



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:04 AM GMT

PDB ID : 1ZHI  
Title : Complex of the *S. cerevisiae* Orc1 and Sir1 interacting domains  
Authors : Hou, Z.; Bernstein, D.A.; Fox, C.A.; Keck, J.L.  
Deposited on : 2005-04-25  
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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

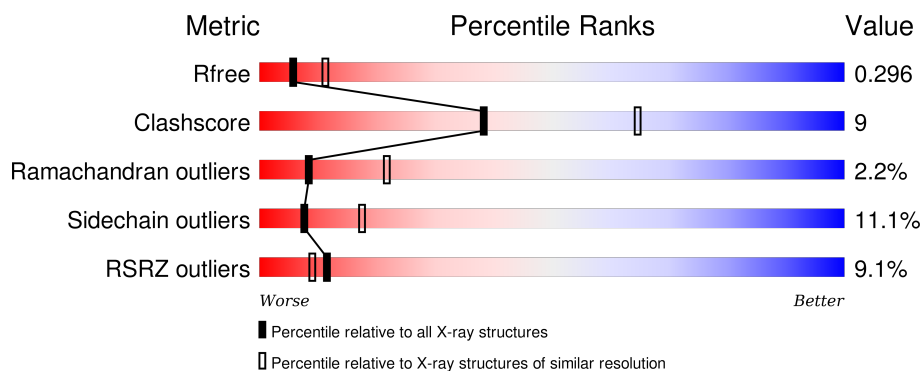
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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.

Mol	Chain	Length	Quality of chain
1	A	225	<div> <div>8%</div> <div>63%</div> <div>22%</div> <div>•</div> <div>13%</div> </div>
2	B	138	<div> <div>7%</div> <div>64%</div> <div>22%</div> <div>• •</div> <div>9%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2699 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 Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1597	1020	268	305	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	CLONING ARTIFACT	UNP P54784
A	-4	SER	-	CLONING ARTIFACT	UNP P54784
A	-3	HIS	-	CLONING ARTIFACT	UNP P54784
A	-2	MET	-	CLONING ARTIFACT	UNP P54784
A	-1	ALA	-	CLONING ARTIFACT	UNP P54784
A	0	SER	-	CLONING ARTIFACT	UNP P54784

- Molecule 2 is a protein called Regulatory protein SIR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	125	Total	C	N	O	S	0	0	0
			1036	675	170	186	5			

There are 7 discrepancies between the modelled and reference sequences:

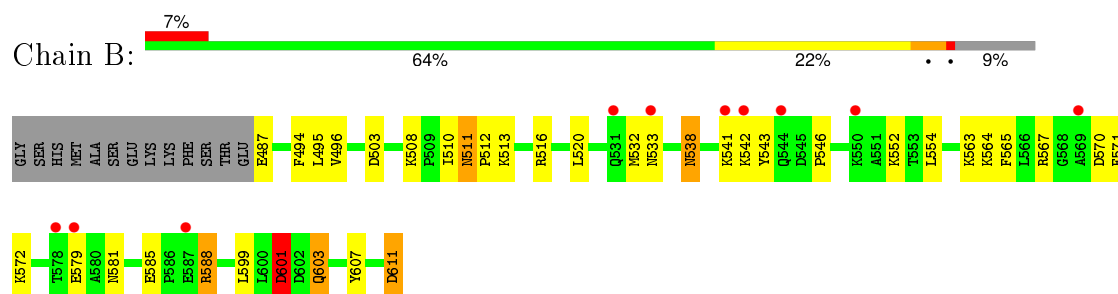
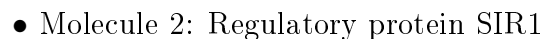
Chain	Residue	Modelled	Actual	Comment	Reference
B	474	GLY	-	CLONING ARTIFACT	UNP P21691
B	475	SER	-	CLONING ARTIFACT	UNP P21691
B	476	HIS	-	CLONING ARTIFACT	UNP P21691
B	477	MET	-	CLONING ARTIFACT	UNP P21691
B	478	ALA	-	CLONING ARTIFACT	UNP P21691
B	479	SER	-	CLONING ARTIFACT	UNP P21691
B	593	ALA	CYS	ENGINEERED	UNP P21691

