



# wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 04:34 AM GMT

PDB ID : 2H0Q  
Title : Crystal Structure of the PGM domain of the Suppressor of T-Cell receptor (Sts-1)  
Authors : Nassar, N.; Ford, B.; Carpino, N.  
Deposited on : 2006-05-15  
Resolution : 1.82 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

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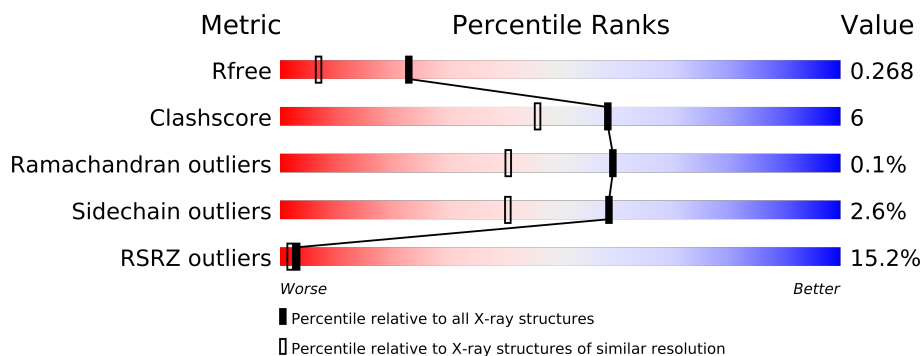
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.82 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))
$R_{free}$	66092	4101 (1.84-1.80)
Clashscore	79885	5140 (1.84-1.80)
Ramachandran outliers	78287	5077 (1.84-1.80)
Sidechain outliers	78261	5077 (1.84-1.80)
RSRZ outliers	66119	4103 (1.84-1.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	261	
1	B	261	
1	C	261	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6472 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Suppressor of T-cell receptor signaling 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	6	0
			2066	1311	361	375	19			
1	B	256	Total	C	N	O	S	0	9	0
			2032	1287	356	372	17			
1	C	261	Total	C	N	O	S	0	2	0
			2071	1314	363	377	17			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	132	Total	O	0	0
			132	132		
2	B	109	Total	O	0	0
			109	109		
2	C	62	Total	O	0	0
			62	62		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.23Å 74.34Å 100.11Å 90.00° 101.46° 90.00°	Depositor
Resolution (Å)	98.06 – 1.82 45.49 – 1.82	Depositor EDS
% Data completeness (in resolution range)	96.2 (98.06-1.82) 96.2 (45.49-1.82)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.196 , 0.236 0.233 , 0.268	Depositor DCC
$R_{free}$ test set	3647 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	27.6	Xtriage
Anisotropy	0.713	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 72282 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.69% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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	0.67	0/2154	0.70	1/2924 (0.0%)
1	B	0.64	1/2128 (0.0%)	0.68	1/2889 (0.0%)
1	C	0.49	0/2140	0.63	2/2905 (0.1%)
All	All	0.60	1/6422 (0.0%)	0.67	4/8718 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	602	CYS	CB-SG	-6.48	1.71	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	597	LEU	CA-CB-CG	-7.45	98.17	115.30
1	B	602	CYS	CB-CA-C	-5.39	99.63	110.40
1	C	405	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	474	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2066	0	2038	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2032	0	2023	40	1
1	C	2071	0	2051	24	1
2	A	132	0	0	0	0
2	B	109	0	0	3	0
2	C	62	0	0	3	0
All	All	6472	0	6112	77	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

The worst 5 of 77 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:436[B]:MET:CE	1:B:436[B]:MET:HE2	1.55	1.35
1:B:570:GLU:HG2	2:B:738:HOH:O	1.36	1.22
1:A:436[B]:MET:CE	1:B:436[B]:MET:CE	2.16	1.15
1:C:462[B]:ARG:HH12	1:C:565:HIS:CE1	1.74	1.04
1:A:436[B]:MET:SD	1:B:436[B]:MET:HE3	1.67	1.02

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:391:TYR:OH	1:C:540:ASN:ND2[3_555]	2.16	0.04

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	265/261 (102%)	259 (98%)	6 (2%)	0	100	100
1	B	263/261 (101%)	252 (96%)	10 (4%)	1 (0%)	43	25
1	C	262/261 (100%)	252 (96%)	10 (4%)	0	100	100
All	All	790/783 (101%)	763 (97%)	26 (3%)	1 (0%)	59	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	608	THR

### 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	234/229 (102%)	228 (97%)	6 (3%)	59	40
1	B	233/229 (102%)	226 (97%)	7 (3%)	53	34
1	C	232/229 (101%)	225 (97%)	7 (3%)	53	34
All	All	699/687 (102%)	679 (97%)	20 (3%)	59	36

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	531	ILE
1	B	532	SER
1	C	558	ASN
1	B	405[A]	ARG
1	B	405[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	582	GLN
1	C	630	ASN
1	C	412	HIS
1	B	577	GLN
1	B	612	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

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, 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	261/261 (100%)	0.65	19 (7%)	15 11	20, 30, 43, 50	0
1	B	256/261 (98%)	0.82	32 (12%)	5 3	23, 31, 45, 51	0
1	C	261/261 (100%)	1.41	67 (25%)	1 1	26, 38, 49, 55	0
All	All	778/783 (99%)	0.96	118 (15%)	3 2	20, 33, 46, 55	0

The worst 5 of 118 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	ALA	9.7
1	C	610	ILE	7.5
1	C	531	ILE	7.2
1	C	606	GLY	7.0
1	C	555	SER	6.8

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.