Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2024 – 08:05 PM EST

PDB ID	:	8UDT
Title	:	The X-RAY co-crystal structure of human FGFR3 and KIN-3248
Authors	:	Tyhonas, J.S.; Arnold, L.D.; Cox, J.; Franovic, A.; Gardiner, E.; Grandinetti, K.; Kania, R.; Kanouni, T.; Lardy, M.; Li, C.; Martin, E.S.; Miller, N.; Mohan, A.; Murphy, E.A.; Perez, M.; Soroceanu, L.; Timple, N.; Uryu, S.; Womble, S.; Kaldor, S.W.
Deposited on	:	2023-09-29
Resolution	:	2.83 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 (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 (1)) were used in the production of this report:

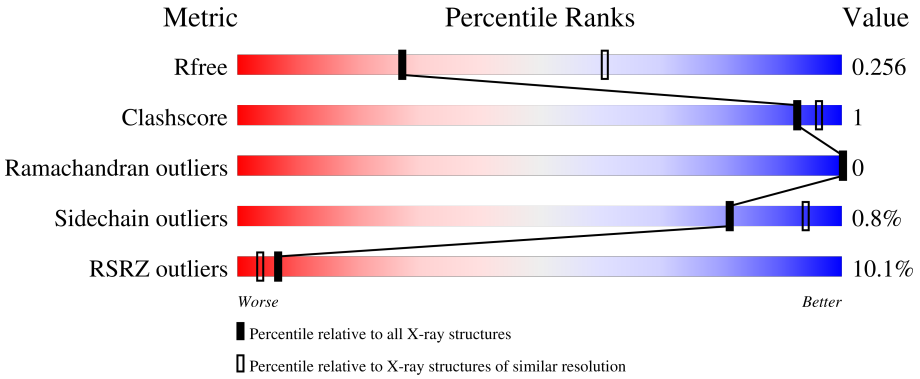
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.83 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	297	9% 94%
1	B	297	9% 92% 5%
1	C	297	10% 92%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13854 atoms, of which 6833 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 Fibroblast growth factor receptor 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	H	N	O	S	2271	0	0
			4520	1434	2271	387	410	18			
1	B	283	Total	C	H	N	O	S	2271	0	0
			4518	1433	2271	389	407	18			
1	C	286	Total	C	H	N	O	S	2291	0	0
			4564	1448	2291	396	411	18			

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	454	MET	-	initiating methionine	UNP P22607
A	?	-	PRO	deletion	UNP P22607
A	?	-	PRO	deletion	UNP P22607
A	?	-	GLY	deletion	UNP P22607
A	?	-	LEU	deletion	UNP P22607
A	?	-	ASP	deletion	UNP P22607
A	?	-	TYR	deletion	UNP P22607
A	?	-	SER	deletion	UNP P22607
A	?	-	PHE	deletion	UNP P22607
A	?	-	ASP	deletion	UNP P22607
A	?	-	THR	deletion	UNP P22607
A	?	-	CYS	deletion	UNP P22607
A	?	-	LYS	deletion	UNP P22607
A	572	SER	PRO	engineered mutation	UNP P22607
A	573	GLY	PRO	engineered mutation	UNP P22607
A	757	HIS	-	expression tag	UNP P22607
A	758	HIS	-	expression tag	UNP P22607
A	759	HIS	-	expression tag	UNP P22607
A	760	HIS	-	expression tag	UNP P22607
A	761	HIS	-	expression tag	UNP P22607
A	762	HIS	-	expression tag	UNP P22607
B	454	MET	-	initiating methionine	UNP P22607
B	?	-	PRO	deletion	UNP P22607

