



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:27 pm BST

PDB ID : 6EUV
Title : Structure of the midlink and cap-binding domains of influenza A polymerase PB2 subunit with a bound azaindole cap-binding inhibitor (VX-787)
Authors : Cusack, S.; Lethier, M.
Deposited on : 2017-10-31
Resolution : 2.70 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

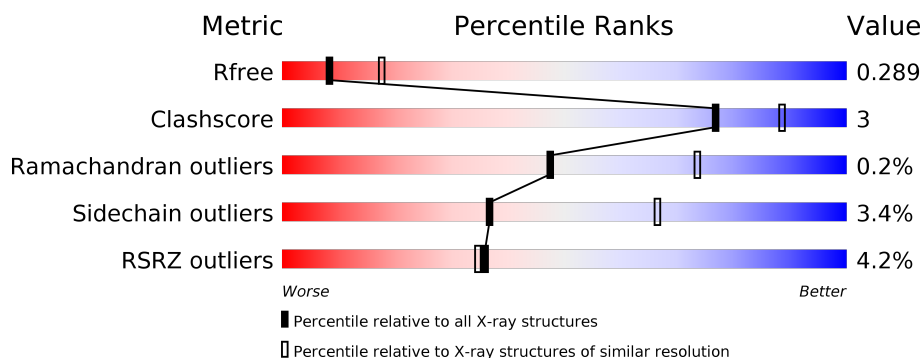
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	290	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>5%</div> <div>.</div> </div> </div>
1	C	290	<div> <div>3%</div> <div> <div></div> <div>92%</div> <div>5%</div> <div>..</div> </div> </div>
1	F	290	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>6%</div> <div>5%</div> </div> </div>
1	I	290	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>.</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	21G	A	602[A]	-	-	X	-

2 Entry composition [i](#)

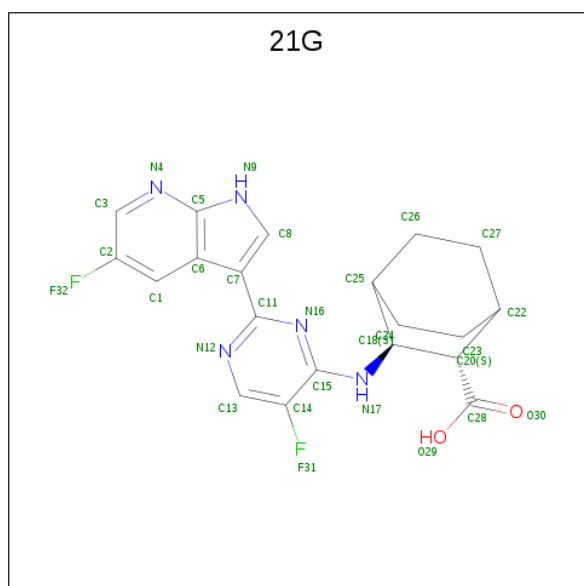
There are 4 unique types of molecules in this entry. The entry contains 9091 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	1	0
			2179	1348	405	410	16			
1	C	283	Total	C	N	O	S	0	1	0
			2224	1373	414	421	16			
1	F	275	Total	C	N	O	S	0	1	0
			2166	1340	403	407	16			
1	I	278	Total	C	N	O	S	0	1	0
			2184	1349	406	413	16			

- Molecule 2 is (2S,3S)-3-[[5-fluoranyl-2-(5-fluoranyl-1H-pyrrolo[2,3-b]pyridin-3-yl)pyrimidin-4-yl]amino]bicyclo[2.2.2]octane-2-carboxylic acid (three-letter code: 21G) (formula: C₂₀H₁₉F₂N₅O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			29	20	2	5	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	1
			58	40	4	10	4		
2	C	1	Total	C	F	N	O	0	0
			29	20	2	5	2		
2	C	1	Total	C	F	N	O	0	1
			58	40	4	10	4		
2	F	1	Total	C	F	N	O	0	0
			29	20	2	5	2		
2	I	1	Total	C	F	N	O	0	0
			29	20	2	5	2		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Ni	0	0
			1	1		
3	A	1	Total	Ni	0	0
			1	1		
3	C	1	Total	Ni	0	0
			1	1		
3	F	1	Total	Ni	0	0
			1	1		

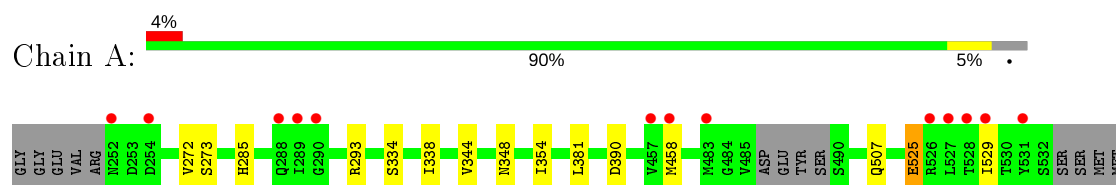
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	C	31	Total	O	0	0
			31	31		
4	F	25	Total	O	0	0
			25	25		
4	I	27	Total	O	0	0
			27	27		

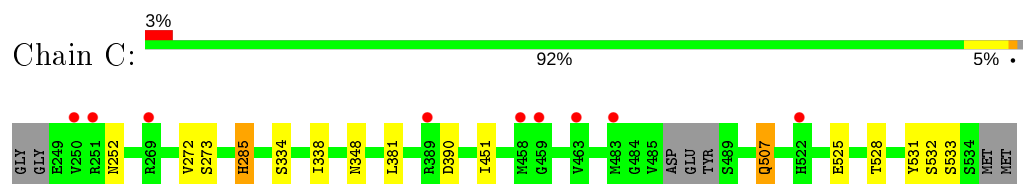
3 Residue-property plots [i](#)

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.

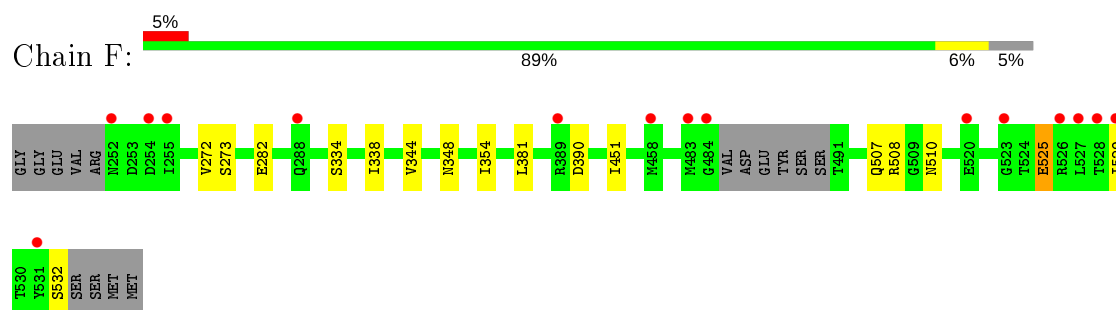
- Molecule 1: Polymerase basic protein 2



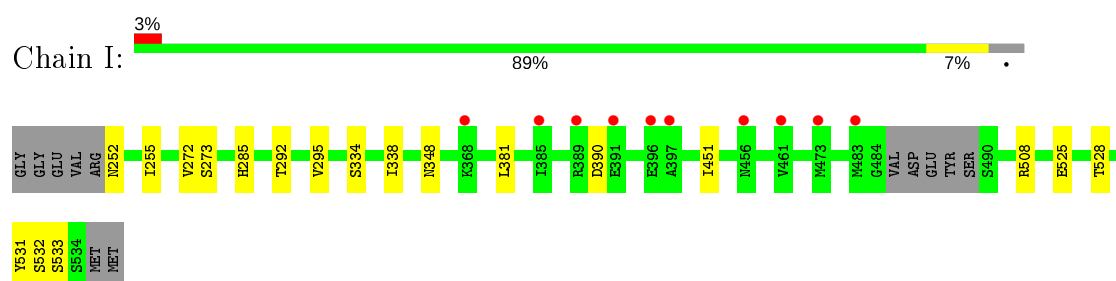
- Molecule 1: Polymerase basic protein 2



- Molecule 1: Polymerase basic protein 2



- Molecule 1: Polymerase basic protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.49 Å 80.32 Å 92.32 Å 89.54° 107.12° 99.11°	Depositor
Resolution (Å)	43.35 – 2.70 46.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.8 (43.35-2.70) 94.9 (46.73-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.69 Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.243 , 0.282 0.246 , 0.289	Depositor DCC
R_{free} test set	1837 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 64.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,h+1	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9091	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.05 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3970e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: NI, 21G

