



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:53 am BST

PDB ID : 4G0V  
Title : Human topoisomerase iibeta in complex with DNA and mitoxantrone  
Authors : Wu, C.C.; Li, T.K.; Li, Y.C.; Chan, N.L.  
Deposited on : 2012-07-10  
Resolution : 2.55 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

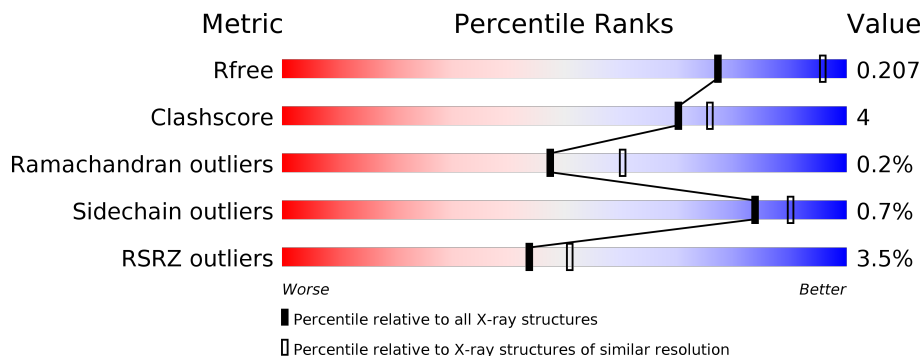
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	803	 3% 74% 8% 17%
1	B	803	 2% 75% 8% 17%
2	C	8	 13% 63% 38%
2	E	8	 75% 25%
3	D	12	 42% 50% 8%
3	F	12	 33% 67%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12243 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 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	663	Total	C	N	O	S	0	8	0
			5391	3432	932	1003	24			
1	B	666	Total	C	N	O	S	0	4	0
			5403	3438	939	1002	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	EXPRESSION TAG	UNP Q02880
A	420	ALA	-	EXPRESSION TAG	UNP Q02880
A	421	SER	-	EXPRESSION TAG	UNP Q02880
A	422	TRP	-	EXPRESSION TAG	UNP Q02880
A	423	SER	-	EXPRESSION TAG	UNP Q02880
A	424	HIS	-	EXPRESSION TAG	UNP Q02880
A	425	PRO	-	EXPRESSION TAG	UNP Q02880
A	426	GLN	-	EXPRESSION TAG	UNP Q02880
A	427	PHE	-	EXPRESSION TAG	UNP Q02880
A	428	GLU	-	EXPRESSION TAG	UNP Q02880
A	429	LYS	-	EXPRESSION TAG	UNP Q02880
A	430	GLY	-	EXPRESSION TAG	UNP Q02880
A	431	ALA	-	EXPRESSION TAG	UNP Q02880
A	432	ASP	-	EXPRESSION TAG	UNP Q02880
A	433	ASP	-	EXPRESSION TAG	UNP Q02880
A	434	ASP	-	EXPRESSION TAG	UNP Q02880
A	435	ASP	-	EXPRESSION TAG	UNP Q02880
A	436	LYS	-	EXPRESSION TAG	UNP Q02880
A	437	VAL	-	EXPRESSION TAG	UNP Q02880
A	438	PRO	-	EXPRESSION TAG	UNP Q02880
A	439	ASP	-	EXPRESSION TAG	UNP Q02880
A	440	PRO	-	EXPRESSION TAG	UNP Q02880
A	441	THR	-	EXPRESSION TAG	UNP Q02880
A	442	SER	-	EXPRESSION TAG	UNP Q02880
A	443	VAL	-	EXPRESSION TAG	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASP	-	EXPRESSION TAG	UNP Q02880
A	1202	GLY	-	EXPRESSION TAG	UNP Q02880
A	1203	ALA	-	EXPRESSION TAG	UNP Q02880
A	1204	PRO	-	EXPRESSION TAG	UNP Q02880
A	1205	GLY	-	EXPRESSION TAG	UNP Q02880
A	1206	PHE	-	EXPRESSION TAG	UNP Q02880
A	1207	SER	-	EXPRESSION TAG	UNP Q02880
A	1208	SER	-	EXPRESSION TAG	UNP Q02880
A	1209	ILE	-	EXPRESSION TAG	UNP Q02880
A	1210	SER	-	EXPRESSION TAG	UNP Q02880
A	1211	ALA	-	EXPRESSION TAG	UNP Q02880
A	1212	HIS	-	EXPRESSION TAG	UNP Q02880
A	1213	HIS	-	EXPRESSION TAG	UNP Q02880
A	1214	HIS	-	EXPRESSION TAG	UNP Q02880
A	1215	HIS	-	EXPRESSION TAG	UNP Q02880
A	1216	HIS	-	EXPRESSION TAG	UNP Q02880
A	1217	HIS	-	EXPRESSION TAG	UNP Q02880
A	1218	HIS	-	EXPRESSION TAG	UNP Q02880
A	1219	HIS	-	EXPRESSION TAG	UNP Q02880
A	1220	HIS	-	EXPRESSION TAG	UNP Q02880
A	1221	HIS	-	EXPRESSION TAG	UNP Q02880
B	419	MET	-	EXPRESSION TAG	UNP Q02880
B	420	ALA	-	EXPRESSION TAG	UNP Q02880
B	421	SER	-	EXPRESSION TAG	UNP Q02880
B	422	TRP	-	EXPRESSION TAG	UNP Q02880
B	423	SER	-	EXPRESSION TAG	UNP Q02880
B	424	HIS	-	EXPRESSION TAG	UNP Q02880
B	425	PRO	-	EXPRESSION TAG	UNP Q02880
B	426	GLN	-	EXPRESSION TAG	UNP Q02880
B	427	PHE	-	EXPRESSION TAG	UNP Q02880
B	428	GLU	-	EXPRESSION TAG	UNP Q02880
B	429	LYS	-	EXPRESSION TAG	UNP Q02880
B	430	GLY	-	EXPRESSION TAG	UNP Q02880
B	431	ALA	-	EXPRESSION TAG	UNP Q02880
B	432	ASP	-	EXPRESSION TAG	UNP Q02880
B	433	ASP	-	EXPRESSION TAG	UNP Q02880
B	434	ASP	-	EXPRESSION TAG	UNP Q02880
B	435	ASP	-	EXPRESSION TAG	UNP Q02880
B	436	LYS	-	EXPRESSION TAG	UNP Q02880
B	437	VAL	-	EXPRESSION TAG	UNP Q02880
B	438	PRO	-	EXPRESSION TAG	UNP Q02880
B	439	ASP	-	EXPRESSION TAG	UNP Q02880

