



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 09:47 PM EDT

PDB ID : 6OKO
Title : Crystal structure of mRIPK3 complexed with N-(3-fluoro-4-{1H-pyrrolo[2,3-b]pyridin-4-yloxy}phenyl)-1-(4-fluorophenyl)-2-oxo-1,2-dihydropyridine-3-carboxamide
Authors : Pokross, M.E.
Deposited on : 2019-04-14
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

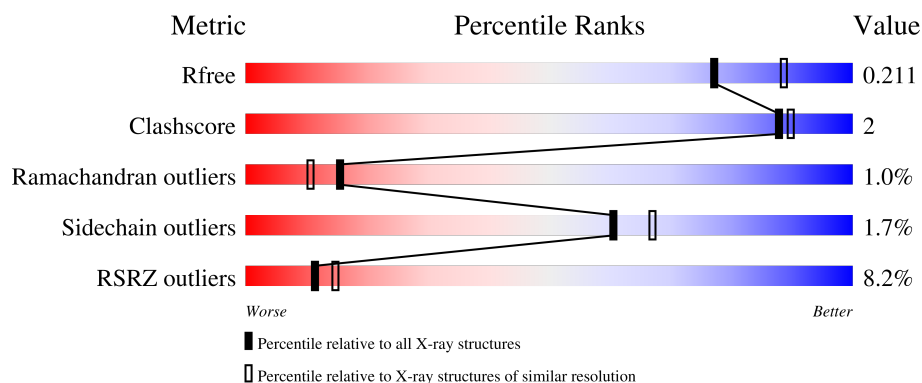
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	325	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>5%</div> <div>19%</div> </div> </div>
1	B	325	<div> <div>10%</div> <div> <div></div> <div>75%</div> <div>6%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4296 atoms, of which 32 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 Receptor-interacting serine/threonine-protein kinase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	1	0
			2035	1309	348	370	8			
1	B	261	Total	C	N	O	S	0	0	0
			1959	1262	336	353	8			

There are 30 discrepancies between the modelled and reference sequences:

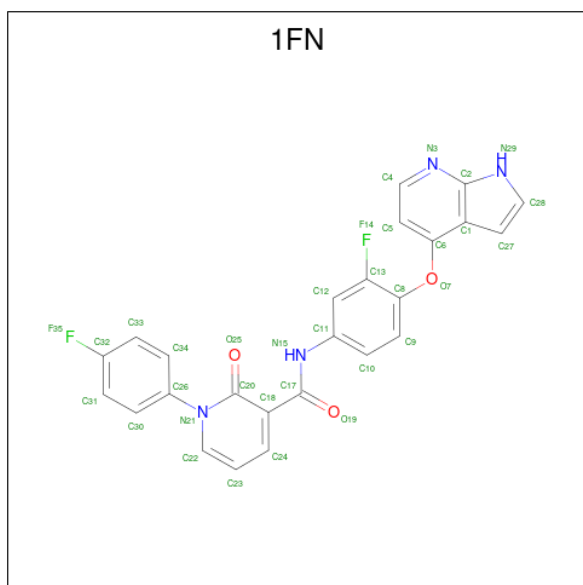
Chain	Residue	Modelled	Actual	Comment	Reference
A	111	ALA	CYS	conflict	UNP Q9QZL0
A	136	ASP	ASN	conflict	UNP Q9QZL0
A	198	LYS	ASP	conflict	UNP Q9QZL0
A	314	LEU	-	expression tag	UNP Q9QZL0
A	315	GLU	-	expression tag	UNP Q9QZL0
A	316	HIS	-	expression tag	UNP Q9QZL0
A	317	HIS	-	expression tag	UNP Q9QZL0
A	318	HIS	-	expression tag	UNP Q9QZL0
A	319	HIS	-	expression tag	UNP Q9QZL0
A	320	HIS	-	expression tag	UNP Q9QZL0
A	321	HIS	-	expression tag	UNP Q9QZL0
A	322	HIS	-	expression tag	UNP Q9QZL0
A	323	HIS	-	expression tag	UNP Q9QZL0
A	324	HIS	-	expression tag	UNP Q9QZL0
A	325	HIS	-	expression tag	UNP Q9QZL0
B	111	ALA	CYS	conflict	UNP Q9QZL0
B	136	ASP	ASN	conflict	UNP Q9QZL0
B	198	LYS	ASP	conflict	UNP Q9QZL0
B	314	LEU	-	expression tag	UNP Q9QZL0
B	315	GLU	-	expression tag	UNP Q9QZL0
B	316	HIS	-	expression tag	UNP Q9QZL0
B	317	HIS	-	expression tag	UNP Q9QZL0
B	318	HIS	-	expression tag	UNP Q9QZL0
B	319	HIS	-	expression tag	UNP Q9QZL0
B	320	HIS	-	expression tag	UNP Q9QZL0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	321	HIS	-	expression tag	UNP Q9QZL0
B	322	HIS	-	expression tag	UNP Q9QZL0
B	323	HIS	-	expression tag	UNP Q9QZL0
B	324	HIS	-	expression tag	UNP Q9QZL0
B	325	HIS	-	expression tag	UNP Q9QZL0

