



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 07:07 AM UTC

PDB ID : 7QA3 / pdb_00007qa3
Title : Crystal structure of PqsR (MvfR) ligand-binding domain in complex with compound N-((2-(4-phenoxyphenyl)thiazol-5-yl)methyl)-2-(trifluoromethyl)pyridin-4-amine
Authors : Schmelz, S.; Blankenfeldt, W.
Deposited on : 2021-11-15
Resolution : 2.67 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

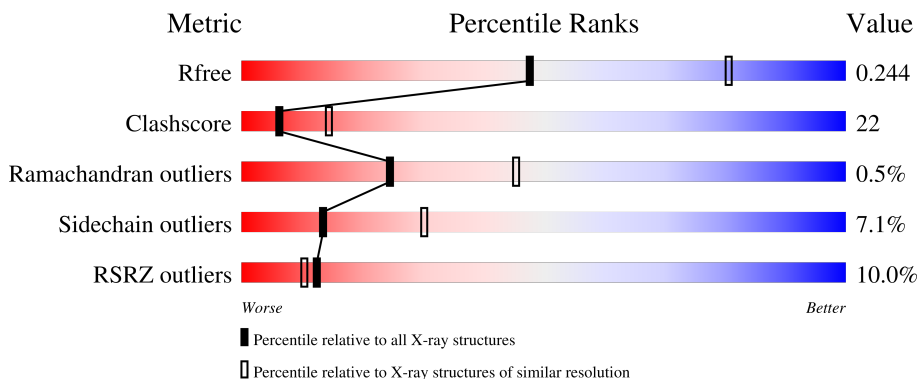
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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}	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	332	 5% 41% 21% 38%
1	B	332	 8% 34% 24% 38%

2 Entry composition [i](#)

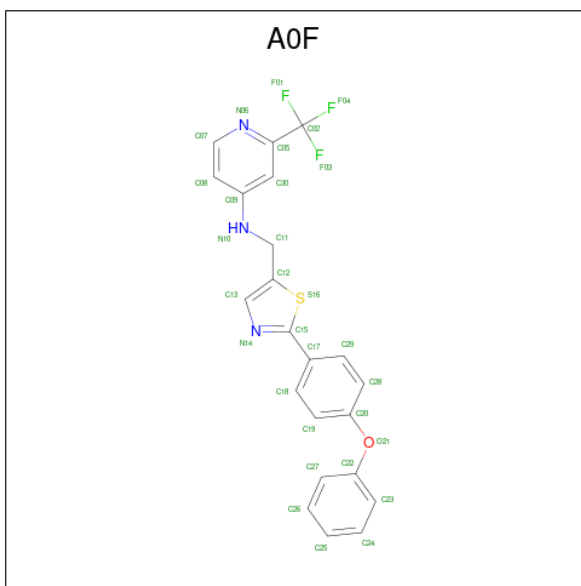
There are 3 unique types of molecules in this entry. The entry contains 6382 atoms, of which 3138 are hydrogens and 0 are deuteriums.

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 Multiple virulence factor regulator MvfR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	206	Total 3141	C 1010	H 1551	N 271	O 303	S 6	13	1	0
1	B	206	Total 3145	C 1011	H 1555	N 271	O 301	S 7	0	2	0

- Molecule 2 is N-[[2-(4-phenoxyphenyl)-1,3-thiazol-5-yl]methyl]-2-(trifluoromethyl)pyridin-4-amine (CCD ID: A0F) (formula: C₂₂H₁₆F₃N₃OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	
			Total	C	F	H	N	O			S
2	A	1	Total 46	C 22	F 3	H 16	N 3	O 1	S 1	0	0
2	B	1	Total 46	C 22	F 3	H 16	N 3	O 1	S 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	O 3	0	0
3	B	1	Total 1	O 1	0	0

