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wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2024 – 10:47 PM EDT

PDB ID	:	3RAD
Title	:	Quinolone(Clinafloxacin)-DNA cleavage complex of type IV topoisomerase from S. pneumoniae
Authors	:	Laponogov, I.; Pan, X.-S.; Veselkov, D.A.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on	:	2011-03-28
Resolution	:	3.35 Å(reported)

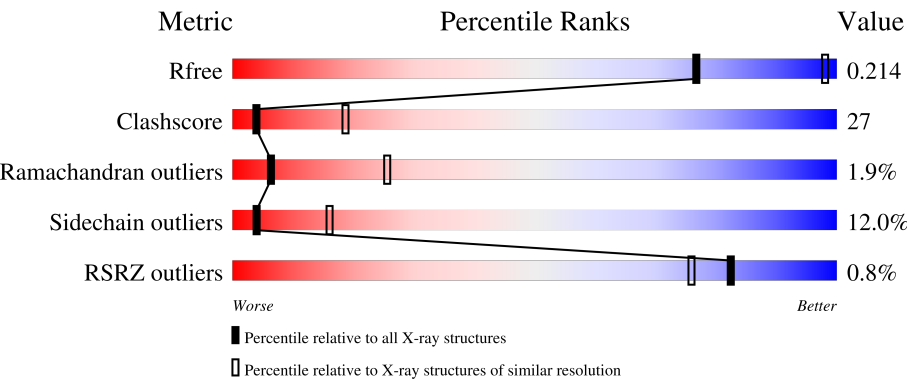The following versions of software and data (see references (i)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.
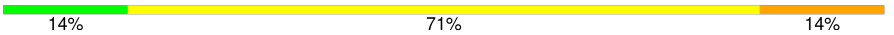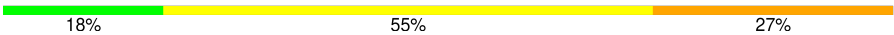
Metric	Percentile Ranks	Value
Rfree		0.214
Clashscore		27
Ramachandran outliers		1.9%
Sidechain outliers		12.0%
RSRZ outliers		0.8%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1012 (3.40-3.32)
Clashscore	180529	1035 (3.40-3.32)
Ramachandran outliers	177936	1037 (3.40-3.32)
Sidechain outliers	177891	1037 (3.40-3.32)
RSRZ outliers	164620	1012 (3.40-3.32)

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	496	57% 34% 6% •
1	B	496	% 50% 40% 7% •
2	C	268	% 47% 26% • 22%
2	D	268	2% 54% 20% • 22%

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Mol	Chain	Length	Quality of chain
3	E	7	86% 14%
4	F	11	9% 45% 45%
5	G	7	14% 71% 14%
6	H	11	18% 55% 27%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 11096 atoms, of which 32 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 A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3702	2343	640	706	13			
1	B	482	Total	C	N	O	S	0	0	0
			3696	2345	635	703	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	SEE REMARK 999	UNP P72525
A	489	LEU	-	expression tag	UNP P72525
A	490	GLU	-	expression tag	UNP P72525
A	491	HIS	-	expression tag	UNP P72525
A	492	HIS	-	expression tag	UNP P72525
A	493	HIS	-	expression tag	UNP P72525
A	494	HIS	-	expression tag	UNP P72525
A	495	HIS	-	expression tag	UNP P72525
A	496	HIS	-	expression tag	UNP P72525
B	257	THR	ILE	SEE REMARK 999	UNP P72525
B	489	LEU	-	expression tag	UNP P72525
B	490	GLU	-	expression tag	UNP P72525
B	491	HIS	-	expression tag	UNP P72525
B	492	HIS	-	expression tag	UNP P72525
B	493	HIS	-	expression tag	UNP P72525
B	494	HIS	-	expression tag	UNP P72525
B	495	HIS	-	expression tag	UNP P72525
B	496	HIS	-	expression tag	UNP P72525

