wwPDB X-ray Structure Validation Summary Report (i)

Dec 4, 2023 – 08:00 am GMT

PDB ID	:	1OIY
Title	:	Structure of human Thr160-phospho CDK2/cyclin A complexed with a 6-cyc lohexylmethyloxy-2-anilino-purine inhibitor
Authors	:	Pratt, D.J.; Endicott, J.A.; Noble, M.E.M.
Deposited on	:	2003-06-26
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

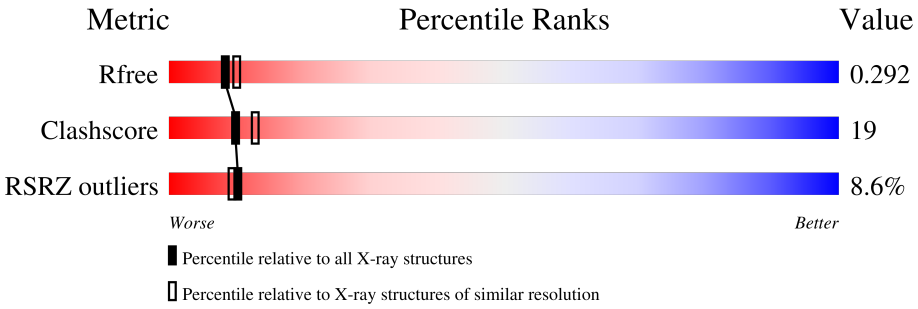
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	302	2% 69% 27%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9273 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.

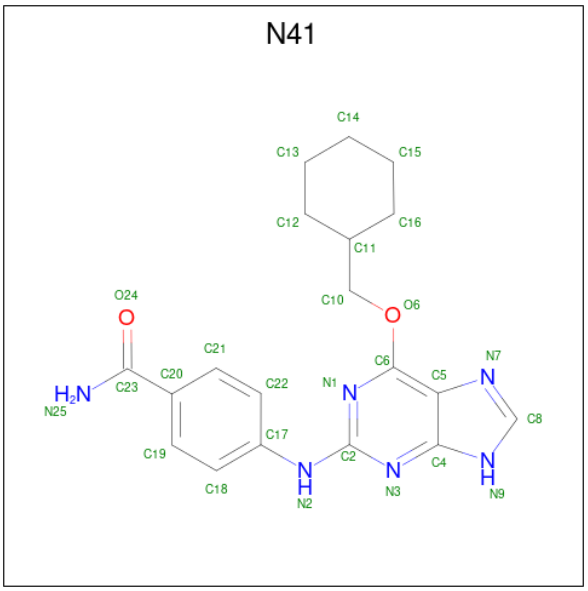
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	P	S	0	1	0
			2366	1538	401	418	1	8			
1	C	297	Total	C	N	O	P	S	0	1	0
			2391	1552	404	426	1	8			

- Molecule 2 is a protein called CYCLIN A2.

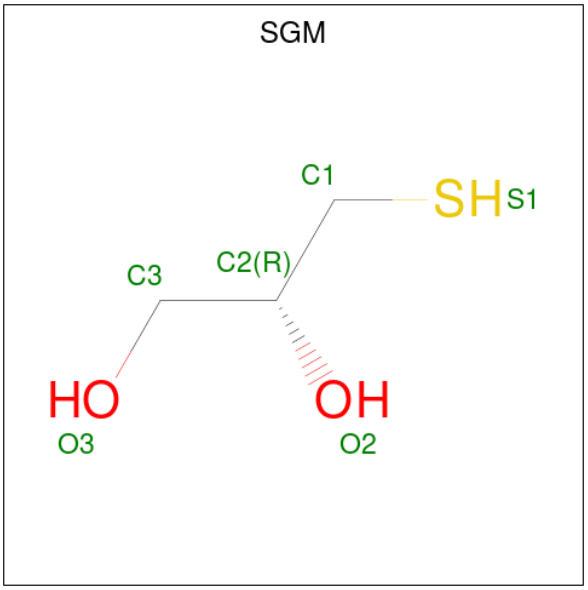
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	1	0
			2088	1354	340	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is 4-(6-CYCLOHEXYLMETHOXY-9H-PURIN-2-YLAMINO)--BENZAMIDE (three-letter code: N41) (formula: $C_{19}H_{22}N_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 27 19 6 2	0	0
3	C	1	Total C N O 27 19 6 2	0	0

