



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:32 AM UTC

PDB ID : 4FHK / pdb_00004fhk
Title : Crystal Structure of PI3K-gamma in Complex with Imidazopyridazine 19e
Authors : Shaffer, P.L.; Tang, J.; Yakowec, P.
Deposited on : 2012-06-06
Resolution : 3.00 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)
Xtriage (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

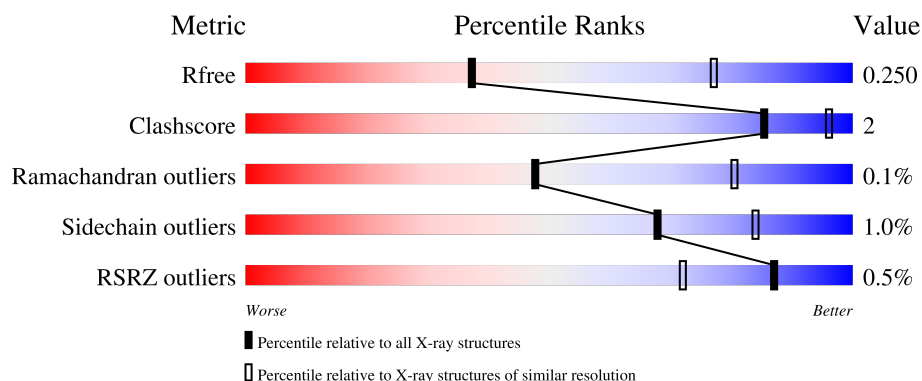
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	960	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6533 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.

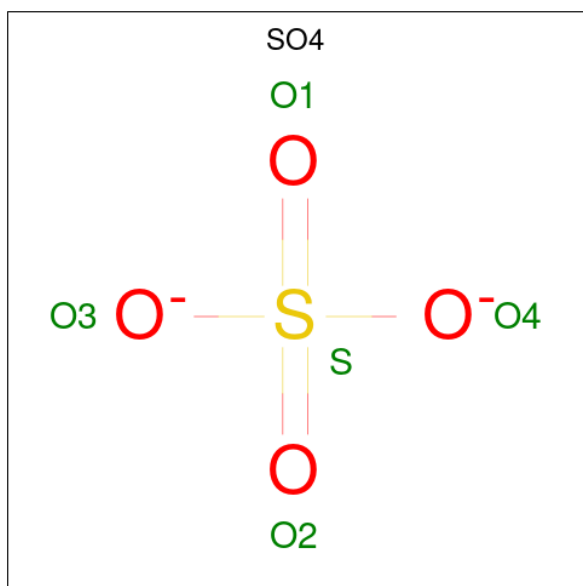
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	819	Total	C	N	O	S	0	0	0
			6460	4151	1086	1189	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	GLY	-	expression tag	UNP P48736

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



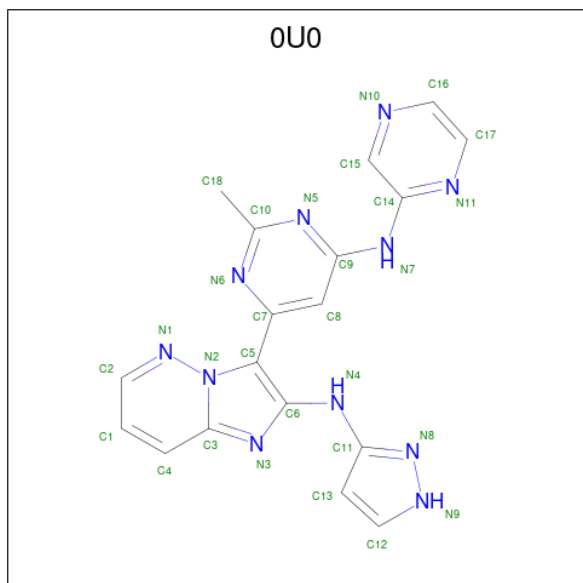
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 3-[2-methyl-6-(pyrazin-2-ylamino)pyrimidin-4-yl]-N-(1H-pyrazol-3-yl)imidazo[1,2-b]pyridazin-2-amine (CCD ID: 0U0) (formula: C₁₈H₁₅N₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			29	18	11		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		

