WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 01:41 PM EDT

PDB ID	:	6CKL
Title	:	N. meningitidis CMP-sialic acid synthetase in the presence of CMP and Neu5Ac2en
Authors	:	Matthews, M.M.; Fisher, A.J.; Chen, X.
Deposited on	:	2018-02-28
Resolution	:	2.68 Å(reported)

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

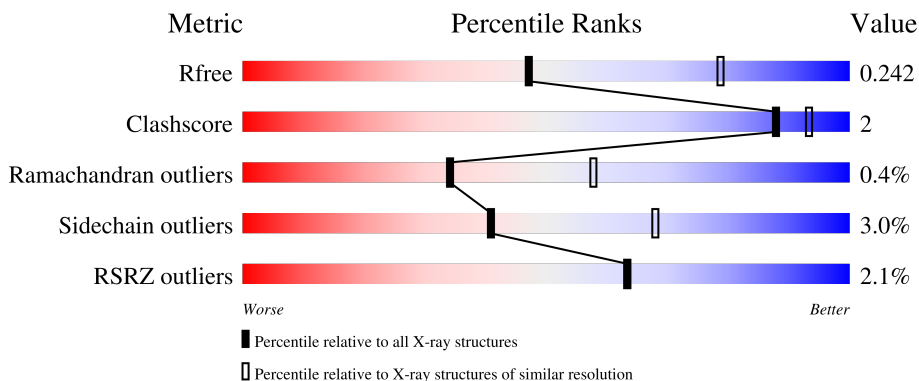|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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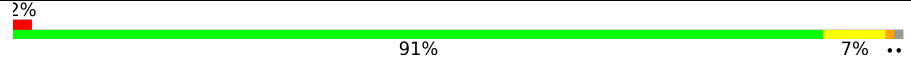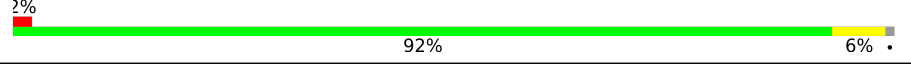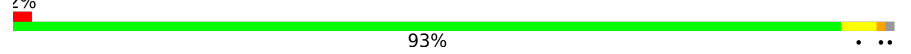*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 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		0.242
Clashscore		2
Ramachandran outliers		0.4%
Sidechain outliers		3.0%
RSRZ outliers		2.1%

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$_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	228	2% / 91% / 7% ··
1	B	228	2% / 92% / 6% ·
1	C	228	2% / 93% / · ··

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:

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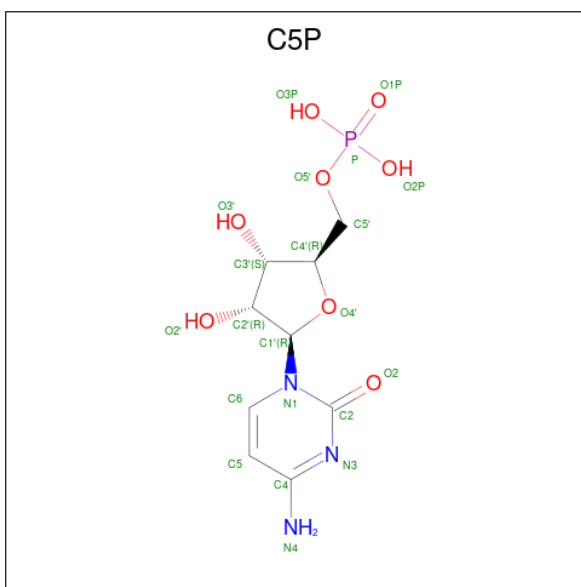| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	A	702	-	-	X	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5437 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 N-acylneuraminate cytidylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total 1722	C 1079	N 304	O 331	S 8	0	0	0
1	B	225	Total 1730	C 1084	N 307	O 331	S 8	0	1	0
1	C	225	Total 1722	C 1079	N 304	O 331	S 8	0	0	0

- Molecule 2 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: $C_9H_{14}N_3O_8P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 21	C 9	N 3	O 8	P 1	0	0
2	B	1	Total 21	C 9	N 3	O 8	P 1	0	0
2	C	1	Total 21	C 9	N 3	O 8	P 1	0	0

• Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total Cl 1 1		0	0
3	B	1	Total Cl 1 1		0	0
3	C	1	Total Cl 1 1		0	0

• Molecule 4 is 2-DEOXY-2,3-DEHYDRO-N-ACETYL-NEURAMINIC ACID (three-letter code: DAN) (formula: $C_{11}H_{17}NO_8$).
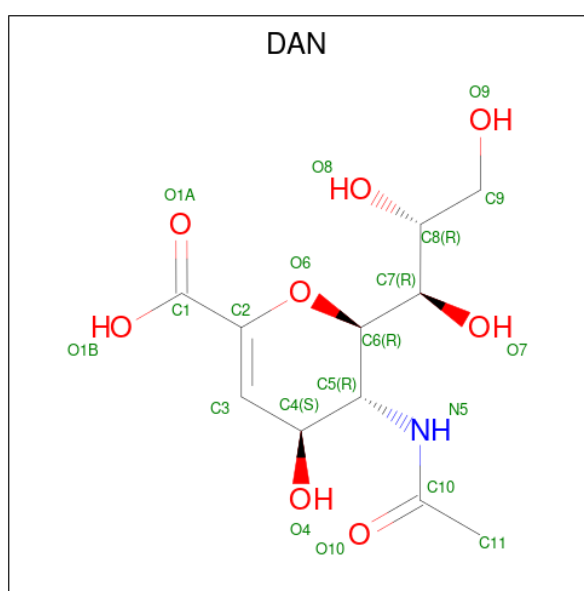
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total C N O 20 11 1 8				0	0
4	B	1	Total C N O 20 11 1 8				0	0
4	C	1	Total C N O 20 11 1 8				0	0

• Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

FLC

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 13	C 6	O 7	0	0
5	C	1	Total 13	C 6	O 7	0	0
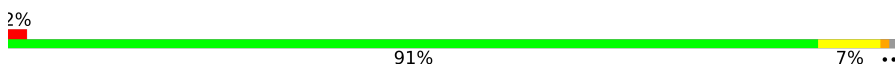
- Molecule 6 is water.

