



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2016 – 01:37 AM EDT

PDB ID : 4Z2C  
Title : Quinolone(Moxifloxacin)-DNA cleavage complex of gyrase from *S. pneumoniae*  
Authors : Laponogov, I.; Veselkov, D.A.; Pan, X.-S.; Selvarajah, J.; Crevel, I.M.-T.; Fisher, L.M.; Sanderson, M.R.  
Deposited on : 2015-03-29  
Resolution : 3.19 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	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

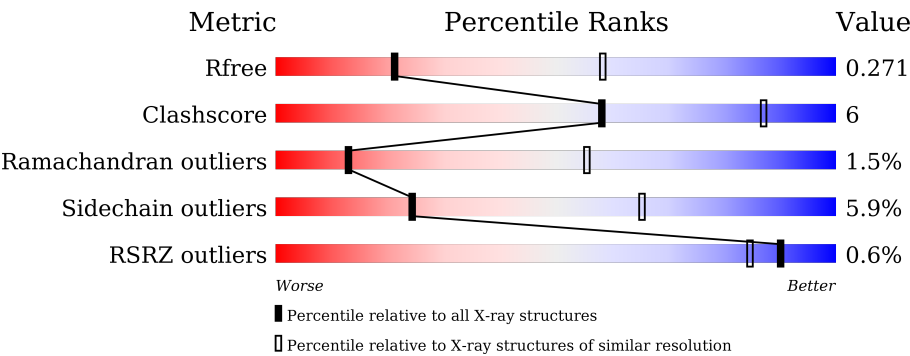
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.19 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.



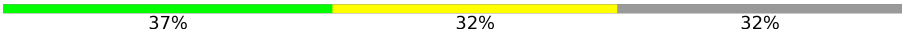
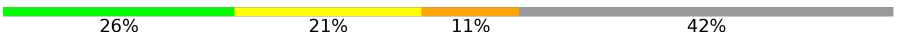
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	499	
1	B	499	
2	C	269	
2	D	269	
3	E	15	
3	G	15	

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Mol	Chain	Length	Quality of chain
4	F	19	
4	H	19	

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
6	MG	G	101	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10598 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 DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	1	0
			3618	2279	648	670	21			
1	B	482	Total	C	N	O	S	0	0	0
			3438	2151	618	651	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	HIS	-	expression tag	UNP Q9R867
A	495	HIS	-	expression tag	UNP Q9R867
A	496	HIS	-	expression tag	UNP Q9R867
A	497	HIS	-	expression tag	UNP Q9R867
A	498	HIS	-	expression tag	UNP Q9R867
A	499	HIS	-	expression tag	UNP Q9R867
B	494	HIS	-	expression tag	UNP Q9R867
B	495	HIS	-	expression tag	UNP Q9R867
B	496	HIS	-	expression tag	UNP Q9R867
B	497	HIS	-	expression tag	UNP Q9R867
B	498	HIS	-	expression tag	UNP Q9R867
B	499	HIS	-	expression tag	UNP Q9R867

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	198	Total	C	N	O	S	0	0	0
			1331	838	235	249	9			
2	D	194	Total	C	N	O	S	0	1	0
			1332	840	229	253	10			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	initiating methionine	UNP Q59957
C	381	GLY	-	expression tag	UNP Q59957
C	382	HIS	-	expression tag	UNP Q59957
C	383	HIS	-	expression tag	UNP Q59957
C	384	HIS	-	expression tag	UNP Q59957
C	385	HIS	-	expression tag	UNP Q59957
C	386	HIS	-	expression tag	UNP Q59957
C	387	HIS	-	expression tag	UNP Q59957
C	388	HIS	-	expression tag	UNP Q59957
C	389	HIS	-	expression tag	UNP Q59957
C	390	HIS	-	expression tag	UNP Q59957
C	391	HIS	-	expression tag	UNP Q59957
C	392	SER	-	expression tag	UNP Q59957
C	393	SER	-	expression tag	UNP Q59957
C	394	GLY	-	expression tag	UNP Q59957
C	395	HIS	-	expression tag	UNP Q59957
C	396	ILE	-	expression tag	UNP Q59957
C	397	ASP	-	expression tag	UNP Q59957
C	398	ASP	-	expression tag	UNP Q59957
C	399	ASP	-	expression tag	UNP Q59957
C	400	ASP	-	expression tag	UNP Q59957
C	401	LYS	-	expression tag	UNP Q59957
C	402	HIS	-	expression tag	UNP Q59957
C	403	MET	-	expression tag	UNP Q59957
D	380	MET	-	initiating methionine	UNP Q59957
D	381	GLY	-	expression tag	UNP Q59957
D	382	HIS	-	expression tag	UNP Q59957
D	383	HIS	-	expression tag	UNP Q59957
D	384	HIS	-	expression tag	UNP Q59957
D	385	HIS	-	expression tag	UNP Q59957
D	386	HIS	-	expression tag	UNP Q59957
D	387	HIS	-	expression tag	UNP Q59957
D	388	HIS	-	expression tag	UNP Q59957
D	389	HIS	-	expression tag	UNP Q59957
D	390	HIS	-	expression tag	UNP Q59957
D	391	HIS	-	expression tag	UNP Q59957
D	392	SER	-	expression tag	UNP Q59957
D	393	SER	-	expression tag	UNP Q59957
D	394	GLY	-	expression tag	UNP Q59957
D	395	HIS	-	expression tag	UNP Q59957
D	396	ILE	-	expression tag	UNP Q59957
D	397	ASP	-	expression tag	UNP Q59957
D	398	ASP	-	expression tag	UNP Q59957

