



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:12 AM 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 full wwPDB validation 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/ValidationPDFNotes.html>

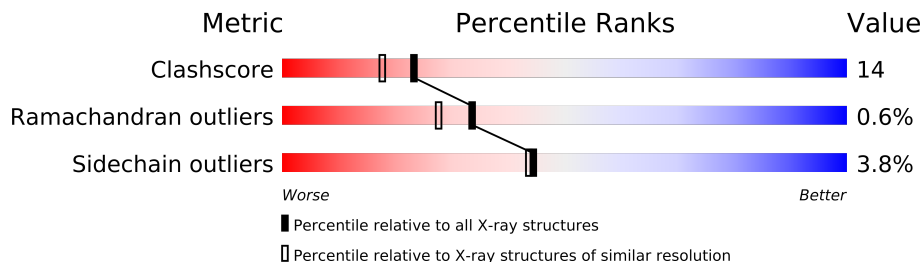
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
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 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	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 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 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		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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

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	0.37	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 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	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

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 14.

All (114) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:325:LEU:HD13	1:B:333:LEU:HB3	1.43	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(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
1:B:239:PRO:HG2	1:B:313:PRO:HD3	1.59	0.83
1:B:256:ARG:HB3	1:B:295:LEU:HD21	1.58	0.82
1:A:228:SER:HB3	1:A:229:PRO:HD2	1.61	0.82
1:A:418:TRP:HE3	1:A:419:ILE:HD12	1.45	0.82
1:B:325:LEU:HD12	1:B:337:LEU:HD22	1.62	0.81
1:A:301:ASP:O	1:A:304:PRO:HD3	1.81	0.79
1:B:312:ILE:HD12	1:B:313:PRO:HD2	1.64	0.77
1:B:241:VAL:HB	1:B:312:ILE:HD13	1.66	0.76
1:A:311:ASN:ND2	1:A:343:ASN:H	1.84	0.76
1:B:297:GLN:HG3	2:B:578:HOH:O	1.86	0.75
1:A:471:ASP:CG	1:A:479:ARG:HH22	1.92	0.73
1:B:325:LEU:HD12	1:B:337:LEU:CD2	2.19	0.72
1:A:418:TRP:CE3	1:A:419:ILE:HD12	2.29	0.68
1:B:244:ASN:O	1:B:248:MET:HG2	1.94	0.67
1:B:256:ARG:CD	1:B:295:LEU:HD11	2.24	0.67
1:B:345:LEU:HD22	1:B:383:LEU:HD21	1.75	0.67
1:B:367:SER:OG	1:B:414:ILE:HD11	1.95	0.66
1:A:232:ILE:HD12	2:A:544:HOH:O	1.97	0.64
1:B:386:SER:HB2	2:B:548:HOH:O	1.99	0.63
1:B:402:THR:HG22	1:B:403:GLY:H	1.64	0.63
1:B:384:GLU:CG	1:B:388:ASN:HA	2.30	0.61
1:A:239:PRO:HG2	1:A:313:PRO:HD3	1.83	0.61
1:A:257:LEU:HD23	1:A:295:LEU:HD13	1.82	0.60
1:B:294:SER:O	1:B:297:GLN:HG2	2.02	0.59
1:A:241:VAL:HG21	1:A:312:ILE:HG12	1.85	0.59
1:A:419:ILE:HG12	1:A:458:ILE:HG13	1.87	0.56
