wwPDB X-ray Structure Validation Summary Report (i)

Feb 10, 2024 – 08:15 PM EST

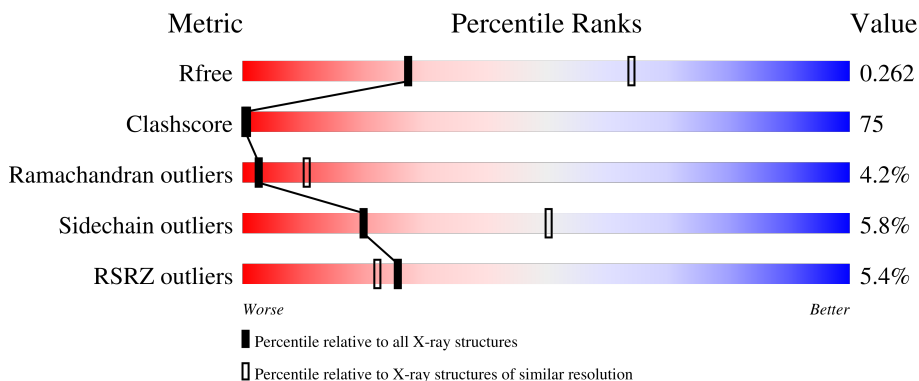|		
PDB ID	:	2OVP
Title	:	Structure of the Skp1-Fbw7 complex
Authors	:	Hao, B.; Oehlmann, S.; Sowa, M.E.; Harper, J.W.; Pavletich, N.P.
Deposited on	:	2007-02-14
Resolution	:	2.90 Å(reported)

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 2.90 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		75
Ramachandran outliers		4.2%
Sidechain outliers		5.8%
RSRZ outliers		5.4%

Worse .... *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	149	11% 16% 69% 5% 10%
2	B	445	3% 20% 71% 7% ••

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4676 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 S-phase kinase-associated protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total 1073	C 686	N 174	O 208	S 5	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	GLY	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	ASN	deletion	UNP P63208
A	1078	GLY	LYS	linker	UNP P63208
A	1079	GLY	GLU	linker	UNP P63208
A	1080	SER	LYS	linker	UNP P63208
A	1081	GLY	ARG	linker	UNP P63208

- Molecule 2 is a protein called F-box/WD repeat protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	441	Total 3484	C 2187	N 627	O 648	S 22	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	109	Total 109	O 109	0	0

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3 Residue-property plots ⓘ

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 and electron density. Residues are co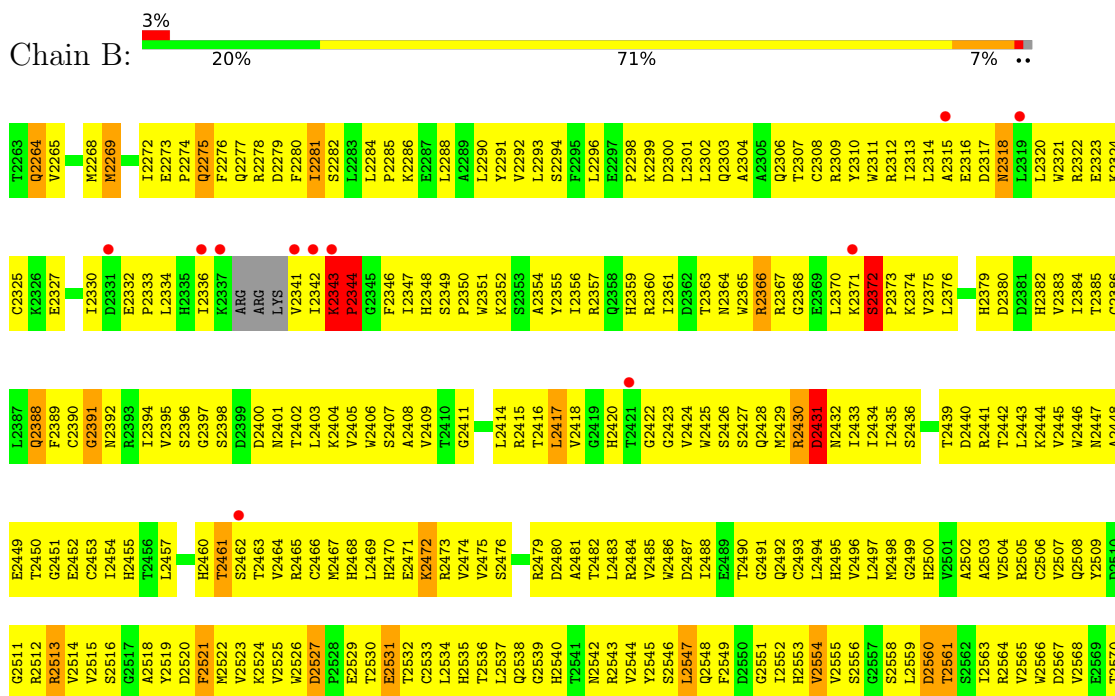lor-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: S-phase kinase-associated protein 1A

