



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2017 – 02:09 PM EDT

PDB ID : 4Z3O
Title : Quinolone(Moxifloxacin)-DNA cleavage complex of topoisomerase IV 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 : unknown
Resolution : 3.44 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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 : rb-20029824
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) : rb-20029824

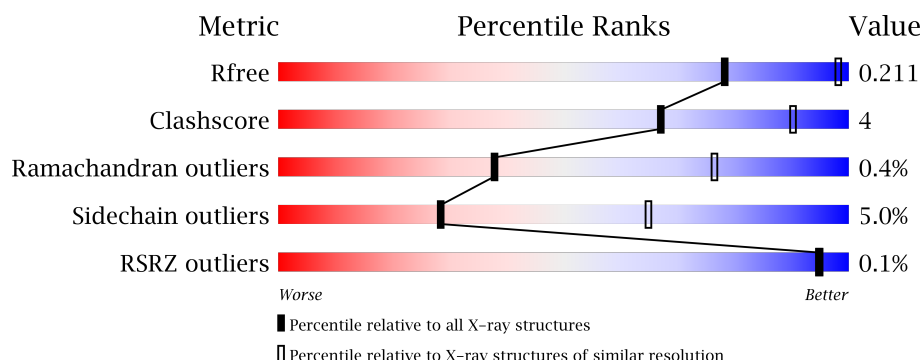
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1082 (3.52-3.36)
Clashscore	112137	1025 (3.50-3.38)
Ramachandran outliers	110173	1155 (3.52-3.36)
Sidechain outliers	110143	1156 (3.52-3.36)
RSRZ outliers	101464	1107 (3.52-3.36)

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 ≥ 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	742	
1	B	742	
2	E	7	
3	F	11	
4	G	7	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	H	11	

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	B	1502	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11053 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 topoisomerase 4 subunit B,ParE30-ParC55 fused topo IV from *S. pneumoniae*.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	689	Total	C	N	O	S	0	0	0
			5136	3252	895	971	18			
1	B	689	Total	C	N	O	S	0	0	0
			5111	3241	885	967	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	403	MET	-	expression tag	UNP Q59961
A	460	ILE	VAL	engineered mutation	UNP Q59961
A	996	ALA	-	linker	UNP Q59961
A	997	THR	-	linker	UNP Q59961
A	998	VAL	-	linker	UNP Q59961
A	999	PHE	-	linker	UNP Q59961
A	1000	HIS	-	linker	UNP Q59961
A	1001	MET	-	linker	UNP Q59961
A	1002	SER	-	linker	UNP Q59961
A	1257	THR	ILE	engineered mutation	UNP P72525
A	1485	THR	-	expression tag	UNP P72525
A	1486	ALA	-	expression tag	UNP P72525
A	1487	LYS	-	expression tag	UNP P72525
A	1488	ALA	-	expression tag	UNP P72525
A	1489	LEU	-	expression tag	UNP P72525
A	1490	GLU	-	expression tag	UNP P72525
A	1491	HIS	-	expression tag	UNP P72525
A	1492	HIS	-	expression tag	UNP P72525
A	1493	HIS	-	expression tag	UNP P72525
A	1494	HIS	-	expression tag	UNP P72525
A	1495	HIS	-	expression tag	UNP P72525
A	1496	HIS	-	expression tag	UNP P72525
B	403	MET	-	expression tag	UNP Q59961
B	460	ILE	VAL	engineered mutation	UNP Q59961

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	996	ALA	-	linker	UNP Q59961
B	997	THR	-	linker	UNP Q59961
B	998	VAL	-	linker	UNP Q59961
B	999	PHE	-	linker	UNP Q59961
B	1000	HIS	-	linker	UNP Q59961
B	1001	MET	-	linker	UNP Q59961
B	1002	SER	-	linker	UNP Q59961
B	1257	THR	ILE	engineered mutation	UNP P72525
B	1485	THR	-	expression tag	UNP P72525
B	1486	ALA	-	expression tag	UNP P72525
B	1487	LYS	-	expression tag	UNP P72525
B	1488	ALA	-	expression tag	UNP P72525
B	1489	LEU	-	expression tag	UNP P72525
B	1490	GLU	-	expression tag	UNP P72525
B	1491	HIS	-	expression tag	UNP P72525
B	1492	HIS	-	expression tag	UNP P72525
B	1493	HIS	-	expression tag	UNP P72525
B	1494	HIS	-	expression tag	UNP P72525
B	1495	HIS	-	expression tag	UNP P72525
B	1496	HIS	-	expression tag	UNP P72525

