



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:21 am GMT

PDB ID : 5BS8  
Title : Crystal structure of a topoisomerase II complex  
Authors : Blower, T.R.; Williamson, B.H.; Kerns, R.J.; Berger, J.M.  
Deposited on : 2015-06-01  
Resolution : 2.40 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

<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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

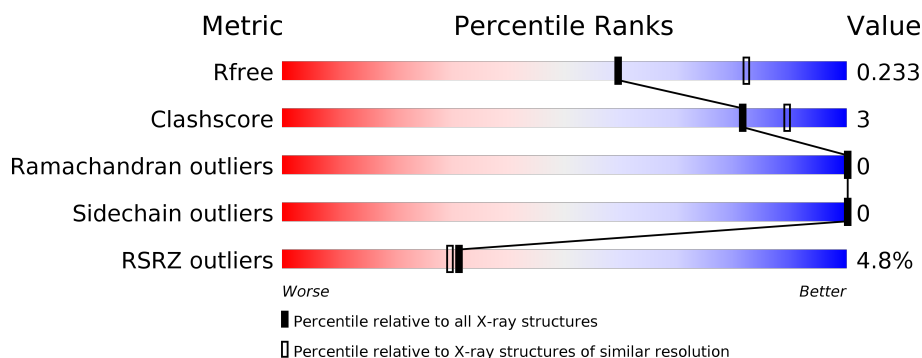
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	503	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>
1	C	503	<div> <div>5%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>.</div> </div> </div>
2	B	253	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>.</div> <div>.</div> </div> </div>
2	D	253	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>
3	E	24	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>13%</div> </div> </div>
3	H	24	<div> <div></div> <div> <div></div> <div>79%</div> <div>8%</div> <div>13%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	24	
4	G	24	

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
1	PTR	A	129	-	-	X	-
1	PTR	C	129	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26152 atoms, of which 12493 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	487	Total	C	H	N	O	P	S	0	1	0
			7646	2388	3808	704	732	1	13			
1	C	487	Total	C	H	N	O	P	S	0	1	0
			7689	2388	3851	704	732	1	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	ILE	-	expression tag	UNP P9WG47
A	502	GLY	-	expression tag	UNP P9WG47
A	503	SER	-	expression tag	UNP P9WG47
A	504	GLY	-	expression tag	UNP P9WG47
C	501	ILE	-	expression tag	UNP P9WG47
C	502	GLY	-	expression tag	UNP P9WG47
C	503	SER	-	expression tag	UNP P9WG47
C	504	GLY	-	expression tag	UNP P9WG47

- Molecule 2 is a protein called DNA gyrase subunit B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	245	Total	C	H	N	O	S	0	0	0
			3906	1217	1974	348	360	7			
2	D	247	Total	C	H	N	O	S	0	0	0
			3930	1224	1984	351	364	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	423	SER	-	expression tag	UNP P9WG45
B	424	ASN	-	expression tag	UNP P9WG45
B	425	ALA	-	expression tag	UNP P9WG45
D	423	SER	-	expression tag	UNP P9WG45

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Chain	Residue	Modelled	Actual	Comment	Reference
D	424	ASN	-	expression tag	UNP P9WG45
D	425	ALA	-	expression tag	UNP P9WG45

- Molecule 3 is a DNA chain called DNA substrate 24-mer GGTCATGAATGACTATGCAC GTAA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	21	Total	C	H	N	O	P	0	21	0
			616	196	206	74	120	20			
3	H	21	Total	C	H	N	O	P	0	21	0
			619	196	209	74	120	20			

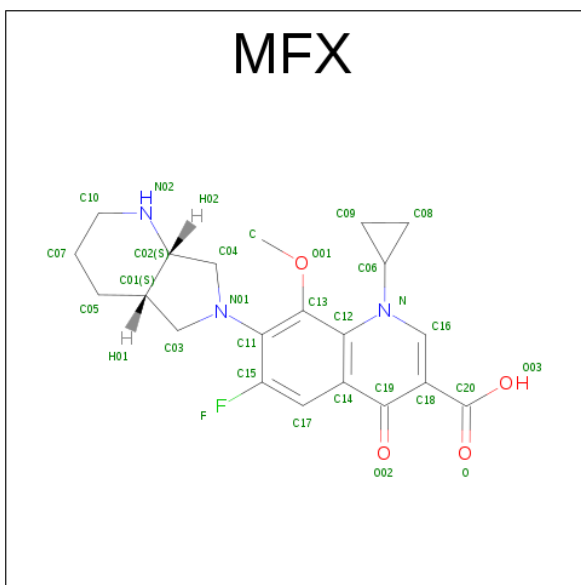
- Molecule 4 is a DNA chain called DNA substrate 24-mer TTACGTGCATAGTCATTCAT GACC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	21	Total	C	H	N	O	P	0	21	0
			617	196	207	74	120	20			
4	G	21	Total	C	H	N	O	P	0	21	0
			618	196	208	74	120	20			

