



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:46 AM BST

PDB ID : 6LD4
Title : Zika NS5 polymerase domain
Authors : El Sahili, A.; Lescar, J.
Deposited on : 2019-11-20
Resolution : 1.50 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 : **FAILED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

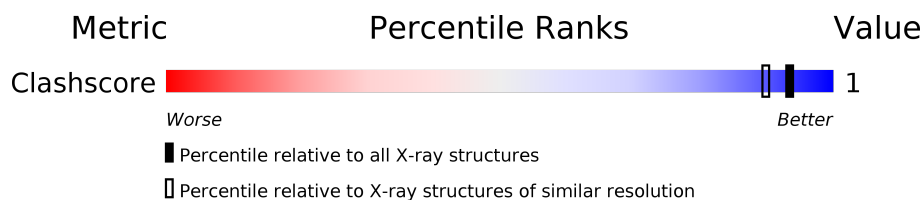
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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))
Clashscore	141614	3144 (1.50-1.50)

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 $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	645	 84% • 13%

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
3	G8O	A	903[B]	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5408 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 RNA-directed RNA polymerase NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	562	Total	C	N	O	S	0	6	0
			4674	2955	856	831	32			

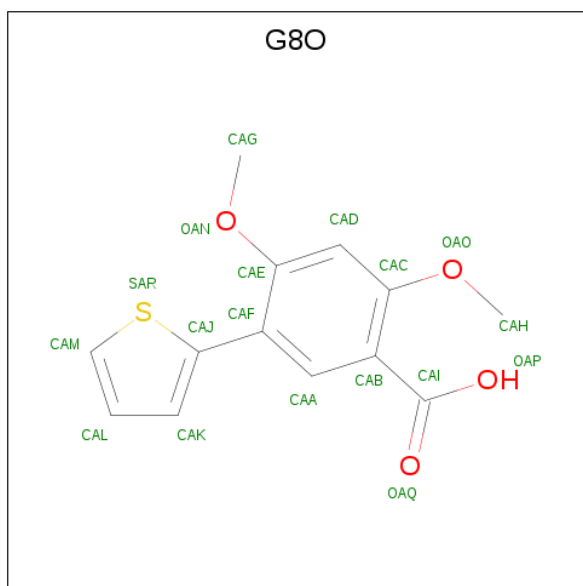
There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	MET	-	expression tag	UNP A0A024B7W1
A	248	HIS	-	expression tag	UNP A0A024B7W1
A	249	HIS	-	expression tag	UNP A0A024B7W1
A	250	HIS	-	expression tag	UNP A0A024B7W1
A	251	HIS	-	expression tag	UNP A0A024B7W1
A	252	HIS	-	expression tag	UNP A0A024B7W1
A	253	HIS	-	expression tag	UNP A0A024B7W1
A	254	SER	-	expression tag	UNP A0A024B7W1
A	255	SER	-	expression tag	UNP A0A024B7W1
A	256	GLY	-	expression tag	UNP A0A024B7W1
A	257	VAL	-	expression tag	UNP A0A024B7W1
A	258	ASP	-	expression tag	UNP A0A024B7W1
A	259	LEU	-	expression tag	UNP A0A024B7W1
A	260	GLY	-	expression tag	UNP A0A024B7W1
A	261	THR	-	expression tag	UNP A0A024B7W1
A	262	GLU	-	expression tag	UNP A0A024B7W1
A	263	ASN	-	expression tag	UNP A0A024B7W1
A	264	LEU	-	expression tag	UNP A0A024B7W1
A	265	TYR	-	expression tag	UNP A0A024B7W1
A	266	PHE	-	expression tag	UNP A0A024B7W1
A	267	GLN	-	expression tag	UNP A0A024B7W1
A	268	SER	-	expression tag	UNP A0A024B7W1
A	269	MET	-	expression tag	UNP A0A024B7W1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

