



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 03:50 AM BST

PDB ID : 6LD2
Title : Zika NS5 polymerase domain
Authors : El Sahili, A.; Lescar, J.
Deposited on : 2019-11-20
Resolution : 1.40 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 : 2.14.4.dev1
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) : 2.14.4.dev1

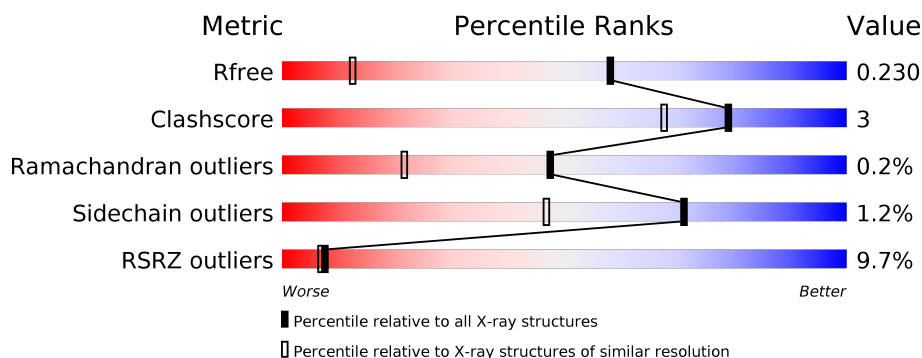
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	645	<div> <div>9%</div> <div>81%</div> <div>6%</div> <div>12%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	KY3	A	903	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5347 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	565	Total	C	N	O	S	0	8	0
			4709	2978	857	842	32			

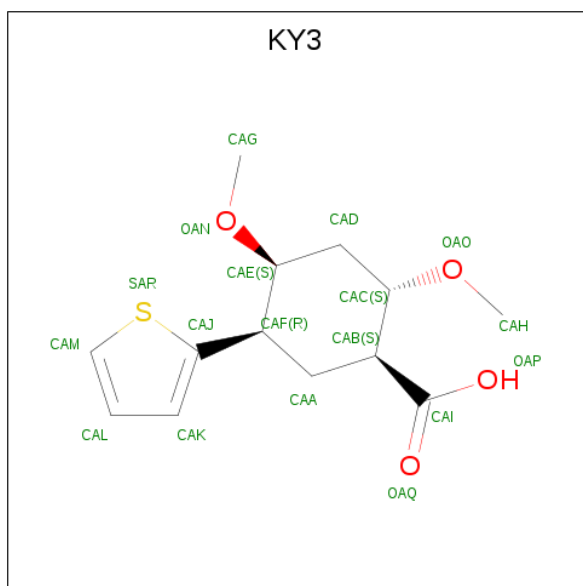
There are 23 discrepancies between the modelled and reference sequences:

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 (1S,2S,4S,5R)-2,4-dimethoxy-5-thiophen-2-yl-cyclohexane-1-carboxylic acid (three-letter code: KY3) (formula: C₁₃H₁₈O₄S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			18	13	4	1		

