WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2024 – 02:46 PM EDT

PDB ID	:	4C62
Title	:	Inhibitors of Jak2 Kinase domain
Authors	:	Read, J.; Green, I.; Pollard, H.; Howard, T.
Deposited on	:	2013-09-17
Resolution	:	2.75 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.

The following versions of software and data (see references ⓘ) were used in the production of this report:

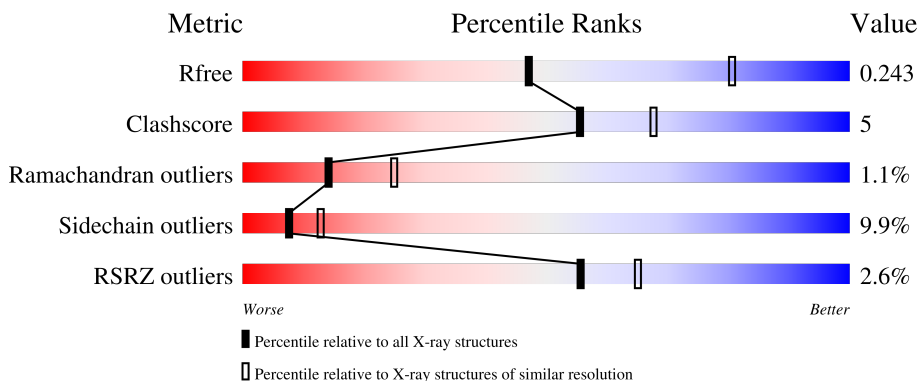|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1   Overall quality at a glance ⓘ

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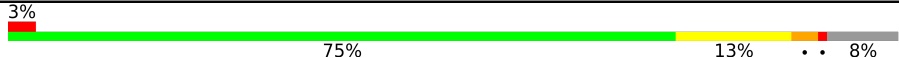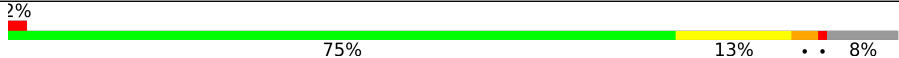*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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		0.243
Clashscore		5
Ramachandran outliers		1.1%
Sidechain outliers		9.9%
RSRZ outliers		2.6%

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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	298	3% / 75% 13% ·· 8%
1	B	298	2% / 75% 13% ·· 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4604 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 TYROSINE-PROTEIN KINASE JAK2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	275	Total	C	N	O	P	S	0	0	0
			2221	1411	376	418	2	14			
1	B	273	Total	C	N	O	P	S	0	0	0
			2199	1403	374	406	2	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	943	ALA	LYS	engineered mutation	UNP O60674
A	945	ALA	LYS	engineered mutation	UNP O60674
A	1129	GLN	ASN	conflict	UNP O60674
B	943	ALA	LYS	engineered mutation	UNP O60674
B	945	ALA	LYS	engineered mutation	UNP O60674
B	1129	GLN	ASN	conflict	UNP O60674