- Molecule 2 is a protein called DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	209	Total	C	N	O	S	0	0	0
			1429	905	252	266	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	D	208	1417	898	247	267	5	0	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	expression tag	UNP Q59961
C	381	GLY	-	expression tag	UNP Q59961
C	382	HIS	-	expression tag	UNP Q59961
C	383	HIS	-	expression tag	UNP Q59961
C	384	HIS	-	expression tag	UNP Q59961
C	385	HIS	-	expression tag	UNP Q59961
C	386	HIS	-	expression tag	UNP Q59961
C	387	HIS	-	expression tag	UNP Q59961
C	388	HIS	-	expression tag	UNP Q59961
C	389	HIS	-	expression tag	UNP Q59961
C	390	HIS	-	expression tag	UNP Q59961
C	391	HIS	-	expression tag	UNP Q59961
C	392	SER	-	expression tag	UNP Q59961
C	393	SER	-	expression tag	UNP Q59961
C	394	GLY	-	expression tag	UNP Q59961
C	395	HIS	-	expression tag	UNP Q59961
C	396	ILE	-	expression tag	UNP Q59961
C	397	ASP	-	expression tag	UNP Q59961
C	398	ASP	-	expression tag	UNP Q59961
C	399	ASP	-	expression tag	UNP Q59961
C	400	ASP	-	expression tag	UNP Q59961
C	401	LYS	-	expression tag	UNP Q59961
C	402	HIS	-	expression tag	UNP Q59961
C	403	MET	-	expression tag	UNP Q59961
C	460	ILE	VAL	SEE REMARK 999	UNP Q59961
C	644	ALA	THR	SEE REMARK 999	UNP Q59961
D	380	MET	-	expression tag	UNP Q59961
D	381	GLY	-	expression tag	UNP Q59961
D	382	HIS	-	expression tag	UNP Q59961
D	383	HIS	-	expression tag	UNP Q59961
D	384	HIS	-	expression tag	UNP Q59961
D	385	HIS	-	expression tag	UNP Q59961
D	386	HIS	-	expression tag	UNP Q59961
D	387	HIS	-	expression tag	UNP Q59961
D	388	HIS	-	expression tag	UNP Q59961
D	389	HIS	-	expression tag	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
D	390	HIS	-	expression tag	UNP Q59961
D	391	HIS	-	expression tag	UNP Q59961
D	392	SER	-	expression tag	UNP Q59961
D	393	SER	-	expression tag	UNP Q59961
D	394	GLY	-	expression tag	UNP Q59961
D	395	HIS	-	expression tag	UNP Q59961
D	396	ILE	-	expression tag	UNP Q59961
D	397	ASP	-	expression tag	UNP Q59961
D	398	ASP	-	expression tag	UNP Q59961
D	399	ASP	-	expression tag	UNP Q59961
D	400	ASP	-	expression tag	UNP Q59961
D	401	LYS	-	expression tag	UNP Q59961
D	402	HIS	-	expression tag	UNP Q59961
D	403	MET	-	expression tag	UNP Q59961
D	460	ILE	VAL	SEE REMARK 999	UNP Q59961
D	644	ALA	THR	SEE REMARK 999	UNP Q59961

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

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

- Molecule 4 is a DNA chain called 5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*G)-3'.

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

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

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

- Molecule 6 is a DNA chain called 5'-D(P*GP*AP*CP*TP*AP*TP*GP*CP*AP*CP*G)-3'.

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	Mg 2	0	0
7	B	2	Total 2	Mg 2	0	0
7	C	1	Total 1	Mg 1	0	0
7	D	1	Total 1	Mg 1	0	0

- Molecule 8 is 7-[(3R)-3-aminopyrrolidin-1-yl]-8-chloro-1-cyclopropyl-6-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid (three-letter code: NFX) (formula: $C_{17}H_{17}ClFN_3O_3$).
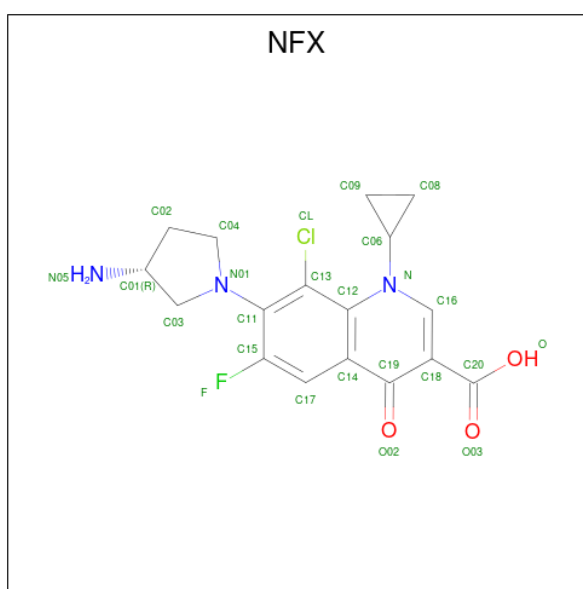
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	F	1	Total 41	C 17	Cl 1	F 1	H 16	N 3	O 3	0	0
8	H	1	Total 41	C 17	Cl 1	F 1	H 16	N 3	O 3	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	18	Total 18	O 18	0	0
9	B	11	Total 11	O 11	0	0
9	C	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	2	Total 2	O 2	0	0
9	G	1	Total 1	O 1	0	0