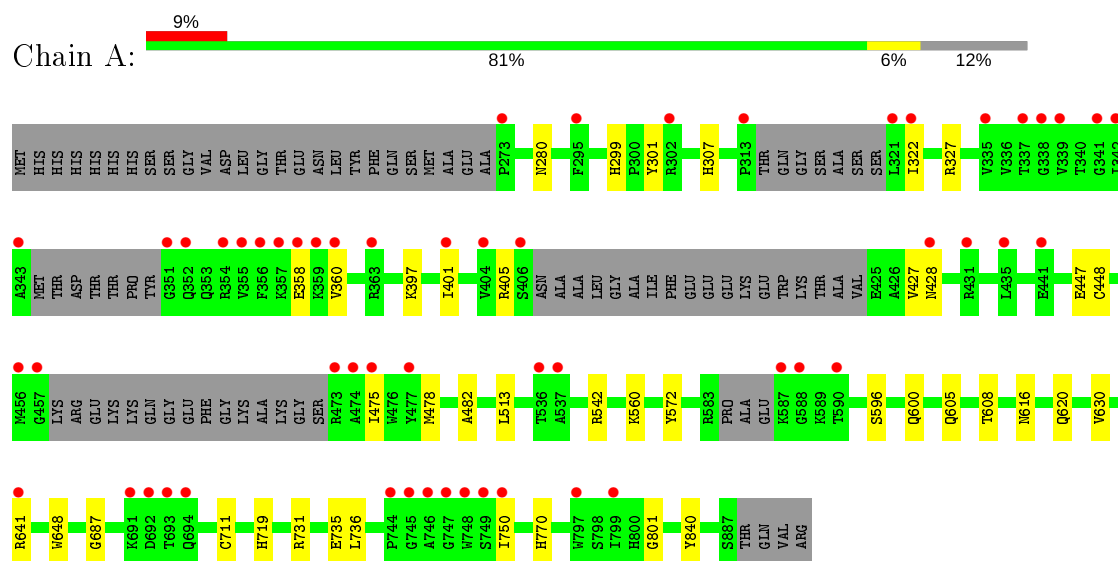
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	618	Total	O	0	0
			618	618		

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: RNA-directed RNA polymerase NS5



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.94Å 85.06Å 69.74Å 90.00° 113.44° 90.00°	Depositor
Resolution (Å)	55.65 – 1.40 55.65 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (55.65-1.40) 98.7 (55.65-1.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 1.40Å)	Xtriage
Refinement program	BUSTER 2.10.3 (3-OCT-2019)	Depositor
R, R_{free}	0.202 , 0.227 0.203 , 0.230	Depositor DCC
R_{free} test set	6639 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
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
F_o, F_c correlation	0.97	EDS
Total number of atoms	5347	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: KY3, 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	0.42	0/4828	0.57	0/6526

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	4709	0	4600	26	0
2	A	2	0	0	0	0
3	A	18	0	0	7	0
4	A	618	0	0	2	0
All	All	5347	0	4600	26	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 (26) 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:405:ARG:NH2	1:A:428:ASN:HD21	1.88	0.71
1:A:401:ILE:HG12	1:A:427:VAL:CG2	2.24	0.67
1:A:280:ASN:ND2	1:A:447:GLU:OE2	2.29	0.66
1:A:478[B]:MET:HG2	1:A:482:ALA:HB3	1.79	0.63
1:A:542:ARG:HD3	1:A:687:GLY:O	2.01	0.60
1:A:513:LEU:HD12	3:A:903:KY3:SAR	2.42	0.60
1:A:360:VAL:HG13	1:A:600:GLN:HE22	1.69	0.58
1:A:801:GLY:HA2	3:A:903:KY3:CAM	2.33	0.57
1:A:513:LEU:CD1	3:A:903:KY3:SAR	2.92	0.57
1:A:307:HIS:HE1	1:A:596:SER:OG	1.88	0.56
1:A:630:VAL:HG21	1:A:648:TRP:CD1	2.40	0.56
1:A:605:GLN:HB2	1:A:608:THR:OG1	2.10	0.51
1:A:513:LEU:HD12	3:A:903:KY3:CAM	2.42	0.50
1:A:513:LEU:HD11	3:A:903:KY3:CAJ	2.42	0.50
1:A:299:HIS:HD2	1:A:301:TYR:H	1.59	0.49
1:A:397:LYS:O	1:A:401:ILE:HG13	2.15	0.47
1:A:719:HIS:HE1	4:A:1516:HOH:O	1.97	0.45
1:A:731:ARG:HD3	1:A:736:LEU:HD21	1.99	0.45
1:A:735:GLU:HG3	4:A:1361:HOH:O	2.16	0.45
1:A:711:CYS:HB3	3:A:903:KY3:CAG	2.50	0.42
1:A:405:ARG:HH21	1:A:428:ASN:HD21	1.63	0.41
1:A:616:ASN:O	1:A:620:GLN:HG2	2.19	0.41
1:A:513:LEU:CD1	3:A:903:KY3:CAJ	2.97	0.41
1:A:401:ILE:HG12	1:A:427:VAL:HG21	1.98	0.41
1:A:770:HIS:HA	1:A:840:TYR:HA	2.02	0.41
1:A:448:CYS:HB2	1:A:572:TYR:CD2	2.57	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	561/645 (87%)	548 (98%)	12 (2%)	1 (0%)	47 21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	322	ILE

