Full wwPDB X-ray Structure Validation 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 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:

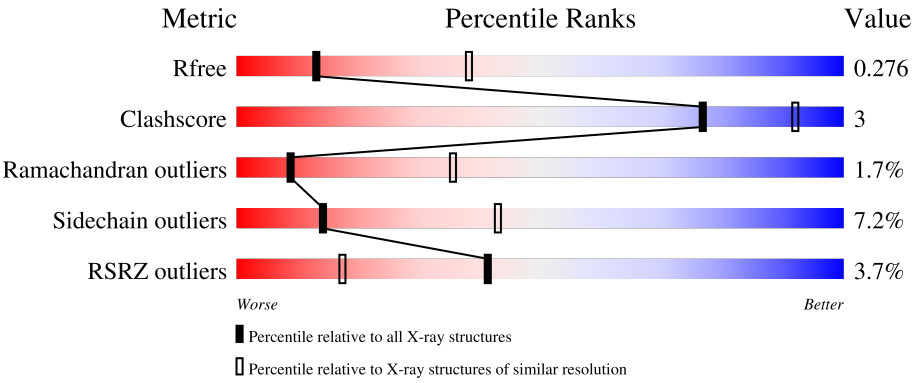
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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.



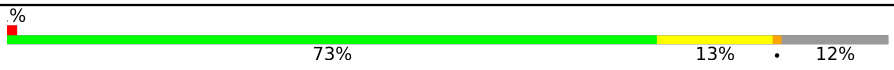
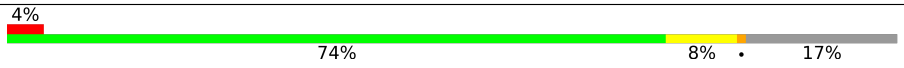
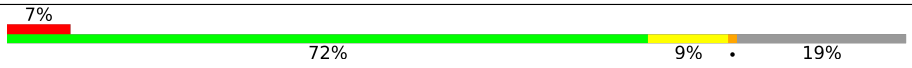
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

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 >=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	497	% 75% 13% • 11%
1	B	497	% 73% 14% • 11%
1	C	497	6% 70% 13% • 16%
1	D	497	3% 71% 12% • 16%
1	E	497	% 73% 12% • 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	497	
1	G	497	
1	H	497	

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
1	A	441	Total	C	N	O	S	0	0	0
			3624	2334	622	646	22			
1	B	441	Total	C	N	O	S	0	0	0
			3624	2334	622	646	22			
1	C	418	Total	C	N	O	S	0	0	0
			3433	2211	588	612	22			
1	D	417	Total	C	N	O	S	0	0	0
			3423	2208	587	606	22			
1	E	427	Total	C	N	O	S	0	0	0
			3516	2271	602	622	21			
1	F	436	Total	C	N	O	S	0	0	0
			3586	2311	616	637	22			
1	G	411	Total	C	N	O	S	0	0	0
			3375	2179	578	597	21			
1	H	405	Total	C	N	O	S	0	0	0
			3336	2154	573	588	21			

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

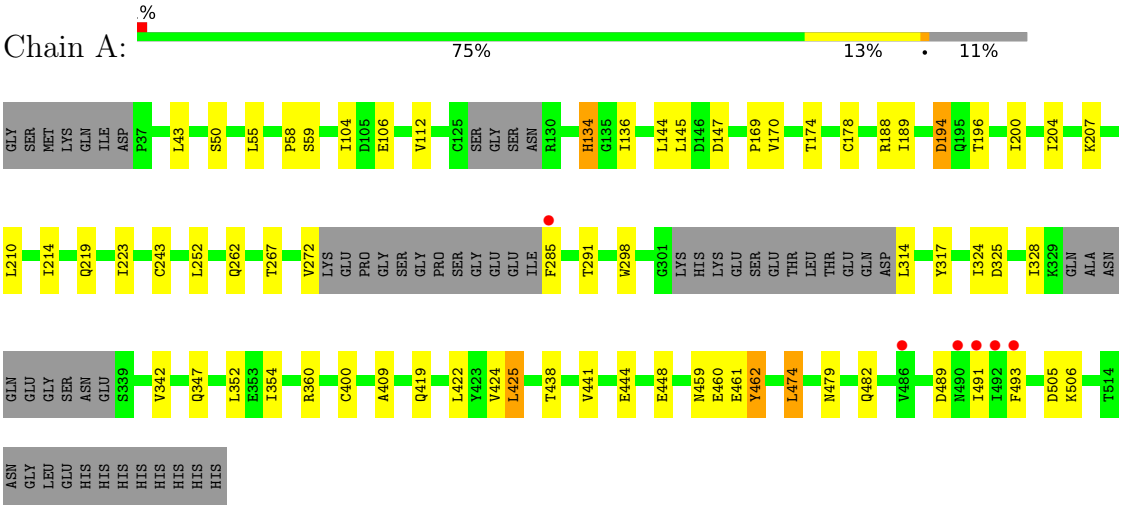
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O 1 1	0	0
2	F	1	Total O 1 1	0	0