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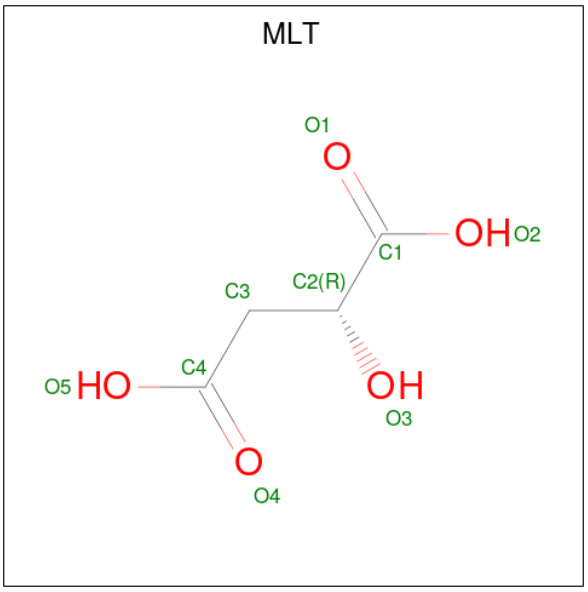
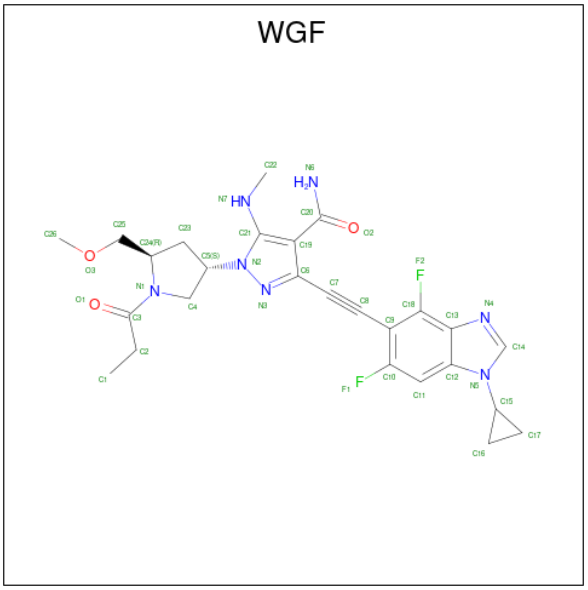
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP P22607
B	?	-	GLY	deletion	UNP P22607
B	?	-	LEU	deletion	UNP P22607
B	?	-	ASP	deletion	UNP P22607
B	?	-	TYR	deletion	UNP P22607
B	?	-	SER	deletion	UNP P22607
B	?	-	PHE	deletion	UNP P22607
B	?	-	ASP	deletion	UNP P22607
B	?	-	THR	deletion	UNP P22607
B	?	-	CYS	deletion	UNP P22607
B	?	-	LYS	deletion	UNP P22607
B	572	SER	PRO	engineered mutation	UNP P22607
B	573	GLY	PRO	engineered mutation	UNP P22607
B	757	HIS	-	expression tag	UNP P22607
B	758	HIS	-	expression tag	UNP P22607
B	759	HIS	-	expression tag	UNP P22607
B	760	HIS	-	expression tag	UNP P22607
B	761	HIS	-	expression tag	UNP P22607
B	762	HIS	-	expression tag	UNP P22607
C	454	MET	-	initiating methionine	UNP P22607
C	?	-	PRO	deletion	UNP P22607
C	?	-	PRO	deletion	UNP P22607
C	?	-	GLY	deletion	UNP P22607
C	?	-	LEU	deletion	UNP P22607
C	?	-	ASP	deletion	UNP P22607
C	?	-	TYR	deletion	UNP P22607
C	?	-	SER	deletion	UNP P22607
C	?	-	PHE	deletion	UNP P22607
C	?	-	ASP	deletion	UNP P22607
C	?	-	THR	deletion	UNP P22607
C	?	-	CYS	deletion	UNP P22607
C	?	-	LYS	deletion	UNP P22607
C	572	SER	PRO	engineered mutation	UNP P22607
C	573	GLY	PRO	engineered mutation	UNP P22607
C	757	HIS	-	expression tag	UNP P22607
C	758	HIS	-	expression tag	UNP P22607
C	759	HIS	-	expression tag	UNP P22607
C	760	HIS	-	expression tag	UNP P22607
C	761	HIS	-	expression tag	UNP P22607
C	762	HIS	-	expression tag	UNP P22607

- Molecule 2 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 4 5	0	0
2	A	1	Total C O 9 4 5	0	0

- Molecule 3 is 3-[(1-cyclopropyl-4,6-difluoro-1H-benzimidazol-5-yl)ethynyl]-1-[(3R,5R)-5-(methoxymethyl)-1-propanoylpyrrolidin-3-yl]-5-(methylamino)-1H-pyrazole-4-carboxamide (three-letter code: WGF) (formula: $C_{26}H_{29}F_2N_7O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	26	2	7	3		
3	B	1	Total	C	F	N	O	0	0
			38	26	2	7	3		
3	C	1	Total	C	F	N	O	0	0
			38	26	2	7	3		

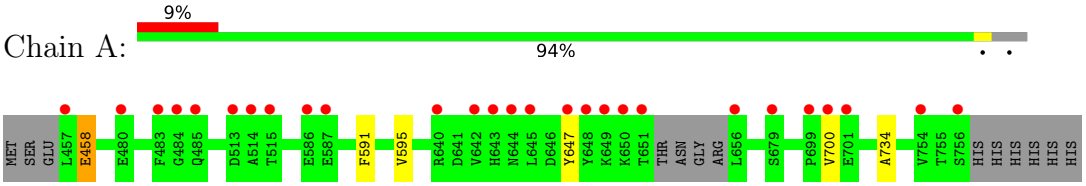
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	30	Total	O	0	0
			30	30		
4	C	28	Total	O	0	0
			28	28		

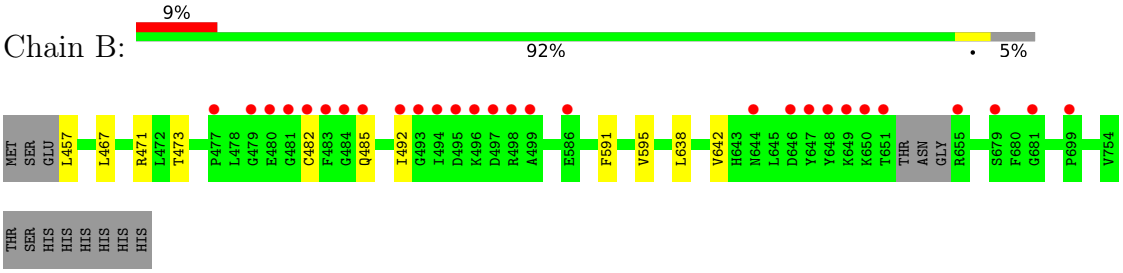
3 Residue-property plots (i)

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.

