



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2021 – 06:03 PM EDT

PDB ID : 7KGA
Title : Crystal structure of a mosquito-borne flavivirus dumbbell RNA
Authors : Akiyama, B.M.; Graham, M.E.; O'Donoghue, Z.; Beckham, J.D.; Kieft, J.S.
Deposited on : 2020-10-16
Resolution : 2.10 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 : 2.20
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) : 2.20

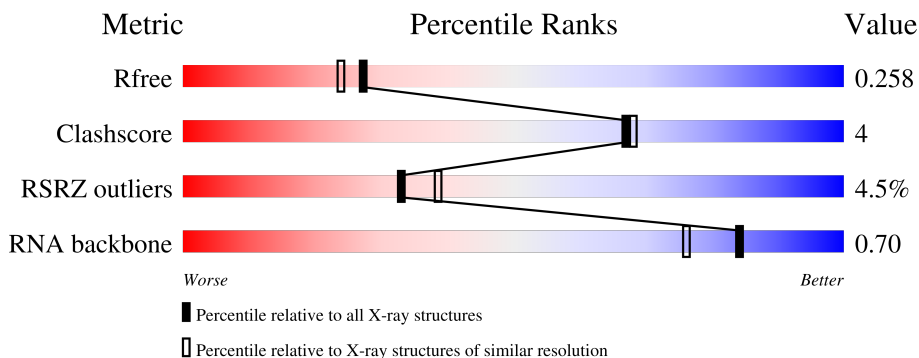
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

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 $\leq 5\%$. 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	90	 6% 76% 22% ..
1	B	90	 3% 80% 18% .

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
2	IRI	A	117	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IRI	B	126	-	-	-	X

2 Entry composition [i](#)

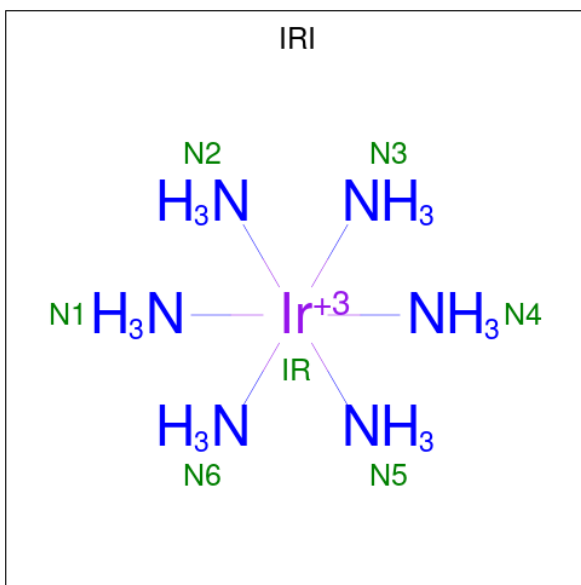
There are 3 unique types of molecules in this entry. The entry contains 4306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RNA chain called RNA (90-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	A	89	Total 1901	C 850	N 348	O 614	P 89	0	0	0
1	B	90	Total 1921	C 859	N 350	O 622	P 90	0	0	0

- Molecule 2 is IRIDIUM HEXAMMINE ION (three-letter code: IRI) (formula: $\text{H}_{18}\text{IrN}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Ir	N		
2	A	1	Total 7	Ir 1	N 6	0	0
2	A	1	Total 7	Ir 1	N 6	0	0
2	A	1	Total 7	Ir 1	N 6	0	0
2	A	1	Total 14	Ir 2	N 12	0	1

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Ir	N		
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	A	1	14	2	12	0	1
2	A	1	7	1	6	0	0
2	A	1	14	2	12	0	1
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	A	1	14	2	12	0	1
2	A	1	7	1	6	0	0
2	A	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Ir	N		
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	14	2	12	0	1
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	14	2	12	0	1
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0
2	B	1	7	1	6	0	0

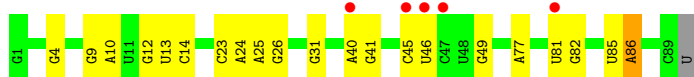
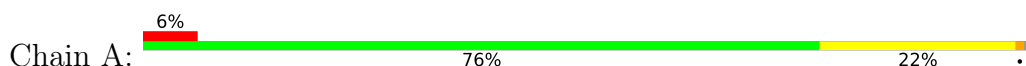
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	76	Total 76	O 76	0	0

