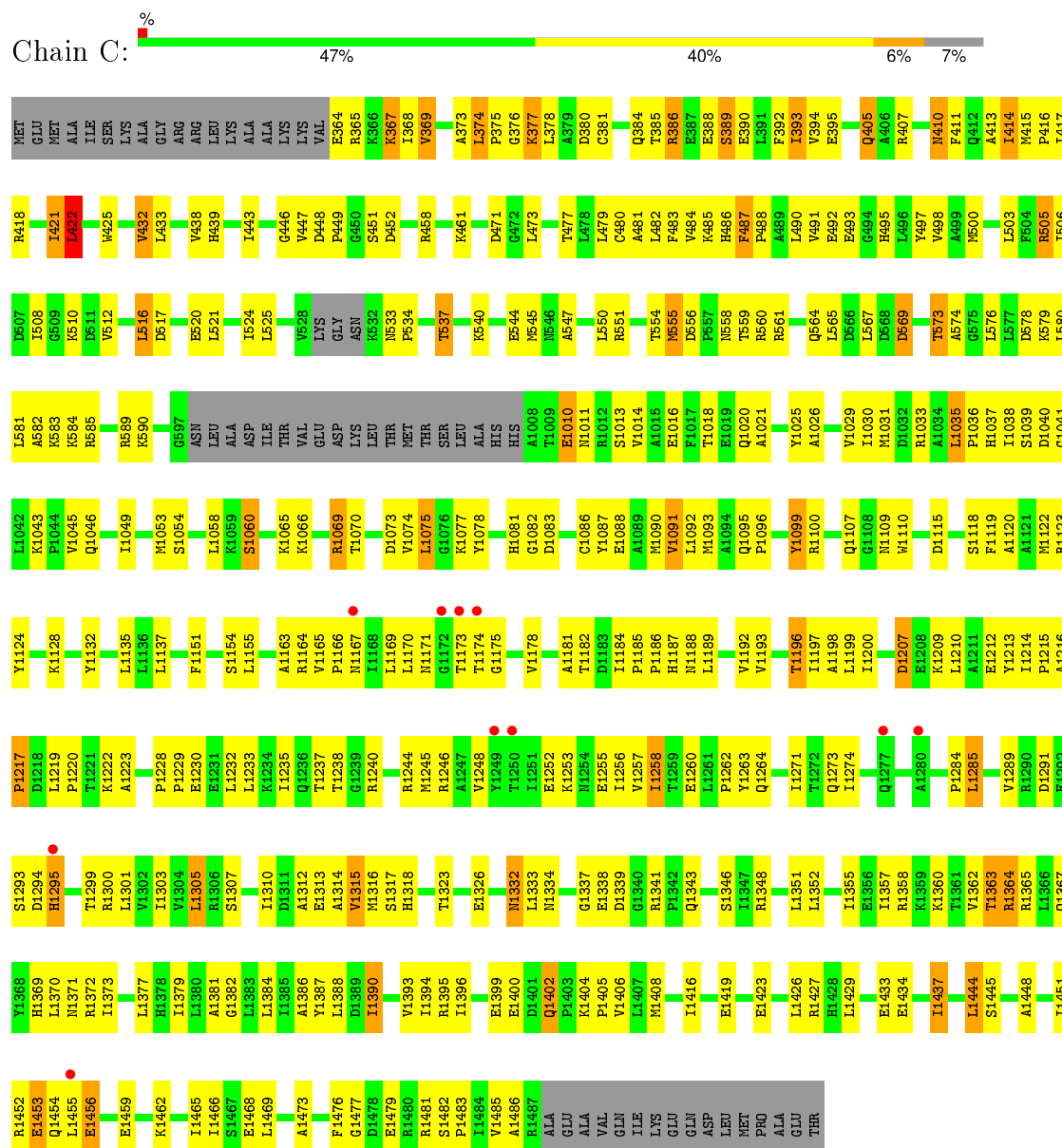


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
5	F	1	Total	C	F	N	O	0	0
			29	21	1	3	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	11	Total	O	0	0
			11	11		
6	C	20	Total	O	0	0
			20	20		
6	E	4	Total	O	0	0
			4	4		
6	F	5	Total	O	0	0
			5	5		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	199.78Å 95.57Å 118.09Å 90.00° 108.27° 90.00°	Depositor
Resolution (Å)	36.17 – 3.25 36.17 – 3.26	Depositor EDS
% Data completeness (in resolution range)	96.8 (36.17-3.25) 96.9 (36.17-3.26)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 3.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.194 , 0.270 0.193 , 0.273	Depositor DCC
$R_{free}$ test set	1317 reflections (4.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	109.1	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 87.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 32260 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11873	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 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: MFX, MG, PTR

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	0.41	0/5320	0.61	0/7231
1	C	0.43	0/5537	0.64	1/7514 (0.0%)
2	E	0.93	0/600	1.92	21/923 (2.3%)
3	F	0.85	0/584	1.77	19/897 (2.1%)
All	All	0.49	0/12041	0.85	41/16565 (0.2%)

There are no bond length outliers.

