



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2023 – 05:41 PM EDT

PDB ID : 4Z32  
Title : Crystal Structure of the FERM-SH2 Domains of Jak2  
Authors : McNally, R.; Eck, M.J.  
Deposited on : 2015-03-30  
Resolution : 3.04 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](mailto:validation@mail.wwpdb.org)

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

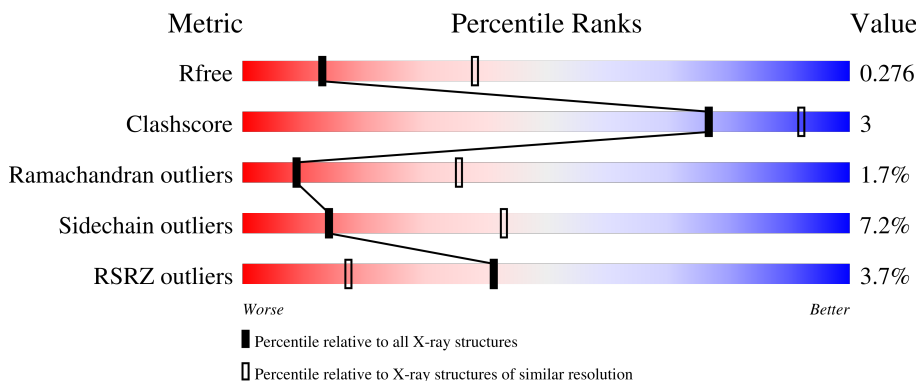
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.04 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.



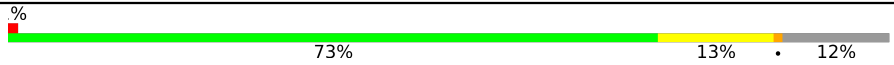


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	497	 6% 75% 13% • 11%
1	B	497	 6% 73% 14% • 11%
1	C	497	 6% 70% 13% • 16%
1	D	497	 3% 71% 12% • 16%
1	E	497	 6% 73% 12% • 14%

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Mol	Chain	Length	Quality of chain
1	F	497	 <p>% 73% 13% • 12%</p>
1	G	497	 <p>4% 74% 8% • 17%</p>
1	H	497	 <p>7% 72% 9% • 19%</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 27929 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
			Total	C	N	O	S			
1	A	441	Total 3624	C 2334	N 622	O 646	S 22	0	0	0
1	B	441	Total 3624	C 2334	N 622	O 646	S 22	0	0	0
1	C	418	Total 3433	C 2211	N 588	O 612	S 22	0	0	0
1	D	417	Total 3423	C 2208	N 587	O 606	S 22	0	0	0
1	E	427	Total 3516	C 2271	N 602	O 622	S 21	0	0	0
1	F	436	Total 3586	C 2311	N 616	O 637	S 22	0	0	0
1	G	411	Total 3375	C 2179	N 578	O 597	S 21	0	0	0
1	H	405	Total 3336	C 2154	N 573	O 588	S 21	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP O60674
A	517	LEU	-	expression tag	UNP O60674
A	518	GLU	-	expression tag	UNP O60674
A	519	HIS	-	expression tag	UNP O60674
A	520	HIS	-	expression tag	UNP O60674
A	521	HIS	-	expression tag	UNP O60674
A	522	HIS	-	expression tag	UNP O60674
A	523	HIS	-	expression tag	UNP O60674
A	524	HIS	-	expression tag	UNP O60674
A	525	HIS	-	expression tag	UNP O60674
A	526	HIS	-	expression tag	UNP O60674
B	30	GLY	-	expression tag	UNP O60674
B	517	LEU	-	expression tag	UNP O60674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	518	GLU	-	expression tag	UNP O60674
B	519	HIS	-	expression tag	UNP O60674
B	520	HIS	-	expression tag	UNP O60674
B	521	HIS	-	expression tag	UNP O60674
B	522	HIS	-	expression tag	UNP O60674
B	523	HIS	-	expression tag	UNP O60674
B	524	HIS	-	expression tag	UNP O60674
B	525	HIS	-	expression tag	UNP O60674
B	526	HIS	-	expression tag	UNP O60674
C	30	GLY	-	expression tag	UNP O60674
C	517	LEU	-	expression tag	UNP O60674
C	518	GLU	-	expression tag	UNP O60674
C	519	HIS	-	expression tag	UNP O60674
C	520	HIS	-	expression tag	UNP O60674
C	521	HIS	-	expression tag	UNP O60674
C	522	HIS	-	expression tag	UNP O60674
C	523	HIS	-	expression tag	UNP O60674
C	524	HIS	-	expression tag	UNP O60674
C	525	HIS	-	expression tag	UNP O60674
C	526	HIS	-	expression tag	UNP O60674
D	30	GLY	-	expression tag	UNP O60674
D	517	LEU	-	expression tag	UNP O60674
D	518	GLU	-	expression tag	UNP O60674
D	519	HIS	-	expression tag	UNP O60674
D	520	HIS	-	expression tag	UNP O60674
D	521	HIS	-	expression tag	UNP O60674
D	522	HIS	-	expression tag	UNP O60674
D	523	HIS	-	expression tag	UNP O60674
D	524	HIS	-	expression tag	UNP O60674
D	525	HIS	-	expression tag	UNP O60674
D	526	HIS	-	expression tag	UNP O60674
E	30	GLY	-	expression tag	UNP O60674
E	517	LEU	-	expression tag	UNP O60674
E	518	GLU	-	expression tag	UNP O60674
E	519	HIS	-	expression tag	UNP O60674
E	520	HIS	-	expression tag	UNP O60674
E	521	HIS	-	expression tag	UNP O60674
E	522	HIS	-	expression tag	UNP O60674
E	523	HIS	-	expression tag	UNP O60674
E	524	HIS	-	expression tag	UNP O60674
E	525	HIS	-	expression tag	UNP O60674
E	526	HIS	-	expression tag	UNP O60674