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Chain	Residue	Modelled	Actual	Comment	Reference
D	399	ASP	-	expression tag	UNP Q59957
D	400	ASP	-	expression tag	UNP Q59957
D	401	LYS	-	expression tag	UNP Q59957
D	402	HIS	-	expression tag	UNP Q59957
D	403	MET	-	expression tag	UNP Q59957

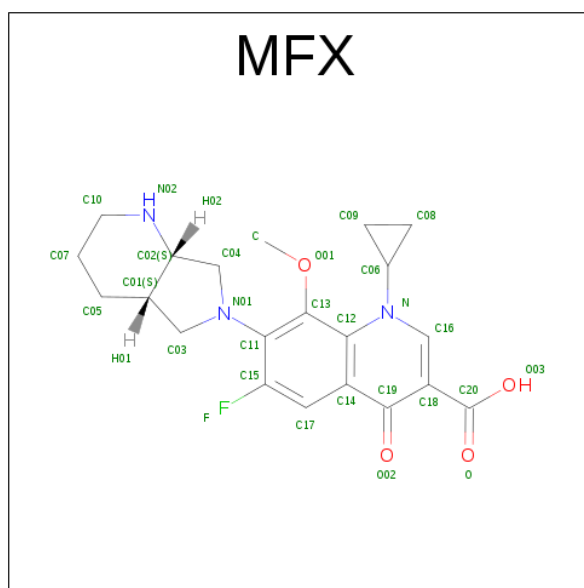
- Molecule 3 is a DNA chain called Symmetrized E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	9	Total	C	N	O	P	0	0	0
			185	89	31	56	9			
3	G	7	Total	C	N	O	P	0	0	0
			141	70	23	42	6			

- Molecule 4 is a DNA chain called Symmetrized E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	13	Total	C	N	O	P	0	0	0
			263	127	50	74	12			
4	H	11	Total	C	N	O	P	0	0	0
			221	107	43	61	10			

- 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	F	1	Total	C	F	N	O	0	0
			29	21	1	3	4		
5	H	1	Total	C	F	N	O	0	0
			29	21	1	3	4		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Mg	0	0
			1	1		
6	G	1	Total	Mg	0	0
			1	1		

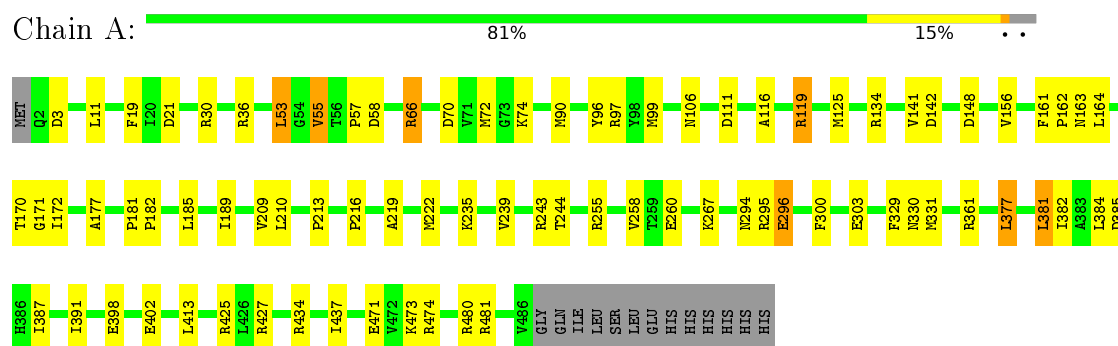
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	2	Total	O	0	0
			2	2		
7	F	1	Total	O	0	0
			1	1		