1:B:499:ALA:HB2	1:B:505:ARG:HG2	1.86	0.56
1:A:241:VAL:HG21	1:A:312:ILE:CG2	2.34	0.56
1:B:499:ALA:HB2	1:B:505:ARG:CG	2.36	0.55
1:B:496:PRO:HB2	1:B:507:VAL:HG13	1.89	0.55
1:A:311:ASN:HD21	1:A:343:ASN:N	1.95	0.54
1:B:297:GLN:HB2	2:B:563:HOH:O	2.06	0.54
1:A:366:ASP:HB3	1:B:483:ILE:HG13	1.88	0.54
1:A:471:ASP:OD1	1:A:479:ARG:NH2	2.41	0.54
1:B:384:GLU:HG2	1:B:388:ASN:HA	1.89	0.54
1:B:387:MET:O	1:B:467:ASP:HB2	2.08	0.54
1:B:335:LYS:HE2	1:B:376:TYR:CE2	2.43	0.54
1:A:325:LEU:HD13	1:A:333:LEU:HB3	1.91	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:378:TYR:N	1:B:379:PRO:CD	2.71	0.53
1:A:328:ILE:O	1:A:328:ILE:HG23	2.07	0.53
1:B:257:LEU:O	1:B:258:LEU:HB3	2.09	0.53
1:B:402:THR:HG22	1:B:403:GLY:N	2.23	0.52
1:B:240:VAL:HG13	1:B:240:VAL:O	2.09	0.52
1:A:241:VAL:CG2	1:A:312:ILE:HG23	2.36	0.52
1:B:258:LEU:HD13	2:B:539:HOH:O	2.10	0.51
1:B:239:PRO:HG2	1:B:313:PRO:CD	2.37	0.51
1:B:343:ASN:HB3	1:B:346:TYR:CD2	2.45	0.51
1:A:328:ILE:CD1	1:B:401:MET:HA	2.40	0.51
1:A:499:ALA:HB2	1:A:505:ARG:HG2	1.94	0.50
1:B:326:THR:HG21	1:B:354:CYS:O	2.11	0.50
1:A:223:SER:HB2	1:A:226:LEU:HG	1.92	0.50
1:A:249:LYS:NZ	1:A:300:ASN:ND2	2.60	0.50
1:A:392:LEU:HG	1:A:462:MET:SD	2.52	0.50
1:B:343:ASN:HB3	1:B:346:TYR:CE2	2.47	0.50
1:B:239:PRO:HD3	1:B:346:TYR:CD1	2.47	0.49
1:B:225:PHE:N	1:B:225:PHE:CD2	2.79	0.49
1:A:213:PRO:HB3	1:A:426:PRO:HG2	1.95	0.49
1:B:331:LEU:HD11	1:B:369:THR:HG23	1.95	0.49
1:A:215:ILE:CG2	1:A:430:GLY:HA3	2.42	0.49
1:A:452:ASN:N	1:A:452:ASN:HD22	2.10	0.49
1:A:471:ASP:CG	1:A:479:ARG:NH2	2.64	0.48
1:B:226:LEU:O	1:B:448:SER:HB2	2.14	0.48
1:A:253:PHE:HB2	1:A:299:VAL:HG21	1.96	0.48
1:A:475:ASN:HA	1:A:506:PRO:HG3	1.96	0.48
1:B:258:LEU:HD22	1:B:258:LEU:C	2.34	0.47
1:A:417:GLY:O	1:A:421:LYS:HG3	2.14	0.47
1:B:380:CYS:HA	1:B:383:LEU:HG	1.96	0.47
1:A:422:LYS:HA	1:A:425:ARG:HD3	1.96	0.47
1:B:219:HIS:HD2	2:B:559:HOH:O	1.97	0.47
1:A:378:TYR:CG	1:A:379:PRO:HD3	2.50	0.46
1:A:450:LEU:O	1:A:450:LEU:HD23	2.15	0.46
1:B:333:LEU:O	1:B:337:LEU:HD13	2.16	0.46
1:B:392:LEU:CD1	1:B:462:MET:HG2	2.46	0.46
1:B:255:GLN:HA	1:B:255:GLN:OE1	2.15	0.45
1:A:314:VAL:O	1:A:314:VAL:HG12	2.16	0.45
1:B:392:LEU:HD12	1:B:462:MET:HG2	1.98	0.45
1:A:393:HIS:O	1:A:397:ILE:HG12	2.17	0.45
1:A:314:VAL:CG1	1:A:314:VAL:O	2.65	0.44
1:A:476:ILE:O	1:A:480:LEU:HG	2.17	0.44