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	0.52	0/2204	0.76	0/2963
1	C	0.53	0/2249	0.76	0/3023
1	F	0.52	0/2191	0.75	0/2945
1	I	0.53	0/2209	0.76	0/2969
All	All	0.53	0/8853	0.75	0/11900

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	2179	0	2217	20	0
1	C	2224	0	2260	11	0
1	F	2166	0	2202	6	0
1	I	2184	0	2218	10	0
2	A	87	0	53	21	0
2	C	87	0	51	9	0
2	F	29	0	18	1	0
2	I	29	0	18	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
4	A	19	0	0	0	0
4	C	31	0	0	1	0
4	F	25	0	0	0	0
4	I	27	0	0	2	0
All	All	9091	0	9037	54	0

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

All (54) 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:285[B]:HIS:CE1	2:A:602[B]:21G:N12	1.69	1.37
1:A:285[A]:HIS:HE1	2:A:602[A]:21G:C27	1.26	1.25
1:A:285[A]:HIS:CE1	2:A:602[A]:21G:C26	2.30	1.14
1:A:285[A]:HIS:CE1	2:A:602[A]:21G:H16	1.83	1.13
1:A:285[A]:HIS:NE2	2:A:602[A]:21G:H16	1.65	1.10
1:A:285[A]:HIS:CE1	2:A:602[A]:21G:C27	2.11	1.09
1:A:285[A]:HIS:CD2	2:A:602[A]:21G:F32	1.96	1.08
2:A:602[B]:21G:O30	2:A:602[B]:21G:H17	1.58	1.01
1:A:285[A]:HIS:CE1	2:A:602[A]:21G:H17	1.57	1.00
2:A:602[A]:21G:O30	2:A:602[A]:21G:H16	1.66	0.94
1:A:285[A]:HIS:HE1	2:A:602[A]:21G:C26	1.78	0.91
1:A:285[A]:HIS:HE2	2:A:602[A]:21G:H16	1.36	0.90
2:C:602[A]:21G:O29	2:C:602[A]:21G:H17	1.71	0.88
1:A:285[B]:HIS:HE1	2:A:602[B]:21G:N12	1.30	0.84
1:C:285[B]:HIS:CD2	2:C:602[B]:21G:C5	2.61	0.84
1:I:285[B]:HIS:CG	1:I:285[B]:HIS:O	2.32	0.83
1:I:285[B]:HIS:O	1:I:285[B]:HIS:ND1	2.23	0.71
2:C:602[A]:21G:O29	2:C:602[A]:21G:C27	2.38	0.71
2:A:602[B]:21G:O30	2:A:602[B]:21G:C27	2.32	0.70
1:C:285[B]:HIS:CD2	2:C:602[B]:21G:N9	2.61	0.69
1:A:285[A]:HIS:HD2	2:A:602[A]:21G:F32	1.66	0.68
1:A:285[A]:HIS:CD2	2:A:602[A]:21G:C2	2.82	0.62
1:C:285[B]:HIS:HD2	2:C:602[B]:21G:N9	2.01	0.59
1:I:252:ASN:HB3	1:I:255:ILE:HD12	1.87	0.55
1:A:293:ARG:NH2	2:A:602[A]:21G:O29	2.40	0.54
1:C:285[B]:HIS:CD2	2:C:602[B]:21G:N4	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:GLU:OE2	1:A:529:ILE:HD12	2.10	0.51
1:F:525:GLU:OE2	1:F:529:ILE:HD12	2.11	0.51
1:I:525:GLU:OE2	1:I:528:THR:HA	2.12	0.49
1:C:525:GLU:OE2	1:C:528:THR:HA	2.13	0.49
1:A:285[B]:HIS:ND1	2:A:602[B]:21G:C11	2.50	0.49
2:A:602[A]:21G:H7	2:A:602[A]:21G:H1	1.95	0.48
2:C:602[A]:21G:F31	1:F:282:GLU:HG3	2.04	0.47
1:C:285[B]:HIS:NE2	2:C:602[B]:21G:N4	2.63	0.47
2:C:602[B]:21G:N16	2:C:602[B]:21G:H1	2.31	0.46
1:I:338:ILE:HD12	1:I:338:ILE:C	2.36	0.46
1:A:338:ILE:C	1:A:338:ILE:HD12	2.37	0.45
1:C:338:ILE:C	1:C:338:ILE:HD12	2.36	0.45
1:F:338:ILE:HD12	1:F:338:ILE:C	2.37	0.45
1:C:285[A]:HIS:CD2	1:C:285[A]:HIS:C	2.90	0.45
1:I:292:THR:HG23	4:I:714:HOH:O	2.16	0.45
2:A:602[B]:21G:C28	1:I:295:VAL:HG11	2.47	0.44
1:A:285[B]:HIS:ND1	2:A:602[B]:21G:N12	2.45	0.44
1:I:390:ASP:OD1	1:I:390:ASP:N	2.53	0.42
1:C:531:TYR:O	1:C:533:SER:N	2.52	0.42
1:C:390:ASP:OD1	1:C:390:ASP:N	2.53	0.42
1:C:507:GLN:HG3	4:C:710:HOH:O	2.19	0.42
1:A:390:ASP:N	1:A:390:ASP:OD1	2.53	0.42
1:F:390:ASP:N	1:F:390:ASP:OD1	2.53	0.42
1:F:510:ASN:HB3	2:F:601:21G:C14	2.50	0.42
1:I:531:TYR:O	1:I:533:SER:N	2.53	0.41
1:I:508:ARG:HD2	4:I:704:HOH:O	2.21	0.41
1:A:344:VAL:CG2	1:A:354:ILE:HD12	2.52	0.40
1:F:344:VAL:CG2	1:F:354:ILE:HD12	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/290 (94%)	265 (97%)	9 (3%)	0	100	100
1	C	280/290 (97%)	270 (96%)	9 (3%)	1 (0%)	34	60
1	F	272/290 (94%)	264 (97%)	8 (3%)	0	100	100
1	I	275/290 (95%)	265 (96%)	9 (3%)	1 (0%)	34	60
All	All	1101/1160 (95%)	1064 (97%)	35 (3%)	2 (0%)	47	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	532	SER
1	I	532	SER

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	243/253 (96%)	235 (97%)	8 (3%)	38	67
1	C	249/253 (98%)	239 (96%)	10 (4%)	31	60
1	F	241/253 (95%)	231 (96%)	10 (4%)	30	59
1	I	244/253 (96%)	238 (98%)	6 (2%)	47	76
All	All	977/1012 (96%)	943 (96%)	34 (4%)	37	65

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	VAL
1	A	273	SER
1	A	334	SER
1	A	348	ASN
1	A	381	LEU
1	A	458	MET
1	A	507	GLN
1	A	525	GLU
1	C	252	ASN

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Mol	Chain	Res	Type
1	C	272	VAL
1	C	273	SER
1	C	285[A]	HIS
1	C	285[B]	HIS
1	C	334	SER
1	C	348	ASN
1	C	381	LEU
1	C	451	ILE
1	C	507	GLN
1	F	272	VAL
1	F	273	SER
1	F	334	SER
1	F	348	ASN
1	F	381	LEU
1	F	451	ILE
1	F	507	GLN
1	F	508	ARG
1	F	525	GLU
1	F	532	SER
1	I	272	VAL
1	I	273	SER
1	I	334	SER
1	I	348	ASN
1	I	381	LEU
1	I	451	ILE

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

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
2	21G	F	601	-	28,33,33	1.27	4 (14%)	33,49,49	2.00	10 (30%)
2	21G	I	601	-	28,33,33	1.21	1 (3%)	33,49,49	1.79	12 (36%)
2	21G	C	601	-	28,33,33	1.21	3 (10%)	33,49,49	1.93	8 (24%)
2	21G	A	602[B]	1	28,33,33	1.16	2 (7%)	33,49,49	1.75	8 (24%)
2	21G	A	601	-	28,33,33	1.23	5 (17%)	33,49,49	1.98	10 (30%)
2	21G	C	602[A]	-	28,33,33	1.20	4 (14%)	33,49,49	1.78	7 (21%)
2	21G	A	602[A]	1	28,33,33	1.28	5 (17%)	33,49,49	1.95	9 (27%)
2	21G	C	602[B]	-	28,33,33	1.09	3 (10%)	33,49,49	1.80	10 (30%)

