



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:15 PM UTC

PDB ID : 5BTI / pdb_00005bti
Title : Crystal structure of a topoisomerase II complex
Authors : Blower, T.R.; Williamson, B.H.; Kerns, R.J.; Berger, J.M.
Deposited on : 2015-06-03
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

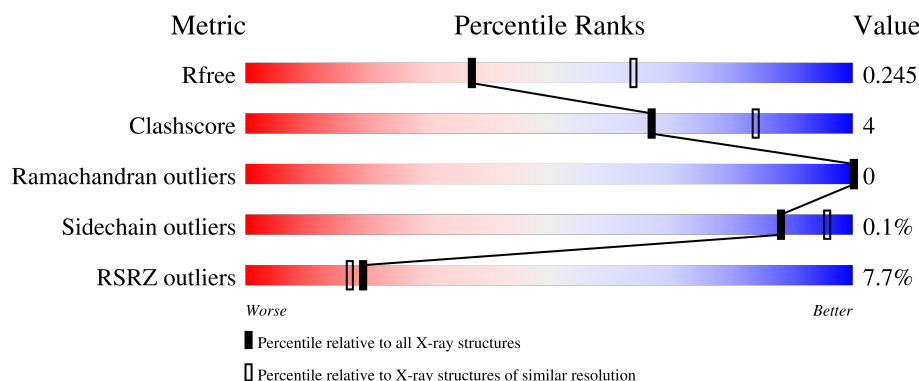
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



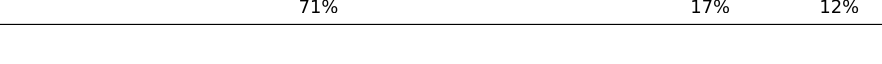
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	503	8% 88% 8% .
1	C	503	4% 90% 6% .
2	B	253	9% 91% 6% .
2	D	253	7% 92% 5% .
3	E	24	50% 75% 12% 12%

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Mol	Chain	Length	Quality of chain
3	H	24	
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	C	129	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26069 atoms, of which 12523 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
			7690	2388	3851	704	733	1	13			
1	C	487	Total	C	H	N	O	P	S	0	1	0
			7690	2388	3851	704	733	1	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	SER	ALA	engineered mutation	UNP P9WG47
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	90	SER	ALA	engineered mutation	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	425	ALA	-	expression tag	UNP P9WG45
D	423	SER	-	expression tag	UNP P9WG45
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
			618	196	208	74	120	20			
3	H	21	Total	C	H	N	O	P	0	21	0
			614	196	204	74	120	20			

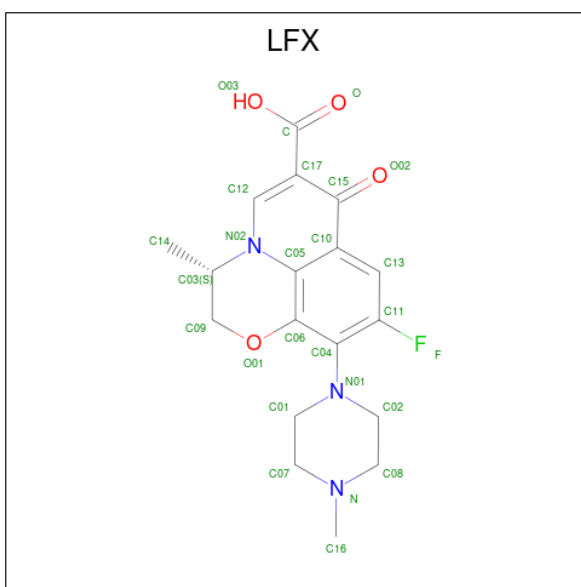
- Molecule 4 is a DNA chain called DNA substrate 24-mer TTACGTGCATAGTCATTCAT GACC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	21	Total	C	H	N	O	P	0	21	0
			619	196	209	74	120	20			
4	G	21	Total	C	H	N	O	P	0	21	0
			614	196	204	74	120	20			

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

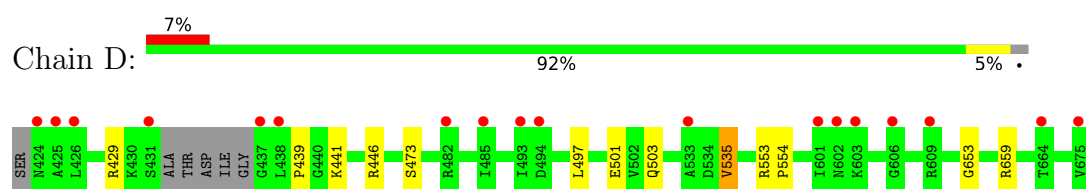
- Molecule 6 is (3S)-9-fluoro-3-methyl-10-(4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (CCD ID: LFX) (formula: C₁₈H₂₀FN₃O₄).