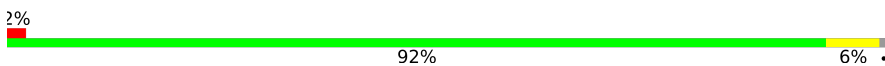| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total 37	O 37	0	0
6	B	40	Total 40	O 40	0	0
6	C	34	Total 34	O 34	0	0

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.
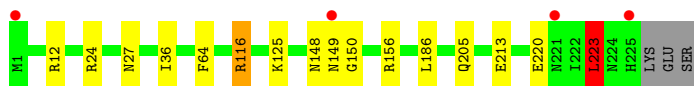
• Molecule 1: N-acylneuraminate cytidylyltransferase
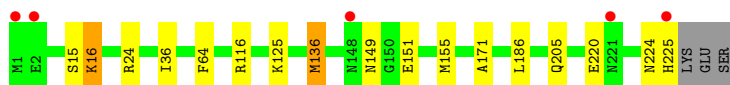
• Molecule 1: N-acylneuraminate cytidylyltransferase

• Molecule 1: N-acylneuraminate cytidylyltransferase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	128.48Å 151.01Å 84.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.86 – 2.68 37.07 – 2.68	Depositor EDS
% Data completeness (in resolution range)	97.1 (97.86-2.68) 97.2 (37.07-2.68)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.194 , 0.242 0.197 , 0.242	Depositor DCC
R_{free} test set	1118 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.309	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5437	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: C5P, CL, DAN, FLC

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	0.56	0/1750	0.77	4/2372 (0.2%)
1	B	0.60	0/1761	0.75	3/2386 (0.1%)
1	C	0.59	0/1750	0.74	1/2372 (0.0%)
All	All	0.58	0/5261	0.75	8/7130 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	136	MET	CG-SD-CE	-6.50	89.81	100.20
1	C	136	MET	CG-SD-CE	-6.10	90.43	100.20
1	B	116	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	223	LEU	CB-CG-CD2	5.73	120.74	111.00
1	A	24	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	A	116	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	16	LYS	CA-CB-CG	5.18	124.81	113.40
1	B	24	ARG	NE-CZ-NH1	-5.03	117.78	120.30

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.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1722	0	1744	7	0
1	B	1730	0	1757	5	0
1	C	1722	0	1744	4	0
2	A	21	0	12	3	0
2	B	21	0	12	1	0
2	C	21	0	12	2	0
3	A	1	0	0	2	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	20	0	16	1	0
4	B	20	0	16	3	0
4	C	20	0	16	2	0
5	B	13	0	5	0	0
5	C	13	0	5	1	0
6	A	37	0	0	1	0
6	B	40	0	0	0	0
6	C	34	0	0	0	0
All	All	5437	0	5339	21	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 2.

All (21) 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)
2:A:701:C5P:O2P	4:B:301:DAN:C2	2.08	1.01
4:A:703:DAN:C2	2:B:303:C5P:O1P	2.31	0.78
4:C:301:DAN:C2	2:C:302:C5P:O2P	2.46	0.64
2:A:701:C5P:O2P	4:B:301:DAN:C3	2.48	0.61
5:C:303:FLC:OB2	5:C:303:FLC:CGC	2.50	0.59
4:C:301:DAN:C3	2:C:302:C5P:O2P	2.51	0.59
1:A:15:SER:HB3	3:A:702:CL:CL	2.39	0.59
1:A:136:MET:HE3	1:A:171:ALA:HB1	1.92	0.51
1:A:205:GLN:HB2	6:A:825:HOH:O	2.13	0.48
1:B:213:GLU:HG2	1:C:214:LEU:HD11	1.94	0.48
1:A:224:ASN:O	1:A:225:HIS:CG	2.68	0.46
1:B:27:ASN:HD22	1:B:223:LEU:HD12	1.81	0.46
1:C:136:MET:HE3	1:C:171:ALA:HB1	1.97	0.46
1:A:15:SER:CB	3:A:702:CL:CL	3.01	0.46
2:A:701:C5P:O2P	4:B:301:DAN:C1	2.64	0.43
1:A:36:ILE:HG21	1:A:64:PHE:HB3	2.01	0.43
1:B:36:ILE:HG21	1:B:64:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ILE:HG21	1:C:64:PHE:HB3	2.01	0.42
1:C:148:ASN:O	1:C:150:GLY:N	2.54	0.41
1:A:155:MET:CE	1:B:156[A]:ARG:NE	2.85	0.40
1:B:148:ASN:O	1:B:150:GLY:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/228 (98%)	218 (98%)	4 (2%)	1 (0%)	34	58
1	B	224/228 (98%)	219 (98%)	4 (2%)	1 (0%)	34	58
1	C	223/228 (98%)	219 (98%)	3 (1%)	1 (0%)	34	58
All	All	670/684 (98%)	656 (98%)	11 (2%)	3 (0%)	34	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	ASN
1	C	149	ASN
1	A	149	ASN

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	192/195 (98%)	187 (97%)	5 (3%)	46	73
1	B	193/195 (99%)	186 (96%)	7 (4%)	35	61
1	C	192/195 (98%)	187 (97%)	5 (3%)	46	73
All	All	577/585 (99%)	560 (97%)	17 (3%)	41	69

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	125	LYS
1	A	151	GLU
1	A	186	LEU
1	A	220	GLU
1	B	12	ARG
1	B	116	ARG
1	B	125	LYS
1	B	186	LEU
1	B	205	GLN
1	B	220	GLU
1	B	223	LEU
1	C	125	LYS
1	C	149	ASN
1	C	186	LEU
1	C	220	GLU
1	C	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	B	63	ASN
1	C	63	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 3 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	C5P	B	303	-	22,22,22	0.96	1 (4%)	33,33,33	1.23	4 (12%)
4	DAN	C	301	-	20,20,20	1.30	3 (15%)	23,28,28	1.55	5 (21%)
2	C5P	A	701	-	22,22,22	0.94	0	33,33,33	1.11	3 (9%)
5	FLC	B	302	-	12,12,12	1.17	1 (8%)	17,17,17	1.43	3 (17%)
5	FLC	C	303	-	12,12,12	1.02	0	17,17,17	1.29	1 (5%)
4	DAN	B	301	-	20,20,20	1.07	1 (5%)	23,28,28	1.42	3 (13%)
2	C5P	C	302	-	22,22,22	0.91	1 (4%)	33,33,33	1.05	1 (3%)
4	DAN	A	703	-	20,20,20	1.13	1 (5%)	23,28,28	1.30	2 (8%)

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	C5P	B	303	-	-	2/10/26/26	0/2/2/2
4	DAN	C	301	-	-	0/18/34/34	0/1/1/1
2	C5P	A	701	-	-	2/10/26/26	0/2/2/2
5	FLC	B	302	-	-	7/16/16/16	-
5	FLC	C	303	-	-	5/16/16/16	-
4	DAN	B	301	-	-	2/18/34/34	0/1/1/1
2	C5P	C	302	-	-	2/10/26/26	0/2/2/2
4	DAN	A	703	-	-	0/18/34/34	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	DAN	O6-C6	-3.18	1.40	1.46
4	C	301	DAN	C4-C3	2.69	1.53	1.50
4	C	301	DAN	C3-C2	2.44	1.36	1.33
4	C	301	DAN	O6-C2	2.33	1.46	1.37
4	A	703	DAN	O6-C6	-2.31	1.42	1.46
5	B	302	FLC	OA2-CAC	-2.24	1.23	1.30
2	C	302	C5P	C6-C5	2.23	1.40	1.35
2	B	303	C5P	C5-C4	-2.21	1.37	1.42

