



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:02 AM UTC

PDB ID : 9FR6 / pdb\_00009fr6  
Title : Crystal structure of human GSK3B in complex with ARN25641  
Authors : Dalle Vedove, A.; Demuro, S.; Di Martino, R.M.C.; Balboni, B.; Tripathi, S.K.; Storici, P.; Girotto, S.; Cavalli, A.  
Deposited on : 2024-06-18  
Resolution : 2.30 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](mailto: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>.

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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

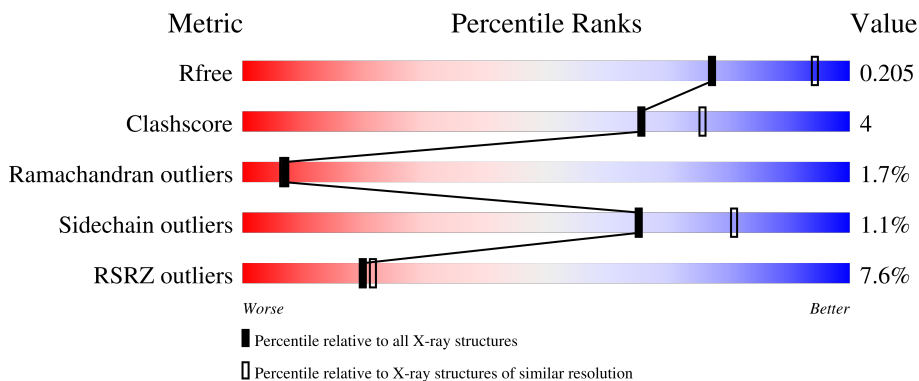
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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  $\geq 3$ , 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	442	 7% 72% 10% 18%
1	B	442	 5% 71% 7% 21%

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6004 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 Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2889	1853	498	526	12	0	0	0
1	B	347	2779	1789	475	504	11	0	0	0

There are 46 discrepancies between the modelled and reference sequences:

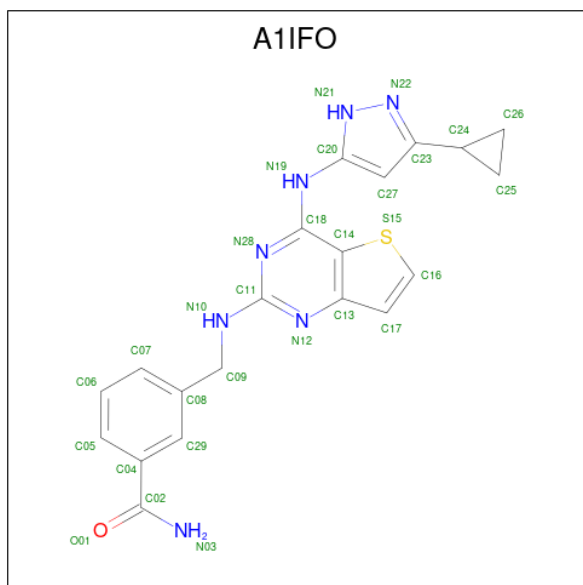
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P49841
A	-20	GLY	-	expression tag	UNP P49841
A	-19	HIS	-	expression tag	UNP P49841
A	-18	HIS	-	expression tag	UNP P49841
A	-17	HIS	-	expression tag	UNP P49841
A	-16	HIS	-	expression tag	UNP P49841
A	-15	HIS	-	expression tag	UNP P49841
A	-14	HIS	-	expression tag	UNP P49841
A	-13	SER	-	expression tag	UNP P49841
A	-12	SER	-	expression tag	UNP P49841
A	-11	GLY	-	expression tag	UNP P49841
A	-10	VAL	-	expression tag	UNP P49841
A	-9	ASP	-	expression tag	UNP P49841
A	-8	LEU	-	expression tag	UNP P49841
A	-7	GLY	-	expression tag	UNP P49841
A	-6	THR	-	expression tag	UNP P49841
A	-5	GLU	-	expression tag	UNP P49841
A	-4	ASN	-	expression tag	UNP P49841
A	-3	LEU	-	expression tag	UNP P49841
A	-2	TYR	-	expression tag	UNP P49841
A	-1	PHE	-	expression tag	UNP P49841
A	0	GLN	-	expression tag	UNP P49841
A	1	SER	-	expression tag	UNP P49841
B	-21	MET	-	initiating methionine	UNP P49841
B	-20	GLY	-	expression tag	UNP P49841