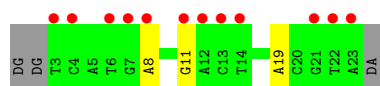
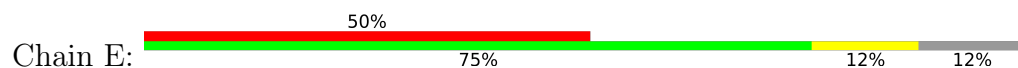
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total	C	F	H	N	O	0	0
			45	18	1	19	3	4		
6	F	1	Total	C	F	H	N	O	0	0
			45	18	1	19	3	4		

- Molecule 7 is water.

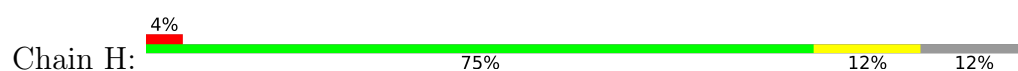
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	100	Total	O	0	0
			100	100		
7	B	37	Total	O	0	0
			37	37		
7	C	89	Total	O	0	0
			89	89		
7	D	37	Total	O	0	0
			37	37		
7	E	11	Total	O	0	0
			11	11		
7	F	12	Total	O	0	0
			12	12		
7	G	3	Total	O	0	0
			3	3		
7	H	5	Total	O	0	0
			5	5		



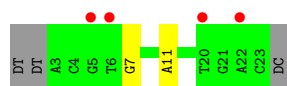
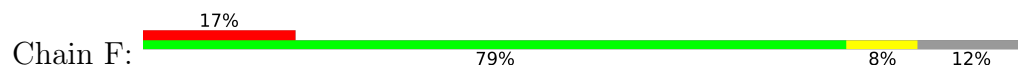
- Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA



- Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA



- Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC



- Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.39Å 83.28Å 129.70Å 90.00° 108.73° 90.00°	Depositor
Resolution (Å)	49.43 – 2.50 49.43 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.2 (49.43-2.50) 95.5 (49.43-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.240 0.222 , 0.245	Depositor DCC
R_{free} test set	3660 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26069	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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: LFX, 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	0.32	0/3882	0.65	0/5254
1	C	0.31	0/3882	0.66	1/5254 (0.0%)
2	B	0.29	0/1960	0.60	0/2634
2	D	0.30	0/1974	0.60	0/2653
3	E	0.19	0/458	0.46	0/704
3	H	0.21	0/458	0.49	0/704
4	F	0.18	0/458	0.46	0/704
4	G	0.21	0/458	0.47	0/704
All	All	0.30	0/13530	0.61	1/18611 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	VAL	N-CA-C	-7.93	105.47	111.90

