



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:02 pm BST

PDB ID : 5EIX
Title : QUINOLONE-STABILIZED CLEAVAGE COMPLEX OF TOPOISOMERASE IV FROM KLEBSIELLA PNEUMONIAE
Authors : Veselkov, D.A.; Laponogov, I.; Pan, X.-S.; Selvarajah, J.; Branstrom, A.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2015-10-30
Resolution : 3.35 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 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

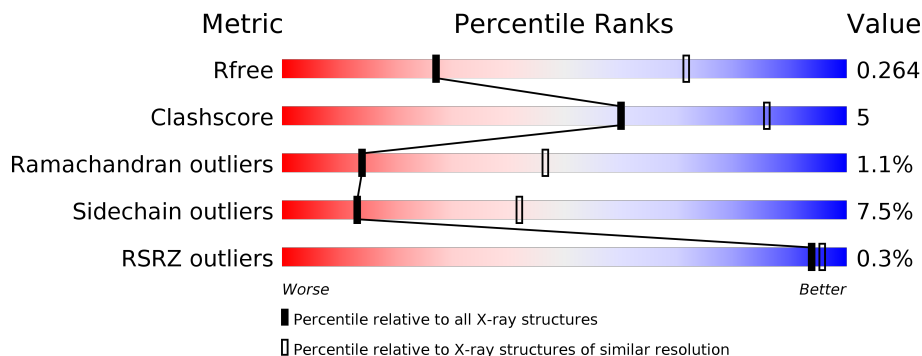
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.




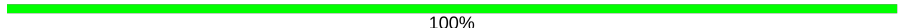




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	741	79% 14% • 5%
1	B	741	81% 12% • 5%
1	G	741	79% 11% • 9%
1	J	741	81% 10% • 8%
2	C	8	100%
2	E	8	100%

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Mol	Chain	Length	Quality of chain
2	H	8	 100%
2	K	8	 100%
3	D	12	 83% 17%
3	F	12	 83% 17%
3	I	12	 83% 17%
3	L	12	 83% 17%

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 20461 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	702	Total 4962	C 3129	N 904	O 907	S 22	0	0	0
1	B	701	Total 4848	C 3059	N 891	O 876	S 22	0	0	0
1	G	671	Total 4468	C 2811	N 827	O 812	S 18	0	0	0
1	J	679	Total 4463	C 2807	N 826	O 811	S 19	0	0	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	389	MET	-	initiating methionine	UNP R4YHS8
A	999	GLU	-	linker	UNP R4YHS8
A	1000	PHE	-	linker	UNP R4YHS8
A	1100	GLY	VAL	conflict	UNP R4YE07
A	1255	THR	SER	conflict	UNP R4YE07
A	1491	HIS	-	expression tag	UNP R4YE07
A	1492	HIS	-	expression tag	UNP R4YE07
A	1493	HIS	-	expression tag	UNP R4YE07
A	1494	HIS	-	expression tag	UNP R4YE07
A	1495	HIS	-	expression tag	UNP R4YE07
A	1496	HIS	-	expression tag	UNP R4YE07
B	389	MET	-	initiating methionine	UNP R4YHS8
B	999	GLU	-	linker	UNP R4YHS8
B	1000	PHE	-	linker	UNP R4YHS8
B	1100	GLY	VAL	conflict	UNP R4YE07
B	1255	THR	SER	conflict	UNP R4YE07
B	1491	HIS	-	expression tag	UNP R4YE07
B	1492	HIS	-	expression tag	UNP R4YE07
B	1493	HIS	-	expression tag	UNP R4YE07
B	1494	HIS	-	expression tag	UNP R4YE07

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1495	HIS	-	expression tag	UNP R4YE07
B	1496	HIS	-	expression tag	UNP R4YE07
G	389	MET	-	initiating methionine	UNP R4YHS8
G	999	GLU	-	linker	UNP R4YHS8
G	1000	PHE	-	linker	UNP R4YHS8
G	1100	GLY	VAL	conflict	UNP R4YE07
G	1255	THR	SER	conflict	UNP R4YE07
G	1491	HIS	-	expression tag	UNP R4YE07
G	1492	HIS	-	expression tag	UNP R4YE07
G	1493	HIS	-	expression tag	UNP R4YE07
G	1494	HIS	-	expression tag	UNP R4YE07
G	1495	HIS	-	expression tag	UNP R4YE07
G	1496	HIS	-	expression tag	UNP R4YE07
J	389	MET	-	initiating methionine	UNP R4YHS8
J	999	GLU	-	linker	UNP R4YHS8
J	1000	PHE	-	linker	UNP R4YHS8
J	1100	GLY	VAL	conflict	UNP R4YE07
J	1255	THR	SER	conflict	UNP R4YE07
J	1491	HIS	-	expression tag	UNP R4YE07
J	1492	HIS	-	expression tag	UNP R4YE07
J	1493	HIS	-	expression tag	UNP R4YE07
J	1494	HIS	-	expression tag	UNP R4YE07
J	1495	HIS	-	expression tag	UNP R4YE07
J	1496	HIS	-	expression tag	UNP R4YE07

- Molecule 2 is a DNA chain called SYMMETRISED E-SITE (PRE-CUT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	P	0	0	0
			160	79	26	48	7			
2	C	8	Total	C	N	O	P	0	0	0
			160	79	26	48	7			
2	H	8	Total	C	N	O	P	0	0	0
			160	79	26	48	7			
2	K	8	Total	C	N	O	P	0	0	0
			160	79	26	48	7			

- Molecule 3 is a DNA chain called SYMMETRISED E-SITE (PRE-CUT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	12	Total	C	N	O	P	0	0	0
			242	117	48	66	11			

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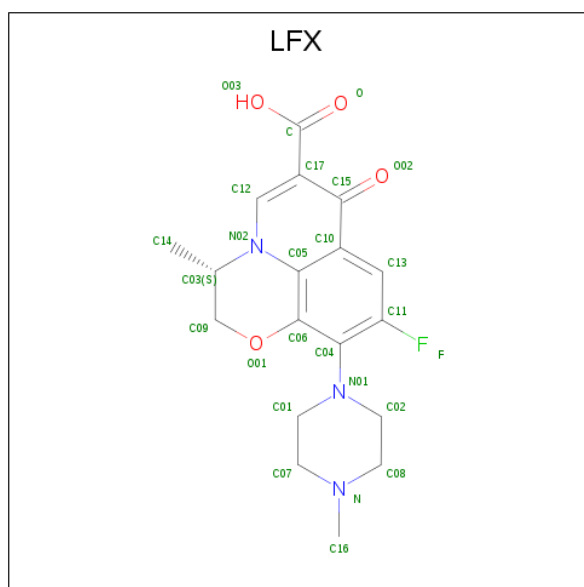
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total	C	N	O	P	0	0	0
			242	117	48	66	11			
3	I	12	Total	C	N	O	P	0	0	0
			242	117	48	66	11			
3	L	12	Total	C	N	O	P	0	0	0
			242	117	48	66	11			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Mg	0	0
			2	2		
4	B	1	Total	Mg	0	0
			1	1		
4	A	2	Total	Mg	0	0
			2	2		
4	L	2	Total	Mg	0	0
			2	2		
4	J	1	Total	Mg	0	0
			1	1		

- Molecule 5 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: C₁₈H₂₀FN₃O₄).