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	HIS	-	expression tag	UNP P49841
B	-18	HIS	-	expression tag	UNP P49841
B	-17	HIS	-	expression tag	UNP P49841
B	-16	HIS	-	expression tag	UNP P49841
B	-15	HIS	-	expression tag	UNP P49841
B	-14	HIS	-	expression tag	UNP P49841
B	-13	SER	-	expression tag	UNP P49841
B	-12	SER	-	expression tag	UNP P49841
B	-11	GLY	-	expression tag	UNP P49841
B	-10	VAL	-	expression tag	UNP P49841
B	-9	ASP	-	expression tag	UNP P49841
B	-8	LEU	-	expression tag	UNP P49841
B	-7	GLY	-	expression tag	UNP P49841
B	-6	THR	-	expression tag	UNP P49841
B	-5	GLU	-	expression tag	UNP P49841
B	-4	ASN	-	expression tag	UNP P49841
B	-3	LEU	-	expression tag	UNP P49841
B	-2	TYR	-	expression tag	UNP P49841
B	-1	PHE	-	expression tag	UNP P49841
B	0	GLN	-	expression tag	UNP P49841
B	1	SER	-	expression tag	UNP P49841

- Molecule 2 is 3-[[[4-[(3-cyclopropyl-1 {H}-pyrazol-5-yl)amino]thieno[3,2-d]pyrimidin-2-yl]amino]methyl]benzamide (CCD ID: A1IFO) (formula: C<sub>20</sub>H<sub>19</sub>N<sub>7</sub>OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			29	20	7	1	1		
2	B	1	Total	C	N	O	S	0	0
			29	20	7	1	1		

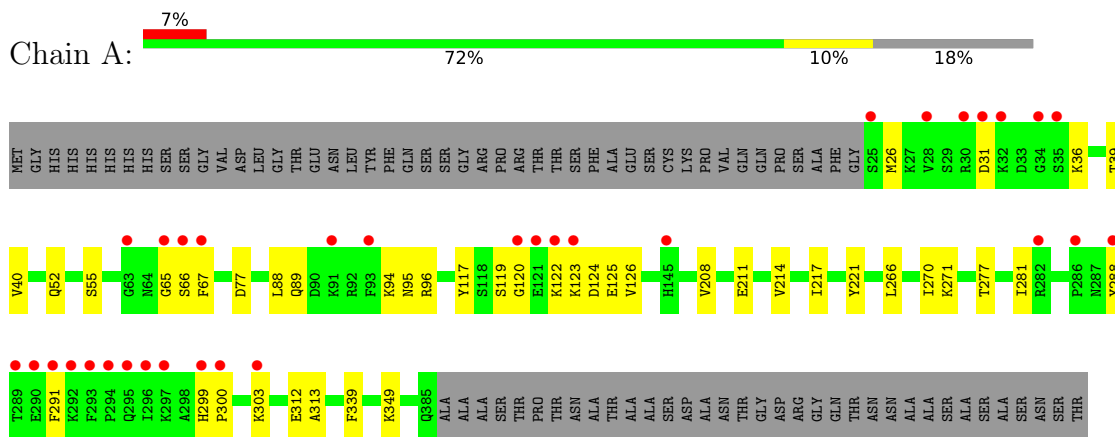
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	150	Total	O	0	0
			150	150		

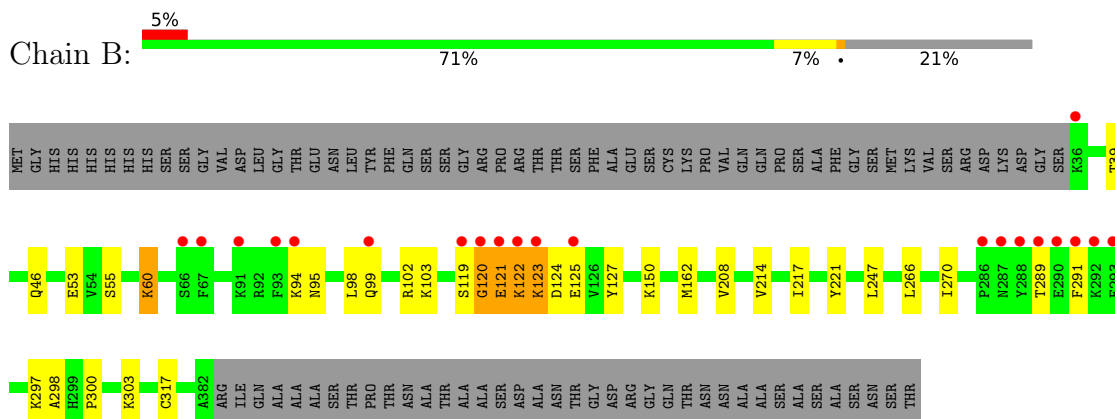
### 3 Residue-property plots [i](#)