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	3839	3851	3853	39	0
1	C	3839	3851	3853	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1932	1974	1973	8	0
2	D	1946	1984	1984	9	0
3	E	410	208	208	5	0
3	H	410	204	204	4	0
4	F	410	209	209	4	0
4	G	410	204	204	7	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	E	26	19	19	0	0
6	F	26	19	19	0	0
7	A	100	0	0	3	0
7	B	37	0	0	1	0
7	C	89	0	0	1	0
7	D	37	0	0	0	0
7	E	11	0	0	0	0
7	F	12	0	0	0	0
7	G	3	0	0	0	0
7	H	5	0	0	0	0
All	All	13546	12523	12526	81	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 (81) 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:C:129:PTR:O2P	4:G:11[B]:DA:C5'	1.68	1.41
1:C:129:PTR:O2P	3:E:11[A]:DG:C5'	1.98	1.12
1:A:266:ARG:HD3	1:A:317:GLU:OE2	1.59	1.03
1:C:129:PTR:O2P	3:E:11[A]:DG:H4'	1.61	1.01
1:C:129:PTR:O2P	3:E:11[A]:DG:C4'	2.12	0.96
1:A:129:PTR:O3P	3:H:11[B]:DG:C5'	2.13	0.96
2:D:653:GLY:O	2:D:659:ARG:NH2	2.11	0.84
1:A:290:GLN:HE22	1:A:334:HIS:HB3	1.44	0.83
1:A:262:ASP:OD1	1:A:263:SER:N	2.14	0.81
1:A:129:PTR:O3P	4:F:11[A]:DA:C5'	2.30	0.79
1:C:98:ARG:NH1	4:F:7[A]:DG:OP1	2.19	0.74
1:A:266:ARG:CD	1:A:317:GLU:OE2	2.34	0.74
1:C:288:ALA:O	1:C:292:ARG:HG3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:GLU:HA	1:C:292:ARG:HD3	1.75	0.68
1:C:357:ARG:NH1	1:C:359:ASP:OD1	2.28	0.66
1:C:129:PTR:P	4:G:11[B]:DA:C5'	2.84	0.65
1:C:128[B]:ARG:NH1	7:C:701:HOH:O	2.21	0.63
2:D:497:LEU:O	2:D:503:GLN:NE2	2.32	0.62
2:B:429:ARG:NH1	2:B:442:LEU:O	2.31	0.62
2:D:429:ARG:NH1	2:D:439:PRO:O	2.33	0.61
1:A:129:PTR:O3P	4:F:11[A]:DA:H4'	2.01	0.61
1:C:129:PTR:O2P	4:G:11[B]:DA:C4'	2.24	0.61
1:A:287:ILE:O	1:A:291:VAL:HG23	2.02	0.60
1:A:391:LEU:HD12	1:A:458:ILE:HD12	1.83	0.60
1:A:290:GLN:OE1	1:A:296:LEU:HD11	2.03	0.58
1:A:128[B]:ARG:NH1	7:A:603:HOH:O	2.35	0.57
1:C:129:PTR:O2P	4:G:11[B]:DA:H4'	2.00	0.56
1:C:291:VAL:O	1:C:294:GLY:HA2	2.06	0.56
1:A:129:PTR:O3P	4:F:11[A]:DA:C4'	2.54	0.56
1:A:441:ARG:NE	1:C:437:ASP:OD1	2.37	0.55
2:D:446:ARG:NH2	2:D:473:SER:OG	2.40	0.54
4:G:7[B]:DG:N2	3:H:18[B]:DC:O2	2.37	0.53
1:C:98:ARG:NH1	3:H:7[B]:DG:OP1	2.42	0.52
1:C:262:ASP:OD1	1:C:263:SER:N	2.38	0.51
1:A:288:ALA:O	1:A:292:ARG:HG3	2.10	0.51
2:D:441:LYS:NZ	2:D:501:GLU:OE1	2.43	0.51
2:B:446:ARG:NH1	2:B:473:SER:OG	2.43	0.51
2:D:659:ARG:NH1	3:E:19[A]:DA:OP1	2.44	0.50
1:A:387:ARG:HD2	1:A:458:ILE:HD11	1.92	0.50
1:A:427:ILE:CG2	1:A:431:GLN:HB2	2.42	0.50
1:A:51:VAL:HG11	3:E:8[A]:DA:H5'	1.94	0.49
1:C:428:ASP:OD1	1:C:429:GLU:N	2.41	0.49
2:D:659:ARG:NH1	4:G:19[B]:DA:OP1	2.46	0.48
1:A:428:ASP:OD1	1:A:429:GLU:N	2.44	0.48
1:A:290:GLN:NE2	1:A:334:HIS:HB3	2.21	0.48
2:B:609:ARG:NH2	7:B:805:HOH:O	2.46	0.48
1:A:23:GLU:OE1	2:B:634:ARG:NH1	2.47	0.47
1:C:442:ARG:HA	1:C:447:GLU:HB3	1.96	0.47
1:C:389:HIS:O	1:C:431:GLN:NE2	2.47	0.46
1:A:415:ASP:OD1	1:A:418:ARG:NH2	2.49	0.46
1:A:402:ASP:N	7:A:601:HOH:O	2.49	0.46
1:C:60:PHE:HB2	1:C:142:LEU:HD13	1.98	0.46
1:A:186:ALA:O	1:A:344:ASN:ND2	2.49	0.46
1:A:394:LEU:HD22	1:A:438:MET:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ILE:HD12	1:C:479:VAL:HG22	1.98	0.45
1:A:441:ARG:HH21	1:C:437:ASP:CG	2.25	0.44
1:A:389:HIS:NE2	1:A:431:GLN:OE1	2.51	0.44
1:A:373:ILE:HD12	1:A:479:VAL:HG22	2.00	0.44
1:A:391:LEU:HD23	1:A:394:LEU:HD12	1.99	0.43
1:A:407:LEU:HD21	1:A:420:GLY:HA3	2.00	0.43
1:C:343:ALA:HB1	1:C:345:MET:HE3	2.00	0.43
2:B:553:ARG:N	2:B:554:PRO:CD	2.82	0.43
1:A:425:LEU:HB2	1:A:427:ILE:CD1	2.49	0.43
1:A:128[B]:ARG:HH21	3:H:11[B]:DG:C5'	2.32	0.42
1:A:52:HIS:NE2	4:G:8[B]:DC:OP1	2.48	0.42
1:C:275:PRO:HG2	1:C:278:VAL:HG21	2.01	0.42
1:C:226:PRO:O	1:C:494:ARG:NH2	2.52	0.42
1:A:262:ASP:CG	1:A:263:SER:N	2.78	0.42
1:A:275:PRO:HG2	1:A:278:VAL:HG21	2.01	0.42
1:C:65:ARG:HB3	1:C:66:PRO:HD2	2.00	0.42
2:B:441:LYS:NZ	2:B:501:GLU:OE1	2.52	0.42
2:B:627:ASP:HB3	2:B:630:VAL:HG22	2.02	0.42
1:A:441:ARG:NH2	1:C:437:ASP:OD1	2.52	0.42
1:A:313:ARG:NH1	7:A:609:HOH:O	2.47	0.42
1:A:407:LEU:HD21	1:A:420:GLY:C	2.45	0.42
1:A:387:ARG:CD	1:A:458:ILE:HD11	2.50	0.41
2:D:553:ARG:N	2:D:554:PRO:CD	2.83	0.41
1:A:473:GLU:OE1	1:A:476:ARG:NH2	2.53	0.41
1:C:31:TYR:HA	2:D:535:VAL:HG13	2.03	0.41
2:B:601:ILE:HG22	2:B:606:GLY:HA2	2.03	0.41
1:C:427:ILE:CG2	1:C:431:GLN:HB2	2.51	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%)	466 (96%)	19 (4%)	0	100	100
1	C	485/503 (96%)	468 (96%)	17 (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%)	1402 (96%)	52 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	408/421 (97%)	408 (100%)	0	100	100
1	C	408/421 (97%)	408 (100%)	0	100	100
2	B	205/211 (97%)	205 (100%)	0	100	100
2	D	207/211 (98%)	206 (100%)	1 (0%)	81	92
All	All	1228/1264 (97%)	1227 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	535	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	GLN
1	A	207	ASN
1	A	238	GLN
1	A	277	GLN
1	A	449	GLN
2	B	514	HIS