- Molecule 2 is 1-(4-fluorophenyl)-N-[3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4-yloxy)phenyl]-2-oxo-1,2-dihydropyridine-3-carboxamide (three-letter code: 1FN) (formula: C₂₅H₁₆F₂N₄O₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	16	0
			50	25	2	16	4	3		
2	B	1	Total	C	F	H	N	O	16	0
			50	25	2	16	4	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total	O	0	0
			140	140		
3	B	62	Total	O	0	0
			62	62		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.76Å 52.75Å 103.75Å 90.00° 130.82° 90.00°	Depositor
Resolution (Å)	39.26 – 2.10 39.26 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (39.26-2.10) 99.2 (39.26-2.10)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.10Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.180 , 0.198 0.183 , 0.211	Depositor DCC
R_{free} test set	1807 reflections (5.25%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4296	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% 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: 1FN

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	0.45	0/2086	0.61	0/2844
1	B	0.42	0/2005	0.62	0/2739
All	All	0.44	0/4091	0.61	0/5583

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	2035	0	2014	8	0
1	B	1959	0	1890	9	0
2	A	34	16	16	0	0
2	B	34	16	16	0	0
3	A	140	0	0	0	0
3	B	62	0	0	0	0
All	All	4264	32	3936	16	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 (16) 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:B:35:VAL:CG1	1:B:88:VAL:HG11	2.13	0.78
1:B:35:VAL:HG11	1:B:88:VAL:HG11	1.72	0.71
1:A:14:VAL:HG13	1:A:78:GLY:HA2	1.76	0.67
1:A:154:GLU:HG2	1:B:154:GLU:HG2	1.76	0.67
1:B:35:VAL:HG12	1:B:88:VAL:HG11	1.90	0.54
1:A:31:GLY:HA2	1:A:34:GLY:O	2.12	0.49
1:A:120:ARG:HD3	1:A:299:VAL:HG11	1.95	0.48
1:B:35:VAL:HG11	1:B:88:VAL:HG21	1.96	0.47
1:B:120:ARG:HD3	1:B:299:VAL:HG11	1.97	0.47
1:B:292:TYR:HE1	1:B:299:VAL:HG21	1.80	0.46
1:A:292:TYR:HE1	1:A:299:VAL:HG21	1.81	0.44
1:B:103:LEU:HD13	1:B:121:LEU:HD13	2.00	0.43
1:A:132:LEU:HD22	1:A:139:LEU:HD23	2.01	0.42
1:B:132:LEU:HD22	1:B:139:LEU:HD23	2.01	0.42
1:A:118:LEU:HD22	1:A:219:VAL:HG13	2.01	0.42
1:A:103:LEU:HD13	1:A:121:LEU:HD13	2.03	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	258/325 (79%)	252 (98%)	5 (2%)	1 (0%)	34	32
1	B	255/325 (78%)	245 (96%)	6 (2%)	4 (2%)	9	5
All	All	513/650 (79%)	497 (97%)	11 (2%)	5 (1%)	15	11

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	14	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	202	LYS
1	A	31	GLY
1	B	31	GLY
1	B	199	VAL

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	220/283 (78%)	217 (99%)	3 (1%)	67	73
1	B	200/283 (71%)	196 (98%)	4 (2%)	55	60
All	All	420/566 (74%)	413 (98%)	7 (2%)	60	67