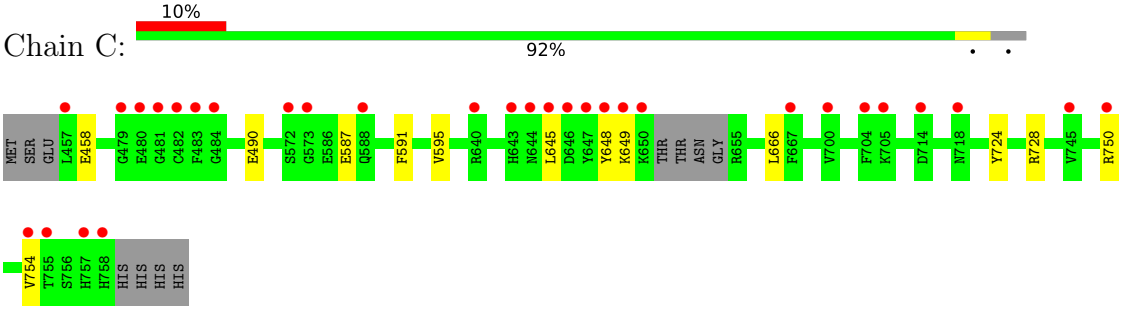
• Molecule 1: Fibroblast growth factor receptor 3



• Molecule 1: Fibroblast growth factor receptor 3



• Molecule 1: Fibroblast growth factor receptor 3



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	89.98Å 160.44Å 179.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.29 – 2.83 33.29 – 2.83	Depositor EDS
% Data completeness (in resolution range)	100.0 (33.29-2.83) 100.0 (33.29-2.83)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.33 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.262 , 0.274 0.247 , 0.256	Depositor DCC
R_{free} test set	1548 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	82.9	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 64.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13854	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLT, WGF

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	0.23	0/2295	0.44	0/3100
1	B	0.23	0/2293	0.44	0/3096
1	C	0.23	0/2321	0.44	0/3134
All	All	0.23	0/6909	0.44	0/9330

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

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	2249	2271	2270	4	0
1	B	2247	2271	2271	4	0
1	C	2273	2291	2290	10	0
2	A	18	0	8	0	0
3	A	38	0	0	1	0
3	B	38	0	0	1	0
3	C	38	0	0	2	0
4	A	62	0	0	0	0
4	B	30	0	0	0	0
4	C	28	0	0	1	0
All	All	7021	6833	6839	20	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 1.

All (20) 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:750:ARG:NH1	1:C:754:VAL:HG22	2.04	0.72
1:B:471:ARG:HD2	1:B:492:ILE:O	1.96	0.65
1:C:750:ARG:CZ	1:C:754:VAL:HG22	2.34	0.58
1:B:482:CYS:O	1:B:485:GLN:HG2	2.06	0.56
3:C:2001:WGF:N4	4:C:2101:HOH:O	2.33	0.56
1:B:642:VAL:O	1:C:458:GLU:HB2	2.07	0.54
3:B:2001:WGF:C5	3:B:2001:WGF:C22	2.89	0.51
1:A:734:ALA:HB1	1:C:490:GLU:OE2	2.13	0.49
3:A:1003:WGF:C5	3:A:1003:WGF:C22	2.92	0.48
3:C:2001:WGF:C5	3:C:2001:WGF:C22	2.92	0.47
1:C:648:TYR:O	1:C:649:LYS:HB2	2.17	0.45
1:C:750:ARG:O	1:C:754:VAL:HG23	2.16	0.45
1:C:750:ARG:NH1	1:C:754:VAL:CG2	2.78	0.44
1:A:591:PHE:O	1:A:595:VAL:HG23	2.18	0.43
1:A:458:GLU:OE2	1:A:458:GLU:O	2.37	0.42
1:B:591:PHE:O	1:B:595:VAL:HG23	2.19	0.41
1:C:724:TYR:CZ	1:C:728:ARG:HD3	2.56	0.41
1:C:591:PHE:O	1:C:595:VAL:HG23	2.20	0.41
1:C:645:LEU:HD21	1:C:666:LEU:HG	2.02	0.41
1:A:647:TYR:CD1	1:A:700:VAL:HG21	2.56	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	280/297 (94%)	276 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	279/297 (94%)	274 (98%)	5 (2%)	0	100	100
1	C	282/297 (95%)	277 (98%)	5 (2%)	0	100	100
All	All	841/891 (94%)	827 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	242/254 (95%)	241 (100%)	1 (0%)	91	97
1	B	241/254 (95%)	237 (98%)	4 (2%)	60	86
1	C	244/254 (96%)	243 (100%)	1 (0%)	91	97
All	All	727/762 (95%)	721 (99%)	6 (1%)	81	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	GLU
1	B	457	LEU
1	B	467	LEU
1	B	473	THR
1	B	638	LEU
1	C	587	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	743	GLN
1	C	540	ASN
1	C	600	GLN
1	C	721	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 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	WGF	C	2001	1	34,42,42	0.68	0	34,62,62	1.29	3 (8%)
2	MLT	A	1002	-	8,8,8	1.02	0	10,10,10	1.35	2 (20%)
2	MLT	A	1001	-	8,8,8	1.03	0	10,10,10	1.19	1 (10%)
3	WGF	A	1003	1	34,42,42	0.78	2 (5%)	34,62,62	1.31	3 (8%)
3	WGF	B	2001	1	34,42,42	0.73	1 (2%)	34,62,62	1.29	2 (5%)

