



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:05 PM UTC

PDB ID : 4FA6 / pdb\_00004fa6  
Title : Design and Synthesis of a Novel Pyrrolidinyl Pyrido Pyrimidinone Derivative as a Potent Inhibitor of PI3Ka and mTOR  
Authors : Pannifer, A.; Greasley, S.E.  
Deposited on : 2012-05-21  
Resolution : 2.70 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

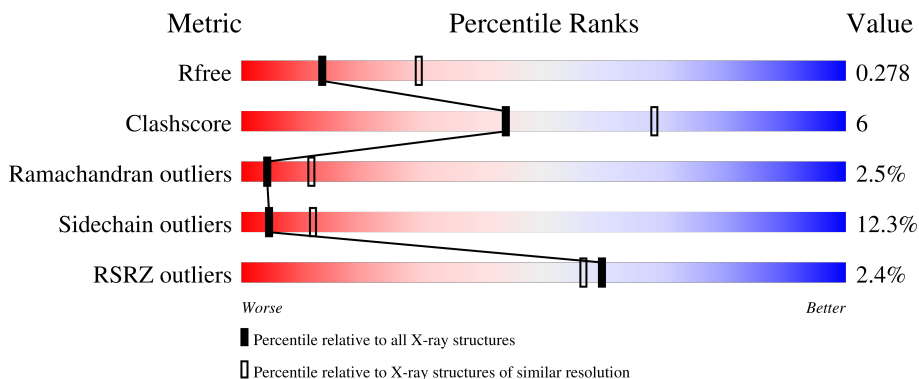
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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 <sub>free</sub>	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	966	 2% 64% 20% •• 13%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 6863 atoms, of which 18 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.

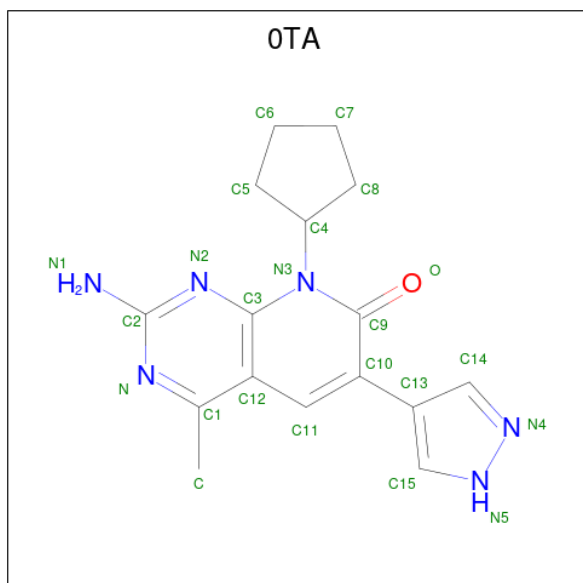
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	842	6818	4375	1165	1242	36	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	expression tag	UNP P48736
A	1103	HIS	-	expression tag	UNP P48736
A	1104	HIS	-	expression tag	UNP P48736
A	1105	HIS	-	expression tag	UNP P48736
A	1106	HIS	-	expression tag	UNP P48736
A	1107	HIS	-	expression tag	UNP P48736
A	1108	HIS	-	expression tag	UNP P48736

- Molecule 2 is 2-amino-8-cyclopentyl-4-methyl-6-(1H-pyrazol-4-yl)pyrido[2,3-d]pyrimidin-7(8H)-one (CCD ID: OTA) (formula: C<sub>16</sub>H<sub>18</sub>N<sub>6</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	41	16	18	6	1	0	0