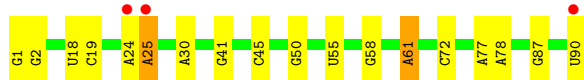
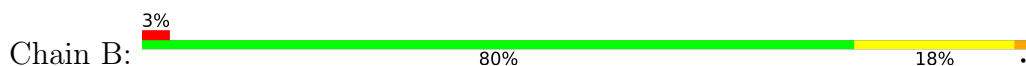
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: RNA (90-MER)



- Molecule 1: RNA (90-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.93Å 49.67Å 73.46Å 90.00° 99.74° 90.00°	Depositor
Resolution (Å)	44.74 – 2.10 44.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.74-2.10) 91.0 (44.74-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.10Å)	Xtrriage
Refinement program	PHENIX Phenixdev-3758	Depositor
R, R_{free}	0.228 , 0.259 0.228 , 0.258	Depositor DCC
R_{free} test set	1938 reflections (7.26%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtrriage
Anisotropy	0.415	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4306	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IRI

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	0.17	0/2127	0.72	0/3313
1	B	0.18	0/2149	0.72	0/3347
All	All	0.18	0/4276	0.72	0/6660

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	1901	0	963	12	0
1	B	1921	0	973	9	2
2	A	154	0	0	8	1
2	B	203	0	0	8	0
3	A	51	0	0	3	0
3	B	76	0	0	4	0
All	All	4306	0	1936	24	2

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 4.

All (24) 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:108:IRI:N2	3:A:201:HOH:O	2.13	0.81
2:B:108:IRI:N2	3:B:201:HOH:O	2.15	0.77
2:B:108:IRI:N3	3:B:201:HOH:O	2.19	0.75
1:B:2:G:N7	3:B:201:HOH:O	2.21	0.73
1:B:25:A:O2'	2:B:118:IRI:N2	2.26	0.69
1:A:49:G:O6	2:A:114:IRI:N3	2.29	0.65
1:A:26:G:OP1	2:A:104[B]:IRI:N5	2.33	0.61
1:A:13:U:OP1	2:A:118:IRI:N5	2.39	0.56
1:A:14:C:OP1	2:A:111:IRI:N4	2.42	0.52
1:B:87:G:N7	2:B:109:IRI:N3	2.57	0.51
1:A:23:C:OP2	1:A:24:A:O2'	2.17	0.50
1:A:12:G:O6	2:A:108:IRI:N5	2.45	0.49
1:A:86:A:H5''	3:A:216:HOH:O	2.12	0.49
1:A:9:G:OP2	3:A:202:HOH:O	2.20	0.48
1:B:1:G:OP1	3:B:203:HOH:O	2.20	0.47
1:B:30:A:OP1	2:B:113:IRI:N6	2.48	0.46
1:B:50:G:N7	2:B:117[B]:IRI:N5	2.65	0.45
1:B:18:U:H2'	1:B:19:C:C6	2.52	0.45
1:A:4:G:N7	2:A:107[A]:IRI:N5	2.67	0.43
1:B:45:C:OP1	2:B:126:IRI:N3	2.52	0.43
1:A:12:G:N7	2:A:108:IRI:N3	2.68	0.41
1:A:31:G:H1'	1:A:85:U:O2	2.21	0.41
1:A:9:G:H2'	1:A:10:A:C8	2.57	0.40
1:B:58:G:O6	2:B:102:IRI:N2	2.55	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:A:OP2	2:A:117:IRI:N5[2_353]	1.30	0.90
1:B:61:A:O2'	1:B:87:G:O2'[1_556]	2.15	0.05

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	88/90 (97%)	9 (10%)	0
1	B	89/90 (98%)	8 (8%)	0
All	All	177/180 (98%)	17 (9%)	0

All (17) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	25	A
1	A	40	A
1	A	41	G
1	A	45	C
1	A	46	U
1	A	77	A
1	A	81	U
1	A	82	G
1	A	86	A
1	B	24	A
1	B	25	A
1	B	41	G
1	B	55	U
1	B	61	A
1	B	72	C
1	B	78	A
1	B	90	U

There are no RNA pucker outliers to report.