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Chain	Residue	Modelled	Actual	Comment	Reference
B	440	PRO	-	EXPRESSION TAG	UNP Q02880
B	441	THR	-	EXPRESSION TAG	UNP Q02880
B	442	SER	-	EXPRESSION TAG	UNP Q02880
B	443	VAL	-	EXPRESSION TAG	UNP Q02880
B	444	ASP	-	EXPRESSION TAG	UNP Q02880
B	1202	GLY	-	EXPRESSION TAG	UNP Q02880
B	1203	ALA	-	EXPRESSION TAG	UNP Q02880
B	1204	PRO	-	EXPRESSION TAG	UNP Q02880
B	1205	GLY	-	EXPRESSION TAG	UNP Q02880
B	1206	PHE	-	EXPRESSION TAG	UNP Q02880
B	1207	SER	-	EXPRESSION TAG	UNP Q02880
B	1208	SER	-	EXPRESSION TAG	UNP Q02880
B	1209	ILE	-	EXPRESSION TAG	UNP Q02880
B	1210	SER	-	EXPRESSION TAG	UNP Q02880
B	1211	ALA	-	EXPRESSION TAG	UNP Q02880
B	1212	HIS	-	EXPRESSION TAG	UNP Q02880
B	1213	HIS	-	EXPRESSION TAG	UNP Q02880
B	1214	HIS	-	EXPRESSION TAG	UNP Q02880
B	1215	HIS	-	EXPRESSION TAG	UNP Q02880
B	1216	HIS	-	EXPRESSION TAG	UNP Q02880
B	1217	HIS	-	EXPRESSION TAG	UNP Q02880
B	1218	HIS	-	EXPRESSION TAG	UNP Q02880
B	1219	HIS	-	EXPRESSION TAG	UNP Q02880
B	1220	HIS	-	EXPRESSION TAG	UNP Q02880
B	1221	HIS	-	EXPRESSION TAG	UNP Q02880

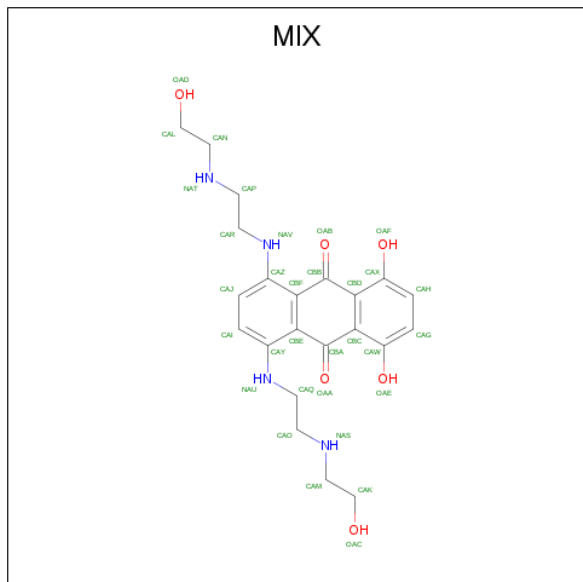
- Molecule 2 is a DNA chain called DNA (5'-D(P\*AP\*GP\*CP\*CP\*GP\*AP\*GP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			
2	E	8	Total	C	N	O	P	0	0	0
			165	77	34	46	8			

- Molecule 3 is a DNA chain called DNA (5'-D(P\*TP\*GP\*CP\*AP\*GP\*CP\*TP\*CP\*GP\*GP\*CP\*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total	C	N	O	P	0	0	0
			245	116	43	74	12			
3	F	12	Total	C	N	O	P	0	0	0
			245	116	43	74	12			