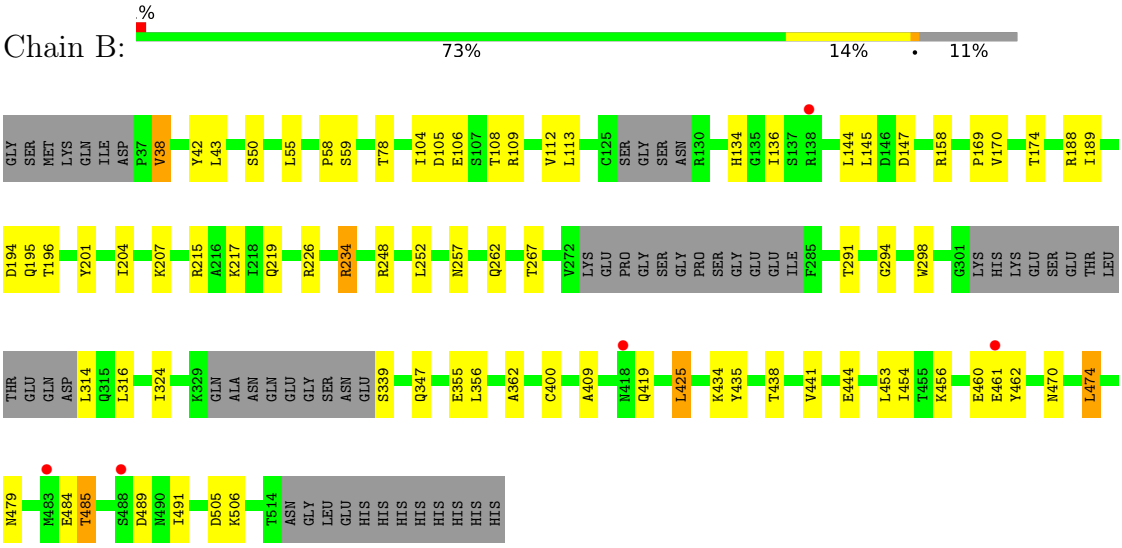
3 Residue-property plots (i)

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.

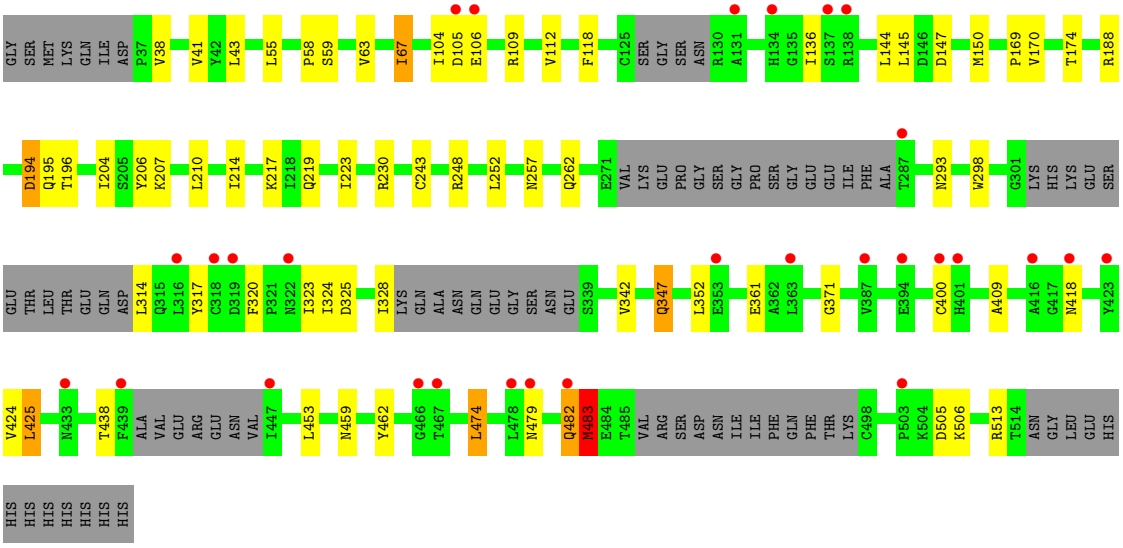
• Molecule 1: Tyrosine-protein kinase JAK2



