wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 03:10 pm BST

PDB ID	:	2XCT
Title	:	The twinned 3.35A structure of S. aureus Gyrase complex with Ciprofloxacin and DNA
Authors	:	Bax, B.D.; Chan, P.; Eggleston, D.S.; Fosberry, A.; Gentry, D.R.; Gorrec, F.; Giordano, I.; Hann, M.M.; Hennessy, A.; Hibbs, M.; Huang, J.; Jones, E.; Jones, J.; Brown, K.K.; Lewis, C.J.; May, E.; Singh, O.; Spitzfaden, C.; Shen, C.; Shillings, A.; Theobald, A.; Wohlkonig, A.; Pearson, N.D.; Gwynn, M.N.
Deposited on	:	2010-04-25
Resolution	:	3.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

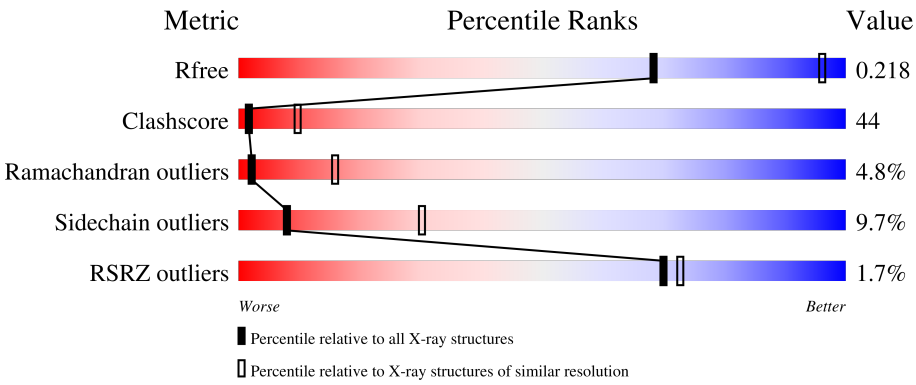
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 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	B	692	% 38% 52% 6% •
1	D	692	% 39% 50% 8% •
1	S	692	3% 33% 55% 9% •

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

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Mol	Chain	Length	Quality of chain
1	U	692	2% 37% 51% 9%
2	E	8	50% 38% 12%
2	V	8	12% 50% 25% 12%
3	F	8	12% 50% 25% 12%
3	W	8	12% 38% 25% 25%
4	G	12	58% 33% 8%
4	X	12	8% 25% 58% 8%
5	H	12	25% 75%
5	Y	12	25% 67% 8%

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
7	CPF	H	1020	-	-	X	-
7	CPF	X	1020	-	-	X	-
7	CPF	Y	1020	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 22370 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 GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	669	5262	3277	944	1015	26	0	2	0
1	D	669	5151	3212	913	1001	25	0	1	0
1	S	667	5199	3247	920	1007	25	0	0	1
1	U	665	5193	3239	926	1003	25	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	409	MET	-	expression tag	UNP P66937
B	544	THR	-	insertion	UNP P66937
B	545	GLY	-	insertion	UNP P66937
B	1123	PHE	TYR	engineered mutation	UNP Q99XG5
D	409	MET	-	expression tag	UNP P66937
D	544	THR	-	insertion	UNP P66937
D	545	GLY	-	insertion	UNP P66937
D	1123	PHE	TYR	engineered mutation	UNP Q99XG5
S	409	MET	-	expression tag	UNP P66937
S	544	THR	-	insertion	UNP P66937
S	545	GLY	-	insertion	UNP P66937
S	1123	PHE	TYR	engineered mutation	UNP Q99XG5
U	409	MET	-	expression tag	UNP P66937
U	544	THR	-	insertion	UNP P66937
U	545	GLY	-	insertion	UNP P66937
U	1123	PHE	TYR	engineered mutation	UNP Q99XG5

- Molecule 2 is a DNA chain called 5'-D(TP*GP*TP*GP*CP*GP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	7	147	69	27	44	7	0	0	0
2	V	7	147	69	27	44	7	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	F	7	145	68	28	42	7	0	0	0
3	W	6	123	58	23	36	6	0	0	0

- Molecule 4 is a DNA chain called 5'-D(GP*TP*AP*CP*CP*CP*AP*CP*GP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	G	11	220	105	42	63	10	0	0	0
4	X	11	220	105	42	63	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
5	H	12	240	115	47	67	11	0	0	0
5	Y	11	219	105	42	62	10	0	0	0

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
6	B	1	1	1	0	0
6	D	1	1	1	0	0
6	F	1	1	1	0	0
6	G	1	1	1	0	0

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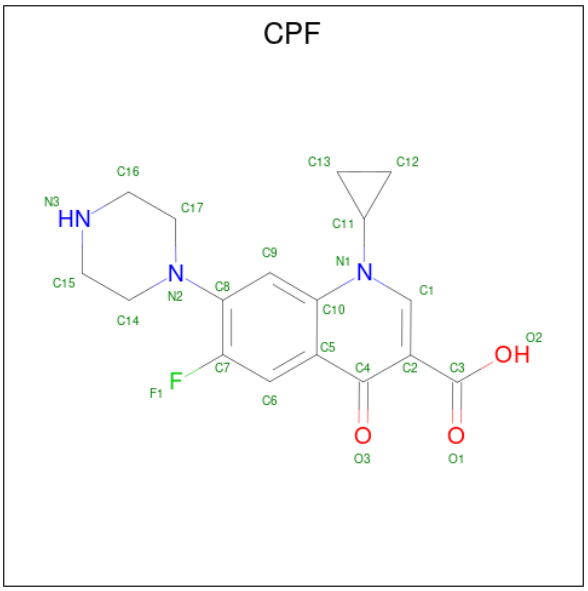
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
6	S	1	1	1	0	0
			Total	Mn		
6	U	1	1	1	0	0
			Total	Mn		
6	W	2	2	2	0	0

- Molecule 7 is 1-CYCLOPROPYL-6-FLUORO-4-OXO-7-PIPERAZIN-1-YL-1,4-DIHYDRO QUINOLINE-3-CARBOXYLIC ACID (three-letter code: CPF) (formula: $C_{17}H_{18}FN_3O_3$).