- Molecule 2 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	P	0	0	0
			140	69	27	38	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	11	Total	C	N	O	P	0	0	0
			225	108	39	67	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	P	0	0	0
			139	68	25	40	6			

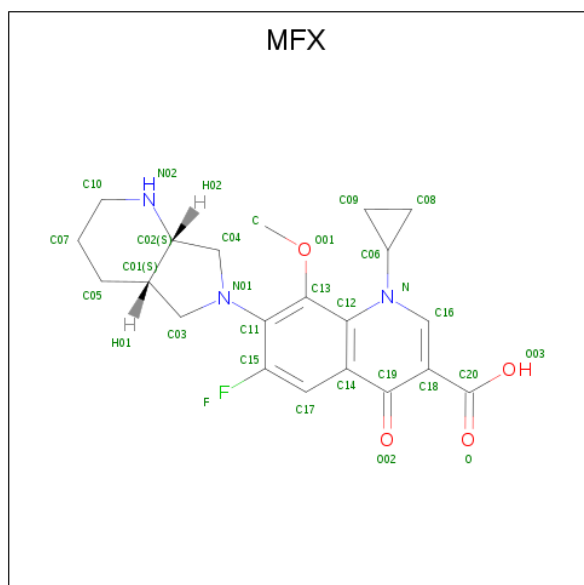
- Molecule 5 is a DNA chain called E-site DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		
6	A	2	Total	Mg	0	0
			2	2		

- Molecule 7 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: C₂₁H₂₄FN₃O₄).



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

- Molecule 8 is water.

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

Continued on next page...

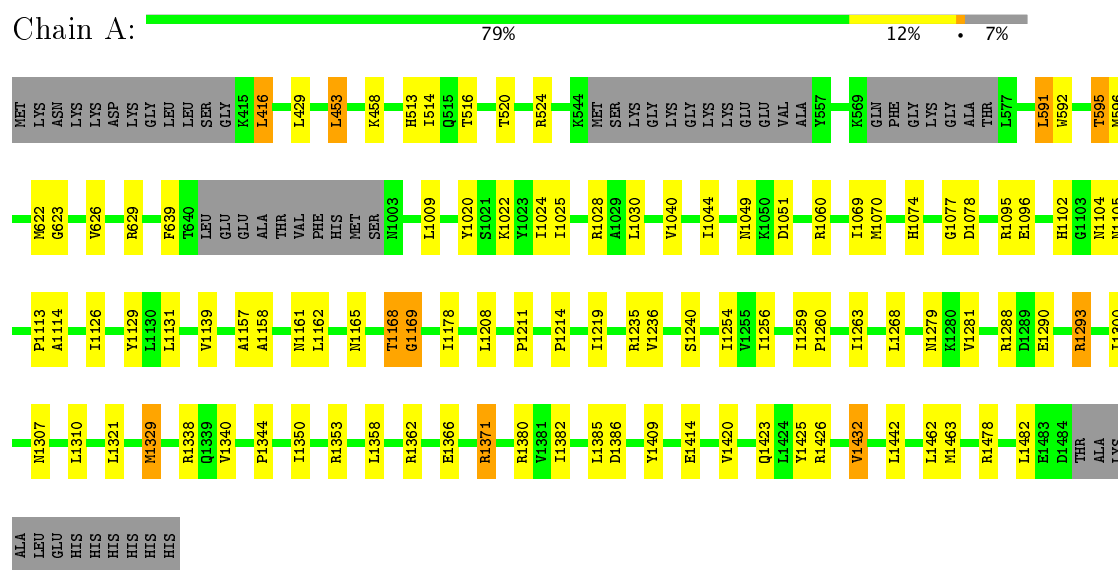
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	8	Total	O	0	0
			8	8		
8	F	1	Total	O	0	0
			1	1		