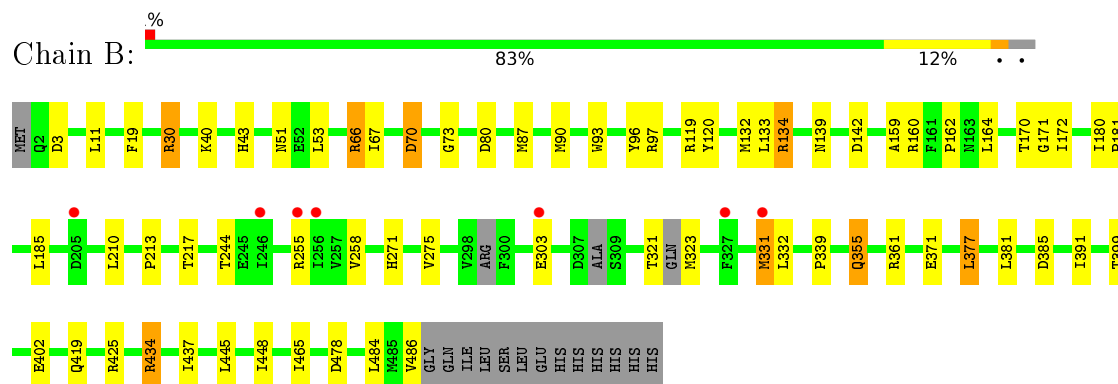
### 3 Residue-property plots

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.