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
2	21G	F	601	-	-	0/4/34/34	0/6/5/5
2	21G	I	601	-	-	0/4/34/34	0/6/5/5
2	21G	C	601	-	-	0/4/34/34	0/6/5/5
2	21G	A	602[B]	1	-	0/4/34/34	0/6/5/5
2	21G	A	601	-	-	0/4/34/34	0/6/5/5
2	21G	C	602[A]	-	-	0/4/34/34	0/6/5/5
2	21G	A	602[A]	1	-	0/4/34/34	0/6/5/5
2	21G	C	602[B]	-	-	0/4/34/34	0/6/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602[A]	21G	C20-C22	-3.65	1.51	1.55
2	F	601	21G	C20-C22	-2.62	1.52	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	21G	C3-N4	2.60	1.36	1.31
2	I	601	21G	C20-C22	-2.55	1.52	1.55
2	F	601	21G	C3-C2	2.52	1.40	1.37
2	A	602[A]	21G	C3-C2	2.46	1.40	1.37
2	A	602[B]	21G	C20-C22	-2.45	1.52	1.55
2	A	601	21G	C20-C22	-2.45	1.52	1.55
2	F	601	21G	C1-C2	2.38	1.40	1.36
2	C	602[A]	21G	C20-C22	-2.36	1.52	1.55
2	C	601	21G	C3-N4	2.30	1.35	1.31
2	C	601	21G	C20-C22	-2.30	1.52	1.55
2	A	601	21G	C13-C14	2.23	1.41	1.37
2	C	602[A]	21G	C15-C14	-2.23	1.37	1.40
2	C	602[B]	21G	C3-C2	2.22	1.40	1.37
2	A	602[A]	21G	C6-C5	-2.19	1.37	1.43
2	A	601	21G	C1-C2	2.18	1.39	1.36
2	C	602[B]	21G	C6-C5	-2.18	1.37	1.43
2	C	602[A]	21G	C3-C2	2.13	1.40	1.37
2	A	602[A]	21G	C3-N4	2.11	1.35	1.31
2	A	601	21G	C11-N12	2.10	1.37	1.34
2	A	602[A]	21G	C1-C6	-2.07	1.38	1.42
2	C	602[A]	21G	C3-N4	2.07	1.35	1.31
2	A	602[B]	21G	C6-C5	-2.06	1.37	1.43
2	A	601	21G	C3-N4	2.05	1.35	1.31
2	C	601	21G	C11-N12	2.02	1.37	1.34
2	C	602[B]	21G	C20-C22	-2.00	1.53	1.55

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	21G	N12-C11-N16	-5.20	120.16	125.25
2	F	601	21G	N12-C11-N16	-5.07	120.29	125.25
2	C	602[A]	21G	C14-C13-N12	-4.63	118.69	122.77
2	C	601	21G	C14-C13-N12	-4.60	118.72	122.77
2	C	601	21G	C14-C15-N16	-4.42	116.84	119.41
2	A	601	21G	C3-N4-C5	4.23	120.94	116.69
2	A	602[B]	21G	C14-C13-N12	-4.03	119.22	122.77
2	A	602[A]	21G	N12-C11-N16	-3.99	121.35	125.25
2	C	602[B]	21G	C14-C13-N12	-3.98	119.27	122.77
2	A	602[A]	21G	C28-C20-C22	-3.88	106.38	113.74
2	C	602[B]	21G	C7-C11-N12	3.85	121.36	117.03
2	A	602[B]	21G	N12-C11-N16	-3.85	121.48	125.25
2	A	602[A]	21G	C14-C13-N12	-3.83	119.39	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	21G	N12-C11-N16	-3.82	121.51	125.25
2	A	602[A]	21G	C7-C11-N12	3.80	121.31	117.03
2	I	601	21G	C14-C15-N16	-3.62	117.31	119.41
2	C	602[A]	21G	N12-C11-N16	-3.61	121.71	125.25
2	F	601	21G	C7-C11-N12	3.48	120.95	117.03
2	A	601	21G	C15-N16-C11	3.45	122.30	116.10
2	A	602[A]	21G	C27-C22-C20	-3.37	103.31	109.24
2	I	601	21G	C14-C13-N12	-3.25	119.90	122.77
2	A	602[B]	21G	C13-N12-C11	3.25	120.52	116.22
2	F	601	21G	C26-C25-C18	-3.24	105.84	110.59
2	C	602[A]	21G	C13-N12-C11	3.21	120.46	116.22
2	A	602[B]	21G	C28-C20-C22	-3.20	107.67	113.74
2	C	602[A]	21G	C2-C1-C6	-3.13	116.35	118.80
2	C	602[B]	21G	N12-C11-N16	-3.10	122.21	125.25
2	F	601	21G	C14-C13-N12	-3.09	120.05	122.77
2	F	601	21G	C15-N16-C11	3.09	121.65	116.10
2	A	602[B]	21G	C2-C1-C6	-3.06	116.41	118.80
2	C	602[A]	21G	N17-C15-N16	3.01	125.31	118.84
2	A	602[A]	21G	C13-N12-C11	3.00	120.18	116.22
2	I	601	21G	N12-C11-N16	-2.94	122.37	125.25
2	C	601	21G	C2-C1-C6	-2.85	116.57	118.80
2	F	601	21G	C13-N12-C11	2.84	119.98	116.22
2	C	602[A]	21G	C28-C20-C22	-2.81	108.41	113.74
2	C	601	21G	C13-N12-C11	2.80	119.92	116.22
2	A	601	21G	C1-C2-C3	-2.77	118.11	121.89
2	A	601	21G	C26-C25-C18	-2.74	106.57	110.59
2	F	601	21G	C14-C15-N16	-2.74	117.82	119.41
2	A	602[B]	21G	C7-C11-N16	2.74	121.92	117.46
2	C	602[B]	21G	C2-C1-C6	-2.70	116.69	118.80
2	A	601	21G	C7-C11-N12	2.69	120.06	117.03
2	A	601	21G	C14-C13-N12	-2.68	120.41	122.77
2	I	601	21G	C27-C26-C25	-2.66	106.24	112.24
2	I	601	21G	C15-N16-C11	2.59	120.76	116.10
2	C	602[B]	21G	C13-N12-C11	2.56	119.60	116.22
2	C	601	21G	C15-N16-C11	2.51	120.62	116.10
2	A	601	21G	C13-N12-C11	2.50	119.53	116.22
2	C	601	21G	C27-C26-C25	-2.45	106.72	112.24
2	F	601	21G	C3-N4-C5	2.38	119.08	116.69
2	C	602[B]	21G	C24-C23-C22	-2.37	106.91	112.24
2	A	602[A]	21G	C15-N16-C11	2.34	120.31	116.10
2	I	601	21G	C2-C1-C6	-2.29	117.01	118.80
2	F	601	21G	C1-C2-C3	-2.27	118.79	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	601	21G	C27-C22-C23	-2.25	105.47	109.44
2	I	601	21G	C27-C22-C20	2.24	113.18	109.24
2	I	601	21G	C25-C18-N17	-2.21	107.57	112.00
2	A	602[A]	21G	C24-C23-C22	-2.20	107.29	112.24
2	C	602[B]	21G	C15-N16-C11	2.20	120.05	116.10
2	A	602[B]	21G	N17-C15-N16	2.16	123.49	118.84
2	A	601	21G	C27-C22-C23	-2.15	105.64	109.44
2	A	602[A]	21G	C2-C1-C6	-2.15	117.12	118.80
2	C	602[B]	21G	C26-C25-C18	-2.14	107.45	110.59
2	I	601	21G	C26-C25-C18	-2.13	107.46	110.59
2	C	602[B]	21G	C3-N4-C5	2.12	118.82	116.69
2	I	601	21G	C24-C23-C22	-2.10	107.51	112.24
2	A	602[B]	21G	C23-C22-C20	2.09	112.92	109.24
2	F	601	21G	C2-C1-C6	-2.07	117.18	118.80
2	A	601	21G	C27-C22-C20	2.07	112.87	109.24
2	C	602[B]	21G	C27-C22-C23	-2.06	105.80	109.44
2	C	602[A]	21G	F31-C14-C15	-2.06	117.57	119.75
2	I	601	21G	N17-C15-N16	2.05	123.26	118.84
2	C	601	21G	C27-C22-C20	2.03	112.81	109.24

There are no chirality outliers.

There are no torsion outliers.