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 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
6	G	1	Total	C	F	H	N	O	0	0
			52	21	1	23	3	4		
6	H	1	Total	C	F	H	N	O	0	0
			52	21	1	23	3	4		

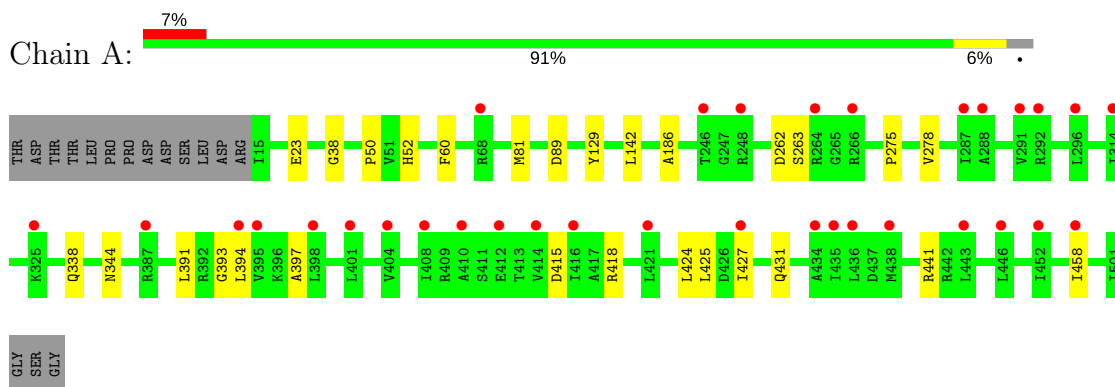
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	139	Total	O	0	0
			139	139		
7	B	53	Total	O	0	0
			53	53		
7	C	115	Total	O	0	0
			115	115		
7	D	54	Total	O	0	0
			54	54		
7	E	7	Total	O	0	0
			7	7		
7	F	12	Total	O	0	0
			12	12		
7	G	13	Total	O	0	0
			13	13		
7	H	10	Total	O	0	0
			10	10		

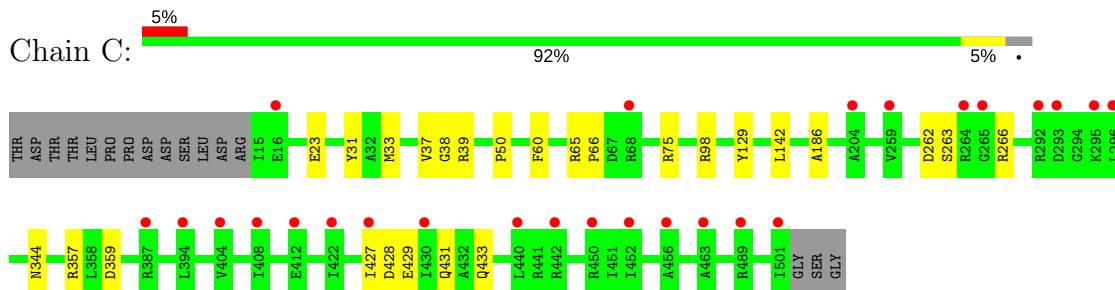
### 3 Residue-property plots [i](#)

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.