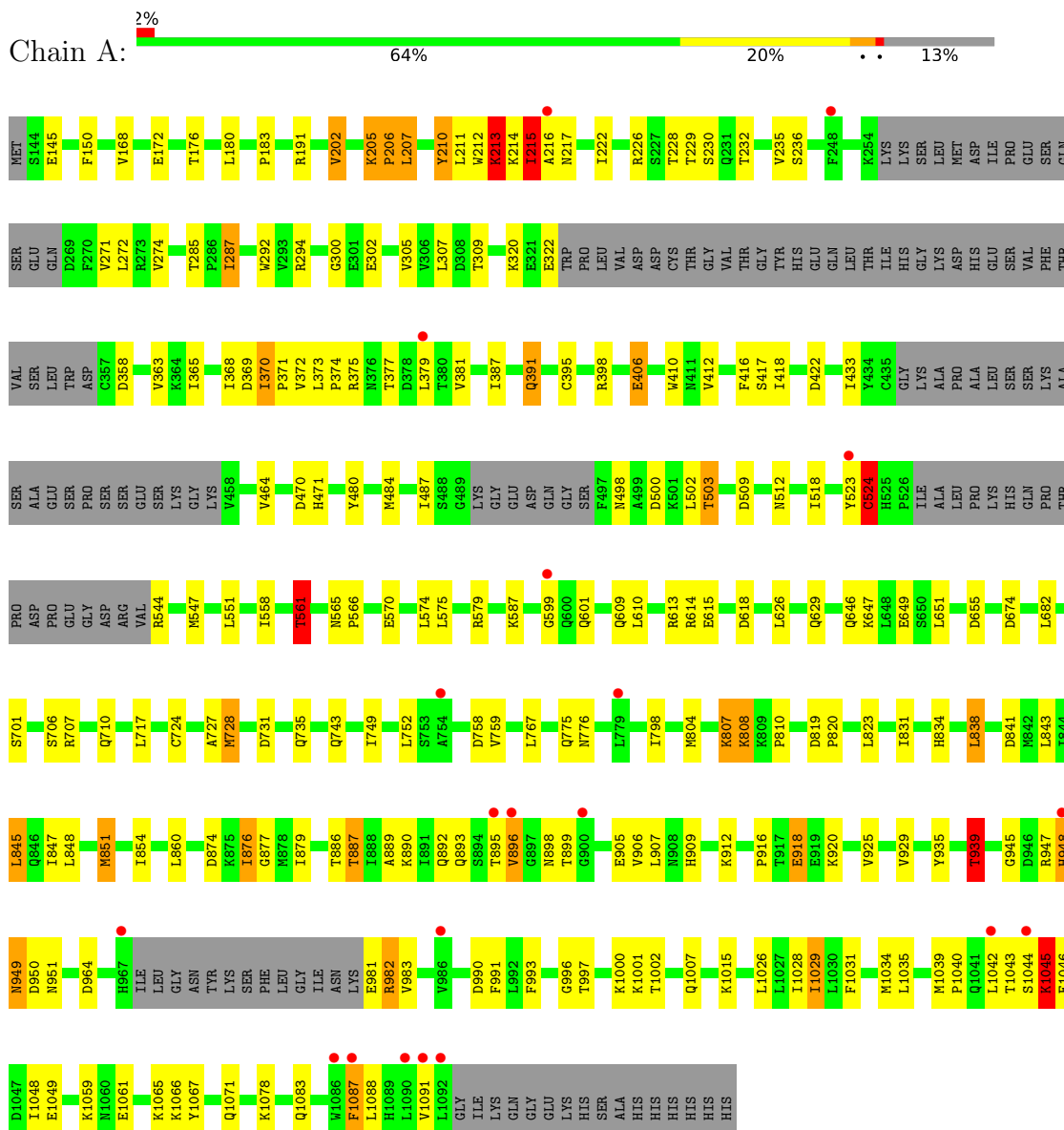
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		

### 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.44Å 68.24Å 106.17Å 90.00° 94.82° 90.00°	Depositor
Resolution (Å)	29.85 – 2.70 29.85 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.85-2.70) 96.6 (29.85-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.68Å)	Xtrriage
Refinement program	REFMAC, BUSTER 2.11.1	Depositor
R, $R_{free}$	0.205 , 0.257 0.217 , 0.278	Depositor DCC
$R_{free}$ test set	1384 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6863	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 0TA