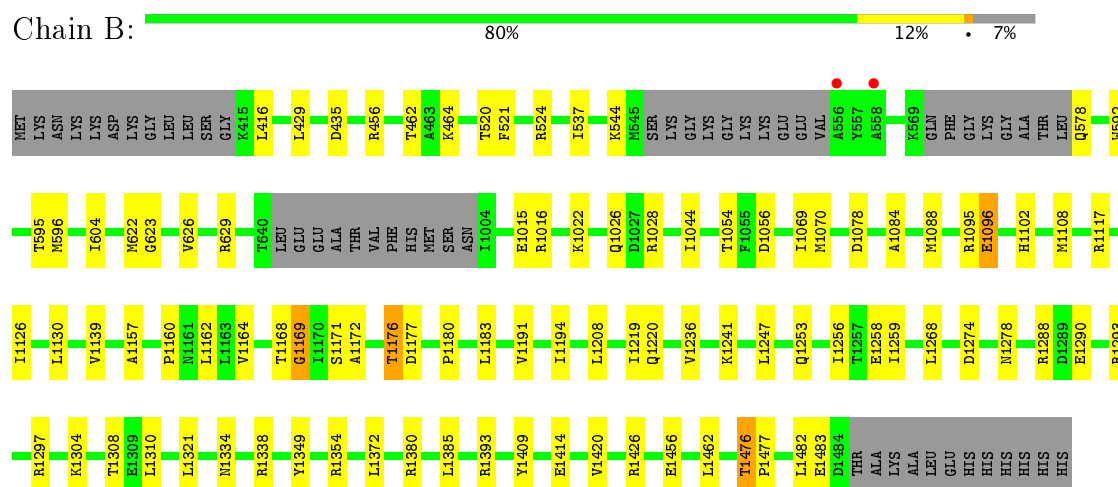
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 topoisomerase 4 subunit B,ParE30-ParC55 fused topo IV from *S. pneumoniae*



- Molecule 1: DNA topoisomerase 4 subunit B,ParE30-ParC55 fused topo IV from *S. pneumoniae*



- Molecule 2: E-site DNA

Chain E:  86% 14%




- Molecule 3: E-site DNA

Chain F:  73% 27%



- Molecule 4: E-site DNA

Chain G:  86% 14%



- Molecule 5: E-site DNA

Chain H:  73% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.76Å 157.76Å 211.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	70.34 – 3.44 70.34 – 3.17	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.34-3.44) 94.7 (70.34-3.17)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.182 , 0.212 0.179 , 0.211	Depositor DCC
R_{free} test set	1932 reflections (4.85%)	DCC
Wilson B-factor (Å ²)	88.1	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11053	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.20	0/5222	0.39	0/7098
1	B	0.20	0/5198	0.38	0/7067
2	E	0.43	0/157	1.01	0/241
3	F	0.45	0/251	1.18	1/385 (0.3%)
4	G	0.44	0/155	1.00	0/238
5	H	0.44	0/253	1.02	0/388
All	All	0.23	0/11236	0.48	1/15417 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	6	DT	O4'-C4'-C3'	-6.55	101.88	104.50

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	5136	0	4805	51	0
1	B	5111	0	4782	42	0
2	E	140	0	78	1	0
3	F	225	0	126	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	139	0	78	1	0
5	H	226	0	124	4	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	F	29	0	23	3	0
7	H	29	0	23	2	0
8	A	5	0	0	0	0
8	B	8	0	0	0	0
8	F	1	0	0	0	0
All	All	11053	0	10039	94	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 4.