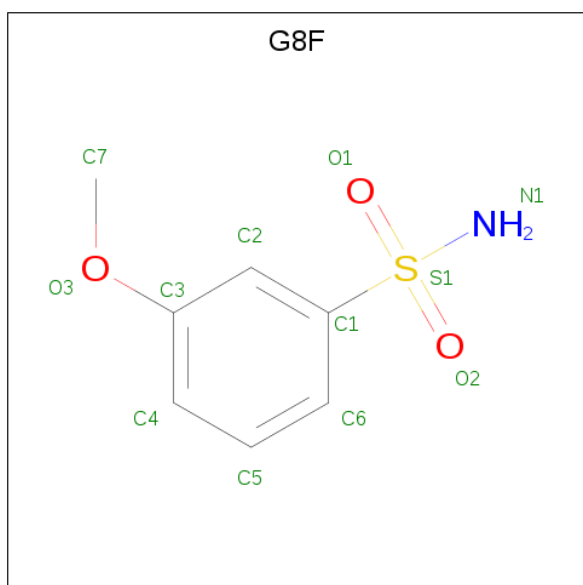
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2,4-dimethoxy-5-thiophen-2-yl-benzoic acid (three-letter code: G8O) (formula: $C_{13}H_{12}O_4S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	1
			34	26	6	2		

- Molecule 4 is 3-methoxybenzenesulfonamide (three-letter code: G8F) (formula: $C_7H_9NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	1
			24	14	2	6	2		

- Molecule 5 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	674	Total	O	0	0
			674	674		

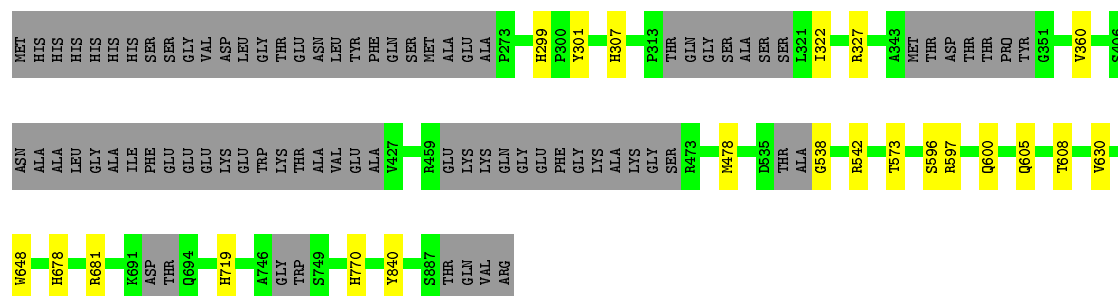
3 Residue-property plots

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. 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. 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.

Note EDS failed to run properly.

- Molecule 1: RNA-directed RNA polymerase NS5

Chain A: 



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.10Å 85.17Å 69.81Å 90.00° 113.34° 90.00°	Depositor
Resolution (Å)	21.91 – 1.50	Depositor
% Data completeness (in resolution range)	99.2 (21.91-1.50)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.50Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.196 , 0.224	Depositor
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.198	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5408	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G8F, G8O, ZN

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	0.51	0/4788	0.59	0/6463

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

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	4674	0	4591	13	0
2	A	2	0	0	0	0
3	A	34	0	0	0	0
4	A	24	0	0	0	0
5	A	674	0	0	3	0
All	All	5408	0	4591	13	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 1.

All (13) 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:605:GLN:HG2	1:A:608:THR:OG1	1.81	0.80
1:A:681:ARG:HD3	5:A:1273:HOH:O	1.93	0.66
1:A:322:ILE:HG21	1:A:327:ARG:HD3	1.79	0.64
1:A:538:GLY:N	1:A:542:ARG:HH12	2.04	0.56
1:A:630:VAL:HG21	1:A:648:TRP:CD1	2.41	0.56
1:A:478:MET:HE1	1:A:573:THR:HG23	1.90	0.54
1:A:299:HIS:HD2	1:A:301:TYR:H	1.61	0.48
1:A:678:HIS:HE1	5:A:1562:HOH:O	1.99	0.45
1:A:597[A]:ARG:HE	1:A:600:GLN:HG3	1.82	0.45
1:A:307:HIS:HE1	1:A:596:SER:OG	2.02	0.43
1:A:360:VAL:HG13	1:A:600:GLN:HE22	1.84	0.43
1:A:719:HIS:HE1	5:A:1543:HOH:O	2.03	0.41
1:A:770:HIS:HA	1:A:840:TYR:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

Of 6 ligands modelled in this entry, 2 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$
3	G8O	A	903[B]	4	18,18,19	3.92	9 (50%)	20,24,26	2.29	6 (30%)
3	G8O	A	903[A]	4	18,18,19	3.77	7 (38%)	20,24,26	1.95	4 (20%)
4	G8F	A	904[B]	3	12,12,12	1.96	2 (16%)	16,17,17	3.29	4 (25%)
4	G8F	A	904[A]	3	12,12,12	1.96	2 (16%)	16,17,17	3.53	5 (31%)