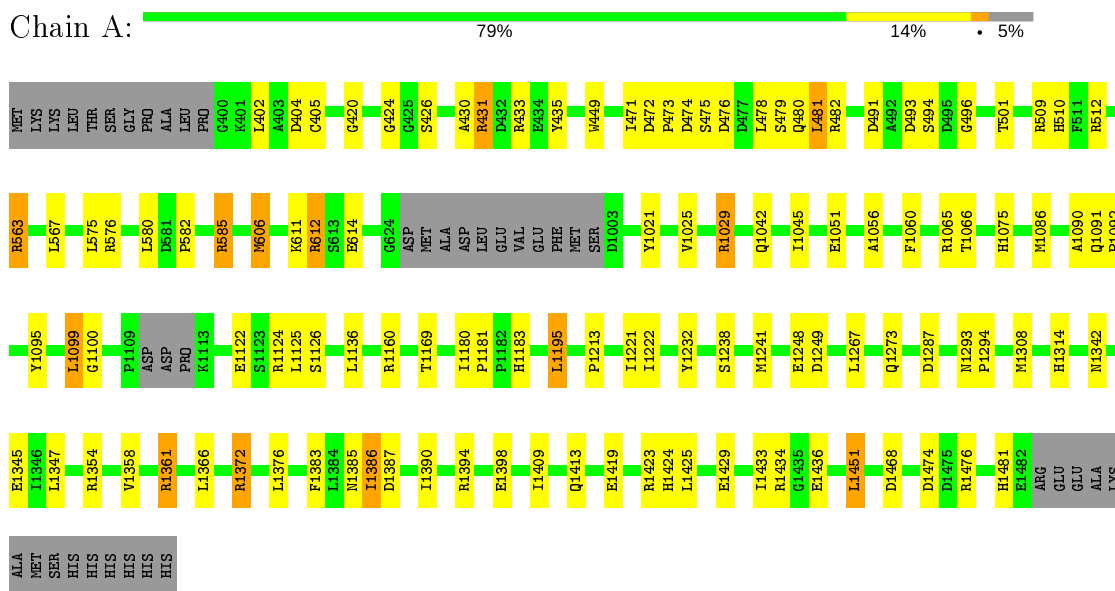


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total 26	C 18	F 1	N 3	O 4	0	0
5	D	1	Total 26	C 18	F 1	N 3	O 4	0	0
5	I	1	Total 26	C 18	F 1	N 3	O 4	0	0
5	L	1	Total 26	C 18	F 1	N 3	O 4	0	0

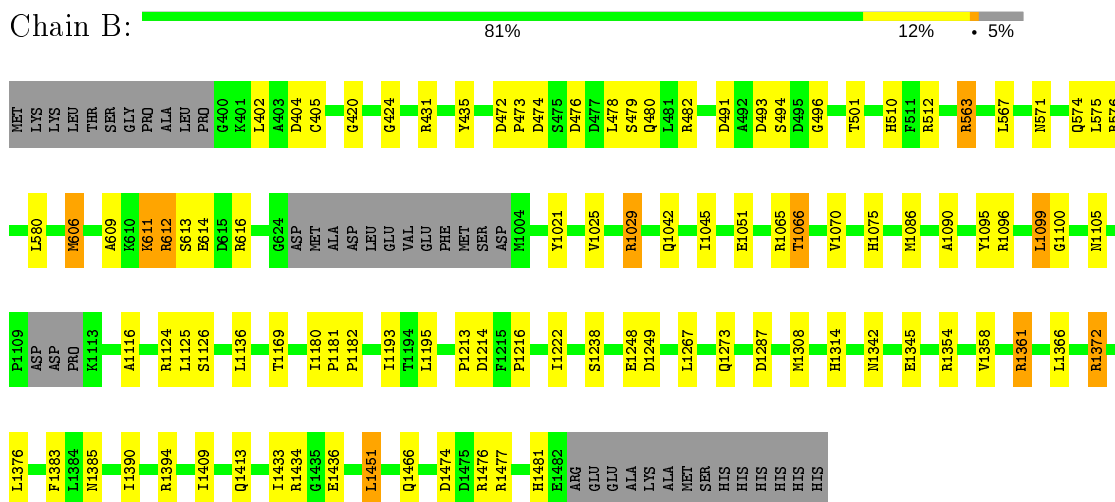
3 Residue-property plots

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

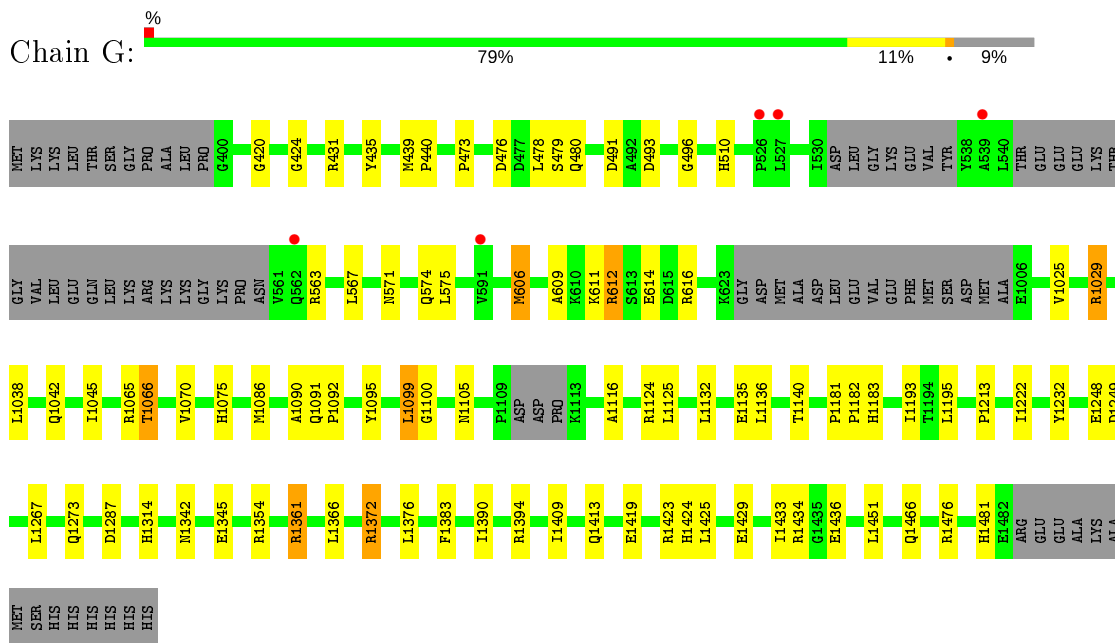
- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A



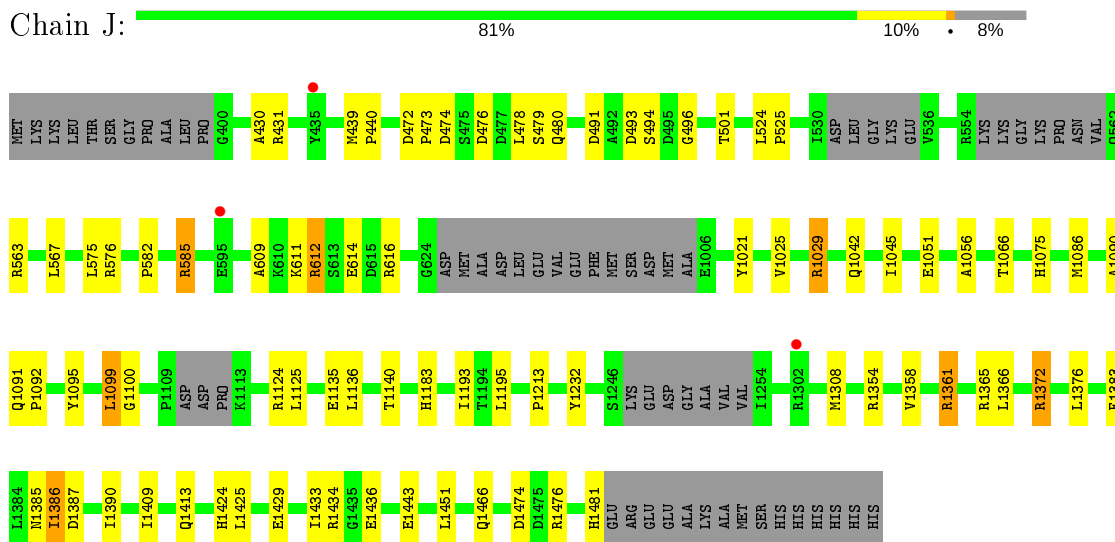
- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A



- Molecule 1: DNA topoisomerase 4 subunit B,DNA topoisomerase 4 subunit A



- Molecule 1: DNA topoisomerase 4 subunit B, DNA topoisomerase 4 subunit A



- Molecule 2: SYMMETRISED E-SITE (PRE-CUT)

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: SYMMETRISED E-SITE (PRE-CUT)

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: SYMMETRISED E-SITE (PRE-CUT)

Chain H:  100%


There are no outlier residues recorded for this chain.

