



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:11 PM GMT

PDB ID : 3BIP
Title : Crystal structure of yeast Spt16 N-terminal Domain
Authors : VanDemark, A.P.; Xin, H.; McCullough, L.; Rawlins, R.; Bentley, S.; Heroux, A.; David, S.J.; Hill, C.P.; Formosa, T.
Deposited on : 2007-11-30
Resolution : 1.94 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>

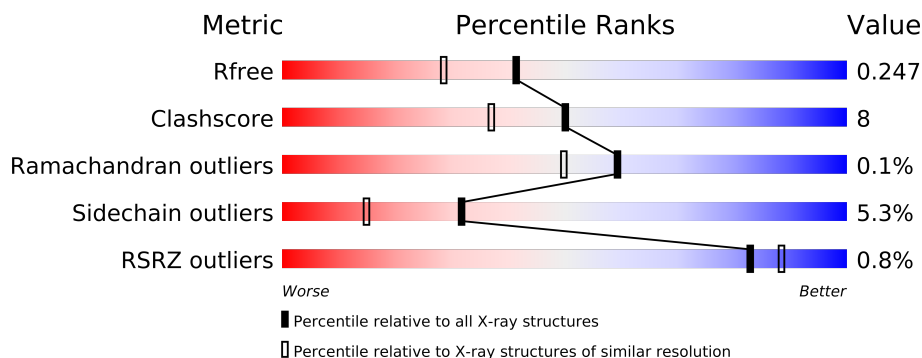
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : 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 1.94 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	2024 (1.96-1.92)
Clashscore	79885	2281 (1.96-1.92)
Ramachandran outliers	78287	2255 (1.96-1.92)
Sidechain outliers	78261	2255 (1.96-1.92)
RSRZ outliers	66119	2024 (1.96-1.92)

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.

Mol	Chain	Length	Quality of chain
1	A	467	
1	B	467	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8034 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 FACT complex subunit SPT16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	10	0
			3668	2353	601	705	9			
1	B	442	Total	C	N	O	S	0	10	0
			3645	2337	594	705	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P32558
A	0	HIS	-	EXPRESSION TAG	UNP P32558
B	-1	GLY	-	EXPRESSION TAG	UNP P32558
B	0	HIS	-	EXPRESSION TAG	UNP P32558

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	360	Total	O	0	0
			360	360		
2	B	361	Total	O	0	0
			361	361		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.14Å 60.14Å 85.93Å 72.59° 77.06° 89.88°	Depositor
Resolution (Å)	38.91 – 1.94 38.91 – 1.94	Depositor EDS
% Data completeness (in resolution range)	73.2 (38.91-1.94) 73.2 (38.91-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.176 , 0.244 0.185 , 0.247	Depositor DCC
R_{free} test set	2657 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.834	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 51629 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8034	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.57	0/3744	0.65	1/5067 (0.0%)
1	B	0.57	0/3719	0.67	2/5031 (0.0%)
All	All	0.57	0/7463	0.66	3/10098 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	LEU	CB-CG-CD1	5.97	121.16	111.00
1	A	100	LEU	CA-CB-CG	5.71	128.44	115.30
1	B	36	LEU	CA-CB-CG	5.70	128.42	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	3668	0	3660	58	0
1	B	3645	0	3625	56	0
2	A	360	0	0	17	0
2	B	361	0	0	7	0
All	All	8034	0	7285	110	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 8.