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	0.88	2/6965 (0.0%)	1.46	42/9423 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	MET	SD-CE	-5.82	1.65	1.79
1	A	983	VAL	CA-C	5.26	1.57	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	949	ASN	CA-C-N	9.95	134.01	120.38
1	A	949	ASN	C-N-CA	9.95	134.01	120.38
1	A	950	ASP	CA-CB-CG	8.11	120.71	112.60
1	A	470	ASP	CA-CB-CG	7.49	120.09	112.60
1	A	939	THR	CB-CA-C	7.33	122.57	110.92
1	A	202	VAL	N-CA-CB	-6.90	102.86	112.52
1	A	417	SER	CA-C-N	6.31	128.95	120.50
1	A	417	SER	C-N-CA	6.31	128.95	120.50
1	A	1031	PHE	CA-C-N	6.07	128.73	120.54
1	A	1031	PHE	C-N-CA	6.07	128.73	120.54
1	A	498	ASN	CA-CB-CG	5.98	118.58	112.60
1	A	191	ARG	N-CA-C	5.81	119.39	110.20
1	A	892	GLN	CA-C-N	5.78	128.34	120.54
1	A	892	GLN	C-N-CA	5.78	128.34	120.54
1	A	216	ALA	N-CA-C	-5.64	106.06	113.17
1	A	150	PHE	CA-CB-CG	5.61	119.41	113.80
1	A	776	ASN	N-CA-C	5.53	117.77	111.02
1	A	804	MET	N-CA-C	5.50	118.55	109.85
1	A	990	ASP	CA-C-N	5.44	127.84	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	990	ASP	C-N-CA	5.44	127.84	120.44
1	A	893	GLN	CA-C-N	5.42	127.81	120.38
1	A	893	GLN	C-N-CA	5.42	127.81	120.38
1	A	216	ALA	CA-C-N	5.34	131.17	121.92
1	A	216	ALA	C-N-CA	5.34	131.17	121.92
1	A	854	ILE	N-CA-C	-5.34	105.30	110.42
1	A	1066	LYS	CA-C-N	5.26	127.64	120.54
1	A	1066	LYS	C-N-CA	5.26	127.64	120.54
1	A	503	THR	N-CA-C	5.25	117.64	110.24
1	A	906	VAL	N-CA-C	5.17	115.79	110.36
1	A	561	THR	CB-CA-C	5.16	120.33	109.65
1	A	727	ALA	CA-C-N	5.13	127.58	120.29
1	A	727	ALA	C-N-CA	5.13	127.58	120.29
1	A	982	ARG	N-CA-C	5.12	116.76	108.41
1	A	470	ASP	CA-C-N	5.11	128.77	120.60
1	A	470	ASP	C-N-CA	5.11	128.77	120.60
1	A	996	GLY	CA-C-N	5.11	128.92	121.31
1	A	996	GLY	C-N-CA	5.11	128.92	121.31
1	A	228	THR	N-CA-C	-5.10	108.08	114.56
1	A	991	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	1087	PHE	CA-C-N	5.03	127.02	120.28
1	A	1087	PHE	C-N-CA	5.03	127.02	120.28
1	A	509	ASP	CA-CB-CG	5.01	117.61	112.60

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	6818	0	6850	83	0
2	A	23	18	18	0	0
3	A	4	0	0	0	0
All	All	6845	18	6868	83	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 6.