- Molecule 2 is N2-[(1S)-1-(5-fluoropyrimidin-2-yl)ethyl]-n4-(1-methylimidazol-4-yl)-6-morpholino-1,3,5-triazine-2,4-diamine (three-letter code: XWW) (formula: $C_{17}H_{21}FN_{10}O$).
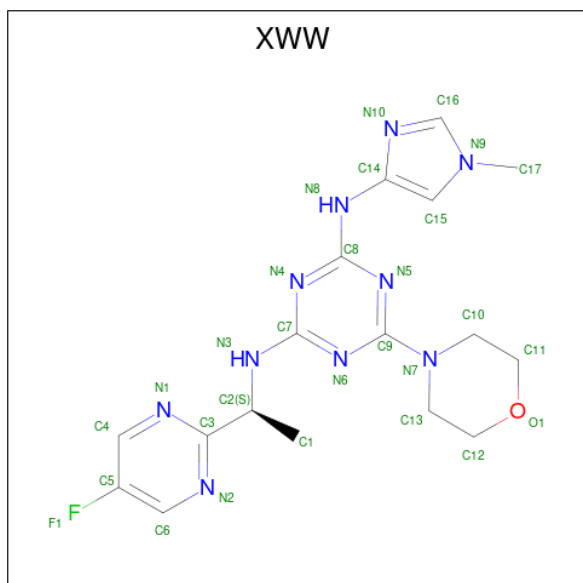
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 29	C 17	F 1	N 10	O 1	0	0
2	B	1	Total 29	C 17	F 1	N 10	O 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 3	C 2	O 1	0	0
3	A	1	Total 3	C 2	O 1	0	0
3	B	1	Total 3	C 2	O 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	44	Total 44	O 44	0	0
4	B	73	Total 73	O 73	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: TYROSINE-PROTEIN KINASE JAK2
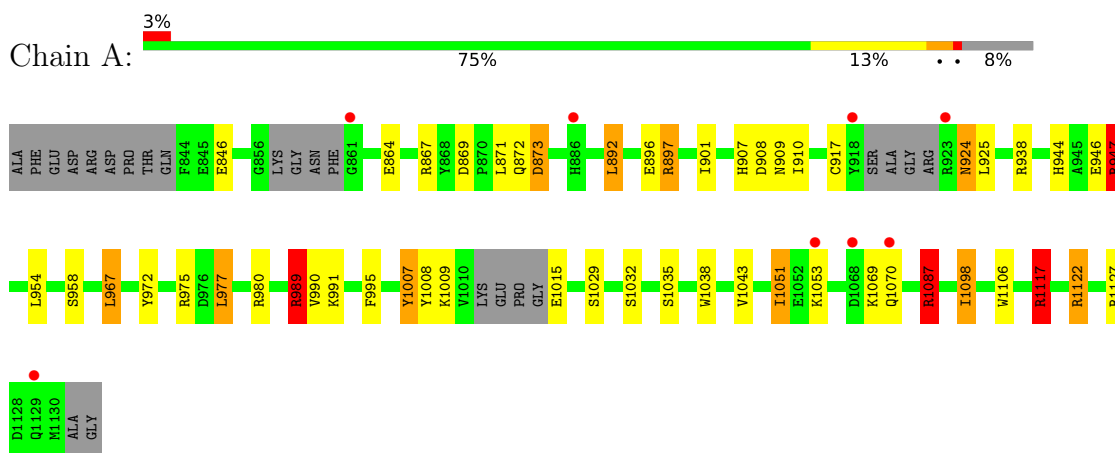
- Molecule 1: TYROSINE-PROTEIN KINASE JAK2
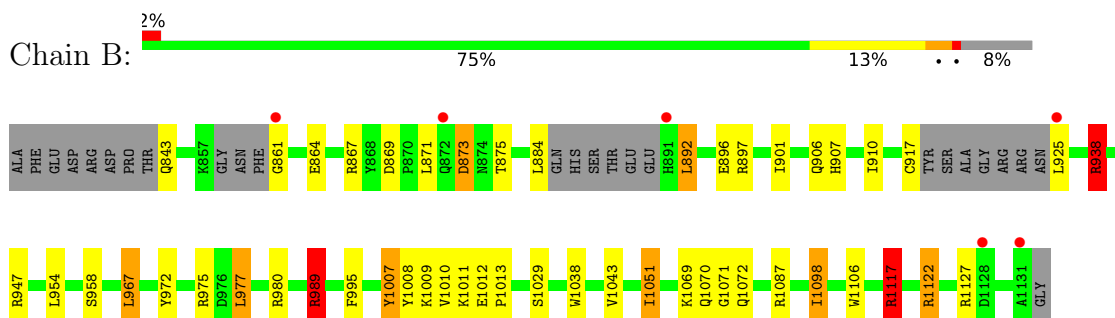
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	44.51Å 126.89Å 135.88Å 90.00° 97.53° 90.00°	Depositor
Resolution (Å)	21.00 – 2.75 20.99 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (21.00-2.75) 99.6 (20.99-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.196 , 0.246 0.200 , 0.243	Depositor DCC
R_{free} test set	991 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å²)	46.5	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.29 , 45.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4604	wwPDB-VP
Average B, all atoms (Å²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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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: PTR, XWW, ACT

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	0.48	0/2231	1.38	26/3012 (0.9%)
1	B	0.52	0/2210	1.40	26/2983 (0.9%)
All	All	0.50	0/4441	1.39	52/5995 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	4
All	All	0	10