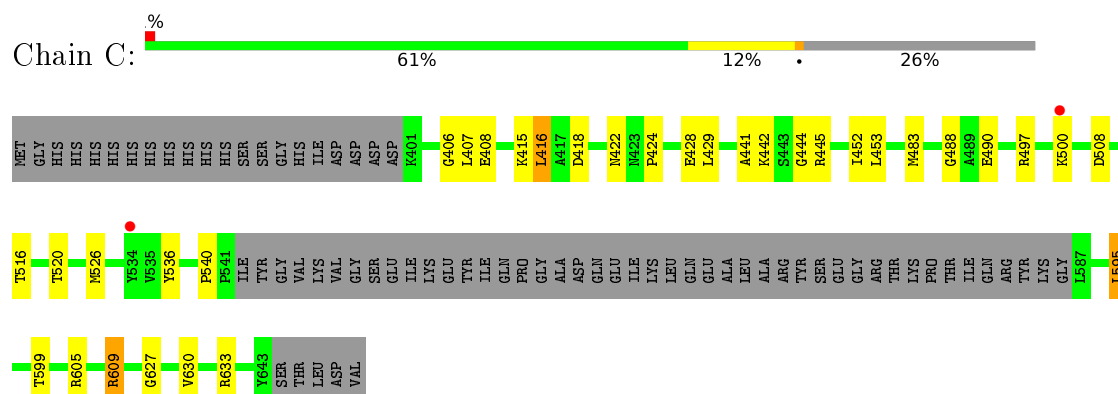
#### • Molecule 1: DNA gyrase subunit A



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

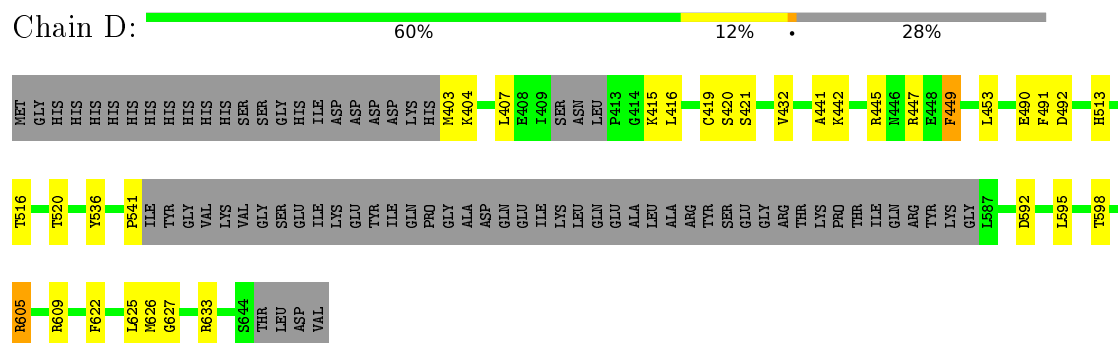


#### • Molecule 2: DNA gyrase subunit B

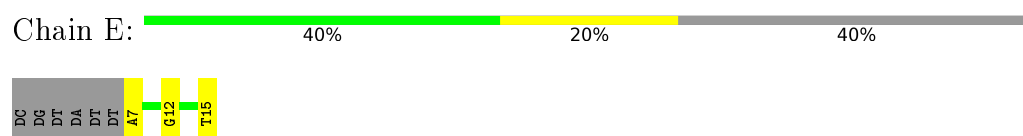




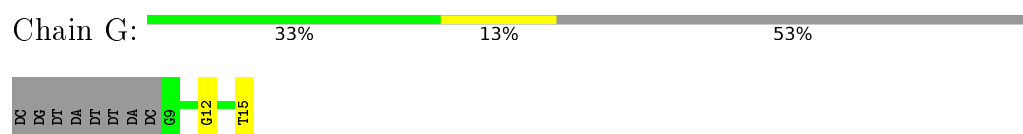
- Molecule 2: DNA gyrase subunit B



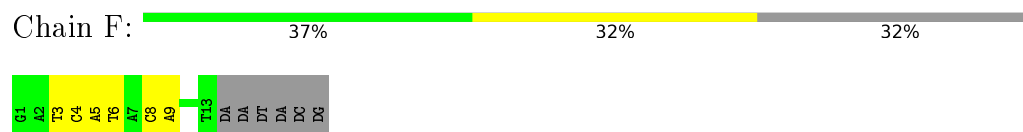
- Molecule 3: Symmetrized E-site DNA



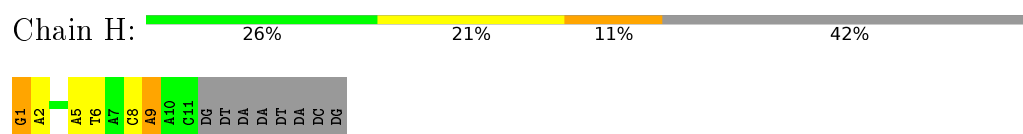
- Molecule 3: Symmetrized E-site DNA



- Molecule 4: Symmetrized E-site DNA



- Molecule 4: Symmetrized E-site DNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.03Å 94.95Å 274.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.25 – 3.19 68.57 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (64.25-3.19) 93.8 (68.57-3.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.223 , 0.268 0.223 , 0.271	Depositor DCC
$R_{free}$ test set	1916 reflections (4.82%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.3	Xtriage
Anisotropy	0.621	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 88.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10598	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.24% 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: MFX, MG

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	0.22	0/3677	0.40	0/4991
1	B	0.22	0/3491	0.40	0/4755
2	C	0.21	0/1352	0.41	0/1846
2	D	0.21	0/1353	0.40	0/1843
3	E	0.47	0/206	1.11	0/316
3	G	0.47	0/157	1.12	0/242
4	F	0.48	0/295	1.15	2/453 (0.4%)
4	H	0.45	0/248	1.19	3/380 (0.8%)
All	All	0.25	0/10779	0.52	5/14826 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	6	DT	O4'-C4'-C3'	-5.99	102.10	104.50
4	H	9	DA	O4'-C4'-C3'	-5.96	102.11	104.50
4	H	1	DG	C3'-C2'-C1'	-5.76	95.59	102.50
4	F	6	DT	O4'-C1'-N1	5.35	111.74	108.00
4	H	6	DT	C1'-O4'-C4'	-5.18	104.92	110.10

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	3618	0	3433	41	0
1	B	3438	0	3061	34	0
2	C	1331	0	1136	18	0
2	D	1332	0	1132	21	0
3	E	185	0	104	3	0
3	G	141	0	80	2	0
4	F	263	0	148	7	0
4	H	221	0	125	7	0
5	F	29	0	22	6	0
5	H	29	0	23	5	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	6	0	0	0	0
7	B	2	0	0	0	0
7	F	1	0	0	0	0
All	All	10598	0	9264	118	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 6.

