wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 7, 2023 – 08:18 AM EDT

PDB ID	:	4GS0
Title	:	Crystal structure of SHP1 catalytic domain with JAK1 activation loop peptide
Authors	:	Alicea-Velazquez, N.L.; Jakoncic, J.; Boggon, T.J.
Deposited on	:	2012-08-27
Resolution	:	1.80 Å(reported)

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

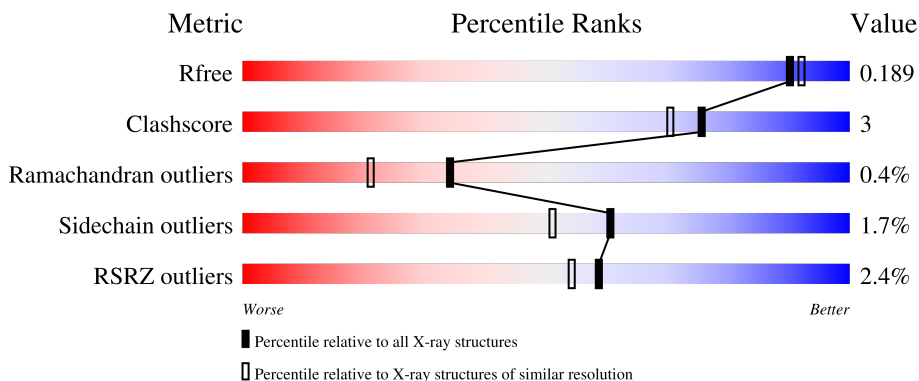|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.80 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		0.189
Clashscore		3
Ramachandran outliers		0.4%
Sidechain outliers		1.7%
RSRZ outliers		2.4%

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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	308	2% / 82% / 8% / 9%
1	B	308	2% / 75% / 8% / 16%
2	C	4	75% / 25%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4734 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 phosphatase non-receptor type 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total 2319	C 1469	N 404	O 433	S 13	0	12	0
1	B	258	Total 2095	C 1322	N 367	O 393	S 13	1	5	0

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	-	expression tag	UNP P29350
A	222	HIS	-	expression tag	UNP P29350
A	223	HIS	-	expression tag	UNP P29350
A	224	HIS	-	expression tag	UNP P29350
A	225	HIS	-	expression tag	UNP P29350
A	226	HIS	-	expression tag	UNP P29350
A	227	HIS	-	expression tag	UNP P29350
A	228	GLY	-	expression tag	UNP P29350
A	229	SER	-	expression tag	UNP P29350
A	230	LEU	-	expression tag	UNP P29350
A	231	VAL	-	expression tag	UNP P29350
A	232	PRO	-	expression tag	UNP P29350
A	233	ARG	-	expression tag	UNP P29350
A	234	SER	-	expression tag	UNP P29350
A	235	GLU	-	expression tag	UNP P29350
A	236	ASN	-	expression tag	UNP P29350
A	237	LEU	-	expression tag	UNP P29350
A	238	TYR	-	expression tag	UNP P29350
A	239	PHE	-	expression tag	UNP P29350
A	240	GLN	-	expression tag	UNP P29350
A	241	GLY	-	expression tag	UNP P29350
A	242	SER	-	expression tag	UNP P29350
B	221	MET	-	expression tag	UNP P29350
B	222	HIS	-	expression tag	UNP P29350
B	223	HIS	-	expression tag	UNP P29350

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Chain	Residue	Modelled	Actual	Comment	Reference
B	224	HIS	-	expression tag	UNP P29350
B	225	HIS	-	expression tag	UNP P29350
B	226	HIS	-	expression tag	UNP P29350
B	227	HIS	-	expression tag	UNP P29350
B	228	GLY	-	expression tag	UNP P29350
B	229	SER	-	expression tag	UNP P29350
B	230	LEU	-	expression tag	UNP P29350
B	231	VAL	-	expression tag	UNP P29350
B	232	PRO	-	expression tag	UNP P29350
B	233	ARG	-	expression tag	UNP P29350
B	234	SER	-	expression tag	UNP P29350
B	235	GLU	-	expression tag	UNP P29350
B	236	ASN	-	expression tag	UNP P29350
B	237	LEU	-	expression tag	UNP P29350
B	238	TYR	-	expression tag	UNP P29350
B	239	PHE	-	expression tag	UNP P29350
B	240	GLN	-	expression tag	UNP P29350
B	241	GLY	-	expression tag	UNP P29350
B	242	SER	-	expression tag	UNP P29350

- Molecule 2 is a protein called Tyrosine-protein kinase JAK1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	F	N	O	P			
2	C	4	33	19	2	4	7	1	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	UNK	GLU	SEE REMARK 999	UNP P23458
C	2	UNK	TYR	SEE REMARK 999	UNP P23458
C	4	UNK	THR	SEE REMARK 999	UNP P23458

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	159	159	159	0	0
3	B	128	Total	O	0	0
			128	128		