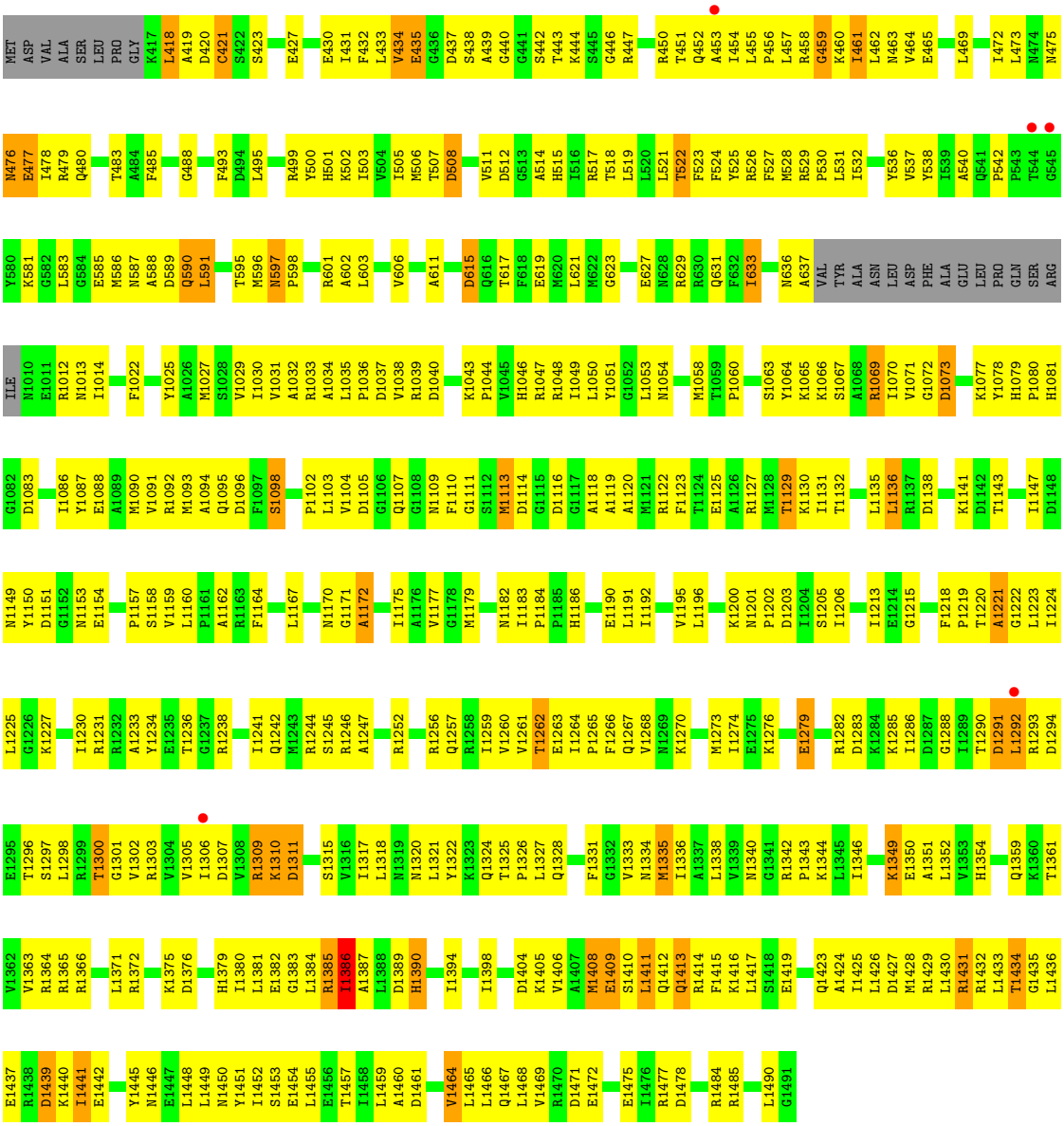
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
7	G	1	24	17	1	3	3	0	0
			Total	C	F	N	O		
7	H	1	24	17	1	3	3	0	0
			Total	C	F	N	O		
7	X	1	24	17	1	3	3	0	0
			Total	C	F	N	O		
7	Y	1	24	17	1	3	3	0	0

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.

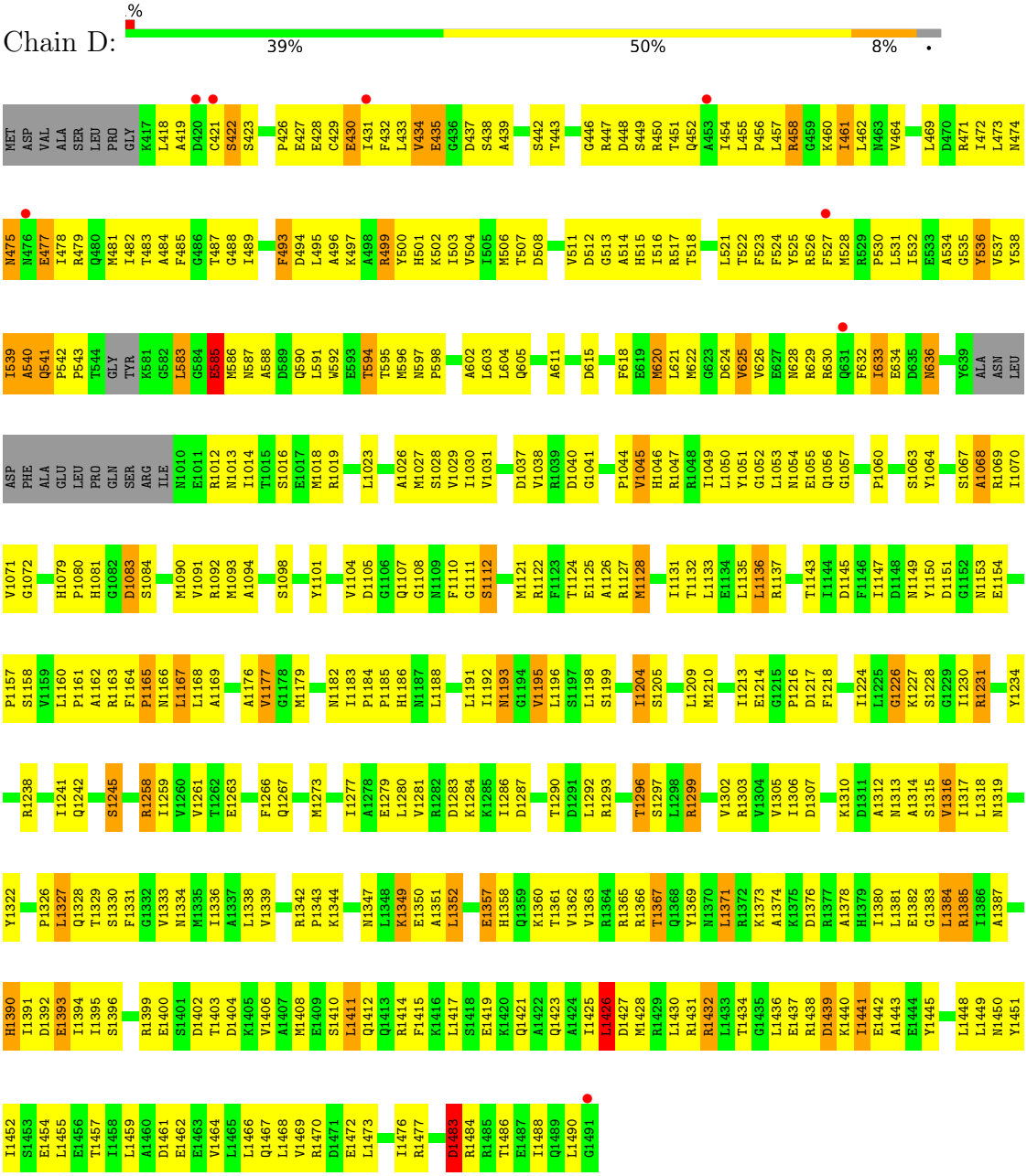
• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain B:



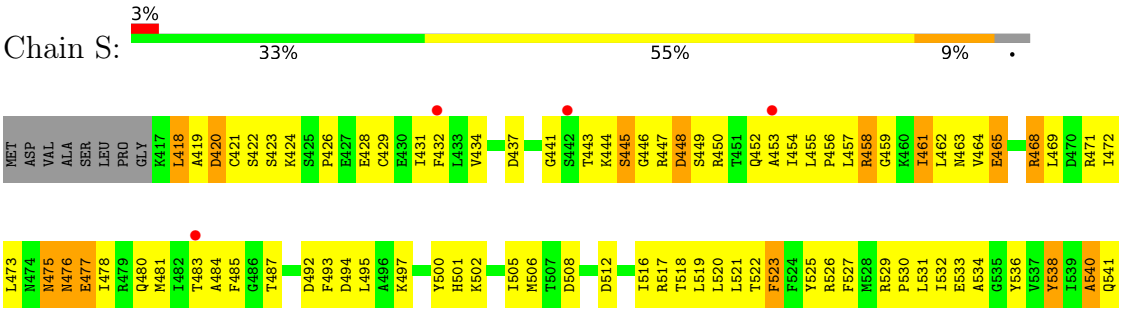
• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

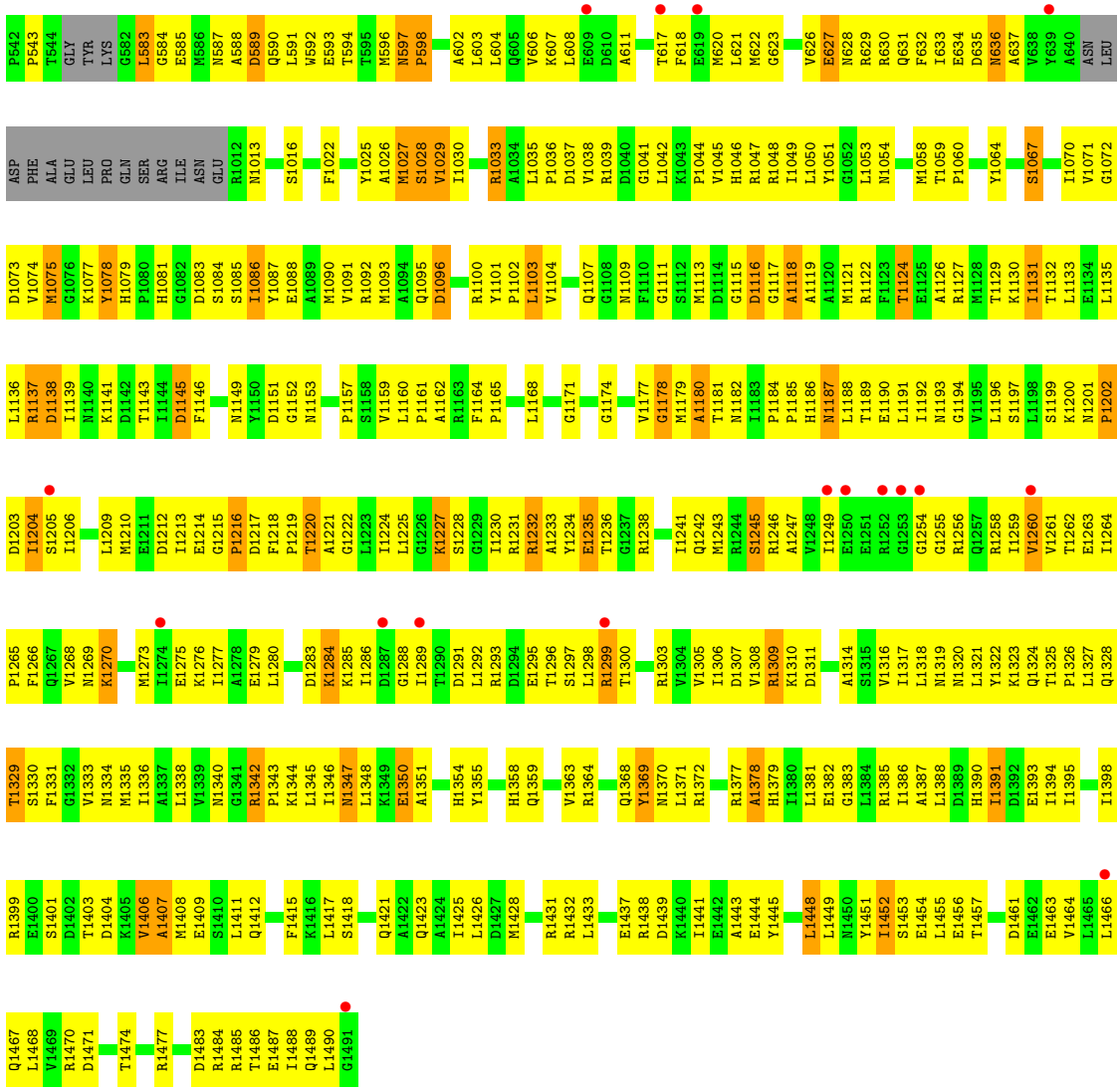
Chain D:



• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

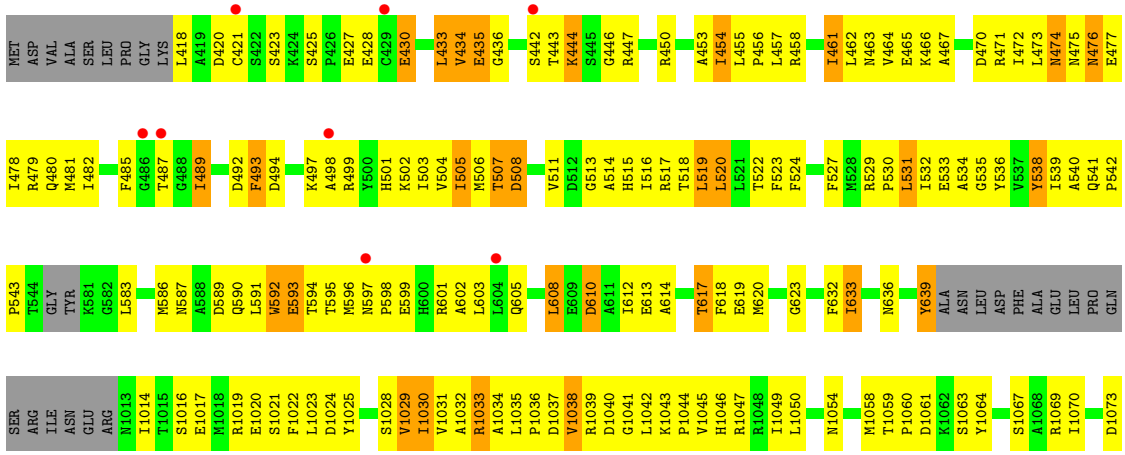
Chain S:

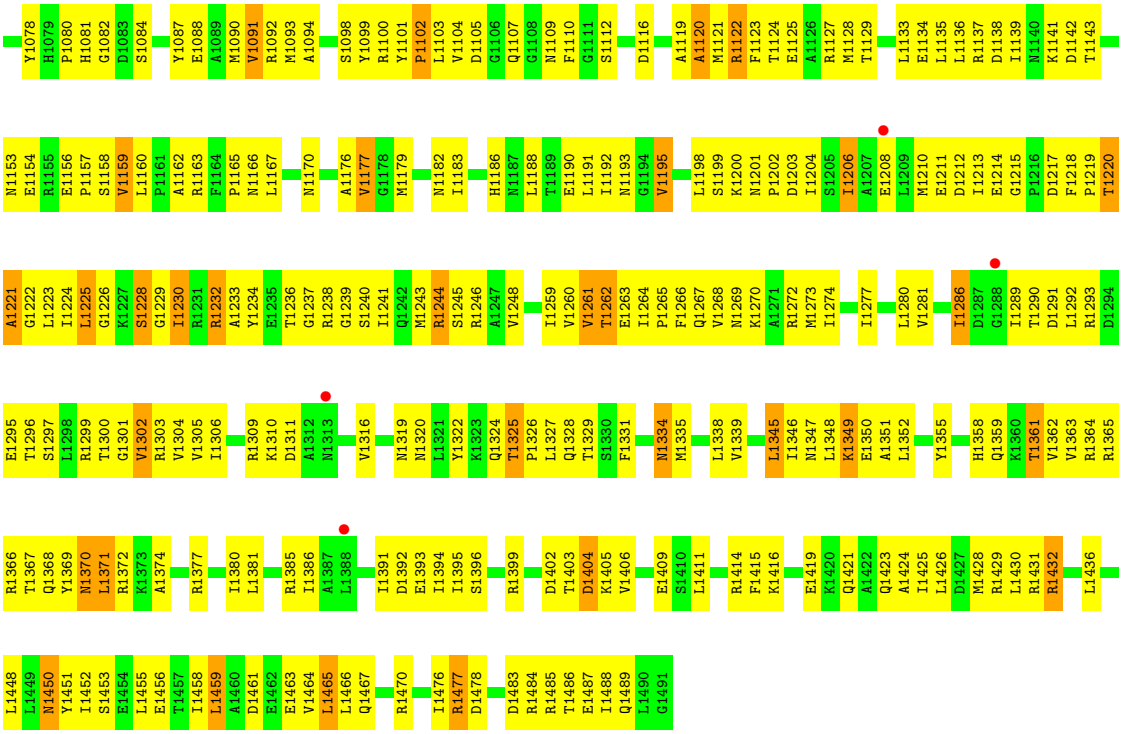




• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain U:



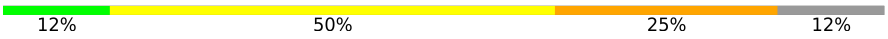


- Molecule 2: 5'-D(TP*GP*TP*GP*CP*GP*GP*T)-3'

Chain E:

- Molecule 2: 5'-D(TP*GP*TP*GP*CP*GP*GP*T)-3'

Chain V:



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

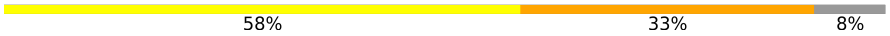
Chain F:

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

Chain W:

- Molecule 4: 5'-D(GP*TP*AP*CP*CP*CP*AP*CP*GP*GP*CP*T)-3'

Chain G:



• Molecule 4: 5'-D(GP*TP*AP*CP*CP*CP*AP*CP*GP*GP*CP*T)-3'

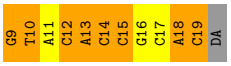
Chain X:

• Molecule 5: 5'-D(GP*TP*AP*CP*AP*CP*CP*GP*CP*AP*CP*A)-3'

Chain H:

• Molecule 5: 5'-D(GP*TP*AP*CP*AP*CP*CP*GP*CP*AP*CP*A)-3'

Chain Y:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.98Å 123.17Å 170.42Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	24.96 – 3.35 24.96 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.5 (24.96-3.35) 97.3 (24.96-3.35)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 3.38Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.166 , 0.236 0.167 , 0.218	Depositor DCC
R_{free} test set	2115 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å^2)	72.1	Xtriage
Anisotropy	0.604	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.277 for h,-k,-l	Xtriage
Reported twinning fraction	0.324 for h,-k,-l	Depositor
Outliers	0 of 52173 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22370	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.16% 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: MN, CPF

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	B	0.49	0/5332	0.70	0/7190
1	D	0.47	0/5220	0.69	1/7063 (0.0%)
1	S	0.45	0/5269	0.68	1/7112 (0.0%)
1	U	0.49	0/5263	0.71	1/7106 (0.0%)
2	E	1.02	0/164	2.13	7/252 (2.8%)
2	V	0.82	0/164	1.77	3/252 (1.2%)
3	F	0.94	1/162 (0.6%)	2.01	7/248 (2.8%)
3	W	0.80	0/137	1.81	6/209 (2.9%)
4	G	0.98	0/246	1.78	10/377 (2.7%)
4	X	1.00	0/246	2.04	17/377 (4.5%)
5	H	1.33	2/269 (0.7%)	2.72	31/412 (7.5%)
5	Y	1.00	0/245	2.42	18/375 (4.8%)
All	All	0.54	3/22717 (0.0%)	0.90	102/30973 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	17	DC	C3'-O3'	-5.51	1.36	1.44
5	H	16	DG	C3'-O3'	-5.48	1.36	1.44
3	F	6	DT	C1'-N1	5.42	1.56	1.49

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	9	DG	O4'-C1'-N9	17.19	120.03	108.00
5	H	17	DC	O4'-C1'-N1	-13.75	98.38	108.00
5	H	9	DG	O4'-C1'-N9	13.50	117.45	108.00
5	H	10	DT	O4'-C1'-N1	13.39	117.37	108.00
5	Y	9	DG	C1'-O4'-C4'	-11.73	98.36	110.10

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	B	5262	0	5259	446	0
1	D	5151	0	5043	443	0
1	S	5199	0	5178	502	0
1	U	5193	0	5163	464	0
2	E	147	0	80	8	0
2	V	147	0	80	8	0
3	F	145	0	79	14	0
3	W	123	0	68	8	0
4	G	220	0	124	27	0
4	X	220	0	124	35	0
5	H	240	0	135	38	0
5	Y	219	0	124	37	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	S	1	0	0	0	0
6	U	1	0	0	0	0
6	W	2	0	0	0	0
7	G	24	0	17	8	0
7	H	24	0	17	9	0
7	X	24	0	17	20	0
7	Y	24	0	17	10	0
All	All	22370	0	21525	1934	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 44.