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	WGF	C	2001	1	-	0/11/42/42	0/5/5/5
2	MLT	A	1002	-	-	0/8/8/8	-
2	MLT	A	1001	-	-	5/8/8/8	-
3	WGF	A	1003	1	-	0/11/42/42	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WGF	B	2001	1	-	2/11/42/42	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	WGF	C19-C20	-2.22	1.47	1.51
3	B	2001	WGF	C19-C20	-2.07	1.47	1.51
3	A	1003	WGF	C11-C10	2.04	1.38	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2001	WGF	C6-N3-N2	5.18	108.02	104.32
3	C	2001	WGF	C6-N3-N2	4.79	107.74	104.32
3	A	1003	WGF	C6-N3-N2	4.45	107.50	104.32
2	A	1002	MLT	O2-C1-C2	2.89	119.07	112.72
2	A	1001	MLT	O2-C1-C2	2.76	118.78	112.72
3	A	1003	WGF	C4-N1-C3	-2.71	123.93	129.33
3	B	2001	WGF	C18-C9-C8	-2.52	118.03	121.62
3	A	1003	WGF	C18-C9-C8	-2.38	118.23	121.62
3	C	2001	WGF	C18-C9-C8	-2.30	118.34	121.62
3	C	2001	WGF	C4-N1-C3	-2.30	124.74	129.33
2	A	1002	MLT	O1-C1-C2	-2.06	118.52	122.54

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	WGF	C1-C2-C3-N1
2	A	1001	MLT	O2-C1-C2-C3
2	A	1001	MLT	O1-C1-C2-O3
2	A	1001	MLT	O1-C1-C2-C3
2	A	1001	MLT	O3-C2-C3-C4
3	B	2001	WGF	C1-C2-C3-O1
2	A	1001	MLT	O2-C1-C2-O3

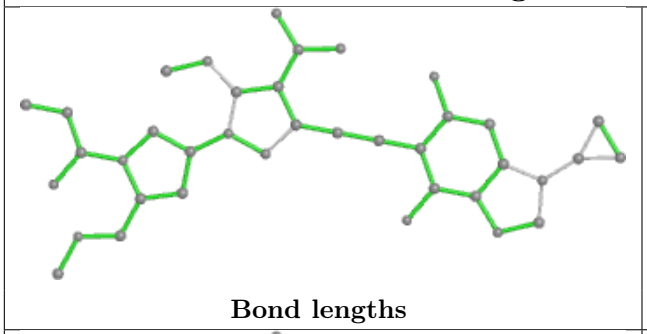
There are no ring outliers.

3 monomers are involved in 4 short contacts:

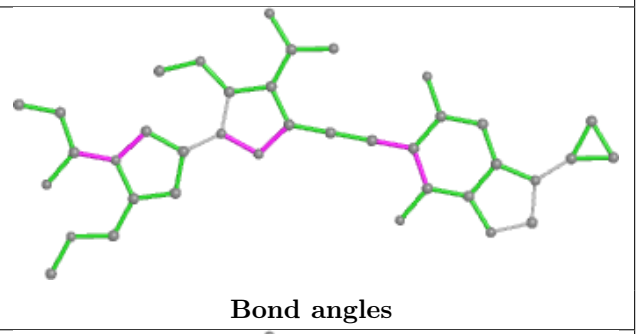
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2001	WGF	2	0
3	A	1003	WGF	1	0
3	B	2001	WGF	1	0

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.