All (110) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:LEU:HD12	1:A:83:HIS:CG	1.91	1.06
1:A:73:ILE:HG13	2:A:820:HOH:O	1.68	0.93
1:A:4:LEU:HD12	1:A:83:HIS:CD2	2.07	0.90
1:B:108:LYS:HD2	1:B:108:LYS:O	1.73	0.88
1:B:106:ASN:H	1:B:113:ASN:HD21	1.20	0.87
1:B:133:ILE:HG21	2:B:994:HOH:O	1.72	0.87
1:B:100:LEU:HD22	1:B:101:GLU:N	1.89	0.86
1:B:89:ASP:HA	1:B:92:LYS:HD2	1.57	0.83
1:A:52:HIS:HD2	1:A:60:PHE:H	1.25	0.82
1:A:249:ASN:HB3	1:A:252:LEU:HD22	1.61	0.81
1:B:363:ASN:HD22	1:B:365:GLY:H	1.28	0.80
1:A:106:ASN:H	1:A:113:ASN:HD21	1.27	0.80
1:A:4:LEU:HD22	1:A:58:TYR:CD2	2.19	0.77
1:B:72:VAL:O	1:B:100:LEU:HD23	1.89	0.72
1:B:52:HIS:HD2	1:B:60:PHE:H	1.39	0.71
1:A:4:LEU:CD2	1:A:58:TYR:CD2	2.73	0.71
1:A:293[B]:ARG:NH1	2:A:473:HOH:O	2.24	0.70
1:B:197:LEU:HD21	1:B:224:LYS:HG3	1.75	0.69
1:A:311:GLU:HG3	2:A:772:HOH:O	1.93	0.68
1:B:154:ALA:O	1:B:158:ASN:HB2	1.93	0.67
1:A:133[A]:ILE:HG12	2:A:517:HOH:O	1.96	0.66
1:A:89:ASP:HA	1:A:92:LYS:HG3	1.77	0.65
1:A:26:GLU:OE1	1:B:390:ARG:NH2	2.30	0.64
1:B:78:SER:O	1:B:82:LYS:HD2	1.97	0.64
1:A:36:LEU:HD13	1:A:139:TYR:CE2	2.32	0.63
1:A:99:THR:HG23	2:A:787:HOH:O	1.98	0.63
1:A:36:LEU:C	1:A:36:LEU:HD12	2.20	0.62
1:A:88:ILE:HD11	1:A:102:LEU:HD22	1.84	0.60
1:B:80:LYS:HE2	2:B:783:HOH:O	2.01	0.60
1:B:404:LYS:HE2	2:B:1057:HOH:O	2.02	0.59
1:A:133[A]:ILE:CG1	2:A:517:HOH:O	2.50	0.59
1:A:23:ASN:HB2	2:A:606:HOH:O	2.02	0.58
1:B:88:ILE:HD11	1:B:102:LEU:HD22	1.85	0.57
1:B:181:GLN:HE22	1:B:424:LEU:HD22	1.69	0.56
1:A:4:LEU:CD1	1:A:83:HIS:CD2	2.87	0.56
1:A:73:ILE:CG1	2:A:820:HOH:O	2.41	0.56
1:A:152:GLU:HG3	2:A:782:HOH:O	2.06	0.56
1:A:189:LYS:HG3	1:A:238:LEU:HD12	1.87	0.55
1:B:231:LEU:HA	1:B:234:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:LEU:HD12	1:A:37:GLY:N	2.21	0.55
1:B:142:LYS:HD2	2:B:1107:HOH:O	2.06	0.54
1:B:219:ASP:CG	2:B:1019:HOH:O	2.47	0.53
1:B:320:LEU:HD22	1:B:414:LEU:HB3	1.90	0.53
1:B:205:ALA:HA	1:B:210:LEU:HG	1.89	0.53
1:A:159:GLU:HG2	2:A:506:HOH:O	2.08	0.53
1:A:74:ILE:HB	1:A:102:LEU:HD12	1.90	0.53
1:B:100:LEU:CD2	1:B:101:GLU:N	2.68	0.53
1:B:108:LYS:O	1:B:108:LYS:CD	2.54	0.52
1:A:106:ASN:HB3	1:A:112:LEU:HD23	1.91	0.52
1:B:260[B]:ILE:CG2	1:B:289:SER:HB2	2.40	0.52
1:A:302:THR:HB	1:A:417:ALA:HB3	1.92	0.51
1:B:78:SER:O	1:B:82:LYS:CD	2.59	0.51
1:B:60:PHE:CD2	1:B:80:LYS:HD3	2.46	0.51
1:B:100:LEU:HD22	1:B:100:LEU:C	2.31	0.51
1:A:336[A]:ARG:HD2	2:A:679:HOH:O	2.11	0.51
1:B:215:ALA:HA	1:B:275:SER:HB3	1.93	0.50
1:B:109:GLU:HG3	1:B:112:LEU:HB3	1.93	0.50
1:A:29:PRO:HA	1:A:130:THR:HG22	1.92	0.50