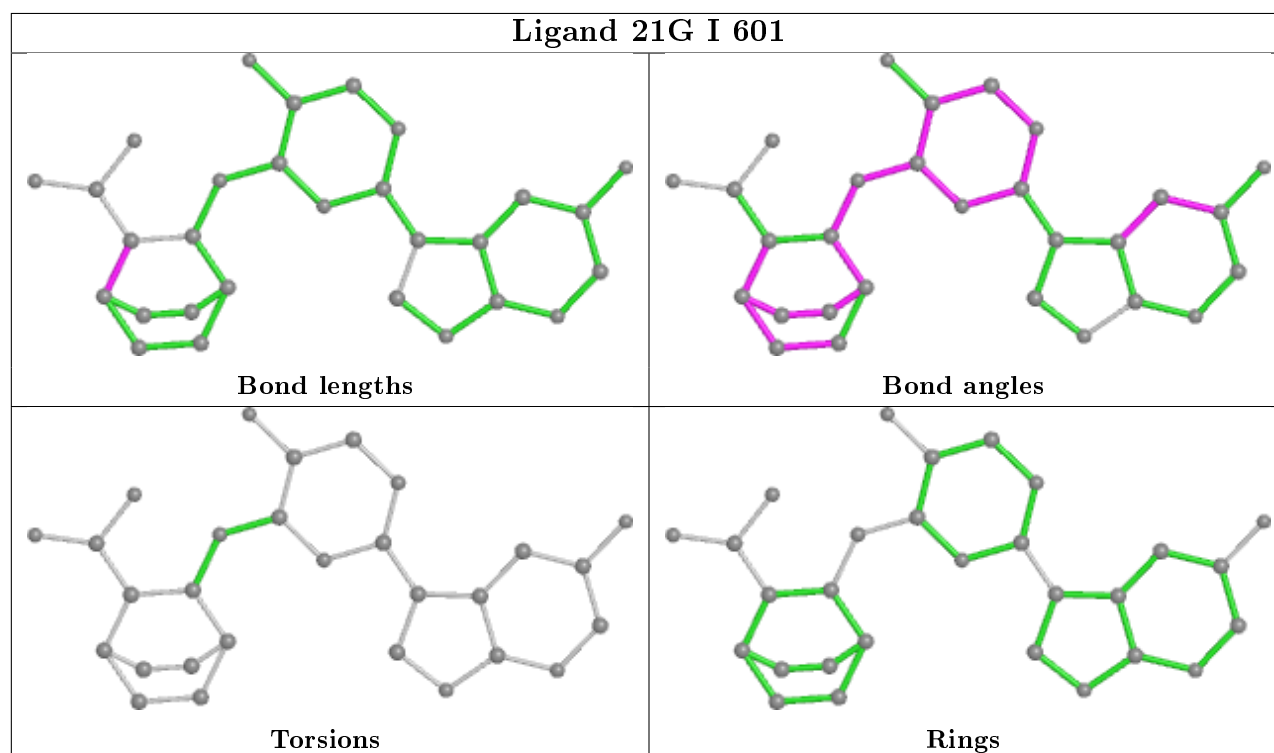
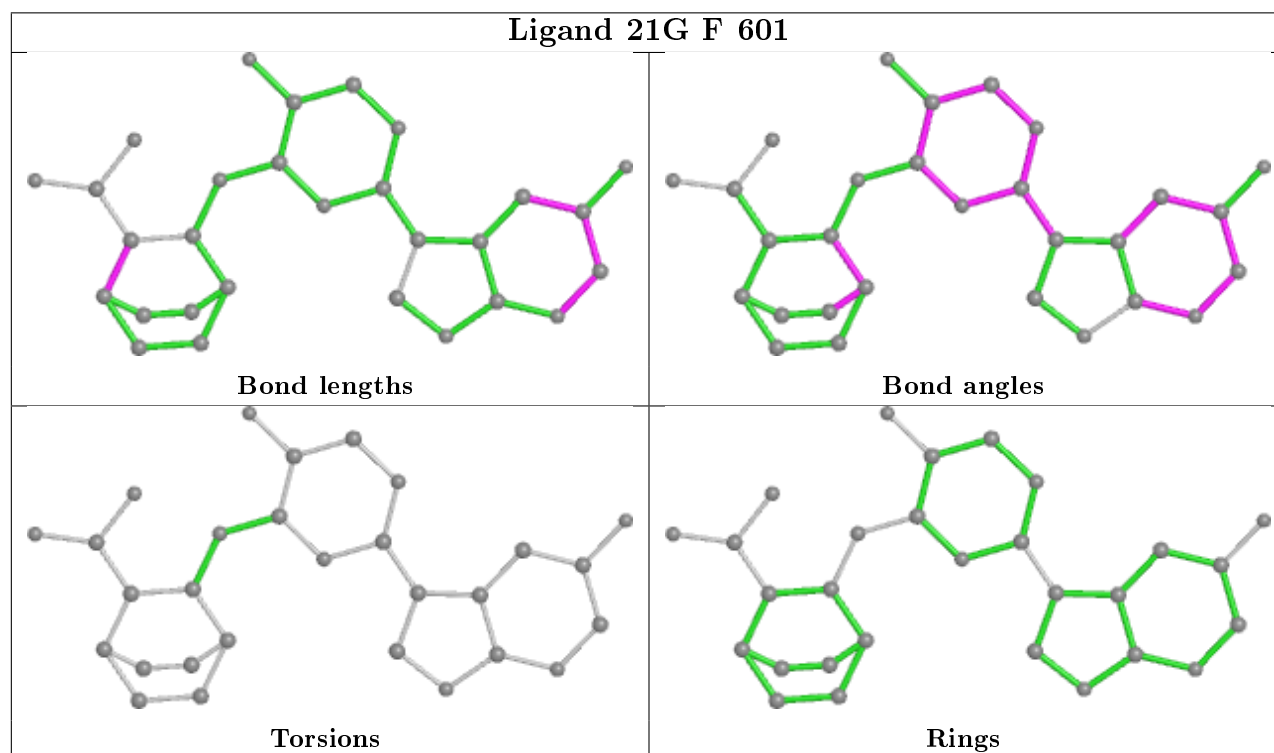
There are no ring outliers.

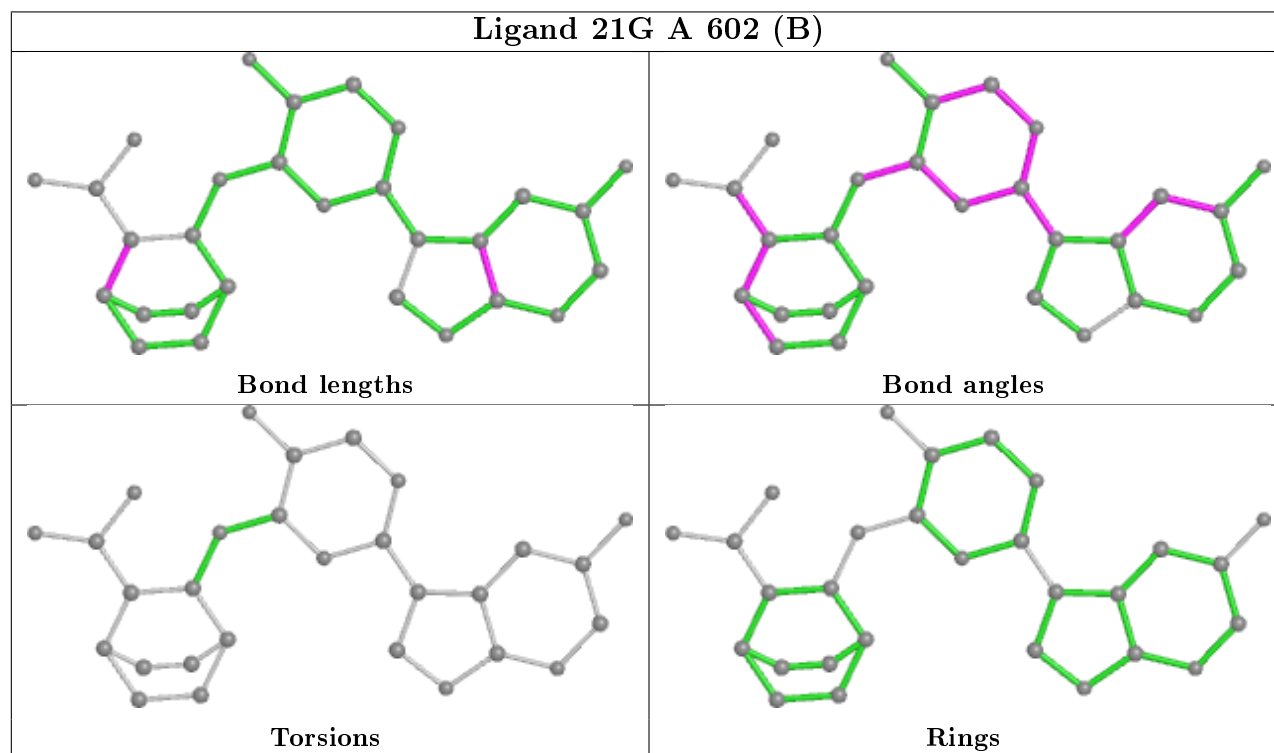
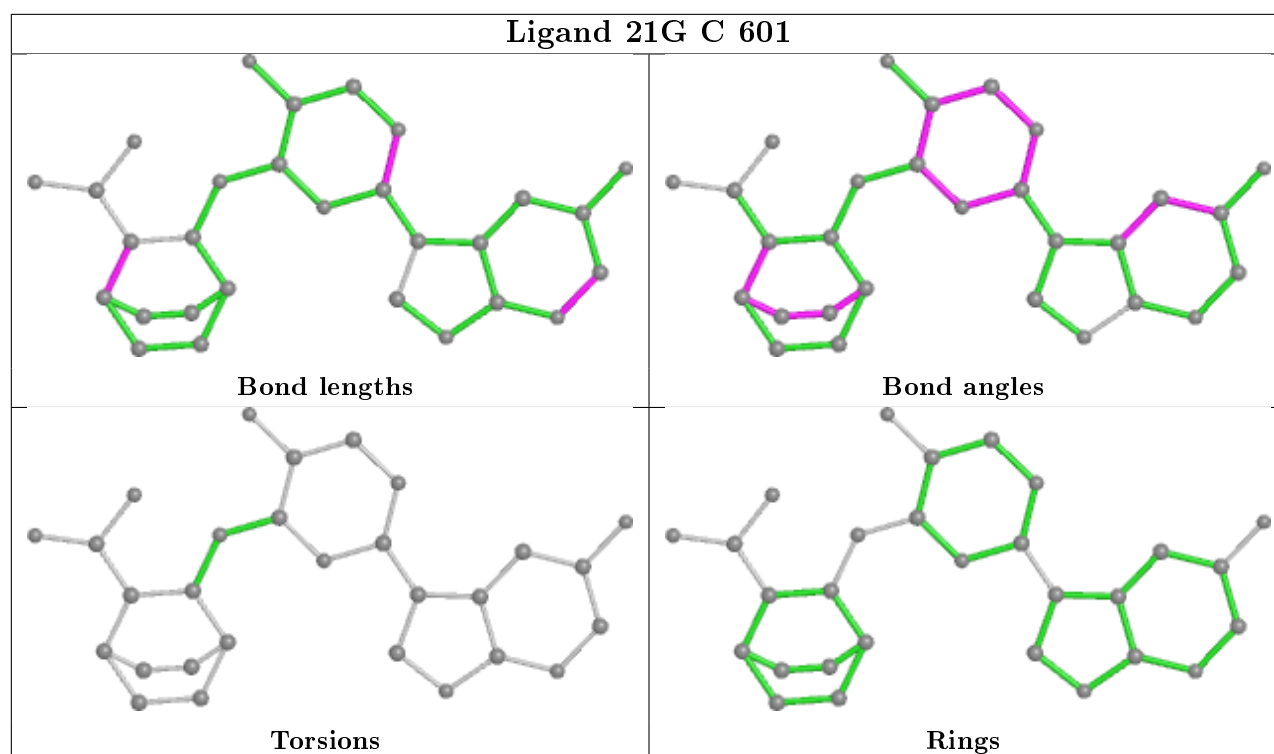
5 monomers are involved in 31 short contacts:

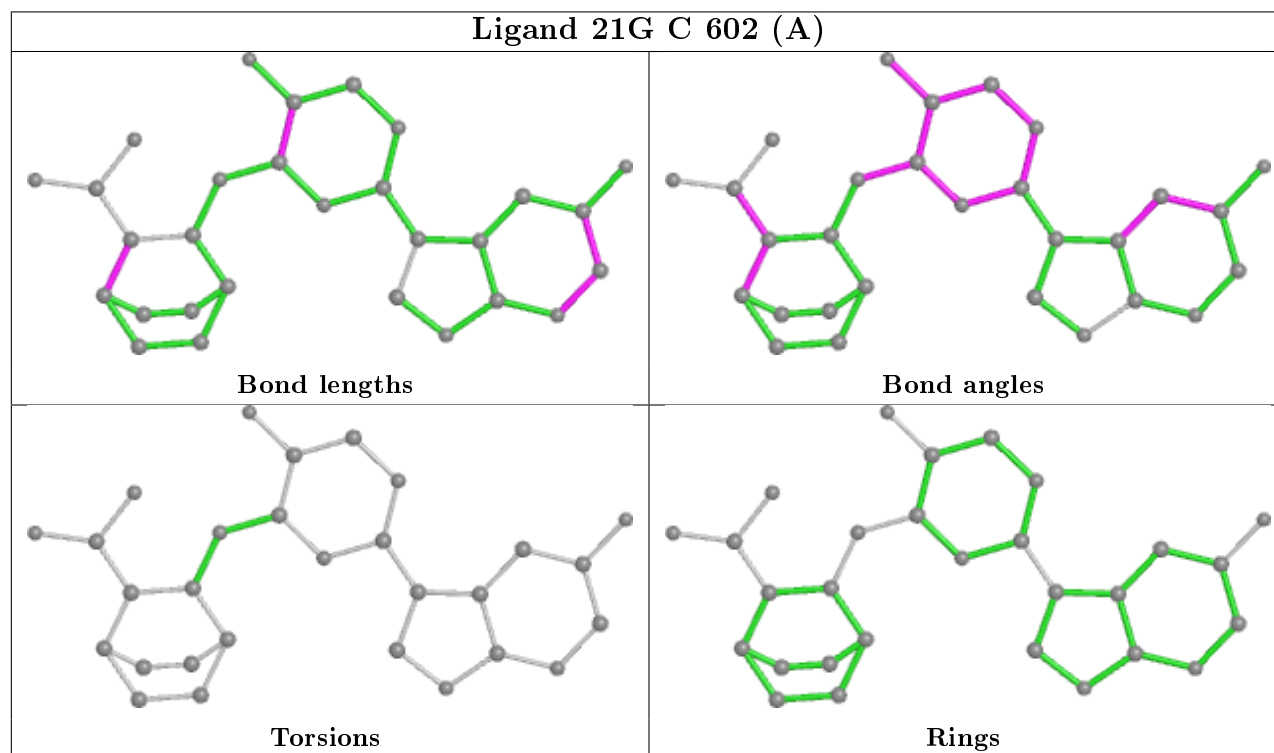
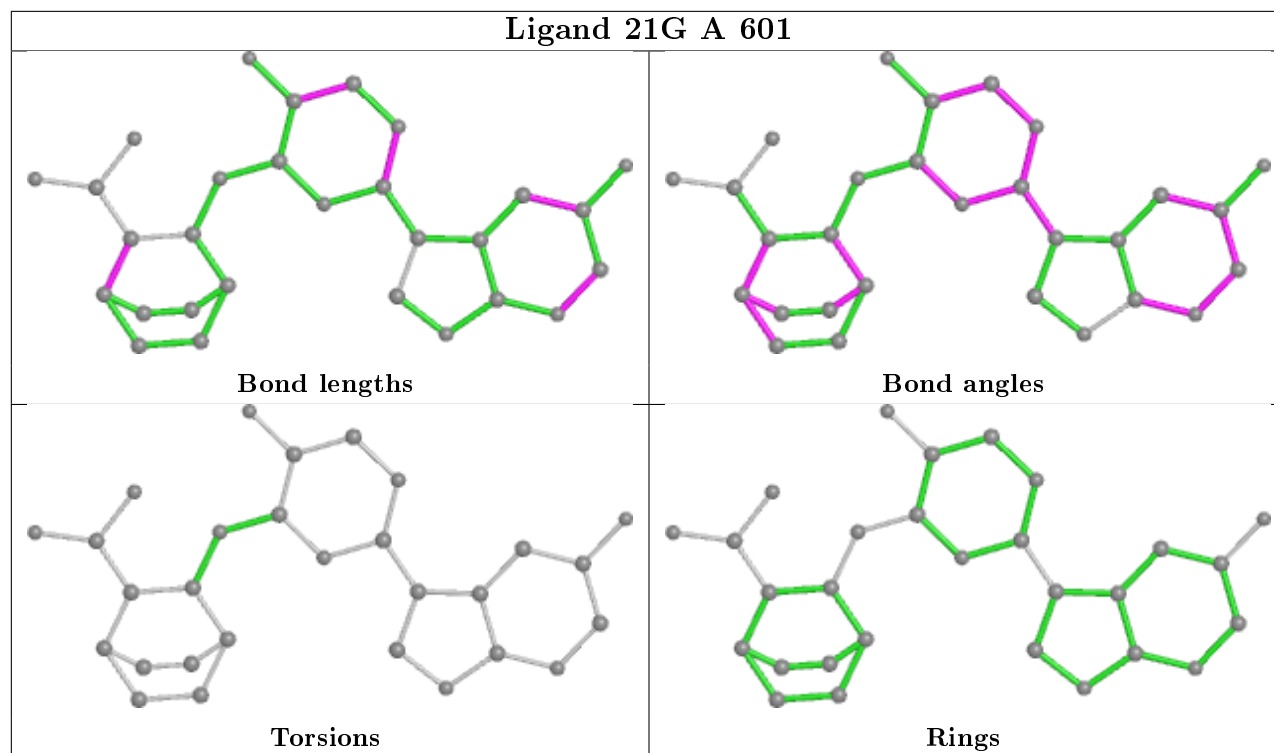
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	21G	1	0
2	A	602[B]	21G	7	0
2	C	602[A]	21G	3	0
2	A	602[A]	21G	14	0
2	C	602[B]	21G	6	0

