



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2018 – 05:23 PM EDT

PDB ID : 5WPA  
Title : Structure of human SFPQ/PSPC1 heterodimer  
Authors : Lee, M.  
Deposited on : 2017-08-04  
Resolution : 2.29 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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-20030736

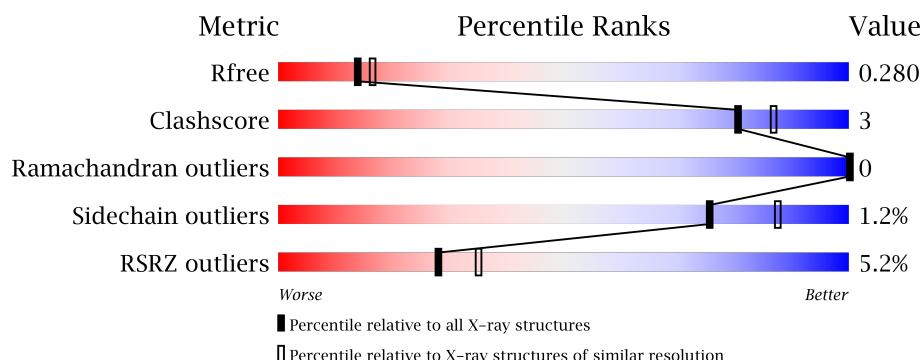
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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))
$R_{free}$	100719	4130 (2.30-2.30)
Clashscore	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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  $\geq 3$ , 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	261	<div> <div>7%</div> <div>79%</div> <div>7%</div> <div>14%</div> </div>
2	B	261	<div> <div>3%</div> <div>90%</div> <div>7%</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4001 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 Splicing factor, proline- and glutamine-rich.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1792	1129	309	348	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	MET	-	initiating methionine	UNP P23246

- Molecule 2 is a protein called Paraspeckle component 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	255	Total	C	N	O	S	0	1	0
			2073	1306	370	389	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	60	GLY	-	expression tag	UNP Q8WXF1

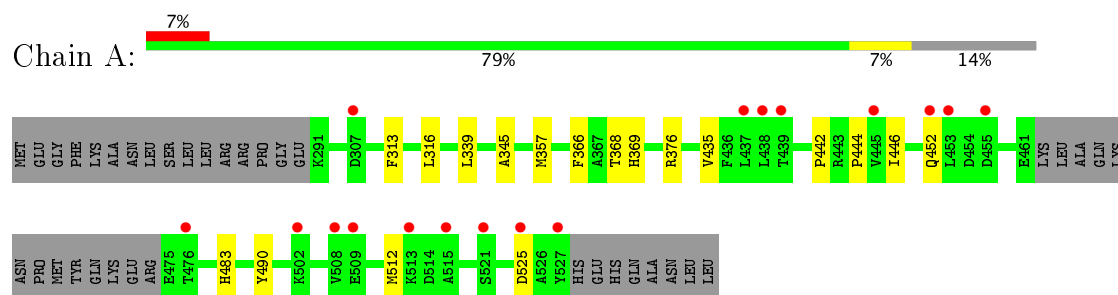
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		
3	B	74	Total	O	0	0
			74	74		

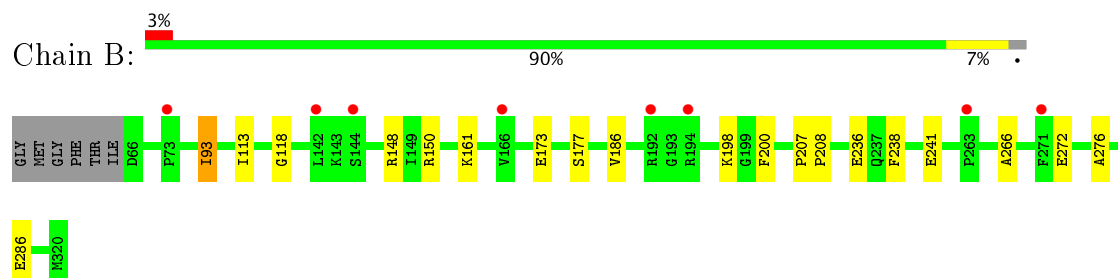
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Splicing factor, proline- and glutamine-rich