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: Glycogen synthase kinase-3 beta



- Molecule 1: Glycogen synthase kinase-3 beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.31Å 85.26Å 178.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.74 – 2.30 74.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (74.74-2.30) 100.0 (74.74-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.18Å)	Xtrriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.199 , 0.232 0.199 , 0.205	Depositor DCC
$R_{free}$ test set	3413 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.5	Xtrriage
Anisotropy	0.560	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.016 for k,h,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6004	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1IFO

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	0.16	0/2960	0.35	0/4022
1	B	0.19	0/2850	0.38	0/3878
All	All	0.17	0/5810	0.36	0/7900

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	2889	0	2919	23	0
1	B	2779	0	2804	23	0
2	A	29	0	0	0	0
2	B	29	0	0	0	0
3	A	128	0	0	2	0
3	B	150	0	0	2	0
All	All	6004	0	5723	43	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 4.

All (43) 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:52:GLN:NE2	3:A:601:HOH:O	2.21	0.72
1:B:94:LYS:NZ	1:B:99:GLN:OE1	2.25	0.69
1:A:214:VAL:HG11	1:B:291:PHE:HB2	1.77	0.65
1:A:96:ARG:NH1	3:A:604:HOH:O	2.30	0.64
1:B:94:LYS:HD2	1:B:95:ASN:N	2.15	0.62
1:A:291:PHE:HB2	1:B:214:VAL:HG11	1.82	0.61
1:B:119:SER:HB2	1:B:123:LYS:HZ1	1.66	0.61
1:A:266:LEU:O	1:A:270:ILE:HG12	2.02	0.60
1:A:89:GLN:HB3	1:A:126:VAL:HG23	1.83	0.59
1:B:266:LEU:O	1:B:270:ILE:HG12	2.02	0.59
1:A:122:LYS:O	1:A:124:ASP:N	2.30	0.59
1:B:39:THR:HG1	1:B:55:SER:HG	1.54	0.56
1:B:122:LYS:O	1:B:124:ASP:N	2.30	0.56
1:A:77:ASP:N	1:A:77:ASP:OD1	2.36	0.56
1:A:88:LEU:HD11	1:A:125:GLU:HB3	1.89	0.55
1:B:103:LYS:NZ	3:B:609:HOH:O	2.39	0.55
1:A:39:THR:HG1	1:A:55:SER:HG	1.51	0.54
1:B:300:PRO:HG2	1:B:303:LYS:HD3	1.89	0.53
1:B:120:GLY:O	1:B:121:GLU:HB2	2.10	0.52
1:B:94:LYS:HE3	1:B:99:GLN:HB2	1.93	0.51
1:B:162:MET:HE2	1:B:247:LEU:HB2	1.92	0.50
1:B:94:LYS:CE	1:B:99:GLN:HB2	2.42	0.50
1:B:297:LYS:HD3	1:B:298:ALA:N	2.28	0.49
1:A:26:MET:HB2	1:A:40:VAL:HG12	1.94	0.48
1:A:94:LYS:HG3	1:A:95:ASN:N	2.29	0.48
1:B:46:GLN:NE2	3:B:619:HOH:O	2.49	0.46
1:B:98:LEU:O	1:B:102:ARG:HG3	2.17	0.45
1:A:89:GLN:HE21	1:A:117:TYR:HE1	1.64	0.45
1:A:277:THR:O	1:A:281:ILE:HG13	2.17	0.45
1:A:349:LYS:HE3	1:A:349:LYS:HB3	1.84	0.44
1:A:208:VAL:HB	1:A:211:GLU:CD	2.41	0.44
1:B:150:LYS:HB2	1:B:150:LYS:HE3	1.72	0.44
1:B:60:LYS:HB2	1:B:60:LYS:HE2	1.67	0.43
1:B:123:LYS:HE2	1:B:125:GLU:HG2	1.99	0.43
1:A:217:ILE:H	1:A:217:ILE:HG13	1.69	0.43
1:B:122:LYS:HG3	1:B:123:LYS:H	1.83	0.43
1:A:65:GLY:O	1:A:67:PHE:N	2.52	0.42
1:A:271:LYS:O	1:A:299:HIS:HB2	2.19	0.41
1:A:300:PRO:HG2	1:A:303:LYS:HG3	2.02	0.41
1:B:123:LYS:HE3	1:B:127:TYR:HE1	1.85	0.41
1:A:312:GLU:H	1:A:312:GLU:CD	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ALA:HB2	1:A:339:PHE:CE1	2.56	0.41
1:A:214:VAL:CG1	1:B:291:PHE:HB2	2.50	0.41