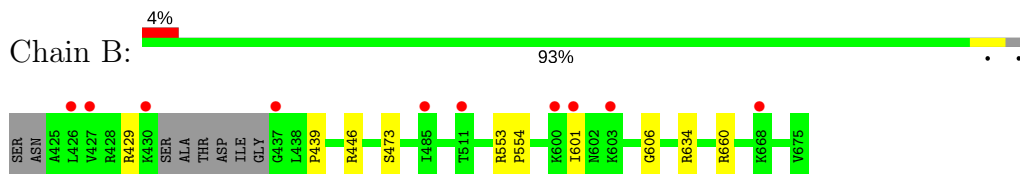
#### • Molecule 1: DNA gyrase subunit A



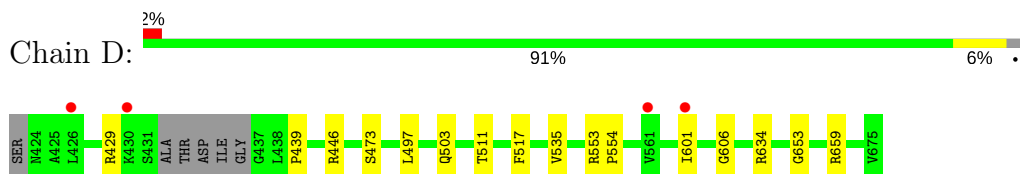
#### • Molecule 1: DNA gyrase subunit A



#### • Molecule 2: DNA gyrase subunit B

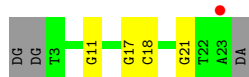


#### • Molecule 2: DNA gyrase subunit B




- Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA

Chain E: 



- Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA

Chain H: 




- Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC

Chain F: 



- Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC

Chain G: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.36Å 83.07Å 129.86Å 90.00° 109.33° 90.00°	Depositor
Resolution (Å)	102.25 – 2.40 102.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (102.25-2.40) 97.7 (102.25-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.196 , 0.233 0.196 , 0.233	Depositor DCC
$R_{free}$ test set	4165 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	26152	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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 [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	0.25	0/3881	0.40	0/5253
1	C	0.24	0/3881	0.40	0/5253
2	B	0.22	0/1960	0.39	0/2634
2	D	0.22	0/1974	0.40	0/2653
3	E	0.52	0/458	0.92	0/704
3	H	0.55	0/458	0.93	0/704
4	F	0.49	0/458	0.90	0/704
4	G	0.55	0/458	0.91	0/704
All	All	0.29	0/13528	0.51	0/18609