- Molecule 4 is MONOTHIOGLYCEROL (three-letter code: SGM) (formula: $C_3H_8O_2S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O S 6 3 2 1	0	0
4	D	1	Total C O S 6 3 2 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	119	Total O 119 119	0	0
6	B	107	Total O 107 107	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	35	Total O 35 35	0	0
6	D	17	Total O 17 17	0	0

SEQUENCE-PLOTS INFOmissingINFO

3 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.00Å 134.87Å 147.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.40 41.02 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.6 (100.00-2.40) 91.6 (41.02-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.244 , 0.309 0.232 , 0.292	Depositor DCC
R_{free} test set	2717 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9273	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SGM, TPO, MG, N41

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	0.86	0/2419	0.98	14/3280 (0.4%)
1	C	0.66	0/2445	0.90	9/3318 (0.3%)
2	B	0.81	0/2142	0.94	9/2908 (0.3%)
2	D	0.64	0/2133	0.87	5/2897 (0.2%)
All	All	0.75	0/9139	0.93	37/12403 (0.3%)

There are no bond length outliers.

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	216	ASP	CB-CG-OD2	8.37	125.83	118.30
2	B	393	ASP	CB-CG-OD2	7.88	125.39	118.30
1	A	68	ASP	CB-CG-OD2	7.33	124.89	118.30
1	C	145	ASP	CB-CG-OD2	6.93	124.54	118.30
1	C	256	ASP	CB-CG-OD2	6.86	124.47	118.30

There are no chirality outliers.

There are no planarity outliers.

4.2 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	2366	0	2413	75	0
1	C	2391	0	2433	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2088	0	2115	61	0
2	D	2083	0	2107	102	0
3	A	27	0	22	4	0
3	C	27	0	22	2	0
4	B	6	0	7	0	0
4	D	6	0	8	1	0
5	B	1	0	0	0	0
6	A	119	0	0	5	0
6	B	107	0	0	7	0
6	C	35	0	0	9	0
6	D	17	0	0	2	0
All	All	9273	0	9127	347	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 19.

The worst 5 of 347 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:C:60:HIS:HD2	1:C:62:ASN:H	1.09	0.99
1:C:162:GLU:OE1	1:C:162:GLU:HA	1.65	0.93
1:A:15:TYR:HE2	1:A:35:ILE:CD1	1.82	0.92
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.00	0.91
1:A:15:TYR:HE2	1:A:35:ILE:HD11	1.40	0.86

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA (i)

There are no RNA molecules in this entry.

4.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	TPO	A	160	1	8,10,11	1.53	1 (12%)	10,14,16	1.22	0
1	TPO	C	160	1	8,10,11	1.22	1 (12%)	10,14,16	1.10	1 (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
1	TPO	A	160	1	-	2/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-O1P	3.17	1.60	1.50
1	C	160	TPO	P-O1P	2.48	1.58	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	TPO	P-OG1-CB	-2.27	116.34	123.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	CB-OG1-P-O1P
1	A	160	TPO	CB-OG1-P-O3P
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	160	TPO	1	0
1	C	160	TPO	1	0

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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	$\#\|Z\| > 2$
3	N41	A	1298	-	27,30,30	1.27	3 (11%)	32,41,41	1.64	6 (18%)
3	N41	C	1298	-	27,30,30	0.77	0	32,41,41	1.84	6 (18%)
4	SGM	D	1193	-	5,5,5	0.27	0	5,5,5	0.65	0
4	SGM	B	1193	2	5,5,5	0.53	0	5,5,5	0.77	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	N41	A	1298	-	-	1/13/21/21	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	N41	C	1298	-	-	6/13/21/21	0/4/4/4
4	SGM	D	1193	-	-	3/4/4/4	-
4	SGM	B	1193	2	-	1/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	N41	O6-C6	3.68	1.38	1.35
3	A	1298	N41	C6-N1	2.68	1.36	1.31
3	A	1298	N41	C4-N9	2.27	1.39	1.34