The worst 5 of 1934 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)
4:G:12:DC:N3	5:H:9:DG:N2	1.82	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:11:DA:N1	5:Y:10:DT:O4	1.78	1.15
5:H:11:DA:H2"	5:H:12:DC:C5'	1.86	1.06
1:U:1122:ARG:HH22	4:X:9:DG:H5"	1.18	1.06
1:D:1192:ILE:HD12	1:D:1477:ARG:HB2	1.39	1.05

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	B	667/692 (96%)	545 (82%)	100 (15%)	22 (3%)	4 24
1	D	664/692 (96%)	526 (79%)	108 (16%)	30 (4%)	2 17
1	S	661/692 (96%)	493 (75%)	123 (19%)	45 (7%)	1 9
1	U	659/692 (95%)	532 (81%)	97 (15%)	30 (5%)	2 16
All	All	2651/2768 (96%)	2096 (79%)	428 (16%)	127 (5%)	2 16

5 of 127 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1150	TYR
1	B	1291	ASP
1	B	1310	LYS
1	B	1409	GLU
1	B	1431	ARG

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	B	563/591 (95%)	518 (92%)	45 (8%)	12	39
1	D	539/591 (91%)	483 (90%)	56 (10%)	7	27
1	S	555/591 (94%)	497 (90%)	58 (10%)	7	26
1	U	553/591 (94%)	499 (90%)	54 (10%)	8	30
All	All	2210/2364 (94%)	1997 (90%)	213 (10%)	8	30

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	591	LEU
1	S	1262	THR
1	U	1306	ILE
1	S	1058	MET
1	S	1143	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 43 such sidechains are listed below:

Mol	Chain	Res	Type
1	S	1390	HIS
1	U	636	ASN
1	S	1412	GLN
1	U	515	HIS
1	U	1107	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
7	CPF	H	1020	6	27,27,27	2.34	7 (25%)	40,40,40	2.89	17 (42%)
7	CPF	X	1020	6	27,27,27	2.29	7 (25%)	40,40,40	2.36	14 (35%)
7	CPF	G	1020	6	27,27,27	2.27	5 (18%)	40,40,40	2.50	17 (42%)
7	CPF	Y	1020	6	27,27,27	2.32	7 (25%)	40,40,40	2.74	20 (50%)

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
7	CPF	H	1020	6	-	6/12/22/22	0/4/4/4
7	CPF	X	1020	6	-	4/12/22/22	0/4/4/4
7	CPF	G	1020	6	-	6/12/22/22	0/4/4/4
7	CPF	Y	1020	6	-	2/12/22/22	0/4/4/4

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1020	CPF	O3-C4	7.17	1.38	1.23
7	X	1020	CPF	O3-C4	6.49	1.36	1.23
7	H	1020	CPF	O3-C4	6.07	1.36	1.23
7	H	1020	CPF	C5-C4	-5.96	1.36	1.48
7	Y	1020	CPF	C5-C4	-5.75	1.37	1.48

The worst 5 of 68 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	1020	CPF	C12-C11-N1	-7.64	107.38	118.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	1020	CPF	C13-C11-N1	-7.26	107.95	118.84
7	Y	1020	CPF	C12-C11-N1	-6.86	108.55	118.84
7	G	1020	CPF	C13-C11-N1	-6.81	108.63	118.84
7	H	1020	CPF	F1-C7-C8	6.15	124.02	118.42

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	H	1020	CPF	C12-C11-N1-C1
7	G	1020	CPF	C9-C8-N2-C14
7	Y	1020	CPF	C9-C8-N2-C14
7	H	1020	CPF	C12-C11-N1-C10
7	G	1020	CPF	C7-C8-N2-C14

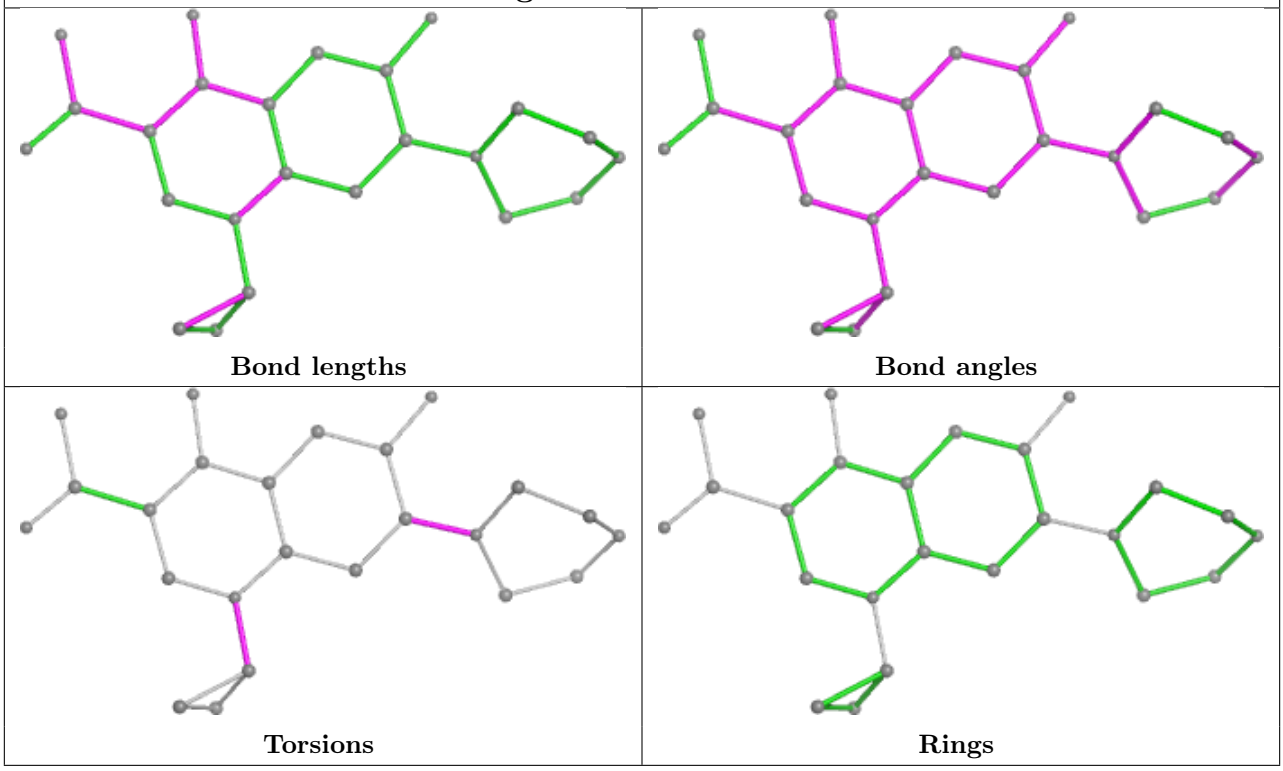
There are no ring outliers.