- Molecule 2: SYMMETRISED E-SITE (PRE-CUT)

Chain K:  100%


There are no outlier residues recorded for this chain.

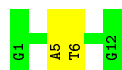
- Molecule 3: SYMMETRISED E-SITE (PRE-CUT)

Chain F:  83% 17%




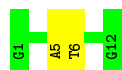
- Molecule 3: SYMMETRISED E-SITE (PRE-CUT)

Chain D:  83% 17%




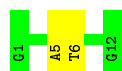
- Molecule 3: SYMMETRISED E-SITE (PRE-CUT)

Chain I:  83% 17%



- Molecule 3: SYMMETRISED E-SITE (PRE-CUT)

Chain L:  83% 17%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.07Å 161.53Å 138.60Å 90.00° 94.22° 90.00°	Depositor
Resolution (Å)	85.01 – 3.35 85.01 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.3 (85.01-3.35) 98.3 (85.01-3.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 3.33Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.224 , 0.259 0.226 , 0.264	Depositor DCC
R_{free} test set	3208 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	71.0	Xtrriage
Anisotropy	0.261	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	20461	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: MG, LFX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/5049	0.38	0/6870
1	B	0.20	0/4935	0.38	0/6730
1	G	0.20	0/4550	0.37	0/6225
1	J	0.20	0/4542	0.38	0/6218
2	C	0.40	0/178	1.14	0/274
2	E	0.40	0/178	1.13	0/274
2	H	0.41	0/178	1.13	0/274
2	K	0.42	0/178	1.15	0/274
3	D	0.43	0/272	0.96	0/418
3	F	0.45	0/272	0.94	0/418
3	I	0.44	0/272	0.95	0/418
3	L	0.44	0/272	0.95	0/418
All	All	0.23	0/20876	0.48	0/28811

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	4962	0	4332	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4848	0	4138	42	0
1	G	4468	0	3575	42	0
1	J	4463	0	3530	33	0
2	C	160	0	91	0	0
2	E	160	0	91	0	0
2	H	160	0	91	0	0
2	K	160	0	91	0	0
3	D	242	0	133	3	0
3	F	242	0	133	1	0
3	I	242	0	133	1	0
3	L	242	0	133	1	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	G	2	0	0	0	0
4	J	1	0	0	0	0
4	L	2	0	0	0	0
5	D	26	0	19	2	0
5	F	26	0	19	0	0
5	I	26	0	19	0	0
5	L	26	0	19	0	0
All	All	20461	0	16547	169	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 5.