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
3	G8O	A	903[B]	4	-	7/9/10/12	0/2/2/2
3	G8O	A	903[A]	4	-	2/9/10/12	0/2/2/2
4	G8F	A	904[B]	3	-	4/8/8/8	0/1/1/1
4	G8F	A	904[A]	3	-	2/8/8/8	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903[B]	G8O	CAJ-SAR	-11.93	1.60	1.72
3	A	903[A]	G8O	CAJ-SAR	-11.32	1.61	1.72
3	A	903[B]	G8O	CAL-CAK	7.86	1.64	1.39
3	A	903[A]	G8O	CAL-CAK	7.85	1.64	1.39
3	A	903[B]	G8O	CAF-CAJ	5.05	1.53	1.48
4	A	904[B]	G8F	S1-N1	4.99	1.70	1.60
4	A	904[A]	G8F	S1-N1	4.70	1.69	1.60
3	A	903[A]	G8O	CAF-CAJ	4.29	1.52	1.48
3	A	903[B]	G8O	CAL-CAM	4.13	1.47	1.34
3	A	903[A]	G8O	CAL-CAM	3.94	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	904[A]	G8F	C1-S1	3.34	1.82	1.77
4	A	904[B]	G8F	C1-S1	3.15	1.82	1.77
3	A	903[A]	G8O	OAO-CAC	2.53	1.41	1.37
3	A	903[B]	G8O	OAO-CAC	2.47	1.41	1.37
3	A	903[B]	G8O	CAB-CAI	2.26	1.52	1.47
3	A	903[B]	G8O	OAN-CAE	2.26	1.40	1.37
3	A	903[A]	G8O	CAK-CAJ	2.23	1.48	1.39
3	A	903[A]	G8O	CAM-SAR	-2.17	1.60	1.71
3	A	903[B]	G8O	CAM-SAR	-2.13	1.60	1.71
3	A	903[B]	G8O	CAK-CAJ	2.05	1.47	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	904[A]	G8F	O2-S1-O1	-10.71	101.15	118.76
4	A	904[B]	G8F	O2-S1-O1	-10.66	101.24	118.76
4	A	904[A]	G8F	O1-S1-C1	6.68	114.81	107.35
3	A	903[A]	G8O	CAL-CAM-SAR	-6.47	107.73	112.98
3	A	903[B]	G8O	CAL-CAM-SAR	-6.21	107.94	112.98
4	A	904[B]	G8F	O2-S1-N1	4.64	114.24	107.36
4	A	904[B]	G8F	O1-S1-C1	4.02	111.84	107.35
3	A	903[B]	G8O	OAO-CAC-CAB	3.93	121.24	115.92
4	A	904[B]	G8F	O2-S1-C1	3.80	111.59	107.35
4	A	904[A]	G8F	O2-S1-N1	3.70	112.85	107.36
4	A	904[A]	G8F	O2-S1-C1	3.67	111.44	107.35
3	A	903[B]	G8O	CAF-CAJ-SAR	3.21	127.35	117.13
3	A	903[B]	G8O	OAN-CAE-CAF	3.18	121.00	116.26
3	A	903[A]	G8O	CAF-CAJ-SAR	3.02	126.76	117.13
3	A	903[B]	G8O	OAN-CAE-CAD	-2.77	119.35	124.12
4	A	904[A]	G8F	O1-S1-N1	2.51	111.08	107.36
3	A	903[B]	G8O	OAO-CAC-CAD	-2.35	120.08	124.12
3	A	903[A]	G8O	OAQ-CAI-CAB	-2.26	118.39	124.36
3	A	903[A]	G8O	OAO-CAC-CAB	2.09	118.75	115.92

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	903[A]	G8O	CAA-CAB-CAI-OAQ
3	A	903[A]	G8O	CAC-CAB-CAI-OAQ
4	A	904[B]	G8F	C2-C3-O3-C7
4	A	904[B]	G8F	C4-C3-O3-C7