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Mol	Chain	Res	Type
2	B	666	ASN
1	C	161	GLN
1	C	207	ASN
1	C	238	GLN
1	C	277	GLN
1	C	336	GLN
1	C	449	GLN
2	D	525	HIS
2	D	558	ASN

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	C	129	1	15,16,17	0.75	0	17,22,24	0.85	0
1	PTR	A	129	1	15,16,17	0.71	0	17,22,24	0.96	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	C	129	1	-	0/10/11/13	0/1/1/1
1	PTR	A	129	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	129	PTR	7	0
1	A	129	PTR	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	LFX	F	101	5	29,29,29	3.22	11 (37%)	44,44,44	1.55	9 (20%)
6	LFX	E	101	5	29,29,29	3.27	12 (41%)	44,44,44	1.70	9 (20%)

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	LFX	F	101	5	-	0/8/27/27	0/4/4/4
6	LFX	E	101	5	-	0/8/27/27	0/4/4/4

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	101	LFX	C12-N02	9.02	1.49	1.34
6	F	101	LFX	C12-N02	8.81	1.49	1.34
6	E	101	LFX	O01-C06	8.45	1.50	1.37
6	F	101	LFX	O01-C06	8.31	1.50	1.37
6	E	101	LFX	C03-N02	-6.77	1.35	1.49
6	F	101	LFX	C03-N02	-6.74	1.35	1.49
6	E	101	LFX	C05-N02	5.43	1.47	1.40
6	F	101	LFX	C05-N02	5.40	1.47	1.40
6	E	101	LFX	C12-C17	3.75	1.48	1.38
6	F	101	LFX	C12-C17	3.73	1.48	1.38
6	E	101	LFX	C02-N01	-3.15	1.41	1.46
6	F	101	LFX	C10-C15	3.15	1.54	1.48
6	E	101	LFX	C10-C15	3.14	1.54	1.48
6	F	101	LFX	C02-N01	-3.08	1.41	1.46
6	F	101	LFX	C04-N01	3.01	1.49	1.40
6	E	101	LFX	C04-N01	3.01	1.49	1.40
6	F	101	LFX	C13-C11	2.76	1.42	1.37
6	E	101	LFX	C13-C11	2.73	1.42	1.37
6	E	101	LFX	O03-C	-2.28	1.24	1.30
6	E	101	LFX	C04-C06	2.23	1.44	1.40
6	F	101	LFX	O03-C	-2.20	1.24	1.30
6	E	101	LFX	C07-N	-2.06	1.41	1.46
6	F	101	LFX	C07-N	-2.03	1.41	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	101	LFX	C08-N-C07	4.98	117.47	109.54
6	F	101	LFX	C17-C12-N02	-3.96	119.68	124.42
6	E	101	LFX	C17-C12-N02	-3.76	119.91	124.42
6	F	101	LFX	C08-N-C07	3.58	115.23	109.54
6	E	101	LFX	C10-C15-C17	3.48	120.03	115.64
6	F	101	LFX	C10-C15-C17	3.38	119.91	115.64
6	F	101	LFX	C09-C03-N02	3.20	113.56	107.34
6	E	101	LFX	C09-C03-N02	3.05	113.27	107.34
6	E	101	LFX	C06-C04-C11	2.99	118.83	115.92
6	F	101	LFX	C06-C04-C11	2.94	118.78	115.92
6	E	101	LFX	C02-C08-N	2.76	115.29	110.86
6	E	101	LFX	O01-C06-C04	2.75	120.79	117.90
6	E	101	LFX	C02-N01-C04	-2.44	112.14	119.73
6	F	101	LFX	C13-C11-C04	-2.32	119.88	123.34
6	F	101	LFX	C06-C04-N01	-2.29	116.48	122.45
6	F	101	LFX	F-C11-C04	2.16	121.84	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	101	LFX	C02-C08-N	2.04	114.13	110.86
6	E	101	LFX	C01-N01-C04	-2.03	113.40	119.73

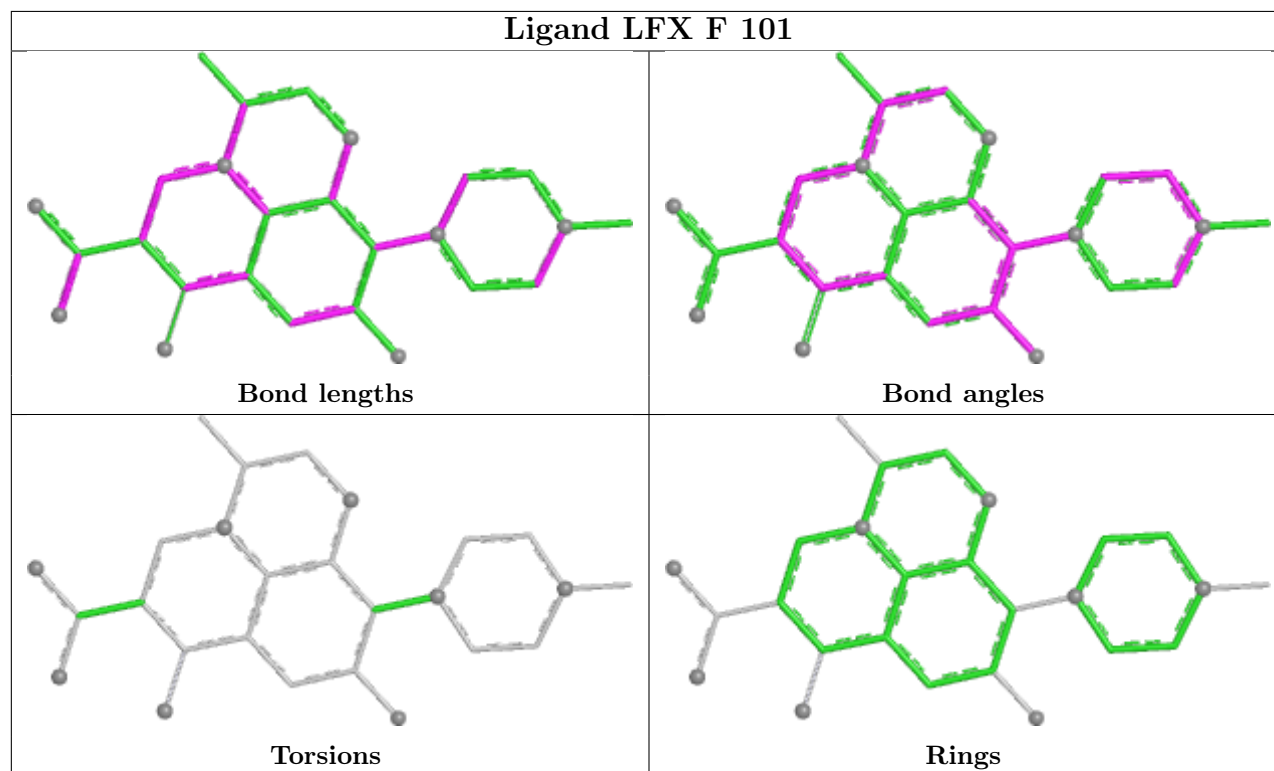
There are no chirality outliers.