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	359/442 (81%)	330 (92%)	22 (6%)	7 (2%)	6	5
1	B	345/442 (78%)	326 (94%)	14 (4%)	5 (1%)	9	9
All	All	704/884 (80%)	656 (93%)	36 (5%)	12 (2%)	7	7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	A	36	LYS
1	A	221	TYR
1	B	221	TYR
1	A	31	ASP
1	B	122	LYS
1	A	123	LYS
1	B	121	GLU
1	B	123	LYS
1	A	288	TYR
1	B	120	GLY
1	A	120	GLY

### 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	322/383 (84%)	321 (100%)	1 (0%)	86	93
1	B	309/383 (81%)	303 (98%)	6 (2%)	50	69
All	All	631/766 (82%)	624 (99%)	7 (1%)	65	81

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

Mol	Chain	Res	Type
1	A	119	SER
1	B	53	GLU
1	B	60	LYS
1	B	208	VAL
1	B	217	ILE
1	B	289	THR
1	B	317	CYS

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	99	GLN
1	A	108	ASN
1	B	46	GLN

### 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	A1IFO	A	501	-	31,33,33	2.76	8 (25%)	35,47,47	2.70	9 (25%)
2	A1IFO	B	501	-	31,33,33	2.72	8 (25%)	35,47,47	2.63	11 (31%)

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	A1IFO	A	501	-	-	4/15/19/19	0/5/5/5
2	A1IFO	B	501	-	-	4/15/19/19	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1IFO	C02-N03	7.73	1.47	1.33
2	B	501	A1IFO	C11-N10	7.66	1.46	1.34
2	A	501	A1IFO	C11-N10	7.64	1.46	1.34
2	B	501	A1IFO	C02-N03	7.57	1.46	1.33
2	B	501	A1IFO	C13-C17	6.35	1.51	1.42
2	A	501	A1IFO	C13-C17	6.18	1.51	1.42
2	A	501	A1IFO	C24-C23	4.56	1.54	1.49
2	B	501	A1IFO	C24-C23	4.15	1.53	1.49
2	B	501	A1IFO	C14-S15	-3.82	1.67	1.73
2	A	501	A1IFO	C14-S15	-3.77	1.67	1.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1IFO	C18-N19	3.44	1.46	1.39
2	A	501	A1IFO	C18-N19	3.42	1.46	1.39
2	A	501	A1IFO	C04-C02	2.86	1.54	1.50
2	B	501	A1IFO	C04-C02	2.77	1.54	1.50
2	A	501	A1IFO	O01-C02	-2.68	1.19	1.24
2	B	501	A1IFO	O01-C02	-2.59	1.19	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	A1IFO	C26-C24-C23	8.76	130.91	119.63
2	B	501	A1IFO	C26-C24-C23	7.97	129.89	119.63
2	A	501	A1IFO	C14-S15-C16	6.70	100.10	91.24
2	B	501	A1IFO	C14-S15-C16	6.62	99.99	91.24
2	A	501	A1IFO	C25-C24-C23	6.47	127.95	119.63
2	B	501	A1IFO	C25-C24-C23	5.64	126.89	119.63
2	A	501	A1IFO	C13-N12-C11	4.90	121.93	116.69
2	B	501	A1IFO	C13-N12-C11	4.37	121.37	116.69
2	B	501	A1IFO	C13-C14-S15	-3.79	106.86	110.75
2	A	501	A1IFO	C13-C14-S15	-3.73	106.92	110.75
2	B	501	A1IFO	C09-N10-C11	-3.63	118.36	123.15
2	A	501	A1IFO	N28-C11-N12	-2.99	121.36	126.26
2	B	501	A1IFO	C24-C23-N22	2.89	126.18	120.56
2	A	501	A1IFO	C17-C16-S15	-2.48	108.79	113.90
2	B	501	A1IFO	N28-C11-N12	-2.47	122.21	126.26
2	A	501	A1IFO	C24-C23-N22	2.42	125.25	120.56
2	B	501	A1IFO	C17-C16-S15	-2.40	108.96	113.90
2	B	501	A1IFO	C24-C23-C27	-2.40	125.53	128.60
2	B	501	A1IFO	C04-C02-N03	2.05	120.27	117.74
2	A	501	A1IFO	C20-C27-C23	2.04	106.58	105.28