- Molecule 4 is 1,4-DIHYDROXY-5,8-BIS({2-[(2-HYDROXYETHYL)AMINO]ETHYL}AMINO)-9,10-ANTHRACENEDIONE (three-letter code: MIX) (formula: C<sub>22</sub>H<sub>28</sub>N<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	32	22	4	6	0	0
4	D	1	32	22	4	6	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	B	2	2	2	0	0
5	A	2	2	2	0	0
5	D	1	1	1	0	0
5	F	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	210	210	210	0	0
6	B	242	242	242	0	0

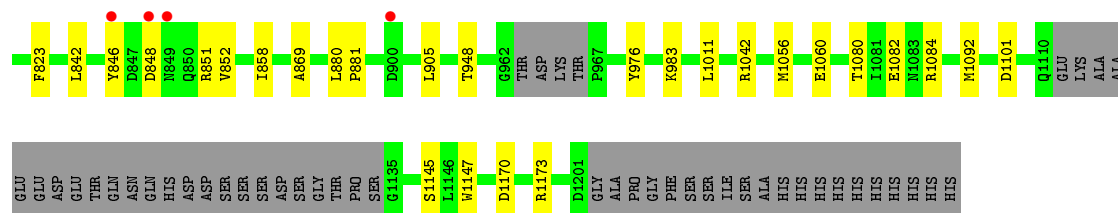
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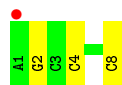
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
6	C	17	Total 17	O 17	0	0
6	D	43	Total 43	O 43	0	0
6	E	14	Total 14	O 14	0	0
6	F	33	Total 33	O 33	0	0







- Molecule 2: DNA (5'-D(P\*AP\*GP\*CP\*CP\*GP\*AP\*GP\*C)-3')



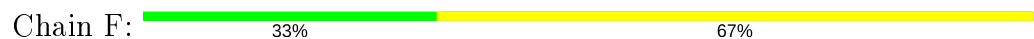
- Molecule 2: DNA (5'-D(P\*AP\*GP\*CP\*CP\*GP\*AP\*GP\*C)-3')



- Molecule 3: DNA (5'-D(P\*TP\*GP\*CP\*AP\*GP\*CP\*TP\*CP\*GP\*GP\*CP\*T)-3')



- Molecule 3: DNA (5'-D(P\*TP\*GP\*CP\*AP\*GP\*CP\*TP\*CP\*GP\*GP\*CP\*T)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.55Å 176.61Å 93.76Å 90.00° 111.53° 90.00°	Depositor
Resolution (Å)	27.94 – 2.55 27.94 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (27.94-2.55) 95.0 (27.94-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.43 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.161 , 0.206 0.162 , 0.207	Depositor DCC
$R_{free}$ test set	3957 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.7	Xtrriage
Anisotropy	0.071	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12243	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: MIX, 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	0.39	0/5516	0.54	0/7430
1	B	0.40	0/5515	0.53	0/7421
2	C	0.77	0/185	1.47	4/283 (1.4%)
2	E	0.81	0/185	1.40	4/283 (1.4%)
3	D	0.72	0/273	1.70	10/419 (2.4%)
3	F	0.77	0/273	1.58	8/419 (1.9%)
All	All	0.43	0/11947	0.69	26/16255 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	10	DG	O4'-C1'-N9	9.97	114.98	108.00
3	F	10	DG	O4'-C1'-N9	9.87	114.91	108.00
2	C	8	DC	O4'-C1'-N1	8.98	114.28	108.00
3	D	14	DC	C4'-C3'-C2'	-8.15	95.77	103.10
3	F	14	DC	O4'-C4'-C3'	-7.97	101.22	106.00
3	F	14	DC	C4'-C3'-C2'	-7.91	95.98	103.10
3	D	14	DC	C1'-O4'-C4'	-6.97	103.13	110.10
2	E	1	DA	C1'-O4'-C4'	-6.89	103.21	110.10
2	E	8	DC	O4'-C1'-N1	6.88	112.81	108.00
3	D	19	DC	C1'-O4'-C4'	-6.71	103.39	110.10
3	F	19	DC	C1'-O4'-C4'	-6.37	103.73	110.10
3	D	20	DT	O4'-C4'-C3'	-6.34	101.96	104.50
3	D	16	DC	O4'-C1'-N1	5.94	112.16	108.00
3	F	14	DC	C1'-O4'-C4'	-5.89	104.21	110.10
3	D	14	DC	O4'-C4'-C3'	-5.35	102.36	104.50
2	E	1	DA	C3'-C2'-C1'	-5.35	96.08	102.50
3	D	17	DG	C5-C6-O6	-5.34	125.40	128.60
3	F	17	DG	O4'-C1'-N9	-5.31	104.28	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	20	DT	C1'-O4'-C4'	-5.29	104.81	110.10
3	F	20	DT	N3-C4-O4	5.28	123.07	119.90
2	E	1	DA	O4'-C1'-N9	5.26	111.69	108.00
2	C	2	DG	C3'-C2'-C1'	-5.26	96.19	102.50
2	C	2	DG	O4'-C1'-N9	5.25	111.67	108.00
3	D	19	DC	O4'-C4'-C3'	-5.15	102.44	104.50
2	C	4	DC	C1'-O4'-C4'	-5.10	105.00	110.10
3	F	19	DC	P-O5'-C5'	-5.07	112.79	120.90