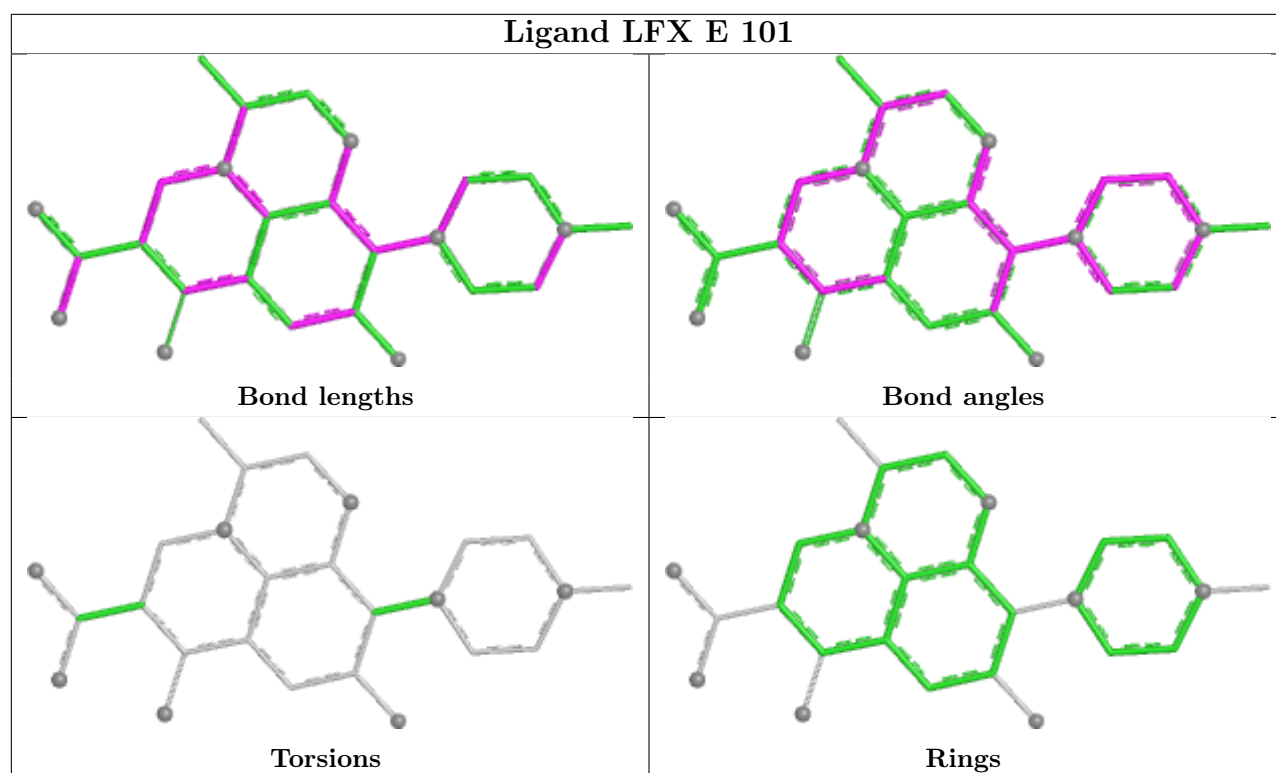
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	486/503 (96%)	0.48	40 (8%) 17 15	23, 61, 113, 179	1 (0%)
1	C	486/503 (96%)	0.45	21 (4%) 40 35	21, 64, 118, 178	1 (0%)
2	B	245/253 (96%)	0.70	22 (8%) 15 13	46, 70, 107, 142	0
2	D	247/253 (97%)	0.60	18 (7%) 21 19	44, 65, 110, 155	0
3	E	21/24 (87%)	1.65	12 (57%) 0 0	28, 49, 93, 98	21 (100%)
3	H	21/24 (87%)	0.14	1 (4%) 35 31	12, 23, 51, 90	21 (100%)
4	F	21/24 (87%)	1.48	4 (19%) 3 2	35, 44, 102, 111	21 (100%)
4	G	21/24 (87%)	0.31	1 (4%) 35 31	11, 24, 70, 76	21 (100%)
All	All	1548/1608 (96%)	0.55	119 (7%) 19 17	11, 64, 113, 179	86 (5%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	426	LEU	6.1
1	C	501	ILE	5.4
2	D	431	SER	5.0
1	A	501	ILE	4.9
2	B	437	GLY	4.7
2	B	426	LEU	4.6
1	A	406	ALA	4.3
2	D	675	VAL	4.2
2	D	437	GLY	4.1
3	E	23[A]	DA	4.0
2	B	601	ILE	4.0
1	A	500	ALA	3.9
1	C	500	ALA	3.8
1	A	412	GLU	3.7
1	A	290	GLN	3.7
2	B	425	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	128[A]	ARG	3.6
2	B	533	ALA	3.6
2	B	606	GLY	3.5
4	G	23[B]	DC	3.5
1	A	458	ILE	3.4
2	B	430	LYS	3.3
1	C	292	ARG	3.3
1	A	413	THR	3.2
2	D	602	ASN	3.2
2	D	424	ASN	3.1
2	B	675	VAL	3.1
1	C	293	ASP	3.0
4	F	22[A]	DA	3.0
3	E	22[A]	DT	3.0
1	C	407	LEU	3.0
2	B	565	GLN	3.0
2	B	481	LEU	3.0
2	B	585	ARG	3.0
2	B	427	VAL	2.9
2	D	601	ILE	2.9
3	H	3[B]	DT	2.9
2	B	605	ASP	2.9
1	A	407	LEU	2.8
1	A	410	ALA	2.8
1	C	16	GLU	2.8
1	A	265	GLY	2.8
3	E	8[A]	DA	2.8
2	B	498	LYS	2.8
2	B	674	ASP	2.8
2	D	494	ASP	2.8
1	A	296	LEU	2.7
1	A	302	ILE	2.7