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	3838	3808	3853	25	0
1	C	3838	3851	3853	24	0
2	B	1932	1974	1973	6	0
2	D	1946	1984	1984	10	0
3	E	410	206	207	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	410	209	209	4	0
4	F	410	207	207	7	0
4	G	410	208	209	6	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	G	29	23	22	0	0
6	H	29	23	22	0	0
7	A	139	0	0	3	0
7	B	53	0	0	1	0
7	C	115	0	0	2	0
7	D	54	0	0	0	0
7	E	7	0	0	0	0
7	F	12	0	0	0	0
7	G	13	0	0	1	0
7	H	10	0	0	0	0
All	All	13659	12493	12539	65	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 (65) 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:129:PTR:O1P	3:H:11[B]:DG:C5'	1.77	1.32
1:C:129:PTR:O2P	4:G:11[B]:DA:C5'	1.82	1.25
1:A:129:PTR:O1P	4:F:11[A]:DA:C5'	1.83	1.23
1:A:38:GLY:O	1:A:50:PRO:HG2	1.42	1.15
1:C:129:PTR:O2P	3:E:11[A]:DG:C5'	1.95	1.13
1:A:129:PTR:O1P	3:H:11[B]:DG:C4'	2.01	1.06
1:A:129:PTR:O1P	3:H:11[B]:DG:H4'	1.61	1.00
1:C:129:PTR:O2P	3:E:11[A]:DG:C4'	2.12	0.98
1:C:38:GLY:O	1:C:50:PRO:HG2	1.64	0.97
1:C:129:PTR:O2P	3:E:11[A]:DG:H4'	1.64	0.96
1:A:129:PTR:O1P	4:F:11[A]:DA:H4'	1.67	0.93
1:C:129:PTR:O2P	4:G:11[B]:DA:C4'	2.15	0.92
1:C:33:MET:O	1:C:37:VAL:HG12	1.76	0.85
1:C:129:PTR:O2P	4:G:11[B]:DA:H4'	1.74	0.83
2:D:653:GLY:O	2:D:659:ARG:NH2	2.16	0.78
4:G:8[B]:DC:OP2	7:G:201:HOH:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PTR:O1P	4:F:11[A]:DA:C4'	2.10	0.70
2:B:429:ARG:NH1	2:B:439:PRO:O	2.25	0.69
1:A:393:GLY:O	7:A:601:HOH:O	2.11	0.69
1:C:98:ARG:NH1	3:H:7[B]:DG:OP1	2.29	0.66
2:D:429:ARG:NH1	2:D:439:PRO:O	2.29	0.66
1:A:38:GLY:C	1:A:50:PRO:HG2	2.18	0.63
1:A:441:ARG:NH2	1:C:433:GLN:OE1	2.31	0.62
2:B:446:ARG:NH1	2:B:473:SER:OG	2.34	0.59
1:C:75:ARG:NH1	7:C:602:HOH:O	2.37	0.58
1:C:262:ASP:OD1	1:C:263:SER:N	2.39	0.56
1:A:415:ASP:OD1	1:A:418:ARG:NH2	2.39	0.55
1:C:357:ARG:NH1	1:C:359:ASP:OD1	2.40	0.54
1:C:428:ASP:OD1	1:C:429:GLU:N	2.41	0.53
1:C:98:ARG:NH1	4:F:7[A]:DG:OP1	2.41	0.53
2:D:446:ARG:NH2	2:D:473:SER:OG	2.43	0.52
1:A:427:ILE:CG2	1:A:431:GLN:HB2	2.41	0.50
1:C:427:ILE:CG2	1:C:431:GLN:HB2	2.43	0.48
2:B:660:ARG:NH1	7:B:806:HOH:O	2.47	0.47
3:E:17[A]:DG:N2	4:F:8[A]:DC:O2	2.48	0.47
3:E:18[A]:DC:O2	4:F:7[A]:DG:N2	2.45	0.46
1:C:60:PHE:HB2	1:C:142:LEU:HD13	1.97	0.46
1:C:186:ALA:O	1:C:344:ASN:ND2	2.49	0.46
3:E:21[A]:DG:N2	4:F:4[A]:DC:O2	2.50	0.45
1:A:391:LEU:HD23	1:A:394:LEU:HD12	1.99	0.45
1:C:39:ARG:NH1	7:C:604:HOH:O	2.41	0.45
1:C:38:GLY:C	1:C:50:PRO:HG2	2.32	0.44
1:A:23:GLU:OE1	2:B:634:ARG:NH1	2.48	0.44
1:A:52:HIS:NE2	4:G:8[B]:DC:OP1	2.46	0.44
1:A:424:LEU:HG	1:A:425:LEU:HG	1.99	0.44
1:C:23:GLU:OE1	2:D:634:ARG:NH1	2.51	0.44
1:A:338:GLN:O	7:A:602:HOH:O	2.21	0.43
1:A:397:ALA:N	7:A:601:HOH:O	2.51	0.43
1:C:262:ASP:N	1:C:266:ARG:O	2.51	0.43
2:D:601:ILE:HG22	2:D:606:GLY:HA2	1.99	0.43
1:A:262:ASP:OD1	1:A:263:SER:N	2.52	0.42
1:A:186:ALA:O	1:A:344:ASN:ND2	2.53	0.42
1:C:65:ARG:HB3	1:C:66:PRO:HD2	2.01	0.42
1:A:81:MET:HE1	1:A:89:ASP:HB3	2.02	0.42
2:D:553:ARG:N	2:D:554:PRO:CD	2.83	0.42
1:C:31:TYR:HA	2:D:535:VAL:HG13	2.02	0.41
2:D:497:LEU:O	2:D:503:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PRO:HG2	1:A:278:VAL:HG21	2.03	0.41
1:A:60:PHE:HB2	1:A:142:LEU:HD13	2.02	0.41
2:B:553:ARG:N	2:B:554:PRO:CD	2.84	0.41
1:A:391:LEU:HD12	1:A:458:ILE:HD12	2.03	0.41
1:A:425:LEU:HB2	1:A:427:ILE:HD11	2.02	0.41
2:D:659:ARG:NH1	4:G:19[B]:DA:OP1	2.54	0.40
2:B:601:ILE:HG22	2:B:606:GLY:HA2	2.04	0.40
2:D:511:THR:HG21	2:D:517:PHE:CE2	2.57	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	485/503 (96%)	469 (97%)	16 (3%)	0	100	100
1	C	485/503 (96%)	466 (96%)	19 (4%)	0	100	100
2	B	241/253 (95%)	233 (97%)	8 (3%)	0	100	100
2	D	243/253 (96%)	235 (97%)	8 (3%)	0	100	100
All	All	1454/1512 (96%)	1403 (96%)	51 (4%)	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	Outliers	Percentiles	
1	A	407/420 (97%)	407 (100%)	0	100	100
1	C	407/420 (97%)	407 (100%)	0	100	100
2	B	205/211 (97%)	205 (100%)	0	100	100
2	D	207/211 (98%)	207 (100%)	0	100	100
All	All	1226/1262 (97%)	1226 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	431	GLN