4 monomers are involved in 47 short contacts:

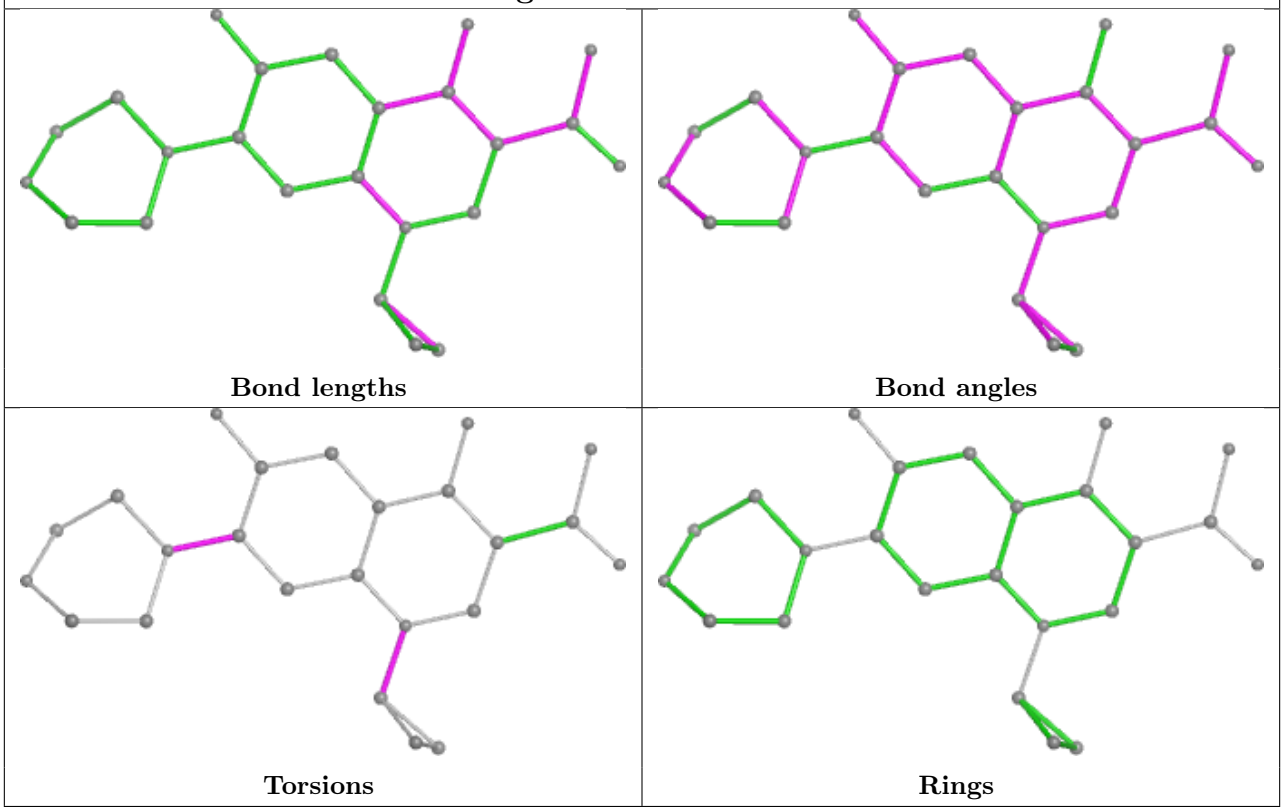
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	1020	CPF	9	0
7	X	1020	CPF	20	0
7	G	1020	CPF	8	0
7	Y	1020	CPF	10	0

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.