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1298	N41	C10-O6-C6	4.43	121.73	117.50
3	C	1298	N41	C2-N1-C6	4.36	122.88	115.18
3	A	1298	N41	C2-N3-C4	4.34	120.20	115.28
3	C	1298	N41	C2-N3-C4	4.25	120.10	115.28
3	A	1298	N41	C2-N1-C6	4.15	122.51	115.18

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1193	SGM	C1-C2-C3-O3
3	C	1298	N41	C19-C20-C23-N25
4	D	1193	SGM	O2-C2-C3-O3
3	C	1298	N41	C19-C20-C23-O24
3	C	1298	N41	C21-C20-C23-N25

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	N41	4	0
3	C	1298	N41	2	0
4	D	1193	SGM	1	0

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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^{th} 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	293/302 (97%)	-0.04	5 (1%) 70 68	11, 22, 45, 55	0
1	C	296/302 (98%)	0.62	35 (11%) 4 4	24, 47, 70, 80	0
2	B	258/260 (99%)	-0.04	5 (1%) 66 64	11, 25, 44, 55	0
2	D	258/260 (99%)	0.82	50 (19%) 1 0	20, 48, 73, 78	0
All	All	1105/1124 (98%)	0.34	95 (8%) 10 9	11, 35, 69, 80	0

The worst 5 of 95 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	175	VAL	5.8
2	D	432	LEU	5.5
1	C	234	PRO	5.5
2	D	399	LEU	5.3
2	D	326	ASN	5.0

5.2 Non-standard residues in protein, DNA, RNA chains

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	RSR	B-factors(Å^2)	Q<0.9
1	TPO	C	160	11/12	0.92	0.15	38,46,48,49	0
1	TPO	A	160	11/12	0.98	0.13	12,16,17,18	0

5.3 Carbohydrates

There are no monosaccharides in this entry.

5.4 Ligands (i)

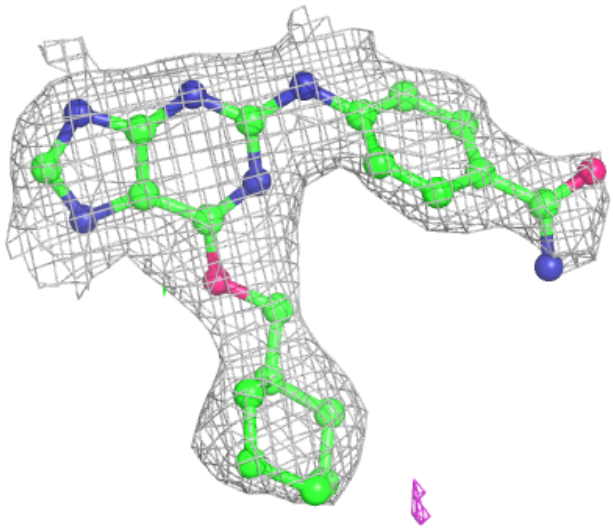
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

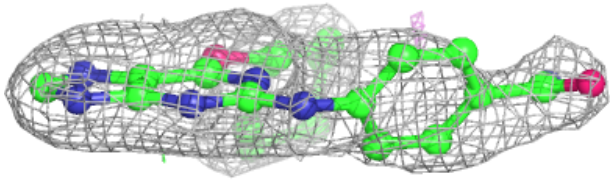
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	N41	C	1298	27/27	0.91	0.22	42,45,59,61	0
4	SGM	D	1193	6/6	0.91	0.15	62,63,64,66	0
4	SGM	B	1193	6/6	0.93	0.21	35,37,39,43	0
3	N41	A	1298	27/27	0.94	0.12	25,30,34,35	0
5	MG	B	1433	1/1	0.95	0.15	19,19,19,19	0

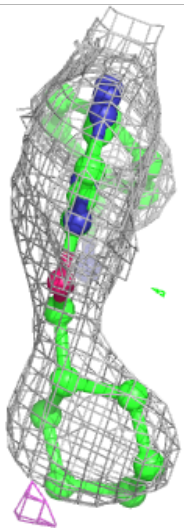
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around N41 C 1298:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