All (94) 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:1380:ARG:NH1	1:A:1409:TYR:O	2.23	0.71
1:B:520:THR:HG21	1:B:622:MET:HG3	1.73	0.70
1:B:1288:ARG:NH1	1:B:1290:GLU:OE2	2.26	0.68
1:B:592:TRP:HA	1:B:596:MET:HB2	1.74	0.68
1:B:1290:GLU:OE1	1:B:1297:ARG:NH1	2.27	0.67
1:A:520:THR:HG21	1:A:622:MET:HG3	1.75	0.67
1:B:623:GLY:O	1:B:629:ARG:NH2	2.29	0.65
1:A:1077:GLY:HA2	1:B:1117:ARG:HD3	1.78	0.64
1:A:623:GLY:O	1:A:629:ARG:NH2	2.31	0.63
1:A:1024:ILE:HD12	1:A:1028:ARG:HE	1.64	0.62
1:B:1220:GLN:HG2	1:B:1483:GLU:HB2	1.84	0.58
1:A:592:TRP:HA	1:A:596:MET:HB2	1.84	0.58
1:A:1288:ARG:NH1	1:A:1290:GLU:OE2	2.33	0.57
1:A:1382:ILE:HD12	1:A:1432:VAL:HG23	1.85	0.57
1:A:1386:ASP:OD1	1:B:1393:ARG:NH2	2.38	0.56
1:A:1371:ARG:HG2	1:A:1442:LEU:HD11	1.87	0.56
1:A:1104:ASN:HB3	1:A:1114:ALA:HB2	1.87	0.56
1:A:1070:MET:HE1	1:A:1078:ASP:HB3	1.89	0.55
1:A:1040:VAL:HG11	4:G:13:DC:H5'	1.89	0.54
1:A:1028:ARG:HH11	1:A:1028:ARG:HG3	1.72	0.54
1:A:1044:ILE:HG12	1:A:1069:ILE:HD13	1.90	0.54
1:B:1256:ILE:HD13	1:B:1321:LEU:HD21	1.90	0.54
1:B:1219:ILE:HB	1:B:1482:LEU:HD23	1.90	0.53
1:B:537:ILE:HB	1:B:604:ILE:HB	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1070:MET:HE1	1:B:1078:ASP:HB3	1.91	0.53
1:A:1235:ARG:NH2	5:H:11:DG:O3'	2.38	0.53
1:B:1380:ARG:NH2	1:B:1409:TYR:O	2.40	0.53
1:A:1051:ASP:O	1:A:1060:ARG:NH2	2.42	0.52
1:B:544:LYS:O	1:B:578:GLN:N	2.43	0.52
1:A:1219:ILE:HB	1:A:1482:LEU:HD23	1.92	0.52
5:H:5:DA:N3	7:H:101:MFX:H03	2.25	0.52
1:A:591:LEU:HD23	1:A:595:THR:HG23	1.93	0.51
1:A:591:LEU:HD22	1:A:596:MET:HG3	1.93	0.51
1:A:626:VAL:HG11	5:H:9:DA:H3'	1.92	0.50
1:B:1054:THR:OG1	1:B:1056:ASP:OD1	2.23	0.50
1:B:1171:SER:OG	1:B:1172:ALA:N	2.43	0.50
1:A:1350:ILE:HA	1:A:1463:MET:HE3	1.94	0.50
1:B:1274:ASP:O	1:B:1278:ASN:ND2	2.37	0.50
1:B:1247:LEU:HD11	1:B:1253:GLN:HB2	1.93	0.49
1:A:1020:TYR:O	1:A:1024:ILE:HG12	2.12	0.49
1:B:1169:GLY:HA2	1:B:1176:THR:HG22	1.95	0.49
1:A:1211:PRO:O	1:A:1478:ARG:NH2	2.44	0.49
1:B:1044:ILE:HG12	1:B:1069:ILE:HD13	1.95	0.49
1:B:462:THR:HG21	1:B:521:PHE:HD2	1.78	0.49
1:A:1340:VAL:HB	1:A:1344:PRO:HG2	1.95	0.48
1:A:458:LYS:HG2	1:A:514:ILE:HD11	1.95	0.48
1:A:1168:THR:HA	1:A:1169:GLY:HA3	1.65	0.47
1:B:1096:GLU:HG2	1:B:1126:ILE:HD13	1.97	0.47
1:A:639:PHE:HA	1:A:1022:LYS:HE3	1.96	0.46
1:A:1161:ASN:OD1	1:A:1165:ASN:ND2	2.46	0.46
1:B:1241:LYS:HB3	1:B:1258:GLU:HB2	1.96	0.46
1:A:1025:ILE:HG23	1:A:1030:LEU:HD12	1.97	0.46
1:A:1129:TYR:HB3	1:A:1158:ALA:HB3	1.98	0.46
1:B:1015:GLU:OE1	1:B:1016:ARG:NH1	2.49	0.46
1:A:1350:ILE:HG12	1:A:1463:MET:HE1	1.97	0.45
1:B:1354:ARG:NE	1:B:1456:GLU:OE1	2.45	0.45
1:B:1028:ARG:NH1	2:E:14:DA:H4'	2.32	0.44
1:B:456:ARG:HB3	7:F:101:MFX:H	1.98	0.44
1:A:1307:ASN:ND2	1:A:1310:LEU:HB2	2.33	0.44
1:A:1425:TYR:HB3	1:B:1420:VAL:HG13	1.99	0.44
3:F:5:DA:N3	7:F:101:MFX:H03	2.33	0.44
1:A:1157:ALA:O	1:A:1353:ARG:HD3	2.18	0.44
1:A:1256:ILE:HD13	1:A:1321:LEU:HD21	1.99	0.44
1:B:626:VAL:HG11	3:F:9:DA:H3'	1.99	0.44
3:F:5:DA:C4	7:F:101:MFX:H03	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:HIS:HB2	1:A:1020:TYR:CD1	2.53	0.43
1:A:1358:LEU:O	1:A:1362:ARG:HG3	2.18	0.43
1:B:1095:ARG:HB2	1:B:1180:PRO:HB3	2.00	0.43
1:A:1049:ASN:HB2	1:A:1131:LEU:HD13	2.00	0.43
1:B:1191:VAL:HA	1:B:1194:ILE:HD12	2.00	0.43
1:B:1164:VAL:HG21	1:B:1183:LEU:HD23	2.01	0.43
1:A:1105:ASN:HA	1:A:1113:PRO:HB3	2.01	0.42
1:B:1168:THR:HA	1:B:1169:GLY:HA3	1.69	0.42
1:B:1426:ARG:HA	1:B:1426:ARG:HD3	1.91	0.42
1:B:435:ASP:OD2	1:B:456:ARG:HG2	2.19	0.42
1:A:1096:GLU:HG2	1:A:1126:ILE:HD13	2.02	0.42
1:A:1259:ILE:HD12	1:A:1263:ILE:HG22	2.01	0.42
1:B:1130:LEU:HD23	1:B:1157:ALA:HA	2.01	0.42
1:A:1423:GLN:H	1:A:1426:ARG:HH21	1.68	0.42
1:A:1240:SER:OG	1:A:1260:PRO:HD3	2.20	0.41
5:H:5:DA:C4	7:H:101:MFX:H03	2.55	0.41
1:A:416:LEU:HD12	1:A:453:LEU:HG	2.01	0.41
1:A:1070:MET:HA	1:A:1074:HIS:O	2.20	0.41
1:B:1022:LYS:O	1:B:1026:GLN:HG2	2.21	0.41
1:B:1084:ALA:O	1:B:1088:MET:HG3	2.21	0.41
1:A:1254:ILE:HB	1:A:1300:ILE:HB	2.03	0.41
1:A:1178:ILE:HG12	1:A:1329:MET:HG2	2.01	0.41
1:A:1095:ARG:HA	1:A:1214:PRO:HB3	2.03	0.41
1:B:1108:MET:HE2	1:B:1259:ILE:HD11	2.02	0.41
1:B:462:THR:HG21	1:B:521:PHE:CD2	2.56	0.41
1:B:1476:THR:HA	1:B:1477:PRO:HD3	1.95	0.40
1:A:1293:ARG:HH11	1:A:1293:ARG:HB3	1.86	0.40
1:A:516:THR:O	1:A:520:THR:HG23	2.22	0.40
1:B:1160:PRO:HG3	1:B:1349:TYR:CE2	2.57	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	681/742 (92%)	645 (95%)	34 (5%)	2 (0%)	44	80
1	B	681/742 (92%)	639 (94%)	39 (6%)	3 (0%)	38	76
All	All	1362/1484 (92%)	1284 (94%)	73 (5%)	5 (0%)	38	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1304	LYS
1	B	1169	GLY
1	A	1169	GLY
1	A	1329	MET
1	B	464	LYS