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Chain	Residue	Modelled	Actual	Comment	Reference
F	30	GLY	-	expression tag	UNP O60674
F	517	LEU	-	expression tag	UNP O60674
F	518	GLU	-	expression tag	UNP O60674
F	519	HIS	-	expression tag	UNP O60674
F	520	HIS	-	expression tag	UNP O60674
F	521	HIS	-	expression tag	UNP O60674
F	522	HIS	-	expression tag	UNP O60674
F	523	HIS	-	expression tag	UNP O60674
F	524	HIS	-	expression tag	UNP O60674
F	525	HIS	-	expression tag	UNP O60674
F	526	HIS	-	expression tag	UNP O60674
G	30	GLY	-	expression tag	UNP O60674
G	517	LEU	-	expression tag	UNP O60674
G	518	GLU	-	expression tag	UNP O60674
G	519	HIS	-	expression tag	UNP O60674
G	520	HIS	-	expression tag	UNP O60674
G	521	HIS	-	expression tag	UNP O60674
G	522	HIS	-	expression tag	UNP O60674
G	523	HIS	-	expression tag	UNP O60674
G	524	HIS	-	expression tag	UNP O60674
G	525	HIS	-	expression tag	UNP O60674
G	526	HIS	-	expression tag	UNP O60674
H	30	GLY	-	expression tag	UNP O60674
H	517	LEU	-	expression tag	UNP O60674
H	518	GLU	-	expression tag	UNP O60674
H	519	HIS	-	expression tag	UNP O60674
H	520	HIS	-	expression tag	UNP O60674
H	521	HIS	-	expression tag	UNP O60674
H	522	HIS	-	expression tag	UNP O60674
H	523	HIS	-	expression tag	UNP O60674
H	524	HIS	-	expression tag	UNP O60674
H	525	HIS	-	expression tag	UNP O60674
H	526	HIS	-	expression tag	UNP O60674

- Molecule 2 is water.