All (83) 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:210:TYR:O	1:A:213:LYS:HE3	1.64	0.95
1:A:213:LYS:NZ	1:A:214:LYS:HG3	1.87	0.88
1:A:213:LYS:HZ3	1:A:214:LYS:HG3	1.42	0.81
1:A:1045:LYS:HG2	1:A:1049:GLU:CD	2.14	0.73
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.69	0.72
1:A:1045:LYS:HZ2	1:A:1045:LYS:HB2	1.57	0.68
1:A:808:LYS:O	1:A:810:PRO:HD3	1.94	0.68
1:A:916:PRO:HD2	1:A:920:LYS:HD3	1.77	0.66
1:A:214:LYS:O	1:A:215:ILE:HG13	1.99	0.63
1:A:214:LYS:C	1:A:215:ILE:HG13	2.24	0.63
1:A:1045:LYS:HB2	1:A:1045:LYS:NZ	2.14	0.62
1:A:523:TYR:O	1:A:524:CYS:HB2	1.99	0.62
1:A:1045:LYS:NZ	1:A:1045:LYS:CB	2.65	0.59
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.37	0.59
1:A:743:GLN:HG2	1:A:876:ILE:HD12	1.84	0.59
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.51	0.59
1:A:213:LYS:HZ2	1:A:214:LYS:HG3	1.66	0.58
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.86	0.58
1:A:724:CYS:HB2	1:A:728:MET:HE3	1.86	0.57
1:A:214:LYS:HZ1	1:A:300:GLY:HA2	1.69	0.57
1:A:935:TYR:O	1:A:939:THR:HB	2.04	0.57
1:A:579:ARG:HD2	1:A:610:LEU:HD11	1.87	0.56
1:A:887:THR:HG22	1:A:890:LYS:H	1.72	0.54
1:A:807:LYS:HE3	1:A:807:LYS:H	1.73	0.54
1:A:205:LYS:O	1:A:206:PRO:O	2.26	0.54
1:A:222:ILE:HD12	1:A:235:VAL:HG21	1.90	0.54
1:A:206:PRO:O	1:A:294:ARG:NH2	2.40	0.53
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.90	0.53
1:A:212:TRP:C	1:A:214:LYS:H	2.16	0.53
1:A:947:ARG:HH21	1:A:951:ASN:HB3	1.74	0.52
1:A:207:LEU:CD2	1:A:211:LEU:HB3	2.40	0.52
1:A:925:VAL:O	1:A:929:VAL:HG23	2.09	0.52
1:A:1045:LYS:O	1:A:1049:GLU:HG3	2.09	0.52
1:A:1043:THR:C	1:A:1045:LYS:H	2.18	0.52
1:A:847:ILE:HG22	1:A:851:MET:HE2	1.93	0.50
1:A:889:ALA:HB2	1:A:949:ASN:HB3	1.94	0.49
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.93	0.49
1:A:558:ILE:O	1:A:561:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:905:GLU:HG2	1:A:909:HIS:CE1	2.48	0.49
1:A:207:LEU:HD21	1:A:211:LEU:HB3	1.95	0.49
1:A:860:LEU:HD11	1:A:1015:LYS:HB3	1.93	0.49
1:A:215:ILE:HA	1:A:217:ASN:OD1	2.12	0.48
1:A:831:ILE:HB	1:A:879:ILE:HB	1.95	0.48
1:A:214:LYS:NZ	1:A:300:GLY:HA2	2.28	0.47
1:A:547:MET:HE2	1:A:551:LEU:C	2.39	0.46
1:A:370:ILE:HD13	1:A:371:PRO:HD2	1.96	0.46
1:A:948:HIS:ND1	1:A:948:HIS:N	2.62	0.46
1:A:706:SER:O	1:A:710:GLN:HB3	2.16	0.46
1:A:180:LEU:C	1:A:183:PRO:HD2	2.42	0.45
1:A:834:HIS:HB2	1:A:876:ILE:HG12	1.97	0.45
1:A:1067:TYR:O	1:A:1071:GLN:HG2	2.17	0.44
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.53	0.44
1:A:213:LYS:CD	1:A:213:LYS:C	2.90	0.44
1:A:1034:MET:HG2	1:A:1039:MET:HE3	1.98	0.44
1:A:422:ASP:HB3	1:A:599:GLY:O	2.18	0.44
1:A:368:ILE:HG21	1:A:433:ILE:HD11	2.00	0.43
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.99	0.43
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.53	0.43
1:A:391:GLN:HE21	1:A:502:LEU:HD21	1.83	0.43
1:A:841:ASP:O	1:A:845:LEU:HD22	2.19	0.43
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.01	0.43
1:A:651:LEU:HD22	1:A:655:ASP:HB3	2.01	0.43
1:A:464:VAL:HG12	1:A:484:MET:HE3	2.00	0.43
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.86	0.43
1:A:912:LYS:HE2	1:A:918:GLU:HG2	2.01	0.43
1:A:287:ILE:H	1:A:287:ILE:HG13	1.74	0.42
1:A:365:ILE:HD13	1:A:518:ILE:HG22	2.02	0.42
1:A:406:GLU:H	1:A:406:GLU:HG2	1.68	0.42
1:A:1045:LYS:C	1:A:1049:GLU:HG3	2.45	0.42
1:A:363:VAL:HG12	1:A:416:PHE:HE1	1.85	0.41
1:A:370:ILE:HD12	1:A:372:VAL:O	2.20	0.41
1:A:808:LYS:H	1:A:808:LYS:HG2	1.74	0.41
1:A:212:TRP:C	1:A:214:LYS:N	2.78	0.41
1:A:731:ASP:O	1:A:735:GLN:HG3	2.20	0.41
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.51	0.41
1:A:819:ASP:HA	1:A:820:PRO:HD3	2.00	0.41
1:A:480:TYR:HB2	1:A:518:ILE:HG13	2.01	0.41
1:A:565:ASN:HA	1:A:566:PRO:HD3	1.89	0.41
1:A:500:ASP:O	1:A:503:THR:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ARG:HB3	1:A:618:ASP:OD2	2.21	0.41
1:A:1045:LYS:CG	1:A:1049:GLU:CD	2.90	0.40
1:A:176:THR:HG23	1:A:674:ASP:HB2	2.04	0.40
1:A:213:LYS:C	1:A:213:LYS:HD2	2.47	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	828/966 (86%)	762 (92%)	45 (5%)	21 (2%)	<b>4</b> <b>11</b>