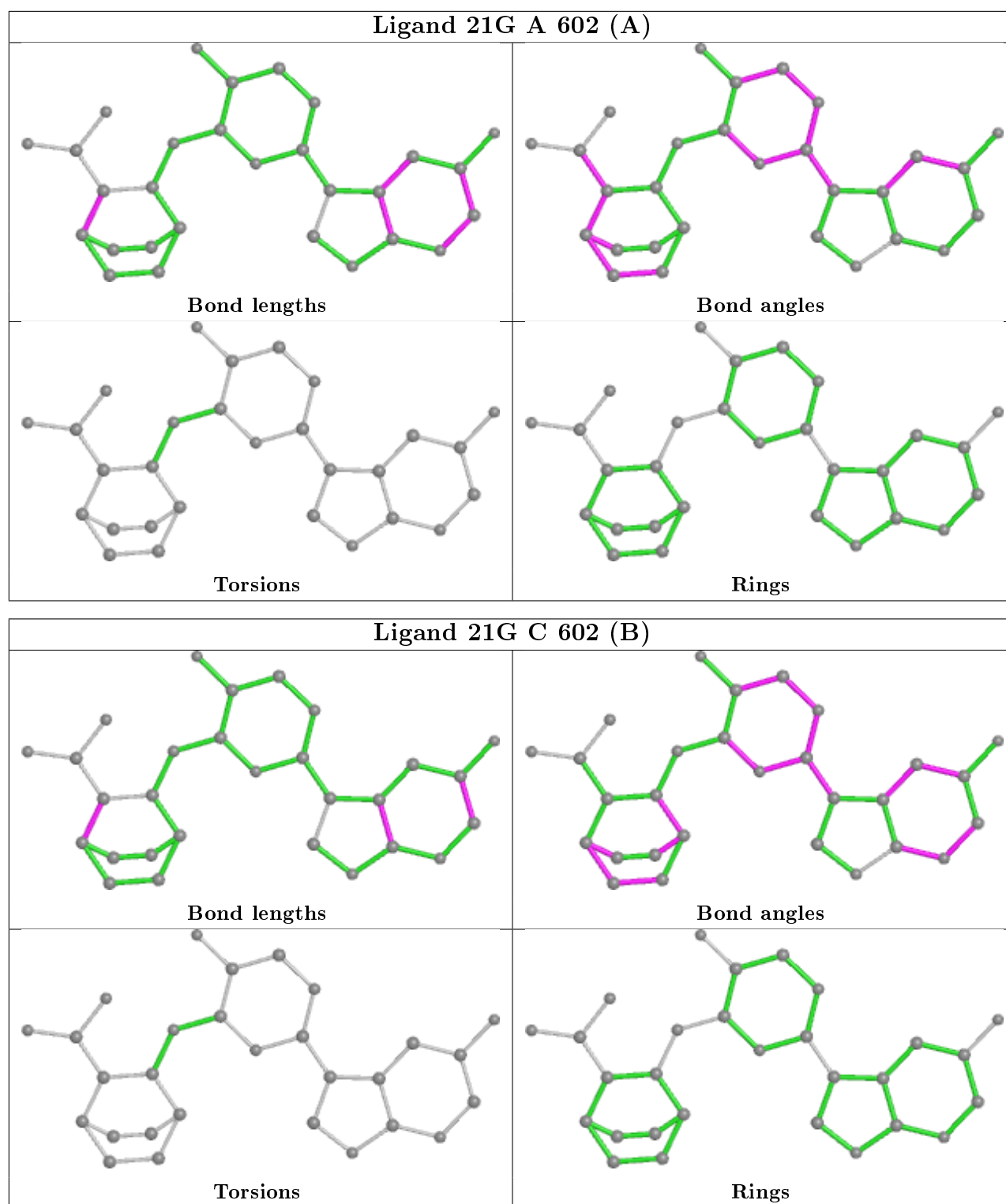
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

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	277/290 (95%)	0.36	13 (4%) 31 30	27, 45, 81, 102	0
1	C	283/290 (97%)	0.33	9 (3%) 47 48	29, 47, 92, 142	0
1	F	275/290 (94%)	0.36	15 (5%) 25 24	27, 46, 84, 126	0
1	I	278/290 (95%)	0.32	10 (3%) 42 42	28, 46, 83, 106	0
All	All	1113/1160 (95%)	0.35	47 (4%) 36 35	27, 46, 86, 142	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	252	ASN	5.0
1	C	483	MET	4.8
1	F	527	LEU	4.7
1	A	252	ASN	4.4
1	I	473	MET	4.0
1	C	250	VAL	4.0
1	C	458	MET	3.9
1	A	527	LEU	3.7
1	I	483	MET	3.6
1	F	531	TYR	3.6
1	A	289	ILE	3.3
1	F	389	ARG	3.2
1	F	529	ILE	3.2
1	F	523	GLY	3.0
1	C	251	ARG	3.0
1	A	531	TYR	2.9
1	A	458	MET	2.9
1	F	526	ARG	2.9
1	F	254	ASP	2.9
1	A	483	MET	2.9
1	A	290	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	529	ILE	2.8
1	I	389	ARG	2.8
1	F	458	MET	2.7
1	F	484	GLY	2.7
1	I	456	ASN	2.7
1	A	457	VAL	2.6
1	I	385	ILE	2.5
1	A	528	THR	2.4
1	F	255	ILE	2.4
1	F	483	MET	2.3
1	A	254	ASP	2.3
1	I	461	VAL	2.3
1	I	391	GLU	2.3
1	A	526	ARG	2.2
1	C	389	ARG	2.2
1	I	368	LYS	2.2
1	F	528	THR	2.2
1	I	397	ALA	2.2
1	C	522	HIS	2.2
1	C	463	VAL	2.1
1	A	288	GLN	2.1
1	C	459	GLY	2.1
1	F	520	GLU	2.1
1	I	396	GLU	2.1
1	F	288	GLN	2.0
1	C	269	ARG	2.0

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](#)

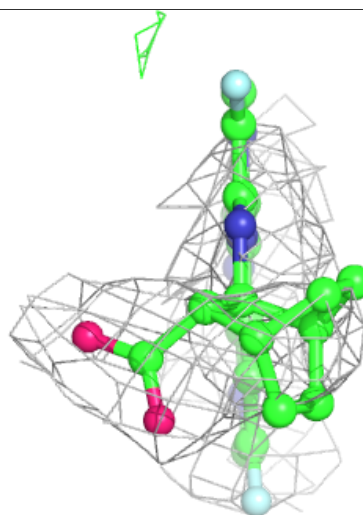
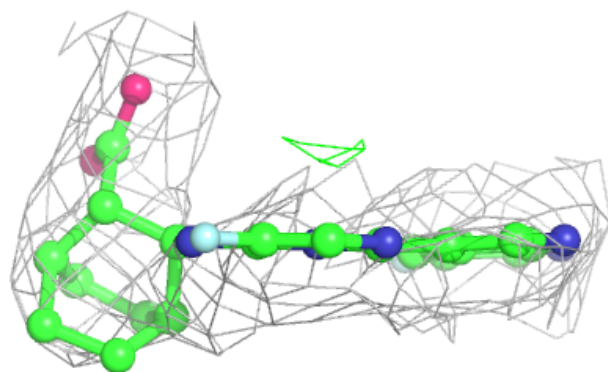
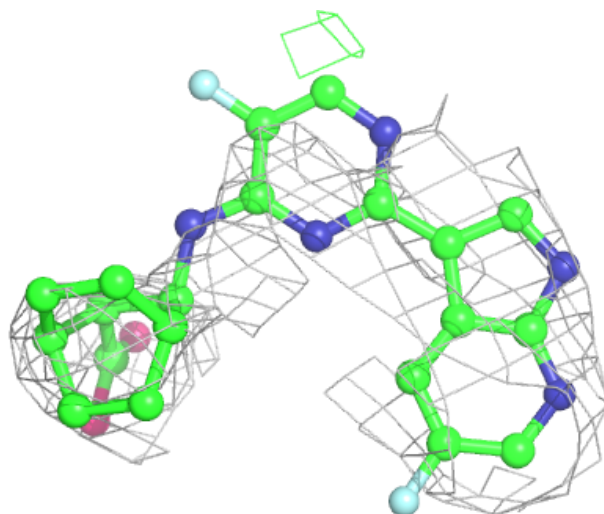
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	21G	A	602[B]	29/29	0.83	0.30	57,64,67,70	29
2	21G	A	602[A]	29/29	0.83	0.30	54,68,79,81	29
2	21G	C	602[A]	29/29	0.87	0.25	45,53,57,60	29
2	21G	C	602[B]	29/29	0.87	0.25	51,56,58,61	29
3	NI	F	602	1/1	0.96	0.07	84,84,84,84	0
2	21G	C	601	29/29	0.96	0.17	28,31,33,39	0
2	21G	I	601	29/29	0.97	0.17	28,32,40,46	0
2	21G	F	601	29/29	0.97	0.18	23,27,35,36	0
3	NI	I	602	1/1	0.97	0.04	77,77,77,77	0
2	21G	A	601	29/29	0.97	0.16	23,28,35,39	0
3	NI	A	603	1/1	0.99	0.07	64,64,64,64	0
3	NI	C	603	1/1	0.99	0.09	68,68,68,68	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.