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	897	ARG	NE-CZ-NH2	-21.23	109.68	120.30
1	B	975	ARG	NE-CZ-NH2	-19.81	110.39	120.30
1	B	1117	ARG	NE-CZ-NH2	-18.70	110.95	120.30
1	A	947	ARG	NE-CZ-NH2	-18.64	110.98	120.30
1	B	989	ARG	NE-CZ-NH2	-18.53	111.03	120.30
1	A	1087	ARG	NE-CZ-NH2	-17.64	111.48	120.30
1	B	938	ARG	NE-CZ-NH2	-17.19	111.71	120.30
1	A	1122	ARG	NE-CZ-NH2	-16.99	111.80	120.30
1	A	1117	ARG	NE-CZ-NH2	-16.85	111.87	120.30
1	B	897	ARG	NE-CZ-NH2	-16.10	112.25	120.30
1	A	975	ARG	NE-CZ-NH2	-15.99	112.30	120.30
1	A	1087	ARG	NE-CZ-NH1	15.94	128.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	989	ARG	NE-CZ-NH2	-15.36	112.62	120.30
1	B	989	ARG	NE-CZ-NH1	14.87	127.74	120.30
1	B	1122	ARG	NE-CZ-NH2	-14.72	112.94	120.30
1	B	1117	ARG	NE-CZ-NH1	14.61	127.60	120.30
1	B	1122	ARG	NE-CZ-NH1	14.60	127.60	120.30
1	A	938	ARG	NE-CZ-NH2	-14.59	113.01	120.30
1	B	947	ARG	NE-CZ-NH2	-14.56	113.02	120.30
1	B	975	ARG	NE-CZ-NH1	14.49	127.55	120.30
1	B	938	ARG	NE-CZ-NH1	14.43	127.52	120.30
1	A	1117	ARG	NE-CZ-NH1	14.15	127.38	120.30
1	A	975	ARG	NE-CZ-NH1	14.11	127.36	120.30
1	B	947	ARG	NE-CZ-NH1	13.88	127.24	120.30
1	B	1087	ARG	NE-CZ-NH1	13.81	127.21	120.30
1	B	1087	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	A	1122	ARG	NE-CZ-NH1	13.65	127.13	120.30
1	B	897	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	A	938	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	947	ARG	NE-CZ-NH1	12.00	126.30	120.30
1	A	897	ARG	CD-NE-CZ	10.76	138.66	123.60
1	A	897	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	A	989	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	A	947	ARG	CD-NE-CZ	9.61	137.05	123.60
1	A	1087	ARG	CD-NE-CZ	9.14	136.40	123.60
1	B	989	ARG	CD-NE-CZ	8.56	135.59	123.60
1	A	1117	ARG	CD-NE-CZ	8.43	135.40	123.60
1	B	975	ARG	CD-NE-CZ	8.27	135.17	123.60
1	B	938	ARG	CD-NE-CZ	8.25	135.15	123.60
1	A	1122	ARG	CD-NE-CZ	8.17	135.03	123.60
1	B	1122	ARG	CD-NE-CZ	7.59	134.23	123.60
1	B	1117	ARG	CD-NE-CZ	7.48	134.07	123.60
1	A	938	ARG	CD-NE-CZ	6.96	133.34	123.60
1	A	989	ARG	CD-NE-CZ	6.92	133.29	123.60
1	B	897	ARG	CD-NE-CZ	6.83	133.16	123.60
1	B	1087	ARG	CD-NE-CZ	6.78	133.09	123.60
1	A	975	ARG	CD-NE-CZ	6.55	132.77	123.60
1	A	989	ARG	CG-CD-NE	-6.33	98.52	111.80
1	B	989	ARG	CG-CD-NE	6.22	124.85	111.80
1	A	897	ARG	CG-CD-NE	5.68	123.73	111.80
1	B	1117	ARG	CG-CD-NE	-5.56	100.13	111.80
1	B	897	ARG	CG-CD-NE	-5.49	100.28	111.80

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1087	ARG	Sidechain
1	A	1117	ARG	Sidechain
1	A	1122	ARG	Sidechain
1	A	897	ARG	Sidechain
1	A	947	ARG	Sidechain
1	A	989	ARG	Sidechain
1	B	1117	ARG	Sidechain
1	B	1122	ARG	Sidechain
1	B	938	ARG	Sidechain
1	B	989	ARG	Sidechain

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	2221	0	2126	25	0
1	B	2199	0	2129	19	0
2	A	29	0	21	1	0
2	B	29	0	21	2	0
3	A	6	0	6	0	0
3	B	3	0	3	0	0
4	A	44	0	0	6	0
4	B	73	0	0	2	0
All	All	4604	0	4306	45	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 5.