i

- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform

1963	GLY	V640	SER	LEU	GLY
1968	LEU	I643	GLU	THR	SER
1969	ASN	L651	GLY	HIS	E145
1970	TYR	D655	GLY	GLY	N167
1971	LYS	Q662	GLY	LYS	T182
1972	PHE	Q711	LYS	ASP	P183
1973	LEU	Q711	V458	HIS	I224
1974	GLY	I749	L468	VAL	S227
1975	ILE	I749	M484	THR	I233
1976	ASN	L752	S488	VAL	L245
1977	K990	SER	GLY	LEU	K252
1978	V983	ALA	LYS	ASP	ALA
1979	S998	GLU	GLY	C357	LYS
1980	GLY	K756	ASP	K360	LYS
1981	LYS	L767	GLN	GLN	LYS
1982	K1001	E799	GLY	K364	SER
1983	I1029	V803	M514	I368	LEU
1984	M1039	K808	L519	L373	ASP
1985	PRO	G835	H522	PRO	ILE
1986	GLN	L838	TYR	ARG	GLU
1987	LEU	M842	CYS	ASN	GLU
1988	S1044	L847	HIS	THR	GLN
1989	I1048	E852	PRO	V381	GLN
1990	V1082	W855	ALA	K386	D269
1991	L1092	L860	LEU	L428	F270
1992	GLY	L864	PRO	L429	V271
1993	ILE	N898	PRO	LYS	I287
1994	LYS	THR	GLY	ALA	F290
1995	SER	ALA	ASP	ALA	E321
1996	ALA	AG01	ARG	GLY	GLY
1997		D904	VAL	LEU	THR
1998		S915	ALA	LYS	VAL
1999		P916	ALA	ALA	THR
2000		L942	L564	GLY	GLY
2001		R947	P566	GLU	CYS
2002		V959	C630	SER	THR
2003				PRO	GLY
2004				SER	GLN

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.54Å 67.93Å 106.49Å 90.00° 95.40° 90.00°	Depositor
Resolution (Å)	40.96 – 3.00 40.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (40.96-3.00) 99.9 (40.96-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.222 , 0.260 0.212 , 0.250	Depositor DCC
R_{free} test set	1050 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6533	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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: SO4, OU0

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	0.58	0/6596	0.76	0/8955

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	6460	0	6284	26	0
2	A	20	0	0	0	0
3	A	29	0	15	2	0
4	A	24	0	0	0	0
All	All	6533	0	6299	28	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.

The worst 5 of 28 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:629:GLN:HG2	1:A:1029:ILE:HG13	1.71	0.72
1:A:182:THR:HB	1:A:183:PRO:HD3	1.76	0.68
1:A:947:ARG:NH2	1:A:963:ILE:O	2.32	0.62
3:A:1205:OUO:H5	3:A:1205:OUO:N11	2.17	0.60
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.85	0.58

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	795/960 (83%)	774 (97%)	20 (2%)	1 (0%)	48 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER

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	692/857 (81%)	685 (99%)	7 (1%)	68 84

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	662	GLN
1	A	749	ILE
1	A	959	ASN
1	A	904	ASP
1	A	381	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1089	HIS
1	A	959	ASN
1	A	893	GLN
1	A	775	GLN
1	A	909	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](#)

5 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	SO4	A	1203	-	4,4,4	0.44	0	6,6,6	0.08	0
3	OU0	A	1205	-	33,33,33	3.15	9 (27%)	39,46,46	2.91	21 (53%)
2	SO4	A	1201	-	4,4,4	0.42	0	6,6,6	0.09	0
2	SO4	A	1202	-	4,4,4	0.44	0	6,6,6	0.08	0
2	SO4	A	1204	-	4,4,4	0.44	0	6,6,6	0.07	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
3	OU0	A	1205	-	-	5/12/12/12	0/5/5/5

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1205	OU0	N2-N1	-12.39	1.24	1.37
3	A	1205	OU0	C7-C5	-8.25	1.40	1.48
3	A	1205	OU0	N9-N8	-6.16	1.23	1.36
3	A	1205	OU0	C13-C11	-4.18	1.32	1.44
3	A	1205	OU0	C11-N4	-3.93	1.34	1.39

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1205	OU0	C11-N8-N9	6.48	108.21	103.76
3	A	1205	OU0	C2-N1-N2	5.96	122.68	113.68
3	A	1205	OU0	C15-C14-N11	-5.78	118.68	121.26
3	A	1205	OU0	N4-C11-N8	5.32	126.43	117.50
3	A	1205	OU0	C3-N2-N1	-5.20	121.62	126.72

There are no chirality outliers.