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

51 ligands are modelled in this entry.

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	IRI	A	106	-	0,6,6	0.00	-	-	-	-
2	IRI	B	126	-	0,6,6	0.00	-	-	-	-
2	IRI	B	101	-	0,6,6	0.00	-	-	-	-
2	IRI	A	118	-	0,6,6	0.00	-	-	-	-
2	IRI	A	108	-	0,6,6	0.00	-	-	-	-
2	IRI	A	107[B]	-	0,6,6	0.00	-	-	-	-
2	IRI	A	111	-	0,6,6	0.00	-	-	-	-
2	IRI	B	105	-	0,6,6	0.00	-	-	-	-
2	IRI	B	117[B]	-	0,6,6	0.00	-	-	-	-
2	IRI	A	109[B]	-	0,6,6	0.00	-	-	-	-
2	IRI	A	110	-	0,6,6	0.00	-	-	-	-
2	IRI	B	116	-	0,6,6	0.00	-	-	-	-
2	IRI	A	105	-	0,6,6	0.00	-	-	-	-
2	IRI	A	104[B]	-	0,6,6	0.00	-	-	-	-
2	IRI	B	102	-	0,6,6	0.00	-	-	-	-
2	IRI	B	117[A]	-	0,6,6	0.00	-	-	-	-
2	IRI	A	115	-	0,6,6	0.00	-	-	-	-
2	IRI	B	118	-	0,6,6	0.00	-	-	-	-
2	IRI	A	116[A]	-	0,6,6	0.00	-	-	-	-
2	IRI	B	120[A]	-	0,6,6	0.00	-	-	-	-
2	IRI	B	123	-	0,6,6	0.00	-	-	-	-
2	IRI	B	107	-	0,6,6	0.00	-	-	-	-
2	IRI	B	114	-	0,6,6	0.00	-	-	-	-
2	IRI	B	124	-	0,6,6	0.00	-	-	-	-
2	IRI	B	122[B]	-	0,6,6	0.00	-	-	-	-
2	IRI	B	106	-	0,6,6	0.00	-	-	-	-
2	IRI	A	101	-	0,6,6	0.00	-	-	-	-
2	IRI	A	107[A]	-	0,6,6	0.00	-	-	-	-
2	IRI	A	109[A]	-	0,6,6	0.00	-	-	-	-
2	IRI	A	102	-	0,6,6	0.00	-	-	-	-
2	IRI	B	112	-	0,6,6	0.00	-	-	-	-
2	IRI	B	125	-	0,6,6	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IRI	A	104[A]	-	0,6,6	0.00	-	-	-	-
2	IRI	A	114	-	0,6,6	0.00	-	-	-	-
2	IRI	B	113	-	0,6,6	0.00	-	-	-	-
2	IRI	B	115	-	0,6,6	0.00	-	-	-	-
2	IRI	A	112	-	0,6,6	0.00	-	-	-	-
2	IRI	B	119	-	0,6,6	0.00	-	-	-	-
2	IRI	A	113	-	0,6,6	0.00	-	-	-	-
2	IRI	B	103	-	0,6,6	0.00	-	-	-	-
2	IRI	A	117	-	0,6,6	0.00	-	-	-	-
2	IRI	B	121	-	0,6,6	0.00	-	-	-	-
2	IRI	B	108	-	0,6,6	0.00	-	-	-	-
2	IRI	B	109	-	0,6,6	0.00	-	-	-	-
2	IRI	B	122[A]	-	0,6,6	0.00	-	-	-	-
2	IRI	B	104	-	0,6,6	0.00	-	-	-	-
2	IRI	B	111	-	0,6,6	0.00	-	-	-	-
2	IRI	B	120[B]	-	0,6,6	0.00	-	-	-	-
2	IRI	A	116[B]	-	0,6,6	0.00	-	-	-	-
2	IRI	B	110	-	0,6,6	0.00	-	-	-	-
2	IRI	A	103	-	0,6,6	0.00	-	-	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 17 short contacts:

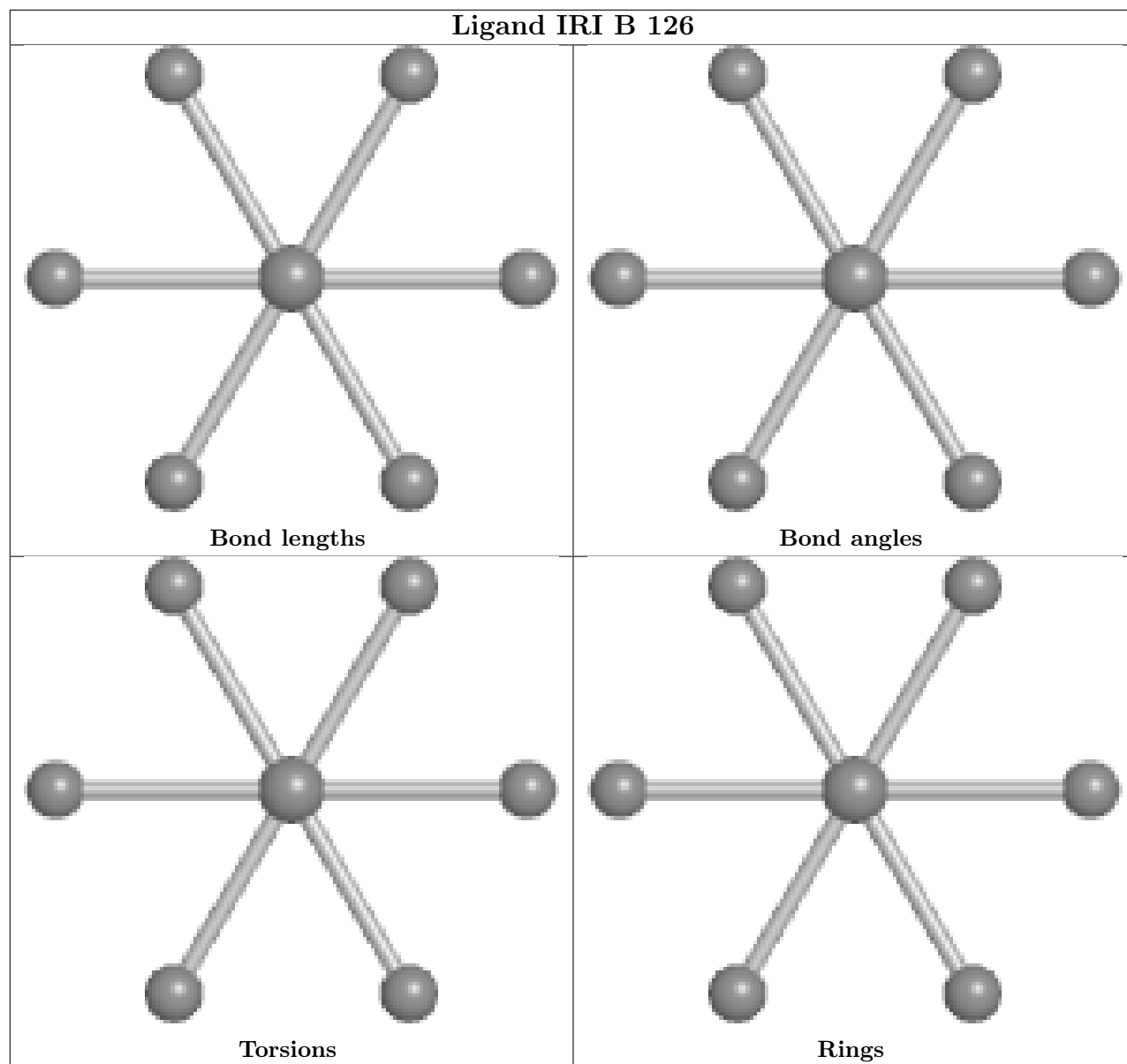
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	126	IRI	1	0
2	A	118	IRI	1	0
2	A	108	IRI	3	0
2	A	111	IRI	1	0
2	B	117[B]	IRI	1	0
2	A	104[B]	IRI	1	0
2	B	102	IRI	1	0
2	B	118	IRI	1	0
2	A	107[A]	IRI	1	0
2	A	114	IRI	1	0
2	B	113	IRI	1	0
2	A	117	IRI	0	1