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	479/635 (75%)	454 (95%)	25 (5%)	27	64
1	B	477/635 (75%)	454 (95%)	23 (5%)	30	67
All	All	956/1270 (75%)	908 (95%)	48 (5%)	28	65

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	416	LEU
1	A	429	LEU
1	A	453	LEU
1	A	524	ARG
1	A	591	LEU
1	A	595	THR
1	A	1009	LEU
1	A	1102	HIS
1	A	1139	VAL
1	A	1162	LEU
1	A	1168	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1208	LEU
1	A	1236	VAL
1	A	1268	LEU
1	A	1279	ASN
1	A	1281	VAL
1	A	1293	ARG
1	A	1338	ARG
1	A	1366	GLU
1	A	1371	ARG
1	A	1385	LEU
1	A	1414	GLU
1	A	1420	VAL
1	A	1432	VAL
1	A	1462	LEU
1	B	416	LEU
1	B	429	LEU
1	B	524	ARG
1	B	595	THR
1	B	1096	GLU
1	B	1102	HIS
1	B	1139	VAL
1	B	1162	LEU
1	B	1176	THR
1	B	1177	ASP
1	B	1208	LEU
1	B	1236	VAL
1	B	1268	LEU
1	B	1293	ARG
1	B	1308	THR
1	B	1310	LEU
1	B	1334	ASN
1	B	1338	ARG
1	B	1372	LEU
1	B	1385	LEU
1	B	1414	GLU
1	B	1462	LEU
1	B	1476	THR

