Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 12:41 AM EST

PDB ID	:	5BTG
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 (i) 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 (i)) were used in the production of this report:

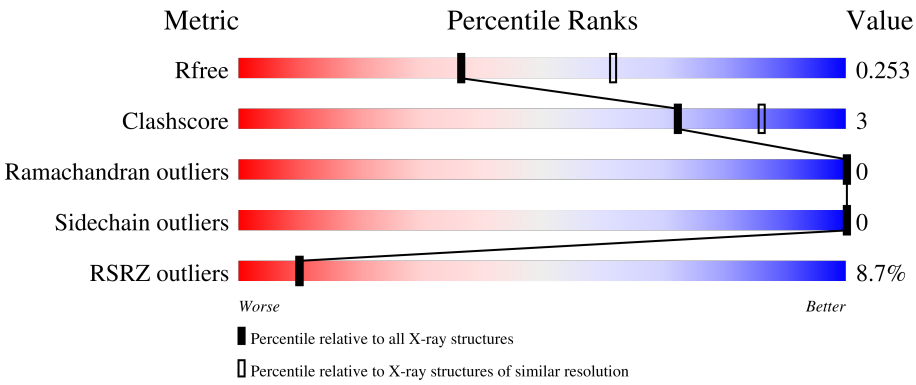
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	7%, 90%, 7% •
1	C	503	9%, 91%, 5% •
2	B	253	8%, 91%, 6% •
2	D	253	5%, 92%, 5% •
3	E	24	21%, 71%, 17%, 12%

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Mol	Chain	Length	Quality of chain
3	H	24	21% 79% 8% 12%
4	F	24	29% 71% 17% 12%
4	G	24	29% 67% 21% 12%

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 (i)

There are 7 unique types of molecules in this entry. The entry contains 25949 atoms, of which 12510 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
			Total	C	H	N	O	P	S			
1	A	487	7691	2388	3853	704	732	1	13	0	1	0
1	C	487	7690	2388	3852	704	732	1	13	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

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

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

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

There are 6 discrepancies between the modelled and reference sequences:

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

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

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
3	E	21	615	196	205	74	120	20	0	21	0
3	H	21	611	196	201	74	120	20	0	21	0

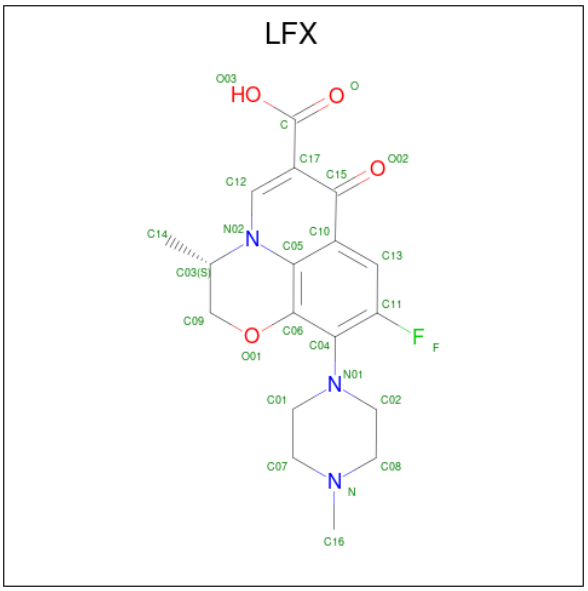
- Molecule 4 is a DNA chain called DNA substrate 24-mer TTACGTGCATAGTCATTCAT GACC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P			
4	F	21	612	196	202	74	120	20	0	21	0
4	G	21	611	196	201	74	120	20	0	21	0

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

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

- 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 (three-letter code: LFX) (formula: $C_{18}H_{20}FN_3O_4$).



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

- Molecule 7 is water.

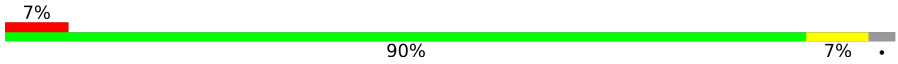
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	87	87	87	0	0
			Total	O		
7	B	34	34	34	0	0
			Total	O		
7	C	26	26	26	0	0
			Total	O		
7	D	24	24	24	0	0
			Total	O		
7	E	7	7	7	0	0
			Total	O		
7	F	8	8	8	0	0
			Total	O		
7	G	3	3	3	0	0

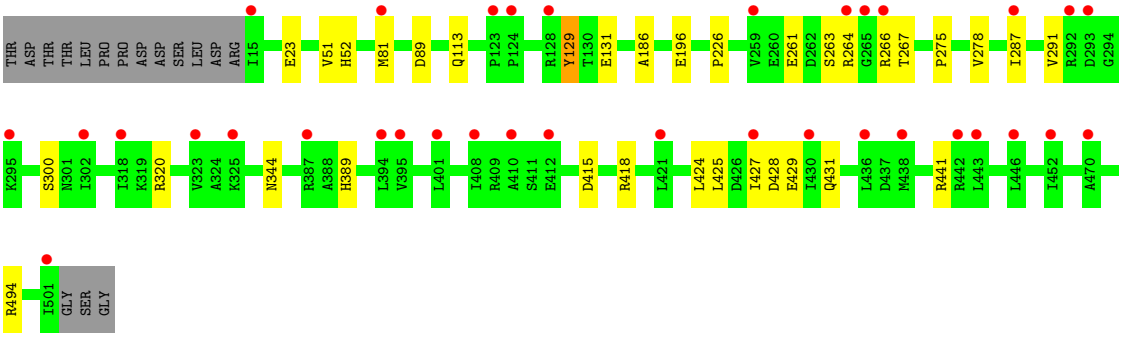
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA gyrase subunit A