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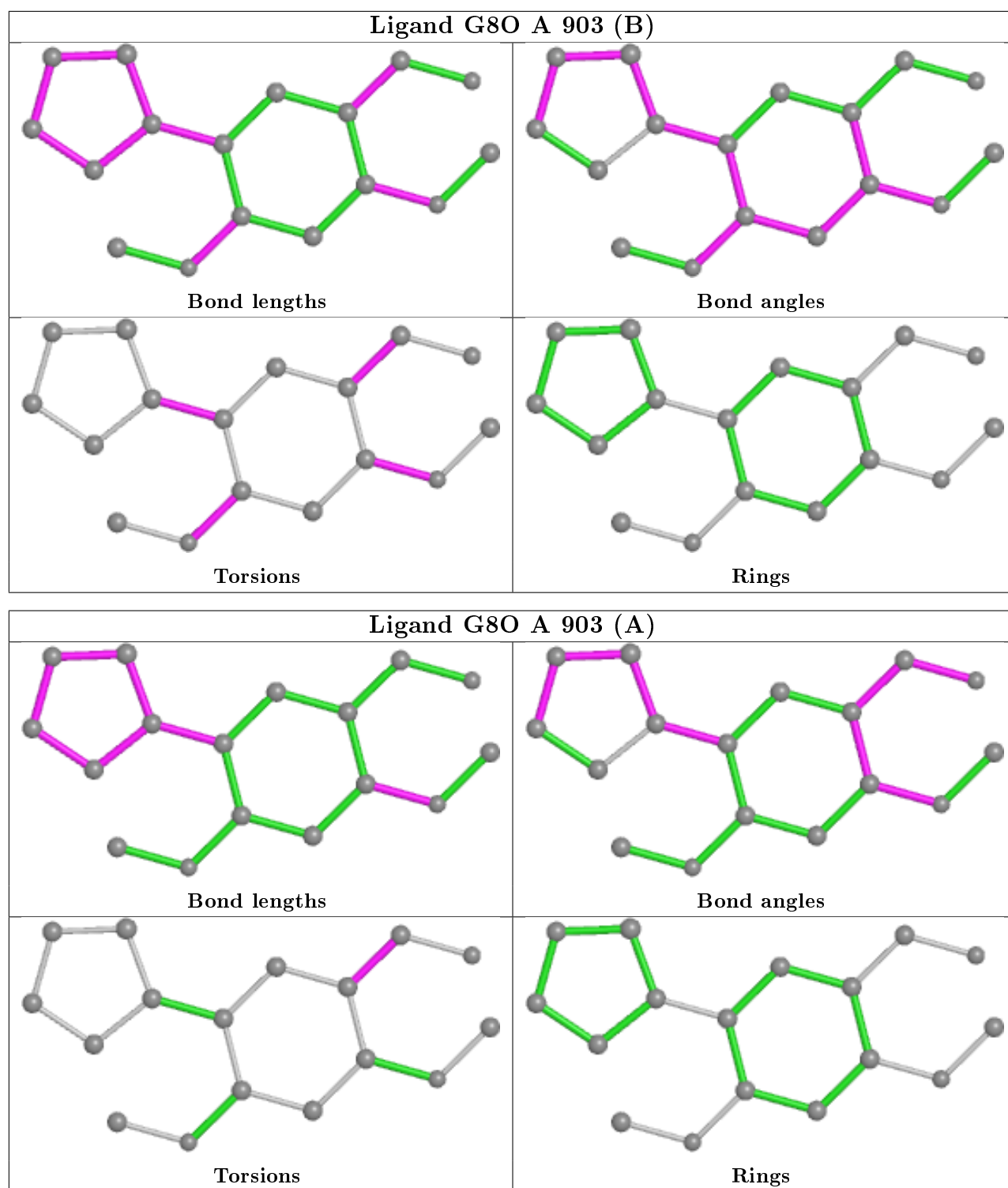
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Mol	Chain	Res	Type	Atoms
4	A	904[A]	G8F	C2-C3-O3-C7
4	A	904[A]	G8F	C4-C3-O3-C7
3	A	903[B]	G8O	CAC-CAB-CAI-OAQ
3	A	903[B]	G8O	CAA-CAB-CAI-OAQ
3	A	903[B]	G8O	CAD-CAC-OAO-CAH
3	A	903[B]	G8O	CAD-CAE-OAN-CAG
3	A	903[B]	G8O	CAB-CAC-OAO-CAH
3	A	903[B]	G8O	CAF-CAE-OAN-CAG
4	A	904[B]	G8F	C6-C1-S1-O1
3	A	903[B]	G8O	CAA-CAF-CAJ-SAR
4	A	904[B]	G8F	C2-C1-S1-O1

