WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2024 – 02:10 PM EST

PDB ID : 7HOE

Title : Group deposition for crystallographic fragment screening of Coxsackievirus A16 (G-10) 2A protease – Crystal structure of Coxsackievirus A16 (G-10) 2A protease in complex with Z1148747945 (A71EV2A-x0487)

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Deposited on : 2024-11-06

Resolution : 1.32 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*
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
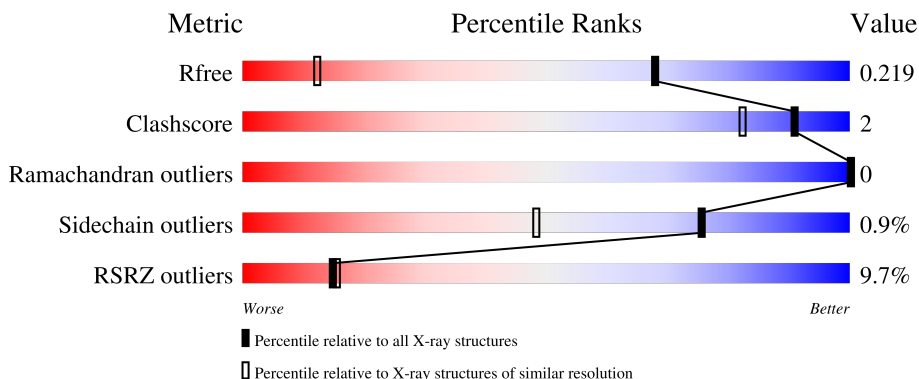http://www.wwpdb.org/validation/2017/FAQs#types.

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1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
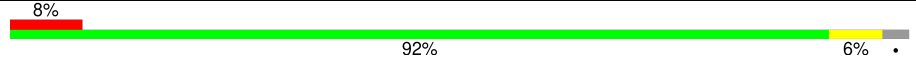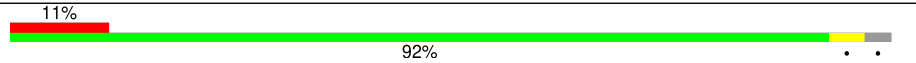*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.32 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	Percentile Ranks	Value
Rfree		0.219
Clashscore		2
Ramachandran outliers		0
Sidechain outliers		0.9%
RSRZ outliers		9.7%

Worse　　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	2202 (1.34-1.30)
Clashscore	180529	2378 (1.34-1.30)
Ramachandran outliers	177936	2325 (1.34-1.30)
Sidechain outliers	177891	2325 (1.34-1.30)
RSRZ outliers	164620	2199 (1.34-1.30)

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 >=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	144	8% ... 92% ... 6% ·
1	B	144	11% ... 92% · ·

Ideal geometry (proteins)	:	Engh & Huber (2001)	
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)	
Validation Pipeline (wwPDB-VP)	:	2.40	

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2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 2625 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 Protease 2A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total 1101	C 685	N 196	O 213	S 7	0	3	0
1	B	139	Total 1074	C 671	N 192	O 204	S 7	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).
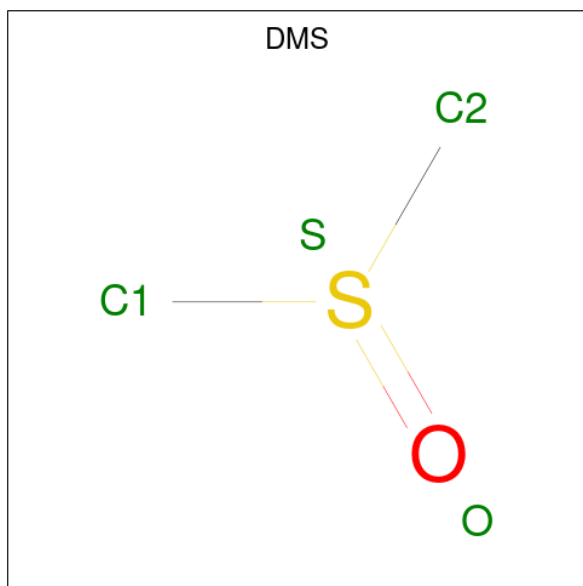
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 4	C 2	O 1	S 1	0	0
3	A	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 4 is N-(3-methylpyridin-4-yl)acetamide (three-letter code: WKY) (formula: $C_8H_{10}N_2O$) (labeled as "Ligand of Interest" by depositor).
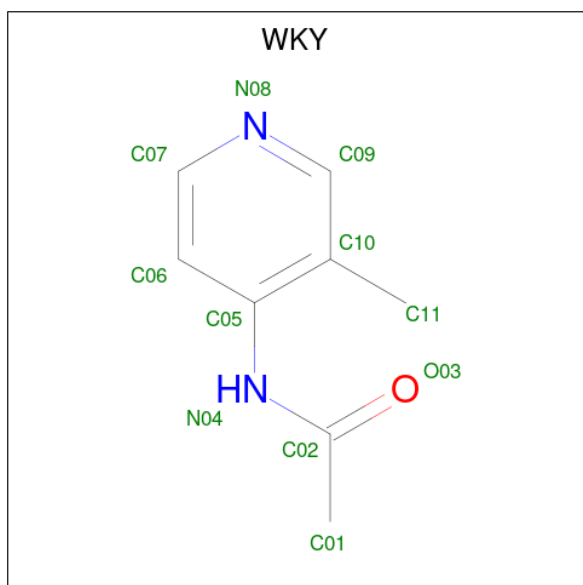
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total 11	C 8	N 2	O 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	217	Total 217	O 217	0	0
5	B	212	Total 212	O 212	0	0