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	PRO
1	A	377	THR
1	A	615	GLU
1	A	896	VAL
1	A	898	ASN
1	A	899	THR
1	A	213	LYS
1	A	215	ILE
1	A	524	CYS
1	A	1040	PRO
1	A	210	TYR
1	A	375	ARG
1	A	758	ASP
1	A	1000	LYS
1	A	1045	LYS
1	A	1046	GLU
1	A	374	PRO

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Mol	Chain	Res	Type
1	A	874	ASP
1	A	1044	SER
1	A	964	ASP
1	A	759	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	Percentiles
1	A	755/864 (87%)	662 (88%)	93 (12%)	<b>4</b> <b>12</b>

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	168	VAL
1	A	202	VAL
1	A	205	LYS
1	A	207	LEU
1	A	213	LYS
1	A	215	ILE
1	A	226	ARG
1	A	229	THR
1	A	230	SER
1	A	232	THR
1	A	236	SER
1	A	271	VAL
1	A	285	THR
1	A	287	ILE
1	A	302	GLU
1	A	307	LEU
1	A	309	THR
1	A	320	LYS
1	A	322	GLU
1	A	358	ASP
1	A	369	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	370	ILE
1	A	373	LEU
1	A	379	LEU
1	A	381	VAL
1	A	387	ILE
1	A	391	GLN
1	A	395	CYS
1	A	398	ARG
1	A	406	GLU
1	A	418	ILE
1	A	487	ILE
1	A	512	ASN
1	A	524	CYS
1	A	544	ARG
1	A	561	THR
1	A	570	GLU
1	A	574	LEU
1	A	575	LEU
1	A	587	LYS
1	A	601	GLN
1	A	609	GLN
1	A	613	ARG
1	A	626	LEU
1	A	646	GLN
1	A	647	LYS
1	A	649	GLU
1	A	682	LEU
1	A	701	SER
1	A	707	ARG
1	A	717	LEU
1	A	728	MET
1	A	749	ILE
1	A	752	LEU
1	A	767	LEU
1	A	775	GLN
1	A	798	ILE
1	A	807	LYS
1	A	808	LYS
1	A	823	LEU
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	848	LEU
1	A	876	ILE
1	A	886	THR
1	A	887	THR
1	A	895	THR
1	A	896	VAL
1	A	907	LEU
1	A	918	GLU
1	A	939	THR
1	A	948	HIS
1	A	981	GLU
1	A	982	ARG
1	A	997	THR
1	A	1001	LYS
1	A	1002	THR
1	A	1007	GLN
1	A	1026	LEU
1	A	1028	ILE
1	A	1029	ILE
1	A	1042	LEU
1	A	1045	LYS
1	A	1048	ILE
1	A	1059	LYS
1	A	1061	GLU
1	A	1065	LYS
1	A	1078	LYS
1	A	1087	PHE
1	A	1088	LEU
1	A	1091	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	225	HIS
1	A	291	GLN
1	A	376	ASN
1	A	389	HIS
1	A	391	GLN
1	A	392	GLN
1	A	396	GLN
1	A	554	GLN
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	634	ASN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	834	HIS
1	A	892	GLN
1	A	959	ASN
1	A	1041	GLN
1	A	1083	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](#)

1 ligand is 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	0TA	A	1201	-	26,26,26	1.70	2 (7%)	29,38,38	1.07	3 (10%)

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	OTA	A	1201	-	-	0/8/15/15	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	OTA	C9-N3	7.65	1.48	1.38
2	A	1201	OTA	C3-N3	3.81	1.43	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	OTA	O-C9-N3	-2.98	116.77	121.39
2	A	1201	OTA	C15-C13-C10	2.48	131.55	127.70
2	A	1201	OTA	C4-N3-C9	2.23	120.87	117.69