All (45) 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:947:ARG:NH2	4:A:2016:HOH:O	2.11	0.84
2:B:2135:XWW:H15	2:B:2135:XWW:N4	2.02	0.74
1:A:967:LEU:HD23	1:A:972:TYR:HB2	1.69	0.74
1:B:967:LEU:HD23	1:B:972:TYR:HB2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:892:LEU:HD12	1:A:892:LEU:O	2.03	0.59
1:A:871:LEU:O	1:A:873:ASP:HB3	2.03	0.58
2:B:2135:XWW:N4	2:B:2135:XWW:C15	2.61	0.57
1:B:892:LEU:HD12	1:B:892:LEU:O	2.06	0.54
1:A:1032:SER:HB2	4:A:2031:HOH:O	2.09	0.51
1:B:871:LEU:O	1:B:873:ASP:HB3	2.10	0.51
1:B:977:LEU:HD22	1:B:1043:VAL:HG21	1.92	0.51
1:B:954:LEU:HD21	1:B:1098:ILE:HD13	1.93	0.51
1:A:989:ARG:HH12	1:B:1117:ARG:CZ	2.25	0.49
1:A:947:ARG:CZ	4:A:2016:HOH:O	2.58	0.47
1:A:977:LEU:HB2	4:A:2025:HOH:O	2.14	0.47
1:A:954:LEU:HD21	1:A:1098:ILE:HD13	1.95	0.47
1:A:967:LEU:HD23	1:A:972:TYR:CB	2.43	0.47
1:B:967:LEU:HD23	1:B:972:TYR:CB	2.44	0.46
1:A:1051:ILE:HG22	1:A:1051:ILE:O	2.14	0.46
1:B:1007:PTR:CD1	1:B:1007:PTR:C	2.92	0.46
1:A:907:HIS:HB3	1:A:910:ILE:HD12	1.97	0.46
1:B:1010:VAL:O	1:B:1012:GLU:N	2.49	0.46
1:B:907:HIS:HB3	1:B:910:ILE:HD12	1.98	0.45
1:A:944:HIS:CG	4:A:2016:HOH:O	2.70	0.44
1:A:977:LEU:HD22	1:A:1043:VAL:HG21	1.98	0.44
1:A:1007:PTR:CD1	1:A:1007:PTR:C	2.96	0.44
1:A:924:ASN:HD22	1:A:924:ASN:HA	1.59	0.44
1:A:989:ARG:NH1	1:B:1117:ARG:NH2	2.67	0.43
1:A:967:LEU:HD11	1:A:995:PHE:HE1	1.82	0.43
1:B:867:ARG:HG2	1:B:869:ASP:HB2	2.01	0.42
1:B:1117:ARG:HD3	4:B:2070:HOH:O	2.18	0.42
1:A:954:LEU:HB2	1:A:1127:ARG:HD3	2.02	0.42
1:A:989:ARG:HG3	1:A:990:VAL:N	2.34	0.42
1:A:909:ASN:HA	1:A:991:LYS:HG2	2.02	0.41
1:B:967:LEU:HD11	1:B:995:PHE:HE1	1.86	0.41
1:A:867:ARG:HG2	1:A:869:ASP:HB2	2.02	0.41
1:A:1053:LYS:N	4:A:2036:HOH:O	2.54	0.41
1:B:861:GLY:HA2	1:B:884:LEU:HA	2.02	0.41
1:B:843:GLN:N	4:B:2001:HOH:O	2.52	0.41
1:B:1051:ILE:HG22	1:B:1051:ILE:O	2.19	0.41
1:B:954:LEU:HB2	1:B:1127:ARG:HD3	2.03	0.41
1:B:1038:TRP:CE3	1:B:1106:TRP:HA	2.56	0.41
1:A:1032:SER:H	1:A:1035:SER:HG	1.69	0.40
1:A:1038:TRP:CE3	1:A:1106:TRP:HA	2.57	0.40
2:A:2133:XWW:N4	2:A:2133:XWW:H15	2.36	0.40

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	265/298 (89%)	255 (96%)	8 (3%)	2 (1%)	19	34
1	B	263/298 (88%)	255 (97%)	4 (2%)	4 (2%)	10	18
All	All	528/596 (89%)	510 (97%)	12 (2%)	6 (1%)	14	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1011	LYS
1	B	1013	PRO
1	B	1071	GLY
1	A	872	GLN
1	A	1051	ILE
1	B	1051	ILE

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	234/267 (88%)	210 (90%)	24 (10%)	7	12
1	B	232/267 (87%)	210 (90%)	22 (10%)	8	15
All	All	466/534 (87%)	420 (90%)	46 (10%)	8	13

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	846	GLU
1	A	864	GLU
1	A	873	ASP
1	A	892	LEU
1	A	896	GLU
1	A	901	ILE
1	A	908	ASP
1	A	917	CYS
1	A	924	ASN
1	A	925	LEU
1	A	946	GLU
1	A	947	ARG
1	A	958	SER
1	A	967	LEU
1	A	977	LEU
1	A	980	ARG
1	A	1009	LYS
1	A	1015	GLU
1	A	1029	SER
1	A	1069	LYS
1	A	1070	GLN
1	A	1087	ARG
1	A	1098	ILE
1	A	1117	ARG
1	B	864	GLU
1	B	873	ASP
1	B	875	THR
1	B	892	LEU
1	B	896	GLU
1	B	901	ILE
1	B	906	GLN
1	B	917	CYS
1	B	925	LEU
1	B	938	ARG
1	B	958	SER
1	B	967	LEU
1	B	977	LEU
1	B	980	ARG
1	B	989	ARG
1	B	1009	LYS
1	B	1029	SER
1	B	1069	LYS

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Mol	Chain	Res	Type
1	B	1070	GLN
1	B	1072	GLN
1	B	1098	ILE
1	B	1117	ARG

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	854	GLN
1	A	924	ASN
1	A	950	HIS
1	B	854	GLN
1	B	944	HIS