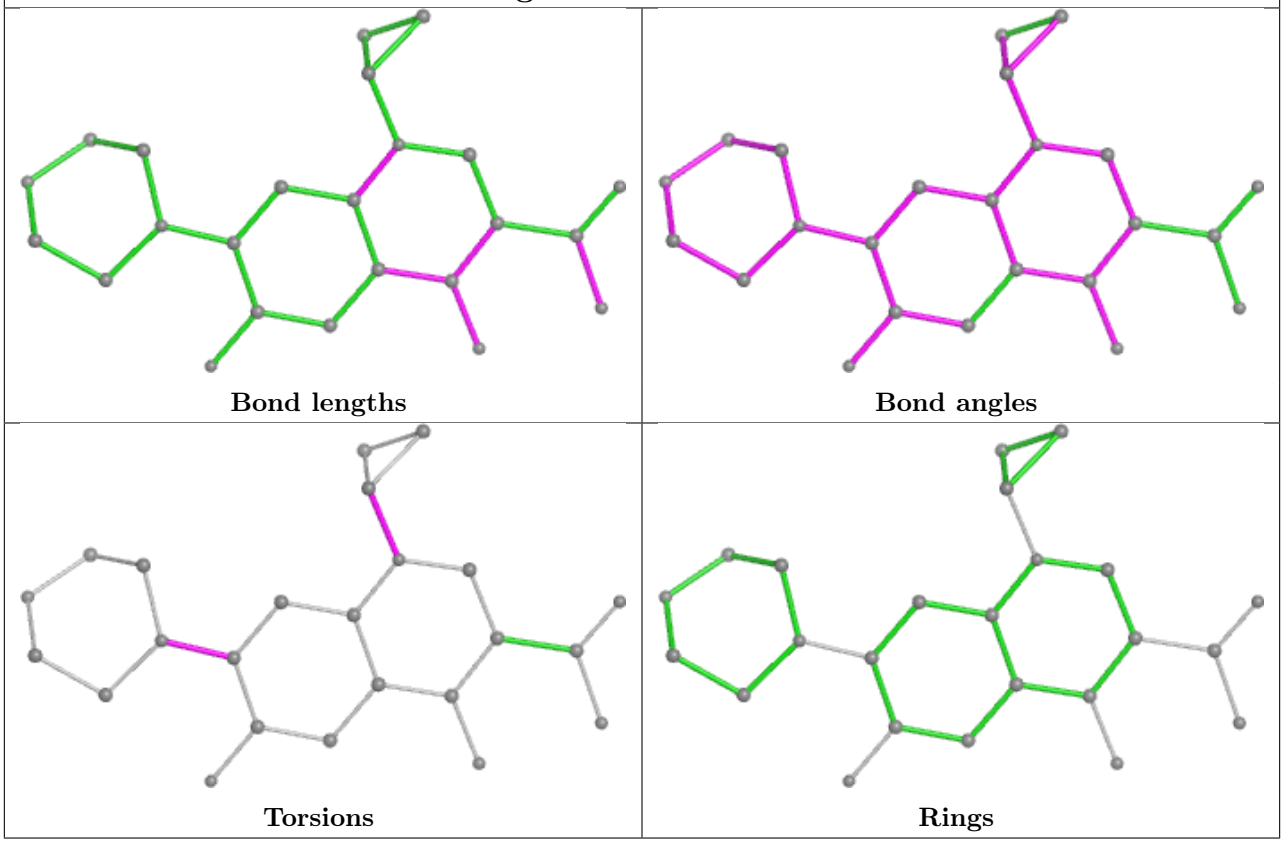
Ligand CPF H 1020



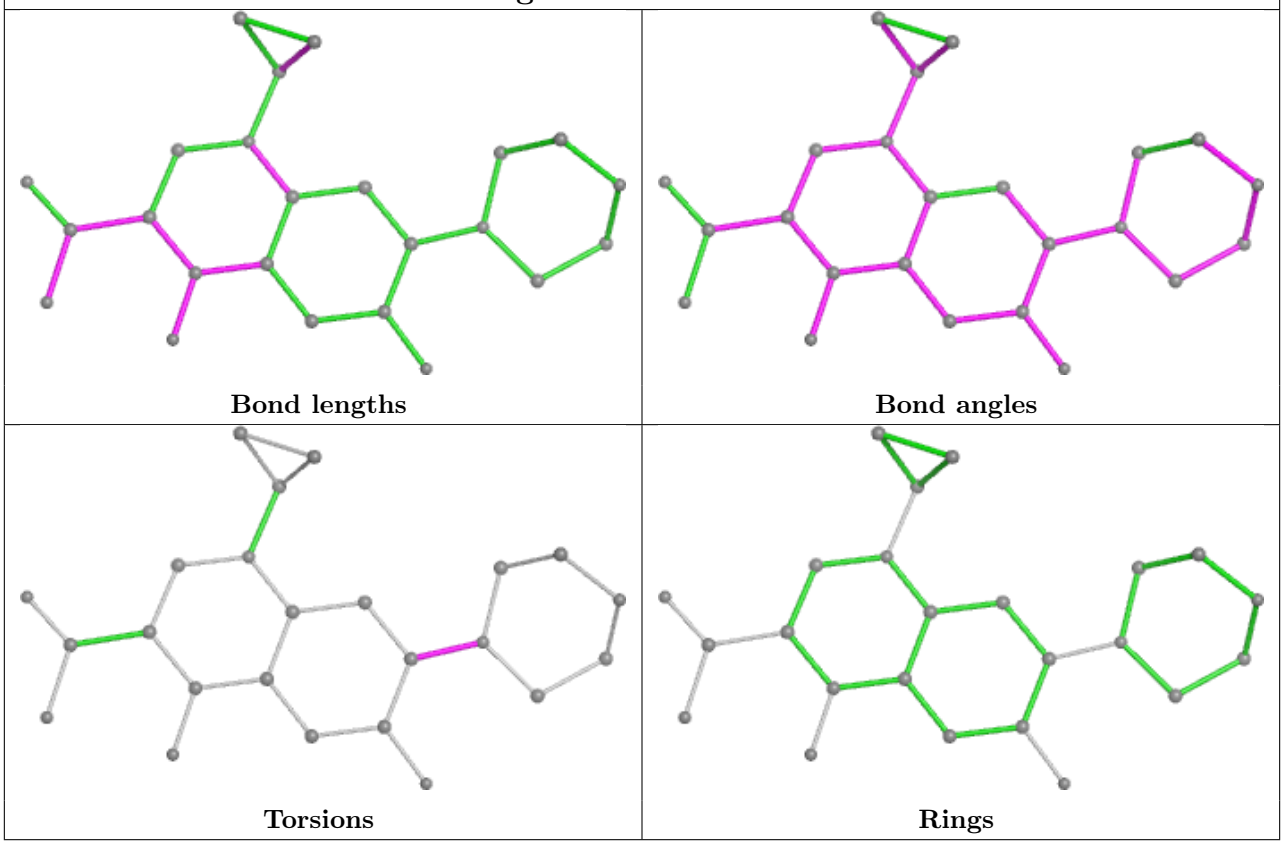
Ligand CPF X 1020



Ligand CPF G 1020



Ligand CPF Y 1020



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	B	669/692 (96%)	-0.03	5 (0%)	87	91	29, 64, 101, 143	0
1	D	669/692 (96%)	-0.02	8 (1%)	79	82	35, 69, 108, 143	0
1	S	667/692 (96%)	0.12	21 (3%)	49	52	43, 78, 119, 218	0
1	U	665/692 (96%)	0.07	12 (1%)	68	71	39, 72, 110, 158	0
2	E	7/8 (87%)	-0.02	0	100	100	48, 52, 83, 89	0
2	V	7/8 (87%)	-0.23	0	100	100	51, 62, 76, 86	0
3	F	7/8 (87%)	-0.20	0	100	100	51, 57, 77, 80	0
3	W	6/8 (75%)	-0.25	0	100	100	62, 75, 86, 86	0
4	G	11/12 (91%)	-0.11	0	100	100	60, 67, 90, 120	0
4	X	11/12 (91%)	0.34	0	100	100	68, 88, 102, 125	0
5	H	12/12 (100%)	0.01	0	100	100	48, 77, 111, 123	0
5	Y	11/12 (91%)	-0.04	0	100	100	67, 75, 106, 117	0
All	All	2742/2848 (96%)	0.03	46 (1%)	70	73	29, 71, 112, 218	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1491	GLY	4.7
1	S	619	GLU	4.6
1	U	486	GLY	3.8
1	U	604	LEU	3.8
1	B	545	GLY	3.7

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 monosaccharides in this entry.