### 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	129	1	15,16,17	1.08	1 (6%)	19,22,24	1.05	1 (5%)
1	PTR	C	129	1	15,16,17	1.37	3 (20%)	19,22,24	1.12	1 (5%)

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	129	1	-	0/9/11/13	0/1/1/1
1	PTR	C	129	1	-	0/9/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	129	PTR	CA-C	-2.66	1.46	1.50
1	A	129	PTR	CA-C	-2.61	1.46	1.50
1	C	129	PTR	CB-CA	-2.30	1.48	1.53
1	C	129	PTR	OH-CZ	-2.02	1.35	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	PTR	CB-CA-C	-3.13	105.38	111.41
1	C	129	PTR	CB-CA-C	-2.95	105.73	111.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	129	PTR	6	0
1	C	129	PTR	6	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
6	MFX	G	101	5	24,33,33	4.45	13 (54%)	28,50,50	1.66	6 (21%)
6	MFX	H	101	5	24,33,33	4.45	13 (54%)	28,50,50	1.64	7 (25%)

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
6	MFX	G	101	5	-	0/10/35/35	0/4/5/5
6	MFX	H	101	5	-	0/10/35/35	0/4/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	101	MFX	C01-C02	-10.74	1.37	1.53
6	G	101	MFX	C01-C02	-10.49	1.37	1.53
6	H	101	MFX	C04-N01	-7.95	1.35	1.46
6	G	101	MFX	C04-N01	-7.86	1.36	1.46
6	G	101	MFX	C07-C05	-2.85	1.45	1.53
6	H	101	MFX	C07-C05	-2.68	1.46	1.53
6	H	101	MFX	C19-C18	2.05	1.45	1.39
6	G	101	MFX	C19-C18	2.08	1.45	1.39
6	G	101	MFX	O01-C13	2.58	1.42	1.38
6	H	101	MFX	O01-C13	2.63	1.42	1.38
6	H	101	MFX	C11-N01	2.69	1.48	1.40
6	G	101	MFX	C11-N01	2.74	1.48	1.40
6	H	101	MFX	C17-C15	3.51	1.40	1.35
6	G	101	MFX	C17-C15	3.53	1.40	1.35
6	H	101	MFX	C03-C01	3.76	1.58	1.53
6	G	101	MFX	C03-C01	3.80	1.58	1.53
6	H	101	MFX	C02-N02	4.30	1.52	1.47
6	G	101	MFX	C02-N02	4.48	1.52	1.47
6	G	101	MFX	C16-C18	5.13	1.48	1.39
6	H	101	MFX	C16-C18	5.14	1.48	1.39
6	H	101	MFX	C04-C02	6.86	1.64	1.52
6	G	101	MFX	C04-C02	6.99	1.64	1.52
6	H	101	MFX	C19-C14	7.42	1.52	1.41
6	G	101	MFX	C19-C14	7.63	1.52	1.41
6	G	101	MFX	C03-N01	9.40	1.59	1.46
6	H	101	MFX	C03-N01	9.43	1.59	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	101	MFX	C03-N01-C11	-3.47	116.44	123.04
6	H	101	MFX	C03-N01-C11	-3.45	116.48	123.04
6	H	101	MFX	C04-N01-C11	-2.82	117.68	123.04
6	G	101	MFX	C04-N01-C11	-2.61	118.09	123.04
6	H	101	MFX	F-C15-C17	-2.50	116.83	120.31
6	G	101	MFX	F-C15-C17	-2.44	116.91	120.31
6	G	101	MFX	C13-C11-N01	-2.18	117.34	122.68
6	H	101	MFX	C17-C15-C11	-2.10	120.32	123.37
6	H	101	MFX	C13-C11-C15	2.05	118.01	116.01
6	H	101	MFX	C07-C05-C01	2.05	115.27	111.95
6	G	101	MFX	C06-N-C12	2.43	123.97	120.87
6	G	101	MFX	F-C15-C11	2.96	122.57	118.30
6	H	101	MFX	F-C15-C11	3.15	122.85	118.30