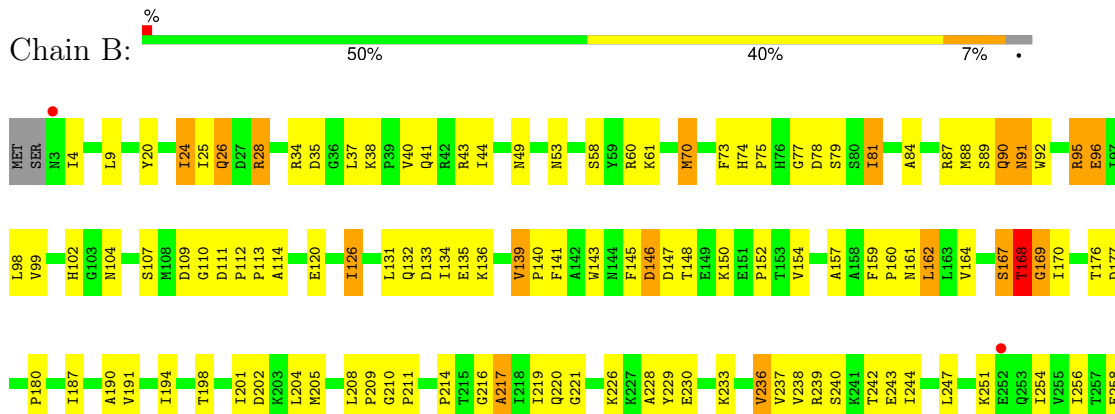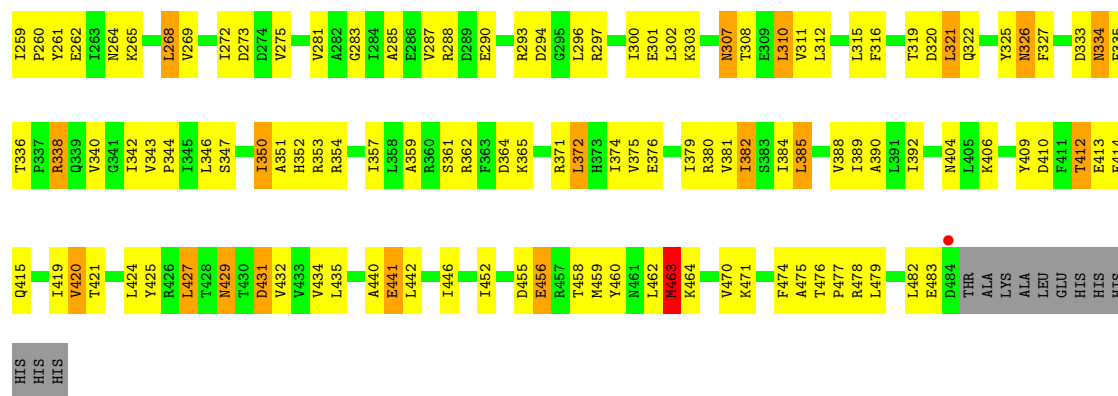# 3 Residue-property plots ⓘ

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.

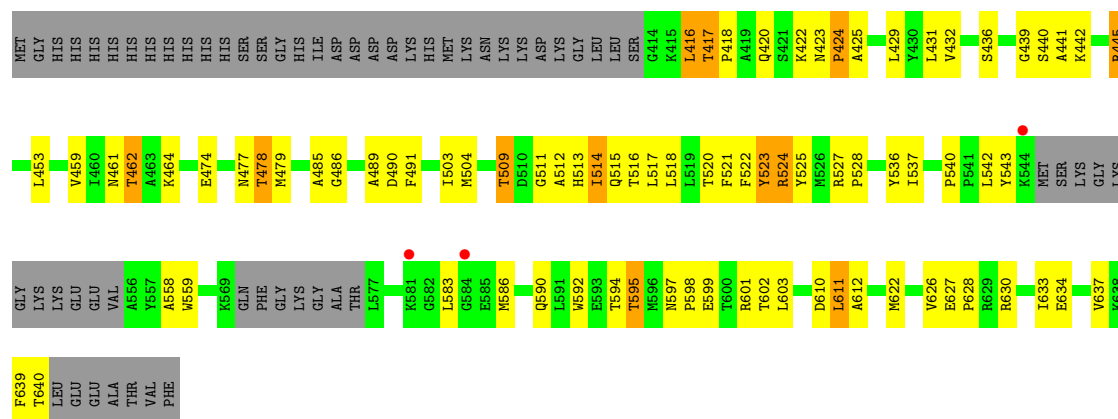• Molecule 1: DNA topoisomerase 4 subunit A
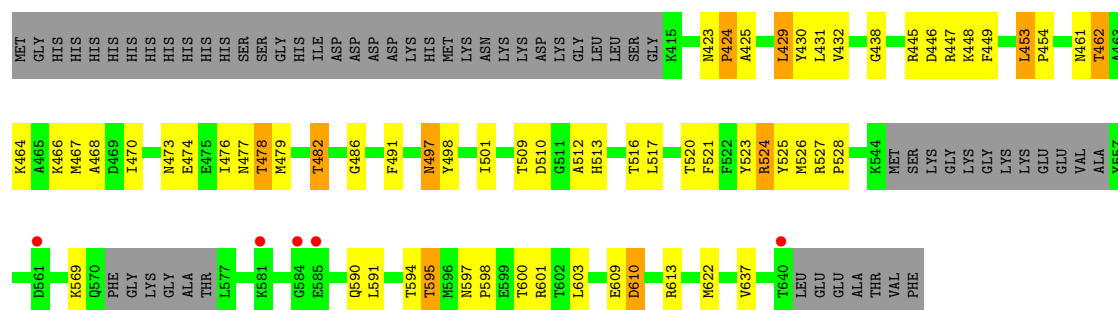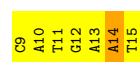
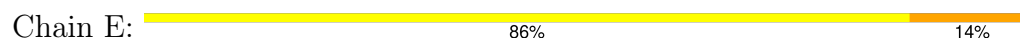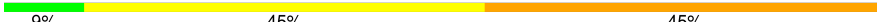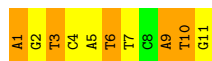Chain A:

• Molecule 1: DNA topoisomerase 4 subunit A

Chain B:

I259 P260 Y261 E262 I263 N264 K265 L268 V269 I272 D273 D274 V275 V281 A282 G283 I284 A285 E286 V287 R288 D289 E290 R293 D294 G295 L296 R297 I300 E301 L302 K303 N307 T308 E309 L310 V311 L312 L315 F316 T319 D320 L321 Q322 Y325 N326 F327 D333 N334 F335

T336 P337 R338 Q339 V340 G341 I342 V343 P344 L346 I345 S347 I350 A351 H352 R353 R354 I357 L358 A359 R360 S361 R362 F363 D364 K365 R371 L372 H373 I374 V375 E376 I379 R380 I382 V381 S383 I384 L385 V388 I389 A390 L391 I392 N404 L405 K406 Y409 D410 F411 T412 E413 E414

Q415 I419 V420 T421 L424 Y425 R426 L427 T428 N429 T430 D431 V432 V433 V434 L435 A440 E441 L442 I446 I452 D455 E456 R457 T458 M459 Y460 N461 L462 M463 K464 V470 K471 F474 A475 T476 P477 R478 L479 L482 E483 D484 THR ALA ALA LEU HIS HIS HIS

HIS HIS HIS

• Molecule 2: DNA topoisomerase 4 subunit B

Chain C:

%

47%　　　　26%　•　22%

MET GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY ILE ASP ASP ASP ASP LYS HIS HIS MET LYS ASN LYS LYS ASP LYS GLY LEU LEU SER G414 K415 L416 T417 P418 A419 Q420 S421 K422 N423 P424 A425 L429 Y430 L431 V432 S436 G439 S440 A441 K442 R445

L453 V459 I460 N461 T462 A463 K464 E474 N477 T478 M479 A485 G486 A489 D490 F491 I503 M504 T509 D510 G511 A512 H513 I514 Q515 T516 L517 L518 L519 T520 F521 F522 Y523 R524 Y525 M526 R527 P528 Y536 I537 P540 P541 L542 Y543 K544 MET SER LYS GLY LYS

GLY LYS LYS GLU VAL A556 Y557 A558 W559 K569 GLN PHE GLY LYS GLY ALA THR L577 K581 G582 L583 G584 E585 M586 Q590 L591 W592 E593 T594 T595 M596 N597 P598 E599 T600 R601 T602 L603 D610 L611 A612 M622 V626 E627 P628 R629 R630 I633 E634 V637 K638

F639 T640 LEU GLU GLU ALA THR VAL PHE

• Molecule 2: DNA topoisomerase 4 subunit B

Chain D:

2%

54%　　　　20%　•　22%

MET GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY ILE ASP ASP ASP ASP LYS HIS HIS MET LYS ASN LYS LYS ASP LYS GLY LEU LEU SER GLY K415 N423 P424 A425 L429 Y430 L431 V432 G438 R445 D446 R447 K448 F449 L453 P454 N461 T462 A463

K464 A465 K466 M467 A468 D469 I470 N473 E474 E475 I476 N477 T478 M479 T482 G486 F491 N497 V498 I501 T509 D510 G511 A512 H513 T516 L517 T520 F521 F522 Y523 R524 Y525 M526 R527 P528 K544 MET SER LYS GLY LYS GLY LYS LYS GLU GLU VAL ALA Y557

D561 K569 Q570 PHE GLY LYS GLY ALA THR L577 K581 G584 E585 Q590 L591 T594 T595 M596 N597 P598 E599 T600 R601 T602 L603 E609 D610 R613 M622 V637 T640 LEU GLU GLU ALA THR VAL PHE

• Molecule 3: 5'-D(*CP*AP*TP*GP*AP*AP*T)-3'

Chain E:

86%　　　　14%

C9 A10 T11 G12 A13 A14 T15

• Molecule 4: 5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*G)-3'

Chain F:

9%   45%   45%

A1 G2 T3 C4 A5 T6 T7 C8 A9 T10 G11

• Molecule 5: 5'-D(*CP*GP*TP*GP*CP*AP*T)-3'

Chain G:

14%   71%   14%

C9 G10 T11 G12 C13 A14 T15

• Molecule 6: 5'-D(P*GP*AP*CP*TP*AP*TP*GP*CP*AP*CP*G)-3'

Chain H:

18%   55%   27%

G1 A2 C3 T4 A5 T6 G7 C8 A9 C10 G11

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	157.13Å 157.13Å 211.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.67 – 3.35 41.67 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.67-3.35) 99.3 (41.67-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.177 , 0.228 0.167 , 0.214	Depositor DCC
R_{free} test set	4351 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	77.9	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 63.3	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11096	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NFX

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	0.44	0/3763	0.66	1/5104 (0.0%)
1	B	0.44	0/3757	0.64	0/5098
2	C	0.34	0/1455	0.54	0/1991
2	D	0.33	0/1443	0.53	0/1976
3	E	0.76	0/157	1.83	7/241 (2.9%)
4	F	0.89	0/251	2.02	14/385 (3.6%)
5	G	0.84	0/155	1.96	7/238 (2.9%)
6	H	0.77	0/253	1.80	10/388 (2.6%)
All	All	0.46	0/11234	0.80	39/15421 (0.3%)