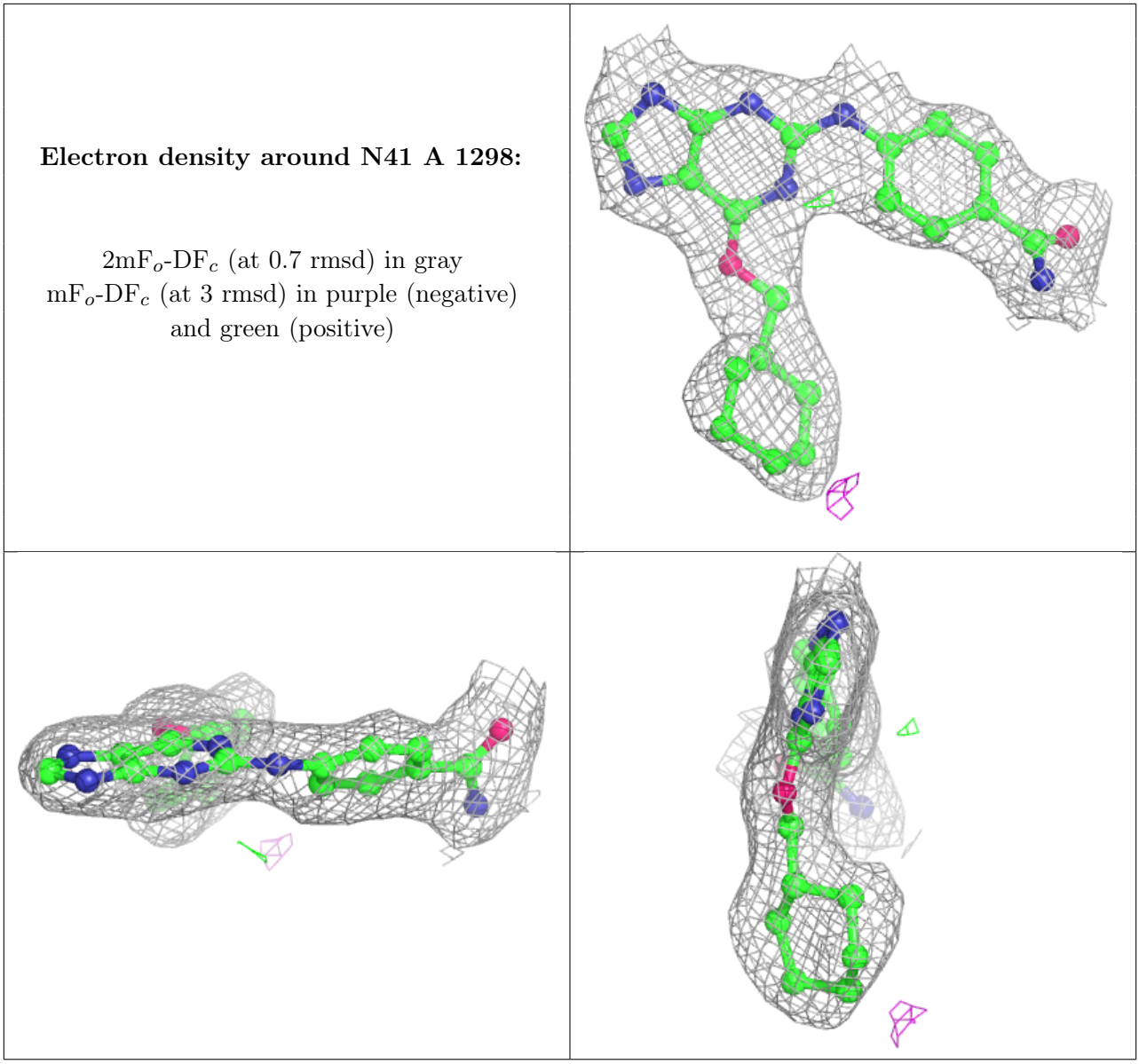






Electron density around N41 A 1298:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



5.5 Other polymers (i)

There are no such residues in this entry.