

Full wwPDB X-ray Structure Validation Report (i)

May 24, 2020 - 01:28 am BST

PDB ID	:	60KO
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-car
		boxamide
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 (i) symbol.

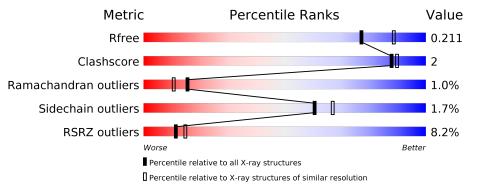
The following versions of software and data (see references (1)) were used in the production of this report:

1 Overall quality at a glance (i)

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries},{ m resolution\ range}({ m \AA}))$
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 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 <=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	А	325	3% 76%	5%	19%
1	В	325	75%	6%	20%



$60 \mathrm{KO}$

2 Entry composition (i)

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.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	263	Total	С	Ν	Ο	S	0	1	0
1		203	2035	1309	348	370	8	0		0
1	D	De 1 Te	Total	С	Ν	Ο	S	0	0	0
T	D	261	1959	1262	336	353	8		U	U

• Molecule 1 is a protein called Receptor-interacting serine/threonine-protein kinase 3.

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

There are 30 discrepancies between the modelled and reference sequences:

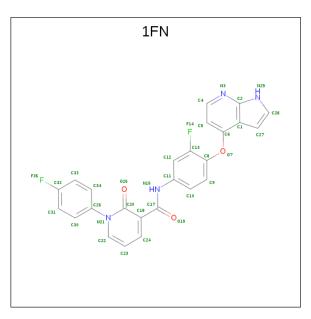
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Contenta	Continued from previous page								
Chain	Residue	Modelled	Actual	Comment	Reference				
В	321	HIS	-	expression tag	UNP Q9QZL0				
В	322	HIS	-	expression tag	UNP Q9QZL0				
В	323	HIS	-	expression tag	UNP Q9QZL0				
В	324	HIS	-	expression tag	UNP Q9QZL0				
В	325	HIS	-	expression tag	UNP Q9QZL0				

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• Molecule 2 is 1-(4-fluorophenyl)-N-[3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4-yloxy)phenyl]-2-o xo-1,2-dihydropyridine-3-carboxamide (three-letter code: 1FN) (formula: $C_{25}H_{16}F_2N_4O_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
0	Δ	1	Total	С	F	Η	Ν	Ο	16	0
	Z A	1	50	25	2	16	4	3	10	0
0	р	1	Total	С	F	Η	Ν	Ο	16	0
	2 В		50	25	2	16	4	3	10	0

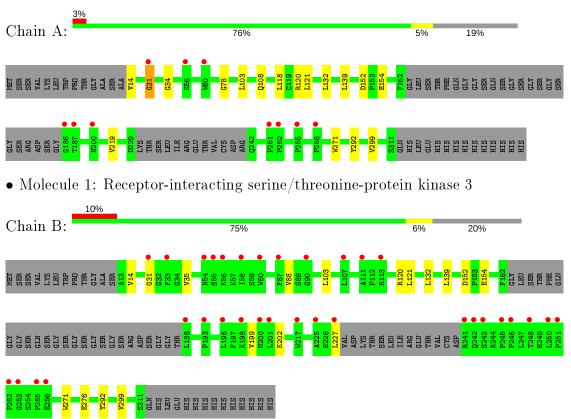
• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	140	Total O 140 140	0	0
3	В	62	$\begin{array}{cc} \text{Total} & \text{O} \\ 62 & 62 \end{array}$	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Receptor-interacting serine/threonine-protein kinase 3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	144.76Å 52.75 Å 103.75 Å	Depositor
a, b, c, α , β , γ	90.00° 130.82° 90.00°	Depositor
Resolution (Å)	39.26 - 2.10	Depositor
Resolution (A)	39.26 - 2.10	EDS
% Data completeness	98.5 (39.26-2.10)	Depositor
(in resolution range)	99.2 (39.26-2.10)	EDS
R _{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.19 (at 2.10 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
D D.	0.180 , 0.198	Depositor
R, R_{free}	0.183 , 0.211	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.

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.



¹Intensities estimated from amplitudes.

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		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.45	0/2086	0.61	0/2844	
1	В	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	А	2035	0	2014	8	0
1	В	1959	0	1890	9	0
2	А	34	16	16	0	0
2	В	34	16	16	0	0
3	А	140	0	0	0	0
3	В	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



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

magnitude.

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	А	258/325~(79%)	252~(98%)	5(2%)	1 (0%)	34 32
1	В	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	\mathbf{Res}	Type
1	В	14	VAL
	a .:	1	

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	J	1	1 0
Mol	Chain	\mathbf{Res}	Type
1	В	202	LYS
1	А	31	GLY
1	В	31	GLY
1	В	199	VAL

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		Outliers	Percentiles		
1	А	220/283~(78%)	217~(99%)	3~(1%)	67 73		
1	В	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	А	108	GLN
1	А	152	ASP
1	А	271	TRP
1	В	152	ASP
1	В	227	LEU
1	В	271	TRP
1	В	276	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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).