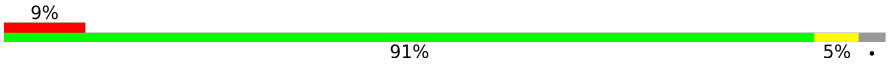
Chain A:

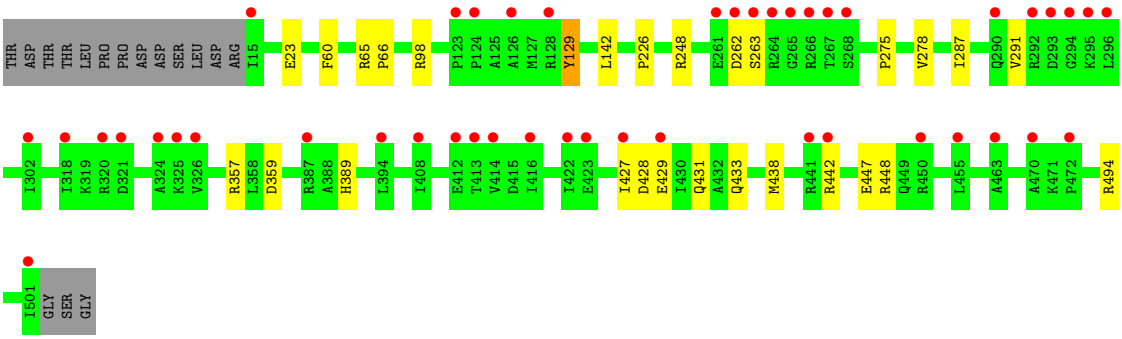




• Molecule 1: DNA gyrase subunit A

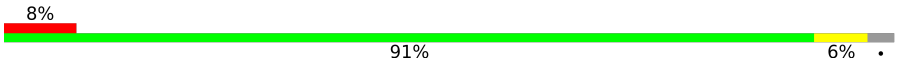
Chain C:

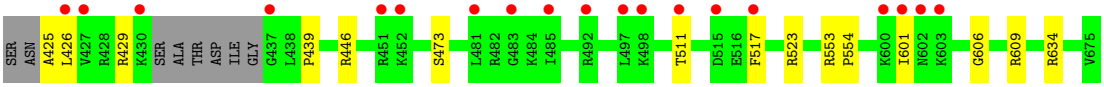




• Molecule 2: DNA gyrase subunit B

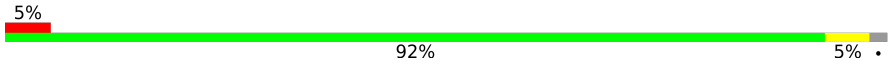
Chain B:

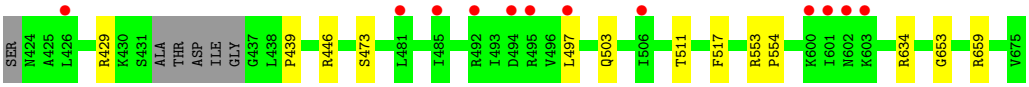




• Molecule 2: DNA gyrase subunit B

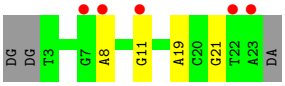
Chain D:





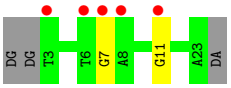
• Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA

Chain E:



• Molecule 3: DNA substrate 24-mer GGTCATGAATGACTATGCACGTAA

Chain H:

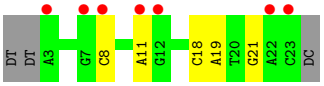


• Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC

Chain F:

• Molecule 4: DNA substrate 24-mer TTACGTGCATAGTCATTCATGACC

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	108.09Å 82.99Å 129.10Å 90.00° 108.76° 90.00°	Depositor
Resolution (Å)	46.33 – 2.50 49.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.33-2.50) 98.5 (49.21-2.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.27 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.249 0.230 , 0.253	Depositor DCC
R_{free} test set	3714 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	40.4	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25949	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: PTR, LFX, 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	0/3881	0.40	0/5253
1	C	0.21	0/3881	0.39	0/5253
2	B	0.22	0/1960	0.40	0/2634
2	D	0.21	0/1974	0.39	0/2653
3	E	0.54	0/458	0.95	0/704
3	H	0.58	0/458	0.98	0/704
4	F	0.53	0/458	0.94	0/704
4	G	0.52	0/458	0.94	0/704
All	All	0.28	0/13528	0.52	0/18609