1	A	446	LEU	2.7
1	A	293	ASP	2.6
1	A	295	LYS	2.6
4	F	6[A]	DT	2.6
1	A	294	GLY	2.6
3	E	12[A]	DA	2.6
1	C	17	PRO	2.6
1	A	27	SER	2.6
1	A	15	ILE	2.6
1	A	297	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	603	LYS	2.6
1	A	387	ARG	2.5
1	C	438	MET	2.5
1	A	16	GLU	2.5
3	E	14[A]	DT	2.5
1	C	296	LEU	2.5
1	C	297	ALA	2.5
2	B	519	ILE	2.5
1	C	404	VAL	2.5
1	A	122	ASP	2.4
2	B	485	ILE	2.4
1	C	290	GLN	2.4
2	D	664	THR	2.4
2	D	485	ILE	2.4
3	E	3[A]	DT	2.4
1	A	219	VAL	2.4
1	A	414	VAL	2.4
1	A	292	ARG	2.4
2	D	533	ALA	2.4
2	D	493	ILE	2.3
2	D	609	ARG	2.3
2	B	495	ARG	2.3
1	A	405	ILE	2.3
1	C	285	THR	2.3
1	A	409	ARG	2.3
1	C	128[A]	ARG	2.3
3	E	11[A]	DG	2.3
1	A	408	ILE	2.3
2	D	438	LEU	2.3
3	E	13[A]	DC	2.3
2	B	602	ASN	2.2
2	D	425	ALA	2.2
3	E	7[A]	DG	2.2
1	A	441	ARG	2.2
1	C	442	ARG	2.2
1	A	434	ALA	2.2
4	F	5[A]	DG	2.2
1	C	122	ASP	2.2
1	C	412	GLU	2.2
1	A	159	ARG	2.2
4	F	20[A]	DT	2.2
1	A	261	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	4[A]	DC	2.1
1	A	425	LEU	2.1
1	C	159	ARG	2.1
1	C	402	ASP	2.1
3	E	21[A]	DG	2.1
2	B	439	PRO	2.1
1	A	262	ASP	2.1
1	A	428	ASP	2.1
2	D	606	GLY	2.1
2	B	604	GLU	2.1
1	A	248	ARG	2.0
2	D	482	ARG	2.0
1	A	329	ASN	2.0
2	D	603	LYS	2.0
1	C	259	VAL	2.0
1	C	408	ILE	2.0
1	A	438	MET	2.0
1	A	263	SER	2.0
3	E	6[A]	DT	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. 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	B-factors(Å ²)	Q<0.9
1	PTR	A	129	16/17	0.94	0.12	41,50,57,60	0
1	PTR	C	129	16/17	0.94	0.11	38,42,60,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