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1IFO	N03-C02-C04-C05
2	A	501	A1IFO	N03-C02-C04-C29
2	A	501	A1IFO	O01-C02-C04-C05
2	A	501	A1IFO	O01-C02-C04-C29
2	B	501	A1IFO	N03-C02-C04-C29
2	B	501	A1IFO	O01-C02-C04-C29
2	B	501	A1IFO	N03-C02-C04-C05

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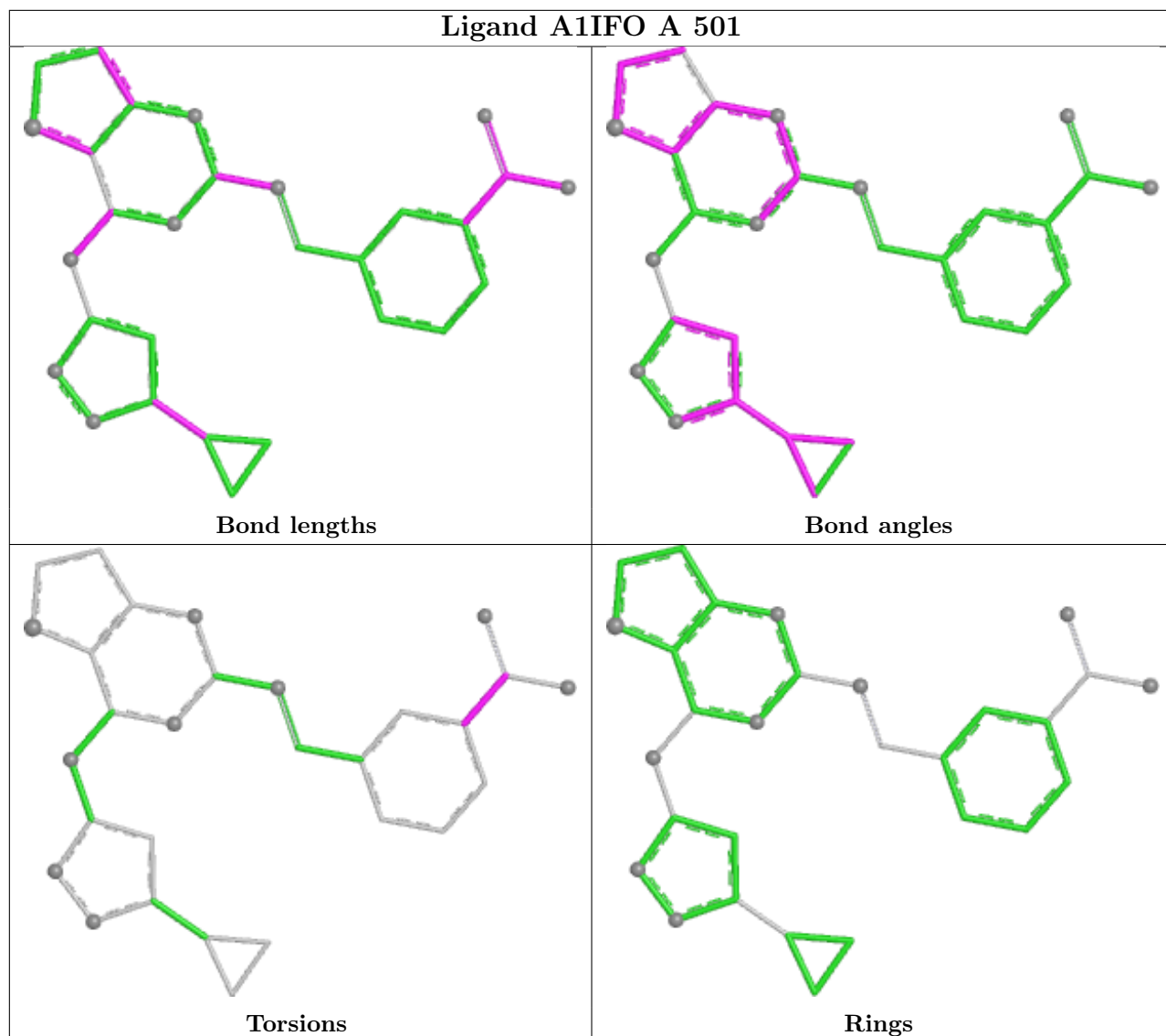
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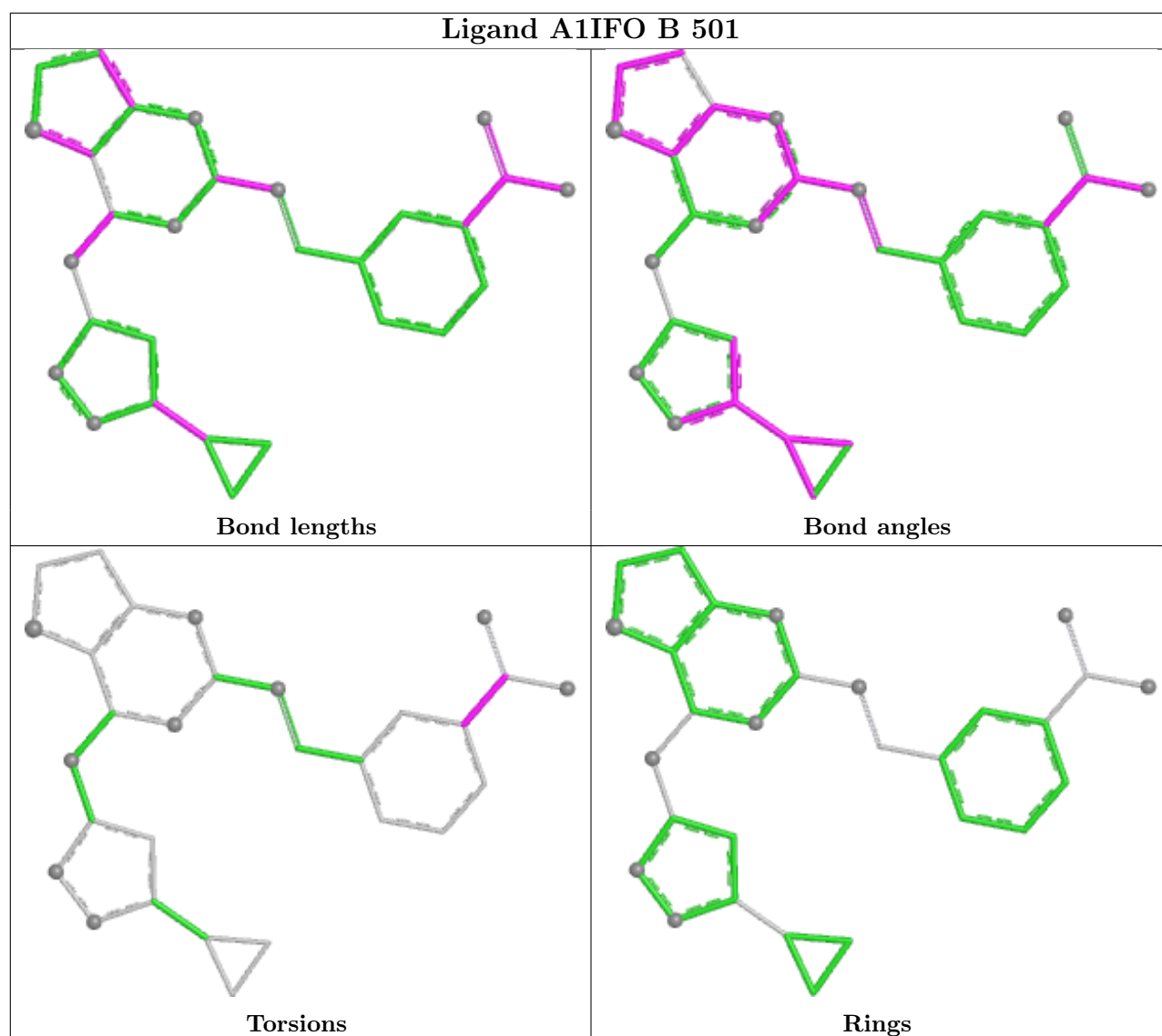
<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
2	B	501	A1IFO	O01-C02-C04-C05

