Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:25 PM GMT

PDB ID	:	4IC4
Title	:	Crystal structure of Osh3 ORD from Saccharomyces cerevisiae
Authors	:	Tong, J.; Im, Y.J.
Deposited on	:	2012-12-09
Resolution	:	1.50 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.50 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.

Worse　　　　　　　　　　　　　　　　　　　Better

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
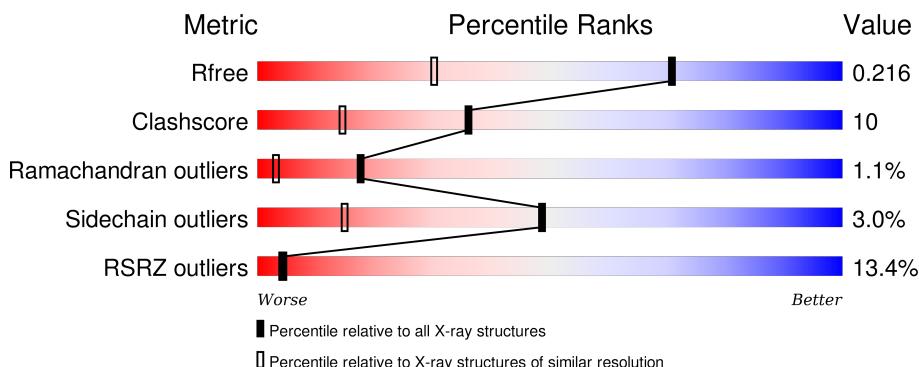
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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 <=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	397	13% / 74% / 18% / · 6%
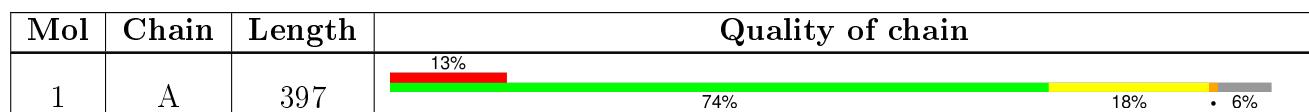
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3332 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 Oxysterol-binding protein homolog 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total	C	N	O	S	0	0	0
			3041	1947	521	568	5			

There are 5 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	600	GLY	-	EXPRESSION TAG	UNP P38713
A	601	ALA	-	EXPRESSION TAG	UNP P38713
A	602	MET	-	EXPRESSION TAG	UNP P38713
A	603	ASP	-	EXPRESSION TAG	UNP P38713
A	604	PRO	-	EXPRESSION TAG	UNP P38713

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	291	Total	O	0	0
			291	291		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. 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: Oxysterol-binding protein homolog 3
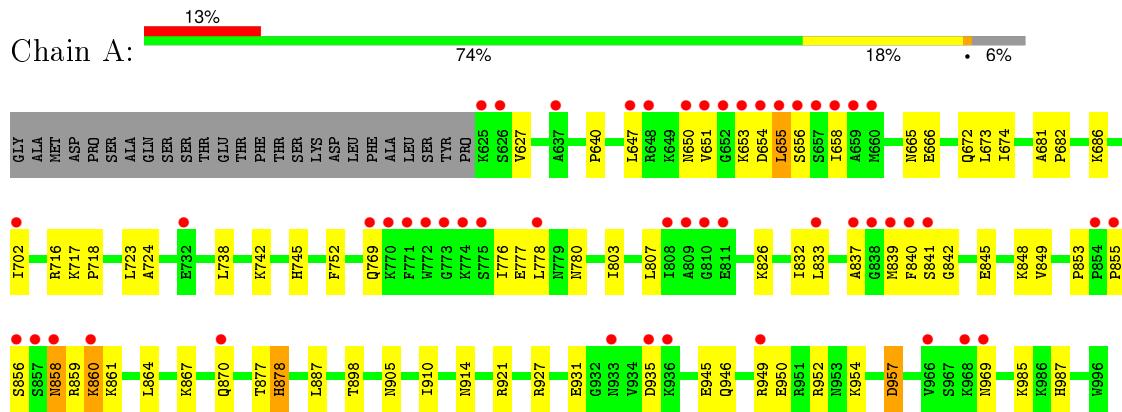
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	40.87Å 89.20Å 96.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.69 – 1.50 32.69 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.69-1.50) 99.6 (32.69-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.66 (at 1.50Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.234 0.218 , 0.216	Depositor DCC
R_{free} test set	2887 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 49.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 56924 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3332	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.30	0/3120	0.60	0/4218

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	3041	0	3034	58	0
2	A	291	0	0	4	0
All	All	3332	0	3034	58	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 10.