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	14	DA	O4'-C4'-C3'	-13.34	98.00	106.00
4	F	9	DA	O4'-C4'-C3'	-11.62	99.03	106.00
6	H	10	DC	O4'-C4'-C3'	-10.87	99.48	106.00
4	F	10	DT	O4'-C4'-C3'	-9.86	100.09	106.00
4	F	3	DT	O4'-C4'-C3'	-9.75	100.15	106.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3702	0	3579	201	0
1	B	3696	0	3589	222	0
2	C	1429	0	1193	80	0
2	D	1417	0	1167	61	0
3	E	140	0	78	6	0
4	F	225	0	126	9	0
5	G	139	0	78	3	0
6	H	226	0	124	7	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	F	25	16	16	4	0
8	H	25	16	16	4	0
9	A	18	0	0	0	0
9	B	11	0	0	1	0
9	C	2	0	0	0	0
9	E	2	0	0	0	0
9	G	1	0	0	0	0
All	All	11064	32	9966	577	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 27.

The worst 5 of 577 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ASP:HB3	1:B:148:THR:HG23	1.27	1.15
1:B:70:MET:HE1	1:B:78:ASP:HB3	1.19	1.11
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.18	1.09
1:B:307:ASN:ND2	1:B:310:LEU:HB2	1.69	1.07
1:A:60:ARG:HH11	1:A:60:ARG:HB2	1.18	1.07

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	480/496 (97%)	432 (90%)	40 (8%)	8 (2%)	7	27
1	B	480/496 (97%)	414 (86%)	57 (12%)	9 (2%)	6	25
2	C	203/268 (76%)	175 (86%)	23 (11%)	5 (2%)	4	21
2	D	202/268 (75%)	176 (87%)	22 (11%)	4 (2%)	6	25
All	All	1365/1528 (89%)	1197 (88%)	142 (10%)	26 (2%)	6	25

5 of 26 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PHE
1	B	168	THR
1	B	217	ALA
2	D	569	LYS
2	D	610	ASP

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	371/431 (86%)	332 (90%)	39 (10%)	5	21
1	B	372/431 (86%)	321 (86%)	51 (14%)	3	11
2	C	104/224 (46%)	91 (88%)	13 (12%)	3	14
2	D	102/224 (46%)	91 (89%)	11 (11%)	5	20
All	All	949/1310 (72%)	835 (88%)	114 (12%)	4	16

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	162	LEU
2	D	501	ILE
1	B	321	LEU

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Mol	Chain	Res	Type
2	D	497	ASN
2	C	514	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	ASN
2	C	477	ASN
1	B	267	ASN
2	D	497	ASN
2	C	420	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
8	NFX	F	101	7	28,28,28	1.21	3 (10%)	35,43,43	1.42	6 (17%)
8	NFX	H	101	7	28,28,28	1.22	3 (10%)	35,43,43	1.41	5 (14%)

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
8	NFX	F	101	7	-	4/12/23/23	0/4/4/4
8	NFX	H	101	7	-	5/12/23/23	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	101	NFX	C11-C13	2.52	1.43	1.40
8	F	101	NFX	C11-C13	2.51	1.43	1.40
8	H	101	NFX	C12-N	2.42	1.43	1.40
8	F	101	NFX	C12-N	2.40	1.43	1.40
8	F	101	NFX	C12-C13	2.19	1.43	1.40

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	F	101	NFX	C06-N-C16	-3.46	114.67	119.74
8	H	101	NFX	C06-N-C16	-3.46	114.67	119.74
8	F	101	NFX	C16-C18-C19	-3.01	117.73	119.94
8	H	101	NFX	C16-C18-C19	-3.00	117.74	119.94
8	F	101	NFX	C09-C06-N	2.68	123.11	118.87