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3838	3853	3853	32	0
1	C	3838	3852	3853	24	0
2	B	1932	1974	1973	10	0
2	D	1946	1984	1984	9	0
3	E	410	205	205	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	410	201	202	5	0
4	F	410	202	202	4	0
4	G	410	201	201	8	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	E	26	19	19	0	0
6	F	26	19	19	0	0
7	A	87	0	0	0	0
7	B	34	0	0	2	0
7	C	26	0	0	1	0
7	D	24	0	0	0	0
7	E	7	0	0	0	0
7	F	8	0	0	0	0
7	G	3	0	0	0	0
All	All	13439	12510	12511	75	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (75) 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:266:ARG:HD3	1:A:320:ARG:HG3	1.44	0.97
1:C:129:PTR:O2P	4:G:11[B]:DA:C5'	2.16	0.93
1:C:98:ARG:NH1	4:F:7[A]:DG:OP1	2.10	0.84
2:D:653:GLY:O	2:D:659:ARG:NH2	2.11	0.83
1:A:266:ARG:HG2	1:A:320:ARG:HG2	1.59	0.82
1:C:129:PTR:O2P	3:E:11[A]:DG:H4'	1.80	0.81
1:A:129:PTR:O1P	3:H:11[B]:DG:C5'	2.29	0.81
1:A:266:ARG:CD	1:A:320:ARG:HG3	2.12	0.79
4:G:18[B]:DC:O2	3:H:7[B]:DG:N2	2.20	0.75
1:A:129:PTR:O1P	3:H:11[B]:DG:H4'	1.89	0.73
1:C:129:PTR:O2P	4:G:11[B]:DA:H4'	1.94	0.68
1:A:129:PTR:O1P	4:F:11[A]:DA:H4'	1.94	0.67
1:C:357:ARG:NH1	1:C:359:ASP:OD1	2.27	0.67
1:A:266:ARG:HG2	1:A:320:ARG:CG	2.25	0.67
1:A:263:SER:O	1:A:264:ARG:HB2	1.96	0.66
2:D:429:ARG:NH1	2:D:439:PRO:O	2.30	0.65
2:B:429:ARG:NH1	2:B:439:PRO:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PTR:O1P	4:F:11[A]:DA:C5'	2.45	0.64
1:A:266:ARG:NH2	1:A:300:SER:OG	2.31	0.63
1:A:129:PTR:O1P	3:H:11[B]:DG:C4'	2.47	0.63
1:C:129:PTR:O2P	4:G:11[B]:DA:C4'	2.45	0.61
1:C:129:PTR:O2P	3:E:11[A]:DG:C4'	2.48	0.61
1:A:441:ARG:NH2	1:C:433:GLN:OE1	2.33	0.60
1:C:248:ARG:NH1	4:G:21[B]:DG:OP1	2.35	0.59
1:A:261:GLU:HG3	1:A:267:THR:HG22	1.87	0.57
1:A:287:ILE:O	1:A:291:VAL:HG23	2.05	0.56
1:A:266:ARG:HH11	1:A:320:ARG:NH1	2.04	0.56
1:A:389:HIS:NE2	1:A:431:GLN:OE1	2.40	0.55
1:C:428:ASP:OD1	1:C:429:GLU:N	2.40	0.54
1:C:287:ILE:O	1:C:291:VAL:HG23	2.07	0.53
1:A:52:HIS:NE2	4:G:8[B]:DC:OP1	2.42	0.51
1:A:428:ASP:OD1	1:A:429:GLU:N	2.42	0.51
2:B:609:ARG:NH2	7:B:804:HOH:O	2.44	0.51
1:C:262:ASP:OD1	1:C:263:SER:N	2.40	0.51
2:D:659:ARG:NH1	3:E:19[A]:DA:OP1	2.43	0.51
2:D:497:LEU:O	2:D:503:GLN:NE2	2.43	0.50
1:C:129:PTR:O2P	3:E:11[A]:DG:C5'	2.59	0.50
1:C:438:MET:HA	1:C:442:ARG:HH21	1.77	0.50
2:B:446:ARG:NH1	2:B:473:SER:OG	2.45	0.49
4:G:18[B]:DC:N3	3:H:7[B]:DG:N1	2.59	0.49
1:A:51:VAL:HG11	3:E:8[A]:DA:H5'	1.95	0.49
2:B:425:ALA:N	7:B:805:HOH:O	2.46	0.49
2:D:659:ARG:NH1	4:G:19[B]:DA:OP1	2.45	0.48
2:B:426:LEU:HD21	2:B:523:ARG:HE	1.78	0.48
1:A:266:ARG:CG	1:A:320:ARG:CG	2.91	0.47
2:D:446:ARG:NH2	2:D:473:SER:OG	2.48	0.47
1:A:427:ILE:CG2	1:A:431:GLN:HB2	2.45	0.46
1:A:266:ARG:CD	1:A:320:ARG:CG	2.88	0.46
1:C:389:HIS:O	1:C:431:GLN:NE2	2.45	0.46
1:A:81:MET:HE1	1:A:89:ASP:HB3	1.97	0.46
1:A:113:GLN:NE2	1:A:131:GLU:OE1	2.50	0.45
1:C:448:ARG:NE	7:C:603:HOH:O	2.49	0.45
1:C:60:PHE:HB2	1:C:142:LEU:HD13	1.99	0.45
1:C:23:GLU:OE1	2:D:634:ARG:NH1	2.50	0.44
1:A:23:GLU:OE1	2:B:634:ARG:NH1	2.50	0.44
1:C:427:ILE:CG2	1:C:431:GLN:HB2	2.48	0.44
2:B:511:THR:HG21	2:B:517:PHE:CE2	2.53	0.44
2:B:426:LEU:HD21	2:B:523:ARG:NE	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:ARG:HB3	1:C:66:PRO:HD2	2.00	0.43
4:F:16[A]:DT:C6	4:F:17[A]:DT:H72	2.53	0.43
1:A:415:ASP:OD1	1:A:418:ARG:NH2	2.52	0.43
1:C:442:ARG:HA	1:C:447:GLU:HB3	2.00	0.42
1:C:226:PRO:O	1:C:494:ARG:NH2	2.52	0.42
1:A:425:LEU:HB2	1:A:427:ILE:CD1	2.49	0.42
1:A:186:ALA:O	1:A:344:ASN:ND2	2.53	0.41
2:B:553:ARG:N	2:B:554:PRO:CD	2.83	0.41
2:B:601:ILE:HG22	2:B:606:GLY:HA2	2.03	0.41
1:A:196:GLU:OE2	1:A:494:ARG:NH1	2.53	0.41
2:D:511:THR:HG21	2:D:517:PHE:CE2	2.56	0.41
1:A:424:LEU:HG	1:A:425:LEU:HG	2.03	0.41
2:D:553:ARG:N	2:D:554:PRO:CD	2.84	0.41
1:A:275:PRO:HG2	1:A:278:VAL:HG21	2.02	0.41
1:C:248:ARG:NH1	3:E:21[A]:DG:OP1	2.53	0.41
1:C:275:PRO:HG2	1:C:278:VAL:HG21	2.02	0.41
1:A:226:PRO:O	1:A:494:ARG:NH2	2.54	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%)	467 (96%)	18 (4%)	0	100	100
1	C	485/503 (96%)	468 (96%)	17 (4%)	0	100	100
2	B	241/253 (95%)	234 (97%)	7 (3%)	0	100	100
2	D	243/253 (96%)	235 (97%)	8 (3%)	0	100	100
All	All	1454/1512 (96%)	1404 (97%)	50 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	407/420 (97%)	407 (100%)	0	100	100
1	C	407/420 (97%)	407 (100%)	0	100	100
2	B	205/211 (97%)	205 (100%)	0	100	100
2	D	207/211 (98%)	207 (100%)	0	100	100
All	All	1226/1262 (97%)	1226 (100%)	0	100	100