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 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$
7	MFX	F	101	6	24,33,33	1.59	5 (20%)	28,50,50	2.10	11 (39%)
7	MFX	H	101	6	24,33,33	1.64	5 (20%)	28,50,50	2.22	11 (39%)

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	MFX	F	101	6	-	0/10/35/35	0/4/5/5
7	MFX	H	101	6	-	0/10/35/35	0/4/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	101	MFX	C01-C02	2.06	1.56	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	101	MF	C14-C12	2.07	1.43	1.41
7	H	101	MF	C14-C12	2.27	1.43	1.41
7	H	101	MF	C01-C02	2.34	1.56	1.53
7	F	101	MF	C09-C08	2.80	1.59	1.48
7	H	101	MF	C09-C08	2.81	1.59	1.48
7	H	101	MF	C17-C15	2.83	1.39	1.35
7	F	101	MF	C17-C15	2.87	1.39	1.35
7	F	101	MF	F-C15	4.04	1.45	1.35
7	H	101	MF	F-C15	4.16	1.45	1.35

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	H	101	MF	C16-C18-C19	-4.12	118.07	119.99
7	F	101	MF	C16-C18-C19	-4.07	118.09	119.99
7	H	101	MF	C17-C14-C19	-3.08	116.65	121.69
7	F	101	MF	C17-C14-C19	-3.04	116.72	121.69
7	H	101	MF	C17-C15-C11	-2.73	119.41	123.37
7	F	101	MF	C17-C15-C11	-2.68	119.48	123.37
7	H	101	MF	C18-C19-C14	-2.66	117.36	122.09
7	F	101	MF	C18-C19-C14	-2.65	117.38	122.09
7	F	101	MF	O01-C13-C11	-2.15	116.17	119.96
7	F	101	MF	C13-C12-N	2.06	125.83	121.43
7	H	101	MF	C13-C12-N	2.15	126.03	121.43
7	F	101	MF	F-C15-C11	2.39	121.76	118.30
7	H	101	MF	F-C15-C11	2.42	121.80	118.30
7	F	101	MF	C-O01-C13	2.46	120.77	114.90
7	H	101	MF	C10-N02-C02	2.51	113.21	111.62
7	F	101	MF	C19-C14-C12	2.57	121.82	119.90
7	H	101	MF	C19-C14-C12	2.61	121.84	119.90
7	H	101	MF	C-O01-C13	2.76	121.49	114.90
7	F	101	MF	C13-C11-C15	4.23	120.14	116.01
7	H	101	MF	C13-C11-C15	4.41	120.31	116.01
7	F	101	MF	C06-N-C12	4.74	126.92	120.87
7	H	101	MF	C06-N-C12	5.39	127.74	120.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	101	MFX	3	0
7	H	101	MFX	2	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, 95th 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 ²)	Q<0.9
1	A	689/742 (92%)	-0.42	0 100 100	47, 86, 145, 174	0
1	B	689/742 (92%)	-0.43	2 (0%) 93 91	46, 82, 146, 171	0
2	E	7/7 (100%)	-0.41	0 100 100	88, 89, 126, 139	0
3	F	11/11 (100%)	-0.30	0 100 100	89, 107, 155, 156	0
4	G	7/7 (100%)	-0.27	0 100 100	94, 99, 123, 172	0
5	H	11/11 (100%)	-0.29	0 100 100	100, 116, 148, 161	0
All	All	1414/1520 (93%)	-0.42	2 (0%) 95 95	46, 85, 147, 174	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	558	ALA	2.9
1	B	556	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [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, 95th 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(\AA^2)	Q<0.9
6	MG	B	1502	1/1	0.95	0.32	4.65	83,83,83,83	0
7	MFX	H	101	29/29	0.94	0.21	0.53	93,126,142,180	0
7	MFX	F	101	29/29	0.95	0.21	0.02	74,108,137,167	0
6	MG	A	1502	1/1	0.96	0.32	-	100,100,100,100	0
6	MG	A	1501	1/1	0.90	0.30	-	83,83,83,83	0
6	MG	B	1501	1/1	0.95	0.40	-	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.