ſ	Mol	Type	Chain	Res	Link	Bo	ond leng	ths	B	ond ang	les
	IVIOI	туре	Chain	nes	LINK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
	2	1FN	В	4000	-	$36,\!38,\!38$	0.87	2(5%)	41,54,54	0.51	0
	2	1FN	А	4000	-	36, 38, 38	0.90	2(5%)	41,54,54	0.55	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	$1 \mathrm{FN}$	В	4000	-	-	5/16/16/16	0/5/5/5
2	1FN	А	4000	-	-	1/16/16/16	0/5/5/5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	А	4000	1FN	C22-N21	2.79	1.40	1.36
2	В	4000	1FN	C20-N21	2.52	1.42	1.37
2	А	4000	1FN	C20-N21	2.40	1.42	1.37
2	В	4000	1FN	C22-N21	2.32	1.39	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

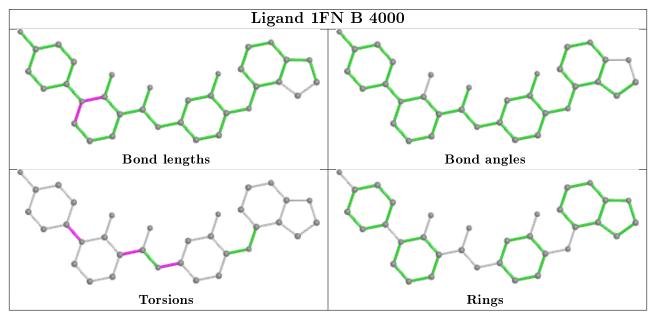


Mol	Chain	Res	Type	Atoms
2	В	4000	1FN	C12-C11-N15-C17
2	В	4000	1FN	N15-C17-C18-C24
2	В	4000	1FN	O19-C17-C18-C24
2	В	4000	1FN	C10-C11-N15-C17
2	В	4000	1FN	C30-C26-N21-C22
2	А	4000	1FN	C30-C26-N21-C22

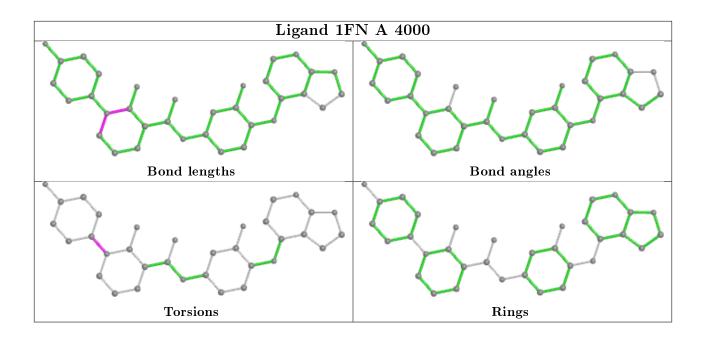
There are no ring outliers.

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 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 similar 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	263/325~(80%)	0.16	10 (3%) 40 46	33, 50, 77, 99	0
1	В	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	В	33	PHE	9.9
1	В	227	LEU	6.9
1	В	196	LEU	5.9
1	В	243	SER	5.6
1	В	241	ARG	5.0
1	В	56	LYS	4.6
1	В	188	LEU	4.5
1	В	251	PRO	4.4
1	В	60	TRP	4.4
1	А	60	TRP	4.2
1	В	198	LYS	4.1
1	В	87	PHE	4.0
1	В	55	SER	3.9
1	В	248	THR	3.9
1	А	200	ASN	3.7
1	В	200	ASN	3.5
1	В	255	PRO	3.5
1	В	256	GLU	3.4
1	А	187	THR	3.4
1	В	242	GLN	3.4
1	В	252	PRO	3.3
1	В	250	LEU	3.2
1	В	111	ALA	3.2
1	В	90	GLY	3.2

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

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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 carbohydrates in this entry.

6.4 Ligands (i)

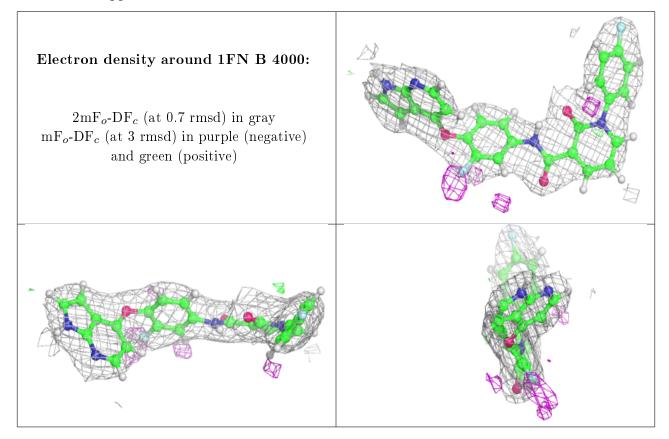
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	\mathbf{RSR}	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	$Q{<}0.9$
2	1FN	В	4000	34/34	0.95	0.12	$43,\!57,\!63,\!65$	16
2	1FN	А	4000	34/34	0.98	0.11	$33,\!40,\!44,\!48$	16

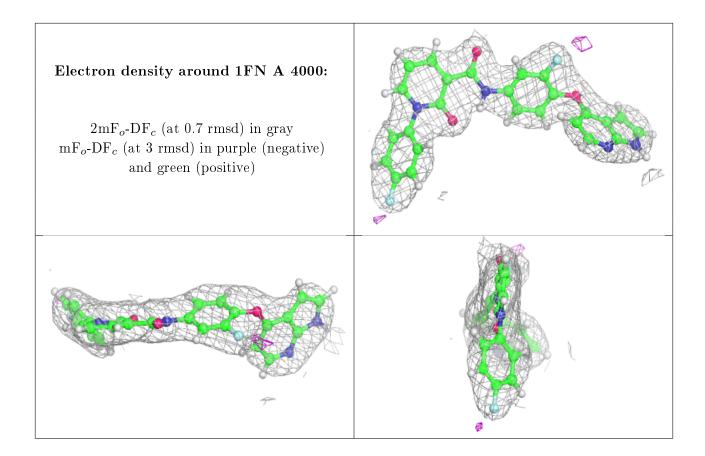
The following is a graphical depiction of the model fit to experimental electron density of all



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.