E297
G296
ARG
PHE
ASP
ASP
ALA
PRO
ALA
TRP
GLN
PRO
SER
ILE
VAL
GLU
THR
ALA
ALA
GLN
ARG
ARG
SER
GLY
PRO
LYS
ALA
LEU
ALA
TYR
ARG
GLN
ARG
ALA
ALA
PRO
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.02Å 122.61Å 112.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.86 – 2.67 53.86 – 2.67	Depositor EDS
% Data completeness (in resolution range)	63.8 (53.86-2.67) 59.5 (53.86-2.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.208 , 0.245 0.208 , 0.244	Depositor DCC
R_{free} test set	692 reflections (3.06%)	wwPDB-VP
Wilson B-factor (Å ²)	57.6	Xtrriage
Anisotropy	0.023	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6382	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: A0F

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	0/1623	0.73	0/2210
1	B	0.60	2/1626 (0.1%)	0.83	5/2214 (0.2%)
All	All	0.56	2/3249 (0.1%)	0.78	5/4424 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	186	ILE	CB-CG2	5.65	1.71	1.52
1	B	258	TYR	C-N	5.47	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	122	VAL	N-CA-C	-7.82	96.34	107.75
1	B	186	ILE	CG1-CB-CG2	6.09	128.97	110.70
1	B	186	ILE	CA-C-O	5.46	126.37	120.47
1	B	293	ARG	NH1-CZ-NH2	-5.22	112.51	119.30
1	B	279	ARG	N-CA-C	-5.17	99.79	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	ARG	Sidechain
1	B	279	ARG	Sidechain
1	B	293	ARG	Sidechain

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	1590	1551	1551	59	0
1	B	1590	1555	1555	84	0
2	A	30	16	0	1	0
2	B	30	16	0	2	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
All	All	3244	3138	3106	141	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 22.

The worst 5 of 141 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:242[A]:VAL:HG13	1:B:251:LEU:HD23	1.60	0.82
1:A:207:LEU:HD23	1:A:208:LEU:HG	1.65	0.77
1:A:165:TYR:OH	1:B:259:GLU:OE2	2.03	0.76
1:B:224:MET:O	1:B:228:VAL:HG23	1.86	0.76
1:B:290:GLN:HA	1:B:293:ARG:HD2	1.73	0.70

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	205/332 (62%)	192 (94%)	13 (6%)	0	100	100
1	B	206/332 (62%)	189 (92%)	15 (7%)	2 (1%)	12	28
All	All	411/664 (62%)	381 (93%)	28 (7%)	2 (0%)	24	45

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	273	THR
1	B	279	ARG

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	171/288 (59%)	163 (95%)	8 (5%)	23	47
1	B	172/288 (60%)	156 (91%)	16 (9%)	8	19
All	All	343/576 (60%)	319 (93%)	24 (7%)	13	31

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	144	ASP
1	B	156	SER
1	B	155	ILE
1	B	166	THR

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Mol	Chain	Res	Type
1	A	183	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	ASN
1	B	160	GLN
1	B	176	HIS

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 oligosaccharides 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	A0F	B	401	-	33,33,33	1.83	5 (15%)	42,46,46	2.85	16 (38%)
2	A0F	A	401	-	33,33,33	2.05	6 (18%)	42,46,46	2.20	14 (33%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A0F	B	401	-	-	1/19/19/19	0/4/4/4
2	A0F	A	401	-	-	3/19/19/19	0/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	A0F	C13-N14	6.12	1.49	1.37
2	B	401	A0F	C15-S16	-4.74	1.63	1.74
2	A	401	A0F	C12-S16	-4.72	1.58	1.73
2	A	401	A0F	C17-C15	4.43	1.54	1.47
2	A	401	A0F	C15-S16	-4.30	1.64	1.74

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	A0F	S16-C15-N14	-6.90	107.96	113.97
2	B	401	A0F	C18-C17-C15	6.28	130.29	120.75
2	B	401	A0F	C29-C17-C15	-6.21	111.30	120.75
2	A	401	A0F	S16-C15-N14	-5.97	108.77	113.97
2	B	401	A0F	C17-C15-S16	5.86	133.93	122.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A0F	C12-C11-N10-C09
2	B	401	A0F	C12-C11-N10-C09
2	A	401	A0F	N14-C15-C17-C18
2	A	401	A0F	N14-C15-C17-C29