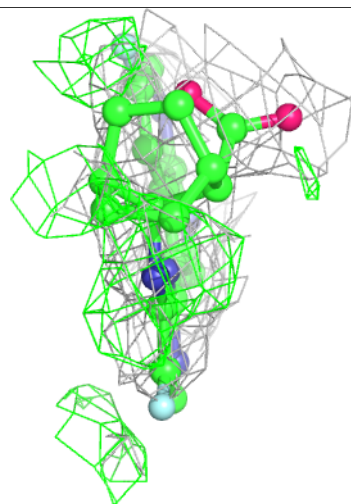
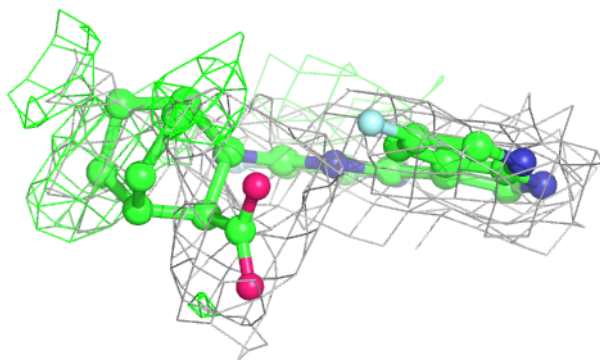
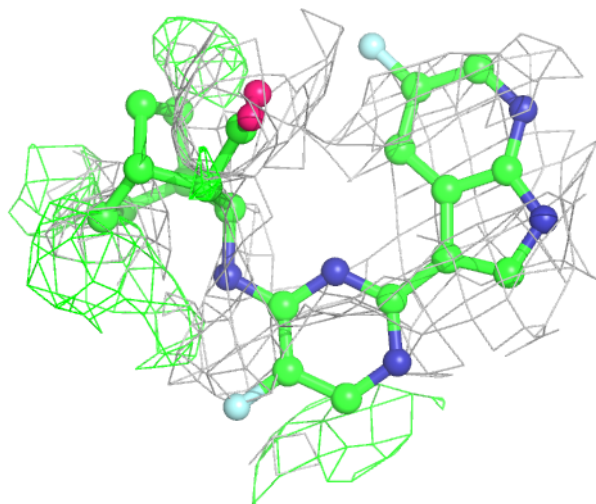
Electron density around 21G A 602 (B):

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



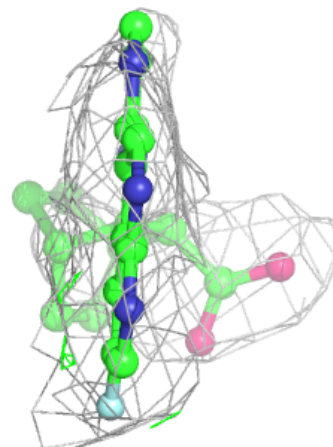
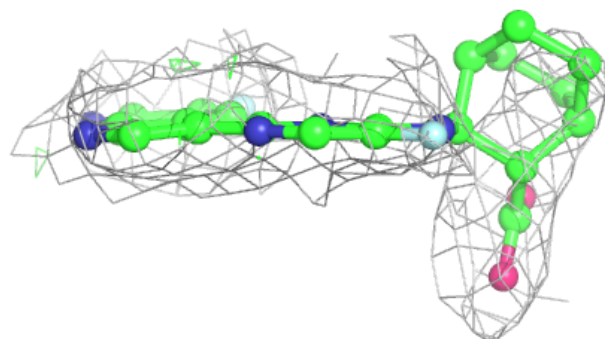
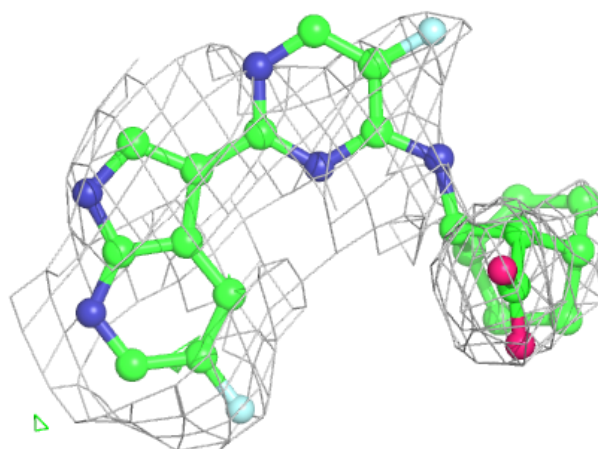
Electron density around 21G A 602 (A):

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



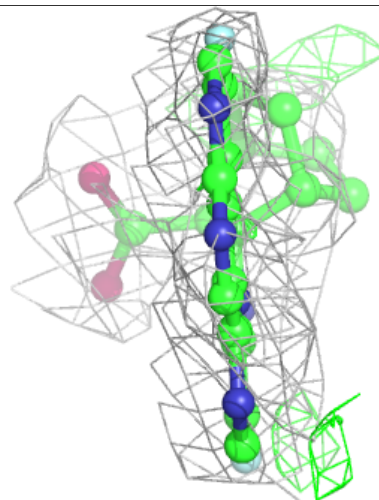
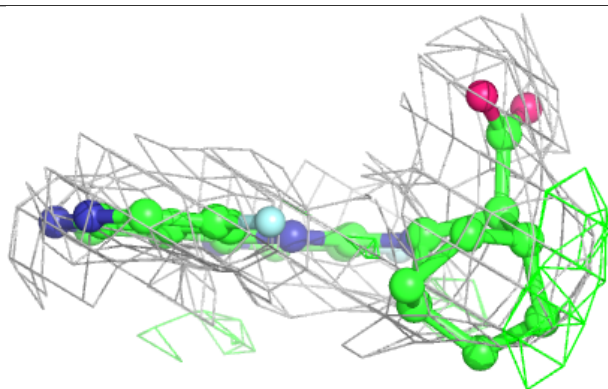
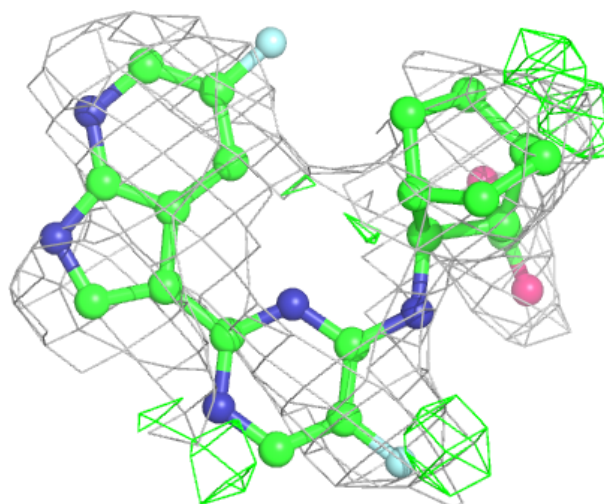
Electron density around 21G C 602 (A):