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	PTR	B	1008	1	15,16,17	0.64	0	19,22,24	1.44	4 (21%)
1	PTR	B	1007	1	15,16,17	0.69	0	19,22,24	1.16	1 (5%)
1	PTR	A	1007	1	15,16,17	0.76	0	19,22,24	1.12	1 (5%)
1	PTR	A	1008	1	15,16,17	0.70	0	19,22,24	1.32	2 (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	PTR	B	1008	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1007	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1008	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1008	PTR	CG-CB-CA	-3.23	107.55	114.10
1	B	1008	PTR	CG-CB-CA	-2.99	108.05	114.10
1	B	1008	PTR	P-OH-CZ	2.65	132.25	123.75
1	B	1008	PTR	O3P-P-O2P	2.47	117.07	107.64
1	B	1007	PTR	CG-CB-CA	-2.26	109.53	114.10
1	A	1007	PTR	CG-CB-CA	-2.18	109.68	114.10
1	B	1008	PTR	O3P-P-OH	-2.10	98.66	105.24
1	A	1008	PTR	O3P-P-O2P	2.01	115.32	107.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1007	PTR	1	0
1	A	1007	PTR	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#|Z| > 2$
3	ACT	A	2134	-	1,2,3	1.20	0	1,1,3	0.84	0
2	XWW	B	2135	-	29,32,32	1.53	2 (6%)	33,44,44	2.85	13 (39%)
3	ACT	A	2135	-	1,2,3	1.26	0	1,1,3	0.59	0
2	XWW	A	2133	-	29,32,32	1.43	3 (10%)	33,44,44	2.61	9 (27%)
3	ACT	B	2134	-	1,2,3	1.36	0	1,1,3	0.70	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
2	XWW	A	2133	-	-	3/14/24/24	0/4/4/4
2	XWW	B	2135	-	-	3/14/24/24	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2135	XWW	C7-N3	5.33	1.41	1.34
2	A	2133	XWW	C7-N3	4.60	1.40	1.34
2	B	2135	XWW	C9-N7	4.51	1.44	1.35
2	A	2133	XWW	C9-N7	4.46	1.44	1.35
2	A	2133	XWW	C8-N8	2.44	1.41	1.36

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2133	XWW	C13-N7-C9	-7.32	109.56	121.69
2	A	2133	XWW	C10-N7-C9	-7.27	109.63	121.69
2	B	2135	XWW	C13-N7-C9	-6.49	110.94	121.69
2	B	2135	XWW	C10-N7-C9	-6.38	111.11	121.69
2	B	2135	XWW	C1-C2-C3	-5.67	104.40	110.95
2	B	2135	XWW	C9-N5-C8	5.56	118.58	113.90
2	A	2133	XWW	C9-N6-C7	5.43	118.46	113.90
2	B	2135	XWW	C9-N6-C7	4.94	118.05	113.90
2	A	2133	XWW	C9-N5-C8	4.92	118.04	113.90
2	B	2135	XWW	N3-C7-N4	3.69	122.73	117.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2135	XWW	C5-C4-N1	-3.58	119.30	121.46
2	B	2135	XWW	N6-C9-N5	-3.54	120.46	126.31
2	A	2133	XWW	N6-C9-N5	-3.23	120.98	126.31
2	B	2135	XWW	N2-C3-N1	2.97	129.87	125.95
2	B	2135	XWW	N3-C7-N6	-2.96	112.73	117.18
2	A	2133	XWW	C11-C10-N7	2.88	115.33	110.02
2	A	2133	XWW	N3-C7-N4	2.63	121.12	117.18
2	B	2135	XWW	C8-N8-C14	-2.53	123.09	129.43
2	B	2135	XWW	C12-C13-N7	2.51	114.65	110.02
2	B	2135	XWW	N6-C9-N7	2.47	120.16	117.11
2	A	2133	XWW	N6-C7-N4	-2.25	122.67	126.23
2	A	2133	XWW	N5-C9-N7	2.01	119.59	117.11

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2135	XWW	N3-C2-C3-N2
2	B	2135	XWW	N6-C9-N7-C10
2	B	2135	XWW	N5-C9-N7-C10
2	A	2133	XWW	N6-C9-N7-C10
2	A	2133	XWW	N5-C9-N7-C10
2	A	2133	XWW	N3-C2-C3-N2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