All (118) 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:243:ARG:HB3	1:A:260:GLU:HB2	1.69	0.74
2:C:627:GLY:O	2:C:633:ARG:NH2	2.25	0.69
1:A:391:ILE:HD13	1:B:391:ILE:HD13	1.74	0.69
2:D:403:MET:HA	2:D:421:SER:HA	1.73	0.68
2:C:406:GLY:O	2:C:408:GLU:N	2.25	0.64
1:A:471:GLU:OE1	1:A:474:ARG:NH2	2.31	0.64
1:A:106:ASN:HB3	1:A:116:ALA:HB2	1.79	0.63
5:F:101:MFX:H03	4:H:5:DA:C4	2.34	0.62
1:A:255:ARG:NH1	1:A:303:GLU:OE2	2.33	0.62
1:A:177:ALA:O	1:A:330:ASN:ND2	2.34	0.61
1:A:222:MET:HB2	1:A:239:VAL:HB	1.82	0.60
5:F:101:MFX:C	5:F:101:MFX:H08A	2.32	0.59
2:C:442:LYS:O	2:C:445:ARG:NH1	2.36	0.59
2:D:627:GLY:O	2:D:633:ARG:NH2	2.36	0.59
1:A:119[B]:ARG:NH1	1:B:80:ASP:OD2	2.36	0.58
2:D:419:CYS:SG	2:D:420:SER:N	2.75	0.58
1:A:111:ASP:OD1	1:A:267:LYS:NZ	2.36	0.58
2:D:490:GLU:O	2:D:492:ASP:N	2.36	0.58
1:A:19:PHE:HZ	2:D:633:ARG:HD3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ASP:OD1	1:B:361:ARG:NH2	2.38	0.56
1:A:427:ARG:NH2	1:B:419:GLN:OE1	2.39	0.55
3:E:15:DT:C2	5:H:101:MFX:H08A	2.42	0.54
1:A:189:ILE:HD12	1:A:473:LYS:HB2	1.88	0.54
1:B:132:MET:HA	1:B:159:ALA:HA	1.89	0.54
1:A:244:THR:HG22	1:A:258:VAL:HA	1.91	0.53
2:C:483:MET:HG3	2:C:526:MET:HE3	1.89	0.53
2:D:625:LEU:O	2:D:633:ARG:NE	2.40	0.53
1:A:385:ASP:OD1	1:A:434:ARG:NH1	2.42	0.52
1:B:377:LEU:HG	1:B:437:ILE:HG23	1.91	0.52
1:B:97:ARG:HH22	1:B:478:ASP:HB2	1.73	0.52
1:A:258:VAL:HB	1:A:300:PHE:HB3	1.92	0.52
2:D:633:ARG:NH1	4:F:9:DA:OP1	2.42	0.52
2:C:441:ALA:O	2:C:445:ARG:HB3	2.10	0.52
2:D:441:ALA:O	2:D:445:ARG:HB3	2.09	0.52
2:C:633:ARG:NH1	4:H:9:DA:OP1	2.43	0.52
1:A:3:ASP:OD1	2:D:605:ARG:NH2	2.44	0.51
1:A:66:ARG:HG3	1:B:73:GLY:HA3	1.93	0.51
4:F:5:DA:C4	5:H:101:MFX:H03	2.47	0.50
4:H:1:DG:H2"	4:H:2:DA:C8	2.46	0.50
1:A:398:GLU:N	1:A:402:GLU:OE2	2.38	0.50
2:C:633:ARG:HD3	1:B:19:PHE:HZ	1.77	0.50
1:B:255:ARG:HG3	1:B:303:GLU:HG2	1.94	0.50
1:A:74:LYS:HD3	1:B:66:ARG:HH21	1.77	0.49
1:A:36:ARG:HH21	1:A:156:VAL:HB	1.77	0.49
5:F:101:MFX:H03	4:H:5:DA:N3	2.27	0.49
4:F:3:DT:H2"	4:F:4:DC:O5'	2.13	0.49
1:A:53:LEU:HB3	1:A:55:VAL:HG22	1.95	0.48
5:F:101:MFX:H01	4:H:5:DA:O4'	2.14	0.48
1:B:180:ILE:HG12	1:B:331:MET:HG2	1.95	0.47
2:D:541:PRO:HG3	2:D:598:THR:HG21	1.97	0.47
1:B:371:GLU:HG2	1:B:448:ILE:HD13	1.96	0.47
1:B:385:ASP:OD1	1:B:434:ARG:NH1	2.47	0.47
4:F:5:DA:N3	5:H:101:MFX:H03	2.30	0.47
2:D:536:TYR:OH	2:D:609:ARG:NH1	2.48	0.47
1:B:139:ASN:O	1:B:361:ARG:NH1	2.48	0.47
1:A:57:PRO:HD3	1:A:125:MET:HB2	1.97	0.46
4:H:8:DC:H2"	4:H:9:DA:H5'	1.98	0.46
1:A:377:LEU:HG	1:A:437:ILE:HG23	1.96	0.46
2:C:605:ARG:NE	1:B:3:ASP:OD1	2.41	0.46
3:E:7:DA:C8	3:E:7:DA:H5"	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:513:HIS:O	2:D:516:THR:OG1	2.26	0.46