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	5391	0	5438	40	0
1	B	5403	0	5449	39	0
2	C	165	0	89	0	0
2	E	165	0	89	0	0
3	D	245	0	136	2	0
3	F	245	0	136	2	0
4	A	32	0	26	3	0
4	D	32	0	28	4	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	210	0	0	3	0
6	B	242	0	0	1	0
6	C	17	0	0	0	0
6	D	43	0	0	0	0
6	E	14	0	0	0	0
6	F	33	0	0	0	0
All	All	12243	0	11391	82	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 (82) 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:B:732:PRO:HG2	1:B:869:ALA:HB1	1.71	0.70
1:A:482:LYS:HG2	1:A:499:VAL:HG12	1.79	0.64
1:A:778[A]:GLN:HG3	6:A:1531:HOH:O	1.98	0.62
1:A:1076:GLN:OE1	1:A:1078:LYS:NZ	2.33	0.61
1:B:757:GLU:HB2	1:B:823:PHE:HB3	1.84	0.59
1:A:551:LYS:NZ	6:A:1566:HOH:O	2.34	0.58
4:D:101:MIX:OAB	4:D:101:MIX:NAV	2.31	0.57
1:B:1080:THR:O	1:B:1084:ARG:NH1	2.37	0.56
1:B:1170:ASP:OD1	1:B:1173[B]:ARG:NH2	2.37	0.56
1:B:507:LEU:HD13	3:D:14:DC:H5''	1.88	0.56
1:A:1002:HIS:HB3	1:A:1008:GLN:HG3	1.88	0.56
1:A:560:GLN:HB3	1:A:722:PHE:HA	1.89	0.54
1:B:1082:GLU:OE1	1:B:1082:GLU:N	2.33	0.53
1:A:485:ALA:O	1:A:489:LEU:HB2	2.07	0.53
1:A:457:LEU:HD22	1:A:529:ILE:HG12	1.89	0.53
1:A:482:LYS:HG2	1:A:499:VAL:CG1	2.39	0.53
3:D:13:DG:O6	4:D:101:MIX:HAN1	2.09	0.53
1:A:752:ARG:HD3	1:A:754:ASP:OD2	2.09	0.52
1:A:757:GLU:HB2	1:A:823:PHE:HB3	1.90	0.52
1:B:461:ASN:HB2	1:B:495:ASP:HA	1.91	0.52
1:A:773:TYR:CE1	1:A:775:HIS:HB2	2.46	0.51
1:A:820:ARG:HH21	1:B:820[B]:ARG:NH2	2.09	0.51
1:B:637:ALA:HB3	1:B:639:GLU:HG3	1.93	0.50
1:A:460:ALA:HB3	1:A:463:ALA:HB2	1.93	0.50
1:A:503:ARG:HD3	6:A:1413:HOH:O	2.10	0.50
1:B:752:ARG:HD3	1:B:754:ASP:OD2	2.11	0.50
1:A:646:ASP:HA	1:A:649:ARG:NH2	2.27	0.49
1:B:673:LYS:NZ	6:B:1451:HOH:O	2.43	0.49
1:B:810:LEU:HD12	1:B:948:THR:HB	1.94	0.49
1:A:762[A]:GLN:NE2	1:B:765:GLY:HA3	2.28	0.49
1:B:846:TYR:CZ	1:B:851:ARG:HG3	2.48	0.49
1:A:846:TYR:CZ	1:A:851:ARG:HG3	2.48	0.48
1:B:759:LYS:HG3	1:B:823:PHE:CE2	2.48	0.48
1:B:673:LYS:HD2	1:B:676:ASP:OD1	2.14	0.48
1:B:482:LYS:HD2	1:B:501:PRO:HD3	1.96	0.47
1:B:587:GLU:HG2	1:B:653:LEU:HG	1.97	0.47
1:B:1084:ARG:CZ	1:B:1092:MET:HE1	2.45	0.47
1:B:976:TYR:HB2	1:B:983:LYS:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:858:ILE:HG13	1:B:1042:ARG:HD2	1.96	0.46
1:B:560:GLN:HB3	1:B:722:PHE:HA	1.98	0.46
1:A:1150:THR:O	1:A:1154:VAL:HG23	2.16	0.46
1:A:472:THR:HB	1:A:497:TYR:CD2	2.50	0.45
4:A:1301:MIX:NAV	4:A:1301:MIX:OAB	2.42	0.45
1:B:1084:ARG:NE	1:B:1092:MET:HE1	2.32	0.45
1:A:768:ALA:HA	1:A:773:TYR:HB3	1.99	0.45
1:A:858:ILE:HG13	1:A:1042:ARG:HD2	1.98	0.45
1:A:777:GLU:OE1	1:B:820[B]:ARG:NH1	2.51	0.44
4:D:101:MIX:OAA	4:D:101:MIX:NAU	2.49	0.44
4:A:1301:MIX:HAK1	3:F:13:DG:O6	2.17	0.44
1:A:1026:LYS:HB3	1:A:1026:LYS:HE2	1.70	0.44
1:B:881:PRO:HB3	1:B:1011:LEU:HD21	2.00	0.43
1:B:457:LEU:HD22	1:B:529:ILE:HG12	1.99	0.43
1:B:480:SER:O	1:B:484:LEU:HG	2.17	0.43
1:A:503:ARG:O	4:A:1301:MIX:HAP1	2.18	0.43
1:A:524:ASN:O	1:A:528:LYS:HD3	2.18	0.43
1:A:469:LEU:HD21	1:A:544:LEU:O	2.19	0.42
1:A:807:GLY:HA3	1:A:813:GLY:HA2	2.01	0.42
1:B:731:ILE:HA	1:B:732:PRO:HD3	1.75	0.42
1:A:456:LYS:HE2	1:A:479:ASP:OD2	2.19	0.42
1:A:818:SER:C	1:A:820:ARG:H	2.23	0.42
1:A:939:ILE:HB	1:A:984:PHE:HB2	2.01	0.42
3:F:11:DC:H2'	3:F:12:DA:C8	2.53	0.42
1:A:773:TYR:CZ	1:A:775:HIS:HB2	2.54	0.42
1:A:844:PHE:HA	1:A:854:PRO:HA	2.01	0.42
1:B:460:ALA:HB3	1:B:463:ALA:HB2	2.01	0.42
1:B:768:ALA:HA	1:B:773:TYR:HB3	2.01	0.42
1:A:883:TYR:CZ	1:A:1031:VAL:HG21	2.54	0.42
1:B:807:GLY:HA3	1:B:813:GLY:HA2	2.01	0.42
1:B:842:LEU:HD21	1:B:858:ILE:HG22	2.02	0.42
1:B:1145:SER:OG	1:B:1147:TRP:HB2	2.20	0.41
1:A:680:TRP:CE2	1:A:720:ILE:HD12	2.55	0.41
1:A:869:ALA:HB3	1:A:880:LEU:HB2	2.03	0.41
1:A:969:LEU:HD12	1:A:969:LEU:O	2.20	0.41
1:A:731:ILE:HA	1:A:732:PRO:HD3	1.87	0.41
1:A:842:LEU:HD21	1:A:858:ILE:HG22	2.02	0.41
1:B:1080:THR:OG1	1:B:1084:ARG:NH1	2.54	0.41
1:B:1056:MET:O	1:B:1060:GLU:HG3	2.21	0.41
1:B:492:ILE:HG13	1:B:492:ILE:H	1.71	0.40
1:B:522:GLU:OE1	4:D:101:MIX:HAK1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762[A]:GLN:HA	1:A:762[A]:GLN:NE2	2.37	0.40
1:B:654:PHE:HB3	1:B:711:TYR:CZ	2.56	0.40
1:B:539:ASP:OD1	1:B:540:ASP:N	2.52	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	663/803 (83%)	637 (96%)	25 (4%)	1 (0%)	47 60
1	B	660/803 (82%)	639 (97%)	19 (3%)	2 (0%)	41 51
All	All	1323/1606 (82%)	1276 (96%)	44 (3%)	3 (0%)	47 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	VAL
1	B	852	VAL
1	B	1101	ASP