All (169) 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:582:PRO:HA	1:A:585:ARG:HD2	1.66	0.77
1:A:1376:LEU:HD22	1:A:1433:ILE:HG23	1.68	0.74
1:B:1376:LEU:HD22	1:B:1433:ILE:HG23	1.71	0.73
1:J:1376:LEU:HD22	1:J:1433:ILE:HG23	1.72	0.71
1:G:1424:HIS:HA	1:G:1429:GLU:HG3	1.73	0.70
1:G:1376:LEU:HD22	1:G:1433:ILE:HG23	1.74	0.69
1:J:582:PRO:HA	1:J:585:ARG:HD2	1.76	0.68
1:A:509:ARG:HA	1:A:512:ARG:HH21	1.58	0.68
1:A:430:ALA:HB1	1:A:576:ARG:HB2	1.75	0.66
1:A:576:ARG:HA	1:A:580:LEU:HB2	1.78	0.66
1:B:1342:ASN:ND2	1:B:1345:GLU:OE2	2.28	0.66
1:A:1409:ILE:HG23	1:A:1413:GLN:HB2	1.76	0.66
1:B:1409:ILE:HG23	1:B:1413:GLN:HB2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:1099:LEU:N	1:J:1100:GLY:HA3	2.11	0.65
1:A:1099:LEU:N	1:A:1100:GLY:HA3	2.12	0.65
3:D:5:DA:H2"	3:D:6:DT:H5"	1.78	0.65
1:B:1099:LEU:N	1:B:1100:GLY:HA3	2.11	0.64
1:G:1342:ASN:ND2	1:G:1345:GLU:OE2	2.31	0.63
1:A:1342:ASN:ND2	1:A:1345:GLU:OE2	2.31	0.63
1:J:1424:HIS:HA	1:J:1429:GLU:HG3	1.80	0.63
1:G:1099:LEU:N	1:G:1100:GLY:HA3	2.14	0.63
1:J:1090:ALA:HA	1:J:1100:GLY:HA2	1.79	0.62
1:A:433:ARG:NH2	1:G:1287:ASP:OD2	2.32	0.62
1:A:1160:ARG:NH1	1:A:1468:ASP:OD1	2.33	0.62
1:J:494:SER:HB3	1:J:1021:TYR:HA	1.83	0.61
1:A:1042:GLN:NE2	1:A:1095:TYR:OH	2.35	0.60
1:J:1409:ILE:HG23	1:J:1413:GLN:HB2	1.84	0.60
1:J:1042:GLN:NE2	1:J:1095:TYR:OH	2.35	0.59
1:B:1273:GLN:OE1	1:B:1314:HIS:NE2	2.36	0.59
3:L:5:DA:H2"	3:L:6:DT:H5"	1.84	0.58
1:A:1183:HIS:NE2	1:A:1232:TYR:OH	2.29	0.58
1:G:1090:ALA:HA	1:G:1100:GLY:HA2	1.84	0.58
1:B:1169:THR:H	1:B:1180:ILE:HB	1.69	0.57
1:J:1383:PHE:HE2	1:J:1433:ILE:HD12	1.68	0.57
3:F:5:DA:H2"	3:F:6:DT:H5"	1.86	0.57
1:A:1273:GLN:OE1	1:A:1314:HIS:NE2	2.38	0.57
1:G:1213:PRO:O	1:G:1476:ARG:NH2	2.38	0.57
1:B:1213:PRO:O	1:B:1476:ARG:NH2	2.38	0.57
1:J:1213:PRO:O	1:J:1476:ARG:NH2	2.37	0.56
1:A:1424:HIS:HA	1:A:1429:GLU:HG3	1.87	0.56
1:A:1090:ALA:HA	1:A:1100:GLY:HA2	1.85	0.56
1:A:606:MET:HA	1:A:612:ARG:HD3	1.87	0.55
1:G:1105:ASN:HB3	1:G:1116:ALA:HB2	1.89	0.55
1:G:1383:PHE:HE2	1:G:1433:ILE:HD12	1.72	0.55
1:B:1372:ARG:NH1	1:B:1436:GLU:OE1	2.39	0.55
1:B:1090:ALA:HA	1:B:1100:GLY:HA2	1.89	0.55
1:J:1372:ARG:NH1	1:J:1436:GLU:OE1	2.40	0.55
1:G:1409:ILE:HG23	1:G:1413:GLN:HB2	1.89	0.54
1:B:1096:ARG:NE	1:B:1214:ASP:OD1	2.35	0.53
1:B:1358:VAL:HG13	1:B:1361:ARG:HH21	1.73	0.53
1:B:576:ARG:HA	1:B:580:LEU:HB2	1.91	0.53
1:A:1358:VAL:HG13	1:A:1361:ARG:HH21	1.73	0.53
1:B:1267:LEU:HD21	1:B:1287:ASP:HB2	1.89	0.53
1:G:1042:GLN:NE2	1:G:1095:TYR:OH	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1181:PRO:HB2	1:A:1213:PRO:HB3	1.91	0.52
3:D:5:DA:C4	5:D:100:LFX:H01A	2.44	0.52
1:A:1267:LEU:HD21	1:A:1287:ASP:HB2	1.90	0.52
1:B:493:ASP:HB2	1:B:496:GLY:H	1.74	0.52
1:B:1045:ILE:HD13	1:B:1086:MET:HB2	1.90	0.52
3:I:5:DA:H2"	3:I:6:DT:H5"	1.91	0.52
1:A:1419:GLU:OE2	1:G:1423:ARG:NH1	2.40	0.51
1:B:609:ALA:O	1:B:616:ARG:NH2	2.43	0.51
1:G:609:ALA:O	1:G:616:ARG:NH2	2.44	0.51
1:A:1372:ARG:NH1	1:A:1436:GLU:OE1	2.43	0.51
1:B:1390:ILE:HD13	1:J:1390:ILE:HD13	1.93	0.51
1:G:1372:ARG:NH1	1:G:1436:GLU:OE1	2.44	0.51
1:G:1038:LEU:HD11	1:G:1132:LEU:HD13	1.92	0.50
1:B:404:ASP:OD2	1:B:482:ARG:NH2	2.44	0.50
1:G:491:ASP:HB3	1:G:567:LEU:HG	1.92	0.50
1:B:494:SER:HB3	1:B:1021:TYR:HA	1.93	0.50
1:B:420:GLY:O	1:B:424:GLY:N	2.42	0.50
1:B:571:ASN:HB2	1:B:574:GLN:HG3	1.94	0.50
1:J:1358:VAL:HG13	1:J:1361:ARG:HH21	1.76	0.50
1:A:1045:ILE:HD13	1:A:1086:MET:HB2	1.93	0.50
1:B:1042:GLN:NE2	1:B:1095:TYR:OH	2.44	0.50
1:J:1365:ARG:NE	1:J:1443:GLU:OE2	2.38	0.50
1:A:478:LEU:O	1:A:480:GLN:N	2.46	0.49
1:B:606:MET:HA	1:B:612:ARG:HD3	1.94	0.49
1:A:493:ASP:HB2	1:A:496:GLY:H	1.78	0.49
1:A:1423:ARG:NH1	1:G:1419:GLU:OE2	2.39	0.48
1:A:420:GLY:O	1:A:424:GLY:N	2.44	0.48
1:G:493:ASP:HB2	1:G:496:GLY:H	1.78	0.48
1:B:491:ASP:HB3	1:B:567:LEU:HG	1.95	0.48
1:G:612:ARG:O	1:G:614:GLU:N	2.45	0.48
1:J:1045:ILE:HD13	1:J:1086:MET:HB2	1.95	0.48
1:A:404:ASP:OD2	1:A:482:ARG:NH2	2.46	0.48
1:A:491:ASP:HB3	1:A:567:LEU:HG	1.95	0.48
1:B:613:SER:H	1:B:616:ARG:HH21	1.62	0.47
1:J:1056:ALA:HA	1:J:1124:ARG:HD3	1.97	0.47
1:A:1248:GLU:HA	1:A:1249:ASP:HA	1.56	0.47
1:G:478:LEU:O	1:G:480:GLN:N	2.48	0.47
1:G:1025:VAL:HA	1:G:1029:ARG:HB2	1.97	0.46
1:A:494:SER:HB3	1:A:1021:TYR:HA	1.97	0.46
1:A:426:SER:OG	1:G:1105:ASN:HB2	2.16	0.46
1:B:478:LEU:O	1:B:480:GLN:N	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1183:HIS:NE2	1:G:1232:TYR:OH	2.33	0.46
1:A:1390:ILE:HD13	1:G:1390:ILE:HD13	1.98	0.46
1:B:1248:GLU:HA	1:B:1249:ASP:HA	1.55	0.46
1:G:439:MET:HA	1:G:440:PRO:HD3	1.82	0.46
1:A:449:TRP:HA	1:A:509:ARG:HD2	1.98	0.46
1:A:1383:PHE:HE2	1:A:1433:ILE:HD12	1.81	0.46
1:A:612:ARG:O	1:A:614:GLU:N	2.44	0.46
1:A:1213:PRO:O	1:A:1476:ARG:NH2	2.49	0.45
1:A:471:ILE:HD11	1:A:481:LEU:HG	1.98	0.45
1:G:1267:LEU:HD21	1:G:1287:ASP:HB2	1.97	0.45
1:J:493:ASP:HB2	1:J:496:GLY:H	1.80	0.45
1:J:472:ASP:O	1:J:474:ASP:N	2.43	0.45
1:J:478:LEU:O	1:J:480:GLN:N	2.49	0.45
1:A:431:ARG:CZ	1:A:433:ARG:HG2	2.46	0.45
1:B:404:ASP:OD1	1:B:405:CYS:N	2.48	0.45
1:J:1025:VAL:HA	1:J:1029:ARG:HB2	1.99	0.45
1:B:1105:ASN:HB3	1:B:1116:ALA:HB2	1.98	0.44
1:G:420:GLY:O	1:G:424:GLY:N	2.46	0.44
1:A:1169:THR:H	1:A:1180:ILE:HB	1.82	0.44
1:G:571:ASN:HB2	1:G:574:GLN:HG3	2.00	0.44
1:J:1124:ARG:HG2	1:J:1125:LEU:N	2.31	0.44
1:B:1025:VAL:HA	1:B:1029:ARG:HB2	1.99	0.44
1:G:1045:ILE:HD13	1:G:1086:MET:HB2	2.00	0.44
1:J:1183:HIS:NE2	1:J:1232:TYR:OH	2.40	0.44
1:B:1216:PRO:HA	1:B:1477:ARG:HD3	1.99	0.44
1:G:1193:ILE:HD13	1:G:1466:GLN:HG2	1.99	0.44
1:B:612:ARG:O	1:B:614:GLU:N	2.46	0.44
1:G:1361:ARG:HB3	1:G:1361:ARG:HE	1.56	0.44
1:J:609:ALA:O	1:J:616:ARG:NH2	2.51	0.44
1:A:1056:ALA:HA	1:A:1124:ARG:HD3	1.98	0.44
1:J:612:ARG:O	1:J:614:GLU:N	2.46	0.43
1:B:1124:ARG:HG2	1:B:1125:LEU:N	2.32	0.43
1:G:606:MET:HA	1:G:612:ARG:HD3	2.01	0.43
1:J:491:ASP:HB3	1:J:567:LEU:H	1.82	0.43
1:A:1394:ARG:HD3	1:G:1425:LEU:HB3	2.00	0.43
3:D:5:DA:N3	5:D:100:LFX:H01A	2.34	0.43
1:G:1181:PRO:HB2	1:G:1213:PRO:HB3	2.01	0.43
1:A:404:ASP:OD1	1:A:405:CYS:N	2.52	0.43
1:G:1248:GLU:HA	1:G:1249:ASP:HA	1.53	0.43
1:B:1451:LEU:HD13	1:B:1451:LEU:HA	1.87	0.42
1:A:1060:PHE:HB3	1:A:1122:GLU:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1124:ARG:HG2	1:A:1125:LEU:N	2.32	0.42
1:A:1099:LEU:HA	1:A:1126:SER:HB3	2.01	0.42
1:J:430:ALA:HB1	1:J:576:ARG:HB2	2.00	0.42
1:G:1066:THR:O	1:G:1070:VAL:HG23	2.20	0.42
1:A:1221:ILE:HG12	1:A:1241:MET:HG2	2.01	0.42
1:J:439:MET:HA	1:J:440:PRO:HD3	1.82	0.42
1:A:472:ASP:O	1:A:474:ASP:N	2.44	0.42
1:G:1124:ARG:HG2	1:G:1125:LEU:N	2.34	0.42
1:B:1181:PRO:HA	1:B:1182:PRO:HD3	1.89	0.42
1:B:472:ASP:O	1:B:474:ASP:N	2.44	0.41
1:A:1386:ILE:HD12	1:A:1387:ASP:H	1.85	0.41
1:B:1383:PHE:HE2	1:B:1433:ILE:HD12	1.83	0.41
1:B:611:LYS:O	1:B:616:ARG:NH2	2.54	0.41
1:J:1091:GLN:HA	1:J:1092:PRO:HD3	1.86	0.41
1:A:1293:ASN:HA	1:A:1294:PRO:HD2	1.88	0.41
1:A:404:ASP:O	1:A:431:ARG:NH2	2.54	0.41
1:A:1425:LEU:HB3	1:G:1394:ARG:HD3	2.02	0.41
1:J:1193:ILE:HD13	1:J:1466:GLN:HG2	2.01	0.41
1:B:1066:THR:O	1:B:1070:VAL:HG23	2.21	0.41
1:A:1195:LEU:HD12	1:A:1347:LEU:HB3	2.03	0.41
1:B:1099:LEU:HA	1:B:1126:SER:HB3	2.03	0.41
1:G:1273:GLN:OE1	1:G:1314:HIS:NE2	2.54	0.41
1:B:1394:ARG:HD3	1:J:1425:LEU:HB3	2.02	0.41
1:A:1451:LEU:HD13	1:A:1451:LEU:HA	1.88	0.41
1:G:1135:GLU:O	1:G:1140:THR:OG1	2.28	0.41
1:J:1386:ILE:HD12	1:J:1387:ASP:H	1.86	0.41
1:B:1193:ILE:HD13	1:B:1466:GLN:HG2	2.02	0.40
1:A:1091:GLN:HA	1:A:1092:PRO:HD3	1.86	0.40
1:A:1025:VAL:HA	1:A:1029:ARG:HB2	2.03	0.40
1:G:1091:GLN:HA	1:G:1092:PRO:HD3	1.84	0.40
1:G:1181:PRO:HA	1:G:1182:PRO:HD3	1.95	0.40
1:J:1135:GLU:O	1:J:1140:THR:OG1	2.31	0.40
1:J:524:LEU:HA	1:J:525:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	696/741 (94%)	646 (93%)	41 (6%)	9 (1%)	12	42
1	B	695/741 (94%)	645 (93%)	43 (6%)	7 (1%)	15	49
1	G	661/741 (89%)	614 (93%)	40 (6%)	7 (1%)	14	46
1	J	667/741 (90%)	619 (93%)	42 (6%)	6 (1%)	17	51
All	All	2719/2964 (92%)	2524 (93%)	166 (6%)	29 (1%)	14	46