• Molecule 1: Tyrosine-protein kinase JAK2

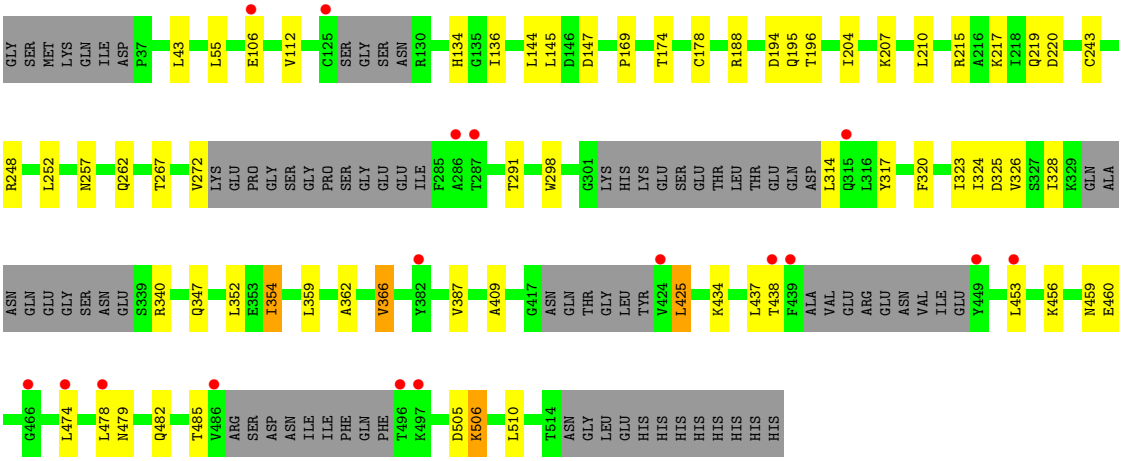


• Molecule 1: Tyrosine-protein kinase JAK2



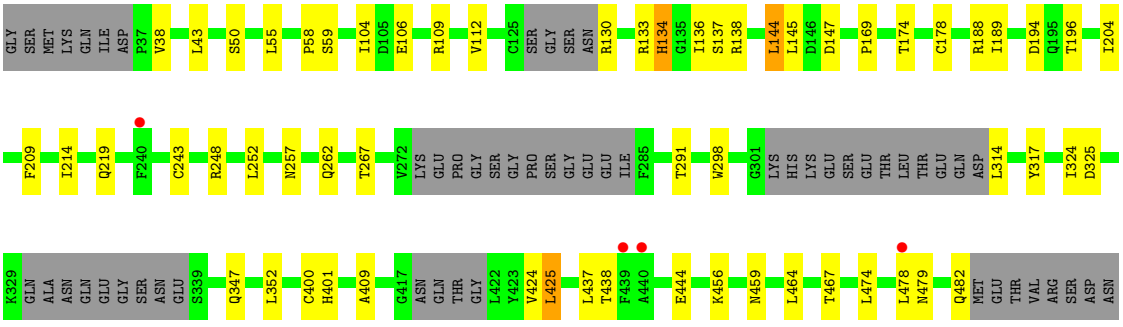
• Molecule 1: Tyrosine-protein kinase JAK2

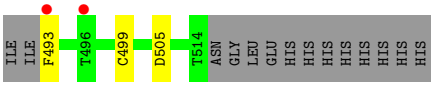
Chain D:



• Molecule 1: Tyrosine-protein kinase JAK2

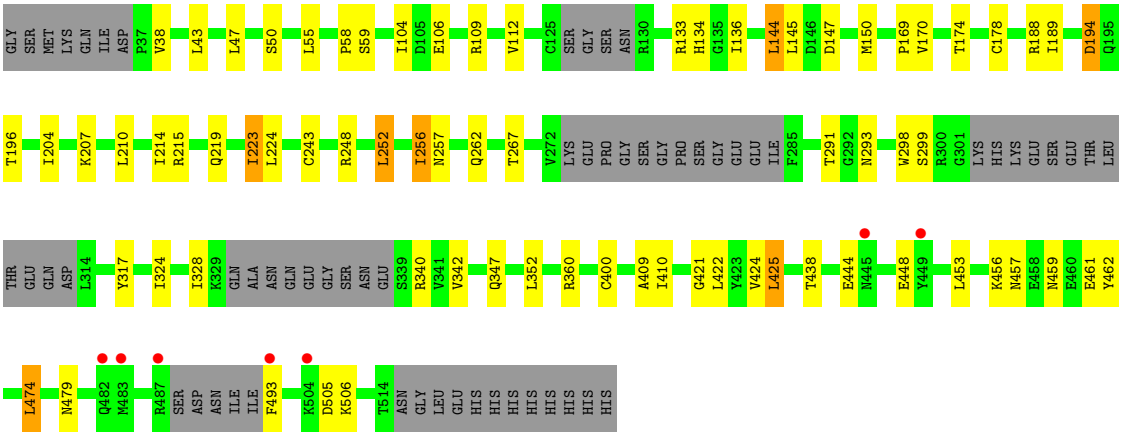
Chain E:





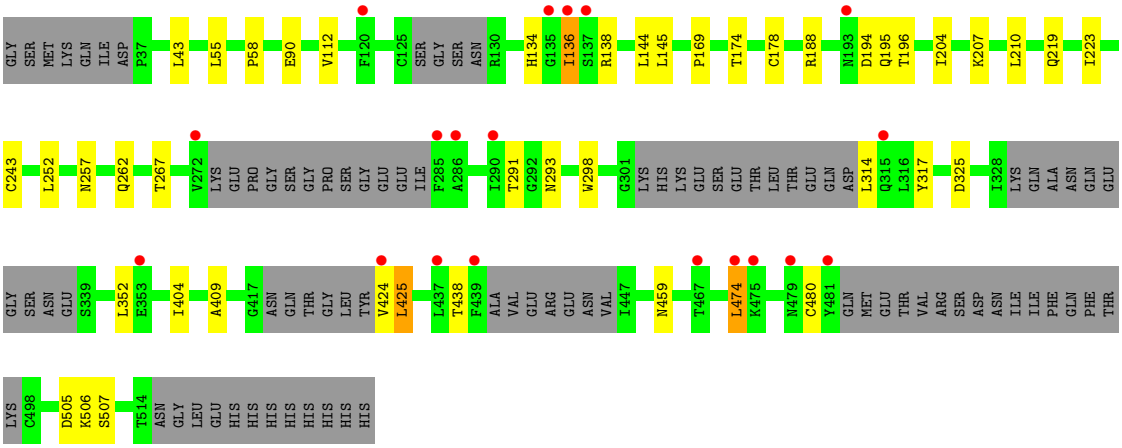
• Molecule 1: Tyrosine-protein kinase JAK2

Chain F:



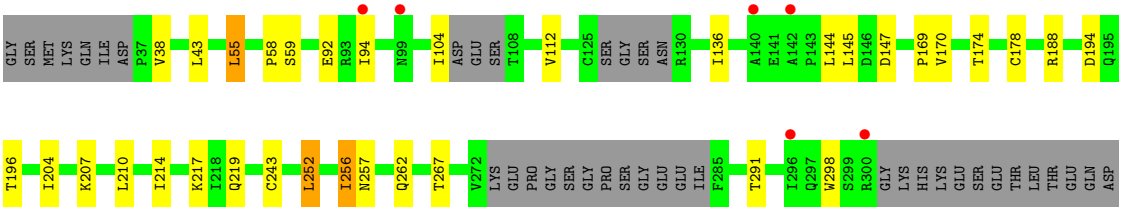
• Molecule 1: Tyrosine-protein kinase JAK2