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	A	503/560 (90%)	497 (99%)	6 (1%)	71 47

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	ARG
1	A	358	GLU
1	A	475	ILE
1	A	560	LYS
1	A	641	ARG
1	A	750	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	299	HIS
1	A	307	HIS
1	A	352	GLN
1	A	402	ASN
1	A	428	ASN
1	A	600	GLN
1	A	605	GLN
1	A	719	HIS
1	A	762	GLN

5.3.3 RNA [i](#)

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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	KY3	A	903	-	16,19,19	5.31	8 (50%)	12,26,26	3.73	6 (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
3	KY3	A	903	-	-	2/5/28/28	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	KY3	CAB-CAC	-10.43	1.41	1.52
3	A	903	KY3	CAJ-CAF	-10.04	1.37	1.51
3	A	903	KY3	CAF-CAE	-7.79	1.44	1.52
3	A	903	KY3	CAA-CAB	-7.79	1.42	1.53
3	A	903	KY3	CAA-CAF	-7.06	1.43	1.53
3	A	903	KY3	CAD-CAC	-5.49	1.41	1.52
3	A	903	KY3	CAD-CAE	-5.23	1.42	1.52
3	A	903	KY3	OAO-CAC	-2.27	1.37	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	KY3	CAK-CAJ-CAF	-6.91	120.91	129.00
3	A	903	KY3	CAF-CAA-CAB	6.21	118.35	108.35
3	A	903	KY3	CAL-CAM-SAR	-5.23	108.74	112.98
3	A	903	KY3	CAE-CAD-CAC	4.86	122.40	110.71
3	A	903	KY3	CAH-OAO-CAC	4.32	125.68	114.03
3	A	903	KY3	CAG-OAN-CAE	2.37	120.41	114.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

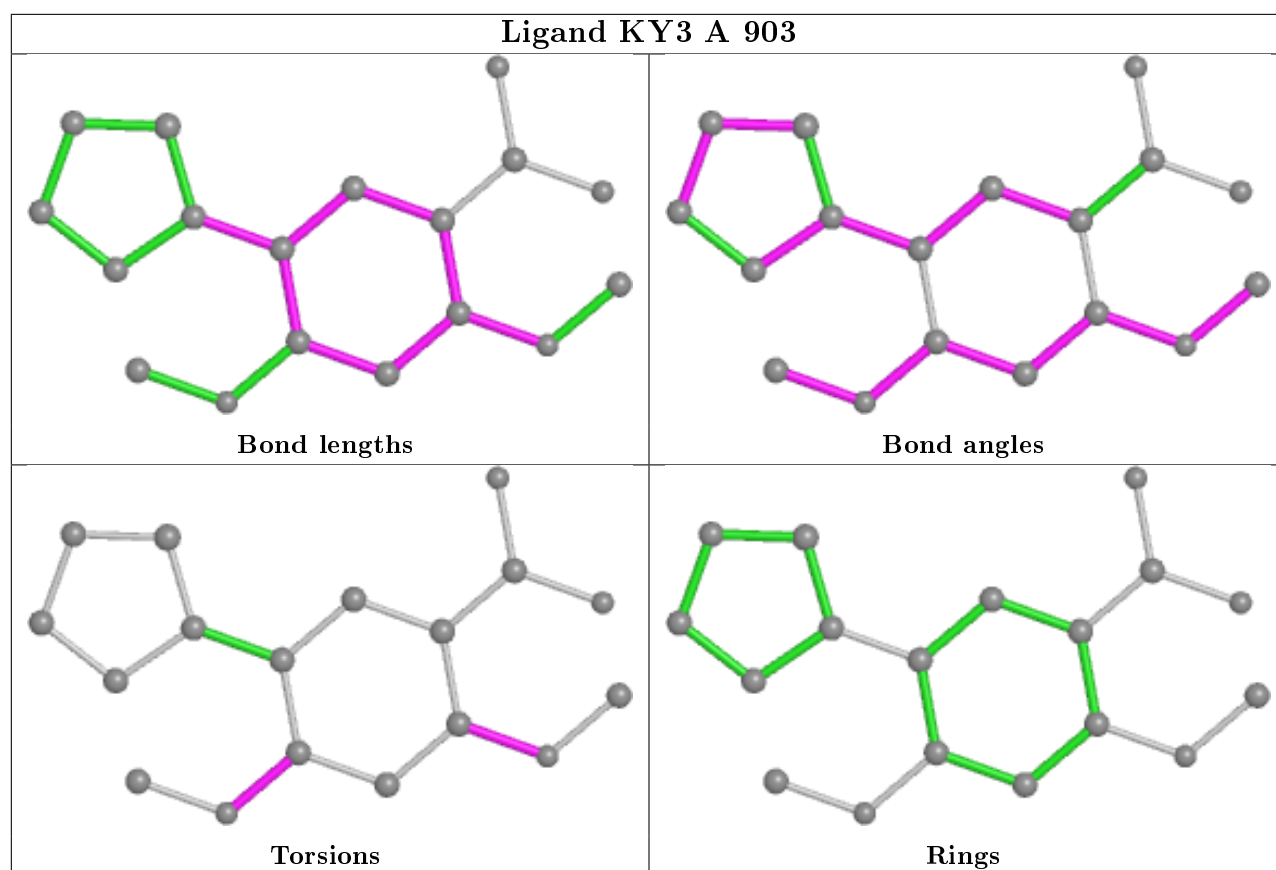
Mol	Chain	Res	Type	Atoms
3	A	903	KY3	CAD-CAE-OAN-CAG
3	A	903	KY3	CAD-CAC-OAO-CAH