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	152	ASP
1	A	271	TRP
1	B	152	ASP
1	B	227	LEU
1	B	271	TRP
1	B	276	GLU

Sometimes 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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	1FN	B	4000	-	36,38,38	0.54	0	46,54,54	0.37	0
2	1FN	A	4000	-	36,38,38	0.57	0	46,54,54	0.44	0

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	1FN	B	4000	-	-	2/16/16/16	0/5/5/5
2	1FN	A	4000	-	-	0/16/16/16	0/5/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

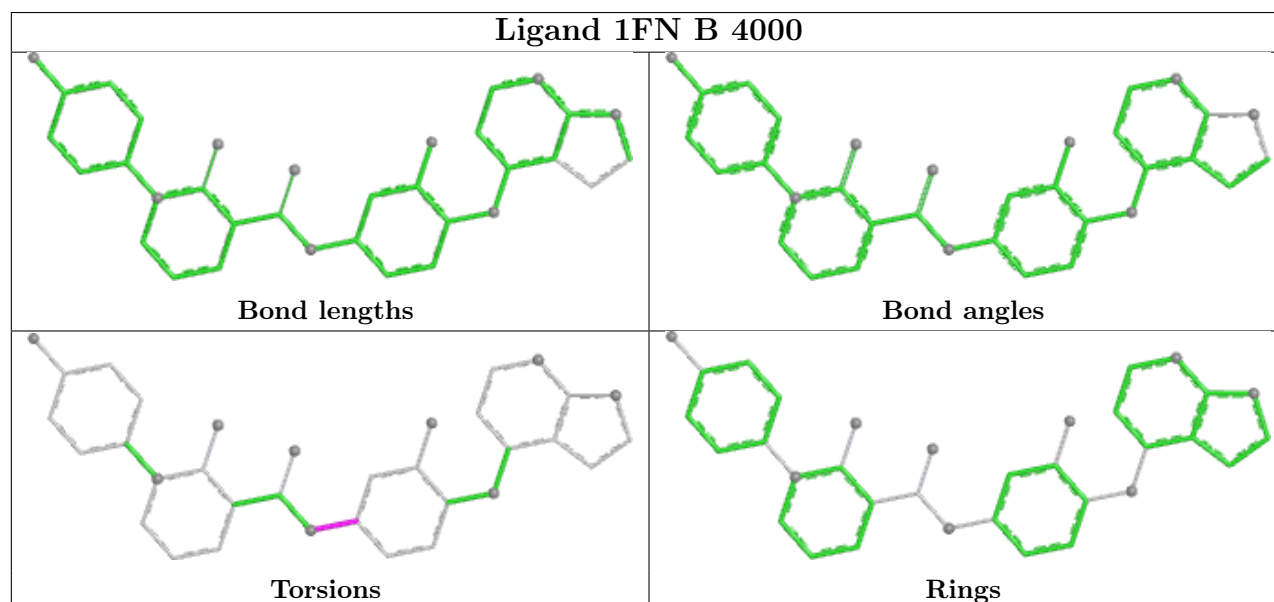
Mol	Chain	Res	Type	Atoms
2	B	4000	1FN	C12-C11-N15-C17
2	B	4000	1FN	C10-C11-N15-C17

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 [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	263/325 (80%)	0.16	10 (3%) 40 46	33, 50, 77, 99	0
1	B	261/325 (80%)	0.70	33 (12%) 3 5	36, 72, 116, 136	0
All	All	524/650 (80%)	0.43	43 (8%) 11 15	33, 60, 105, 136	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	PHE	9.9
1	B	227	LEU	6.9
1	B	196	LEU	5.9
1	B	243	SER	5.6
1	B	241	ARG	5.0
1	B	56	LYS	4.6
1	B	188	LEU	4.5
1	B	251	PRO	4.4
1	B	60	TRP	4.4
1	A	60	TRP	4.2
1	B	198	LYS	4.1
1	B	87	PHE	4.0
1	B	55	SER	3.9
1	B	248	THR	3.9
1	A	200	ASN	3.7
1	B	200	ASN	3.5
1	B	255	PRO	3.5
1	B	256	GLU	3.4
1	A	187	THR	3.4
1	B	242	GLN	3.4
1	B	252	PRO	3.3
1	B	250	LEU	3.2
1	B	111	ALA	3.2
1	B	90	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	255	PRO	3.1
1	A	251	PRO	2.8
1	B	246	PRO	2.8
1	B	193	PRO	2.7
1	A	31	GLY	2.6
1	B	113	ARG	2.6
1	B	201	LEU	2.6
1	A	252	PRO	2.5
1	A	56	LYS	2.5
1	B	54	ASN	2.4
1	A	186	GLY	2.4
1	B	58	ILE	2.4
1	B	217	TRP	2.3
1	B	31	GLY	2.3
1	B	225	ALA	2.1
1	B	107	LEU	2.1
1	B	245	PRO	2.1
1	A	258	PRO	2.0
1	B	253	GLY	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.