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	DAN	C6-C5-N5	-4.22	103.90	110.91
2	B	303	C5P	O2P-P-O3P	3.74	121.93	107.64
5	C	303	FLC	OB2-CBC-CB	3.56	119.23	113.05
4	A	703	DAN	C9-C8-C7	-3.49	104.85	112.41
4	C	301	DAN	O6-C2-C3	-3.12	120.97	124.61
4	C	301	DAN	O9-C9-C8	-3.01	104.52	111.07
2	B	303	C5P	O5'-P-O1P	-2.88	98.41	106.47
2	A	701	C5P	O2P-P-O3P	2.82	118.41	107.64
4	B	301	DAN	O1B-C1-C2	2.78	121.13	114.20
4	A	703	DAN	O1B-C1-C2	2.69	120.92	114.20
2	C	302	C5P	O2P-P-O5'	-2.59	99.83	106.73
2	A	701	C5P	O2P-P-O5'	-2.54	99.98	106.73
2	B	303	C5P	O3P-P-O5'	-2.50	100.07	106.73
5	B	302	FLC	OB2-CBC-CB	2.45	117.31	113.05
2	B	303	C5P	O3'-C3'-C4'	-2.43	104.02	111.05
4	C	301	DAN	C6-C5-N5	-2.33	107.04	110.91
2	A	701	C5P	O4'-C1'-N1	-2.29	103.14	108.36
5	B	302	FLC	OG2-CGC-CG	2.20	121.41	114.35
4	C	301	DAN	O7-C7-C8	-2.19	103.53	108.81
4	C	301	DAN	O1B-C1-O1A	-2.17	118.65	123.61
5	B	302	FLC	OG1-CGC-CG	-2.05	116.97	122.94
4	B	301	DAN	O9-C9-C8	-2.01	106.69	111.07

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	303	FLC	CA-CB-CBC-OB1
5	C	303	FLC	CA-CB-CBC-OB2

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Mol	Chain	Res	Type	Atoms
5	C	303	FLC	OHB-CB-CBC-OB1
5	C	303	FLC	OHB-CB-CBC-OB2
2	B	303	C5P	C3'-C4'-C5'-O5'
5	B	302	FLC	CBC-CB-CG-CGC
5	B	302	FLC	OHB-CB-CG-CGC
2	B	303	C5P	O4'-C4'-C5'-O5'
2	A	701	C5P	C3'-C4'-C5'-O5'
2	A	701	C5P	O4'-C4'-C5'-O5'
2	C	302	C5P	O4'-C4'-C5'-O5'
2	C	302	C5P	C3'-C4'-C5'-O5'
5	B	302	FLC	CA-CB-CG-CGC
5	B	302	FLC	CA-CB-CBC-OB1
5	B	302	FLC	CA-CB-CBC-OB2
5	B	302	FLC	CAC-CA-CB-OHB
5	C	303	FLC	CBC-CB-CG-CGC
4	B	301	DAN	O1A-C1-C2-C3
4	B	301	DAN	C6-C5-N5-C10
5	B	302	FLC	CAC-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	303	C5P	1	0
4	C	301	DAN	2	0
2	A	701	C5P	3	0
5	C	303	FLC	1	0
4	B	301	DAN	3	0
2	C	302	C5P	2	0
4	A	703	DAN	1	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
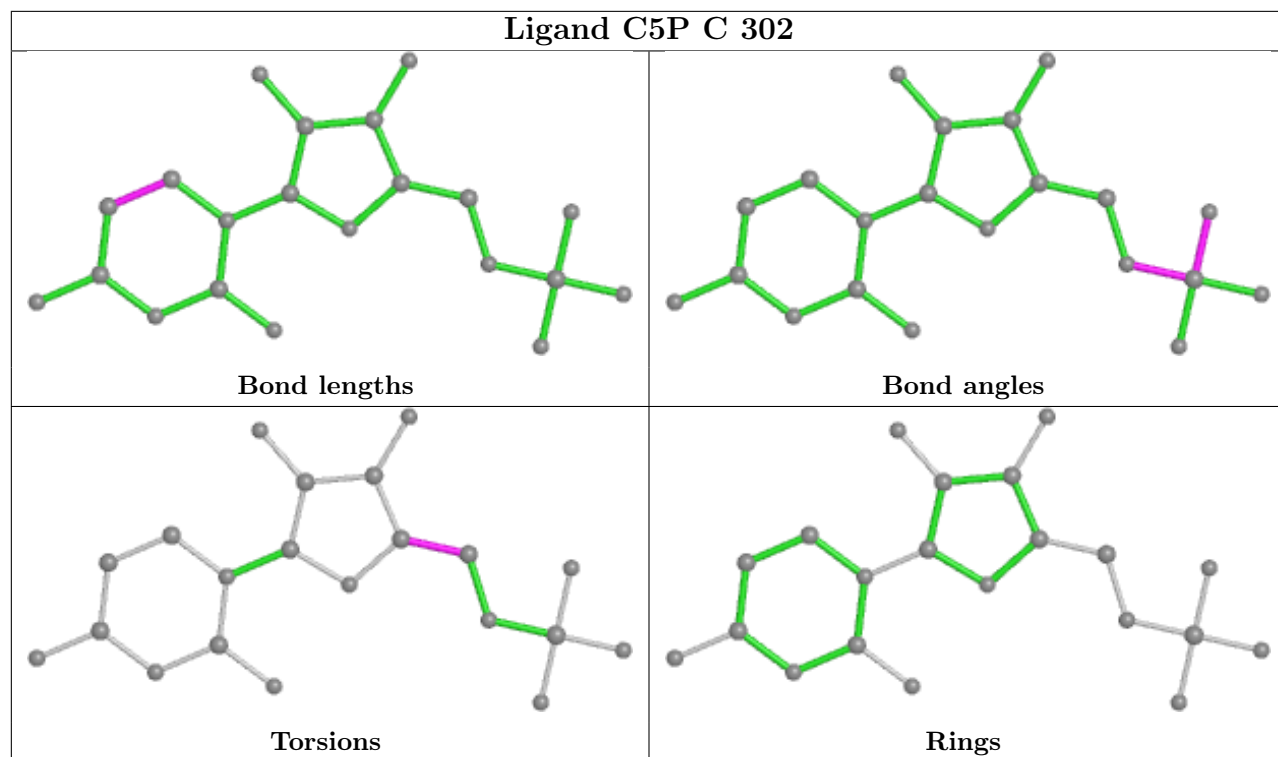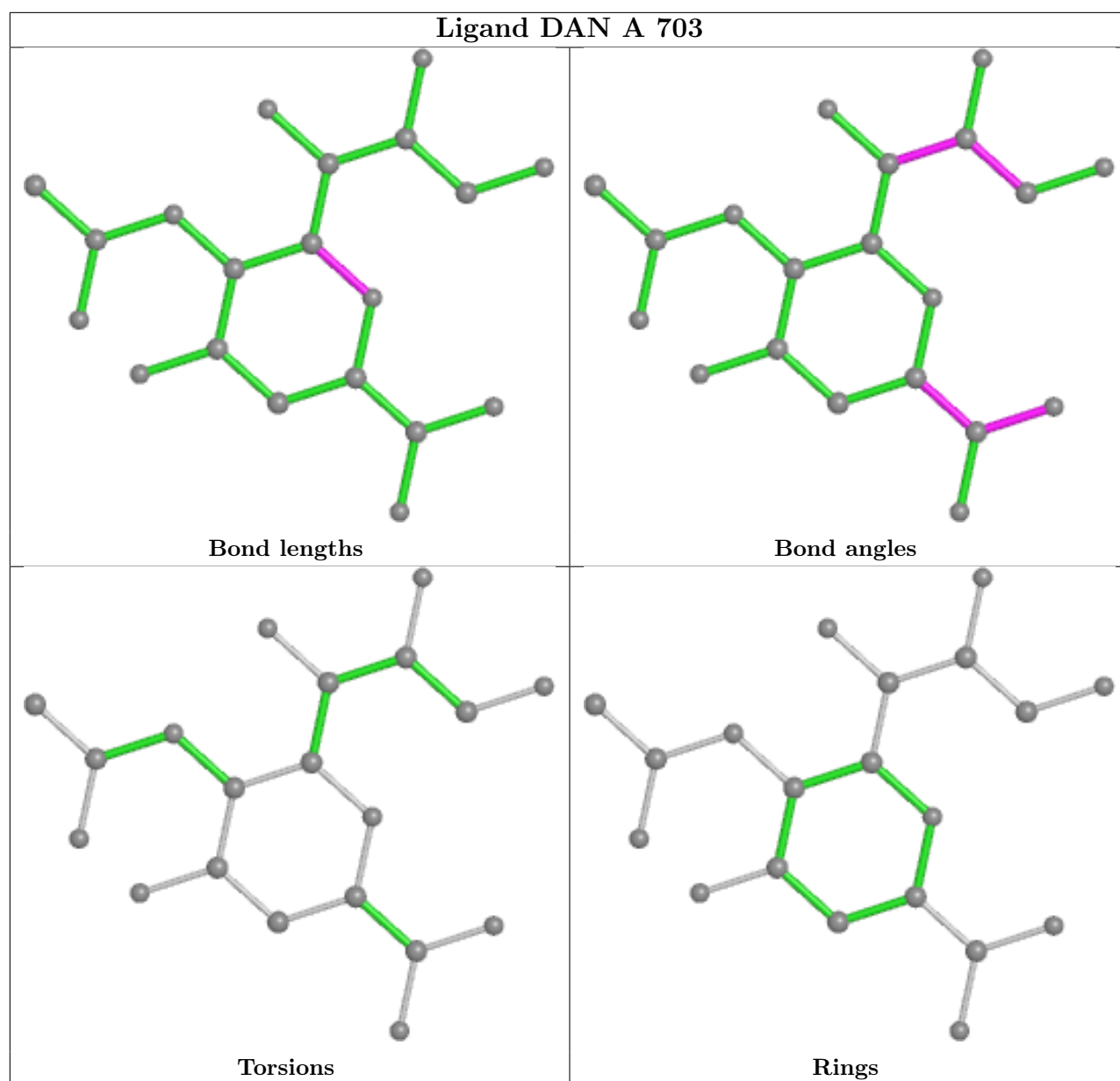
equivalents in the CSD to analyse the geometry.

