Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 05:03 PM JST

PDB ID	:	5XN3
Title	:	Crystal structure of SPSB2 in complex with a rational designed RGD containing cyclic peptide inhibitor of SPSB2-iNOS interaction
Authors	:	You, T.; Kuang, Z.
Deposited on	:	2017-05-17
Resolution	:	1.34 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 (i) 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 (1)) were used in the production of this report:

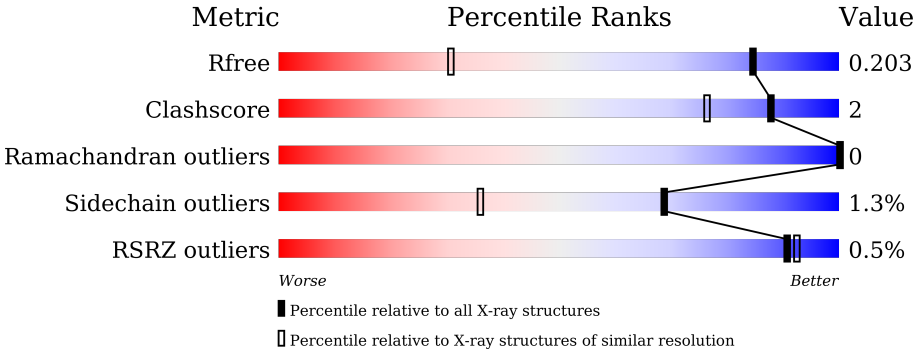
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.34 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	1385 (1.36-1.32)
Clashscore	141614	1417 (1.36-1.32)
Ramachandran outliers	138981	1397 (1.36-1.32)
Sidechain outliers	138945	1397 (1.36-1.32)
RSRZ outliers	127900	1369 (1.36-1.32)

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	209	84% 10% • 5%
2	B	8	88% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1620 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
			Total	C	N	O	S			
1	A	199	1504	946	275	279	4	0	0	1

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	cloning artifact	UNP Q99619
A	21	GLY	-	cloning artifact	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 cR8 peptide from NOS2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	8	62	35	14	13	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	52	52	52	0	0
3	B	2	2	2	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: SPRY domain-containing SOCS box protein 2

Chain A:

• Molecule 2: cR8 peptide from NOS2

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	32.49Å 64.60Å 47.59Å 90.00° 102.95° 90.00°	Depositor
Resolution (Å)	46.38 – 1.34 37.68 – 1.34	Depositor EDS
% Data completeness (in resolution range)	90.3 (46.38-1.34) 90.3 (37.68-1.34)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.34Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.180 , 0.200 0.187 , 0.203	Depositor DCC
R_{free} test set	1933 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	11.6	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1620	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (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	1.29	6/1543 (0.4%)	1.34	16/2096 (0.8%)
2	B	1.06	0/61	1.30	1/81 (1.2%)
All	All	1.28	6/1604 (0.4%)	1.34	17/2177 (0.8%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	GLU	CD-OE1	8.05	1.34	1.25
1	A	92	GLU	CD-OE2	-6.27	1.18	1.25
1	A	128	SER	CA-CB	6.24	1.62	1.52
1	A	27	GLU	CD-OE2	-5.27	1.19	1.25
1	A	98	GLU	CD-OE2	5.07	1.31	1.25
1	A	213	ARG	N-CA	-5.06	1.36	1.46

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	ARG	NE-CZ-NH1	10.80	125.70	120.30
1	A	166	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	A	192	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	A	166	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	A	69	ARG	NE-CZ-NH1	-9.13	115.73	120.30
1	A	39	ASP	CB-CG-OD1	8.15	125.63	118.30
1	A	197	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	A	69	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	A	197	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	162	GLU	OE1-CD-OE2	-7.32	114.51	123.30
1	A	79	ARG	NE-CZ-NH1	-6.76	116.92	120.30
2	B	3	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	A	68	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	A	52	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	98	GLU	CG-CD-OE2	-5.59	107.12	118.30
1	A	213	ARG	NE-CZ-NH1	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	ARG	CG-CD-NE	5.19	122.70	111.80

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	1504	0	1439	6	0
2	B	62	0	58	0	0
3	A	52	0	0	1	0
3	B	2	0	0	0	0
All	All	1620	0	1497	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:89:HIS:HD2	3:A:301:HOH:O	1.68	0.77
1:A:134:ASP:HB2	1:A:141:TYR:CE2	2.42	0.55
1:A:94:SER:HB2	1:A:213:ARG:HB3	1.97	0.46
1:A:161:LEU:C	1:A:161:LEU:HD12	2.36	0.46
1:A:49:ASN:ND2	1:A:51:LYS:H	2.18	0.41
1:A:128:SER:HA	1:A:143:GLN:HG2	2.03	0.41

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	197/209 (94%)	193 (98%)	4 (2%)	0	100	100
2	B	6/8 (75%)	6 (100%)	0	0	100	100
All	All	203/217 (94%)	199 (98%)	4 (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	147/162 (91%)	145 (99%)	2 (1%)	67	34
2	B	7/7 (100%)	7 (100%)	0	100	100
All	All	154/169 (91%)	152 (99%)	2 (1%)	69	36

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

Mol	Chain	Res	Type
1	A	49	ASN
1	A	209	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN

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Mol	Chain	Res	Type
1	A	89	HIS
1	A	209	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, 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	199/209 (95%)	0.13	1 (0%) 91 92	7, 13, 28, 43	0
2	B	8/8 (100%)	0.69	0 100 100	15, 22, 26, 37	0
All	All	207/217 (95%)	0.15	1 (0%) 91 92	7, 13, 28, 43	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	147	PRO	2.6

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 (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.