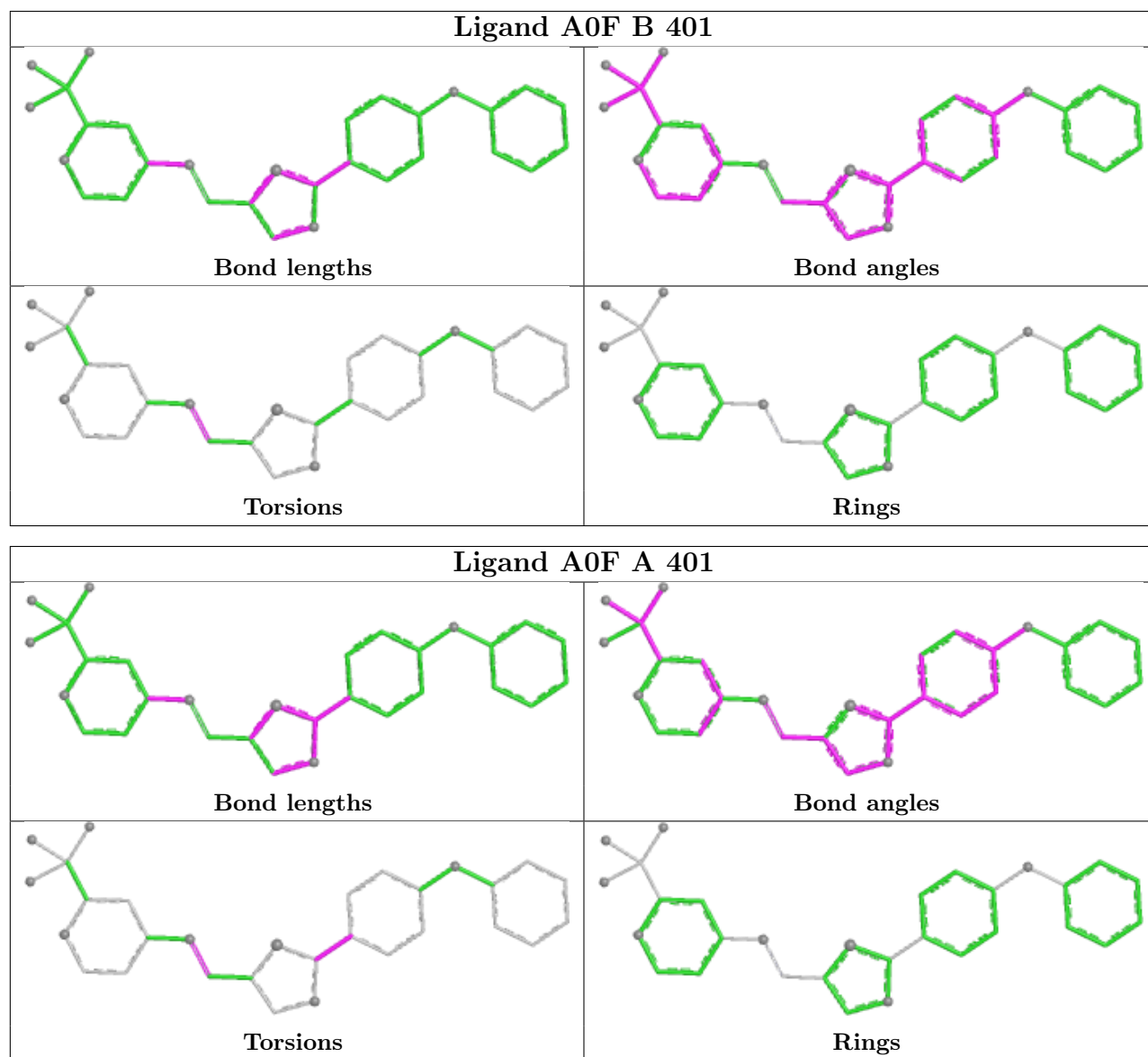
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	A0F	2	0
2	A	401	A0F	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