Ligand C5P B 303

Bond lengths

Bond angles

Torsions

Rings

Ligand DAN C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand C5P A 701

Bond lengths

Bond angles

Torsions

Rings

Ligand DAN B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand C5P C 302

Bond lengths

Bond angles

Torsions

Rings

Ligand DAN A 703

Bond lengths

Bond angles

Torsions

Rings
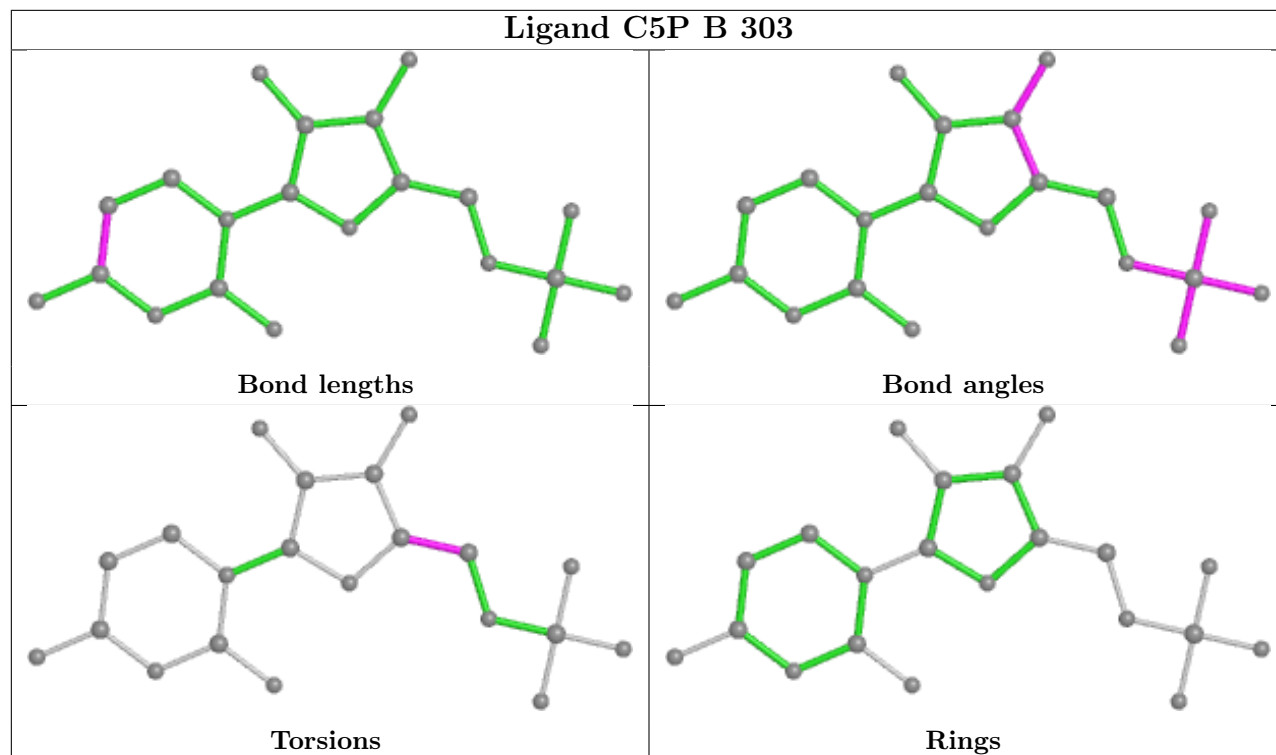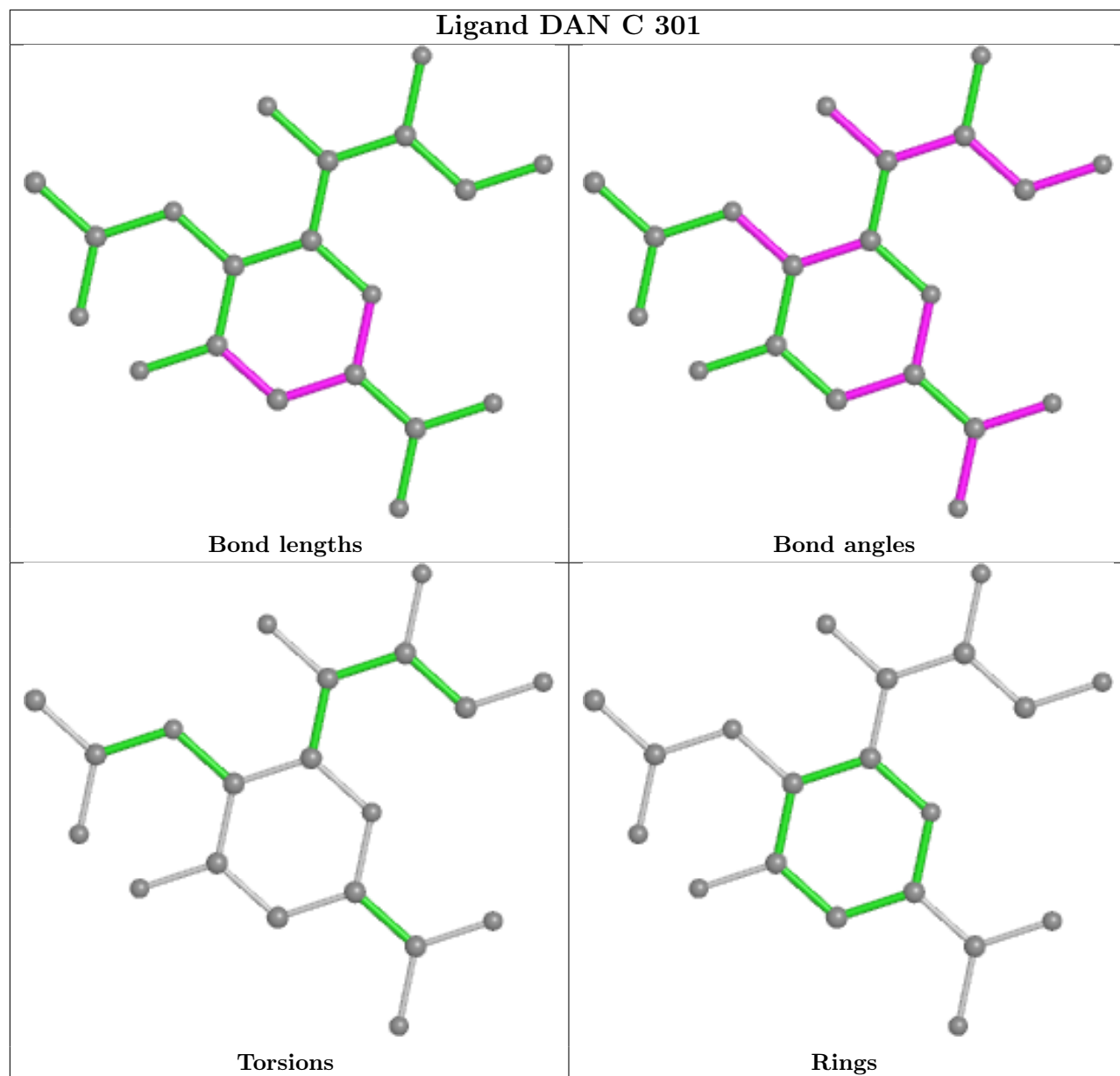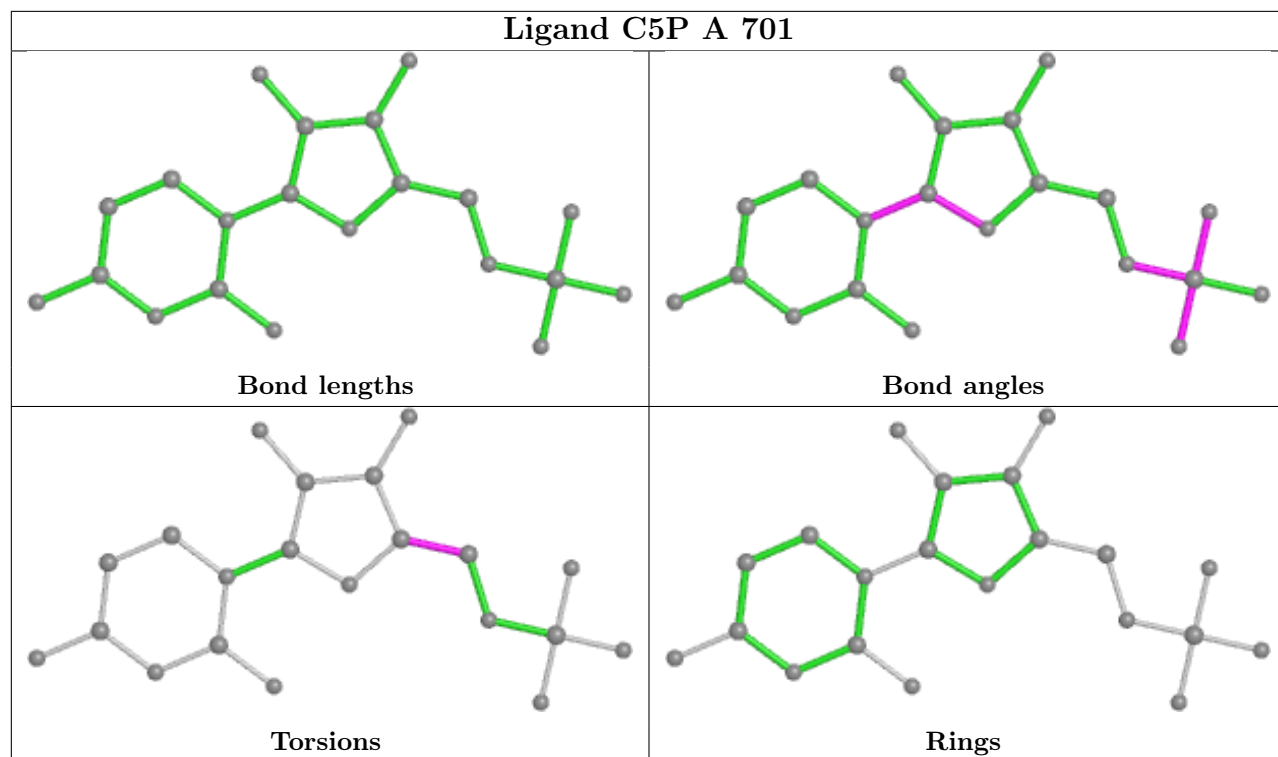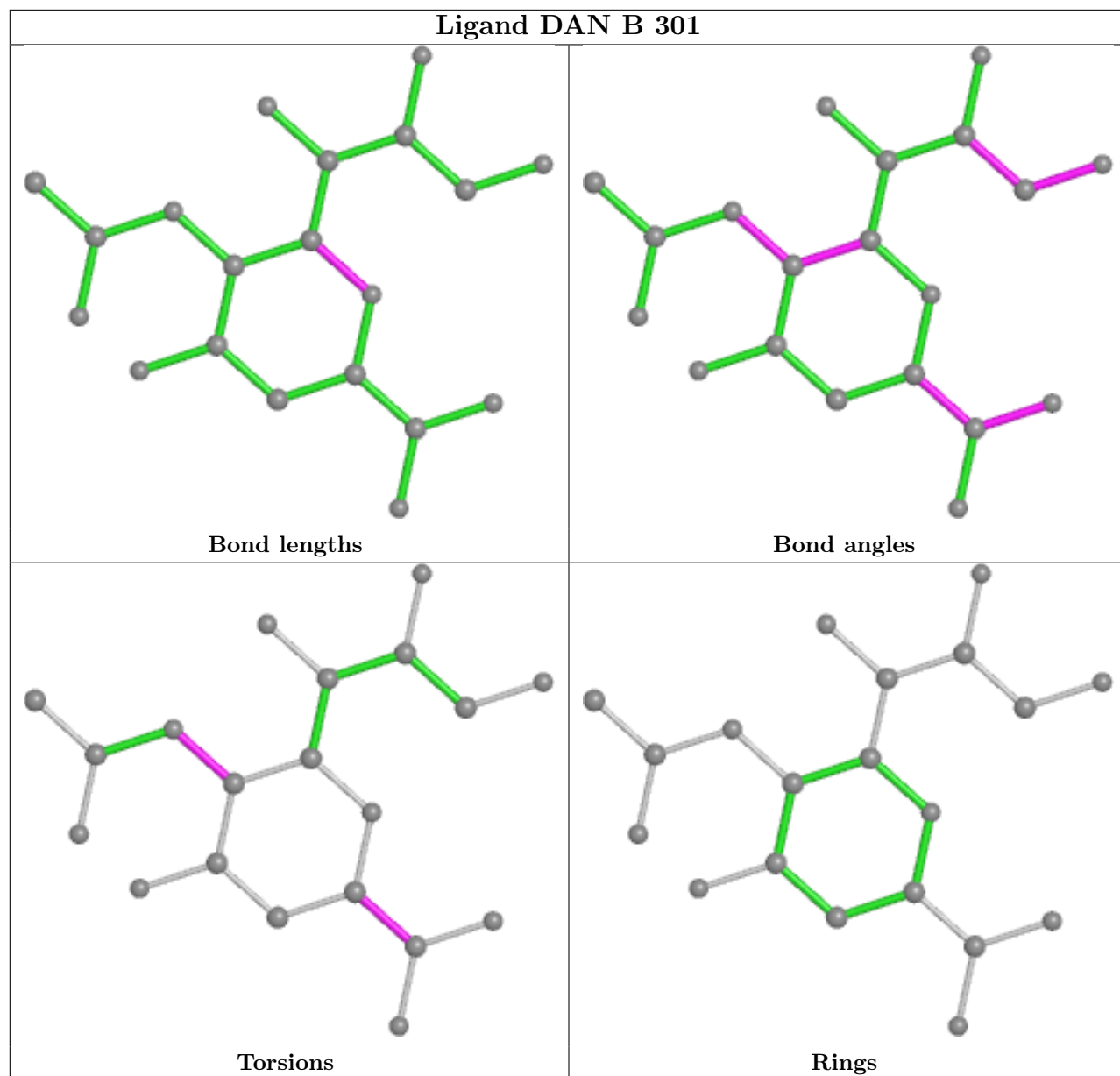
5.7 Other polymers (i)