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	591/704 (84%)	587 (99%)	4 (1%)	84	90
1	B	588/704 (84%)	584 (99%)	4 (1%)	84	90
All	All	1179/1408 (84%)	1171 (99%)	8 (1%)	84	90

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	ILE
1	A	653	LEU
1	A	766	SER
1	A	1092	MET
1	B	480	SER
1	B	848	ASP
1	B	880	LEU
1	B	905	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	811	HIS
1	A	922	GLN
1	B	1076	GLN

### 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

Of 8 ligands modelled in this entry, 6 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
4	MIX	D	101	-	34,34,34	1.24	4 (11%)	44,46,46	0.87	1 (2%)
4	MIX	A	1301	-	34,34,34	1.25	4 (11%)	44,46,46	0.91	1 (2%)

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
4	MIX	D	101	-	-	5/14/30/30	0/3/3/3
4	MIX	A	1301	-	-	7/14/30/30	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	101	MIX	CBF-CBB	-3.40	1.39	1.47
4	A	1301	MIX	CBC-CBA	-3.39	1.39	1.47
4	A	1301	MIX	CBF-CBB	-3.16	1.40	1.47
4	A	1301	MIX	CBD-CBB	-3.10	1.40	1.47
4	A	1301	MIX	CBE-CBA	-3.09	1.40	1.47
4	D	101	MIX	CBE-CBA	-2.98	1.40	1.47
4	D	101	MIX	CBD-CBB	-2.87	1.40	1.47
4	D	101	MIX	CBC-CBA	-2.65	1.41	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	MIX	CAQ-NAU-CAY	-2.15	118.22	123.39
4	D	101	MIX	OAB-CBB-CBF	-2.04	118.13	121.43

There are no chirality outliers.