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	486/503 (96%)	0.71	33 (6%) 18 16	35, 59, 117, 170	0
1	C	486/503 (96%)	0.77	26 (5%) 27 25	37, 62, 118, 182	0
2	B	245/253 (96%)	0.76	10 (4%) 38 36	48, 66, 104, 131	0
2	D	247/253 (97%)	0.65	4 (1%) 72 70	44, 63, 102, 138	0
3	E	21/24 (87%)	0.76	1 (4%) 31 30	64, 116, 224, 263	21 (100%)
3	H	21/24 (87%)	0.62	0 100 100	31, 47, 113, 128	21 (100%)
4	F	21/24 (87%)	0.65	0 100 100	76, 112, 192, 244	21 (100%)
4	G	21/24 (87%)	0.80	1 (4%) 31 30	31, 51, 113, 130	21 (100%)
All	All	1548/1608 (96%)	0.73	75 (4%) 31 30	31, 63, 119, 263	84 (5%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	ARG	8.9
1	A	414	VAL	5.9
2	B	426	LEU	5.9
1	A	387	ARG	5.7
1	C	292	ARG	5.1
1	C	442	ARG	5.0
1	A	421	LEU	4.8
1	A	412	GLU	4.7
1	C	404	VAL	4.6
2	B	603	LYS	4.3
2	D	601	ILE	4.2
1	C	387	ARG	4.2
4	G	23[B]	DC	4.1
2	B	601	ILE	4.1
2	B	430	LYS	4.1
1	C	440	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	293	ASP	3.8
1	A	427	ILE	3.7
1	A	395	VAL	3.7
1	A	264	ARG	3.5
1	C	264	ARG	3.5
2	D	426	LEU	3.5
1	A	68	ARG	3.4
1	C	295	LYS	3.3
1	C	427	ILE	3.3
1	C	394	LEU	3.2
1	A	401	LEU	3.2
1	A	452	ILE	3.1
1	C	501	ILE	3.1
1	C	452	ILE	2.9
1	A	398	LEU	2.9
2	B	437	GLY	2.9
1	A	416	ILE	2.8
1	A	443	LEU	2.8
1	C	489	ARG	2.7
1	A	266	ARG	2.6
1	A	438	MET	2.6
1	A	446	LEU	2.6
1	C	408	ILE	2.6
1	A	408	ILE	2.6
1	C	450	ARG	2.5
3	E	23[A]	DA	2.5
1	C	265	GLY	2.5
1	C	430	ILE	2.5
1	C	68	ARG	2.5
1	C	259	VAL	2.5
2	D	430	LYS	2.4
1	A	458	ILE	2.4
1	A	435	ILE	2.4
1	C	296	LEU	2.3
1	A	436	LEU	2.3
1	A	288	ALA	2.3
2	B	600	LYS	2.3
1	C	463	ALA	2.3
2	B	485	ILE	2.3
1	A	394	LEU	2.2
1	A	404	VAL	2.2
1	A	248	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	204	ALA	2.2
1	C	422	ILE	2.2
1	A	296	LEU	2.2
1	A	291	VAL	2.2
1	A	410	ALA	2.2
1	A	434	ALA	2.2
1	C	412	GLU	2.1
2	B	427	VAL	2.1
2	B	668	LYS	2.1
1	A	314	ILE	2.1
1	C	456	ALA	2.1
1	C	16	GLU	2.1
2	D	561	VAL	2.1
1	A	325	LYS	2.1
1	A	246	THR	2.1
1	A	287	ILE	2.0
2	B	511	THR	2.0

## 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	129	16/17	0.95	0.18	-	43,50,76,86	0
1	PTR	C	129	16/17	0.94	0.19	-	47,58,70,153	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
6	MFX	G	101	29/29	0.94	0.19	0.26	42,52,73,73	0
6	MFX	H	101	29/29	0.94	0.17	-0.79	40,50,62,62	0
5	MG	B	701	1/1	0.94	0.15	-1.23	47,47,47,47	0
5	MG	E	101	1/1	0.99	0.14	-1.37	53,53,53,53	0
5	MG	D	701	1/1	0.91	0.14	-2.78	35,35,35,35	0
5	MG	F	101	1/1	0.96	0.12	-2.84	44,44,44,44	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.