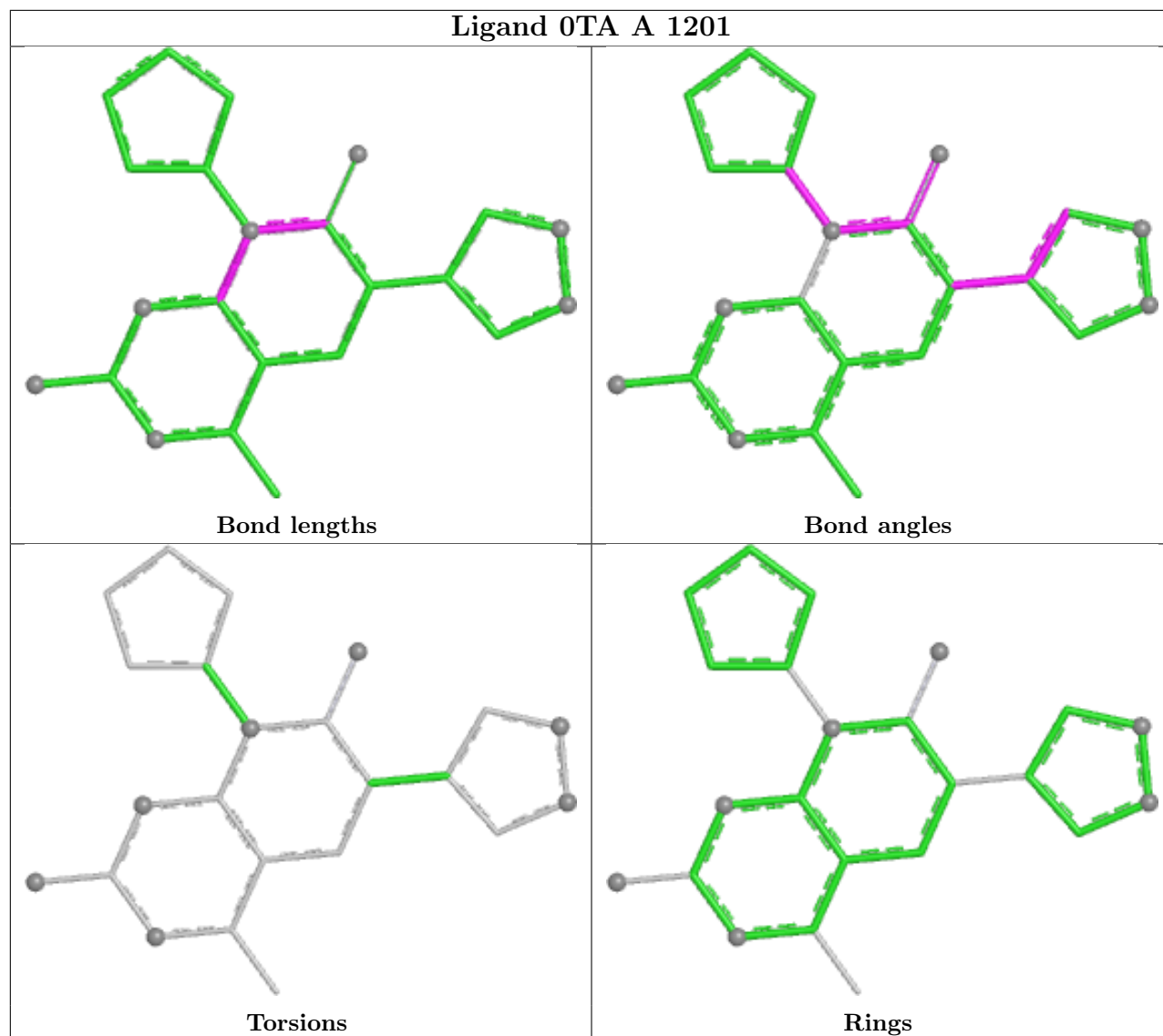
There are no chirality outliers.

There are no torsion outliers.