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

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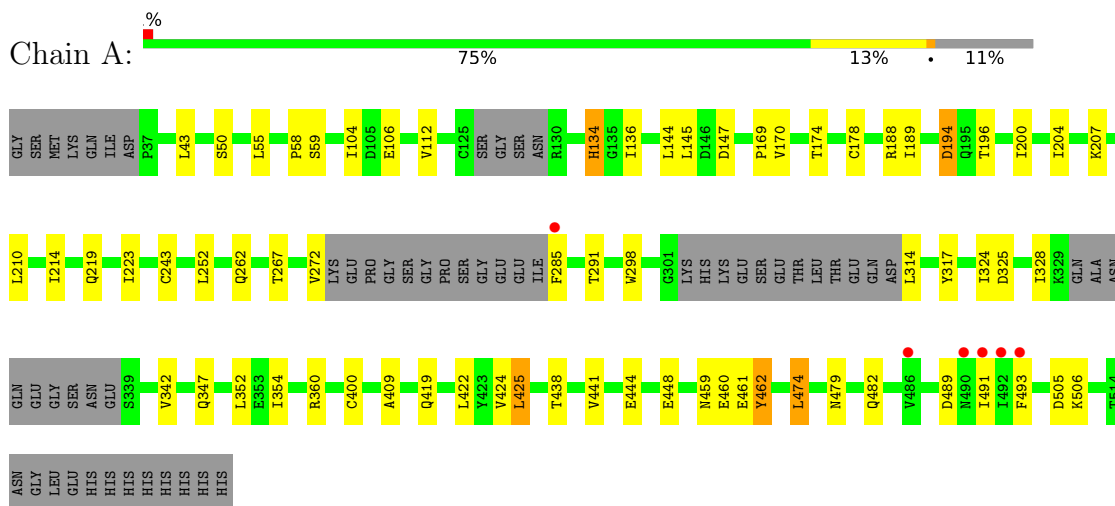
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
2	E	1	Total O 1 1	0	0
2	F	1	Total O 1 1	0	0

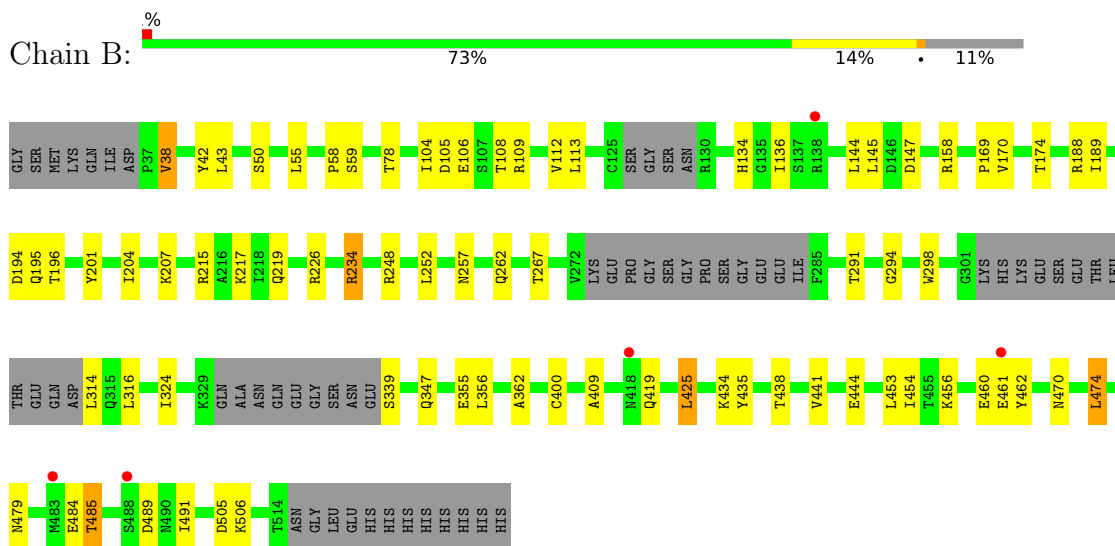
### 3 Residue-property plots [i](#)

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: Tyrosine-protein kinase JAK2



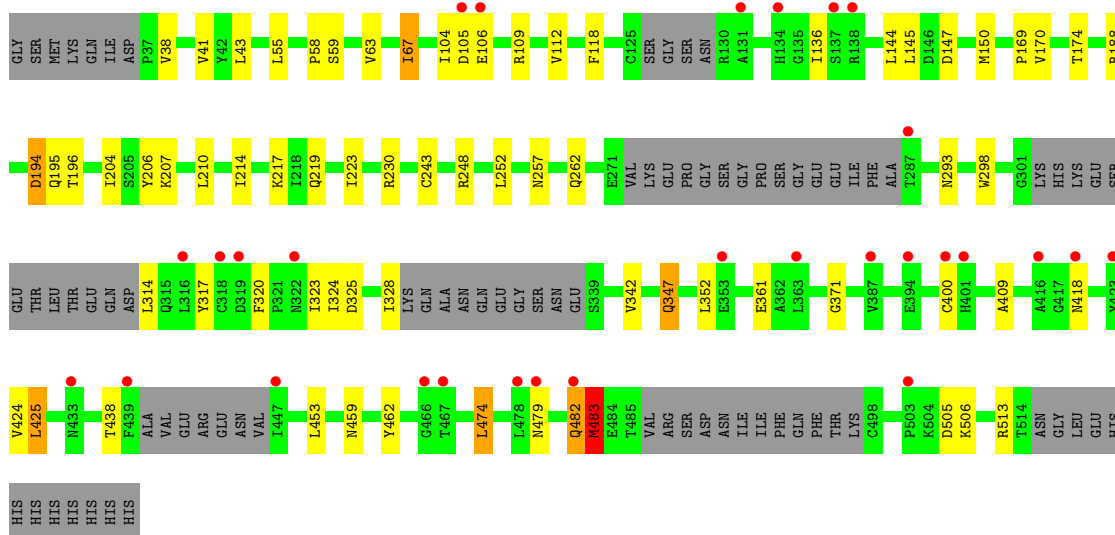
- Molecule 1: Tyrosine-protein kinase JAK2