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	ASP
1	B	476	ASP
1	G	476	ASP
1	J	476	ASP
1	A	479	SER
1	A	612	ARG
1	B	479	SER
1	B	612	ARG
1	G	479	SER
1	G	612	ARG
1	J	479	SER
1	J	612	ARG
1	A	563	ARG
1	B	563	ARG
1	G	563	ARG
1	J	563	ARG
1	A	475	SER
1	A	611	LYS
1	A	435	TYR
1	B	435	TYR
1	B	611	LYS
1	G	435	TYR

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Mol	Chain	Res	Type
1	G	611	LYS
1	J	611	LYS
1	A	473	PRO
1	B	473	PRO
1	G	473	PRO
1	J	473	PRO
1	A	1398	GLU

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	385/637 (60%)	355 (92%)	30 (8%)	12	40
1	B	356/637 (56%)	328 (92%)	28 (8%)	12	40
1	G	290/637 (46%)	271 (93%)	19 (7%)	16	47
1	J	282/637 (44%)	260 (92%)	22 (8%)	12	40
All	All	1313/2548 (52%)	1214 (92%)	99 (8%)	13	42

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	LEU
1	A	431	ARG
1	A	481	LEU
1	A	501	THR
1	A	510	HIS
1	A	563	ARG
1	A	575	LEU
1	A	585	ARG
1	A	606	MET
1	A	1029	ARG
1	A	1051	GLU
1	A	1065	ARG
1	A	1066	THR
1	A	1075	HIS

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Mol	Chain	Res	Type
1	A	1099	LEU
1	A	1136	LEU
1	A	1195	LEU
1	A	1222	ILE
1	A	1238	SER
1	A	1308	MET
1	A	1354	ARG
1	A	1361	ARG
1	A	1366	LEU
1	A	1372	ARG
1	A	1385	ASN
1	A	1386	ILE
1	A	1434	ARG
1	A	1451	LEU
1	A	1474	ASP
1	A	1481	HIS
1	B	402	LEU
1	B	431	ARG
1	B	501	THR
1	B	510	HIS
1	B	512	ARG
1	B	563	ARG
1	B	575	LEU
1	B	606	MET
1	B	1029	ARG
1	B	1051	GLU
1	B	1065	ARG
1	B	1066	THR
1	B	1075	HIS
1	B	1099	LEU
1	B	1136	LEU
1	B	1195	LEU
1	B	1222	ILE
1	B	1238	SER
1	B	1308	MET
1	B	1354	ARG
1	B	1361	ARG
1	B	1366	LEU
1	B	1372	ARG
1	B	1385	ASN
1	B	1434	ARG
1	B	1451	LEU

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Mol	Chain	Res	Type
1	B	1474	ASP
1	B	1481	HIS
1	G	431	ARG
1	G	510	HIS
1	G	575	LEU
1	G	606	MET
1	G	1029	ARG
1	G	1065	ARG
1	G	1066	THR
1	G	1075	HIS
1	G	1099	LEU
1	G	1136	LEU
1	G	1195	LEU
1	G	1222	ILE
1	G	1354	ARG
1	G	1361	ARG
1	G	1366	LEU
1	G	1372	ARG
1	G	1434	ARG
1	G	1451	LEU
1	G	1481	HIS
1	J	431	ARG
1	J	501	THR
1	J	575	LEU
1	J	585	ARG
1	J	1029	ARG
1	J	1051	GLU
1	J	1066	THR
1	J	1075	HIS
1	J	1099	LEU
1	J	1136	LEU
1	J	1195	LEU
1	J	1308	MET
1	J	1354	ARG
1	J	1361	ARG
1	J	1366	LEU
1	J	1372	ARG
1	J	1385	ASN
1	J	1386	ILE
1	J	1434	ARG
1	J	1451	LEU
1	J	1474	ASP

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Mol	Chain	Res	Type
1	J	1481	HIS