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	842/966 (87%)	0.16	20 (2%) 59 56	38, 71, 117, 147	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	4.9
1	A	379	LEU	3.5
1	A	599	GLY	3.2
1	A	895	THR	3.1
1	A	1091	VAL	2.9
1	A	779	LEU	2.8
1	A	523	TYR	2.7
1	A	896	VAL	2.6
1	A	1092	LEU	2.6
1	A	900	GLY	2.5
1	A	754	ALA	2.5
1	A	1086	TRP	2.4
1	A	986	VAL	2.4
1	A	1090	LEU	2.2
1	A	216	ALA	2.2
1	A	967	HIS	2.1
1	A	248	PHE	2.1
1	A	1042	LEU	2.1
1	A	1087	PHE	2.0
1	A	948	HIS	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates

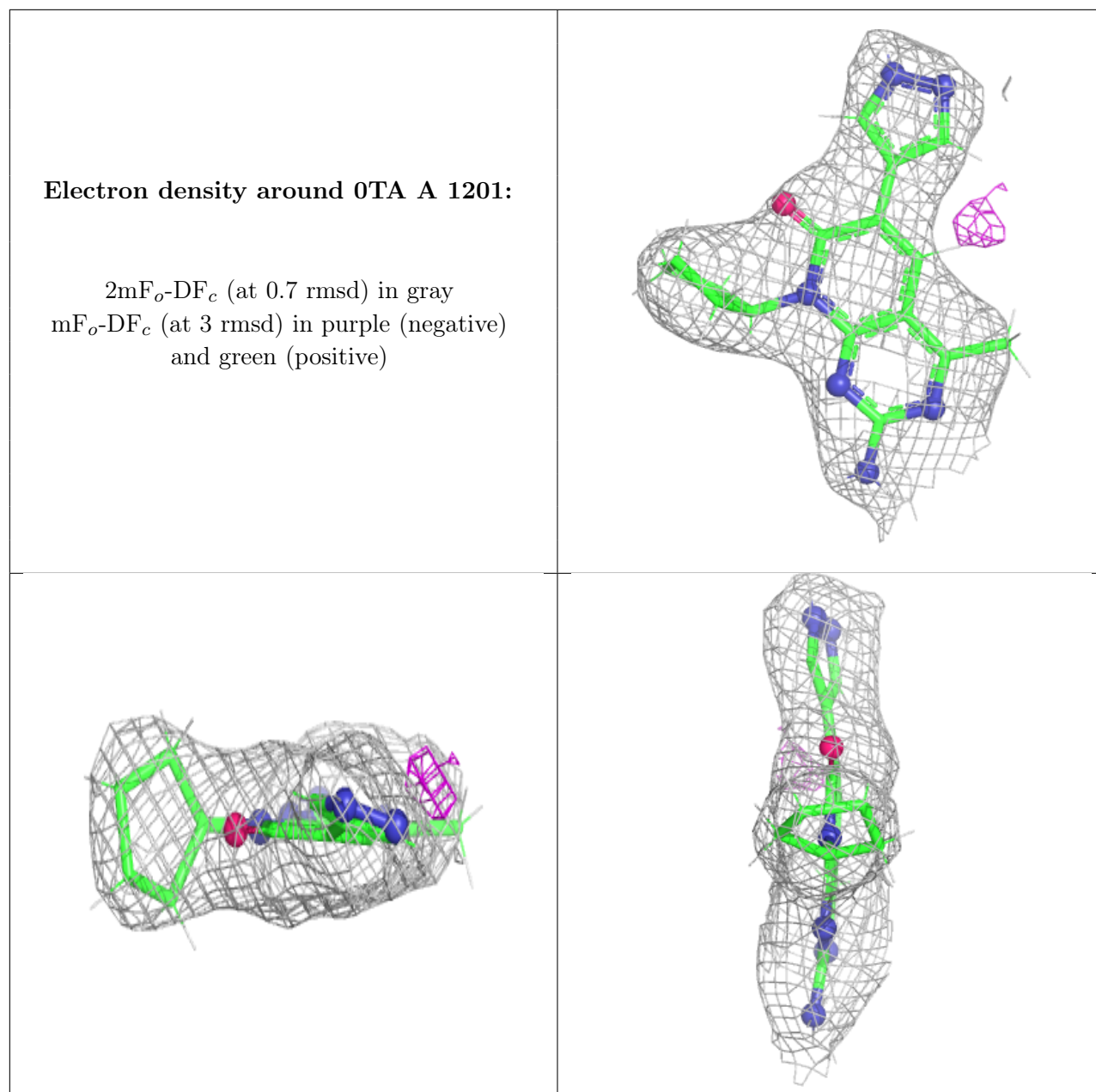
There are no oligosaccharides in this entry.

### 6.4 Ligands

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( $\text{\AA}^2$ )	Q<0.9
2	OTA	A	1201	23/23	0.92	0.09	59,68,72,72	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.