

wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2023 – 07:56 PM EDT

PDB ID 2IKQ

> Title : Crystal structure of mouse Sts-1 PGM domain in complex with phosphate

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2006-10-02 Deposited on

2.61 Å(reported) Resolution

This is a wwPDB X-ray Structure Validation Summary 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

> 1.8.5 (274361), CSD as541be (2020) Mogul

Xtriage (Phenix) 1.13

EDS 2.35

20191225.v01 (using entries in the PDB archive December 25th 2019) Percentile statistics

> Refmac 5.8.0158

CCP47.0.044 (Gargrove)

Ideal geometry (proteins) Engh & Huber (2001) Ideal geometry (DNA, RNA) Parkinson et al. (1996)

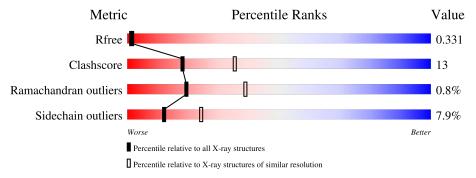
Validation Pipeline (wwPDB-VP) : 2.35

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 2.61 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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%

Mol	Chain	Length	Quality of chain				
1	A	270	67%	26%			
1	В	270	69%	23%	• 5%		
1	M	270	69%	24%			



2 Entry composition (i)

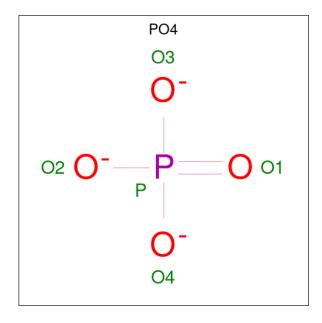
There are 3 unique types of molecules in this entry. The entry contains 6128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Suppressor of T-cell receptor signaling 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	262	Total	Total C N O S	0	0	0			
1	A	202	2065	1312	362	376	15	U	U	0
1	В	256	Total	С	N	О	S	0	0	0 0
1	Б	250	2012	1277	351	369	15	0		
1	M	258	Total	С	N	О	S	0	0	0
1	IVI	250	2026	1286	353	372	15	U		U

• Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	В	1	Total O P 5 4 1	0	0
2	M	1	Total O P 5 4 1	0	0



• Molecule 3 is water.

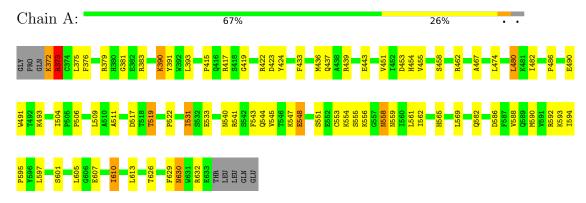
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	В	3	Total O 3 3	0	0
3	M	3	Total O 3 3	0	0



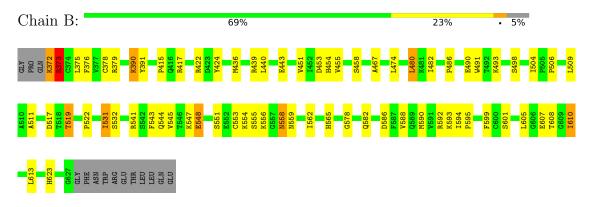
3 Residue-property plots (i)

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. 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. 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.

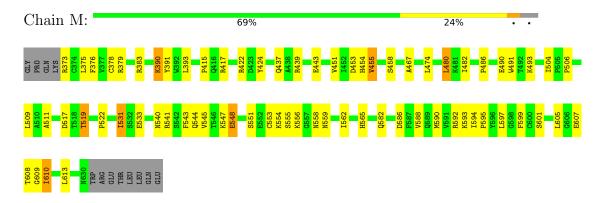
• Molecule 1: Suppressor of T-cell receptor signaling 1