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 ⓘ

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	225/228 (98%)	-0.22	5 (2%)	62	61	27, 41, 71, 75	0
1	B	225/228 (98%)	-0.36	4 (1%)	68	69	27, 40, 67, 75	0
1	C	225/228 (98%)	-0.30	5 (2%)	62	61	26, 39, 69, 75	0
All	All	675/684 (98%)	-0.29	14 (2%)	63	63	26, 40, 70, 75	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	6.8
1	C	1	MET	4.3
1	C	149	ASN	3.9
1	B	1	MET	3.3
1	C	225	HIS	3.0
1	C	223	LEU	2.8
1	A	225	HIS	2.6
1	B	221	ASN	2.5
1	A	148	ASN	2.5
1	B	225	HIS	2.4
1	A	2	GLU	2.4
1	A	221	ASN	2.3
1	C	125	LYS	2.1
1	B	149	ASN	2.0

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

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

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6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

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
5	FLC	B	302	13/13	0.90	0.17	63,69,75,75	0
3	CL	C	304	1/1	0.94	0.08	48,48,48,48	0
4	DAN	C	301	20/20	0.95	0.16	32,41,55,62	0
5	FLC	C	303	13/13	0.95	0.31	55,62,67,69	13
2	C5P	C	302	21/21	0.97	0.13	32,35,42,46	0
4	DAN	A	703	20/20	0.97	0.11	34,36,41,47	0
4	DAN	B	301	20/20	0.97	0.13	32,40,42,49	0