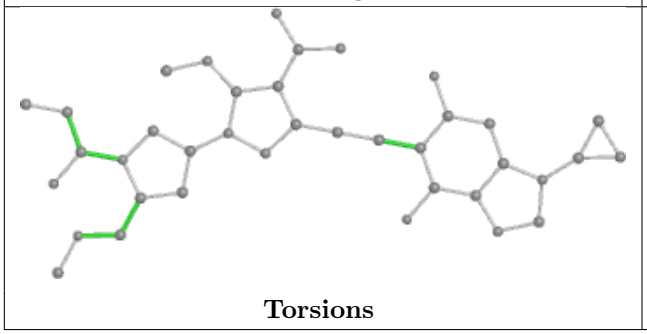
Ligand WGF C 2001



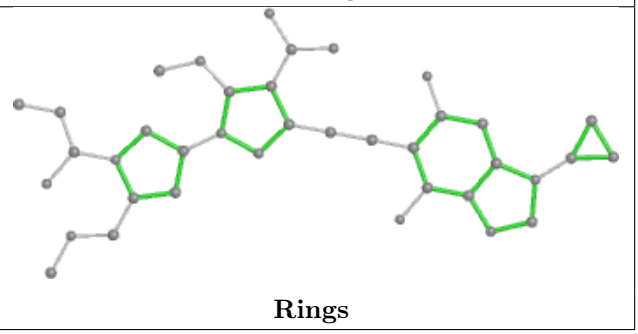
Bond lengths



Bond angles

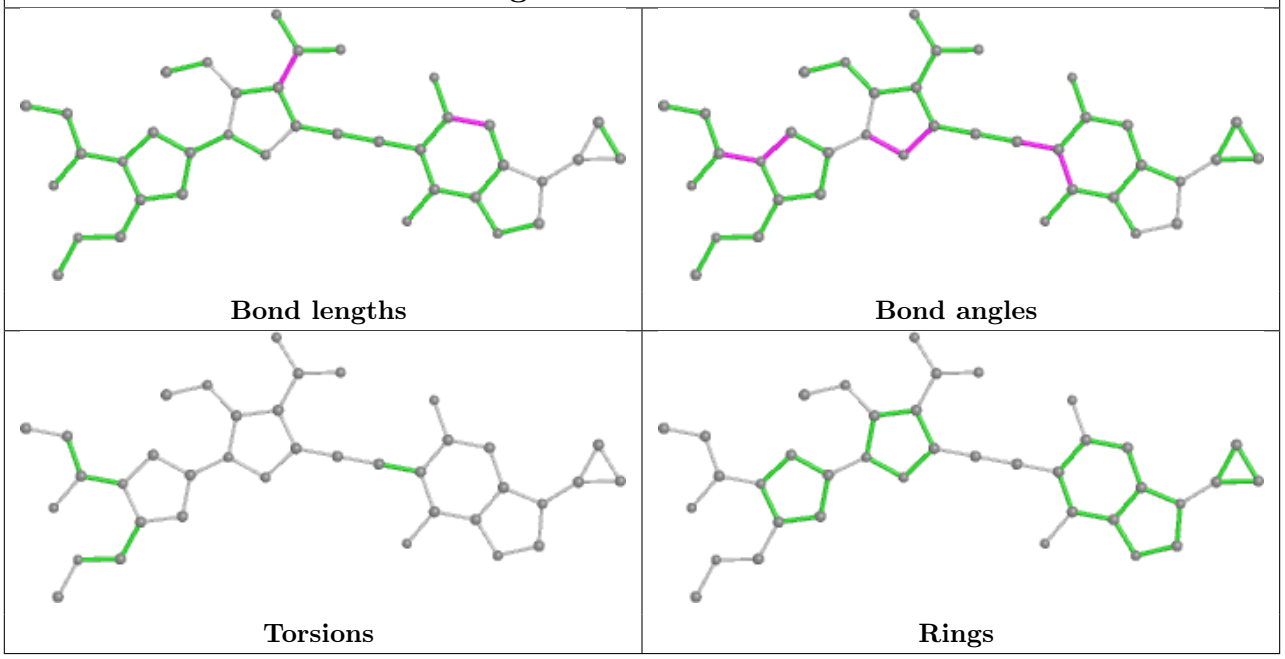


Torsions

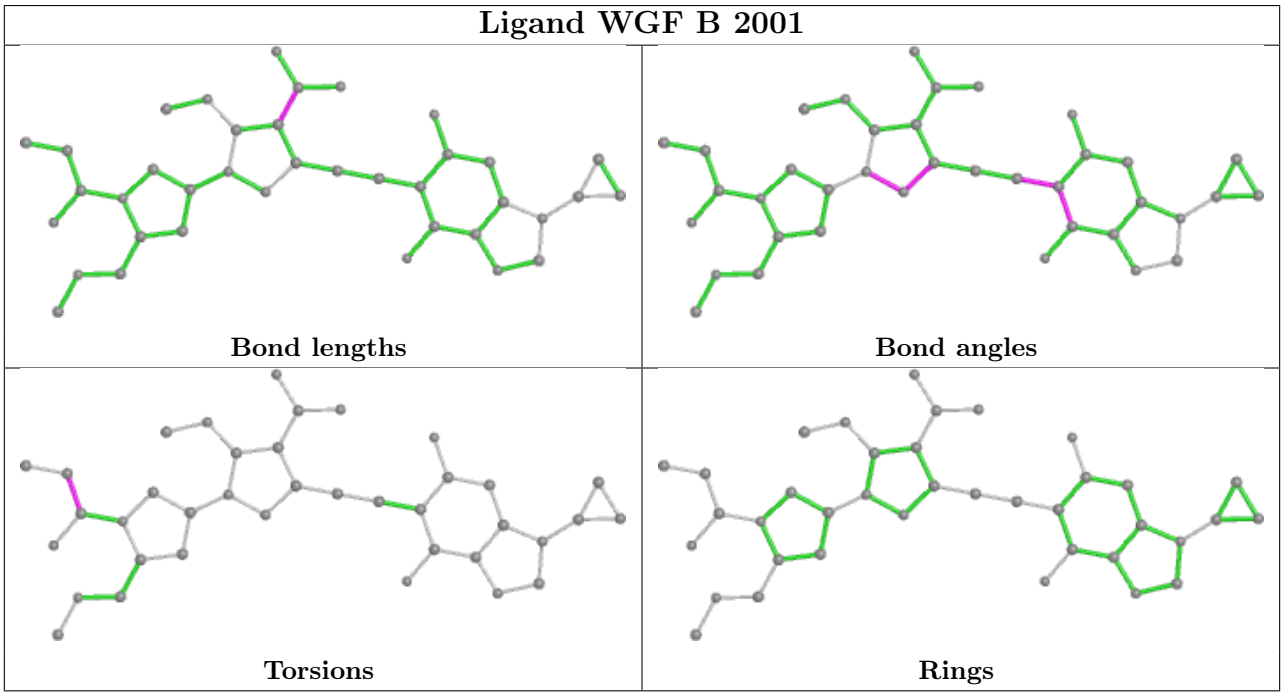


Rings

Ligand WGF A 1003



Ligand WGF B 2001



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^{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	284/297 (95%)	0.45	27 (9%)	8	4	65, 85, 138, 169	0
1	B	283/297 (95%)	0.58	28 (9%)	7	4	69, 101, 167, 186	0
1	C	286/297 (96%)	0.61	31 (10%)	5	3	68, 108, 173, 189	0
All	All	853/891 (95%)	0.55	86 (10%)	7	4	65, 98, 167, 189	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	483	PHE	8.7
1	C	483	PHE	7.5
1	A	651	THR	7.4
1	B	651	THR	5.9
1	C	646	ASP	5.8
1	A	648	TYR	5.7
1	A	644	ASN	5.4
1	C	648	TYR	5.3
1	B	497	ASP	5.2
1	C	480	GLU	5.2
1	C	750	ARG	5.1
1	C	645	LEU	4.9
1	C	667	PHE	4.9
1	A	656	LEU	4.8
1	B	482	CYS	4.7
1	B	480	GLU	4.6
1	C	644	ASN	4.5
1	B	483	PHE	4.5
1	C	649	LYS	4.3
1	A	649	LYS	4.3
1	C	484	GLY	4.1
1	A	480	GLU	4.0
1	C	758	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	704	PHE	3.8
1	C	482	CYS	3.8
1	C	572	SER	3.8
1	A	513	ASP	3.7
1	A	645	LEU	3.7
1	B	485	GLN	3.6
1	B	494	ILE	3.6
1	C	643	HIS	3.5