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	E	23	DC	O4'-C4'-C3'	-16.48	96.11	106.00
2	E	12	DG	O4'-C4'-C3'	-13.03	98.18	106.00
2	E	21	DT	C1'-O4'-C4'	-11.64	98.46	110.10
2	E	25	DC	O4'-C1'-N1	8.82	114.17	108.00
3	F	21	DT	O4'-C1'-N1	8.31	113.82	108.00

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	5249	0	5092	274	0
1	C	5464	0	5392	279	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	534	0	292	49	0
3	F	524	0	296	33	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
5	E	29	0	23	12	0
5	F	29	0	23	17	0
6	A	11	0	0	0	0
6	C	20	0	0	0	0
6	E	4	0	0	1	0
6	F	5	0	0	0	0
All	All	11873	0	11118	629	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 27.

The worst 5 of 629 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)
5:F:1100:MFX:C03	5:F:1100:MFX:HB	1.81	1.11
1:A:1300:ARG:HH11	1:A:1300:ARG:HG3	1.15	1.07
1:A:1256:ILE:HD13	1:A:1316:MET:HG2	1.31	1.06
1:C:386:ARG:HG2	1:C:386:ARG:HH21	1.12	1.05
5:F:1100:MFX:C03	5:F:1100:MFX:C	2.35	1.03

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	682/767 (89%)	564 (83%)	103 (15%)	15 (2%)	8	43
1	C	705/767 (92%)	615 (87%)	70 (10%)	20 (3%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1387/1534 (90%)	1179 (85%)	173 (12%)	35 (2%)	7	40

5 of 35 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	LEU
1	C	508	ILE
1	A	509	GLY
1	A	1066	LYS
1	C	374	LEU

### 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	537/656 (82%)	488 (91%)	49 (9%)	12	41
1	C	572/656 (87%)	507 (89%)	65 (11%)	7	30
All	All	1109/1312 (84%)	995 (90%)	114 (10%)	9	35

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	369	VAL
1	C	432	VAL
1	C	1390	ILE
1	C	384	GLN
1	C	394	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1332	ASN
1	C	486	HIS
1	C	1367	GLN

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Mol	Chain	Res	Type
1	A	1367	GLN
1	A	1428	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	PTR	A	1124	1,3	14,16,17	1.84	1 (7%)	18,22,24	0.75	0
1	PTR	C	1124	1,2	14,16,17	1.98	1 (7%)	18,22,24	0.75	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
1	PTR	A	1124	1,3	-	0/9/11/13	0/1/1/1
1	PTR	C	1124	1,2	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1124	PTR	OH-CZ	-7.18	1.23	1.40
1	A	1124	PTR	OH-CZ	-6.63	1.24	1.40

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1124	PTR	1	0
1	C	1124	PTR	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
5	MFX	E	1100	4	26,33,33	1.68	3 (11%)	29,50,50	2.33	11 (37%)
5	MFX	F	1100	4	26,33,33	1.72	5 (19%)	29,50,50	1.91	9 (31%)

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
5	MFX	E	1100	4	-	0/6/35/35	1/4/5/5
5	MFX	F	1100	4	-	0/6/35/35	1/4/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1100	MFX	C14-C12	-4.82	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1100	MFX	C14-C12	-4.80	1.37	1.41
5	F	1100	MFX	C16-C18	-2.84	1.32	1.38
5	E	1100	MFX	C16-C18	-2.78	1.33	1.38
5	F	1100	MFX	C01-C02	-2.33	1.50	1.53

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1100	MFX	C-O01-C13	-5.37	101.70	115.06
5	E	1100	MFX	C10-N02-C02	-4.72	108.39	111.55
5	E	1100	MFX	C16-N-C06	-4.32	114.34	119.25
5	E	1100	MFX	C-O01-C13	-4.03	105.04	115.06
5	E	1100	MFX	C17-C14-C19	-3.50	115.69	121.47

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	1100	MFX	C01-C02-C05-C07-C10-N02
5	E	1100	MFX	C01-C02-C05-C07-C10-N02

2 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1100	MFX	12	0
5	F	1100	MFX	17	0

## 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<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	691/767 (90%)	-0.03	24 (3%) 48 38	74, 138, 203, 247	0
1	C	710/767 (92%)	-0.16	10 (1%) 78 69	74, 125, 185, 222	0
2	E	26/34 (76%)	0.12	1 (3%) 44 34	105, 127, 234, 250	0
3	F	26/34 (76%)	0.10	1 (3%) 44 34	98, 142, 225, 251	0
All	All	1453/1602 (90%)	-0.09	36 (2%) 61 51	74, 131, 197, 251	0

The worst 5 of 36 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	PRO	4.9
1	A	1172	GLY	4.2
1	A	1173	THR	3.5
1	A	533	ASN	3.5
1	C	1172	GLY	3.4

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	A	1124	16/17	0.98	0.15	-	84,90,97,104	0
1	PTR	C	1124	16/17	0.97	0.17	-	112,119,127,129	0

### 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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	MFX	F	1100	29/29	0.93	0.24	0.04	123,139,149,153	0
5	MFX	E	1100	29/29	0.96	0.19	-0.50	92,109,119,124	0
4	MG	C	2488	1/1	0.98	0.24	-0.85	75,75,75,75	0
4	MG	C	1504	1/1	0.99	0.08	-	89,89,89,89	0
4	MG	A	2487	1/1	0.99	0.40	-	114,114,114,114	0
4	MG	A	1504	1/1	0.95	0.13	-	103,103,103,103	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.