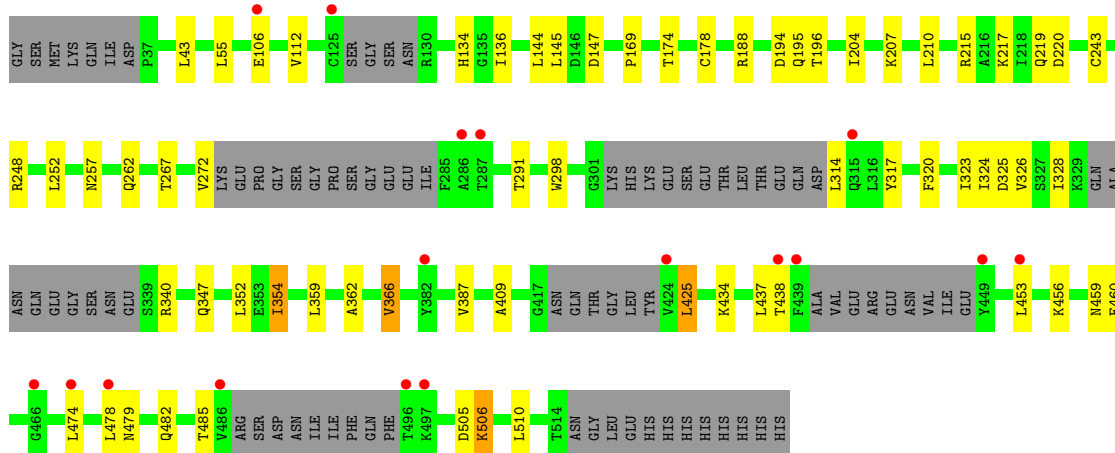
- Molecule 1: Tyrosine-protein kinase JAK2



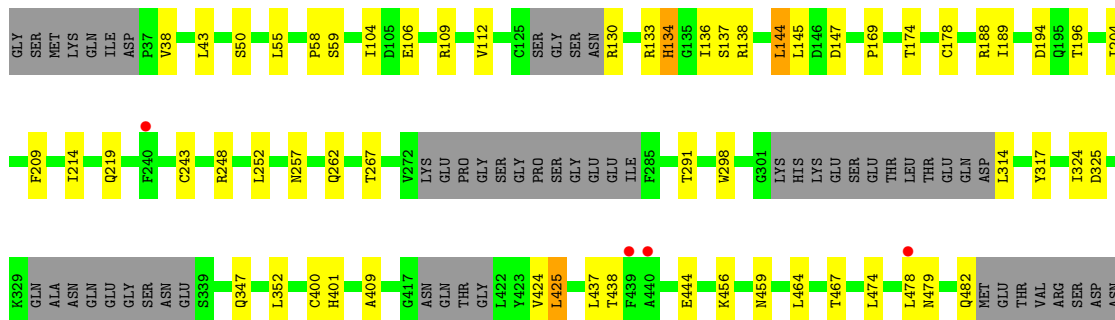
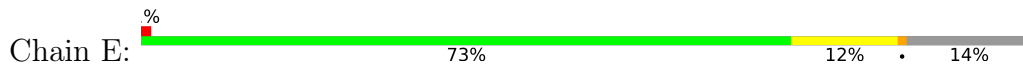