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

Sometimes 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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PTR	A	129	1	15,16,17	0.76	0	19,22,24	1.01	1 (5%)
1	PTR	C	129	1	15,16,17	0.78	0	19,22,24	0.99	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	PTR	CB-CA-C	-2.78	106.27	111.47
1	C	129	PTR	CB-CA-C	-2.49	106.79	111.47

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	A	129	PTR	5	0
1	C	129	PTR	6	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	E	101	5	29,29,29	3.39	11 (37%)	44,44,44	1.74	12 (27%)
6	LFX	F	101	5	29,29,29	3.35	10 (34%)	44,44,44	1.98	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LFX	E	101	5	-	0/8/27/27	0/4/4/4
6	LFX	F	101	5	-	0/8/27/27	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	101	LFX	C12-N02	9.63	1.49	1.34
6	F	101	LFX	C12-N02	9.47	1.49	1.34
6	E	101	LFX	O01-C06	7.96	1.50	1.37
6	F	101	LFX	O01-C06	7.86	1.50	1.37
6	F	101	LFX	C03-N02	-7.46	1.35	1.49
6	E	101	LFX	C03-N02	-7.43	1.35	1.49
6	F	101	LFX	C05-N02	6.14	1.47	1.40
6	E	101	LFX	C05-N02	6.12	1.47	1.40
6	E	101	LFX	C12-C17	3.73	1.48	1.38
6	F	101	LFX	C12-C17	3.67	1.48	1.38
6	F	101	LFX	C02-N01	-3.33	1.41	1.46
6	E	101	LFX	C04-N01	3.25	1.50	1.40
6	E	101	LFX	C10-C15	3.23	1.54	1.48
6	F	101	LFX	C10-C15	3.21	1.54	1.48
6	E	101	LFX	C02-N01	-3.16	1.41	1.46
6	F	101	LFX	C04-N01	3.12	1.49	1.40
6	E	101	LFX	C13-C11	2.84	1.42	1.37
6	F	101	LFX	C13-C11	2.81	1.42	1.37
6	E	101	LFX	C07-N	-2.14	1.41	1.46
6	E	101	LFX	O03-C	-2.09	1.24	1.30
6	F	101	LFX	C07-N	-2.07	1.41	1.46