Chain A:
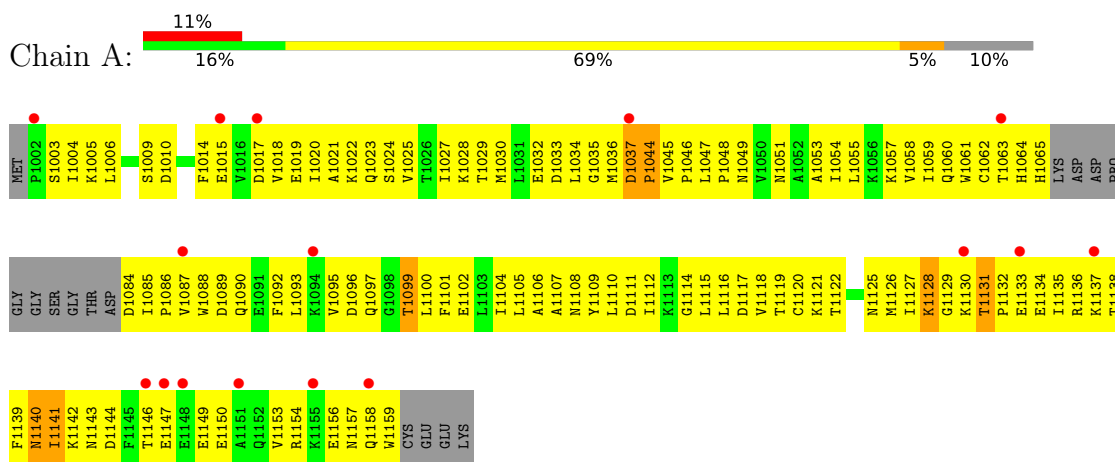
• Molecule 2: F-box/WD repeat protein 7

Chain B:

G2571 N2572 C2573 I2574 H2575 T2576 L2577 H2580 Q2581 S2582 L2583 T2584 S2585 G2586 M2587 E2588 L2589 K2590 D2591 N2592 I2593 L2594 V2595 S2596 G2597 N2598 A2599 D2600 S2601 T2602 V2603 K2604 I2605 W2606 D2607 I2608 K2609 T2610 G2611 L2614 Q2615 T2616 L2617 Q2618 G2619 K2622 H2623 A2626 V2627 T2628 C2629 L2630 K2634 V2637

I2638 T2639 S2640 S2641 D2642 D2643 V2646 K2647 L2648 W2649 D2650 L2651 K2652 T2653 G2654 E2655 F2656 I2657 R2658 N2659 L2660 V2661 T2662 L2663 E2664 S2665 G2666 G2667 S2668 G2669 G2670 V2671 V2672 W2673 R2674 I2675 R2676 A2677 S2678 N2679 T2680 K2681 L2682 V2683 C2684 A2685 V2686 G2687 S2688 R2689 N2690 G2691 T2692 E2693 T2694 T2695 K2696 L2697 L2698

V2699 L2700 D2701 F2702 D2703 V2704 D2705 M2706 LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	222.70Å 222.70Å 102.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.90 19.94 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-2.90) 97.9 (19.94-2.88)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$<I/\sigma(I)>$ [1]	5.10 (at 2.88Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.268 0.233 , 0.262	Depositor DCC
R_{free} test set	1959 reflections (6.72%)	wwPDB-VP
Wilson B-factor (Å^2)	37.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.6	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	4676	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical 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.

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	0.34	0/1091	0.61	0/1476
2	B	0.48	0/3554	0.76	3/4815 (0.1%)
All	All	0.45	0/4645	0.73	3/6291 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2372	SER	N-CA-C	-5.73	95.52	111.00
2	B	2527	ASP	N-CA-C	-5.36	96.54	111.00
2	B	2678	SER	N-CA-C	-5.18	97.01	111.00

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	1073	0	1083	168	0
2	B	3484	0	3468	557	0
3	A	10	0	0	2	0
3	B	109	0	0	12	0
All	All	4676	0	4551	687	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 75.

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The worst 5 of 687 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)
2:B:2343:LYS:HB3	2:B:2344:PRO:HD2	1.16	1.13
2:B:2487:ASP:HB2	2:B:2494:LEU:HD11	1.29	1.12
1:A:1037:ASP:HB2	1:A:1044:PRO:HD3	1.27	1.09
2:B:2642:ASP:HA	2:B:2671:VAL:HG23	1.07	1.07
2:B:2554:VAL:HG13	2:B:2566:TRP:HB2	1.35	1.02

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	130/149 (87%)	102 (78%)	19 (15%)	9 (7%)	1	3
2	B	437/445 (98%)	360 (82%)	62 (14%)	15 (3%)	3	15
All	All	567/594 (96%)	462 (82%)	81 (14%)	24 (4%)	3	10

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2275	GLN
2	B	2344	PRO
2	B	2366	ARG
2	B	2391	GLY
2	B	2431	ASP

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	122/134 (91%)	120 (98%)	2 (2%)	62	86
2	B	391/395 (99%)	363 (93%)	28 (7%)	14	39
All	All	513/529 (97%)	483 (94%)	30 (6%)	20	50

5 of 30 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	2521	PHE
2	B	2680	THR
2	B	2560	ASP
2	B	2705	ASP
2	B	2660	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	2432	ASN
2	B	2538	GLN
2	B	2659	ASN
2	B	2470	HIS
2	B	2540	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 monosaccharides 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(Å²)	Q<0.9
1	A	134/149 (89%)	0.40	16 (11%)	4	3	34, 58, 83, 91	0
2	B	441/445 (99%)	0.09	15 (3%)	45	40	9, 36, 73, 89	0
All	All	575/594 (96%)	0.17	31 (5%)	25	22	9, 41, 77, 91	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	VAL	5.0
2	B	2341	VAL	4.9
1	A	1002	PRO	4.2
2	B	2343	LYS	4.0
2	B	2705	ASP	3.4

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 monosaccharides 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.