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	LFX	I	100	4	21,29,29	1.01	2 (9%)	25,44,44	1.14	2 (8%)
5	LFX	L	103	4	21,29,29	1.01	2 (9%)	25,44,44	1.36	4 (16%)
5	LFX	F	100	4	21,29,29	0.97	2 (9%)	25,44,44	1.12	1 (4%)
5	LFX	D	100	4	21,29,29	1.03	2 (9%)	25,44,44	1.16	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
5	LFX	I	100	4	-	0/4/27/27	0/3/4/4
5	LFX	L	103	4	-	0/4/27/27	0/3/4/4
5	LFX	F	100	4	-	0/4/27/27	0/3/4/4
5	LFX	D	100	4	-	1/4/27/27	0/3/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	100	LFX	C17-C	3.39	1.50	1.47
5	D	100	LFX	C17-C	3.35	1.50	1.47
5	L	103	LFX	C17-C	3.34	1.50	1.47
5	F	100	LFX	C17-C	3.14	1.50	1.47
5	D	100	LFX	O02-C15	2.31	1.27	1.23
5	L	103	LFX	O02-C15	2.26	1.27	1.23
5	I	100	LFX	O02-C15	2.25	1.27	1.23
5	F	100	LFX	O02-C15	2.22	1.27	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	103	LFX	C02-C08-N	2.55	113.69	110.80
5	L	103	LFX	C08-N-C07	2.51	113.03	109.52
5	I	100	LFX	C02-N01-C01	2.28	116.55	111.52
5	F	100	LFX	C02-N01-C01	2.27	116.52	111.52
5	I	100	LFX	C12-C17-C15	-2.18	118.87	119.97
5	L	103	LFX	C01-C07-N	2.08	113.15	110.80
5	L	103	LFX	C02-N01-C01	2.02	115.97	111.52

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	100	LFX	C06-C04-N01-C02

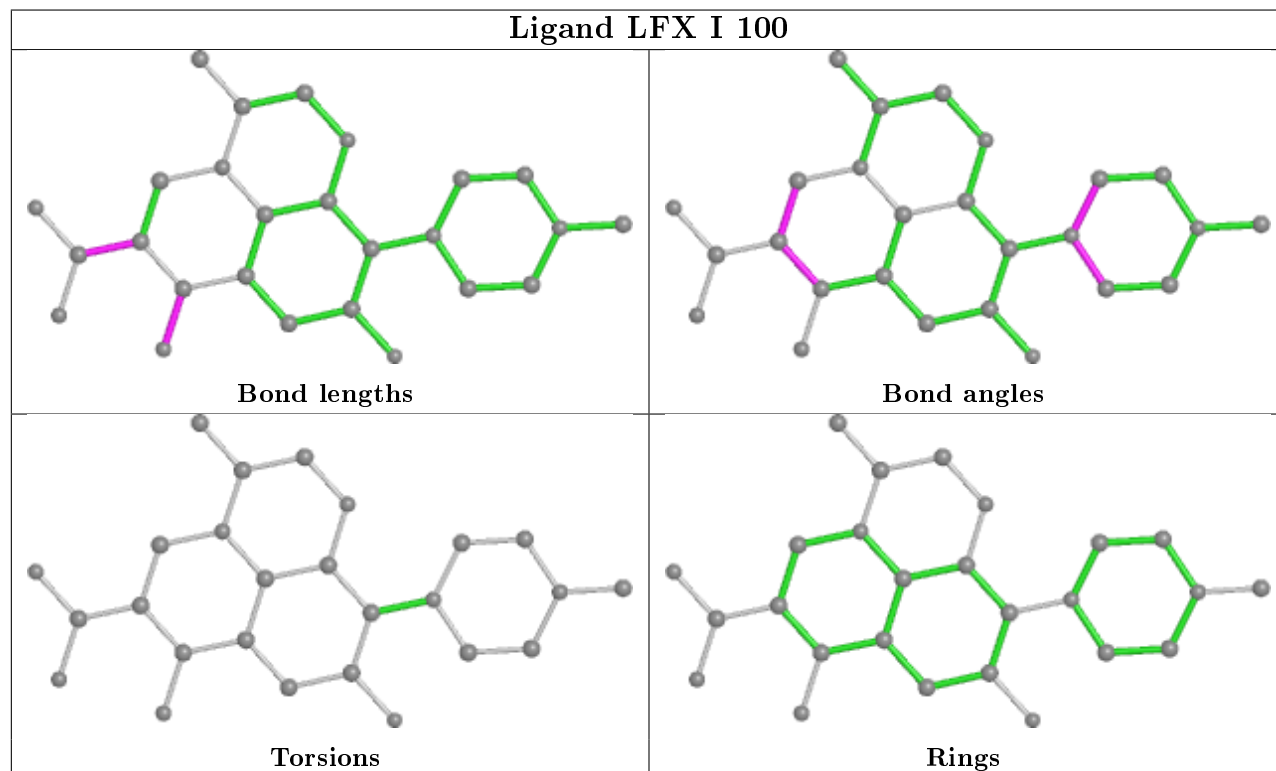
There are no ring outliers.