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



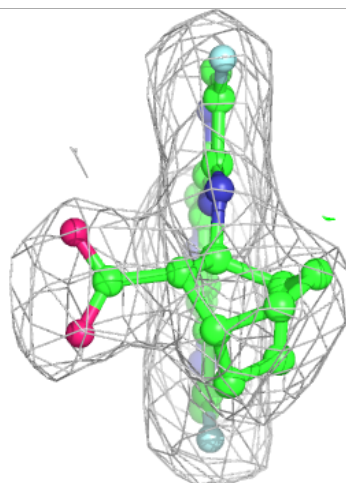
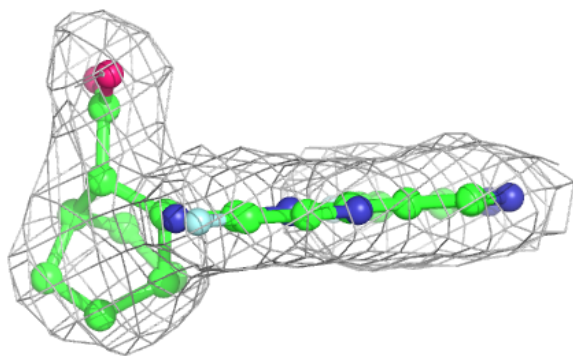
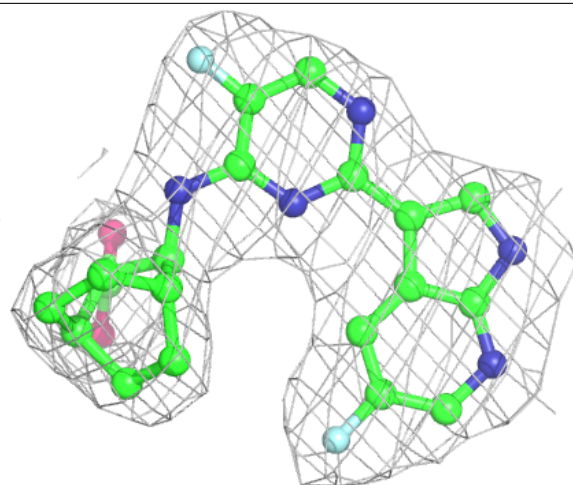
Electron density around 21G C 602 (B):

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



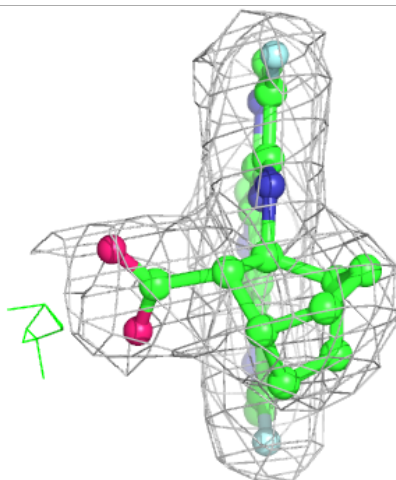
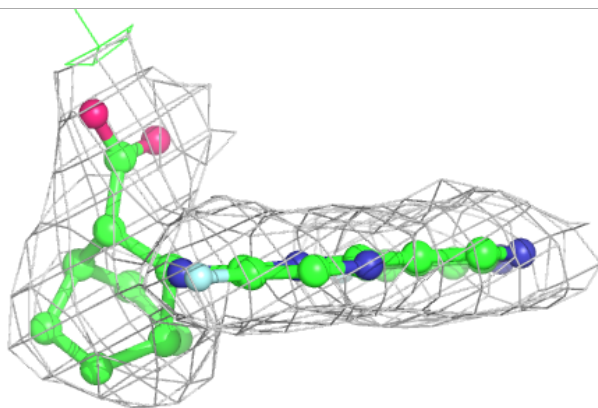
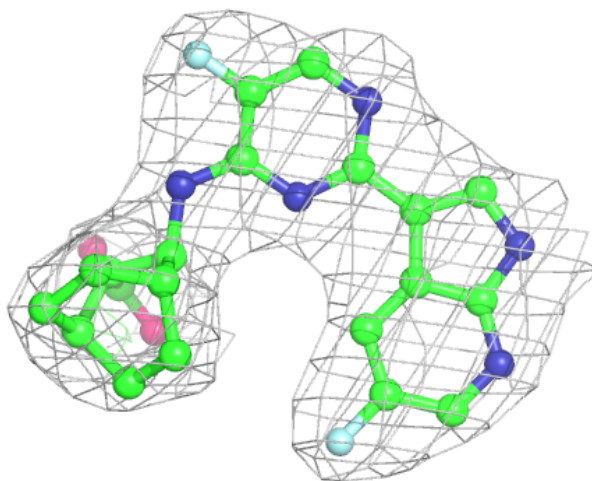
Electron density around 21G C 601:

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



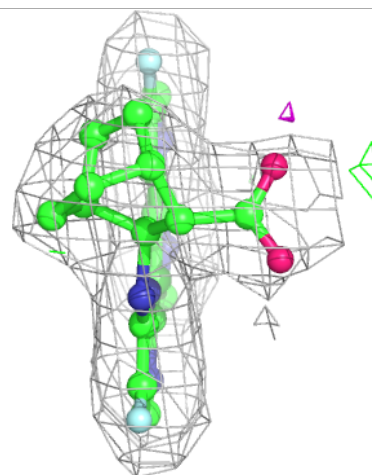
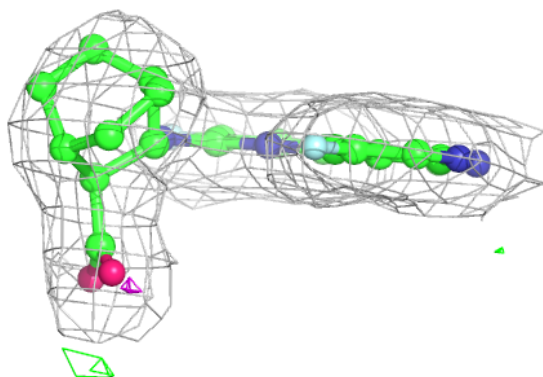
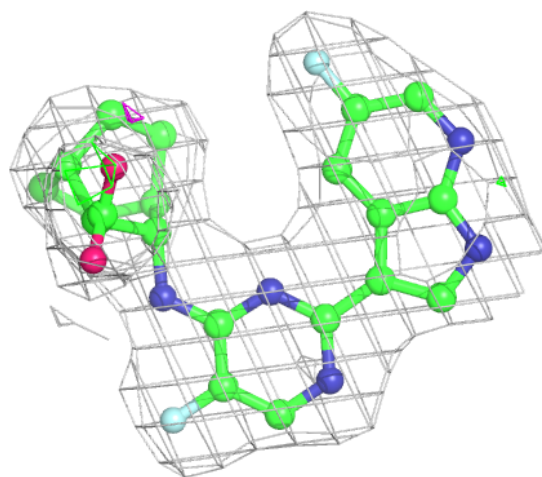
Electron density around 21G I 601:

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



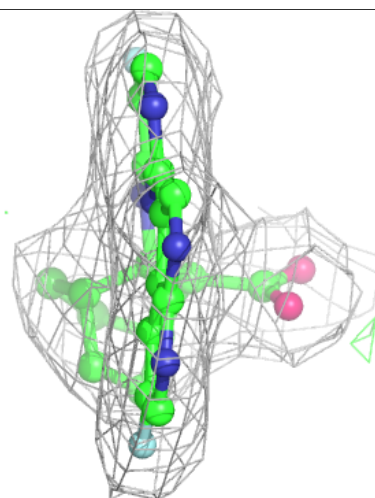
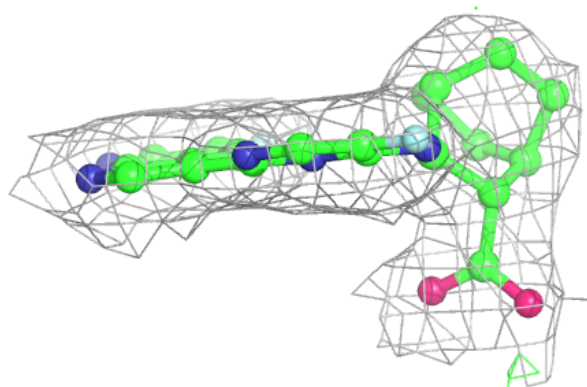
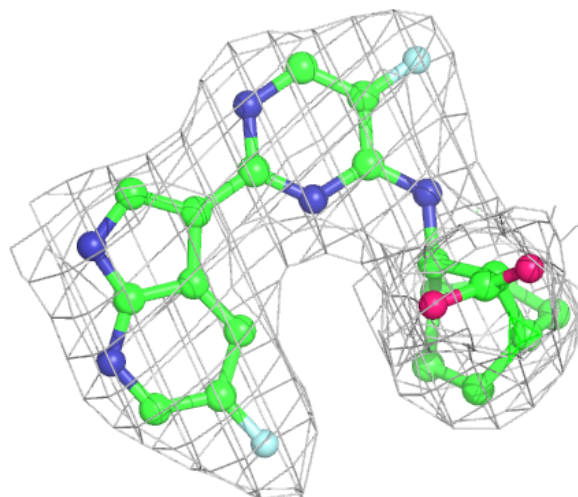
Electron density around 21G F 601:

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



Electron density around 21G A 601:

$2mF_o-DF_c$ (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.