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	101	LFX	C08-N-C07	6.51	118.63	109.52
6	E	101	LFX	C08-N-C07	4.63	116.00	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	101	LFX	C17-C12-N02	-4.29	119.68	124.49
6	F	101	LFX	C02-C08-N	4.21	115.56	110.80
6	E	101	LFX	C17-C12-N02	-4.14	119.86	124.49
6	F	101	LFX	C01-C07-N	3.86	115.16	110.80
6	E	101	LFX	C10-C15-C17	3.41	119.92	115.59
6	F	101	LFX	C10-C15-C17	3.35	119.85	115.59
6	E	101	LFX	C09-C03-N02	3.20	113.65	107.41
6	F	101	LFX	C09-C03-N02	3.11	113.46	107.41
6	F	101	LFX	C06-C04-C11	3.05	118.61	116.02
6	E	101	LFX	C01-C07-N	2.98	114.17	110.80
6	E	101	LFX	F-C11-C04	2.80	122.44	118.36
6	E	101	LFX	C06-C04-C11	2.66	118.27	116.02
6	F	101	LFX	C01-N01-C04	-2.50	111.61	119.44
6	E	101	LFX	C06-C04-N01	-2.45	116.86	122.81
6	F	101	LFX	F-C11-C04	2.27	121.66	118.36
6	F	101	LFX	C06-C04-N01	-2.19	117.48	122.81
6	E	101	LFX	C02-C08-N	2.16	113.24	110.80
6	F	101	LFX	C13-C11-C04	-2.13	120.14	123.22
6	E	101	LFX	C13-C11-C04	-2.12	120.16	123.22
6	E	101	LFX	C01-N01-C04	-2.05	113.04	119.44
6	E	101	LFX	O02-C15-C17	-2.00	119.86	123.22

There are no chirality outliers.

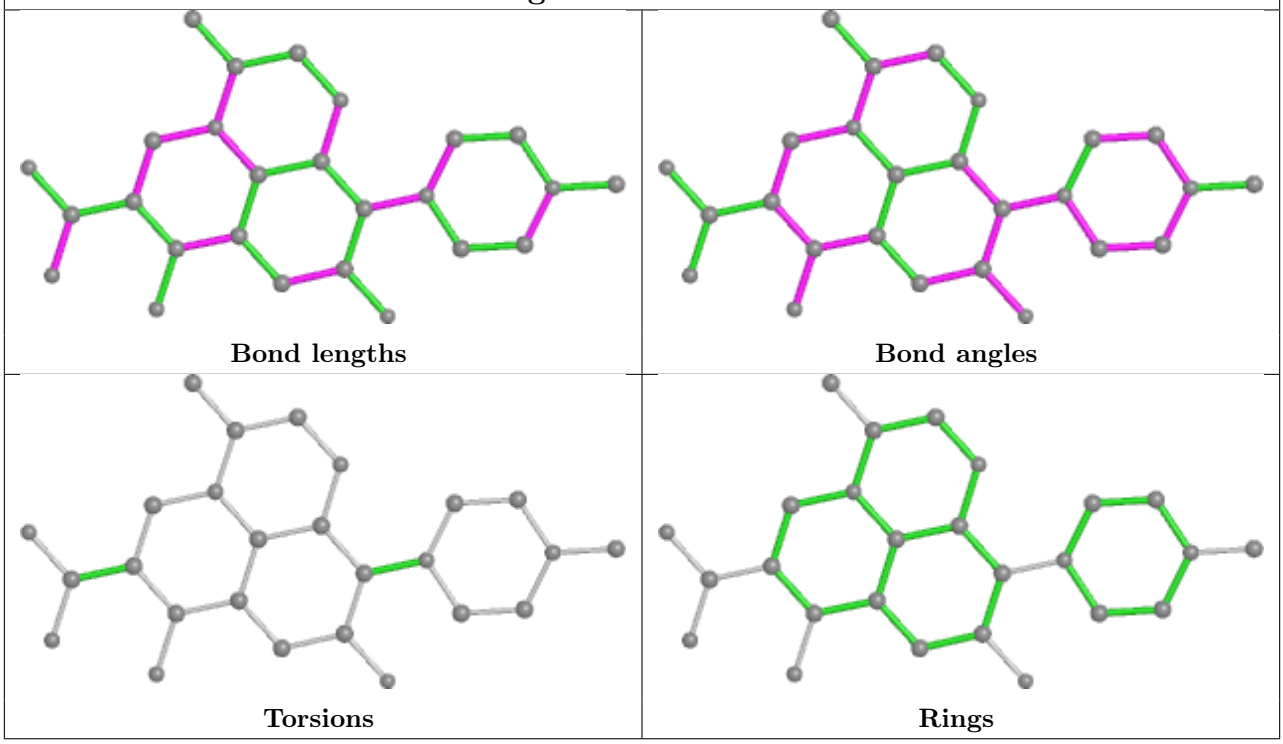
There are no torsion outliers.

There are no ring outliers.