1:A:213:PRO:O	1:A:480:ARG:NH2	2.48	0.46
1:A:36:ARG:HE	1:A:156:VAL:HG21	1.81	0.46
5:F:101:MFX:HA	5:F:101:MFX:H08A	1.98	0.46
1:B:90:MET:HG2	1:B:96:TYR:CE2	2.50	0.45
2:C:516:THR:O	2:C:520:THR:HG23	2.16	0.45
2:D:404:LYS:N	2:D:420:SER:O	2.49	0.45
1:B:119:ARG:NH2	1:B:120:TYR:OH	2.50	0.45
4:F:5:DA:O4'	5:H:101:MFX:H01	2.17	0.45
1:A:66:ARG:HD3	1:B:70:ASP:HA	1.98	0.45
2:D:520:THR:HG21	2:D:626:MET:HG3	1.98	0.44
1:B:332:LEU:HD11	1:B:339:PRO:HB2	1.99	0.44
1:A:19:PHE:CZ	2:D:633:ARG:HD3	2.52	0.44
1:A:382:ILE:HD12	1:A:413:LEU:HD21	1.99	0.44
1:B:355:GLN:HB3	1:B:465:ILE:HD13	2.00	0.44
2:C:416:LEU:HA	2:C:452:ILE:O	2.18	0.44
1:A:235:LYS:HA	1:A:329:PHE:O	2.18	0.44
1:B:67:ILE:HG21	1:B:87:MET:HE1	2.00	0.44
1:B:321:THR:HG1	1:B:323:MET:N	2.16	0.43
2:D:449:PHE:H	2:D:449:PHE:HD1	1.66	0.43
1:A:142:ASP:OD1	1:A:361:ARG:NH2	2.51	0.43
2:C:422:ASN:O	2:C:424:PRO:HD3	2.19	0.43
1:A:219:ALA:N	1:A:260:GLU:OE1	2.41	0.43
1:A:90:MET:HA	1:A:96:TYR:CD1	2.54	0.43
1:B:160:ARG:NE	1:B:355:GLN:OE1	2.44	0.42
1:B:40:LYS:HG3	1:B:43:HIS:ND1	2.34	0.42
1:B:134:ARG:HB2	1:B:160:ARG:HG2	2.01	0.42
1:A:172:ILE:HD12	3:E:12:DG:C2	2.54	0.42
5:H:101:MFX:H16	5:H:101:MFX:H09	1.80	0.42
5:F:101:MFX:H09A	3:G:15:DT:H2"	2.00	0.42
2:D:516:THR:O	2:D:520:THR:HG23	2.19	0.42
4:F:9:DA:C8	4:F:9:DA:H5'	2.55	0.42
2:D:442:LYS:HA	2:D:445:ARG:HD3	2.02	0.42
1:B:275:VAL:HG13	2:D:407:LEU:HA	2.02	0.42
4:F:8:DC:H2'	4:F:8:DC:H6	1.70	0.42
1:B:51:ASN:HB2	1:B:133:LEU:HD13	2.01	0.42
1:A:294:ASN:O	1:A:296:GLU:N	2.44	0.41
1:B:40:LYS:NZ	1:B:170:THR:O	2.35	0.41
2:C:630:VAL:HG11	4:H:9:DA:H3'	2.01	0.41
1:A:425:ARG:HE	1:B:425:ARG:NE	2.18	0.41
2:C:540:PRO:HA	2:C:599:THR:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:THR:O	1:B:402:GLU:HG2	2.20	0.41
2:C:418:ASP:OD2	2:C:497:ARG:NH2	2.44	0.41
1:B:172:ILE:HD12	3:G:12:DG:C2	2.55	0.41
2:C:442:LYS:HA	2:C:445:ARG:HD3	2.02	0.41
2:D:520:THR:HG22	2:D:622:PHE:CD2	2.55	0.41
1:A:381:LEU:HD12	1:A:381:LEU:HA	1.85	0.41
1:A:97:ARG:HB2	1:A:182:PRO:HB3	2.03	0.41
2:C:536:TYR:OH	2:C:609:ARG:NH1	2.54	0.41
1:A:161:PHE:O	1:A:163:ASN:N	2.54	0.41
1:A:58:ASP:N	1:A:58:ASP:OD1	2.45	0.41
1:B:181:PRO:HB2	1:B:213:PRO:HB3	2.04	0.40
2:C:595:LEU:HD23	2:C:595:LEU:HA	1.91	0.40
1:A:216:PRO:HA	1:A:481:ARG:HH11	1.86	0.40
2:C:428:GLU:HG2	2:C:500:LYS:HB3	2.03	0.40
1:A:181:PRO:HG3	1:A:329:PHE:CZ	2.57	0.40
2:D:595:LEU:HA	2:D:595:LEU:HD23	1.76	0.40
1:B:244:THR:HG22	1:B:258:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	484/499 (97%)	452 (93%)	26 (5%)	6 (1%)	16	60
1	B	474/499 (95%)	446 (94%)	24 (5%)	4 (1%)	24	69
2	C	194/269 (72%)	170 (88%)	18 (9%)	6 (3%)	5	34
2	D	189/269 (70%)	164 (87%)	21 (11%)	4 (2%)	9	46
All	All	1341/1536 (87%)	1232 (92%)	89 (7%)	20 (2%)	13	55