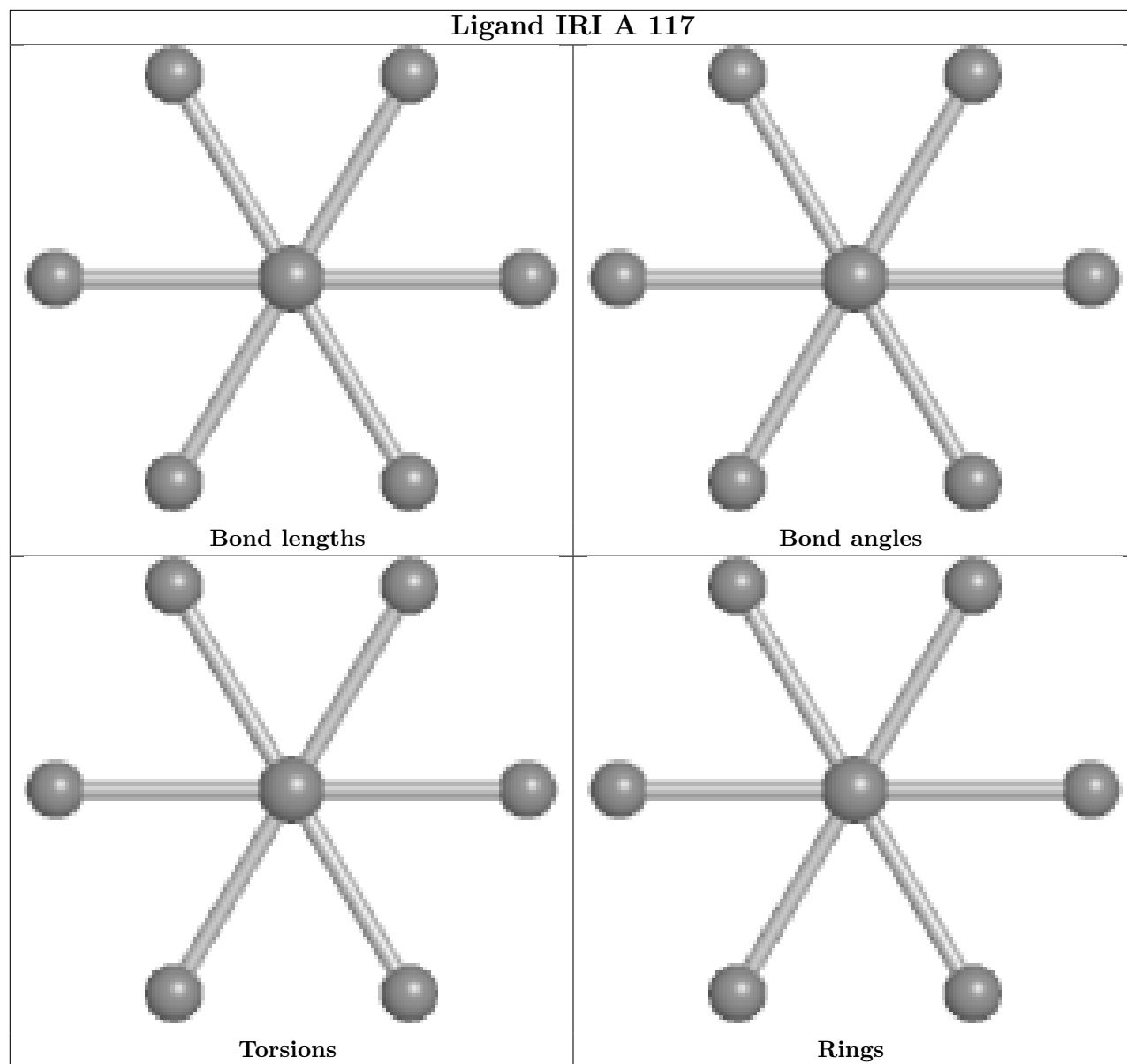
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	108	IRI	2	0
2	B	109	IRI	1	0

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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	89/90 (98%)	0.19	5 (5%) 24 29	20, 38, 77, 104	0
1	B	90/90 (100%)	-0.12	3 (3%) 46 53	18, 27, 57, 103	0
All	All	179/180 (99%)	0.03	8 (4%) 33 38	18, 33, 76, 104	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	A	5.8
1	A	40	A	3.9
1	A	46	U	3.5
1	A	45	C	3.4
1	A	47	C	3.4
1	B	24	A	3.2
1	A	81	U	2.2
1	B	90	U	2.1

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.