There are no chirality outliers.
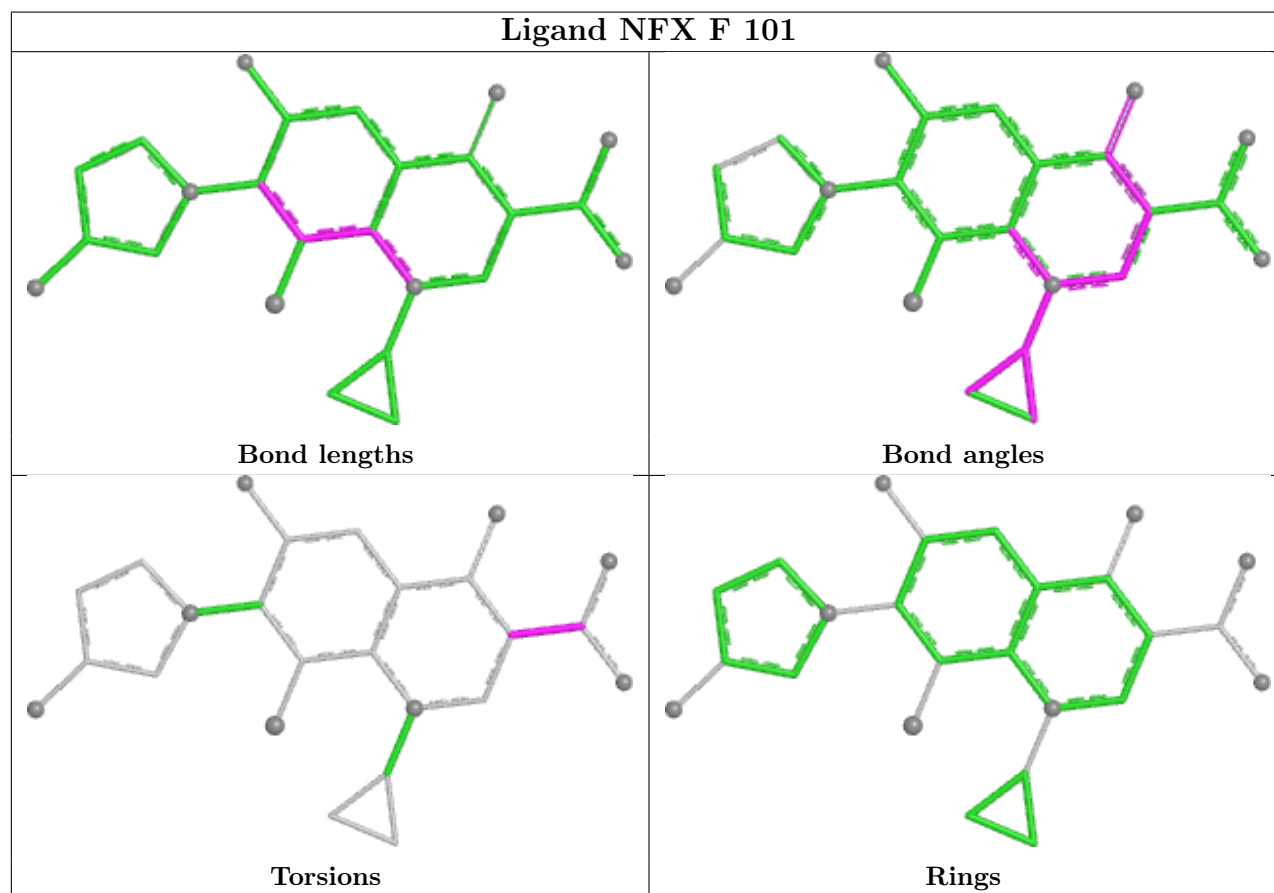
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	101	NFX	C19-C18-C20-O03
8	H	101	NFX	C19-C18-C20-O03
8	F	101	NFX	C19-C18-C20-O
8	H	101	NFX	C19-C18-C20-O
8	F	101	NFX	C16-C18-C20-O03

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	101	NFX	4	0
8	H	101	NFX	4	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 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 NFX F 101

Bond lengths

Bond angles

Torsions

Rings

Ligand NFX H 101

Bond lengths

Bond angles

Torsions

Rings
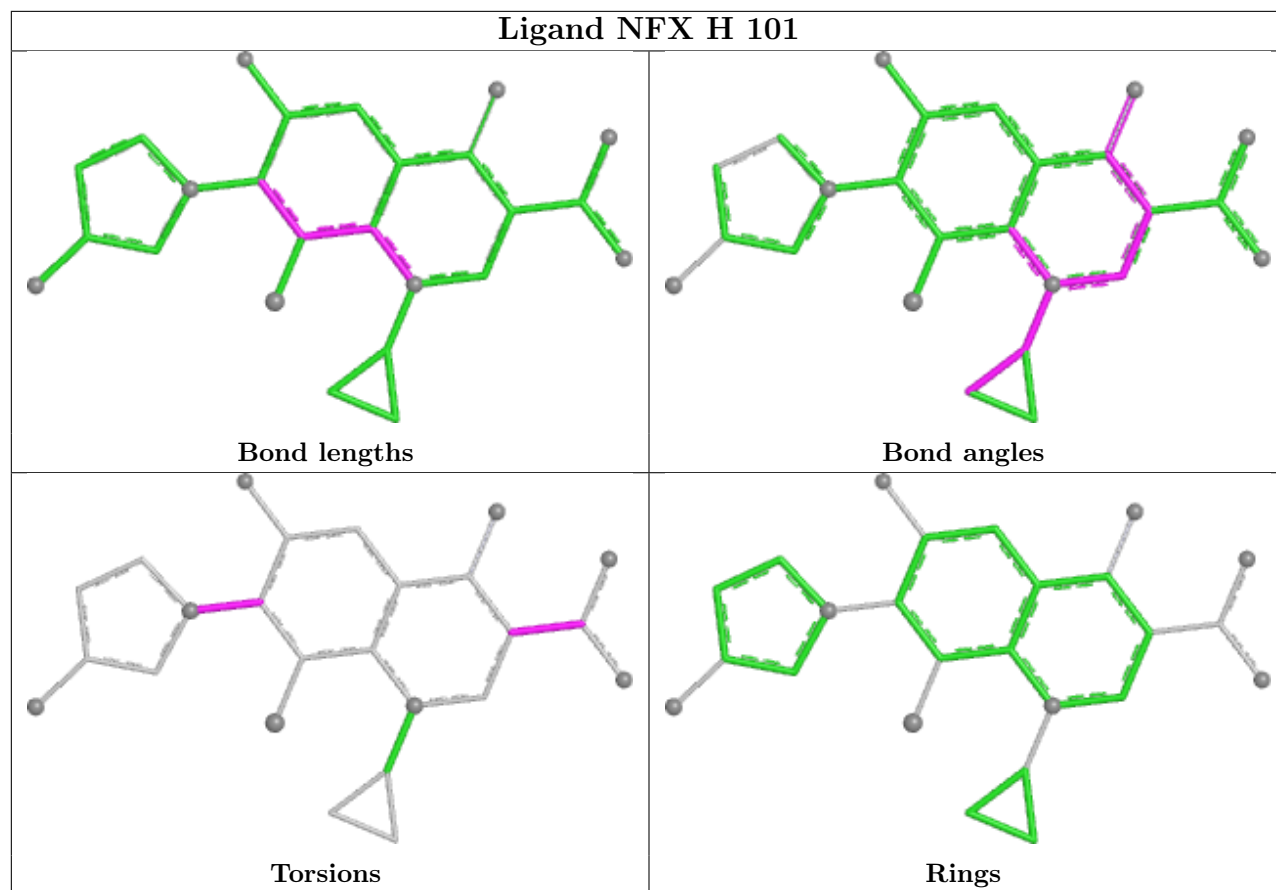
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	482/496 (97%)	-0.74	0	100	100	55, 80, 119, 141	0
1	B	482/496 (97%)	-0.63	3 (0%)	85	81	50, 79, 114, 146	0
2	C	209/268 (77%)	-0.13	3 (1%)	73	66	88, 119, 153, 173	0
2	D	208/268 (77%)	-0.07	5 (2%)	59	50	82, 119, 155, 174	0
3	E	7/7 (100%)	-0.29	0	100	100	86, 91, 128, 158	0
4	F	11/11 (100%)	-0.59	0	100	100	98, 113, 140, 158	0
5	G	7/7 (100%)	0.05	0	100	100	77, 87, 126, 149	0
6	H	11/11 (100%)	-0.84	0	100	100	90, 104, 130, 145	0
All	All	1417/1564 (90%)	-0.51	11 (0%)	82	76	50, 90, 140, 174	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	581	LYS	3.1
2	D	584	GLY	3.0
2	D	640	THR	2.5
1	B	3	ASN	2.5
1	B	252	GLU	2.3