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	361/442 (81%)	0.26	33 (9%) 15 16	22, 42, 88, 113	0
1	B	347/442 (78%)	0.09	21 (6%) 27 29	20, 37, 80, 116	0
All	All	708/884 (80%)	0.18	54 (7%) 20 21	20, 39, 87, 116	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	PHE	7.3
1	A	67	PHE	7.0
1	B	93	PHE	6.7
1	B	291	PHE	6.6
1	A	120	GLY	6.3
1	A	289	THR	5.0
1	A	286	PRO	5.0
1	B	289	THR	4.7
1	B	288	TYR	4.7
1	B	120	GLY	4.5
1	A	93	PHE	4.5
1	A	293	PHE	4.4
1	A	288	TYR	3.9
1	A	34	GLY	3.8
1	B	293	PHE	3.8
1	A	294	PRO	3.6
1	B	36	LYS	3.6
1	A	296	ILE	3.5
1	B	67	PHE	3.5
1	B	121	GLU	3.5
1	A	292	LYS	3.3
1	A	121	GLU	3.3
1	B	94	LYS	3.3
1	A	122	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	65	GLY	3.2
1	A	25	SER	3.1
1	A	66	SER	3.1
1	B	91	LYS	3.1
1	A	63	GLY	3.0
1	B	66	SER	3.0
1	B	286	PRO	3.0
1	A	123	LYS	2.9
1	A	35	SER	2.8
1	B	290	GLU	2.8
1	A	290	GLU	2.7
1	B	287	ASN	2.6
1	A	31	ASP	2.6
1	A	32	LYS	2.6
1	A	91	LYS	2.6
1	B	292	LYS	2.5
1	A	145	HIS	2.4
1	B	122	LYS	2.3
1	A	300	PRO	2.2
1	B	123	LYS	2.2
1	B	119	SER	2.2
1	A	282	ARG	2.1
1	A	28	VAL	2.1
1	B	99	GLN	2.1
1	A	30	ARG	2.1
1	B	125	GLU	2.1
1	A	297	LYS	2.1
1	A	299	HIS	2.0
1	A	303	LYS	2.0
1	A	295	GLN	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](#)