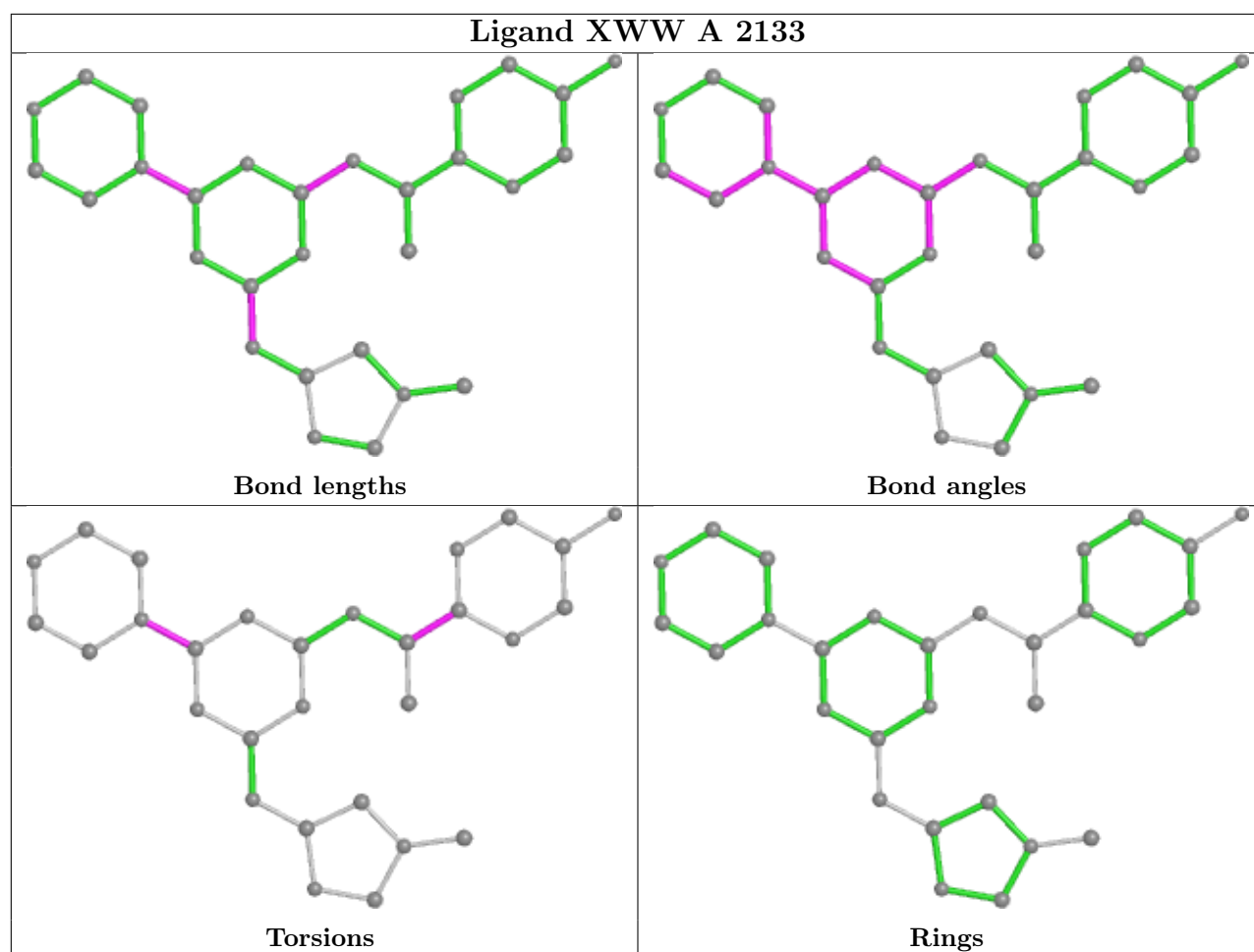| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2135	XWW	2	0
2	A	2133	XWW	1	0

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 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 XWW B 2135	
Bond lengths	**Bond angles**
Torsions	**Rings**