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

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

6.3 Carbohydrates ⓘ

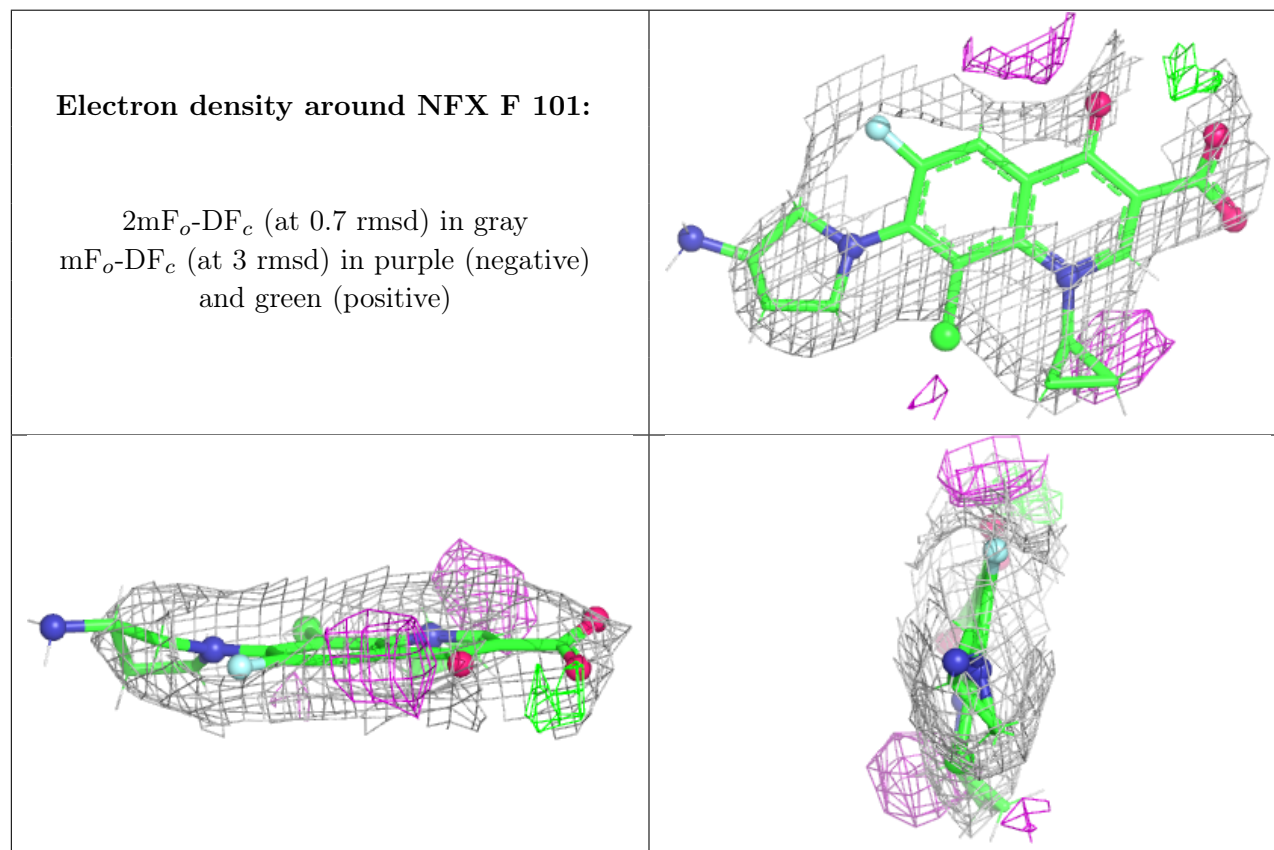There are no monosaccharides in this entry.
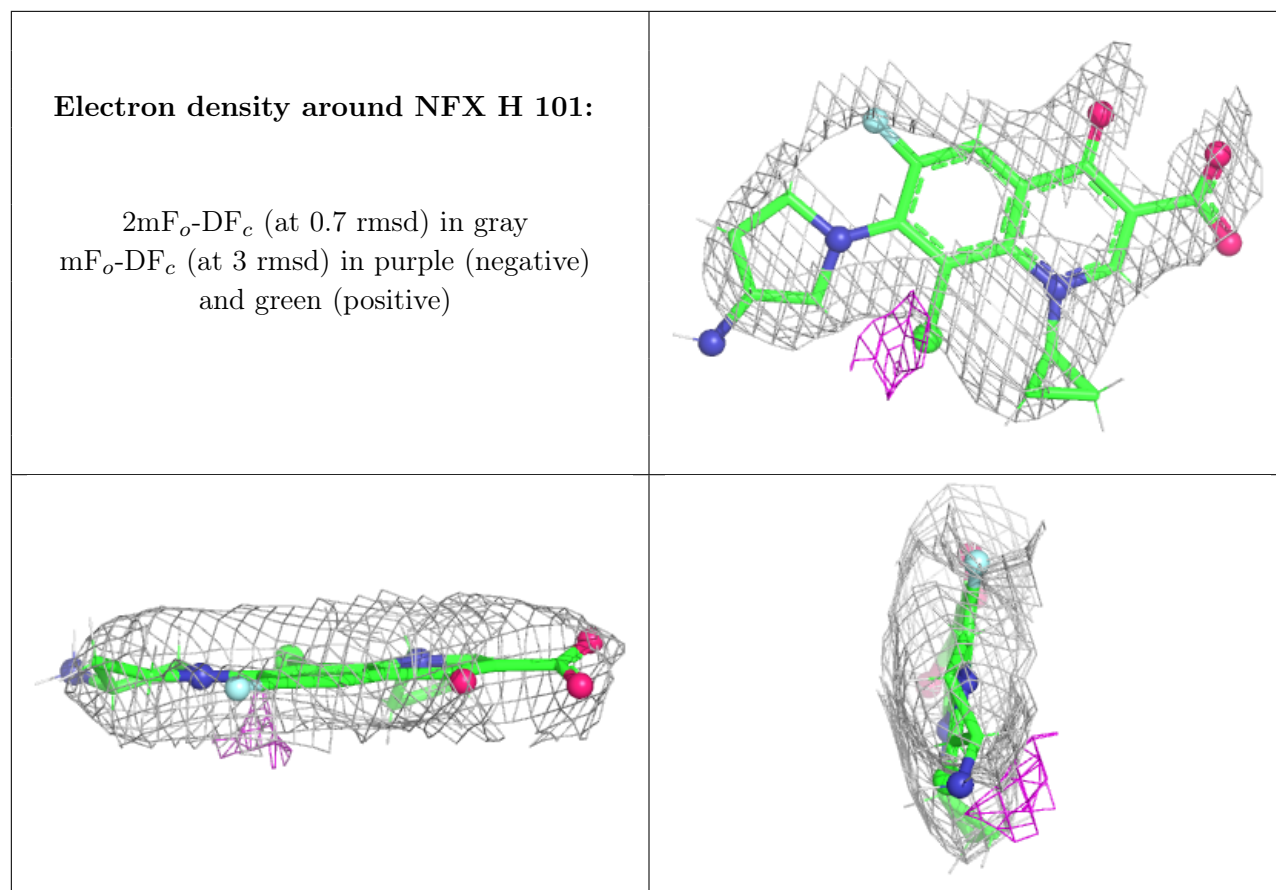
WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

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
7	MG	A	502	1/1	0.84	0.23	121,121,121,121	0
7	MG	C	701	1/1	0.86	0.22	87,87,87,87	0
7	MG	D	701	1/1	0.89	0.23	78,78,78,78	0
7	MG	B	501	1/1	0.90	0.07	101,101,101,101	0
7	MG	B	502	1/1	0.91	0.18	119,119,119,119	0
7	MG	A	501	1/1	0.93	0.06	87,87,87,87	0
8	NFX	F	101	25/25	0.93	0.12	120,135,161,235	0
8	NFX	H	101	25/25	0.94	0.10	118,143,190,200	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 NFX 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 NFX H 101:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.