All (5) torsion outliers are listed below:

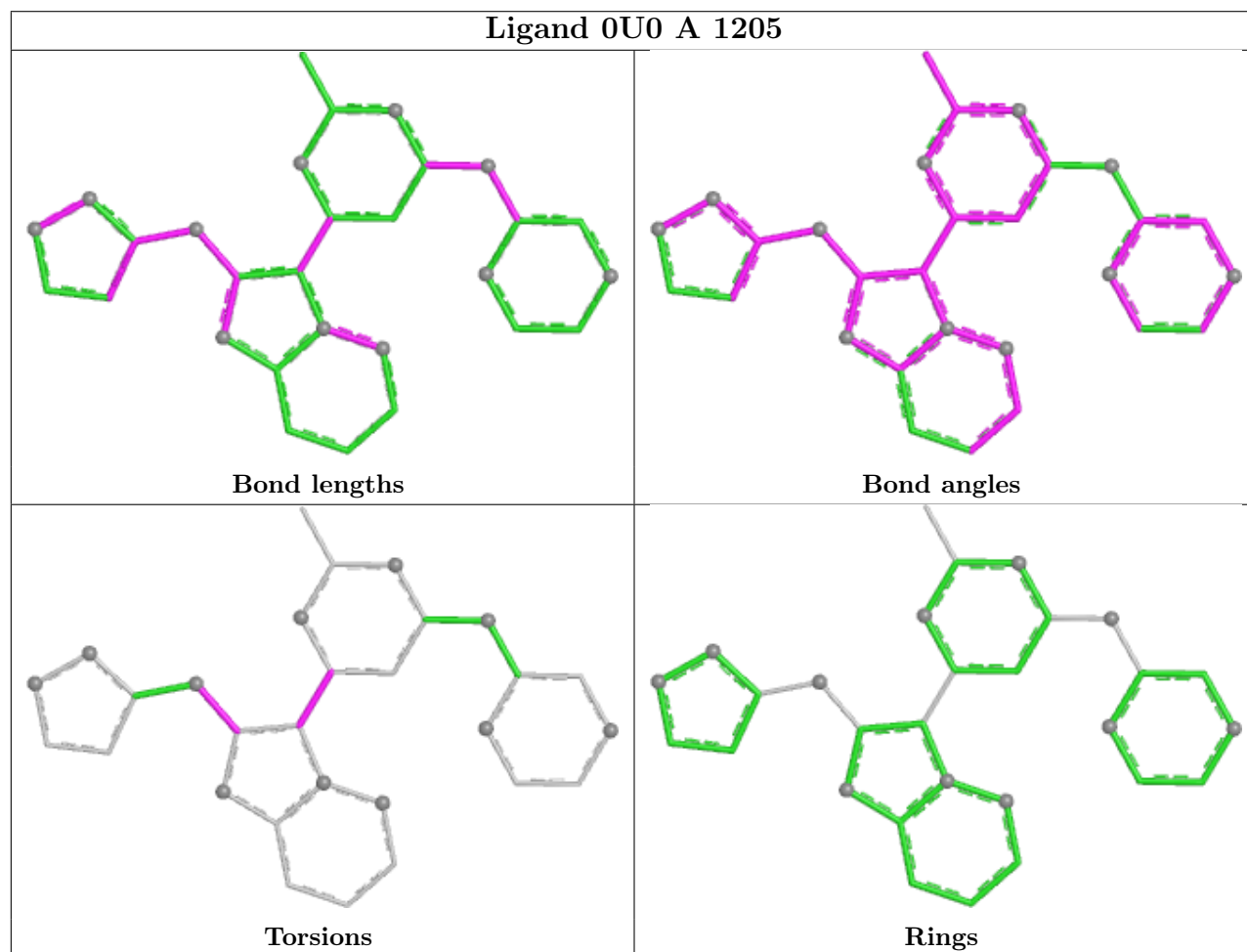
Mol	Chain	Res	Type	Atoms
3	A	1205	OU0	N2-C5-C7-N6
3	A	1205	OU0	N2-C5-C7-C8
3	A	1205	OU0	C6-C5-C7-N6
3	A	1205	OU0	C6-C5-C7-C8
3	A	1205	OU0	C5-C6-N4-C11

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1205	OU0	2	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 [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	OWAB(Å ²)	Q<0.9
1	A	819/960 (85%)	-0.21	4 (0%) 87 72	44, 88, 143, 186	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	901	ALA	3.7
1	A	252	MET	3.0
1	A	898	ASN	2.6
1	A	373	LEU	2.1

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.