Ligand XWW A 2133

Bond lengths

Bond angles

Torsions

Rings
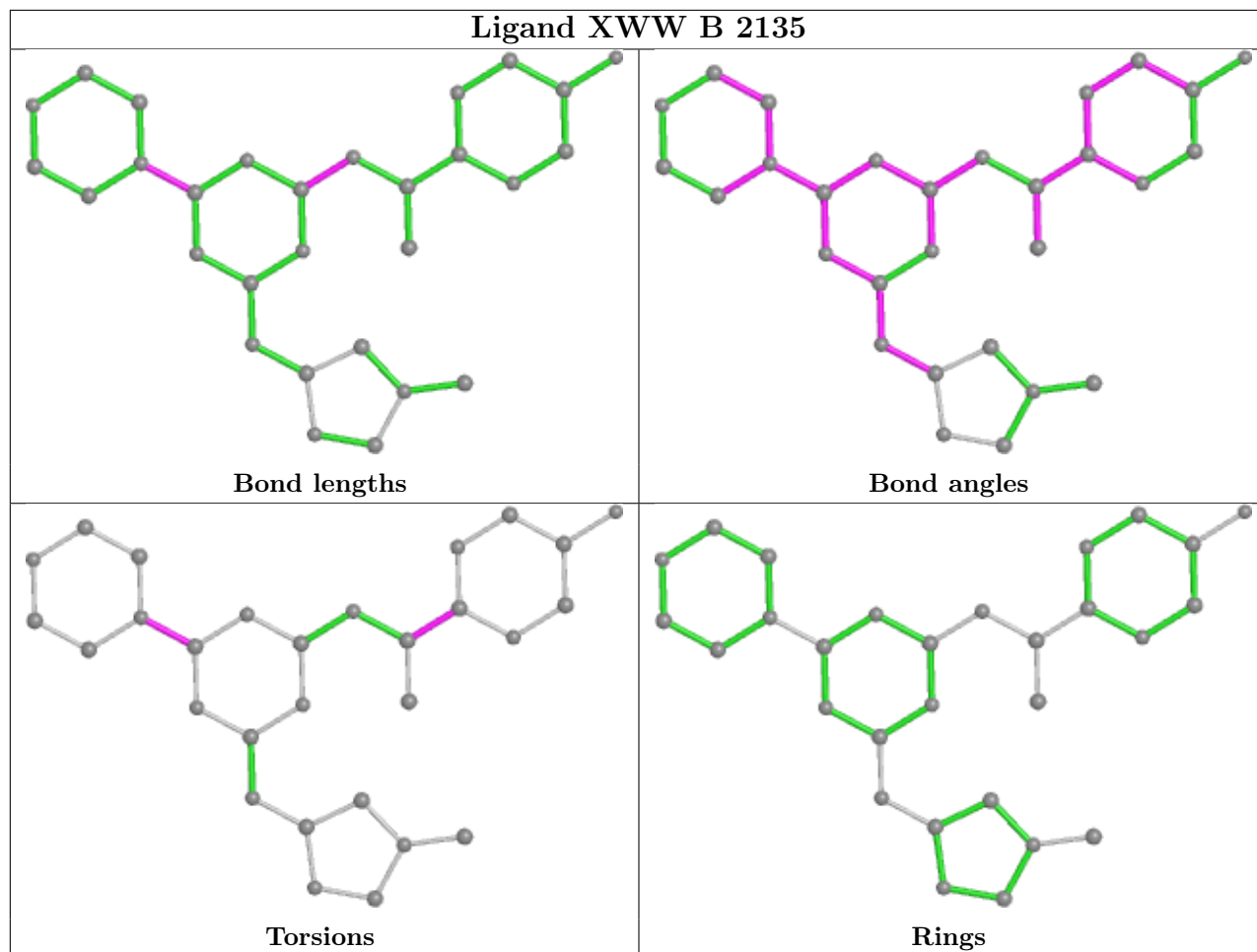
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	273/298 (91%)	0.01	8 (2%)	51	61	26, 52, 90, 102	1 (0%)
1	B	271/298 (90%)	-0.16	6 (2%)	62	70	22, 45, 84, 104	0
All	All	544/596 (91%)	-0.07	14 (2%)	56	65	22, 49, 88, 104	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	891	HIS	3.5
1	B	861	GLY	3.4
1	B	1128	ASP	2.8
1	A	1070	GLN	2.7
1	A	923	ARG	2.7
1	B	1131	ALA	2.6
1	A	886	HIS	2.4
1	A	861	GLY	2.4
1	A	1129	GLN	2.4
1	B	925	LEU	2.4
1	A	918	TYR	2.4
1	A	1053	LYS	2.3
1	A	1068	ASP	2.3
1	B	872	GLN	2.0

## 6.2 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, 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
1	PTR	A	1007	16/17	0.88	0.24	70,86,100,102	0
1	PTR	A	1008	16/17	0.92	0.20	71,78,93,95	0
1	PTR	B	1007	16/17	0.96	0.13	41,49,57,60	0
1	PTR	B	1008	16/17	0.96	0.11	41,45,50,50	0

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	ACT	A	2135	3/4	0.87	0.27	57,57,62,63	0
3	ACT	A	2134	3/4	0.94	0.16	58,58,61,64	0
2	XWW	B	2135	29/29	0.95	0.15	33,40,44,48	0
2	XWW	A	2133	29/29	0.97	0.11	24,27,34,38	0
3	ACT	B	2134	3/4	0.97	0.14	40,40,41,41	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 XWW B 2135:

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

Electron density around XWW A 2133:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
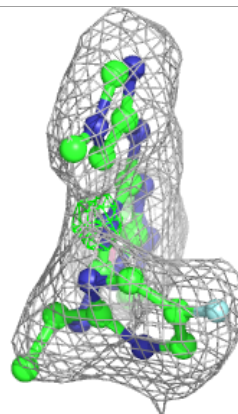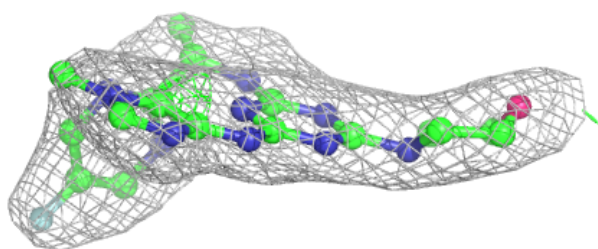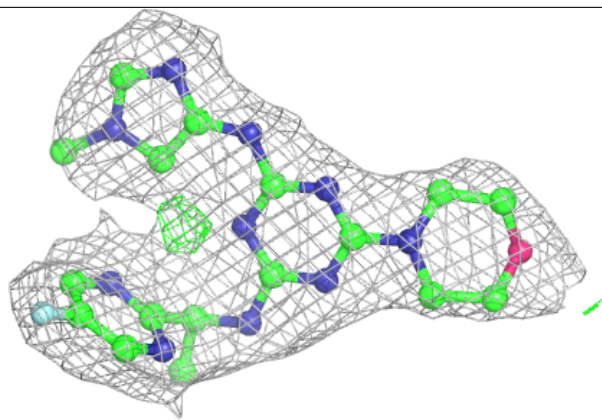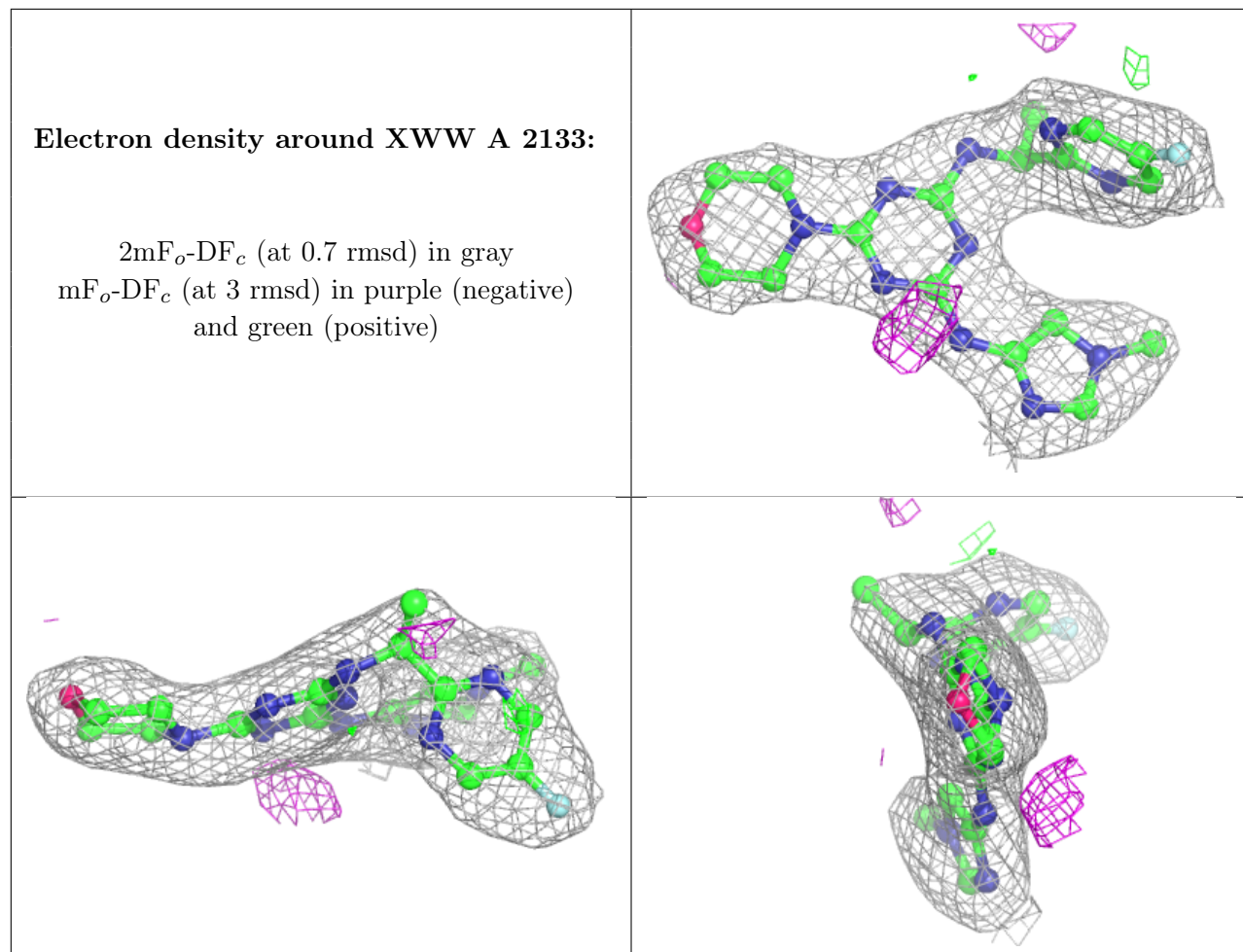
6.5 Other polymers (i)

There are no such residues in this entry.