6.4 Ligands (i)

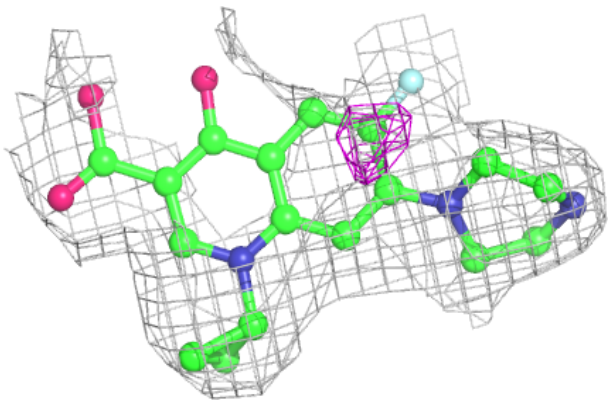
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

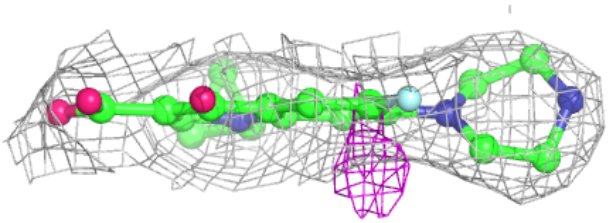
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MN	F	2000	1/1	0.86	0.10	86,86,86,86	0
7	CPF	H	1020	24/24	0.90	0.24	86,86,86,86	0
7	CPF	X	1020	24/24	0.92	0.20	86,86,86,86	0
7	CPF	Y	1020	24/24	0.93	0.18	76,76,76,76	0
7	CPF	G	1020	24/24	0.94	0.19	70,70,70,70	0
6	MN	W	2000	1/1	0.94	0.12	86,86,86,86	0
6	MN	D	2492	1/1	0.95	0.22	85,85,85,85	0
6	MN	W	2001	1/1	0.95	0.07	76,76,76,76	0
6	MN	B	2492	1/1	0.96	0.25	76,76,76,76	0
6	MN	S	2492	1/1	0.98	0.16	70,70,70,70	0
6	MN	U	2492	1/1	0.98	0.22	64,64,64,64	0
6	MN	G	2000	1/1	0.99	0.07	70,70,70,70	0

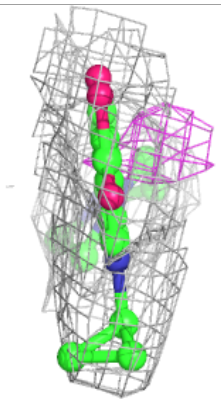
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CPF H 1020:

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

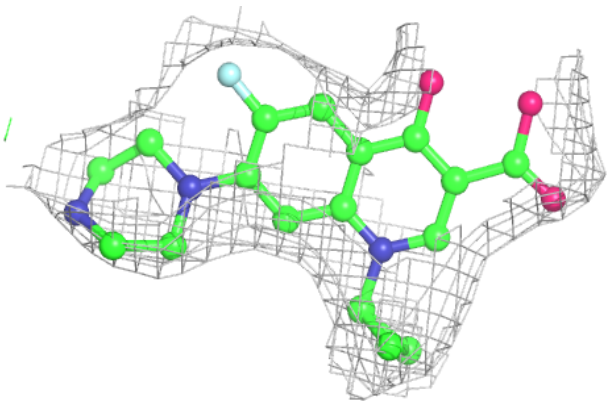


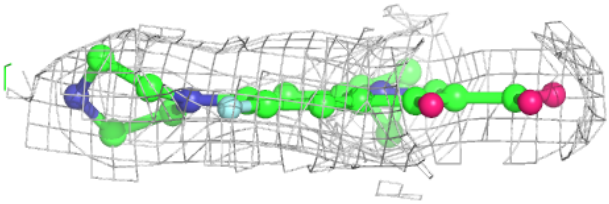


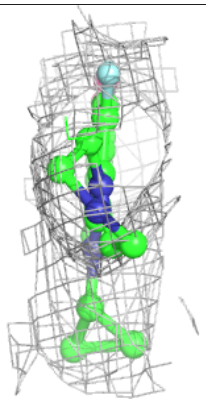


Electron density around CPF X 1020:

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

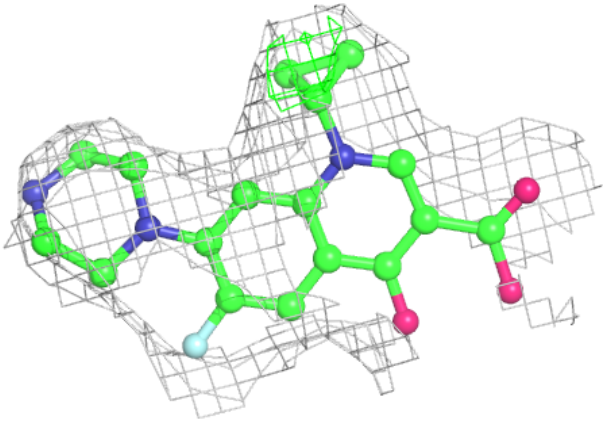


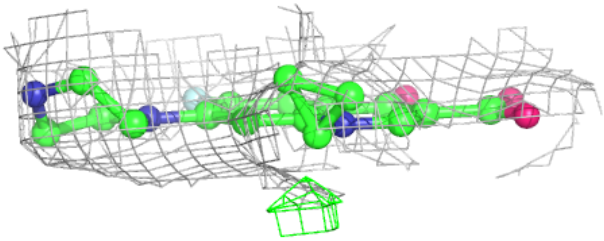


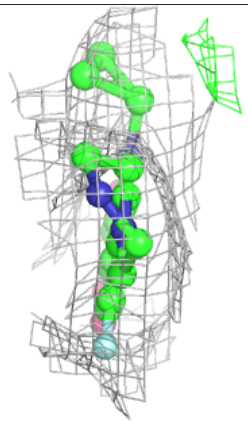


Electron density around CPF Y 1020:

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

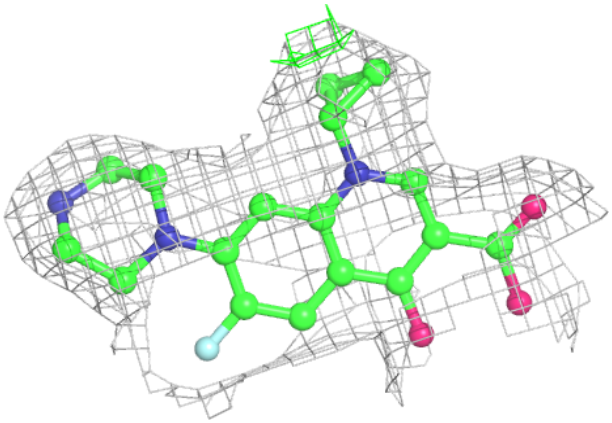


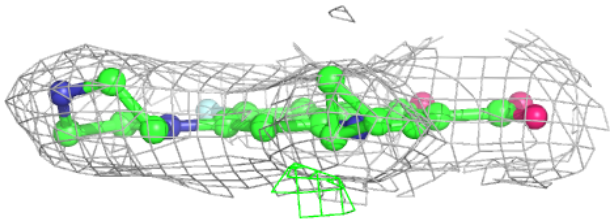


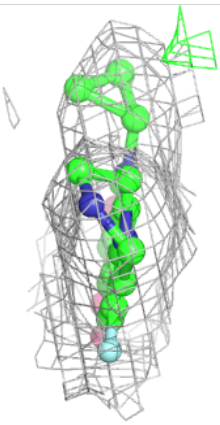


Electron density around CPF G 1020:

$2mF_o$-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.