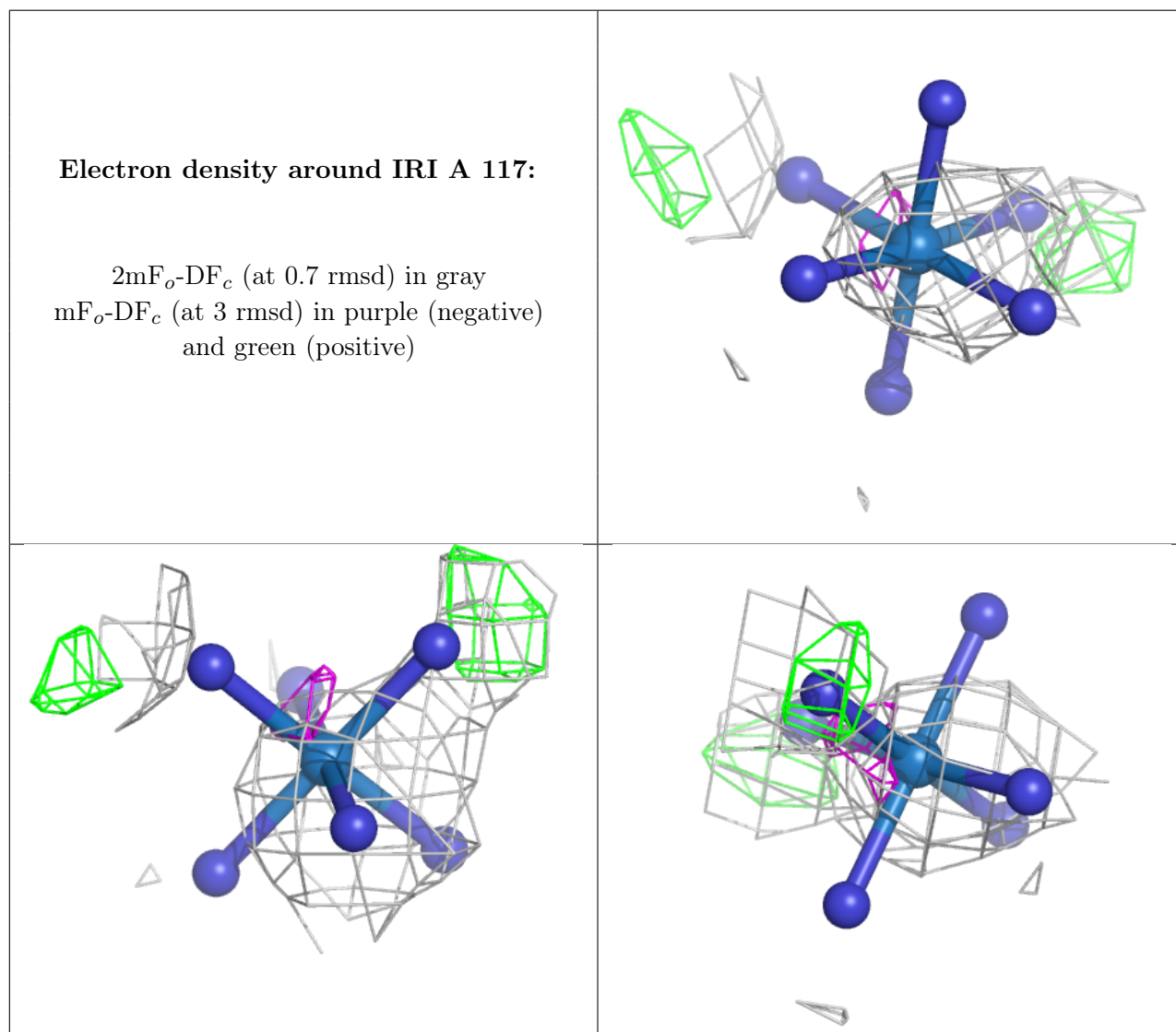
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IRI	A	118	7/7	0.65	0.34	136,138,139,147	7
2	IRI	B	125	7/7	0.69	0.33	125,128,138,148	7
2	IRI	A	117	7/7	0.71	0.47	47,53,62,68	7
2	IRI	B	126	7/7	0.75	0.42	69,75,77,85	7
2	IRI	B	123	7/7	0.78	0.27	116,118,121,128	7
2	IRI	B	124	7/7	0.80	0.33	93,95,98,113	7
2	IRI	A	115	7/7	0.82	0.26	101,103,114,120	7
2	IRI	A	116[A]	7/7	0.83	0.36	78,78,81,88	7
2	IRI	A	116[B]	7/7	0.83	0.36	77,78,87,90	7
2	IRI	B	119	7/7	0.87	0.31	66,67,80,82	7
2	IRI	B	121	7/7	0.87	0.19	102,103,110,121	7
2	IRI	A	111	7/7	0.87	0.20	100,102,109,111	0
2	IRI	A	114	7/7	0.88	0.18	114,118,128,130	0
2	IRI	B	113	7/7	0.88	0.29	49,50,55,67	7
2	IRI	B	122[A]	7/7	0.88	0.30	63,64,75,80	7
2	IRI	B	122[B]	7/7	0.88	0.30	59,60,64,83	7
2	IRI	B	117[B]	7/7	0.89	0.23	87,89,98,98	7
2	IRI	B	118	7/7	0.89	0.24	59,68,80,84	7
2	IRI	B	115	7/7	0.89	0.29	32,34,40,50	7