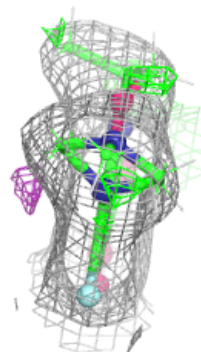
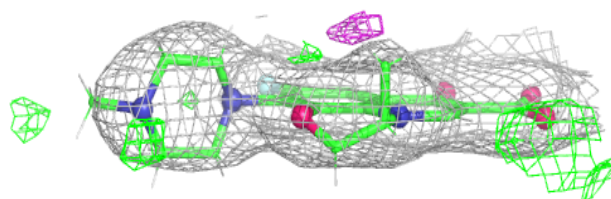
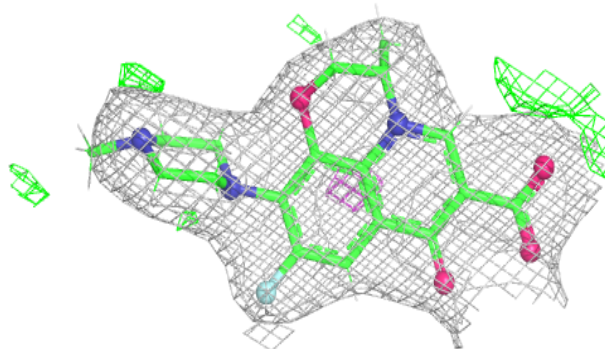
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	LFX	E	101	26/26	0.94	0.09	35,43,58,61	0
6	LFX	F	101	26/26	0.95	0.10	34,48,65,67	0
5	MG	B	701	1/1	0.96	0.08	49,49,49,49	0
5	MG	D	701	1/1	0.97	0.04	31,31,31,31	0
5	MG	C	601	1/1	0.99	0.04	38,38,38,38	0
5	MG	E	102	1/1	0.99	0.05	35,35,35,35	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.