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	491	PHE
1	A	296	GLU
2	C	407	LEU
2	C	415	LYS
2	C	416	LEU
2	C	488	GLY
2	C	490	GLU
1	B	331	MET
2	D	416	LEU
1	A	30	ARG
1	B	171	GLY
2	D	415	LYS
1	A	171	GLY
1	A	295	ARG
1	A	331	MET
2	C	444	GLY
1	B	30	ARG
2	D	605	ARG
1	A	162	PRO
1	B	162	PRO

### 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	341/433 (79%)	319 (94%)	22 (6%)	21	61
1	B	300/433 (69%)	281 (94%)	19 (6%)	22	63
2	C	101/226 (45%)	96 (95%)	5 (5%)	30	71
2	D	103/226 (46%)	98 (95%)	5 (5%)	31	72
All	All	845/1318 (64%)	794 (94%)	51 (6%)	24	65

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	21	ASP

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Mol	Chain	Res	Type
1	A	53	LEU
1	A	55	VAL
1	A	66	ARG
1	A	70	ASP
1	A	72	MET
1	A	99	MET
1	A	119[A]	ARG
1	A	119[B]	ARG
1	A	134	ARG
1	A	141	VAL
1	A	148	ASP
1	A	164	LEU
1	A	170	THR
1	A	185	LEU
1	A	209	VAL
1	A	210	LEU
1	A	377	LEU
1	A	381	LEU
1	A	384	LEU
1	A	387	ILE
2	C	429	LEU
2	C	453	LEU
2	C	508	ASP
2	C	595	LEU
2	C	609	ARG
1	B	11	LEU
1	B	30	ARG
1	B	53	LEU
1	B	66	ARG
1	B	70	ASP
1	B	93	TRP
1	B	134	ARG
1	B	164	LEU
1	B	185	LEU
1	B	210	LEU
1	B	217	THR
1	B	271	HIS
1	B	355	GLN
1	B	377	LEU
1	B	381	LEU
1	B	434	ARG
1	B	445	LEU

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Mol	Chain	Res	Type
1	B	484	LEU
1	B	486	VAL
2	D	432	VAL
2	D	447	ARG
2	D	449	PHE
2	D	453	LEU
2	D	592	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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, 2 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	F	101	6	25,33,33	1.88	7 (28%)	32,50,50	3.70	16 (50%)
5	MFX	H	101	6	25,33,33	1.84	7 (28%)	32,50,50	2.06	11 (34%)

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	F	101	6	-	0/6/35/35	0/4/5/5
5	MFX	H	101	6	-	0/6/35/35	0/4/5/5