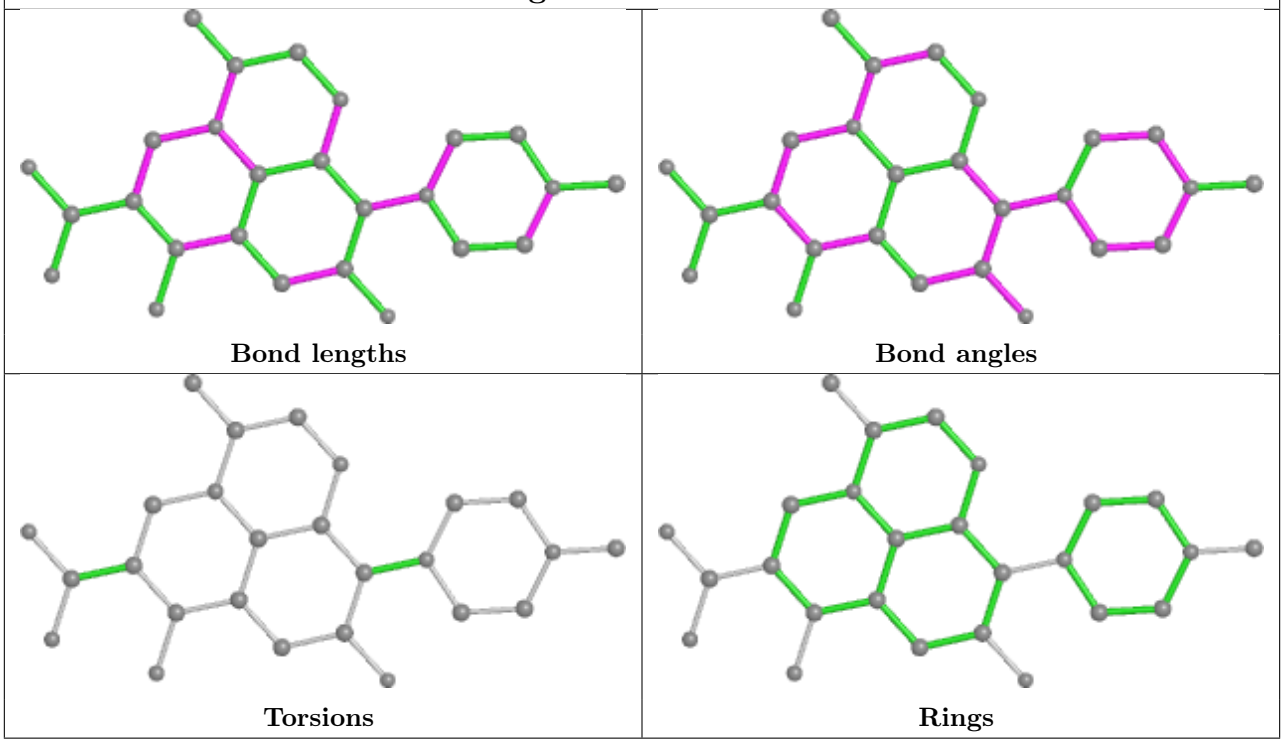
No monomer is involved in short contacts.

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 then 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.

Ligand LFX E 101



Ligand LFX F 101



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	486/503 (96%)	0.70	35 (7%)	15	16	26, 48, 101, 137	0
1	C	486/503 (96%)	0.75	45 (9%)	8	8	27, 50, 106, 137	0
2	B	245/253 (96%)	0.78	19 (7%)	13	13	36, 59, 94, 142	0
2	D	247/253 (97%)	0.55	12 (4%)	29	31	29, 53, 93, 152	0
3	E	21/24 (87%)	1.66	5 (23%)	0	0	57, 99, 170, 207	21 (100%)
3	H	21/24 (87%)	1.46	5 (23%)	0	0	20, 40, 125, 151	21 (100%)
4	F	21/24 (87%)	1.52	7 (33%)	0	0	65, 104, 196, 211	21 (100%)
4	G	21/24 (87%)	1.56	7 (33%)	0	0	20, 32, 132, 147	21 (100%)
All	All	1548/1608 (96%)	0.75	135 (8%)	10	10	20, 53, 111, 211	84 (5%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	23[A]	DA	7.6
1	A	264	ARG	7.3
1	A	292	ARG	7.2
1	C	292	ARG	6.7
4	G	23[B]	DC	6.3
1	A	266	ARG	5.8
2	B	426	LEU	5.5
1	C	264	ARG	5.4
1	A	408	ILE	5.4
1	A	387	ARG	5.1
1	A	412	GLU	4.8
3	H	11[B]	DG	4.6
2	D	601	ILE	4.6
1	C	501	ILE	4.2
1	A	323	VAL	4.1
1	C	412	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	401	LEU	3.9
1	A	452	ILE	3.8
1	A	501	ILE	3.8
1	A	265	GLY	3.8
2	B	515	ASP	3.8
1	C	293	ASP	3.7
1	C	263	SER	3.7
1	C	294	GLY	3.7
1	C	463	ALA	3.7
4	G	8[B]	DC	3.6
4	F	11[A]	DA	3.6
1	A	15	ILE	3.6
1	C	128[A]	ARG	3.5
2	B	427	VAL	3.5
1	C	265	GLY	3.5
3	E	22[A]	DT	3.4
1	C	387	ARG	3.4
2	B	601	ILE	3.4
1	A	128[A]	ARG	3.4
1	C	123	PRO	3.3
1	C	266	ARG	3.3
1	C	15	ILE	3.3
3	H	3[B]	DT	3.2
1	A	123	PRO	3.2
3	E	8[A]	DA	3.2
2	B	481	LEU	3.2
2	B	452	LYS	3.2
1	A	394	LEU	3.1
4	F	3[A]	DA	3.1
3	E	11[A]	DG	3.1
2	B	430	LYS	3.1
2	B	517	PHE	3.1
2	B	437	GLY	3.0
2	D	492	ARG	3.0
2	B	485	ILE	3.0
1	C	126	ALA	2.9
1	C	414	VAL	2.9
1	A	427	ILE	2.9
2	B	603	LYS	2.8
1	A	395	VAL	2.8
2	B	492	ARG	2.8
1	C	470	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	426	LEU	2.8
2	B	602	ASN	2.8
1	C	429	GLU	2.8
4	G	11[B]	DA	2.7
2	D	497	LEU	2.6
2	D	602	ASN	2.6
1	A	287	ILE	2.6
2	D	495	ARG	2.6
1	A	325	LYS	2.6
1	C	442	ARG	2.6
2	B	483	GLY	2.6
1	C	261	GLU	2.5
1	A	446	LEU	2.5
1	C	295	LYS	2.5
2	D	494	ASP	2.5
1	A	295	LYS	2.5
1	A	410	ALA	2.5
2	D	600	LYS	2.5
4	F	8[A]	DC	2.5
4	F	7[A]	DG	2.5
1	C	296	LEU	2.4
2	B	600	LYS	2.4
1	C	324	ALA	2.4
4	F	23[A]	DC	2.4
1	C	268	SER	2.4
1	C	321	ASP	2.4
3	H	7[B]	DG	2.4
1	C	262	ASP	2.4
1	C	290	GLN	2.4
1	C	325	LYS	2.4
1	C	427	ILE	2.4
1	A	442	ARG	2.4
1	C	394	LEU	2.3
1	C	416	ILE	2.3
3	H	6[B]	DT	2.3
2	B	511	THR	2.3
1	C	320	ARG	2.3
1	C	124	PRO	2.3
2	B	497	LEU	2.3
1	A	259	VAL	2.3
2	D	485	ILE	2.3
1	C	450	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	267	THR	2.3
1	A	443	LEU	2.3
2	B	451	ARG	2.2
4	G	7[B]	DG	2.2
1	A	436	LEU	2.2
1	C	302	ILE	2.2
1	C	422	ILE	2.2
1	C	441	ARG	2.2
3	E	7[A]	DG	2.2
2	D	481	LEU	2.2
4	G	22[B]	DA	2.1
1	C	455	LEU	2.1
2	D	603	LYS	2.1
1	A	438	MET	2.1
1	C	423	GLU	2.1
1	C	413	THR	2.1
3	H	8[B]	DA	2.1
1	C	472	PRO	2.1
1	A	293	ASP	2.1
1	A	302	ILE	2.1
1	A	421	LEU	2.1
1	A	81	MET	2.1
1	C	408	ILE	2.1
4	F	12[A]	DG	2.1
1	A	430	ILE	2.1
2	B	498	LYS	2.1
4	F	22[A]	DA	2.1
1	A	470	ALA	2.0
2	D	506	ILE	2.0
4	G	12[B]	DG	2.0
1	A	318	ILE	2.0
1	C	318	ILE	2.0
4	G	3[B]	DA	2.0
1	C	326	VAL	2.0
1	A	124	PRO	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	0.26	32,34,41,43	0
1	PTR	C	129	16/17	0.97	0.28	34,38,47,60	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