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.
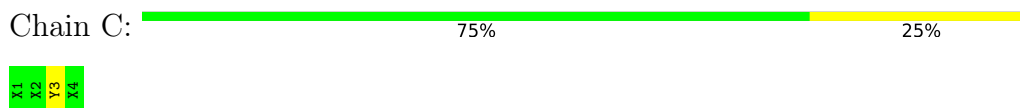
• Molecule 1: Tyrosine-protein phosphatase non-receptor type 6
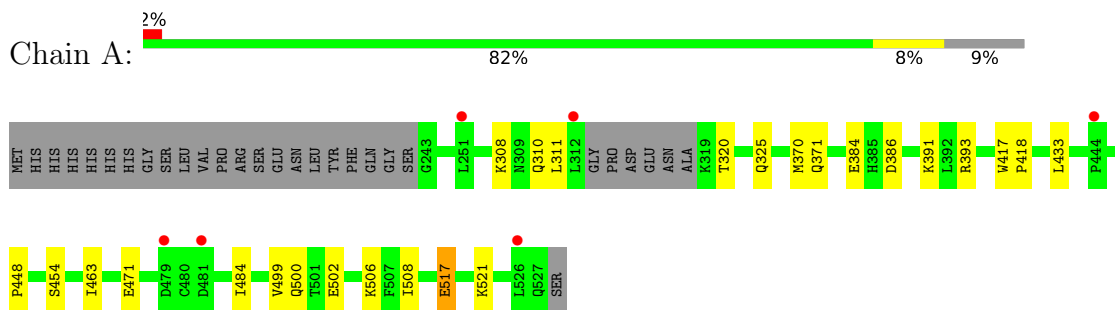
• Molecule 1: Tyrosine-protein phosphatase non-receptor type 6
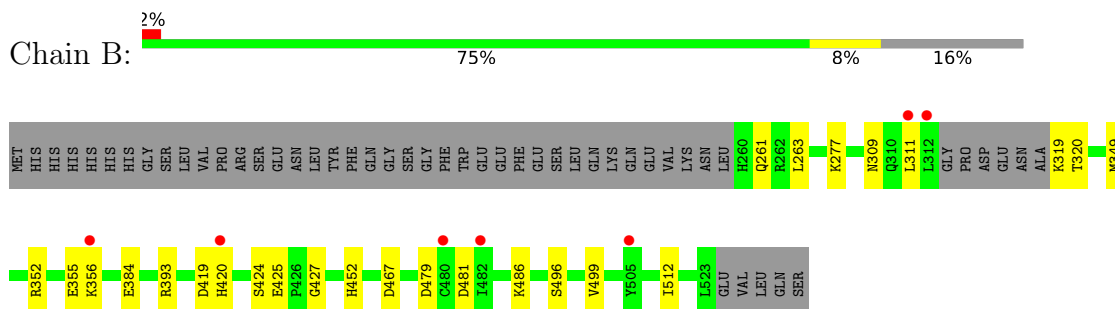
• Molecule 2: Tyrosine-protein kinase JAK1

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	43.94Å 43.94Å 258.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.02 – 1.80 43.02 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.02-1.80) 98.4 (43.02-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 1.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.162 , 0.195 0.159 , 0.189	Depositor DCC
R_{free} test set	2618 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l 0.073 for h,-h-k,-l 0.044 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	4734	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 ⓘ

5.1   Standard geometry ⓘ

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

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	0/2400	0.53	0/3246
1	B	0.36	0/2153	0.53	0/2914
All	All	0.37	0/4553	0.53	0/6160

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	2319	0	2318	14	0
1	B	2095	0	2082	13	0
2	C	33	0	13	0	0
3	A	159	0	0	4	0
3	B	128	0	0	2	0
All	All	4734	0	4413	27	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 27 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:GLU:HG2	1:A:393:ARG:HG2	1.68	0.75
1:A:310[B]:GLN:NE2	3:A:737:HOH:O	2.22	0.70
1:B:384:GLU:HG2	1:B:393:ARG:HG2	1.73	0.70
1:A:500[B]:GLN:OE1	3:A:741:HOH:O	2.15	0.63
1:A:310[A]:GLN:OE1	3:A:737:HOH:O	2.16	0.63

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	287/308 (93%)	278 (97%)	8 (3%)	1 (0%)	41	27
1	B	259/308 (84%)	252 (97%)	6 (2%)	1 (0%)	34	21
All	All	546/616 (89%)	530 (97%)	14 (3%)	2 (0%)	34	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	499	VAL
1	A	499	VAL

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	260/273 (95%)	256 (98%)	4 (2%)	65	56
1	B	232/273 (85%)	228 (98%)	4 (2%)	60	51
All	All	492/546 (90%)	484 (98%)	8 (2%)	60	54

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	496	SER
1	B	481	ASP
1	B	420	HIS
1	A	517	GLU
1	B	424	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\#|Z| > 2$
2	FTY	C	3	2	14,18,19	1.67	2 (14%)	19,27,29	1.31	5 (26%)

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	FTY	C	3	2	-	0/15/21/23	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	FTY	P-O1P	5.05	1.58	1.50
2	C	3	FTY	O-C	2.01	1.27	1.19

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3	FTY	CG-CB-CA	2.21	118.58	114.10
2	C	3	FTY	F2-C1-CZ	-2.13	107.75	110.49
2	C	3	FTY	CE1-CZ-C1	2.11	121.75	119.84
2	C	3	FTY	P-C1-CZ	2.08	115.21	108.95
2	C	3	FTY	F1-C1-CZ	-2.01	107.90	110.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	279/308 (90%)	-0.13	6 (2%) 62	57	15, 27, 62, 84	11 (3%)
1	B	258/308 (83%)	-0.04	7 (2%) 54	49	17, 32, 64, 89	10 (3%)
2	C	0/4	-	-		-	-
All	All	537/620 (86%)	-0.09	13 (2%) 59	54	15, 29, 63, 89	21 (3%)

The worst 5 of 13 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	LEU	5.6
1	B	311	LEU	3.7
1	B	480	CYS	3.4
1	B	482	ILE	2.9
1	B	420	HIS	2.7

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
2	FTY	C	3	18/19	0.90	0.12	44,50,56,57	18

6.3 Carbohydrates ⓘ

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.