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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 ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

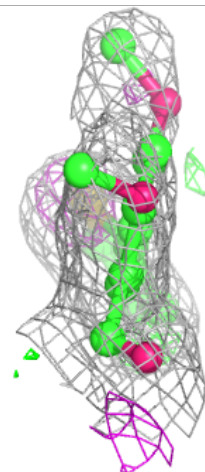
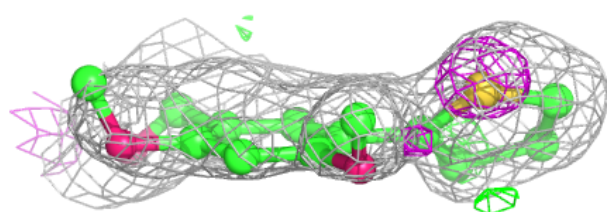
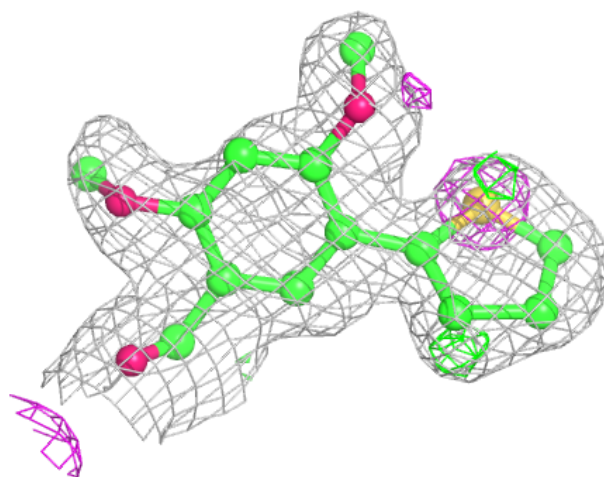
6.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

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.

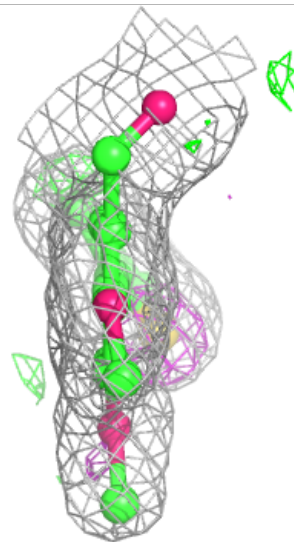
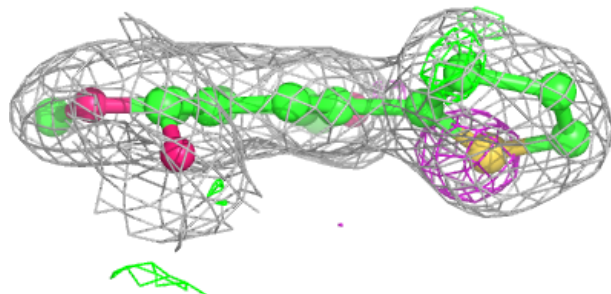
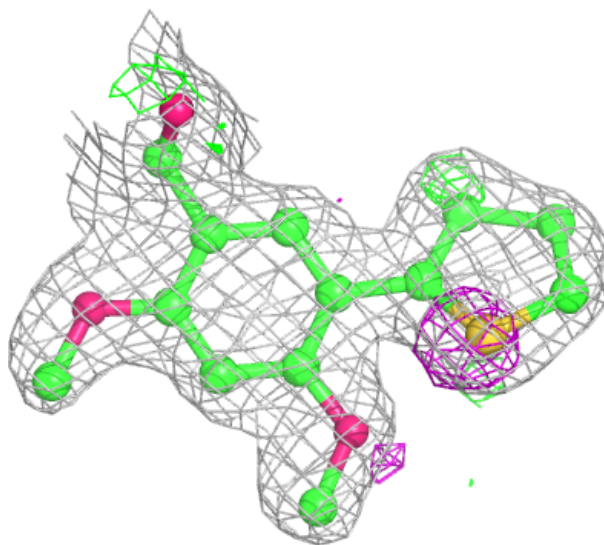
Electron density around G8O A 903 (B):

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



Electron density around G8O A 903 (A):

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



6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.