2	C5P	B	303	21/21	0.98	0.11	32,35,39,43	0
2	C5P	A	701	21/21	0.98	0.13	27,32,34,38	0
3	CL	B	304	1/1	0.98	0.08	42,42,42,42	0
3	CL	A	702	1/1	0.99	0.06	40,40,40,40	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.
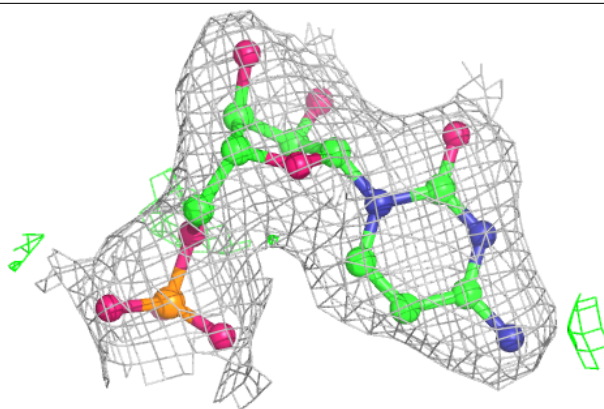
Electron density around DAN C 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
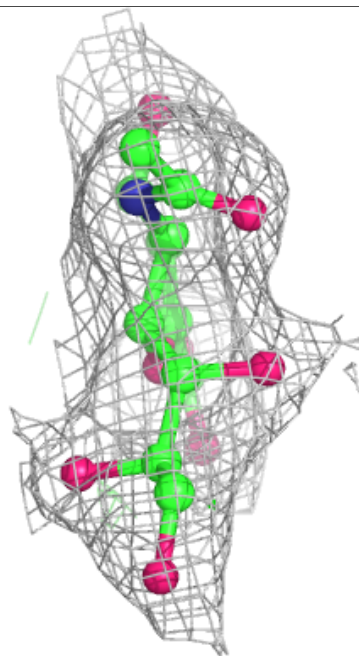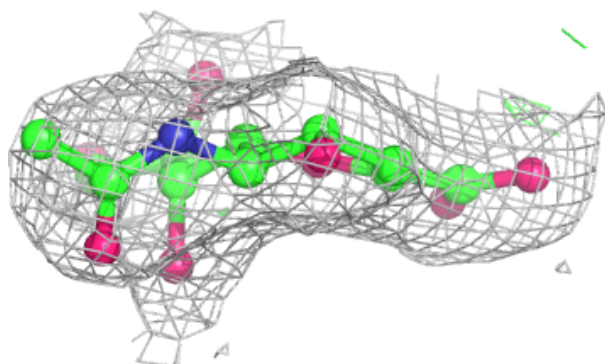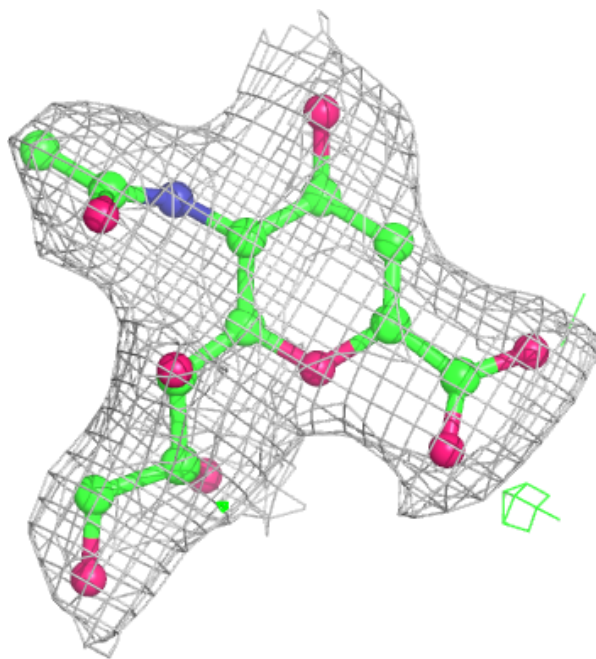$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
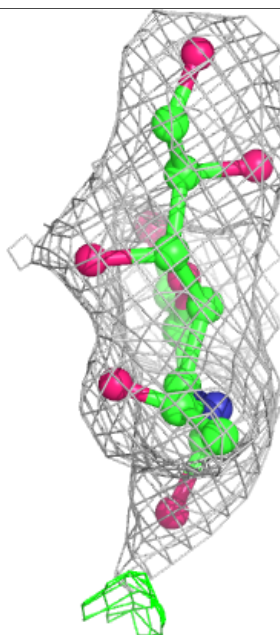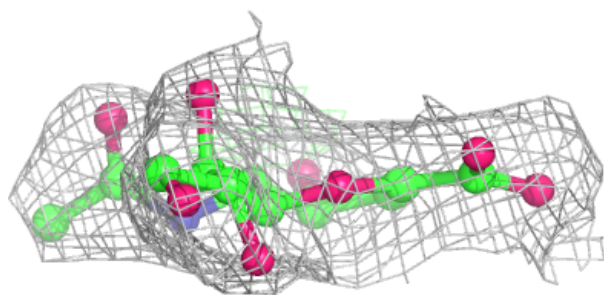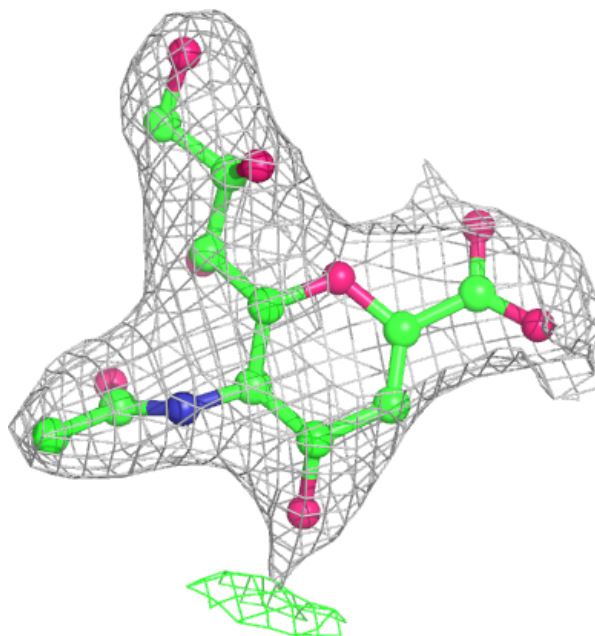
Electron density around C5P C 302:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
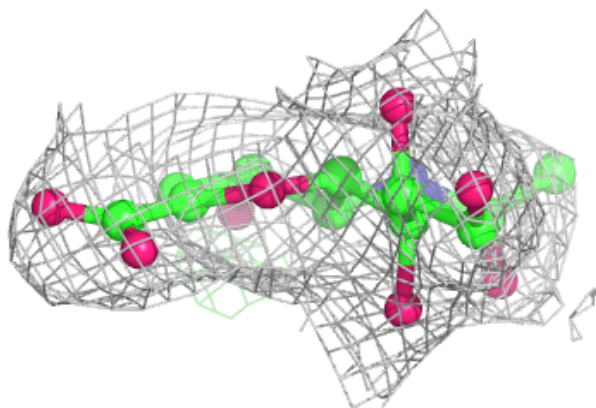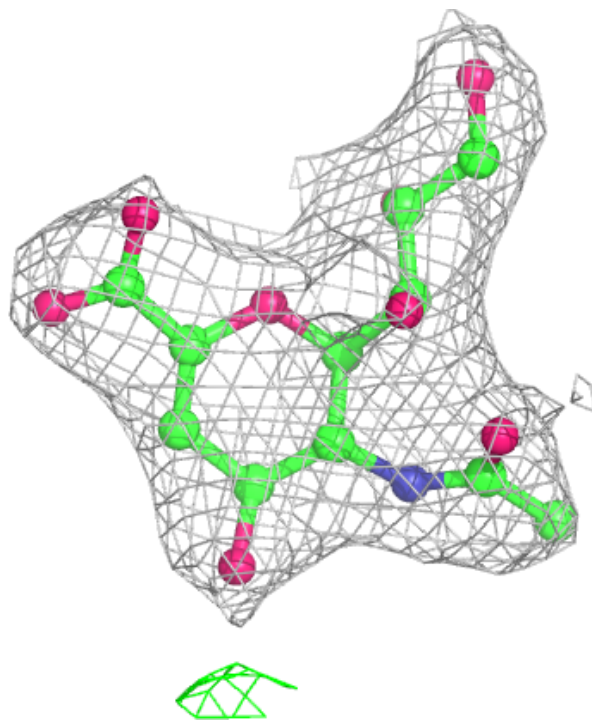mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
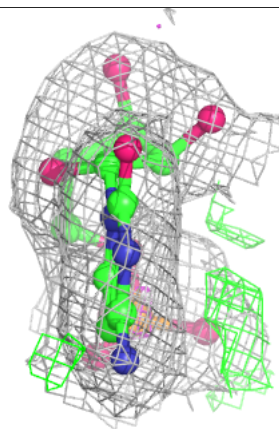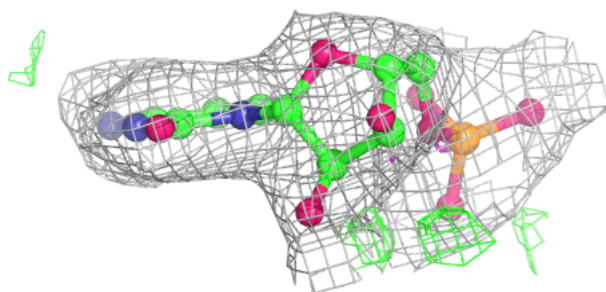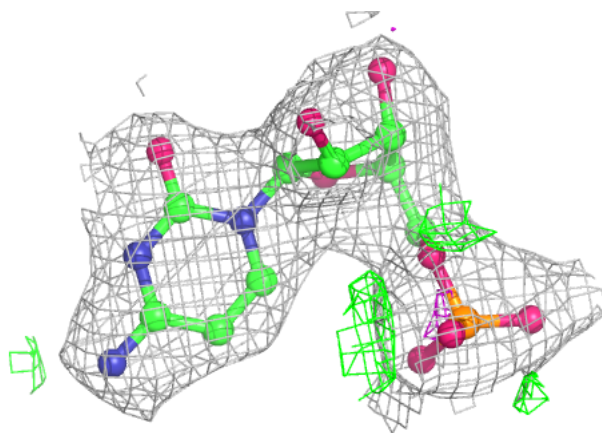and green (positive)
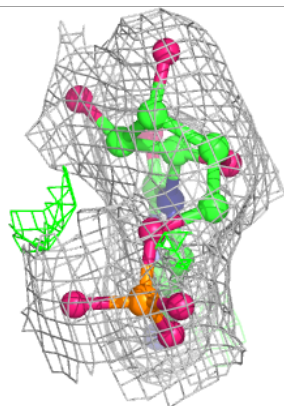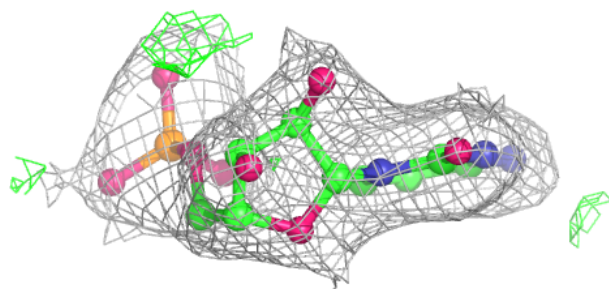
Electron density around DAN A 703:

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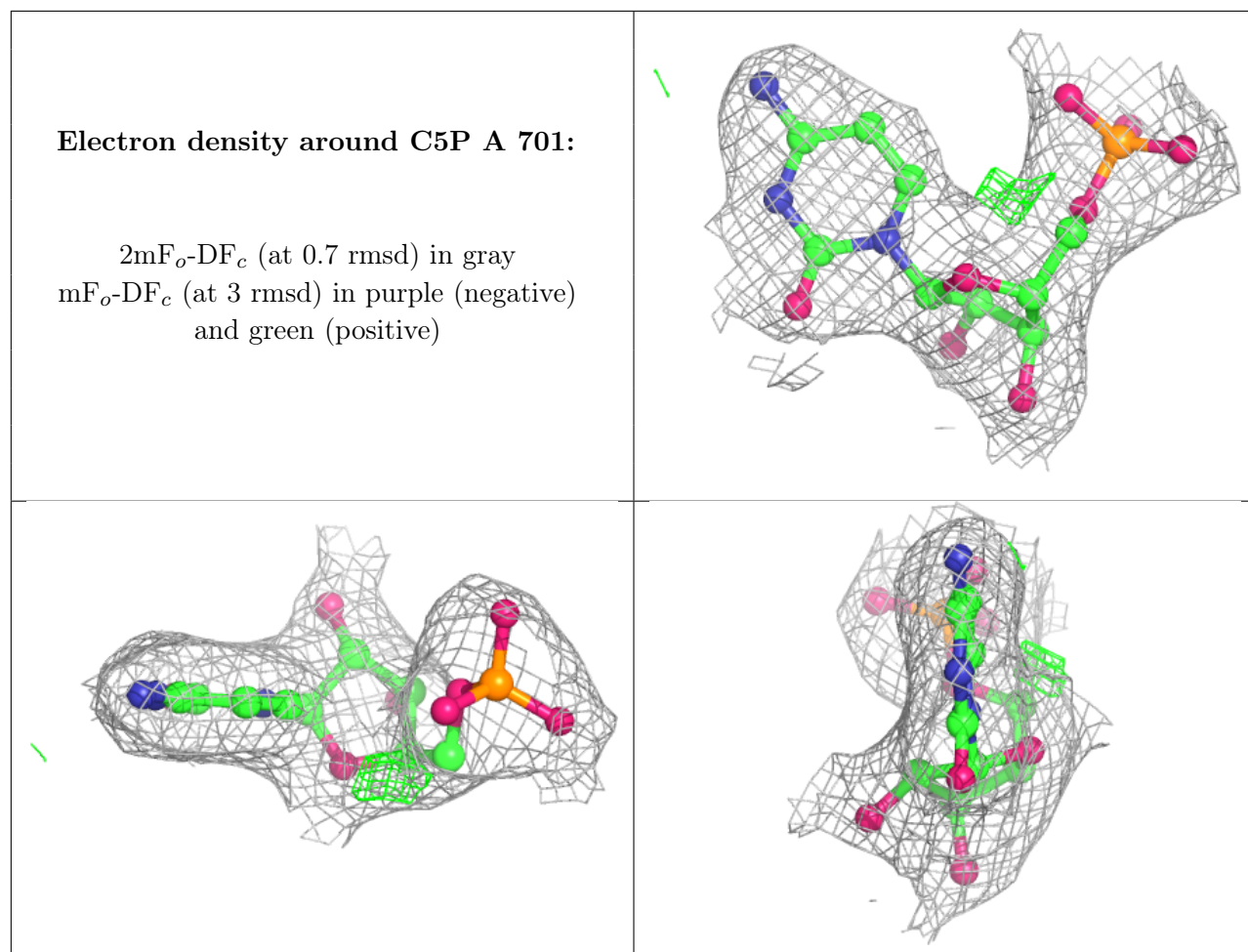and green (positive)

Electron density around DAN B 301:

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

Electron density around C5P B 303:

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

Electron density around C5P A 701:

$2mF_o$-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.