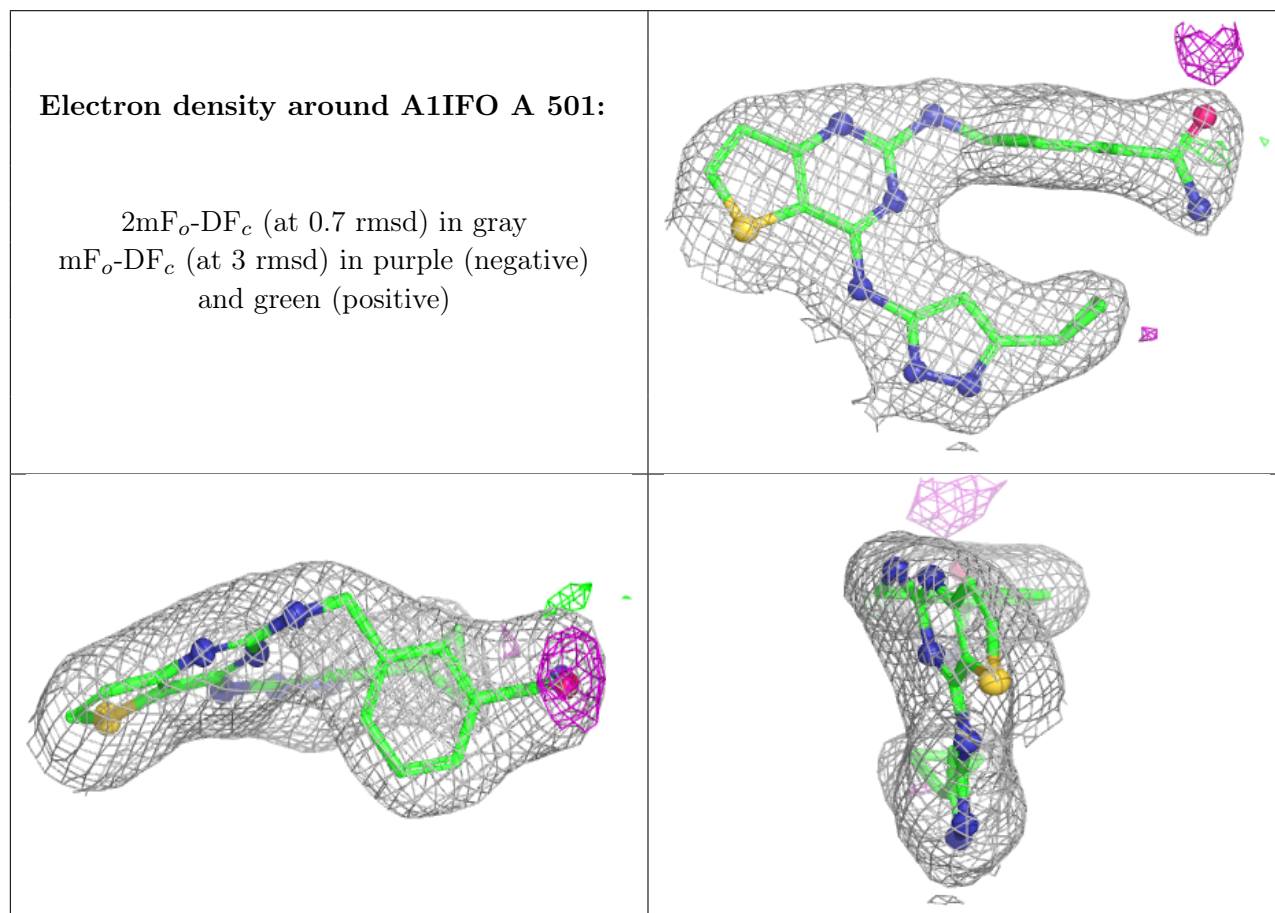
There are no oligosaccharides in this entry.