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	101	MFX	C14-C12	2.18	1.43	1.41
5	H	101	MFX	C01-C02	2.26	1.56	1.53
5	F	101	MFX	C17-C15	2.31	1.39	1.35
5	H	101	MFX	C09-C08	2.38	1.57	1.48
5	F	101	MFX	C09-C08	2.55	1.58	1.48
5	F	101	MFX	C01-C02	2.59	1.57	1.53
5	H	101	MFX	C17-C15	2.80	1.40	1.35
5	F	101	MFX	C14-C12	3.26	1.44	1.41
5	F	101	MFX	C08-C06	3.61	1.58	1.48
5	F	101	MFX	C09-C06	3.65	1.58	1.48
5	H	101	MFX	C08-C06	3.84	1.58	1.48
5	H	101	MFX	C09-C06	3.86	1.59	1.48
5	H	101	MFX	F-C15	3.94	1.45	1.35
5	F	101	MFX	F-C15	4.10	1.45	1.35

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	101	MFX	C16-N-C06	-12.92	104.57	119.25
5	H	101	MFX	C16-N-C06	-5.82	112.63	119.25
5	F	101	MFX	C17-C14-C19	-4.40	114.21	121.47
5	F	101	MFX	O01-C13-C11	-3.69	114.72	120.09
5	F	101	MFX	C17-C15-C11	-2.88	119.08	123.29
5	H	101	MFX	C17-C14-C19	-2.68	117.05	121.47
5	H	101	MFX	C18-C19-C14	-2.67	117.30	121.92
5	F	101	MFX	C18-C19-C14	-2.48	117.63	121.92
5	H	101	MFX	C17-C15-C11	-2.38	119.81	123.29
5	H	101	MFX	O01-C13-C11	-2.27	116.79	120.09
5	F	101	MFX	C13-C12-C14	-2.01	114.55	118.42
5	H	101	MFX	F-C15-C11	2.03	121.21	118.34
5	F	101	MFX	O01-C13-C12	2.17	123.34	119.91
5	F	101	MFX	C-O01-C13	2.20	120.42	115.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	101	MFX	C01-C02-N02	2.22	117.28	111.03
5	H	101	MFX	C-O01-C13	2.36	120.80	115.02
5	H	101	MFX	C19-C14-C12	2.41	121.72	119.73
5	H	101	MFX	C17-C14-C12	2.45	121.23	118.12
5	F	101	MFX	C05-C01-C02	2.72	117.08	113.56
5	F	101	MFX	C07-C05-C01	2.85	116.35	111.91
5	F	101	MFX	F-C15-C11	2.96	122.52	118.34
5	F	101	MFX	C17-C14-C12	3.58	122.67	118.12
5	H	101	MFX	C13-C11-C15	3.77	119.93	115.90
5	H	101	MFX	C06-N-C12	4.05	126.12	120.95
5	F	101	MFX	C13-C11-C15	4.10	120.28	115.90
5	F	101	MFX	C19-C14-C12	4.11	123.12	119.73
5	F	101	MFX	C06-N-C12	10.61	134.52	120.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	101	MFX	6	0
5	H	101	MFX	5	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 ⓘ

### 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	485/499 (97%)	-0.28	0	100	100	76, 105, 137, 178	0
1	B	482/499 (96%)	-0.14	7 (1%)	76	63	80, 118, 169, 206	0
2	C	198/269 (73%)	-0.24	2 (1%)	84	75	92, 130, 160, 192	0
2	D	194/269 (72%)	-0.23	0	100	100	92, 124, 160, 195	0
3	E	9/15 (60%)	-0.08	0	100	100	97, 107, 204, 205	0
3	G	7/15 (46%)	0.11	0	100	100	112, 117, 187, 196	0
4	F	13/19 (68%)	0.27	0	100	100	97, 131, 194, 209	0
4	H	11/19 (57%)	0.09	0	100	100	123, 139, 168, 211	0
All	All	1399/1604 (87%)	-0.21	9 (0%)	90	84	76, 116, 163, 211	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	GLU	3.1
1	B	256	ILE	2.5
2	C	534	TYR	2.5
1	B	327	PHE	2.2
1	B	246	ILE	2.2
1	B	331	MET	2.1
1	B	205	ASP	2.1
1	B	255	ARG	2.1
2	C	500	LYS	2.1

### 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, 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
6	MG	G	101	1/1	0.72	0.35	3.09	175,175,175,175	0
5	MFX	F	101	29/29	0.79	0.30	1.65	156,176,195,214	0
5	MFX	H	101	29/29	0.84	0.29	1.18	87,141,162,188	0
6	MG	H	102	1/1	0.84	0.45	-	151,151,151,151	0

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

There are no such residues in this entry.