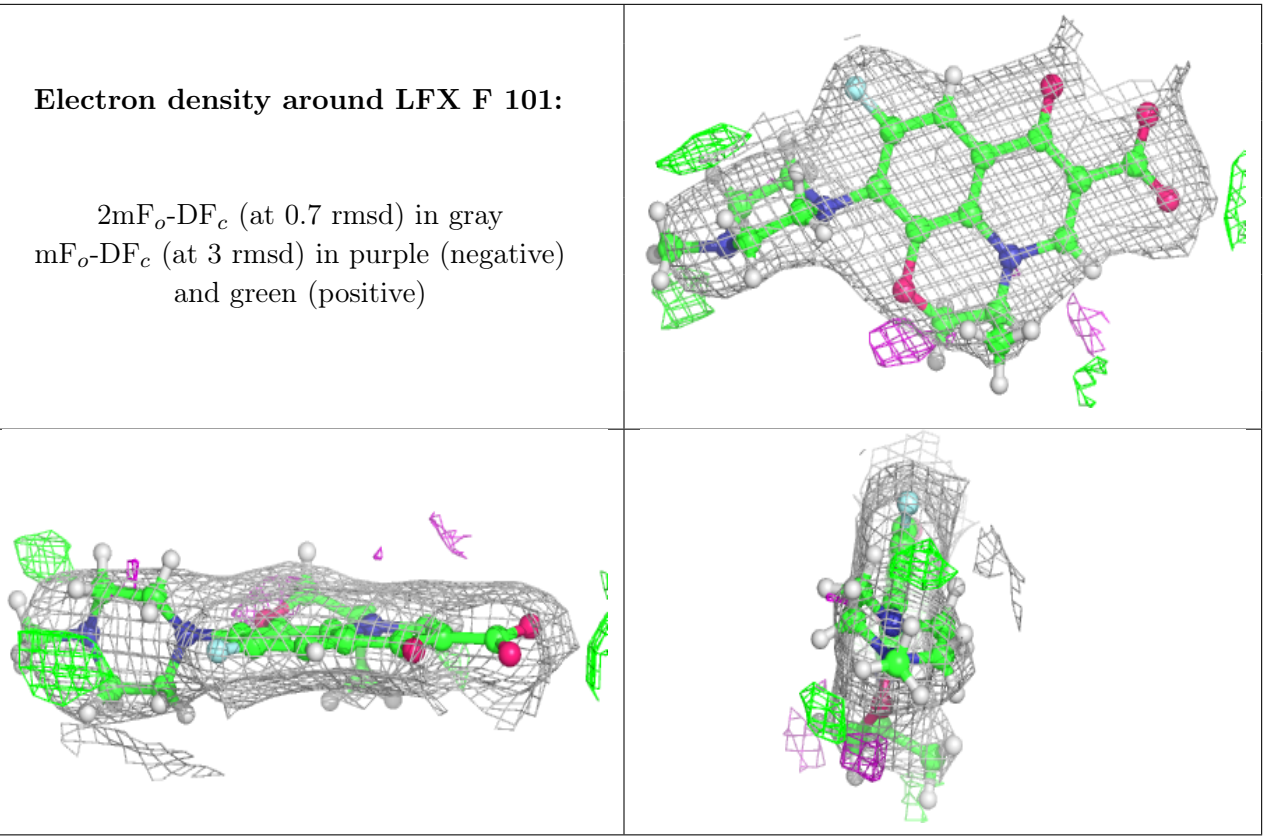
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	LFX	F	101	26/26	0.90	0.22	29,38,47,52	0
6	LFX	E	101	26/26	0.94	0.23	29,36,55,61	0
5	MG	F	102	1/1	0.94	0.20	31,31,31,31	0
5	MG	B	701	1/1	0.96	0.17	32,32,32,32	0
5	MG	E	102	1/1	0.97	0.20	30,30,30,30	0
5	MG	D	701	1/1	0.99	0.13	21,21,21,21	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.