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	903	KY3	7	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 [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	565/645 (87%)	0.49	55 (9%) 7 7	18, 30, 56, 74	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	797	TRP	10.2
1	A	746	ALA	10.0
1	A	748	TRP	7.6
1	A	355	VAL	7.1
1	A	457	GLY	7.0
1	A	747	GLY	6.9
1	A	356	PHE	6.2
1	A	473	ARG	6.2
1	A	343	ALA	5.9
1	A	342	ILE	5.8
1	A	692	ASP	5.7
1	A	354	ARG	5.4
1	A	456	MET	5.4
1	A	406	SER	5.1
1	A	588	GLY	4.9
1	A	321	LEU	4.8
1	A	536[A]	THR	4.8
1	A	313	PRO	4.8
1	A	477	TYR	4.7
1	A	357	LYS	4.6
1	A	358	GLU	4.4
1	A	352	GLN	4.3
1	A	587	LYS	4.0
1	A	693	THR	4.0
1	A	745	GLY	3.6
1	A	431	ARG	3.6
1	A	359	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	799	ILE	3.5
1	A	474	ALA	3.5
1	A	351	GLY	3.5
1	A	641	ARG	3.4
1	A	435	LEU	3.2
1	A	273	PRO	3.1
1	A	691	LYS	3.0
1	A	360	VAL	3.0
1	A	337	THR	3.0
1	A	338	GLY	2.9
1	A	749	SER	2.8
1	A	404	VAL	2.7
1	A	363	ARG	2.7
1	A	750	ILE	2.7
1	A	295	PHE	2.6
1	A	335	VAL	2.6
1	A	302	ARG	2.5
1	A	322	ILE	2.5
1	A	537	ALA	2.4
1	A	441	GLU	2.4
1	A	341	GLY	2.4
1	A	475	ILE	2.4
1	A	590	THR	2.3
1	A	428	ASN	2.2
1	A	744	PRO	2.1
1	A	339	VAL	2.1
1	A	694	GLN	2.1
1	A	401	ILE	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 monosaccharides in this entry.