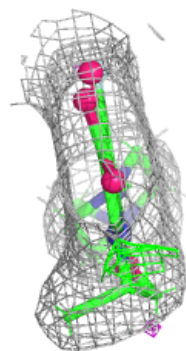
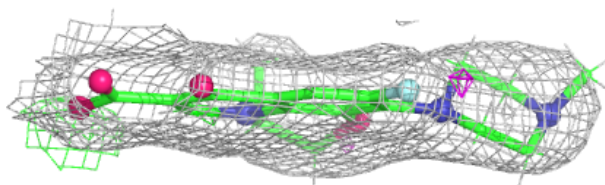
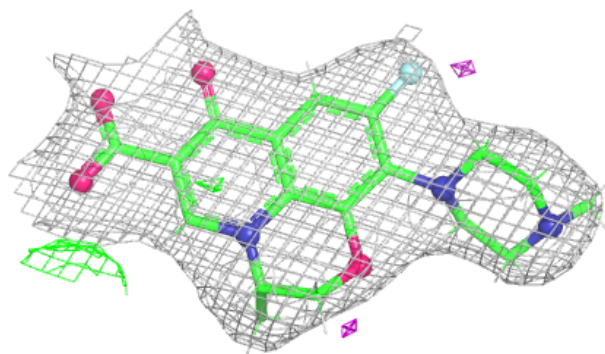
Electron density around LFX E 101:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LFX F 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.