3 Residue-property plots ⓘ

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: Protease 2A
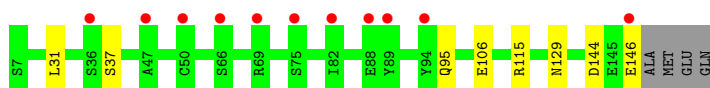
• Molecule 1: Protease 2A
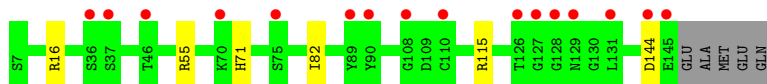
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	86.71Å 56.40Å 64.73Å 90.00° 94.43° 90.00°	Depositor
Resolution (Å)	47.28 – 1.32 47.28 – 1.32	Depositor EDS
% Data completeness (in resolution range)	98.1 (47.28-1.32) 98.1 (47.28-1.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.16 (at 1.32Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.181 , 0.211 0.194 , 0.219	Depositor DCC
R_{free} test set	3534 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å²)	18.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.34 , 37.6	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	2625	wwPDB-VP
Average B, all atoms (Å²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 81.82 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2403e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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.

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: WKY, DMS, ZN

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	0.83	1/1127 (0.1%)	0.94	2/1532 (0.1%)
1	B	0.81	0/1100	0.96	2/1496 (0.1%)
All	All	0.82	1/2227 (0.0%)	0.95	4/3028 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLU	CD-OE2	-5.84	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	16	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	115	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	115	ARG	NE-CZ-NH1	5.17	122.89	120.30

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	1101	0	1035	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1074	0	1017	4	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	8	0	12	0	0
4	B	11	0	0	0	0
5	A	217	0	0	2	0
5	B	212	0	0	2	0
All	All	2625	0	2064	7	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.

All (7) 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:144:ASP:OD1	5:A:301:HOH:O	1.95	0.84
1:A:144:ASP:HA	5:A:301:HOH:O	1.87	0.75
1:B:71:HIS:HE1	5:B:454:HOH:O	1.89	0.55
1:A:37:SER:O	1:A:95:GLN:HG3	2.12	0.48
1:B:55:ARG:HH21	1:B:144:ASP:CG	2.20	0.45
1:B:82:ILE:HD11	5:B:306:HOH:O	2.20	0.41
1:A:31:LEU:HD23	1:B:71:HIS:CD2	2.55	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	141/144 (98%)	137 (97%)	4 (3%)	0	100	100
1	B	137/144 (95%)	135 (98%)	2 (2%)	0	100	100
All	All	278/288 (96%)	272 (98%)	6 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	120/120 (100%)	118 (98%)	2 (2%)	56	21
1	B	116/120 (97%)	116 (100%)	0	100	100
All	All	236/240 (98%)	234 (99%)	2 (1%)	75	53

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	ASN
1	A	146	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	48	GLN
1	A	71	HIS
1	A	129	ASN
1	B	71	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\#|Z| > 2$
4	WKY	B	201	-	11,11,11	0.23	0	13,14,14	0.58	0
3	DMS	A	203	-	3,3,3	0.24	0	3,3,3	0.12	0
3	DMS	A	202	-	3,3,3	0.51	0	3,3,3	0.32	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
4	WKY	B	201	-	-	0/4/4/4	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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 then 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.