All (58) 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:A:655:LEU:HB3	1:A:769:GLN:OE1	1.83	0.78
1:A:640:PRO:HG3	1:A:716:ARG:CZ	2.17	0.75
1:A:686:LYS:HB2	1:A:686:LYS:HZ2	1.54	0.73
1:A:650:ASN:ND2	1:A:658:ILE:HD12	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:ASN:HD22	1:A:658:ILE:HD12	1.56	0.68
1:A:860:LYS:HA	1:A:860:LYS:HZ3	1.61	0.65
1:A:833:LEU:H	1:A:833:LEU:HD23	1.62	0.64
1:A:914:ASN:HD22	1:A:987:HIS:HE1	1.46	0.62
1:A:742:LYS:NZ	1:A:745:HIS:HD2	1.98	0.61
1:A:877:THR:O	1:A:878:HIS:HB2	1.99	0.61
1:A:672:GLN:HE22	1:A:905:ASN:HD22	1.46	0.61
1:A:640:PRO:HG3	1:A:716:ARG:NH2	2.17	0.59
1:A:952:ARG:HG3	1:A:957:ASP:OD2	2.02	0.59
1:A:686:LYS:HB2	1:A:686:LYS:NZ	2.18	0.58
1:A:833:LEU:HD23	1:A:848:LYS:O	2.05	0.57
1:A:837:ALA:HA	2:A:1163:HOH:O	2.04	0.57
1:A:860:LYS:HA	1:A:860:LYS:NZ	2.21	0.56
1:A:777:GLU:HA	1:A:803:ILE:HD13	1.88	0.56
1:A:946:GLN:HE22	1:A:950:GLU:CG	2.20	0.55
1:A:655:LEU:HD23	1:A:656:SER:N	2.22	0.54
1:A:858:ASN:HD22	1:A:859:ARG:N	2.05	0.54
1:A:969:ASN:HA	2:A:1145:HOH:O	2.07	0.54
1:A:849:VAL:HB	1:A:864:LEU:HB2	1.90	0.53
1:A:833:LEU:HD23	1:A:833:LEU:N	2.24	0.53
1:A:702:ILE:HD11	1:A:832:ILE:HG12	1.91	0.53
1:A:914:ASN:ND2	1:A:987:HIS:HE1	2.09	0.51
1:A:723:LEU:O	1:A:724:ALA:HB3	2.11	0.51
1:A:627:VAL:HG11	1:A:910:ILE:HG13	1.92	0.51
1:A:673:LEU:HD22	1:A:718:PRO:HG2	1.92	0.50
1:A:946:GLN:NE2	1:A:950:GLU:HG2	2.27	0.50
1:A:778:LEU:N	1:A:778:LEU:HD12	2.26	0.49
1:A:776:ILE:HG13	1:A:807:LEU:HD11	1.94	0.49
1:A:946:GLN:HE22	1:A:950:GLU:HG2	1.78	0.49
1:A:832:ILE:HD12	1:A:832:ILE:N	2.27	0.48
1:A:672:GLN:HE22	1:A:905:ASN:ND2	2.12	0.47
1:A:914:ASN:HD22	1:A:987:HIS:CE1	2.31	0.47
1:A:666:GLU:OE2	1:A:718:PRO:HG3	2.15	0.47
1:A:887:LEU:HA	1:A:898:THR:HA	1.96	0.47
1:A:905:ASN:HD21	1:A:921:ARG:HA	1.80	0.46
1:A:858:ASN:N	1:A:858:ASN:HD22	2.12	0.46
1:A:742:LYS:HZ3	1:A:745:HIS:HD2	1.62	0.46
1:A:665:ASN:HA	1:A:717:LYS:O	2.15	0.46
1:A:845:GLU:O	1:A:867:LYS:HA	2.15	0.45
1:A:855:PRO:O	1:A:856:SER:HB2	2.15	0.45
1:A:985:LYS:HB2	1:A:985:LYS:HE3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:LEU:C	1:A:738:LEU:HD23	2.37	0.45
1:A:954:LYS:HG3	2:A:1263:HOH:O	2.16	0.44
1:A:905:ASN:ND2	1:A:921:ARG:HA	2.32	0.44
1:A:840:PHE:C	1:A:842:GLY:H	2.21	0.43
1:A:674:ILE:HB	1:A:752:PHE:CZ	2.53	0.43
1:A:681:ALA:N	1:A:682:PRO:CD	2.82	0.43
1:A:826:LYS:HE2	2:A:1096:HOH:O	2.19	0.43
1:A:742:LYS:HE2	1:A:745:HIS:HA	2.01	0.42
1:A:927:ARG:O	1:A:931:GLU:HG3	2.20	0.41
1:A:653:LYS:NZ	1:A:653:LYS:CB	2.83	0.41
1:A:647:LEU:HD11	1:A:776:ILE:HD11	2.03	0.41
1:A:655:LEU:HD21	1:A:717:LYS:HD2	2.02	0.41
1:A:853:PRO:HD2	1:A:861:LYS:HG2	2.03	0.41