• Molecule 1: Suppressor of T-cell receptor signaling 1



• Molecule 1: Suppressor of T-cell receptor signaling 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	116.96Å 74.67Å 101.28Å	Donositor
a, b, c, α , β , γ	90.00° 100.79° 90.00°	Depositor
Resolution (Å)	99.50 - 2.61	Depositor
Resolution (A)	30.77 - 2.61	EDS
% Data completeness	97.6 (99.50-2.61)	Depositor
(in resolution range)	97.6 (30.77-2.61)	EDS
R_{merge}	0.63	Depositor
R_{sym}	0.63	Depositor
$< I/\sigma(I) > 1$	3.57 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
D D.	0.248 , 0.275	Depositor
R, R_{free}	0.310 , 0.331	DCC
R_{free} test set	1293 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32, 42.3	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	0.89	EDS
Total number of atoms	6128	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	
IVIOI	Chain	RMSZ $ \# Z > 5$		RMSZ	# Z > 5
1	A	0.65	0/2118	0.72	$2/2877 \ (0.1\%)$
1	В	0.51	0/2062	0.67	1/2801 (0.0%)
1	M	0.46	0/2077	0.65	1/2822 (0.0%)
All	All	0.55	0/6257	0.68	4/8500 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
1	A	383	ARG	N-CA-CB	-5.95	99.89	110.60
1	A	373	ARG	CG-CD-NE	-5.93	99.35	111.80
1	M	383	ARG	N-CA-CB	-5.11	101.41	110.60
1	В	373	ARG	CG-CD-NE	-5.02	101.26	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	2065	0	2043	75	1
1	В	2012	0	2000	64	4
1	M	2026	0	2005	40	4
2	A	5	0	0	1	0

Continued on next page...



Continued	trom	mmoninonic	maaa
COHABABACA		DIEUIUU	DUIUE
0 0 1000100000			

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	В	5	0	0	0	0
2	M	5	0	0	0	0
3	A	4	0	0	1	0
3	В	3	0	0	0	0
3	M	3	0	0	0	0
All	All	6128	0	6048	163	5

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 13.

The worst 5 of 163 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:372:LYS:O	1:A:373:ARG:HG3	1.53	1.09
1:B:372:LYS:O	1:B:373:ARG:HG3	1.55	1.06
1:M:531:ILE:H	1:M:531:ILE:HD12	1.39	0.88
1:A:531:ILE:H	1:A:531:ILE:HD12	1.39	0.88
1:B:372:LYS:O	1:B:372:LYS:HG2	1.74	0.87

All (5) 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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)	
1:B:578:GLY:O	1:M:391:TYR:OH[1_565]	1.90	0.30	
1:A:540:ASN:ND2	1:A:629:PHE:CE1[4_545]	1.96	0.24	
1:B:391:TYR:OH	1:M:540:ASN:ND2[3_555]	2.05	0.15	
1:B:498:SER:OG	1:M:609:GLY:O[3_555]	2.15	0.05	
1:B:532:SER:OG	1:M:554:LYS:NZ[3_555]	2.16	0.04	

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	in Analysed Favoured Allowed		Outliers	Percentiles	
1	A	$260/270 \ (96\%)$	246 (95%)	12 (5%)	2 (1%)	19 39
1	В	254/270 (94%)	240 (94%)	12 (5%)	2 (1%)	19 39
1	M	$256/270 \ (95\%)$	241 (94%)	13 (5%)	2 (1%)	19 39
All	All	770/810 (95%)	727 (94%)	37 (5%)	6 (1%)	19 39

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	ALA
1	В	511	ALA
1	M	511	ALA
1	A	558	ASN
1	В	558	ASN

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	Chain Analysed Rotameric Outliers		Percentiles		
1	A	$229/237 \ (97\%)$	210 (92%)	19 (8%)	11 22	
1	В	$225/237 \ (95\%)$	208 (92%)	17 (8%)	13 26	
1	M	$226/237 \ (95\%)$	208 (92%)	18 (8%)	12 24	
All	All	680/711 (96%)	626 (92%)	54 (8%)	12 24	

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	548	GLU
1	В	613	LEU
1	M	586	ASP
1	В	555	SER
1	В	605	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol Type Chain Res		Res	es Link	Bond lengths			Bond angles			
MIOI	Type	Chain	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	PO4	M	103	-	4,4,4	0.86	0	6,6,6	0.68	0
2	PO4	A	101	-	4,4,4	0.81	0	6,6,6	0.82	0
2	PO4	В	102	-	4,4,4	0.77	0	6,6,6	0.59	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	101	PO4	1	0



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)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