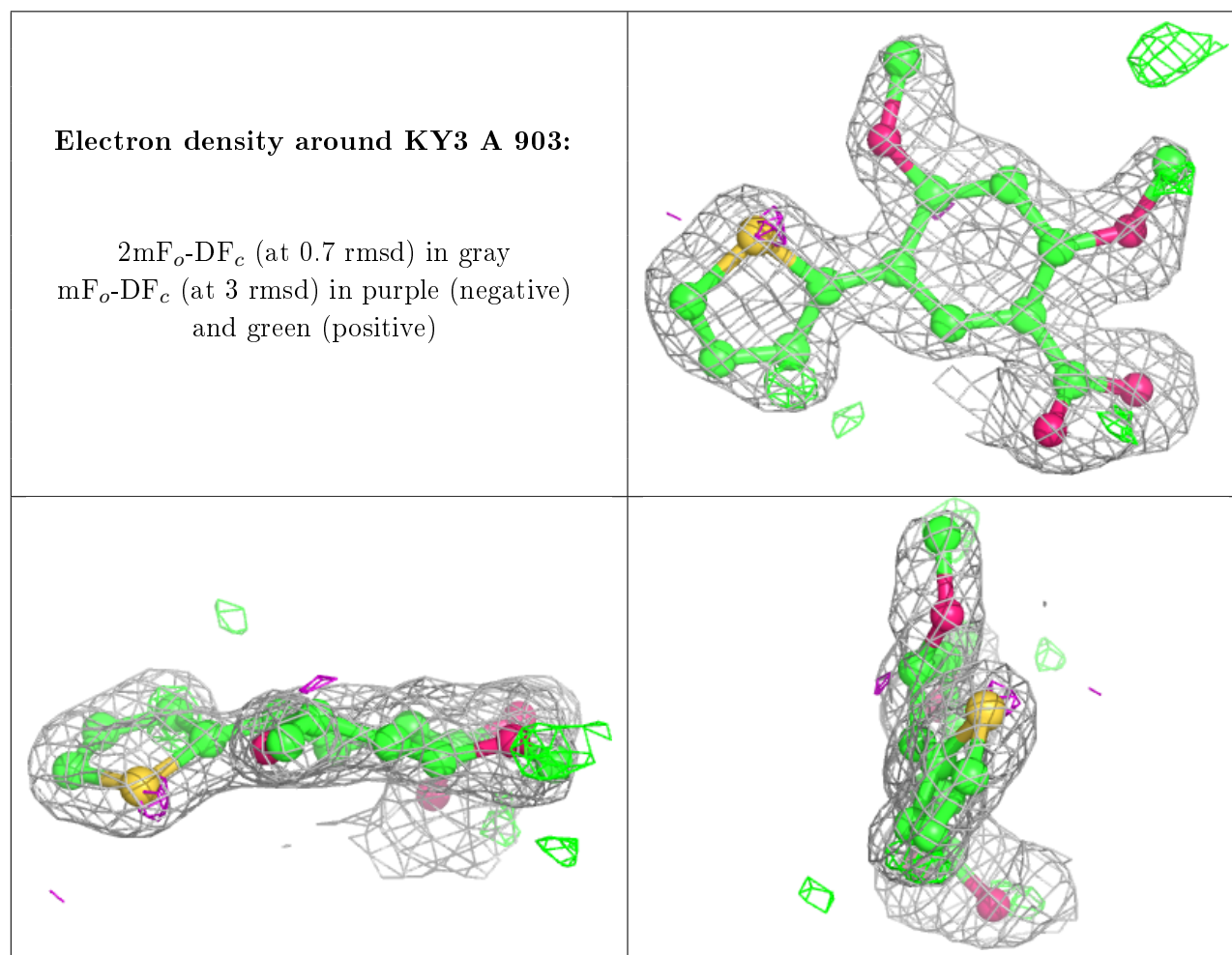
6.4 Ligands [i](#)

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
3	KY3	A	903	18/18	0.81	0.17	29,30,31,32	18
2	ZN	A	901	1/1	0.98	0.09	30,30,30,30	0
2	ZN	A	902	1/1	0.99	0.11	21,21,21,21	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.