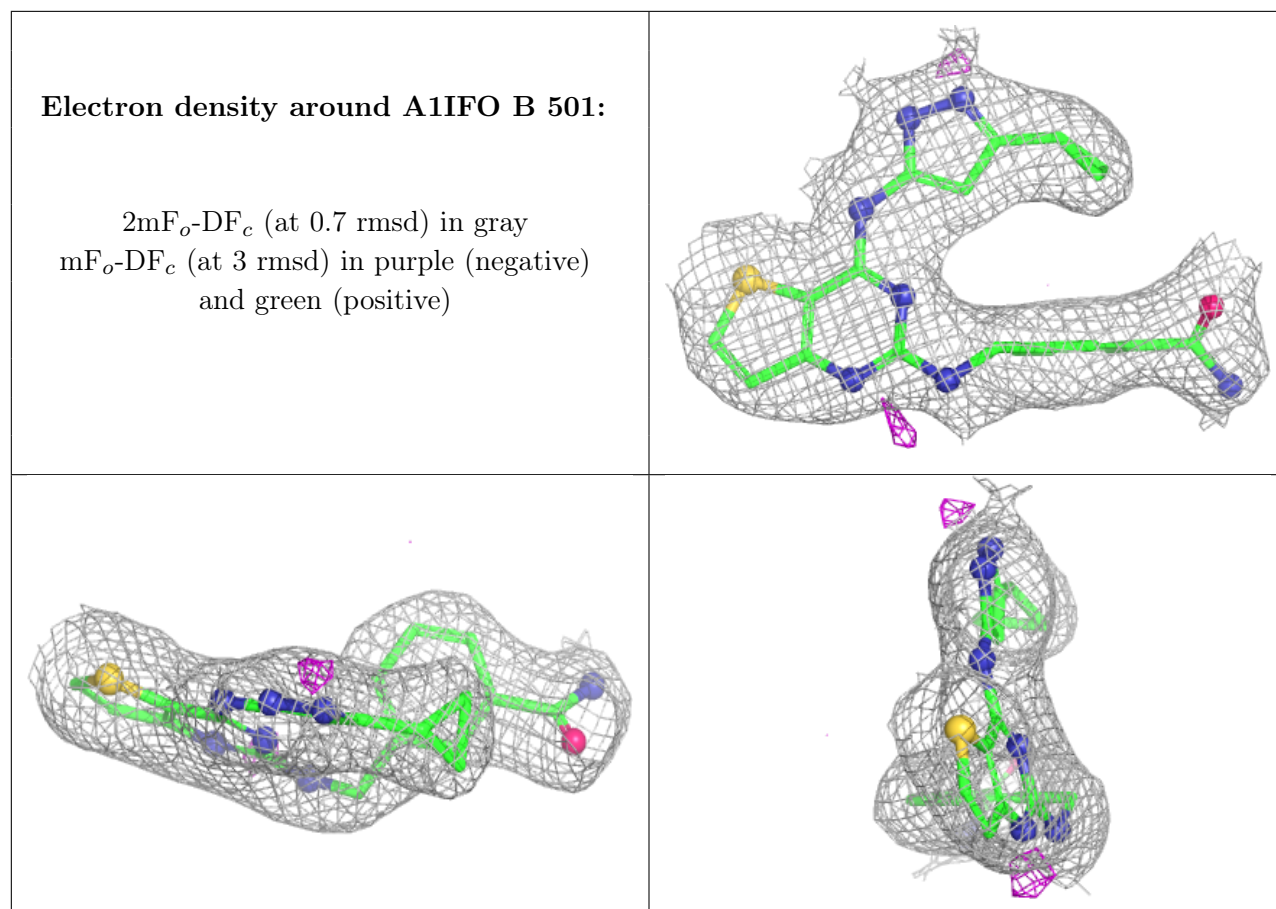
## 6.4 Ligands [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	A1IFO	A	501	29/29	0.97	0.07	27,35,43,50	0
2	A1IFO	B	501	29/29	0.97	0.07	21,30,46,48	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.