



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 27, 2016 – 03:43 PM EDT

PDB ID : 5IXI
Title : Structure of human JAK1 FERM/SH2 in complex with IFNLR1/IL10RA chimera
Authors : Ferrao, R.; Wallweber, H.J.A.; Lupardus, P.J.
Deposited on : 2016-03-23
Resolution : 2.57 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027790
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027790

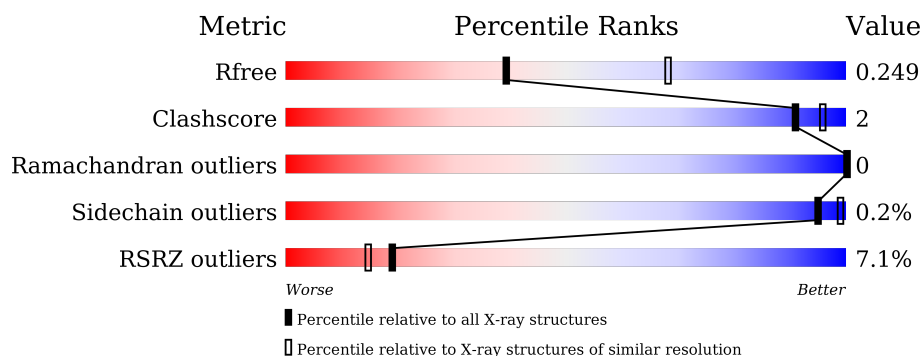
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	544	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>•</div> <div>20%</div> </div> </div>
2	B	53	<div> <div>6%</div> <div> <div></div> <div>45%</div> <div>9%</div> <div>45%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3828 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 JAK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	0	0	0
			3519	2243	604	646	26			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	MET	-	initiating methionine	UNP P23458
A	20	HIS	-	expression tag	UNP P23458
A	21	HIS	-	expression tag	UNP P23458
A	22	HIS	-	expression tag	UNP P23458
A	23	HIS	-	expression tag	UNP P23458
A	24	HIS	-	expression tag	UNP P23458
A	25	HIS	-	expression tag	UNP P23458
A	26	GLY	-	expression tag	UNP P23458
A	27	GLU	-	expression tag	UNP P23458
A	28	ASN	-	expression tag	UNP P23458
A	29	LEU	-	expression tag	UNP P23458
A	30	TYR	-	expression tag	UNP P23458
A	31	PHE	-	expression tag	UNP P23458
A	32	GLN	-	expression tag	UNP P23458
A	33	GLY	-	expression tag	UNP P23458
A	34	SER	-	expression tag	UNP P23458
A	350	ASP	HIS	conflict	UNP P23458
A	368	PHE	TYR	conflict	UNP P23458
A	560	GLY	-	expression tag	UNP P23458
A	561	ASN	-	expression tag	UNP P23458
A	562	SER	-	expression tag	UNP P23458

- Molecule 2 is a protein called Chimera protein of Interferon lambda receptor 1 and Interleukin-10 receptor subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	29	Total	C	N	O	S	0	0	0
			240	167	39	33	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	251	GLY	-	expression tag	UNP Q8IU57
B	252	SER	-	expression tag	UNP Q8IU57

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		
3	B	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	81.17Å 110.42Å 94.87Å 90.00° 98.11° 90.00°	Depositor
Resolution (Å)	36.15 – 2.57 47.60 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.4 (36.15-2.57) 91.7 (47.60-2.57)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.213 , 0.255 0.205 , 0.249	Depositor DCC
R_{free} test set	1839 reflections (7.57%)	DCC
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3828	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.28	0/3598	0.42	0/4867
2	B	0.62	0/249	0.69	0/336
All	All	0.31	0/3847	0.44	0/5203

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	3519	0	3410	11	0
2	B	240	0	255	5	0
3	A	68	0	0	0	0
3	B	1	0	0	0	0
All	All	3828	0	3665	16	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 2.

All (16) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:C	1:A:205:LYS:HD2	2.01	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:275:PRO:HG2	2:B:276:SER:H	1.62	0.65
1:A:410:ASP:OD2	1:A:414:ARG:NH2	2.33	0.61
1:A:303:HIS:ND1	1:A:303:HIS:O	2.35	0.60
2:B:273:LYS:O	2:B:274:LYS:HD3	2.03	0.59
2:B:275:PRO:HB2	2:B:277:PRO:HD3	1.83	0.58
1:A:518:SER:OG	1:A:521:ASP:OD2	2.21	0.58
1:A:463:TYR:CZ	1:A:543:CYS:HB2	2.41	0.56
2:B:275:PRO:HG2	2:B:276:SER:N	2.21	0.56
1:A:471:ASP:OD2	1:A:474:ASN:ND2	2.42	0.53
1:A:115:ASN:ND2	1:A:124:GLN:O	2.49	0.44
2:B:274:LYS:HA	2:B:274:LYS:HD3	1.88	0.43
1:A:205:LYS:N	1:A:205:LYS:HD2	2.33	0.43
1:A:463:TYR:N	1:A:542:ARG:O	2.51	0.42
1:A:204:LYS:CA	1:A:205:LYS:HD2	2.50	0.42
1:A:302:PHE:HB3	1:A:313:TYR:CZ	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	420/544 (77%)	413 (98%)	7 (2%)	0	100	100
2	B	27/53 (51%)	26 (96%)	1 (4%)	0	100	100
All	All	447/597 (75%)	439 (98%)	8 (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	386/497 (78%)	385 (100%)	1 (0%)	94	99
2	B	26/50 (52%)	26 (100%)	0	100	100
All	All	412/547 (75%)	411 (100%)	1 (0%)	95	99

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	499	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 carbohydrates 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 ⓘ

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	436/544 (80%)	0.31	30 (6%) 20 16	36, 59, 99, 142	0
2	B	29/53 (54%)	0.61	3 (10%) 9 6	44, 60, 102, 105	0
All	All	465/597 (77%)	0.33	33 (7%) 19 15	36, 59, 100, 142	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	498	PHE	7.9
1	A	538	PHE	7.6
1	A	540	LEU	7.5
2	B	281	ILE	7.1
1	A	535	ASN	4.6
2	B	278	PHE	4.3
1	A	497	ASN	4.1
1	A	450	ILE	4.1
1	A	464	VAL	4.0
1	A	531	LEU	3.6
1	A	448	TYR	3.5
1	A	533	THR	3.4
1	A	446	THR	3.4
1	A	454	ARG	3.4
1	A	537	SER	3.3
1	A	478	THR	3.3
1	A	477	MET	3.3
1	A	453	LEU	3.2
1	A	36	VAL	3.0
1	A	463	TYR	3.0
1	A	95	ILE	3.0
2	B	280	PHE	2.8
1	A	526	LEU	2.7
1	A	131	PRO	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	200	TYR	2.6
1	A	206	MET	2.5
1	A	49	ARG	2.5
1	A	50	LEU	2.4
1	A	177	LYS	2.4
1	A	534	ASP	2.4
1	A	544	CYS	2.3
1	A	522	LEU	2.2
1	A	121	ASP	2.1

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 carbohydrates 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.