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	370/397 (93%)	354 (96%)	12 (3%)	4 (1%)	17 3

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	655	LEU
1	A	839	MET
1	A	841	SER
1	A	651	VAL

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	337/358 (94%)	327 (97%)	10 (3%)	48 15

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	654	ASP
1	A	780	ASN
1	A	858	ASN
1	A	860	LYS
1	A	870	GLN
1	A	878	HIS
1	A	935	ASP
1	A	945	GLU
1	A	949	ARG
1	A	957	ASP

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	650	ASN
1	A	745	HIS
1	A	780	ASN
1	A	799	GLN
1	A	806	ASN
1	A	818	ASN
1	A	858	ASN
1	A	905	ASN
1	A	914	ASN
1	A	933	ASN
1	A	946	GLN
1	A	994	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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)

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	372/397 (93%)	1.00	50 (13%)	4	4	6, 15, 43, 60	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	840	PHE	19.9
1	A	655	LEU	18.0
1	A	771	PHE	16.9
1	A	838	GLY	16.1
1	A	772	TRP	10.6
1	A	837	ALA	8.3
1	A	841	SER	7.5
1	A	658	ILE	7.2
1	A	856	SER	7.1
1	A	839	MET	7.0
1	A	654	ASP	6.7
1	A	855	PRO	6.4
1	A	625	LYS	6.4
1	A	774	LYS	6.4
1	A	651	VAL	5.8
1	A	653	LYS	5.6
1	A	858	ASN	5.1
1	A	626	SER	4.9
1	A	808	ILE	4.8
1	A	656	SER	4.6
1	A	773	GLY	4.6
1	A	833	LEU	4.5
1	A	637	ALA	4.3
1	A	860	LYS	4.2
1	A	650	ASN	3.6
1	A	966	VAL	3.4
1	A	770	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	935	ASP	3.4
1	A	775	SER	3.3
1	A	732	GLU	3.2
1	A	809	ALA	3.1
1	A	659	ALA	2.9
1	A	969	ASN	2.9
1	A	769	GLN	2.9
1	A	810	GLY	2.8
1	A	660	MET	2.8
1	A	647	LEU	2.7
1	A	870	GLN	2.7
1	A	652	GLY	2.6
1	A	657	SER	2.6
1	A	857	SER	2.5
1	A	648	ARG	2.4
1	A	811	GLU	2.2
1	A	933	ASN	2.1
1	A	936	LYS	2.1
1	A	702	ILE	2.1
1	A	968	LYS	2.1
1	A	778	LEU	2.1
1	A	949	ARG	2.0
1	A	854	PRO	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.