1:B:339:LYS:HE3	1:B:343[B]:GLU:OE2	2.11	0.49
1:A:271:VAL:HB	2:A:684:HOH:O	2.12	0.49
1:A:53:ASN:ND2	2:A:652:HOH:O	2.39	0.49
1:B:260[B]:ILE:HG22	1:B:289:SER:HB2	1.95	0.49
1:A:4:LEU:HD12	1:A:83:HIS:CB	2.41	0.48
1:A:323:LEU:HD23	1:A:398:PHE:CE2	2.49	0.48
1:A:390:ARG:HH22	1:B:23:ASN:HD22	1.62	0.48
1:A:336[A]:ARG:NH1	1:A:344:SER:OG	2.47	0.47
1:A:106:ASN:N	1:A:113:ASN:HD21	2.06	0.47
1:B:338:PRO:HB2	1:B:383:ASN:HB3	1.97	0.47
1:B:136:LYS:HB2	2:B:773:HOH:O	2.13	0.47
1:A:52:HIS:CD2	1:A:60:PHE:H	2.17	0.47
1:B:52:HIS:HE1	2:B:772:HOH:O	1.96	0.47
1:B:36:LEU:HD13	1:B:139:TYR:CE2	2.50	0.46
1:B:193:LYS:HE3	1:B:237:ASP:HB2	1.96	0.46
1:A:343[B]:GLU:OE1	2:A:815:HOH:O	2.20	0.46
1:B:247:LYS:HB3	1:B:247:LYS:NZ	2.31	0.46
1:A:168:GLY:O	1:A:172:VAL:HG23	2.16	0.46
1:B:100:LEU:HD22	1:B:101:GLU:H	1.73	0.46
1:A:363:ASN:HD22	1:A:365:GLY:H	1.64	0.46
1:B:181:GLN:NE2	1:B:424:LEU:HD22	2.31	0.45
1:B:89:ASP:HA	1:B:92:LYS:NZ	2.31	0.45
1:B:82:LYS:N	1:B:82:LYS:HD2	2.32	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:GLU:CD	1:B:390:ARG:HH22	2.20	0.44
1:A:302:THR:HB	1:A:417:ALA:CB	2.48	0.44
1:A:4:LEU:CD2	1:A:58:TYR:CG	3.00	0.44
1:B:338:PRO:HB3	1:B:379:LEU:HA	2.00	0.44
1:B:106:ASN:N	1:B:113:ASN:HD21	2.01	0.43
1:B:319:PHE:HE2	1:B:352:THR:HG1	1.61	0.43
1:B:227:ASP:OD1	1:B:229:LYS:HB3	2.17	0.43
1:A:197:LEU:HD21	1:A:224:LYS:HG3	2.01	0.43
1:A:60:PHE:CD2	1:A:80:LYS:HD3	2.54	0.43
1:B:249:ASN:HB3	1:B:252:LEU:HD22	2.01	0.43
2:A:669:HOH:O	1:B:387:LYS:HE2	2.19	0.42
1:B:89:ASP:HA	1:B:92:LYS:CD	2.39	0.42
1:A:21:LYS:HE2	2:A:790:HOH:O	2.19	0.42
1:A:29:PRO:HA	1:A:130:THR:CG2	2.50	0.42
1:A:334:PRO:HB2	1:B:24:GLU:HG2	2.02	0.42
1:A:309:PRO:HB3	1:A:313:MET:HE2	2.00	0.42
1:B:96:SER:C	1:B:98:ILE:H	2.22	0.42
1:A:47[A]:LYS:HA	1:A:47[A]:LYS:HD3	1.89	0.42
1:B:98:ILE:HG22	1:B:99:THR:N	2.35	0.41
1:A:338:PRO:HB2	1:A:383:ASN:HB3	2.02	0.41
1:B:314:ALA:HB1	1:B:440:LYS:HE3	2.02	0.41
1:B:36:LEU:HD21	1:B:59:GLU:HG3	2.02	0.41
1:B:312:GLU:HG2	1:B:313:MET:N	2.35	0.41
1:A:228:VAL:HG23	2:A:728:HOH:O	2.20	0.41
1:A:147:TRP:CE2	1:A:151:TRP:HB2	2.56	0.41
1:A:36:LEU:CD1	1:A:36:LEU:C	2.86	0.41
1:A:339:LYS:O	1:A:343[A]:GLU:HG2	2.21	0.41
1:A:36:LEU:CD1	1:A:139:TYR:CE2	3.03	0.40
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.89	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	452/467 (97%)	436 (96%)	15 (3%)	1 (0%)	56	45
1	B	448/467 (96%)	438 (98%)	10 (2%)	0	100	100
All	All	900/934 (96%)	874 (97%)	25 (3%)	1 (0%)	59	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	GLY