• Molecule 1: Tyrosine-protein kinase JAK2

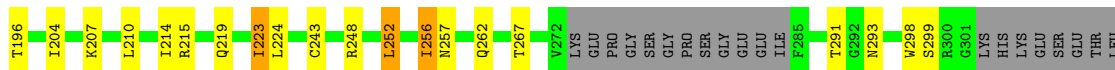
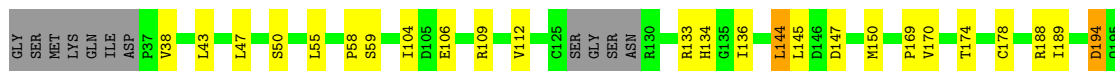
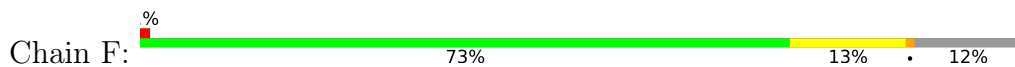


• Molecule 1: Tyrosine-protein kinase JAK2

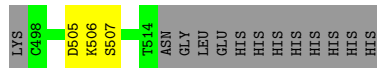
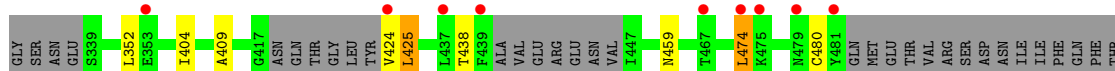
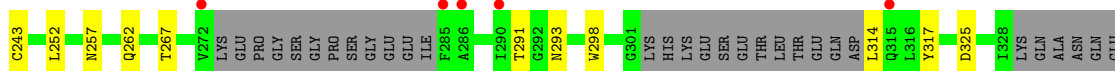
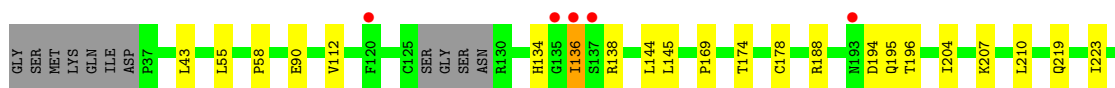
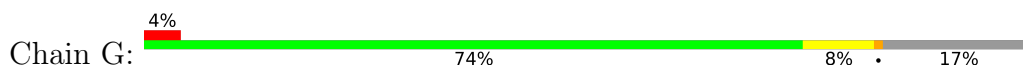




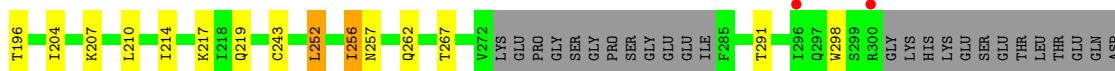
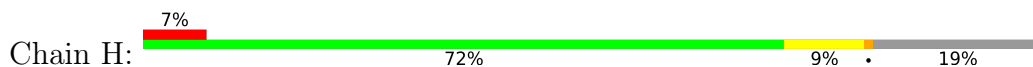
- Molecule 1: Tyrosine-protein kinase JAK2

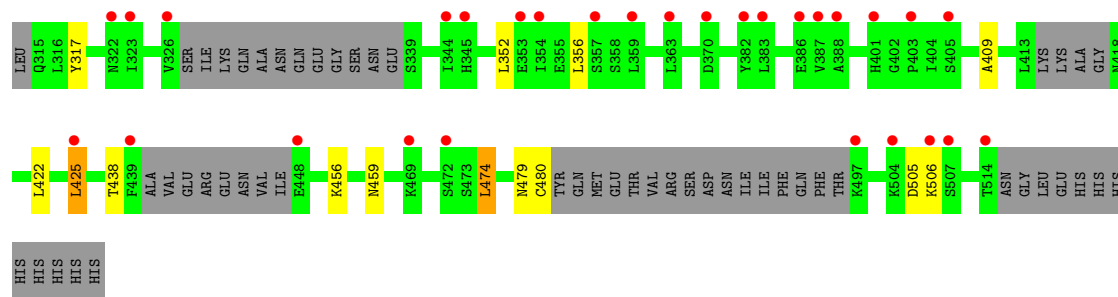


- Molecule 1: Tyrosine-protein kinase JAK2



- Molecule 1: Tyrosine-protein kinase JAK2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.19Å 188.74Å 118.58Å 90.00° 113.87° 90.00°	Depositor
Resolution (Å)	42.95 – 3.04 47.19 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (42.95-3.04) 95.3 (47.19-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.257 , 0.276 0.259 , 0.276	Depositor DCC
$R_{free}$ test set	4470 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.8	Xtrriage
Anisotropy	0.315	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.116 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	27929	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.10 % 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 7.1980e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.39	0/3713	0.59	0/5015
1	B	0.39	0/3713	0.61	0/5015
1	C	0.39	0/3517	0.59	0/4748
1	D	0.38	0/3506	0.58	0/4730
1	E	0.39	0/3603	0.58	0/4863
1	F	0.39	0/3674	0.59	0/4960
1	G	0.39	0/3458	0.59	0/4667
1	H	0.38	0/3418	0.58	0/4613
All	All	0.39	0/28602	0.59	0/38611