2	IRI	B	120[A]	7/7	0.89	0.25	105,108,112,117	7
2	IRI	B	120[B]	7/7	0.89	0.25	107,109,117,122	7
2	IRI	B	117[A]	7/7	0.89	0.23	87,91,101,101	7
2	IRI	A	113	7/7	0.90	0.25	51,56,60,64	7
2	IRI	A	105	7/7	0.91	0.25	46,52,64,66	7
2	IRI	B	114	7/7	0.92	0.29	27,28,30,40	7
2	IRI	B	108	7/7	0.92	0.20	58,59,65,79	0
2	IRI	B	116	7/7	0.92	0.23	71,72,84,87	7
2	IRI	A	108	7/7	0.92	0.33	108,111,127,136	0
2	IRI	A	112	7/7	0.93	0.24	60,67,69,76	7
2	IRI	A	110	7/7	0.93	0.17	74,75,80,88	7
2	IRI	A	107[A]	7/7	0.94	0.21	42,43,58,63	7
2	IRI	B	106	7/7	0.94	0.17	51,54,59,68	7
2	IRI	A	109[A]	7/7	0.94	0.24	27,34,45,47	7
2	IRI	A	109[B]	7/7	0.94	0.24	30,33,46,50	7
2	IRI	A	107[B]	7/7	0.94	0.21	37,41,52,54	7
2	IRI	B	112	7/7	0.95	0.19	45,49,51,61	7
2	IRI	A	106	7/7	0.95	0.21	37,40,44,47	7
2	IRI	A	104[B]	7/7	0.95	0.24	55,57,63,71	7
2	IRI	A	104[A]	7/7	0.95	0.24	47,54,60,60	7
2	IRI	B	109	7/7	0.95	0.23	29,37,58,60	7
2	IRI	B	110	7/7	0.95	0.20	22,25,36,41	7