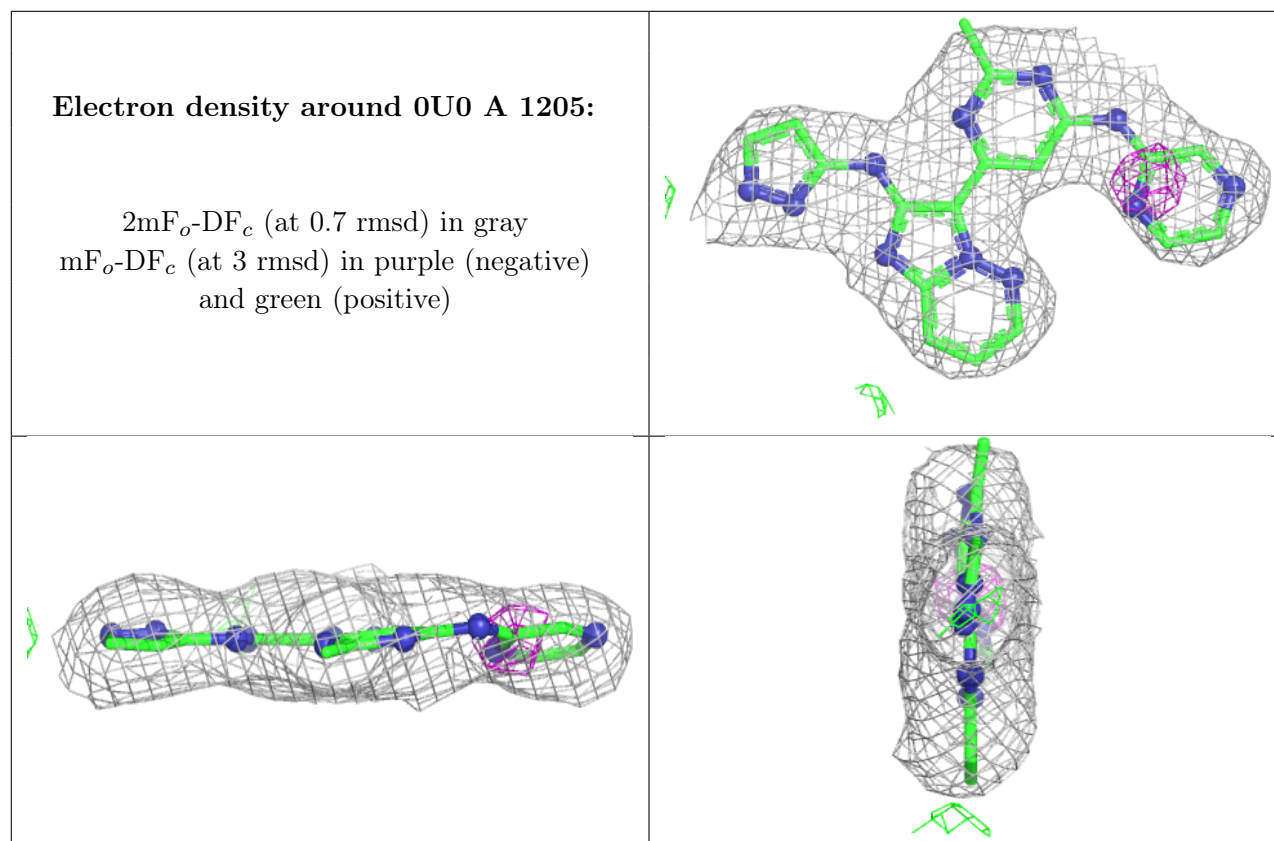
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	1201	5/5	0.80	0.17	105,107,110,111	0
2	SO4	A	1204	5/5	0.83	0.10	128,131,132,135	0
2	SO4	A	1202	5/5	0.84	0.16	116,118,121,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1203	5/5	0.91	0.18	94,95,97,100	0
3	OUO	A	1205	29/29	0.92	0.09	62,69,73,74	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.