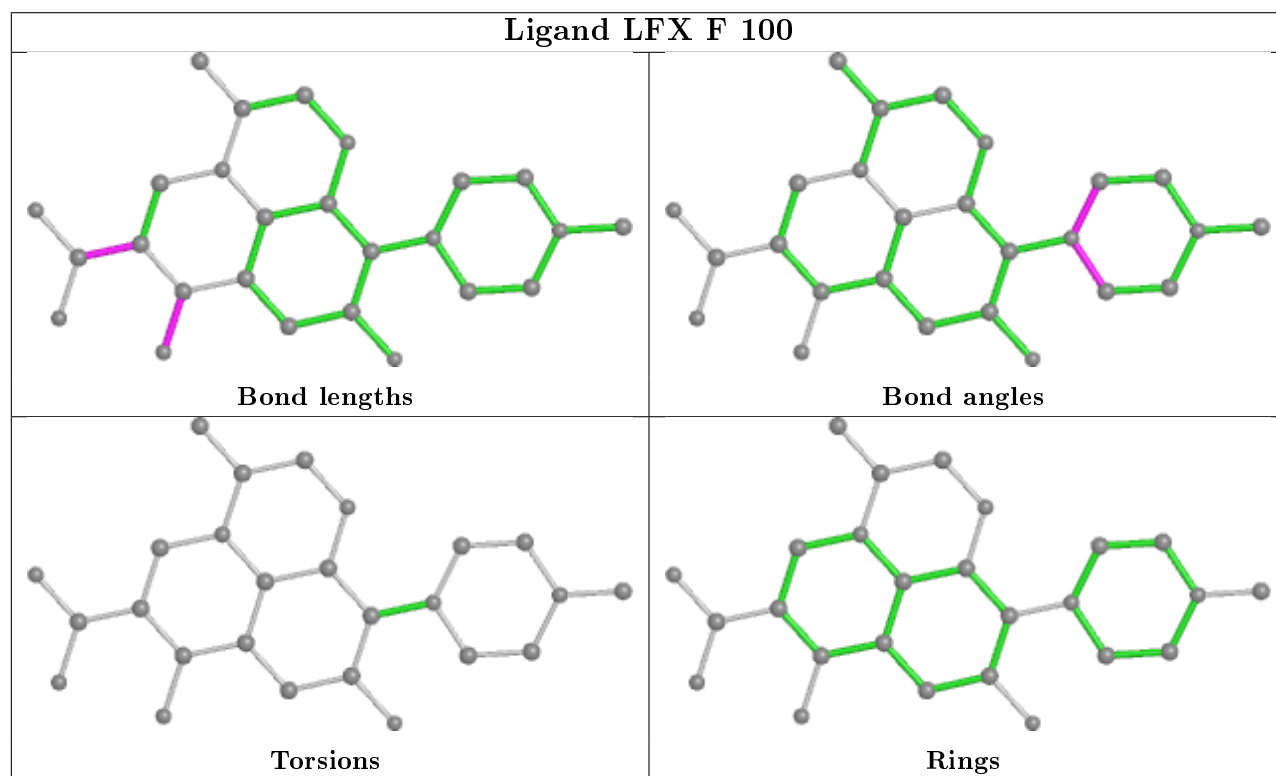
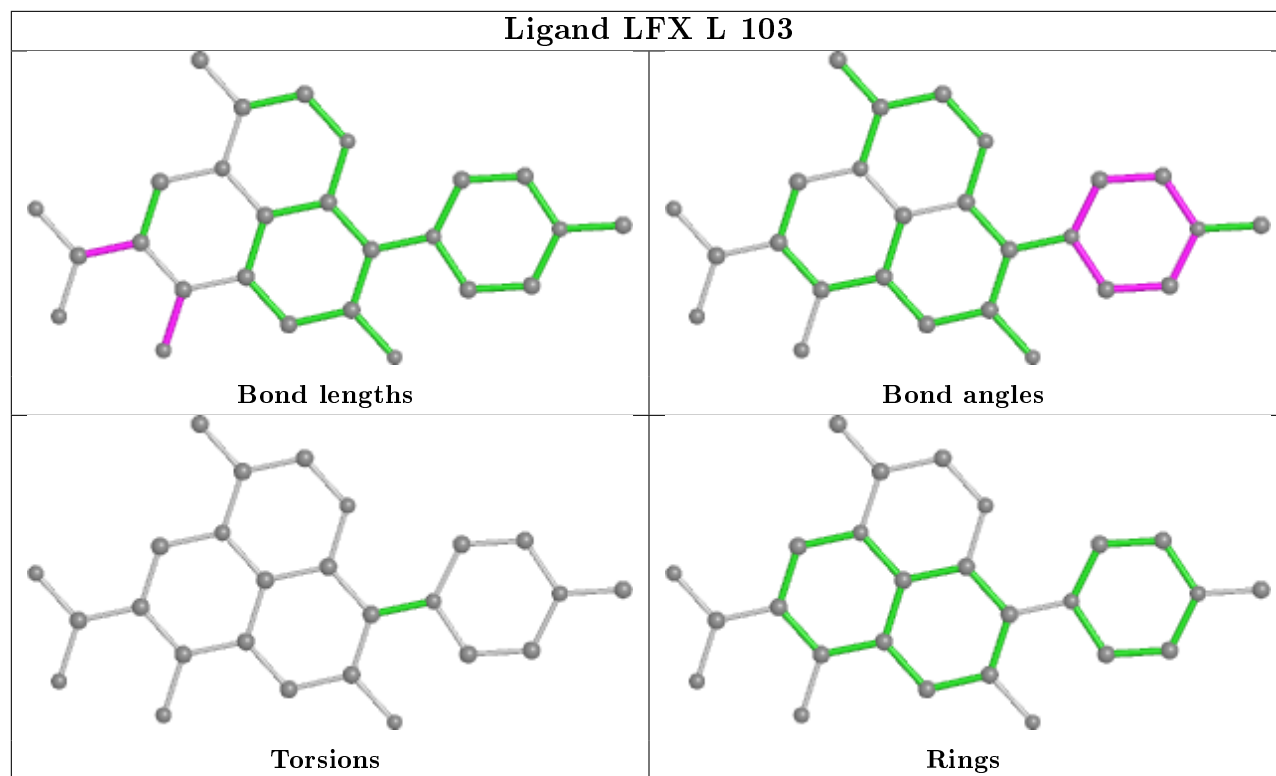
1 monomer is involved in 2 short contacts:

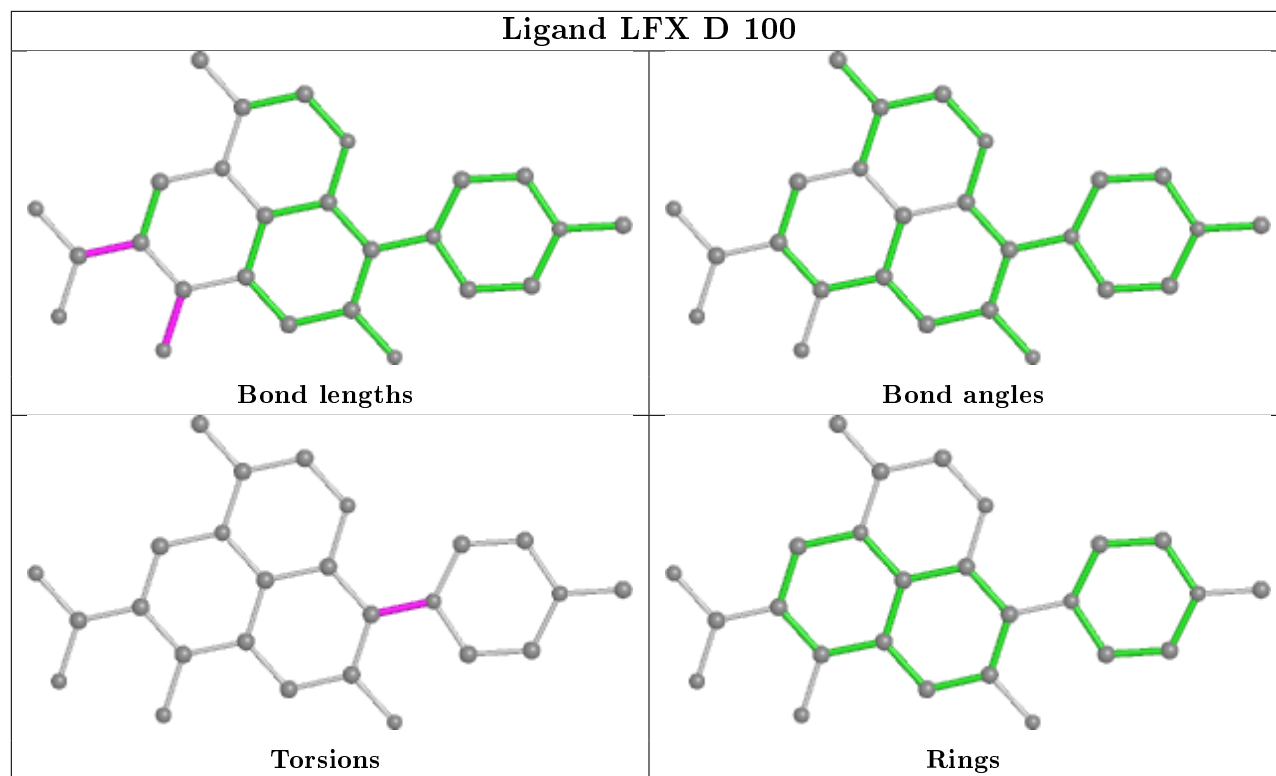
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	100	LFX	2	0

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 [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	702/741 (94%)	-0.33	0 100 100	23, 46, 76, 119	0
1	B	701/741 (94%)	-0.23	0 100 100	28, 52, 89, 138	0
1	G	671/741 (90%)	-0.25	5 (0%) 87 91	26, 61, 106, 140	0
1	J	679/741 (91%)	-0.15	3 (0%) 92 94	26, 65, 121, 152	0
2	C	8/8 (100%)	-0.10	0 100 100	37, 47, 96, 106	0
2	E	8/8 (100%)	-0.15	0 100 100	36, 43, 70, 74	0
2	H	8/8 (100%)	-0.43	0 100 100	47, 59, 96, 108	0
2	K	8/8 (100%)	-0.55	0 100 100	51, 63, 102, 102	0
3	D	12/12 (100%)	-0.16	0 100 100	43, 58, 75, 95	0
3	F	12/12 (100%)	-0.22	0 100 100	37, 52, 68, 91	0
3	I	12/12 (100%)	-0.49	0 100 100	54, 64, 81, 108	0
3	L	12/12 (100%)	-0.35	0 100 100	59, 75, 91, 92	0
All	All	2833/3044 (93%)	-0.24	8 (0%) 94 95	23, 54, 104, 152	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	539	ALA	3.5
1	G	562	GLN	2.9
1	G	591	VAL	2.8
1	G	526	PRO	2.8
1	G	527	LEU	2.6
1	J	595	GLU	2.4
1	J	1302	ARG	2.3
1	J	435	TYR	2.3