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	416/427 (97%)	393 (94%)	23 (6%)	30	14
1	B	414/427 (97%)	394 (95%)	20 (5%)	35	18
All	All	830/854 (97%)	787 (95%)	43 (5%)	32	15

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	18	LEU
1	A	36	LEU
1	A	38	SER
1	A	43	ASN
1	A	52	HIS
1	A	82	LYS
1	A	85	GLN
1	A	92	LYS
1	A	93	ASP
1	A	97	LYS
1	A	98	ILE
1	A	100	LEU
1	A	102	LEU
1	A	108	LYS
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	135	GLU
1	A	187	SER
1	A	219	ASP
1	A	252	LEU
1	A	363	ASN
1	A	377	PHE
1	A	424	LEU
1	B	5	ASN
1	B	18	LEU
1	B	36	LEU
1	B	82	LYS
1	B	90	LEU
1	B	93	ASP
1	B	97	LYS
1	B	100	LEU
1	B	102	LEU
1	B	108	LYS
1	B	112	LEU
1	B	115	LYS
1	B	173	TRP
1	B	219	ASP
1	B	228	VAL
1	B	233	GLN
1	B	235	SER
1	B	377	PHE
1	B	411	ASN
1	B	424	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	52	HIS
1	A	83	HIS
1	A	85	GLN
1	A	113	ASN
1	A	148	ASN
1	A	161	ASN
1	A	214	ASN
1	A	315	ASN
1	A	316	ASN
1	A	330	ASN

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Mol	Chain	Res	Type
1	A	363	ASN
1	A	411	ASN
1	B	5	ASN
1	B	23	ASN
1	B	43	ASN
1	B	52	HIS
1	B	85	GLN
1	B	113	ASN
1	B	148	ASN
1	B	181	GLN
1	B	214	ASN
1	B	223	ASN
1	B	315	ASN
1	B	316	ASN
1	B	330	ASN
1	B	363	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

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, 95th 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 ²)	Q<0.9
1	A	444/467 (95%)	-0.08	3 (0%) 84 90	12, 24, 45, 87	5 (1%)
1	B	442/467 (94%)	-0.10	4 (0%) 81 86	12, 23, 44, 79	7 (1%)
All	All	886/934 (94%)	-0.09	7 (0%) 83 88	12, 23, 45, 87	12 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	LEU	5.4
1	B	448	ASN	3.0
1	B	108	LYS	2.9
1	A	5	ASN	2.7
1	B	85	GLN	2.6
1	A	82	LYS	2.1
1	B	96	SER	2.1

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.