



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 AM GMT

PDB ID : 2FH7  
Title : Crystal structure of the phosphatase domains of human PTP SIGMA  
Authors : Alvarado, J.; Udupi, R.; Smith, D.; Koss, J.; Wasserman, S.R.; Ozyurt, S.; Atwell, S.; Powell, A.; Kearins, M.C.; Rooney, I.; Maletic, M.; Bain, K.T.; Freeman, J.C.; Russell, M.; Thompson, D.A.; Sauder, J.M.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYS-GXRC)  
Deposited on : 2005-12-23  
Resolution : 2.00 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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

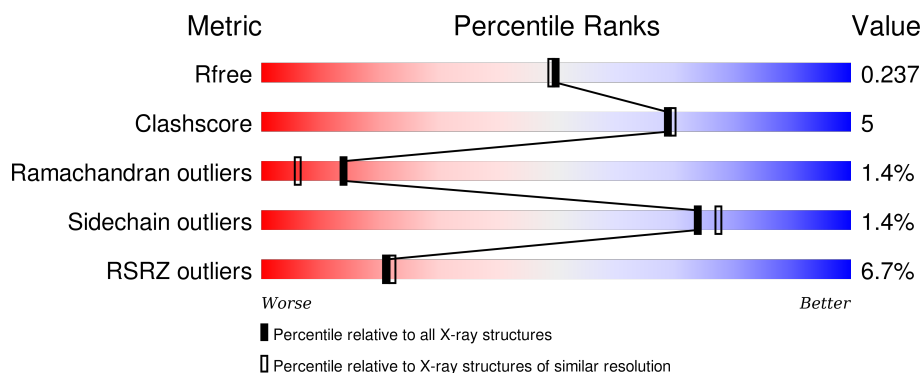
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

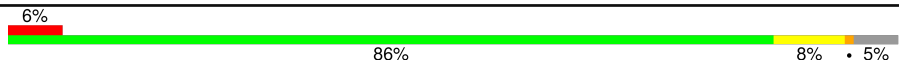
The reported resolution of this entry is 2.00 Å.

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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	595	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5009 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 Receptor-type tyrosine-protein phosphatase S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	568	4648	2945	813	859	31	0	8	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1362	MET	-	CLONING ARTIFACT	UNP Q13332
A	1363	SER	-	CLONING ARTIFACT	UNP Q13332
A	1364	LEU	-	CLONING ARTIFACT	UNP Q13332
A	1949	GLU	-	CLONING ARTIFACT	UNP Q13332
A	1950	GLY	-	CLONING ARTIFACT	UNP Q13332
A	1951	HIS	-	EXPRESSION TAG	UNP Q13332
A	1952	HIS	-	EXPRESSION TAG	UNP Q13332
A	1953	HIS	-	EXPRESSION TAG	UNP Q13332
A	1954	HIS	-	EXPRESSION TAG	UNP Q13332
A	1955	HIS	-	EXPRESSION TAG	UNP Q13332
A	1956	HIS	-	EXPRESSION TAG	UNP Q13332

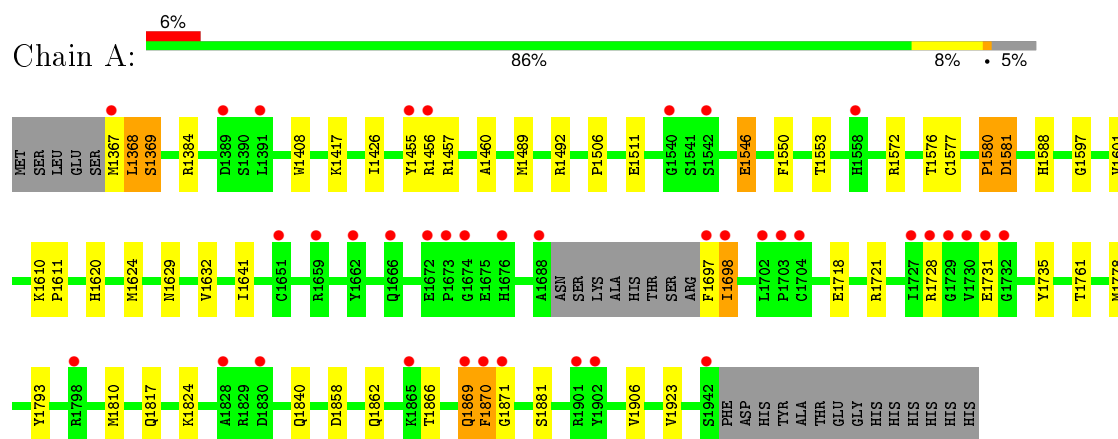
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	361	Total	O	0	0
			361	361		

### 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 errors 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: Receptor-type tyrosine-protein phosphatase S



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.33Å 94.33Å 123.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.67 – 2.00 24.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.67-2.00) 100.0 (24.67-2.00)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.88 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.190 , 0.238 0.190 , 0.237	Depositor DCC
$R_{free}$ test set	2103 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.6	EDS
Estimated twinning fraction	0.051 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 41832 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	0/4761	0.56	0/6453

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 [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	4648	0	4516	42	0
2	A	361	0	0	5	0
All	All	5009	0	4516	42	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 5.