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	206/332 (62%)	0.44	16 (7%) 19 16	31, 64, 108, 139	1 (0%)
1	B	206/332 (62%)	0.80	25 (12%) 8 7	40, 73, 125, 142	2 (0%)
All	All	412/664 (62%)	0.62	41 (9%) 12 10	31, 69, 119, 142	3 (0%)

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	GLN	7.6
1	A	298	GLN	4.9
1	B	107	PHE	4.4
1	A	93	ARG	4.1
1	B	203	GLN	4.0

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](#)

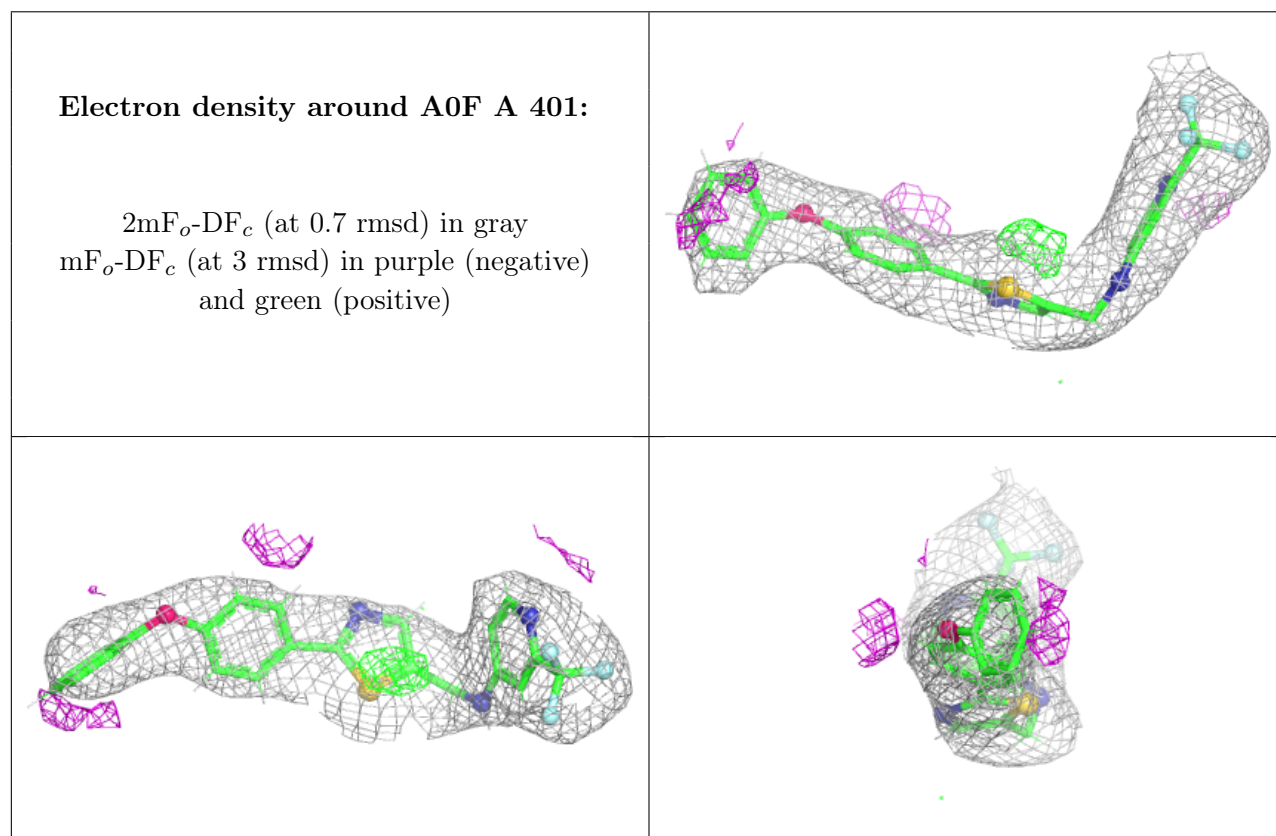
There are no oligosaccharides in this entry.