All (12) torsion outliers are listed below:

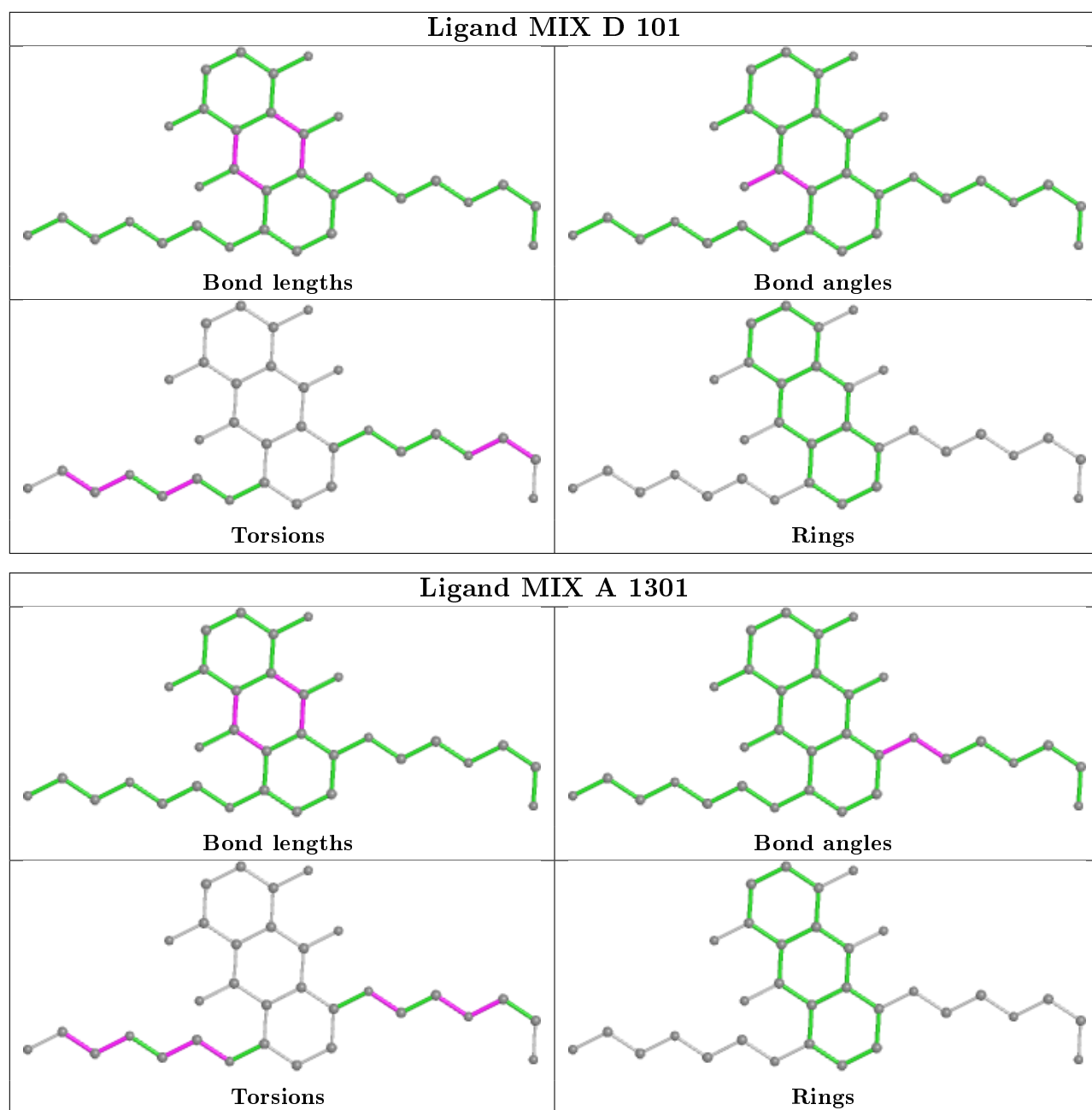
Mol	Chain	Res	Type	Atoms
4	D	101	MIX	OAC-CAK-CAM-NAS
4	A	1301	MIX	CAL-CAN-NAT-CAP
4	A	1301	MIX	OAD-CAL-CAN-NAT
4	A	1301	MIX	NAT-CAP-CAR-NAV
4	D	101	MIX	NAT-CAP-CAR-NAV
4	D	101	MIX	CAK-CAM-NAS-CAO
4	D	101	MIX	OAD-CAL-CAN-NAT
4	A	1301	MIX	CAK-CAM-NAS-CAO
4	A	1301	MIX	CAQ-CAO-NAS-CAM
4	A	1301	MIX	CAP-CAR-NAV-CAZ
4	A	1301	MIX	CAO-CAQ-NAU-CAY
4	D	101	MIX	CAL-CAN-NAT-CAP