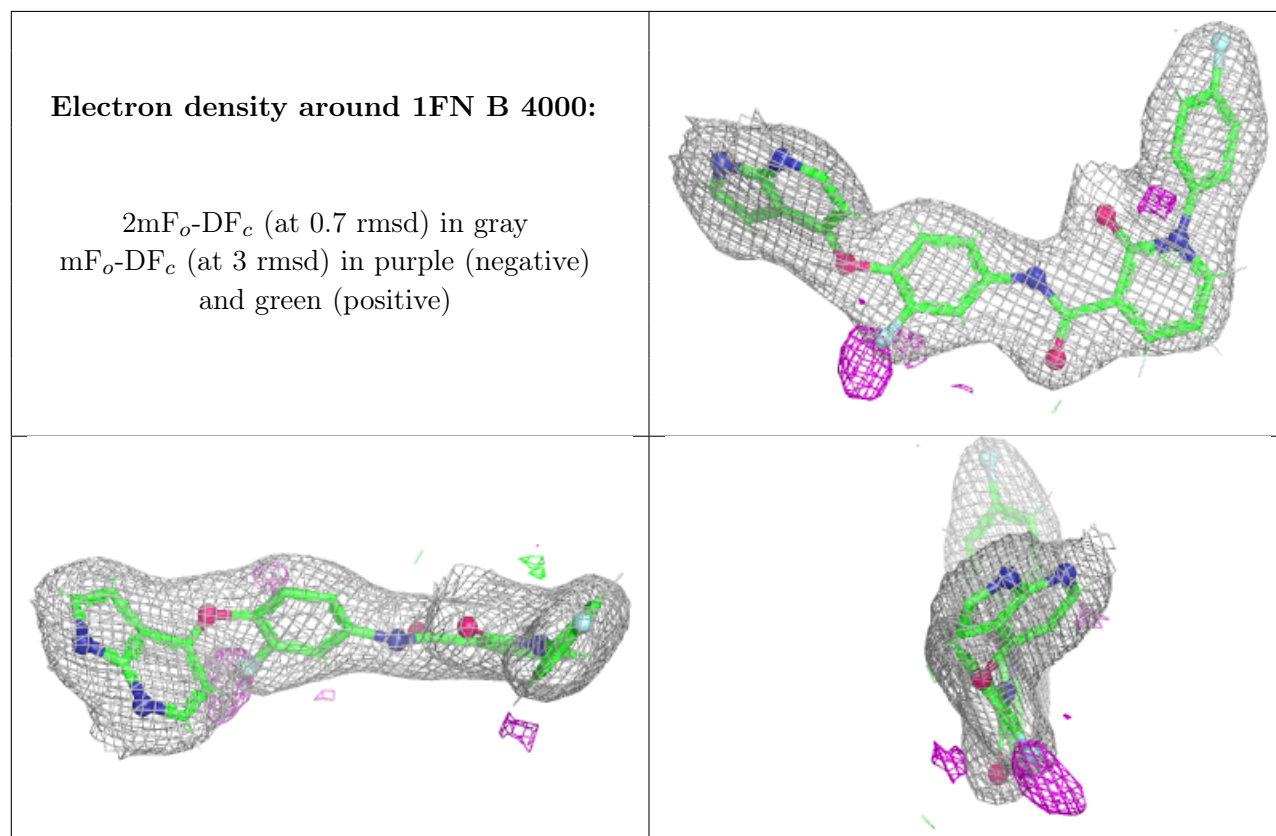
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	1FN	B	4000	34/34	0.95	0.12	43,57,63,65	16
2	1FN	A	4000	34/34	0.98	0.11	33,40,44,48	16

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.