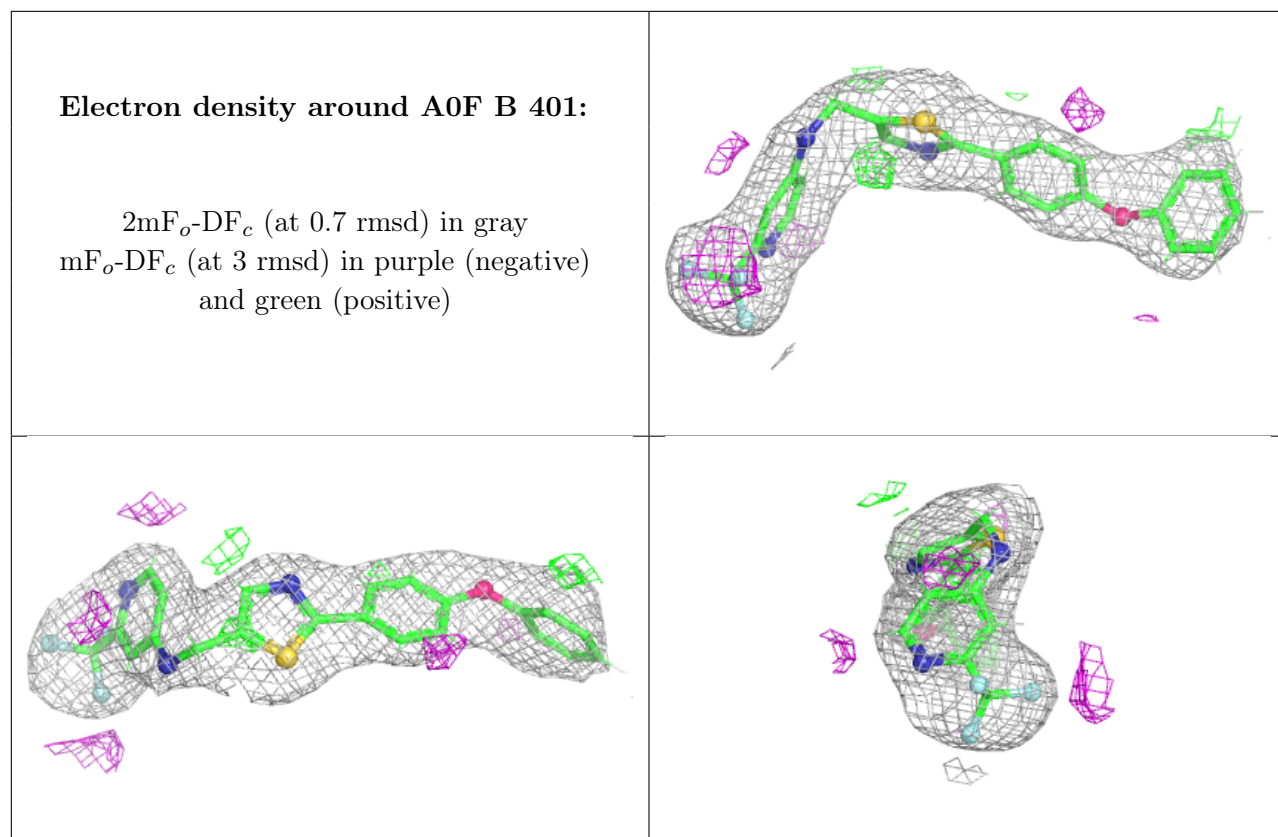
6.4 Ligands [i](#)

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	A0F	A	401	30/30	0.96	0.11	19,49,71,87	0
2	A0F	B	401	30/30	0.96	0.09	32,43,63,77	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.