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	101	MIX	4	0
4	A	1301	MIX	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	663/803 (82%)	-0.21	27 (4%) 37 44	14, 31, 63, 91	0
1	B	666/803 (82%)	-0.25	20 (3%) 50 57	13, 29, 62, 106	0
2	C	8/8 (100%)	-0.31	1 (12%) 3 5	20, 22, 48, 69	0
2	E	8/8 (100%)	-0.50	0 100 100	17, 20, 40, 70	0
3	D	12/12 (100%)	-0.85	0 100 100	19, 24, 29, 33	0
3	F	12/12 (100%)	-0.81	0 100 100	21, 26, 36, 53	0
All	All	1369/1646 (83%)	-0.24	48 (3%) 44 51	13, 30, 63, 106	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	643	TYR	6.4
1	B	644	PHE	5.5
1	A	541	ALA	5.2
1	B	642	GLU	5.1
1	B	638	LYS	5.1
1	A	491	VAL	4.7
1	B	641	LYS	4.5
1	B	645	ALA	4.5
1	A	490	GLY	4.3
1	A	848	ASP	4.1
1	B	849	ASN	3.8
1	B	640	ALA	3.8
1	A	568	LEU	3.8
1	A	692	ARG	3.4
1	A	696	LEU	3.2
1	A	569	LEU	3.1
1	B	692	ARG	3.1
1	A	849	ASN	3.0
1	A	466	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	695	GLY	3.0
1	B	848	ASP	2.9
1	A	539	ASP	2.9
1	A	484	LEU	2.7
2	C	1	DA	2.7
1	A	453	GLY	2.7
1	B	639	GLU	2.7
1	A	487	SER	2.6
1	A	492	ILE	2.6
1	A	646	ASP	2.6
1	A	514	HIS	2.6
1	B	568	LEU	2.5
1	B	491	VAL	2.5
1	B	846	TYR	2.4
1	A	542	GLU	2.4
1	A	567	GLY	2.4
1	A	540	ASP	2.4
1	A	452	LYS	2.3
1	B	693	LEU	2.3
1	A	552	ILE	2.3
1	B	545	LYS	2.2
1	B	900	ASP	2.2
1	B	637	ALA	2.2
1	A	565	ILE	2.2
1	A	467	HIS	2.1
1	A	570	ILE	2.1
1	B	649	ARG	2.1
1	B	492	ILE	2.0
1	A	846	TYR	2.0

## 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](#)

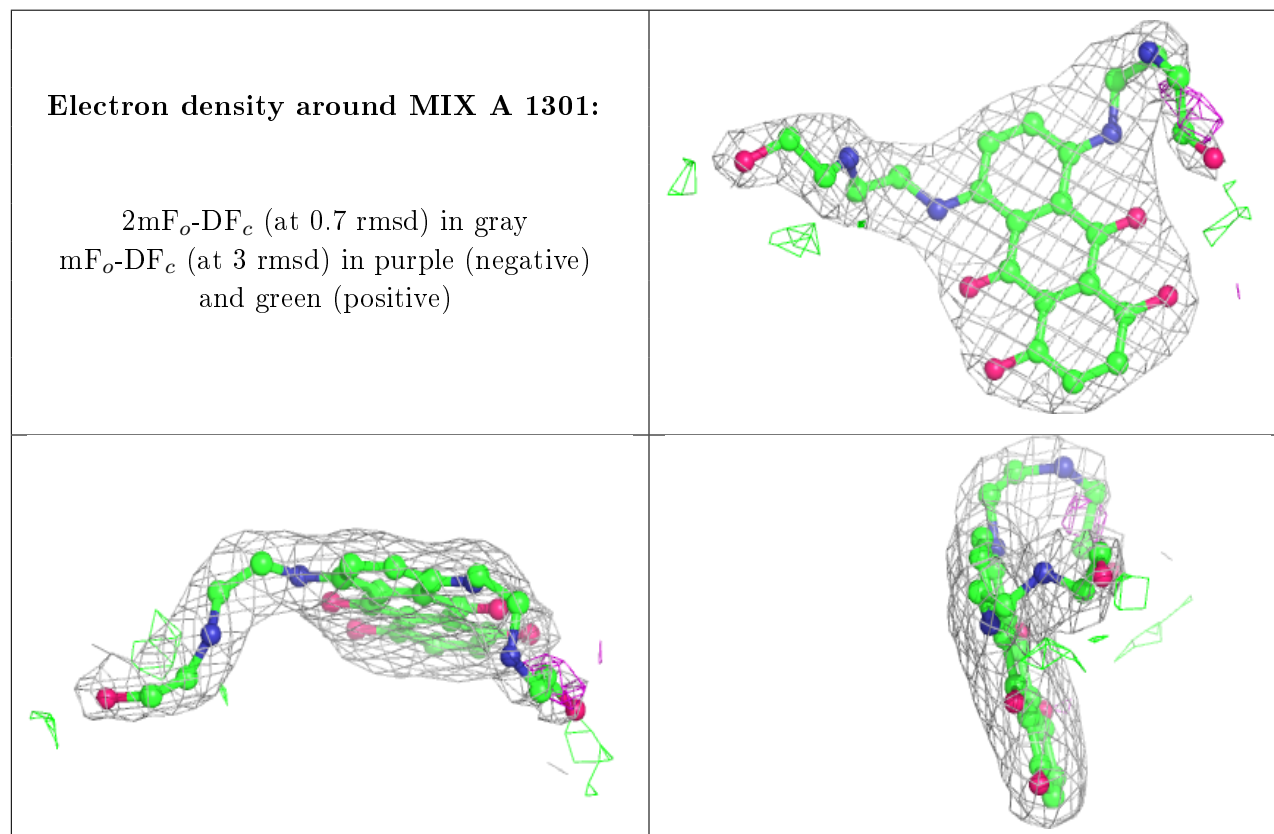
There are no carbohydrates in this entry.