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](#)

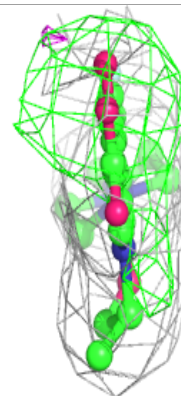
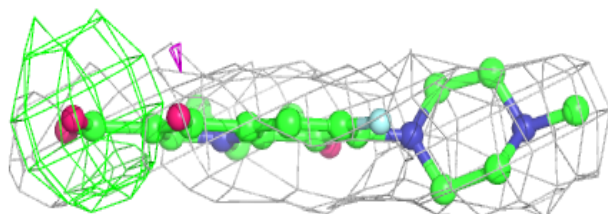
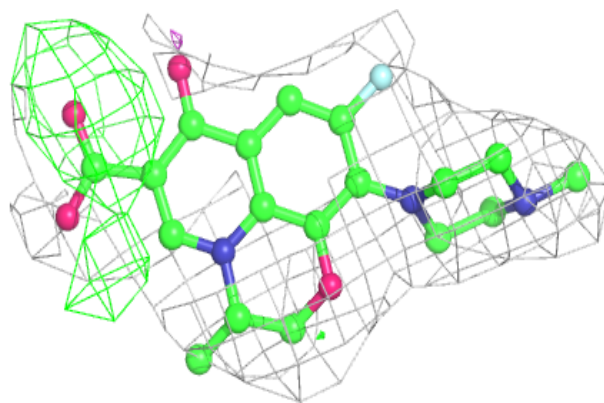
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	MG	J	1501	1/1	0.34	0.22	42,42,42,42	0
4	MG	A	1501	1/1	0.74	0.26	26,26,26,26	0
4	MG	G	1501	1/1	0.85	0.36	54,54,54,54	0
4	MG	B	1501	1/1	0.87	0.32	35,35,35,35	0
4	MG	A	1502	1/1	0.88	0.44	52,52,52,52	0
5	LFX	F	100	26/26	0.89	0.24	27,51,68,73	0
5	LFX	L	103	26/26	0.89	0.24	46,61,70,73	0
5	LFX	D	100	26/26	0.90	0.21	45,69,75,78	0
5	LFX	I	100	26/26	0.92	0.20	40,61,66,69	0
4	MG	G	1502	1/1	0.94	0.29	44,44,44,44	0
4	MG	L	101	1/1	0.95	0.31	36,36,36,36	0
4	MG	L	102	1/1	0.95	0.28	48,48,48,48	0

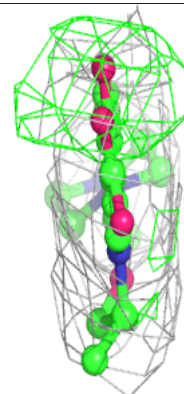
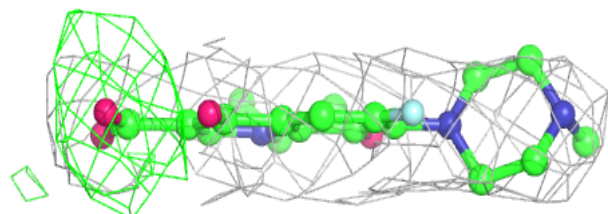
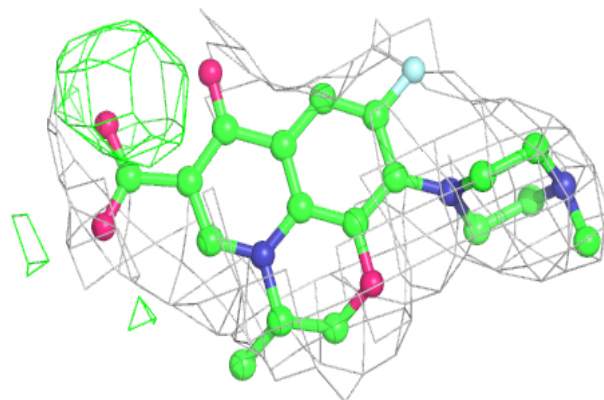
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around LFX F 100:

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

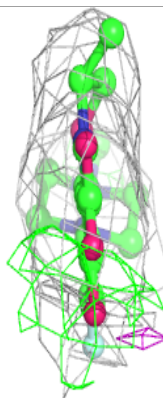
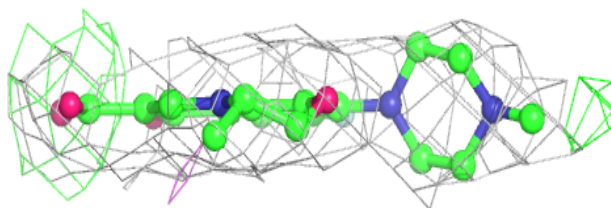
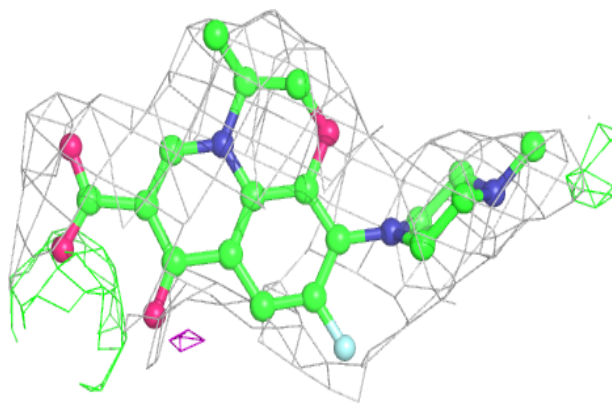
**Electron density around LFX L 103:**

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

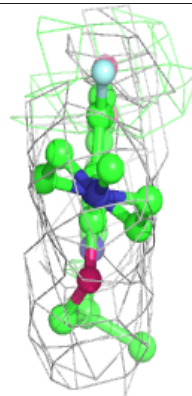
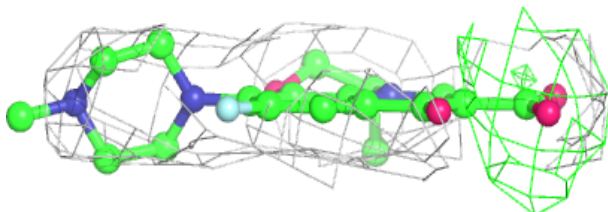
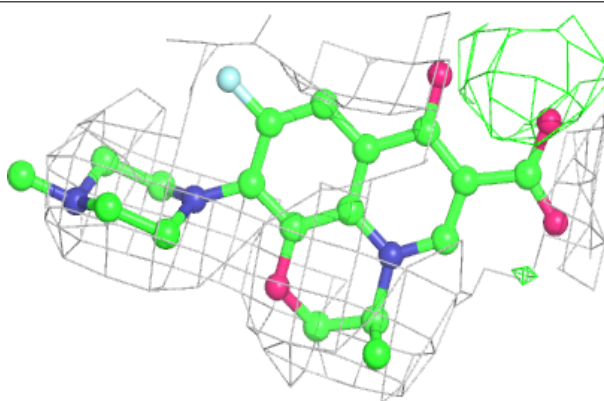


Electron density around LFX D 100:

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

**Electron density around LFX I 100:**

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



6.5 Other polymers

There are no such residues in this entry.