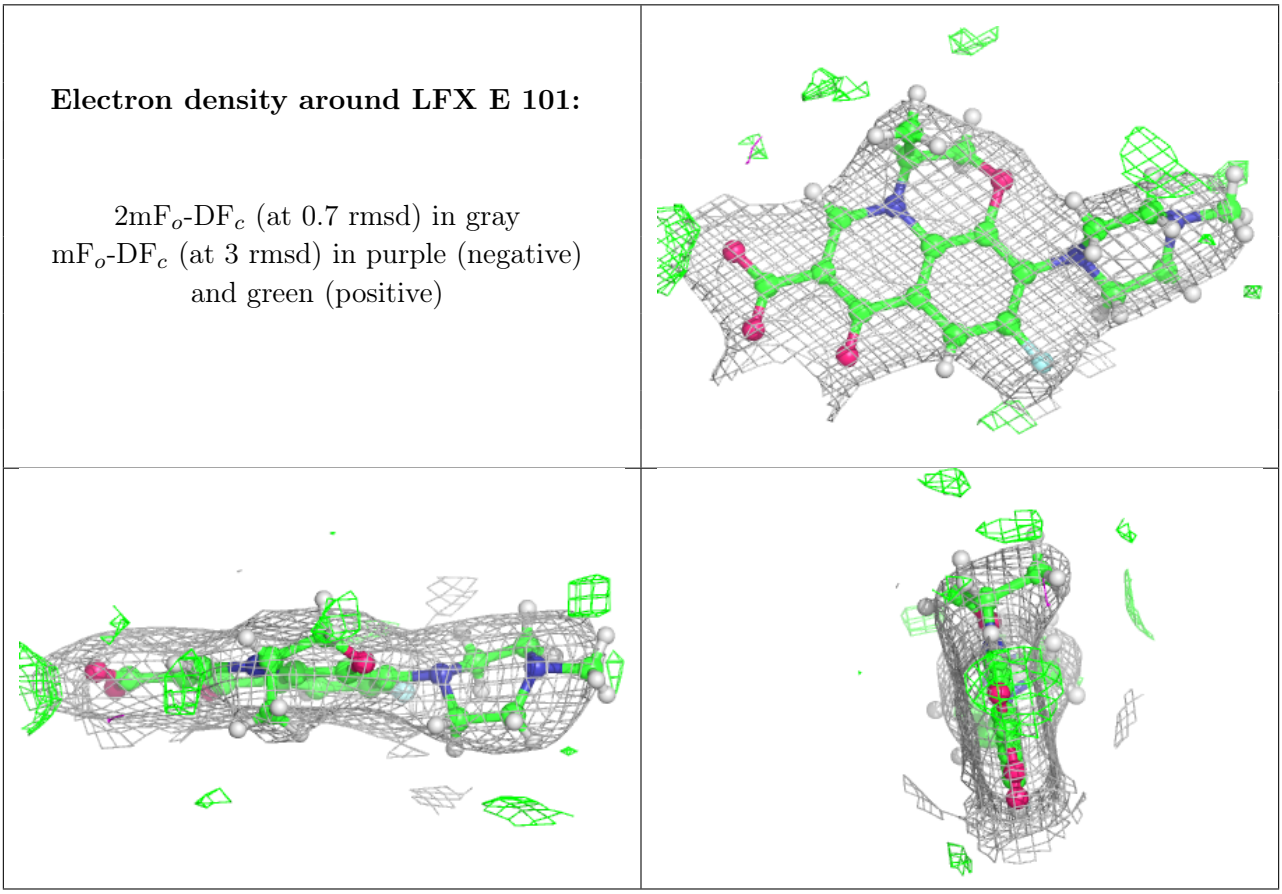
Electron density around LFX F 101:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.