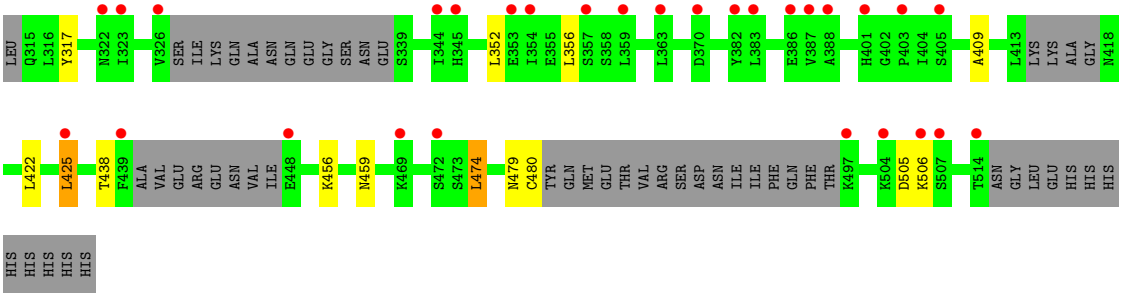
Chain G:



• Molecule 1: Tyrosine-protein kinase JAK2

Chain H:




LEU Q315 L316 Y317 N322 I323 V326 SER ILE LYS GLN ALA ASN GLN GLU GLY SER ASN GLU S339 I344 H345 L352 E353 I354 E355 L356 S357 S358 L359 L363 D370 Y382 L383 E386 V387 A388 H401 G402 P403 I404 S405 A409 L413 LYS LYS ALA GLY N418
L422 L425 T438 P439 ALA VAL GLU ARG GLU ASN VAL ILE E448 K456 N459 K469 S472 S473 L474 N479 C480 TYR GLN MET GLU THR VAL ARG SER ASP ASN ILE ILE PHE GLN PHE THR K497 K504 D505 K506 S507 T514 ASN GLY LEU GLU HIS HIS HIS
HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	2.01 (at 3.01Å)	Xtriage
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^2)	67.8	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.116 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	27929	wwPDB-VP
Average B, all atoms (Å^2)	88.0	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 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.*

[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

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

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

Continued on next page...

Continued from previous page...

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.