Ligand WKY B 201

Bond lengths

Bond angles

Torsions

Rings
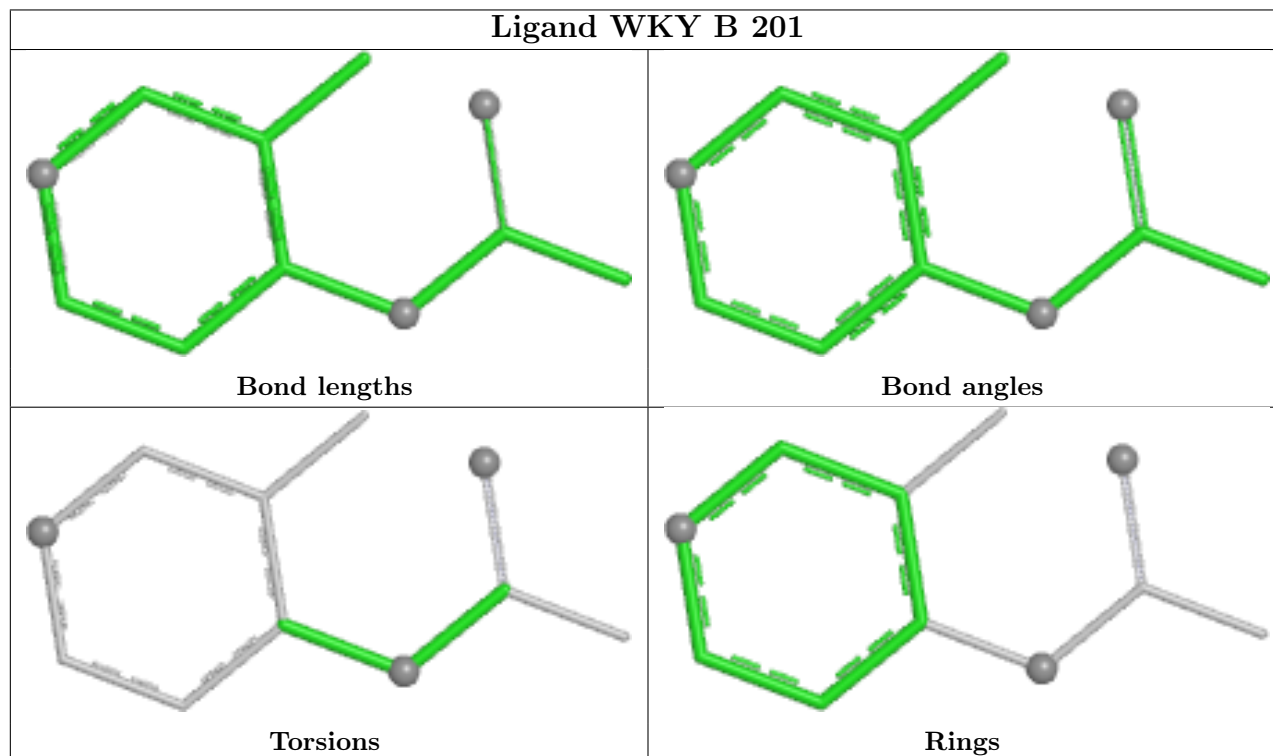
5.7 Other polymers ⓘ

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 ⓘ

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, 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	140/144 (97%)	0.86	11 (7%)	20	22	4, 19, 30, 63	6 (4%)
1	B	139/144 (96%)	0.89	16 (11%)	11	11	9, 18, 26, 33	18 (12%)
All	All	279/288 (96%)	0.87	27 (9%)	15	15	4, 18, 27, 63	24 (8%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	82	ILE	13.0
1	B	37	SER	10.5
1	A	36[A]	SER	9.8
1	B	36	SER	9.3
1	A	66[A]	SER	9.2
1	A	75[A]	SER	8.4
1	B	145	GLU	8.2
1	B	144	ASP	8.2
1	B	75	SER	7.8
1	B	70	LYS	6.9
1	A	69	ARG	6.7
1	A	88	GLU	5.1
1	B	131	LEU	4.8
1	B	129	ASN	3.5
1	B	110	CYS	3.5
1	A	89	TYR	3.1
1	B	128	GLY	3.0
1	A	47	ALA	2.9
1	A	50	CYS	2.9
1	A	146	GLU	2.6
1	B	89	TYR	2.6
1	B	46	THR	2.4
1	A	94	TYR	2.2
1	B	108	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	126	THR	2.0
1	B	90	TYR	2.0
1	B	127	GLY	2.0