- Molecule 2: Paraspeckle component 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.23Å 67.84Å 92.20Å 90.00° 95.06° 90.00°	Depositor
Resolution (Å)	26.19 – 2.29 27.26 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.3 (26.19-2.29) 98.4 (27.26-2.29)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.97 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.219 , 0.272 0.227 , 0.280	Depositor DCC
$R_{free}$ test set	1223 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4001	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.50	0/1826	0.65	0/2457
2	B	0.50	0/2117	0.65	0/2845
All	All	0.50	0/3943	0.65	0/5302

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	1792	0	1750	13	0
2	B	2073	0	2063	17	0
3	A	62	0	0	0	0
3	B	74	0	0	1	0
All	All	4001	0	3813	24	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 (24) 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:316:LEU:HD11	1:A:357:MET:SD	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:MET:HG2	2:B:286:GLU:HB2	1.79	0.64
1:A:442:PRO:HB3	2:B:272:GLU:HG2	1.82	0.62
1:A:369:HIS:CD2	1:A:452:GLN:HG2	2.36	0.59
2:B:236:GLU:HB3	2:B:238:PHE:CE2	2.39	0.58
1:A:435:VAL:HG13	2:B:266:ALA:HB3	1.87	0.56
1:A:435:VAL:HG21	2:B:276:ALA:HB1	1.88	0.55
2:B:207:PRO:HB2	2:B:208:PRO:HD3	1.89	0.55
1:A:435:VAL:HG23	1:A:444:PRO:HB3	1.91	0.53
2:B:93:ILE:HG23	2:B:113:ILE:HD11	1.91	0.50
2:B:148:ARG:NH1	2:B:150:ARG:HG3	2.28	0.48
2:B:161:LYS:HE2	2:B:198:LYS:HE2	1.96	0.47
2:B:236:GLU:HB3	2:B:238:PHE:HE2	1.78	0.47
1:A:435:VAL:CG2	2:B:276:ALA:HB1	2.46	0.45
2:B:118:GLY:HA2	3:B:406:HOH:O	2.16	0.44
2:B:173:GLU:O	2:B:177:SER:HB3	2.16	0.44
1:A:339:LEU:HD12	1:A:345:ALA:HA	2.00	0.44
1:A:376:ARG:HH21	1:A:446:ILE:HD13	1.83	0.43
1:A:366:PHE:HB3	1:A:368:THR:HG23	2.00	0.43
2:B:186:VAL:HB	2:B:200:PHE:CZ	2.54	0.42
2:B:161:LYS:HG2	2:B:198:LYS:HG2	2.01	0.42
2:B:93:ILE:CG2	2:B:113:ILE:HD11	2.51	0.41
1:A:313:PHE:O	1:A:316:LEU:HB2	2.21	0.41
1:A:435:VAL:HG21	2:B:276:ALA:CB	2.52	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	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
2	B	254/261 (97%)	246 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	474/522 (91%)	460 (97%)	14 (3%)	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	189/223 (85%)	186 (98%)	3 (2%)	68	82
2	B	220/223 (99%)	218 (99%)	2 (1%)	82	91
All	All	409/446 (92%)	404 (99%)	5 (1%)	75	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	483	HIS
1	A	490	TYR
1	A	525	ASP
2	B	93	ILE
2	B	241	GLU

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

Mol	Chain	Res	Type
1	A	369	HIS
2	B	288	GLN

### 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 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 [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	224/261 (85%)	0.49	17 (7%) 15 20	23, 55, 86, 119	0
2	B	255/261 (97%)	0.31	8 (3%) 49 56	25, 55, 82, 117	0
All	All	479/522 (91%)	0.39	25 (5%) 28 35	23, 55, 85, 119	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	166	VAL	3.8
2	B	144	SER	3.5
2	B	192	ARG	3.5
1	A	509	GLU	3.3
1	A	527	TYR	3.3
1	A	521	SER	3.0
1	A	515	ALA	3.0
1	A	453	LEU	2.8
1	A	438	LEU	2.8
1	A	452	GLN	2.8
1	A	307	ASP	2.7
1	A	525	ASP	2.7
1	A	439	THR	2.7
2	B	271	PHE	2.6
2	B	263	PRO	2.6
1	A	476	THR	2.6
1	A	437	LEU	2.6
1	A	513	LYS	2.3
2	B	73	PRO	2.3
2	B	194	ARG	2.2
1	A	508	VAL	2.2
1	A	502	LYS	2.1
2	B	142	LEU	2.0
1	A	445	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	455	ASP	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 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.