All (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
1:A:207:LYS:HA	1:A:210:LEU:HD12	1.62	0.81
1:G:207:LYS:HA	1:G:210:LEU:HD12	1.66	0.76
1:C:248:ARG:HH12	1:D:195:GLN:HG2	1.51	0.74
1:H:207:LYS:HA	1:H:210:LEU:HD12	1.68	0.74
1:F:147:ASP:HB3	1:F:248:ARG:HH22	1.53	0.72
1:C:41:VAL:HG21	1:C:67:ILE:CD1	2.19	0.71
1:B:267:THR:HG22	1:B:291:THR:HG22	1.72	0.71
1:D:267:THR:HG22	1:D:291:THR:HG22	1.72	0.70
1:A:267:THR:HG22	1:A:291:THR:HG22	1.74	0.70
1:F:267:THR:HG22	1:F:291:THR:HG22	1.73	0.70
1:C:147:ASP:HB3	1:C:248:ARG:HH22	1.58	0.69
1:E:267:THR:HG22	1:E:291:THR:HG22	1.73	0.69
1:F:147:ASP:HB3	1:F:248:ARG:NH2	2.08	0.68
1:F:133:ARG:HG3	1:F:144:LEU:HA	1.77	0.67
1:G:267:THR:HG22	1:G:291:THR:HG22	1.77	0.66
1:B:147:ASP:HB3	1:B:248:ARG:NH1	2.11	0.65
1:D:328:ILE:HD11	1:D:366:VAL:HG21	1.78	0.65
1:D:326:VAL:HG11	1:D:366:VAL:HG12	1.80	0.64
1:B:147:ASP:CB	1:B:248:ARG:HH12	2.09	0.63
1:C:147:ASP:HB3	1:C:248:ARG:NH2	2.13	0.63
1:E:400:CYS:HA	1:E:425:LEU:HB3	1.81	0.62
1:D:425:LEU:HD21	1:D:478:LEU:HD11	1.83	0.60
1:G:195:GLN:HE22	1:H:147:ASP:HB2	1.65	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:GLN:HE22	1:D:147:ASP:HB2	1.66	0.60
1:D:362:ALA:O	1:D:366:VAL:HG22	2.02	0.60
1:E:178:CYS:SG	1:E:214:ILE:HD13	2.41	0.60
1:E:204:ILE:HD13	1:F:47:LEU:HB3	1.83	0.60
1:H:409:ALA:HB1	1:H:438:THR:HG21	1.83	0.59
1:E:50:SER:HB2	1:F:189:ILE:HG12	1.85	0.59
1:G:425:LEU:HD11	1:G:474:LEU:HD22	1.85	0.58
1:B:147:ASP:CB	1:B:248:ARG:NH1	2.66	0.57
1:B:441:VAL:HG11	1:B:491:ILE:HG21	1.86	0.57
1:E:133:ARG:HG3	1:E:144:LEU:HA	1.87	0.56
1:B:434:LYS:HD3	1:B:453:LEU:HD11	1.88	0.56
1:D:409:ALA:HB1	1:D:438:THR:HG21	1.87	0.56
1:F:409:ALA:HB1	1:F:438:THR:HG21	1.89	0.55
1:D:207:LYS:HA	1:D:210:LEU:HD12	1.89	0.54
1:E:189:ILE:HG12	1:F:50:SER:HB2	1.89	0.54
1:F:178:CYS:HB3	1:F:210:LEU:HD23	1.91	0.53
1:A:272:VAL:HG21	1:A:354:ILE:HG23	1.89	0.53
1:A:194:ASP:O	1:B:248:ARG:NH2	2.35	0.53
1:A:50:SER:HB3	1:B:189:ILE:HG12	1.91	0.52
1:F:207:LYS:HB3	1:F:215:ARG:HG3	1.91	0.52
1:B:409:ALA:HB1	1:B:438:THR:HG21	1.91	0.52
1:E:409:ALA:HB1	1:E:438:THR:HG21	1.90	0.52
1:H:169:PRO:HG2	1:H:174:THR:HG21	1.92	0.52
1:D:169:PRO:HG2	1:D:174:THR:HG21	1.92	0.51
1:C:206:TYR:HE1	1:C:230:ARG:HG2	1.75	0.51
1:C:409:ALA:HB1	1:C:438:THR:HG21	1.92	0.51
1:A:419:GLN:HB3	1:A:422:LEU:HD12	1.92	0.51
1:D:366:VAL:HG23	1:D:387:VAL:HG11	1.92	0.51
1:C:169:PRO:HG2	1:C:174:THR:HG21	1.93	0.51
1:A:147:ASP:HB2	1:B:195:GLN:HE22	1.75	0.51
1:G:169:PRO:HG2	1:G:174:THR:HG21	1.92	0.51
1:B:356:LEU:HD13	1:B:362:ALA:HA	1.92	0.50
1:C:425:LEU:HD11	1:C:474:LEU:HD22	1.92	0.50
1:B:169:PRO:HG2	1:B:174:THR:HG21	1.93	0.50
1:E:38:VAL:HG12	1:E:109:ARG:HG2	1.94	0.50
1:A:178:CYS:HB3	1:A:210:LEU:HD23	1.92	0.50
1:G:409:ALA:HB1	1:G:438:THR:HG21	1.93	0.50
1:C:43:LEU:HD11	1:C:55:LEU:HD13	1.94	0.50
1:B:435:TYR:HE1	1:B:456:LYS:HG3	1.77	0.50
1:G:178:CYS:HB3	1:G:210:LEU:HD23	1.94	0.50
1:D:43:LEU:HD11	1:D:55:LEU:HD13	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:425:LEU:HD21	1:E:478:LEU:HD21	1.93	0.49
1:A:169:PRO:HG2	1:A:174:THR:HG21	1.93	0.49
1:B:38:VAL:HG23	1:B:109:ARG:HG2	1.94	0.49
1:F:43:LEU:HD11	1:F:55:LEU:HD13	1.94	0.49
1:F:169:PRO:HG2	1:F:174:THR:HG21	1.94	0.49
1:G:43:LEU:HD11	1:G:55:LEU:HD13	1.94	0.49
1:H:178:CYS:HB3	1:H:210:LEU:HD23	1.94	0.49
1:C:293:ASN:HA	1:C:513:ARG:HD2	1.95	0.49
1:A:409:ALA:HB1	1:A:438:THR:HG21	1.93	0.49
1:E:169:PRO:HG2	1:E:174:THR:HG21	1.93	0.49
1:H:43:LEU:HD11	1:H:55:LEU:HD23	1.93	0.49
1:B:147:ASP:CG	1:B:248:ARG:NH1	2.67	0.48
1:A:400:CYS:HB2	1:A:425:LEU:HD13	1.96	0.48
1:B:170:VAL:HG12	1:B:217:LYS:HD2	1.96	0.48
1:C:38:VAL:HG12	1:C:109:ARG:HG2	1.95	0.48
1:D:506:LYS:HA	1:D:510:LEU:HD12	1.96	0.48