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

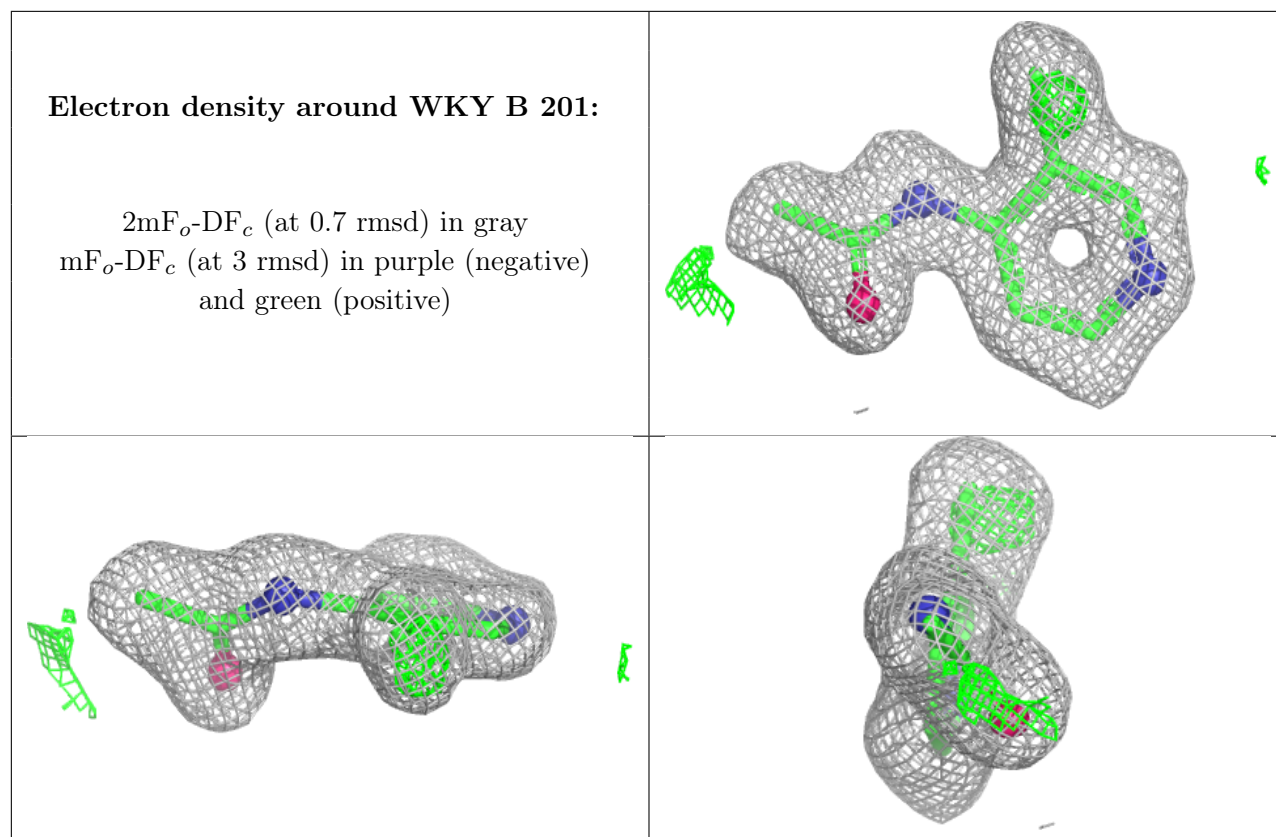There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides 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, 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
3	DMS	A	203	4/4	0.72	0.26	75,79,84,87	0
4	WKY	B	201	11/11	0.91	0.11	18,19,20,21	11
3	DMS	A	202	4/4	0.92	0.14	29,31,36,36	0
2	ZN	B	202	1/1	0.99	0.03	16,16,16,16	0
2	ZN	A	201	1/1	0.99	0.04	16,16,16,16	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 WKY B 201:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.