1	C	755	THR	3.5
1	B	484	GLY	3.4
1	C	705	LYS	3.4
1	B	647	TYR	3.4
1	A	484	GLY	3.3
1	A	457	LEU	3.3
1	C	457	LEU	3.3
1	A	643	HIS	3.3
1	B	477	PRO	3.2
1	B	649	LYS	3.2
1	C	479	GLY	3.1
1	B	496	LYS	3.1
1	B	493	GLY	3.1
1	B	646	ASP	3.1
1	A	756	SER	3.0
1	B	495	ASP	3.0
1	C	650	LYS	3.0
1	A	679	SER	2.9
1	A	647	TYR	2.9
1	B	479	GLY	2.8
1	B	498	ARG	2.8
1	B	499	ALA	2.8
1	A	514	ALA	2.7
1	C	700	VAL	2.7
1	B	679	SER	2.7
1	C	640	ARG	2.7
1	A	700	VAL	2.7
1	A	754	VAL	2.6
1	A	650	LYS	2.6
1	B	586	GLU	2.6
1	C	647	TYR	2.6
1	B	481	GLY	2.5
1	B	492	ILE	2.5
1	C	718	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	714	ASP	2.4
1	A	515	THR	2.4
1	A	640	ARG	2.4
1	C	757	HIS	2.4
1	A	485	GLN	2.4
1	C	588	GLN	2.4
1	A	701	GLU	2.3
1	B	681	GLY	2.3
1	A	587	GLU	2.3
1	B	655	ARG	2.3
1	C	573	GLY	2.2
1	A	642	VAL	2.2
1	B	644	ASN	2.2
1	A	586	GLU	2.2
1	C	481	GLY	2.1
1	C	754	VAL	2.1
1	C	745	VAL	2.1
1	B	648	TYR	2.1
1	A	699	PRO	2.1
1	B	650	LYS	2.0
1	B	699	PRO	2.0

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 monosaccharides 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, 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	WGF	B	2001	38/38	0.70	0.35	118,124,136,141	0
2	MLT	A	1002	9/9	0.78	0.28	131,131,131,131	0