All (42) 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:1546:GLU:HG2	2:A:105:HOH:O	1.78	0.83
1:A:1367:MET:HA	1:A:1368:LEU:O	1.80	0.81
1:A:1870:PHE:CB	1:A:1871:GLY:HA2	2.12	0.79
1:A:1869:GLN:HG3	1:A:1870:PHE:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1601[A]:VAL:HG21	1:A:1641:ILE:HD13	1.66	0.75
1:A:1368:LEU:O	1:A:1369:SER:HB2	1.91	0.69
1:A:1492:ARG:HD3	2:A:92:HOH:O	1.98	0.63
1:A:1455:TYR:O	1:A:1457[A]:ARG:HD2	2.00	0.61
1:A:1550:PHE:HZ	1:A:1577:CYS:HB2	1.67	0.59
1:A:1457[B]:ARG:HB3	1:A:1460:ALA:HB2	1.85	0.58
1:A:1457[A]:ARG:HB3	1:A:1460:ALA:HB2	1.89	0.55
1:A:1601[A]:VAL:HG21	1:A:1641:ILE:CD1	2.37	0.54
1:A:1601[A]:VAL:HG12	1:A:1620:HIS:HD2	1.74	0.53
1:A:1368:LEU:O	1:A:1369:SER:CB	2.57	0.53
1:A:1550:PHE:CZ	1:A:1577:CYS:HB2	2.44	0.53
1:A:1572:ARG:O	1:A:1576:THR:HG23	2.08	0.53
1:A:1367:MET:HA	1:A:1368:LEU:C	2.30	0.52
1:A:1810:MET:HG3	1:A:1824:LYS:HD3	1.90	0.51
1:A:1492:ARG:HD2	1:A:1553:THR:O	2.12	0.50
1:A:1870:PHE:CB	1:A:1871:GLY:CA	2.85	0.50
1:A:1597:GLY:O	1:A:1601[B]:VAL:HG23	2.12	0.50
1:A:1718:GLU:O	1:A:1721:ARG:HG2	2.13	0.48
1:A:1601[A]:VAL:HG13	1:A:1624:MET:SD	2.56	0.46
1:A:1881:SER:HB3	2:A:179:HOH:O	2.16	0.45
1:A:1489:MET:HG3	1:A:1588:HIS:CE1	2.51	0.45
1:A:1858:ASP:O	1:A:1862:GLN:HG2	2.18	0.43
1:A:1869:GLN:CG	1:A:1870:PHE:HA	2.42	0.43
1:A:1721:ARG:HH21	1:A:1735:TYR:HA	1.84	0.43
1:A:1817:GLN:HB3	1:A:1817:GLN:HE21	1.65	0.43
1:A:1778:MET:HG2	1:A:1840:GLN:HG3	2.01	0.43
1:A:1697:PHE:HB3	1:A:1698:ILE:H	1.64	0.42
1:A:1417[A]:LYS:HD2	2:A:119:HOH:O	2.19	0.41
1:A:1580:PRO:HB2	1:A:1581[B]:ASP:H	1.71	0.41
1:A:1492:ARG:NH2	2:A:259:HOH:O	2.54	0.41
1:A:1506:PRO:HB3	1:A:1511:GLU:HB2	2.02	0.41
1:A:1869:GLN:HG3	1:A:1870:PHE:CA	2.44	0.41
1:A:1869:GLN:N	1:A:1870:PHE:CB	2.84	0.41
1:A:1866:THR:O	1:A:1870:PHE:CB	2.68	0.41
1:A:1408:TRP:HB3	1:A:1426:ILE:HD13	2.03	0.41
1:A:1761:THR:HG23	1:A:1793:TYR:HB2	2.03	0.41
1:A:1610:LYS:HB2	1:A:1611:PRO:HD3	2.02	0.41
1:A:1455:TYR:CZ	1:A:1456:ARG:HD2	2.57	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	572/595 (96%)	542 (95%)	22 (4%)	8 (1%)	14 6

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1580	PRO
1	A	1368	LEU
1	A	1369	SER
1	A	1870	PHE
1	A	1728	ARG
1	A	1731	GLU
1	A	1632	VAL
1	A	1923	VAL

### 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	500/522 (96%)	491 (98%)	9 (2%)	66 69

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1384[A]	ARG
1	A	1384[B]	ARG
1	A	1546	GLU

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Mol	Chain	Res	Type
1	A	1581[A]	ASP
1	A	1581[B]	ASP
1	A	1629	ASN
1	A	1698	ILE
1	A	1869	GLN
1	A	1906	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1404	GLN
1	A	1817	GLN
1	A	1864	HIS
1	A	1869	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 [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	568/595 (95%)	0.26	38 (6%) 21 22	10, 27, 46, 60	2 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1367	MET	6.4
1	A	1703	PRO	5.6
1	A	1729	GLY	5.1
1	A	1730	VAL	5.0
1	A	1704	CYS	4.9
1	A	1673	PRO	4.8
1	A	1698	ILE	4.7
1	A	1697	PHE	4.7
1	A	1674	GLY	3.9
1	A	1659	ARG	3.7
1	A	1727	ILE	3.7
1	A	1942	SER	3.7
1	A	1676	HIS	3.6
1	A	1651	CYS	3.4
1	A	1455	TYR	3.4
1	A	1871	GLY	3.2
1	A	1672	GLU	3.0
1	A	1666	GLN	2.9
1	A	1828	ALA	2.8
1	A	1902	TYR	2.8
1	A	1728	ARG	2.8
1	A	1558	HIS	2.6
1	A	1731	GLU	2.6
1	A	1869	GLN	2.6
1	A	1688	ALA	2.5
1	A	1798	ARG	2.5
1	A	1732	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1901	ARG	2.4
1	A	1389	ASP	2.4
1	A	1702	LEU	2.4
1	A	1870	PHE	2.3
1	A	1540	GLY	2.3
1	A	1391	LEU	2.3
1	A	1865	LYS	2.2
1	A	1830	ASP	2.2
1	A	1456	ARG	2.1
1	A	1542	SER	2.0
1	A	1662	TYR	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.