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3624	0	3603	24	0
1	B	3624	0	3603	28	0
1	C	3433	0	3406	29	0
1	D	3423	0	3409	23	0
1	E	3516	0	3496	21	0
1	F	3586	0	3565	28	0
1	G	3375	0	3354	12	0
1	H	3336	0	3311	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
All	All	27929	0	27747	165	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 3.

The worst 5 of 165 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:41:VAL:HG21	1:C:67:ILE:HD11	1.42	1.01
1:H:252:LEU:O	1:H:256:ILE:HD13	1.75	0.87
1:F:252:LEU:O	1:F:256:ILE:HD13	1.76	0.86
1:B:147:ASP:HB3	1:B:248:ARG:HH12	1.42	0.84
1:F:207:LYS:HA	1:F:210:LEU:HD12	1.61	0.83

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	431/497 (87%)	399 (93%)	23 (5%)	9 (2%)	7	30
1	B	431/497 (87%)	400 (93%)	20 (5%)	11 (3%)	5	24
1	C	404/497 (81%)	375 (93%)	21 (5%)	8 (2%)	7	31
1	D	401/497 (81%)	378 (94%)	20 (5%)	3 (1%)	22	57
1	E	413/497 (83%)	388 (94%)	18 (4%)	7 (2%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	424/497 (85%)	393 (93%)	22 (5%)	9 (2%)	7	30
1	G	395/497 (80%)	372 (94%)	19 (5%)	4 (1%)	15	49
1	H	387/497 (78%)	362 (94%)	21 (5%)	4 (1%)	15	49
All	All	3286/3976 (83%)	3067 (93%)	164 (5%)	55 (2%)	9	35

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ILE
1	B	106	GLU
1	B	136	ILE
1	C	106	GLU
1	C	136	ILE

### 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	398/446 (89%)	371 (93%)	27 (7%)	16	46
1	B	398/446 (89%)	368 (92%)	30 (8%)	13	41
1	C	377/446 (84%)	349 (93%)	28 (7%)	13	42
1	D	376/446 (84%)	345 (92%)	31 (8%)	11	37
1	E	385/446 (86%)	358 (93%)	27 (7%)	15	44
1	F	393/446 (88%)	363 (92%)	30 (8%)	13	41
1	G	370/446 (83%)	347 (94%)	23 (6%)	18	49
1	H	366/446 (82%)	341 (93%)	25 (7%)	16	46
All	All	3063/3568 (86%)	2842 (93%)	221 (7%)	14	43

5 of 221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	506	LYS

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Mol	Chain	Res	Type
1	F	112	VAL
1	H	505	ASP
1	H	144	LEU
1	E	137	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	433	ASN
1	F	322	ASN
1	F	195	GLN
1	F	482	GLN
1	B	419	GLN

### 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](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	441/497 (88%)	0.09	6 (1%) 75 49	33, 64, 120, 158	0
1	B	441/497 (88%)	0.05	5 (1%) 80 56	32, 64, 116, 134	0
1	C	418/497 (84%)	0.43	29 (6%) 16 5	52, 104, 152, 167	0
1	D	417/497 (83%)	0.26	17 (4%) 37 15	44, 86, 149, 165	0
1	E	427/497 (85%)	0.12	6 (1%) 75 49	40, 77, 138, 183	0
1	F	436/497 (87%)	0.14	7 (1%) 72 44	34, 73, 127, 167	0
1	G	411/497 (82%)	0.34	19 (4%) 32 12	48, 99, 156, 181	0
1	H	405/497 (81%)	0.56	35 (8%) 10 3	56, 114, 160, 176	0
All	All	3396/3976 (85%)	0.24	124 (3%) 41 17	32, 82, 149, 183	0

The worst 5 of 124 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	496	THR	5.4
1	H	363	LEU	5.0
1	E	493	PHE	4.9
1	C	482	GLN	4.6
1	C	416	ALA	4.6

### 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

There are no ligands in this entry.

## 6.5 Other polymers

There are no such residues in this entry.