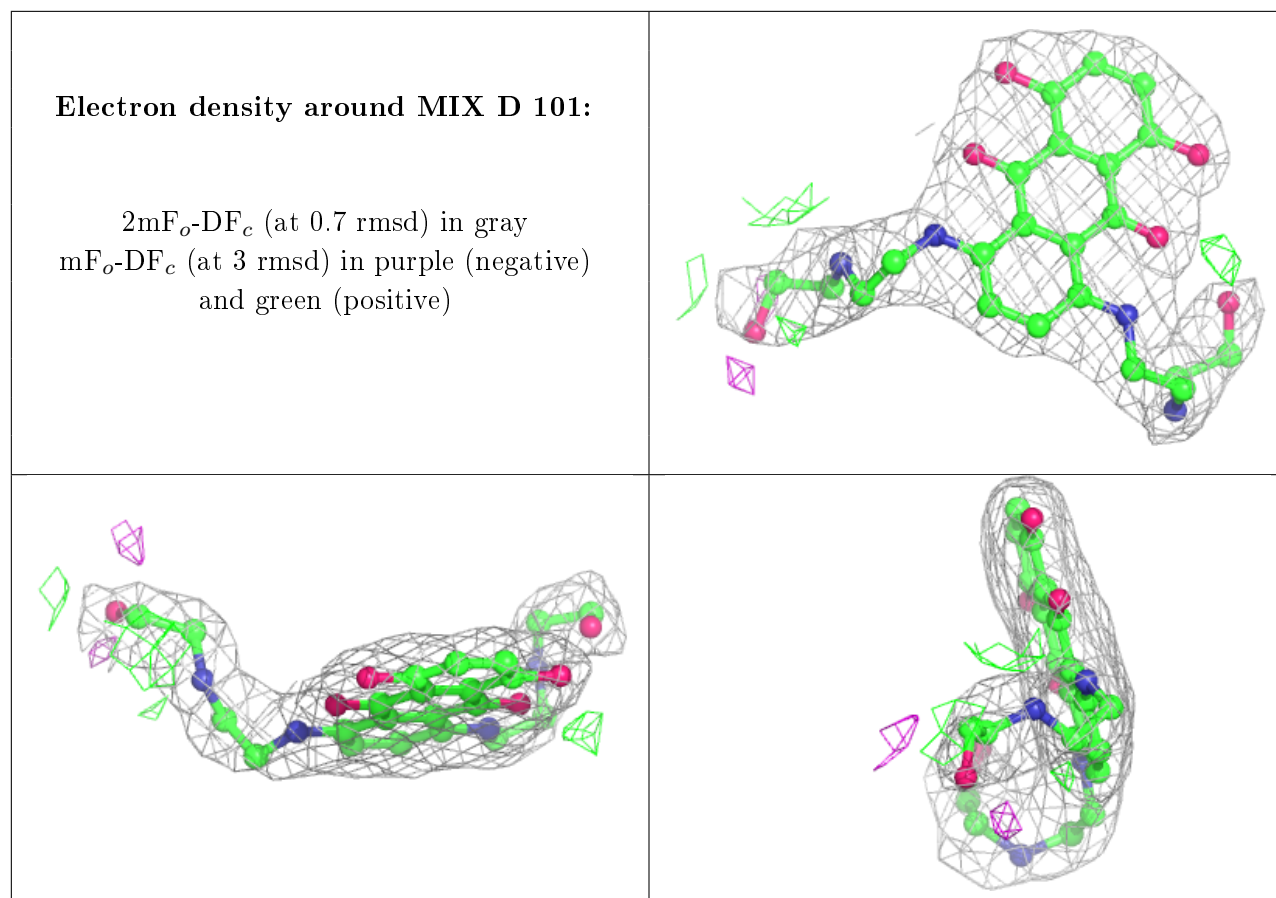
## 6.4 Ligands [i](#)

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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	MG	A	1303	1/1	0.93	0.35	39,39,39,39	0
5	MG	F	101	1/1	0.94	0.15	38,38,38,38	0
5	MG	B	1302	1/1	0.95	0.16	46,46,46,46	0
4	MIX	A	1301	32/32	0.96	0.13	17,26,41,41	0
5	MG	A	1302	1/1	0.97	0.11	27,27,27,27	0
4	MIX	D	101	32/32	0.97	0.12	14,23,38,40	0
5	MG	D	102	1/1	0.98	0.15	39,39,39,39	0
5	MG	B	1301	1/1	0.98	0.10	25,25,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.