1:A:43:LEU:HD11	1:A:55:LEU:HD13	1.96	0.48
1:F:400:CYS:HB2	1:F:425:LEU:HD13	1.95	0.48
1:F:457:ASN:HB2	1:F:461:GLU:H	1.79	0.47
1:E:43:LEU:HD11	1:E:55:LEU:HD13	1.95	0.47
1:D:317:TYR:CZ	1:D:352:LEU:HB2	2.50	0.47
1:B:43:LEU:HD11	1:B:55:LEU:HD13	1.97	0.47
1:B:400:CYS:HB2	1:B:425:LEU:HD13	1.97	0.47
1:F:317:TYR:CZ	1:F:352:LEU:HB2	2.49	0.47
1:B:42:TYR:HB3	1:B:113:LEU:HD23	1.97	0.47
1:C:207:LYS:HA	1:C:210:LEU:HD12	1.97	0.47
1:E:317:TYR:CZ	1:E:352:LEU:HB2	2.50	0.47
1:H:267:THR:HG22	1:H:291:THR:HG22	1.95	0.47
1:B:207:LYS:HZ1	1:B:226:ARG:HH11	1.62	0.47
1:B:461:GLU:HG3	1:B:470:ASN:HB3	1.97	0.47
1:C:400:CYS:HB2	1:C:425:LEU:HD13	1.96	0.47
1:C:482:GLN:O	1:C:483:MET:HB2	2.15	0.47
1:H:425:LEU:HD11	1:H:474:LEU:HD22	1.97	0.47
1:A:441:VAL:HG21	1:A:491:ILE:HG12	1.96	0.46
1:C:324:ILE:HD11	1:C:347:GLN:HA	1.98	0.46
1:B:324:ILE:HD11	1:B:347:GLN:HA	1.97	0.46
1:D:324:ILE:HD11	1:D:347:GLN:HA	1.97	0.46
1:E:147:ASP:HB3	1:E:248:ARG:NH2	2.29	0.46
1:F:324:ILE:HD11	1:F:347:GLN:HA	1.96	0.46
1:G:317:TYR:CZ	1:G:352:LEU:HB2	2.50	0.46
1:A:317:TYR:CZ	1:A:352:LEU:HB2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HD11	1:A:347:GLN:HA	1.97	0.46
1:C:118:PHE:CZ	1:C:371:GLY:HA3	2.51	0.46
1:D:320:PHE:HA	1:D:323:ILE:HD12	1.98	0.46
1:E:324:ILE:HD11	1:E:347:GLN:HA	1.97	0.45
1:B:425:LEU:HD11	1:B:474:LEU:HD22	1.99	0.45
1:A:189:ILE:HG12	1:B:50:SER:HB3	1.97	0.45
1:C:317:TYR:CZ	1:C:352:LEU:HB2	2.52	0.45
1:F:38:VAL:HG12	1:F:109:ARG:HG2	1.98	0.45
1:A:425:LEU:HD11	1:A:474:LEU:HD22	1.98	0.45
1:H:92:GLU:HB3	1:H:94:ILE:HD12	1.98	0.45
1:B:201:TYR:CE2	1:B:234:ARG:HD3	2.52	0.44
1:E:424:VAL:HB	1:E:438:THR:HG23	1.99	0.44
1:C:63:VAL:O	1:C:67:ILE:HG22	2.18	0.44
1:F:425:LEU:HD11	1:F:474:LEU:HD22	2.00	0.44
1:A:461:GLU:O	1:A:462:TYR:HB2	2.18	0.43
1:B:435:TYR:HB2	1:B:454:ILE:HB	2.00	0.43
1:A:272:VAL:CG2	1:A:354:ILE:HG23	2.49	0.43
1:D:340:ARG:HD3	1:D:359:LEU:HB3	2.01	0.43
1:H:317:TYR:CZ	1:H:352:LEU:HB2	2.54	0.43
1:D:178:CYS:HB3	1:D:210:LEU:HD23	2.01	0.43
1:F:424:VAL:HB	1:F:438:THR:HG23	2.01	0.43
1:G:134:HIS:HB2	1:G:507:SER:O	2.19	0.43
1:G:424:VAL:HB	1:G:438:THR:HG23	2.01	0.42
1:F:400:CYS:HA	1:F:425:LEU:HB3	2.01	0.42
1:C:248:ARG:NH1	1:D:195:GLN:HG2	2.29	0.42
1:F:170:VAL:HG13	1:F:214:ILE:HD13	2.01	0.42
1:C:170:VAL:HG13	1:C:214:ILE:HD13	2.02	0.42
1:D:267:THR:HG22	1:D:291:THR:CG2	2.46	0.42
1:C:194:ASP:OD2	1:D:248:ARG:HG2	2.20	0.42
1:E:204:ILE:HD12	1:E:209:PHE:CZ	2.55	0.42
1:H:59:SER:HA	1:H:104:ILE:HG22	2.02	0.42
1:E:248:ARG:HD2	1:F:194:ASP:HB2	2.02	0.42
1:C:170:VAL:HG12	1:C:217:LYS:HD2	2.02	0.42
1:A:59:SER:HA	1:A:104:ILE:HG22	2.03	0.41
1:D:434:LYS:HE3	1:D:453:LEU:HD13	2.01	0.41
1:F:328:ILE:HG12	1:F:342:VAL:HG22	2.03	0.41
1:H:170:VAL:HG13	1:H:214:ILE:HD13	2.01	0.41
1:C:320:PHE:HA	1:C:323:ILE:HD12	2.02	0.41
1:A:170:VAL:HG13	1:A:214:ILE:HD13	2.02	0.41
1:F:59:SER:HA	1:F:104:ILE:HG22	2.02	0.41
1:F:223:ILE:HD13	1:F:224:LEU:HG	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:136:ILE:C	1:G:138:ARG:H	2.24	0.41
1:E:401:HIS:HE1	1:E:499:CYS:O	2.03	0.41
1:C:59:SER:HA	1:C:104:ILE:HG22	2.03	0.40
1:C:424:VAL:HB	1:C:438:THR:HG23	2.02	0.40
1:C:328:ILE:HG12	1:C:342:VAL:HG22	2.02	0.40
1:E:267:THR:HG22	1:E:291:THR:CG2	2.48	0.40
1:A:328:ILE:HG12	1:A:342:VAL:HG22	2.02	0.40
1:B:59:SER:HA	1:B:104:ILE:HG22	2.03	0.40
1:D:272:VAL:HG21	1:D:354:ILE:HG12	2.04	0.40
1:F:267:THR:HG22	1:F:291:THR:CG2	2.48	0.40
1:A:400:CYS:HA	1:A:425:LEU:HB3	2.04	0.40
1:A:424:VAL:HB	1:A:438:THR:HG23	2.04	0.40
1:C:400:CYS:HA	1:C:425:LEU:HB3	2.03	0.40
1:E:59:SER:HA	1:E:104:ILE:HG22	2.03	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	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
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