1:B:240:VAL:HG22	1:B:240:VAL:O	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:ASP:CG	1:A:246:GLN:HG3	2.38	0.44
1:B:310:LEU:O	1:B:321:PRO:HD2	2.18	0.44
1:B:496:PRO:O	1:B:507:VAL:HG22	2.18	0.44
1:B:422:LYS:HA	1:B:425:ARG:HD3	1.99	0.44
1:B:226:LEU:HG	1:B:226:LEU:O	2.17	0.44
1:B:234:LYS:HE2	2:B:583:HOH:O	2.18	0.44
1:A:254:LEU:HD12	1:A:314:VAL:HG21	1.99	0.43
1:A:233:MET:O	1:A:383:LEU:HA	2.18	0.43
1:A:499:ALA:HB2	1:A:505:ARG:CG	2.48	0.43
1:B:226:LEU:HD12	1:B:448:SER:HB3	2.00	0.43
1:A:378:TYR:N	1:A:379:PRO:CD	2.82	0.42
1:B:221:LEU:HB3	1:B:226:LEU:HD22	2.01	0.42
1:B:256:ARG:NH2	1:B:298:GLU:OE1	2.52	0.42
1:B:335:LYS:HG3	1:B:336:HIS:N	2.34	0.42
1:A:328:ILE:CD1	1:B:401:MET:HG2	2.48	0.42
1:B:242:ASN:O	1:B:243:ASP:C	2.58	0.42
1:A:335:LYS:HG2	1:A:376:TYR:CZ	2.54	0.42
1:B:335:LYS:HB2	1:B:335:LYS:HE2	1.86	0.42
1:B:333:LEU:HD12	1:B:333:LEU:HA	1.91	0.41
1:A:325:LEU:HD12	1:A:337:LEU:HD11	2.02	0.41
1:B:402:THR:HG21	1:B:406:ALA:CB	2.51	0.41
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.89	0.41
1:A:478:ALA:HB1	1:A:509:PHE:HB2	2.01	0.41
1:A:249:LYS:HE3	1:A:303:PHE:HB2	2.02	0.41
1:B:365:TYR:CD2	1:B:369:THR:HG22	2.56	0.41
1:A:322:LEU:HA	1:A:322:LEU:HD12	1.97	0.41
1:B:335:LYS:HE2	1:B:376:TYR:HE2	1.85	0.40
1:B:249:LYS:NZ	1:B:306:THR:O	2.53	0.40
1:A:228:SER:CB	1:A:229:PRO:HD2	2.42	0.40

There are no symmetry-related clashes.

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	248/327 (76%)	236 (95%)	11 (4%)	1 (0%)	43	39
1	B	248/327 (76%)	236 (95%)	10 (4%)	2 (1%)	27	20
All	All	496/654 (76%)	472 (95%)	21 (4%)	3 (1%)	33	28

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 ⓘ

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%)	47	46
1	B	221/287 (77%)	212 (96%)	9 (4%)	41	40
All	All	442/574 (77%)	425 (96%)	17 (4%)	44	44

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	LEU
1	A	254	LEU
1	A	293	ASP
1	A	298	GLU
1	A	328	ILE
1	A	333	LEU
1	A	451	GLU
1	A	453	LEU
1	B	251	GLU
1	B	258	LEU
1	B	333	LEU
1	B	335	LYS
1	B	363	ASN
1	B	422	LYS

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Mol	Chain	Res	Type
1	B	424	ASN
1	B	453	LEU
1	B	507	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	ASN
1	A	255	GLN
1	A	300	ASN
1	A	311	ASN
1	A	340	HIS
1	A	452	ASN
1	A	461	ASN
1	B	244	ASN
1	B	340	HIS
1	B	349	ASN
1	B	424	ASN
1	B	452	ASN

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.