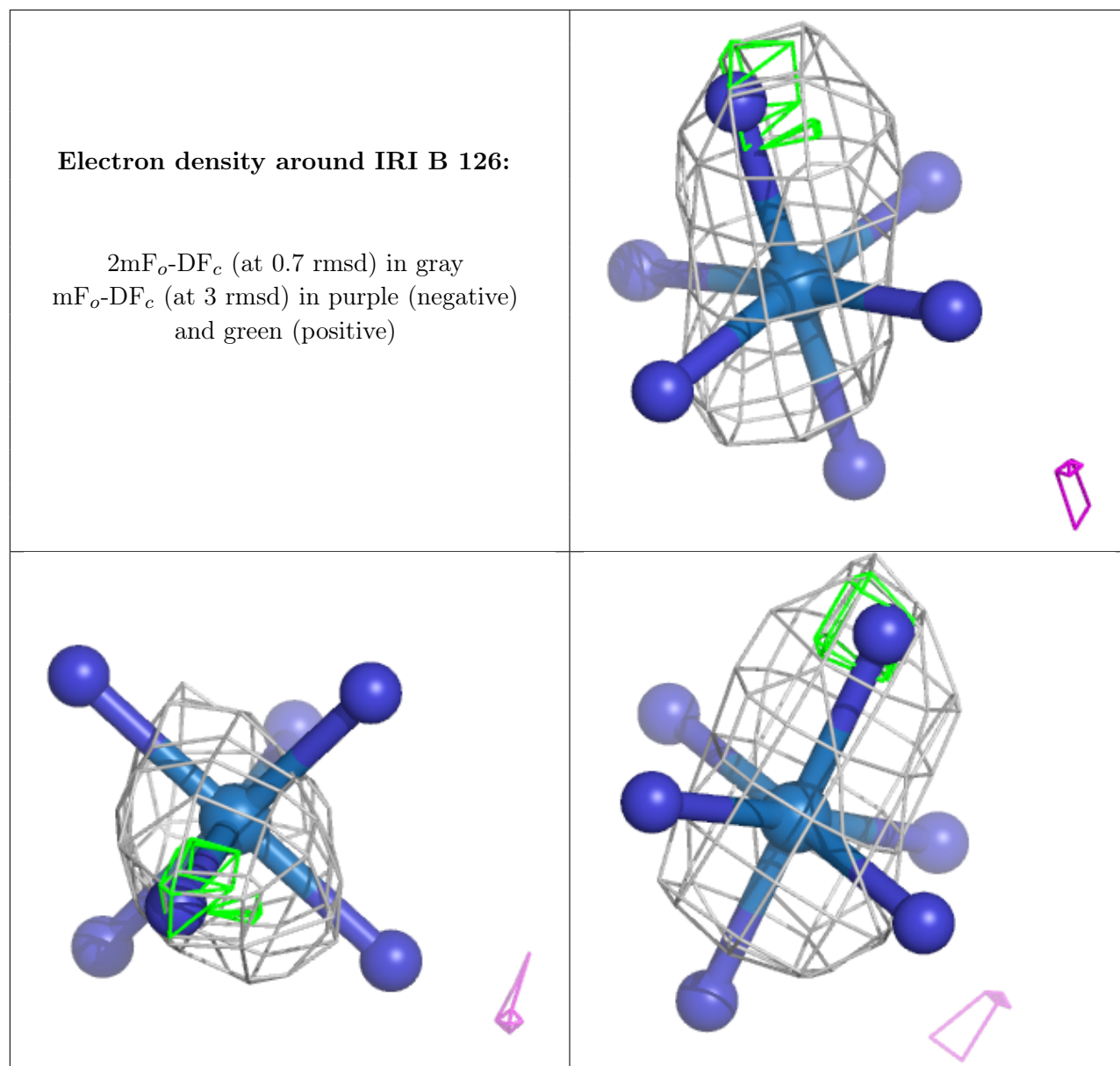
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	IRI	A	103	7/7	0.96	0.22	30,37,48,50	7
2	IRI	B	107	7/7	0.97	0.18	15,20,30,32	7
2	IRI	B	111	7/7	0.97	0.17	51,53,69,71	0
2	IRI	B	104	7/7	0.97	0.18	17,20,25,37	0
2	IRI	A	102	7/7	0.97	0.18	26,28,33,40	7
2	IRI	B	105	7/7	0.98	0.16	22,26,30,44	0
2	IRI	B	101	7/7	0.98	0.20	15,18,20,35	0
2	IRI	B	102	7/7	0.98	0.17	26,31,38,43	0
2	IRI	B	103	7/7	0.98	0.16	25,29,37,47	0
2	IRI	A	101	7/7	0.98	0.15	38,40,47,61	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.