All (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
1	C	483	MET
1	D	136	ILE
1	E	106	GLU
1	E	136	ILE
1	F	106	GLU
1	F	136	ILE
1	F	462	TYR
1	G	136	ILE
1	H	136	ILE
1	A	462	TYR
1	B	134	HIS
1	C	347	GLN
1	A	194	ASP
1	B	444	GLU
1	B	462	TYR
1	B	489	ASP
1	C	462	TYR
1	E	134	HIS
1	F	134	HIS
1	A	106	GLU
1	A	134	HIS
1	A	196	THR
1	A	444	GLU
1	A	489	ASP
1	B	194	ASP
1	B	196	THR
1	B	294	GLY
1	B	485	THR
1	C	196	THR
1	D	196	THR
1	E	194	ASP
1	E	196	THR
1	E	444	GLU
1	F	194	ASP
1	F	196	THR
1	F	421	GLY
1	F	444	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	196	THR
1	H	196	THR
1	D	194	ASP
1	G	194	ASP
1	H	194	ASP
1	C	194	ASP
1	B	58	PRO
1	C	58	PRO
1	A	58	PRO
1	E	58	PRO
1	F	58	PRO
1	H	58	PRO
1	G	58	PRO

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

All (221) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	134	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	LEU
1	A	145	LEU
1	A	188	ARG
1	A	200	ILE
1	A	204	ILE
1	A	219	GLN
1	A	223	ILE
1	A	243	CYS
1	A	252	LEU
1	A	262	GLN
1	A	285	PHE
1	A	298	TRP
1	A	314	LEU
1	A	325	ASP
1	A	360	ARG
1	A	425	LEU
1	A	448	GLU
1	A	459	ASN
1	A	460	GLU
1	A	474	LEU
1	A	479	ASN
1	A	482	GLN
1	A	493	PHE
1	A	505	ASP
1	A	506	LYS
1	B	38	VAL
1	B	78	THR
1	B	105	ASP
1	B	108	THR
1	B	112	VAL
1	B	144	LEU
1	B	145	LEU
1	B	158	ARG
1	B	188	ARG
1	B	204	ILE
1	B	215	ARG
1	B	219	GLN
1	B	234	ARG
1	B	252	LEU
1	B	257	ASN
1	B	262	GLN
1	B	298	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	314	LEU
1	B	316	LEU
1	B	339	SER
1	B	355	GLU
1	B	419	GLN
1	B	425	LEU
1	B	460	GLU
1	B	474	LEU
1	B	479	ASN
1	B	484	GLU
1	B	485	THR
1	B	505	ASP
1	B	506	LYS
1	C	67	ILE
1	C	105	ASP
1	C	112	VAL
1	C	144	LEU
1	C	145	LEU
1	C	150	MET
1	C	188	ARG
1	C	204	ILE
1	C	219	GLN
1	C	223	ILE
1	C	243	CYS
1	C	252	LEU
1	C	257	ASN
1	C	262	GLN
1	C	298	TRP
1	C	314	LEU
1	C	325	ASP
1	C	361	GLU
1	C	418	ASN
1	C	425	LEU
1	C	453	LEU
1	C	459	ASN
1	C	474	LEU
1	C	479	ASN
1	C	482	GLN
1	C	483	MET
1	C	505	ASP
1	C	506	LYS
1	D	106	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	112	VAL
1	D	134	HIS
1	D	144	LEU
1	D	145	LEU
1	D	188	ARG
1	D	204	ILE
1	D	215	ARG
1	D	217	LYS
1	D	219	GLN
1	D	220	ASP
1	D	243	CYS
1	D	252	LEU
1	D	257	ASN
1	D	262	GLN
1	D	298	TRP
1	D	314	LEU
1	D	325	ASP
1	D	354	ILE
1	D	366	VAL
1	D	425	LEU
1	D	437	LEU
1	D	456	LYS
1	D	459	ASN
1	D	460	GLU
1	D	474	LEU
1	D	479	ASN
1	D	482	GLN
1	D	485	THR
1	D	505	ASP
1	D	506	LYS
1	E	112	VAL
1	E	130	ARG
1	E	134	HIS
1	E	137	SER
1	E	138	ARG
1	E	144	LEU
1	E	145	LEU
1	E	188	ARG
1	E	219	GLN
1	E	243	CYS
1	E	252	LEU
1	E	257	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	262	GLN
1	E	298	TRP
1	E	314	LEU
1	E	325	ASP
1	E	425	LEU
1	E	437	LEU
1	E	456	LYS
1	E	459	ASN
1	E	464	LEU
1	E	467	THR
1	E	474	LEU
1	E	479	ASN
1	E	482	GLN
1	E	493	PHE
1	E	505	ASP
1	F	112	VAL
1	F	144	LEU
1	F	145	LEU
1	F	150	MET
1	F	188	ARG
1	F	204	ILE
1	F	219	GLN
1	F	223	ILE
1	F	243	CYS
1	F	252	LEU
1	F	256	ILE
1	F	257	ASN
1	F	262	GLN
1	F	293	ASN
1	F	298	TRP
1	F	299	SER
1	F	340	ARG
1	F	360	ARG
1	F	410	ILE
1	F	422	LEU
1	F	425	LEU
1	F	448	GLU
1	F	453	LEU
1	F	456	LYS
1	F	459	ASN
1	F	474	LEU
1	F	479	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	493	PHE
1	F	505	ASP
1	F	506	LYS
1	G	90	GLU
1	G	112	VAL
1	G	144	LEU
1	G	145	LEU
1	G	188	ARG
1	G	204	ILE
1	G	219	GLN
1	G	223	ILE
1	G	243	CYS
1	G	252	LEU
1	G	257	ASN
1	G	262	GLN
1	G	293	ASN
1	G	298	TRP
1	G	314	LEU
1	G	325	ASP
1	G	404	ILE
1	G	425	LEU
1	G	459	ASN
1	G	474	LEU
1	G	480	CYS
1	G	505	ASP
1	G	506	LYS
1	H	38	VAL
1	H	55	LEU
1	H	112	VAL
1	H	144	LEU
1	H	145	LEU
1	H	188	ARG
1	H	204	ILE
1	H	217	LYS
1	H	219	GLN
1	H	243	CYS
1	H	252	LEU
1	H	256	ILE
1	H	257	ASN
1	H	262	GLN
1	H	298	TRP
1	H	356	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	422	LEU
1	H	425	LEU
1	H	456	LYS
1	H	459	ASN
1	H	474	LEU
1	H	479	ASN
1	H	480	CYS
1	H	505	ASP
1	H	506	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	418	ASN
1	B	175	GLN
1	B	195	GLN
1	B	257	ASN
1	B	322	ASN
1	B	419	GLN
1	C	195	GLN
1	C	322	ASN
1	C	457	ASN
1	D	238	GLN
1	D	322	ASN
1	D	433	ASN
1	E	238	GLN
1	E	433	ASN
1	E	463	ASN
1	F	195	GLN
1	F	322	ASN
1	F	482	GLN
1	G	175	GLN
1	G	195	GLN
1	G	451	HIS
1	H	418	ASN