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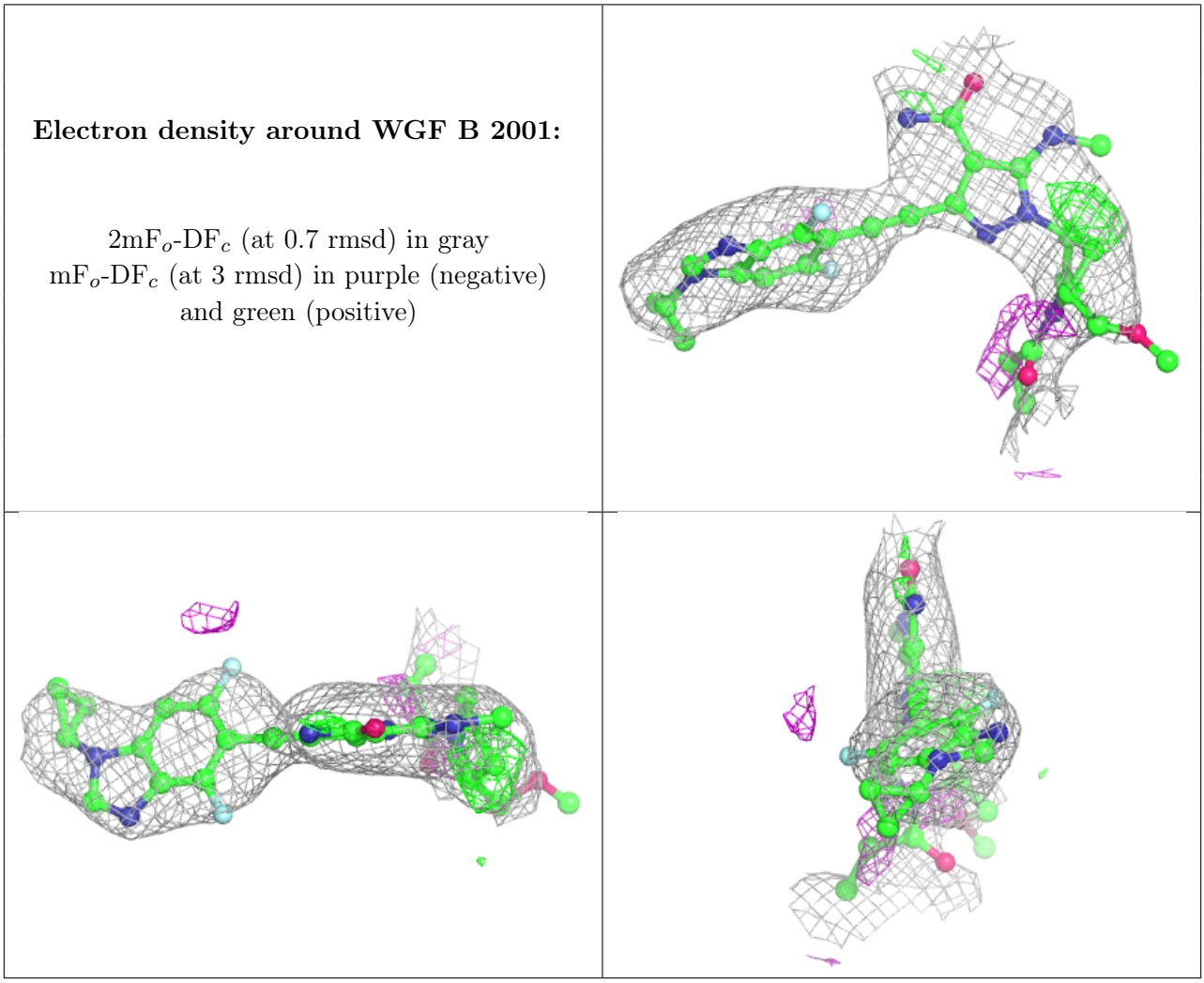
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	WGF	C	2001	38/38	0.79	0.28	105,111,119,120	0
2	MLT	A	1001	9/9	0.81	0.36	92,94,95,95	0
3	WGF	A	1003	38/38	0.88	0.26	92,98,108,110	0

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.

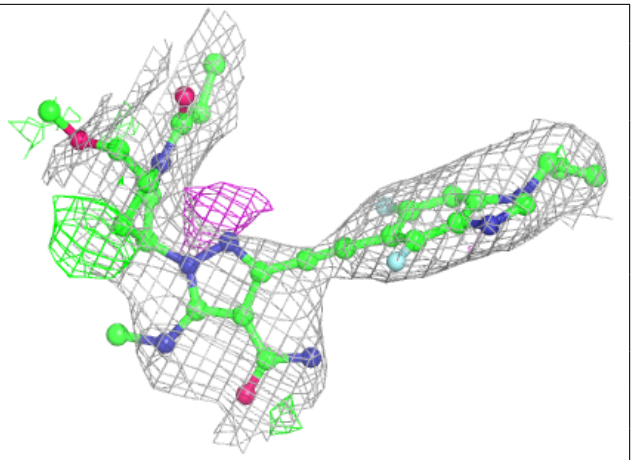
Electron density around WGF B 2001:

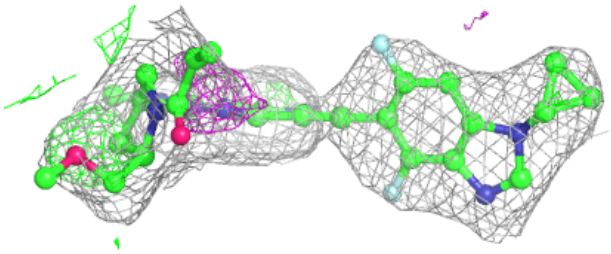
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

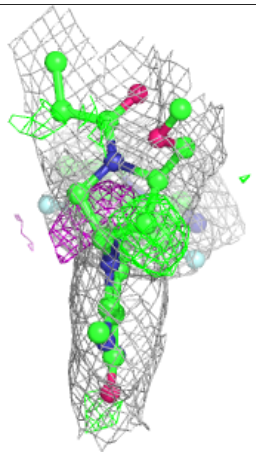


Electron density around WGF C 2001:

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

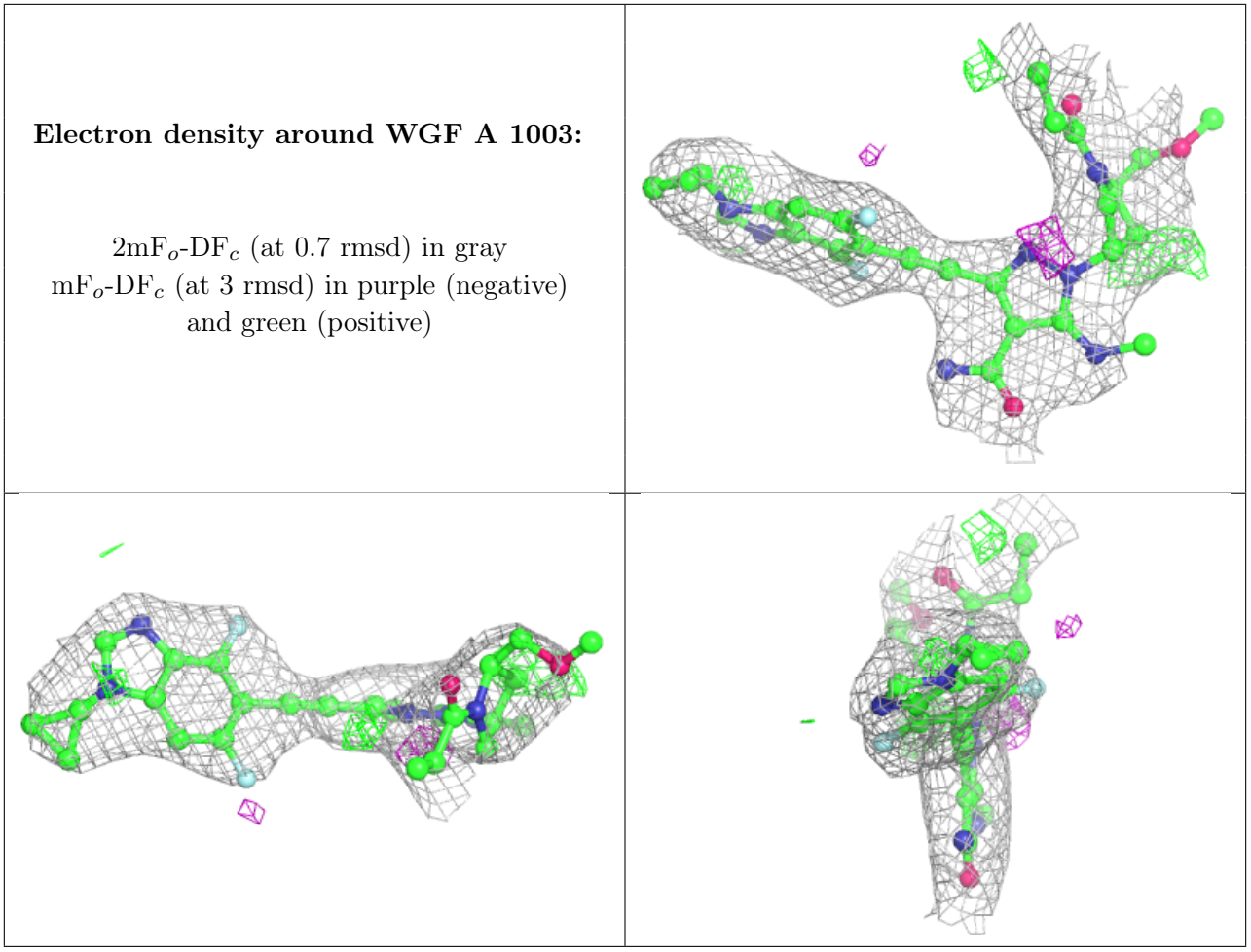






Electron density around WGF A 1003:

$2mF_o$-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.