



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:14 AM EDT

PDB ID : 6JWM
Title : Crystal structure of the SPRY domain of SPSB2 in complex with cR7, a potent cyclic peptide inhibitor of SPSB2-iNOS interaction
Authors : Li, K.; Kuang, Z.
Deposited on : 2019-04-21
Resolution : 1.23 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)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

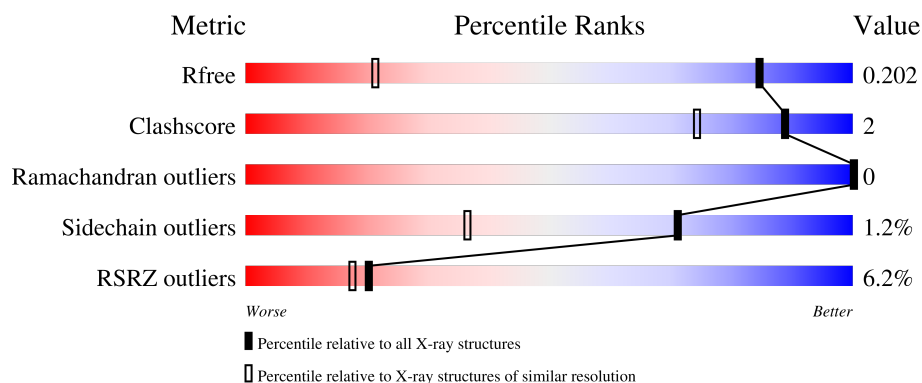
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.23 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	2024 (1.28-1.20)
Clashscore	141614	1007 (1.26-1.22)
Ramachandran outliers	138981	2053 (1.28-1.20)
Sidechain outliers	138945	2051 (1.28-1.20)
RSRZ outliers	127900	1987 (1.28-1.20)

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 $\leq 5\%$. 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	209	<div> <div>6%</div> <div> <div></div> <div>90%</div> <div>6%</div> <div>••</div> </div> </div>
2	B	7	<div> <div>100%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1745 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 SPRY domain-containing SOCS box protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1565	983	289	289	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	expression tag	UNP Q99619
A	21	GLY	-	expression tag	UNP Q99619
A	221	GLY	-	expression tag	UNP Q99619
A	222	SER	-	expression tag	UNP Q99619
A	223	HIS	-	expression tag	UNP Q99619
A	224	HIS	-	expression tag	UNP Q99619
A	225	HIS	-	expression tag	UNP Q99619
A	226	HIS	-	expression tag	UNP Q99619
A	227	HIS	-	expression tag	UNP Q99619
A	228	HIS	-	expression tag	UNP Q99619

- Molecule 2 is a protein called Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	0	0	0
			55	30	13	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ARG	GLU	conflict	UNP P35228
B	2	GLY	LYS	conflict	UNP P35228

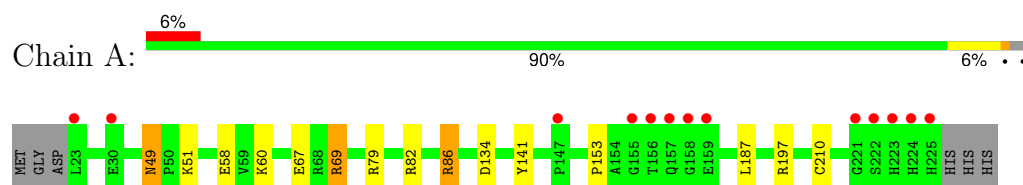
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total 119	O 119	0	0
3	B	6	Total 6	O 6	0	0

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: SPRY domain-containing SOCS box protein 2



- Molecule 2: Nitric oxide synthase, inducible



There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	40.06Å 63.97Å 68.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.86 – 1.23 46.86 – 1.23	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.86-1.23) 99.6 (46.86-1.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.45 (at 1.24Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.177 , 0.200 0.184 , 0.202	Depositor DCC
R_{free} test set	2589 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	7.0	Xtriage
Anisotropy	0.984	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1745	wwPDB-VP
Average B, all atoms (Å ²)	9.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.94% 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	0.78	0/1609	1.04	7/2185 (0.3%)
2	B	0.64	0/54	0.87	0/71
All	All	0.77	0/1663	1.04	7/2256 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	82	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	A	69	ARG	NE-CZ-NH1	-9.37	115.61	120.30
1	A	197	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	A	86	ARG	NE-CZ-NH1	-8.35	116.12	120.30
1	A	197	ARG	NE-CZ-NH2	7.72	124.16	120.30
1	A	86	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	A	82	ARG	NH1-CZ-NH2	5.38	125.32	119.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	79	ARG	Sidechain
1	A	86	ARG	Sidechain

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	1565	0	1511	6	0
2	B	55	0	49	0	0
3	A	119	0	0	0	0
3	B	6	0	0	0	0
All	All	1745	0	1560	6	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 (6) 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:49:ASN:ND2	1:A:51:LYS:H	1.98	0.62
1:A:134:ASP:HB2	1:A:141:TYR:CE2	2.43	0.54
1:A:58:GLU:CD	1:A:60:LYS:HE3	2.34	0.48
1:A:67:GLU:HA	1:A:210:CYS:O	2.19	0.42
1:A:49:ASN:C	1:A:49:ASN:HD22	2.23	0.42
1:A:153:PRO:HG3	1:A:187:LEU:HB3	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	201/209 (96%)	197 (98%)	4 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	5/7 (71%)	5 (100%)	0	0	100	100
All	All	206/216 (95%)	202 (98%)	4 (2%)	0	100	100

There are no Ramachandran outliers to report.

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	157/162 (97%)	155 (99%)	2 (1%)	69	33
2	B	6/6 (100%)	6 (100%)	0	100	100
All	All	163/168 (97%)	161 (99%)	2 (1%)	71	36

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	69	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	151	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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, 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	203/209 (97%)	0.29	13 (6%) 19 16	3, 8, 20, 30	0
2	B	7/7 (100%)	0.45	0 100 100	8, 9, 17, 17	0
All	All	210/216 (97%)	0.29	13 (6%) 20 17	3, 8, 20, 30	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	157	GLN	4.8
1	A	223	HIS	4.2
1	A	156	THR	3.7
1	A	155	GLY	3.6
1	A	224	HIS	2.5
1	A	222	SER	2.4
1	A	159	GLU	2.3
1	A	221	GLY	2.2
1	A	23	LEU	2.2
1	A	225	HIS	2.1
1	A	30	GLU	2.1
1	A	147	PRO	2.1
1	A	158	GLY	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.