5.3.3 RNA

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

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	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

All (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
1	B	418	ASN	4.4
1	F	483	MET	4.4
1	H	323	ILE	4.2
1	C	423	TYR	4.1
1	C	138	ARG	4.0
1	C	479	ASN	4.0
1	H	140	ALA	4.0
1	G	137	SER	3.9
1	H	388	ALA	3.8
1	D	315	GLN	3.7
1	C	105	ASP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	493	PHE	3.7
1	C	106	GLU	3.7
1	H	344	ILE	3.6
1	D	106	GLU	3.6
1	C	418	ASN	3.5
1	H	506	LYS	3.5
1	F	487	ARG	3.5
1	G	467	THR	3.5
1	C	387	VAL	3.4
1	H	322	ASN	3.4
1	C	318	CYS	3.4
1	H	353	GLU	3.3
1	F	493	PHE	3.3
1	D	286	ALA	3.3
1	D	438	THR	3.2
1	G	285	PHE	3.2
1	H	448	GLU	3.2
1	H	296	ILE	3.1
1	F	449	TYR	3.1
1	A	492	ILE	3.1
1	D	486	VAL	3.1
1	G	120	PHE	3.1
1	A	490	ASN	3.1
1	C	466	GLY	3.0
1	C	433	ASN	3.0
1	H	326	VAL	3.0
1	F	504	LYS	3.0
1	C	131	ALA	3.0
1	C	467	THR	3.0
1	C	400	CYS	3.0
1	F	482	GLN	2.9
1	H	386	GLU	2.9
1	H	387	VAL	2.9
1	C	439	PHE	2.8
1	E	439	PHE	2.8
1	C	353	GLU	2.8
1	G	481	TYR	2.8
1	D	424	VAL	2.8
1	G	272	VAL	2.7
1	H	370	ASP	2.7
1	D	478	LEU	2.7
1	D	382	TYR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	478	LEU	2.7
1	D	449	TYR	2.7
1	H	142	ALA	2.7
1	H	357	SER	2.7
1	G	424	VAL	2.7
1	G	136	ILE	2.7
1	D	497	LYS	2.7
1	C	319	ASP	2.7
1	H	359	LEU	2.7
1	G	135	GLY	2.7
1	C	363	LEU	2.7
1	H	405	SER	2.6
1	G	286	ALA	2.6
1	H	514	THR	2.6
1	H	401	HIS	2.6
1	H	425	LEU	2.6
1	H	469	LYS	2.5
1	G	193	ASN	2.5
1	G	353	GLU	2.4
1	H	497	LYS	2.4
1	A	486	VAL	2.4
1	H	99	ASN	2.4
1	F	445	ASN	2.3
1	B	461	GLU	2.3
1	H	507	SER	2.2
1	D	125	CYS	2.2
1	G	474	LEU	2.2
1	H	94	ILE	2.2
1	G	315	GLN	2.2
1	C	322	ASN	2.2
1	D	287	THR	2.2
1	A	491	ILE	2.2
1	B	488	SER	2.2
1	H	354	ILE	2.2
1	C	287	THR	2.2
1	E	496	THR	2.2
1	G	479	ASN	2.2
1	C	137	SER	2.1
1	C	401	HIS	2.1
1	E	478	LEU	2.1
1	E	440	ALA	2.1
1	G	290	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	503	PRO	2.1
1	B	138	ARG	2.1
1	H	504	LYS	2.1
1	C	134	HIS	2.1
1	C	447	ILE	2.1
1	C	316	LEU	2.1
1	C	394	GLU	2.1
1	G	475	LYS	2.1
1	G	437	LEU	2.1
1	D	474	LEU	2.1
1	D	439	PHE	2.1
1	H	300	ARG	2.1
1	A	285	PHE	2.0
1	H	439	PHE	2.0
1	E	240	PHE	2.0
1	H	345	HIS	2.0
1	H	472	SER	2.0
1	H	383	LEU	2.0
1	D	466	GLY	2.0
1	H	403	PRO	2.0
1	H	382	TYR	2.0
1	G	439	PHE	2.0
1	B	483	MET	2.0
1	D	453	LEU	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.