



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 07:53 pm GMT

PDB ID : 1SW6
Title : S. CEREVISIAE SWI6 ANKYRIN-REPEAT FRAGMENT
Authors : Foord, R.; Taylor, I.A.; Sedgwick, S.G.; Smerdon, S.J.
Deposited on : 1998-09-28
Resolution : 2.10 Å(reported)

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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

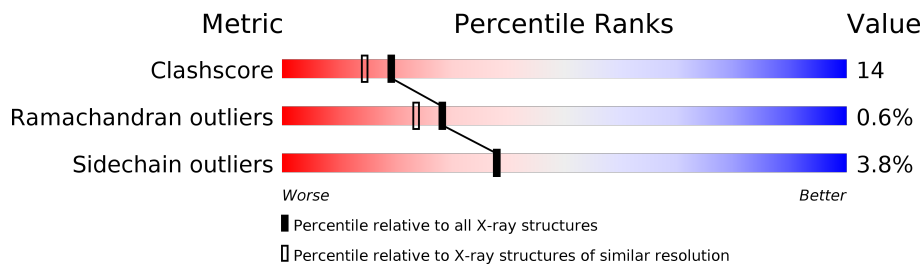
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	327	
1	B	327	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4155 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 REGULATORY PROTEIN SWI6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1971	1255	330	375	11			
1	B	254	Total	C	N	O	S	0	0	0
			1969	1252	331	375	11			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		
2	B	110	Total	O	0	0
			110	110		

Note EDS was not executed.

- Chain A:
-
- | Row 1 | Row 2 | Row 3 |
|-------|-------|-------|
| ASN | GLU | D366 |
| ASP | MET | A499 |
| ASP | PRO | Y376 |
| ILE | THR | L377 |
| ASN | SER | R505 |
| LYS | LEU | P506 |
| GLY | ASN | F509 |
| GLY | ASP | G512 |
| PRO | ASP | LEU |
| ASP | SER | GLU |
| ASN | SER | |
| ASN | ASN | |
| GLU | ARG | I397 |
| ASN | ASN | |
| ASN | SER | G417 |
| GLY | SER | W418 |
| GLY | GLY | I419 |
| ASP | GLY | V420 |
| ASP | SER | K421 |
| ASN | SER | K422 |
| ARG | ASN | R425 |
| THR | GLN | P426 |
| ALA | GLN | G430 |
| G212 | HIS | THR |
| P213 | VAL | GLU |
| I214 | VAL | GLY |
| I215 | S291 | LYS |
| S223 | F292 | SER |
| L226 | D293 | LYS |
| S227 | S294 | PRO |
| S228 | E298 | ASN |
| P229 | P299 | ASP |
| L230 | N300 | LYS |
| K231 | D301 | ASN |
| I232 | A302 | GLY |
| M233 | F303 | GLU |
| P239 | P304 | ARG |
| V240 | N311 | D447 |
| V241 | I312 | |
| N242 | P313 | L450 |
| D243 | V314 | E451 |
| Q246 | L322 | N452 |
| K249 | L326 | L453 |
| F253 | I328 | T458 |
| L254 | I328 | M462 |
| L257 | L333 | D471 |
| L258 | V334 | M475 |
| F259 | K336 | I476 |
| PRO | L337 | A477 |
| GLU | N343 | A478 |
| ILE | | R479 |
| GLN | | L480 |

- Chain B:
-
- 56% 20% 22%
- ASN ASP ASP ILE ASN ASN LYS GLY PRO THR SER SER GLY ASP ASP ASN ASP ARG THR ALA G212 H219 D220 L221 T222 S223 D224 F225 L226 K234 P239 V240 V241 N242 D243 N244 M248 K249 L250 E251 Q255 R256 L257 L258 P258 R259 PRO GLU ILE GLN MET
- PRO THR SER LEU ASN ASP SER ASN ARG ASN SER GLU GLY GLY SER ASN GLN GLN HIS VAL S291 S294 L295 L296 Q297 E298 T306 L310 R311 P312 P313 P321 L325 T326 L331 F332 L333 Y334 K335 H336 L337 N343 R344 Y346 C354
- N363 N364 Y365 D366 S367 G368 T369 Y376 L377 Y378 P379 C380 L383 E384 D385 S386 M387 N388 L392 M401 T402 G403 A406 I414 K422 Q423 N424 R425 G430 THR ASN GLU LYS GLU SER LYS PRO ASN ASP LYS ASN GLY ARG D447 S448 L453 M462
- D467 I483 P496 A499 R505 P506 V507 G512 LEU GLU

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.85Å 91.73Å 90.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10	Depositor
% Data completeness (in resolution range)	86.0 (15.00-2.10)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4155	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

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	0.37	0/2008	0.58	0/2725
1	B	0.36	0/2005	0.60	0/2720
All	All	0.37	0/4013	0.59	0/5445

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	1971	0	1967	52	0
1	B	1969	0	1971	65	0
2	A	105	0	0	1	0
2	B	110	0	0	6	0
All	All	4155	0	3938	114	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 14.

The worst 5 of 114 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:B:325:LEU:HD13	1:B:333:LEU:HB3	1.43	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HD11	1:B:447:ASP:HB2	1.53	0.90
1:B:256:ARG:HD2	1:B:295:LEU:HD11	1.56	0.88
1:A:311:ASN:HD21	1:A:343:ASN:H	1.15	0.87
1:A:241:VAL:HG21	1:A:312:ILE:HG23	1.58	0.84

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	248/327 (76%)	236 (95%)	11 (4%)	1 (0%)	38	35
1	B	248/327 (76%)	236 (95%)	10 (4%)	2 (1%)	22	17
All	All	496/654 (76%)	472 (95%)	21 (4%)	3 (1%)	28	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	SER
1	B	243	ASP
1	B	223	SER

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	221/287 (77%)	213 (96%)	8 (4%)	40	41
1	B	221/287 (77%)	212 (96%)	9 (4%)	35	35
All	All	442/574 (77%)	425 (96%)	17 (4%)	38	38

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	453	LEU
1	B	251	GLU
1	B	422	LYS
1	A	451	GLU
1	B	424	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	ASN
1	A	461	ASN
1	B	349	ASN
1	A	340	HIS
1	B	340	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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 [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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.