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	31	Total 31	O 31	0	0



- Molecule 1: Origin recognition complex subunit 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.15Å 72.15Å 310.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.00 – 2.70 17.97 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.5 (18.00-2.70) 98.5 (17.97-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.70Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.231 , 0.293 0.247 , 0.296	Depositor DCC
$R_{free}$ test set	697 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 13843 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.52	0/1631	0.68	8/2213 (0.4%)
2	B	0.57	0/1060	0.77	2/1432 (0.1%)
All	All	0.54	0/2691	0.72	10/3645 (0.3%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	191	ASP	CB-CG-OD2	6.23	123.91	118.30
2	B	611	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	170	ASP	CB-CG-OD2	5.86	123.57	118.30
1	A	24	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	108	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	54	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	210	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	601	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	186	ASP	CB-CG-OD2	5.08	122.87	118.30

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	1597	0	1559	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1036	0	1064	25	0
3	A	35	0	0	1	0
3	B	31	0	0	1	0
All	All	2699	0	2623	48	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 9.

All (48) 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:503:ASP:HB2	2:B:510:ILE:HD11	1.44	0.97
1:A:18:GLU:O	1:A:19:GLN:HB2	1.67	0.95
2:B:503:ASP:HB2	2:B:510:ILE:CD1	2.10	0.81
1:A:61:GLU:O	2:B:516:ARG:NH1	2.19	0.75
1:A:74:LEU:HD21	1:A:85:LEU:HD13	1.72	0.70
1:A:77:ASN:OD1	1:A:79:LEU:HD23	1.94	0.67
1:A:104:GLN:NE2	3:A:253:HOH:O	2.29	0.65
1:A:106:ASN:HB2	1:A:109:ALA:HB3	1.80	0.64
1:A:71:ILE:HG12	1:A:85:LEU:HD11	1.81	0.62
2:B:496:VAL:HG11	2:B:532:MET:HG2	1.83	0.61
2:B:494:PHE:HE2	2:B:510:ILE:CD1	2.15	0.60
2:B:563:LYS:HD2	3:B:54:HOH:O	2.04	0.57
2:B:511:ASN:ND2	2:B:513:LYS:H	2.04	0.56
1:A:46:ASP:OD1	1:A:48:ILE:HG12	2.07	0.55
1:A:40:TYR:HA	1:A:74:LEU:HD12	1.89	0.55
2:B:503:ASP:CB	2:B:510:ILE:HD11	2.28	0.53
2:B:567:ARG:HD2	2:B:571:PHE:CD2	2.45	0.52
1:A:112:LEU:HD22	1:A:119:TYR:OH	2.10	0.51
2:B:511:ASN:HD22	2:B:513:LYS:H	1.58	0.51
2:B:494:PHE:HE2	2:B:510:ILE:HD12	1.76	0.51
1:A:102:TYR:CE2	1:A:109:ALA:HB1	2.47	0.50
1:A:106:ASN:O	1:A:109:ALA:HB3	2.12	0.49
2:B:585:GLU:HB3	2:B:588:ARG:HG3	1.94	0.49
2:B:494:PHE:CE2	2:B:510:ILE:HD12	2.48	0.49
2:B:511:ASN:HD22	2:B:512:PRO:N	2.10	0.48
1:A:58:MET:SD	1:A:146:PHE:HA	2.54	0.48
2:B:538:ASN:HA	2:B:538:ASN:HD22	1.56	0.48
2:B:563:LYS:HE2	2:B:607:TYR:CZ	2.50	0.46
2:B:511:ASN:HD22	2:B:512:PRO:CD	2.29	0.46
1:A:60:ASN:HB3	1:A:65:THR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:THR:C	1:A:80:ASN:H	2.19	0.45
1:A:121:LYS:O	1:A:125:GLU:HB2	2.15	0.45
1:A:63:ALA:HA	2:B:520:LEU:HD21	1.98	0.45
2:B:511:ASN:ND2	2:B:512:PRO:HD2	2.33	0.44
1:A:106:ASN:HB2	1:A:109:ALA:CB	2.47	0.44
1:A:103:ARG:HG3	1:A:110:ASN:HB3	1.98	0.44
1:A:109:ALA:O	1:A:112:LEU:HD21	2.19	0.43
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.88	0.43
1:A:104:GLN:HE22	1:A:184:PHE:H	1.67	0.43
2:B:599:LEU:HD21	2:B:603:GLN:HE22	1.83	0.42
2:B:511:ASN:HD22	2:B:512:PRO:HD2	1.82	0.42
2:B:570:ASP:O	2:B:571:PHE:HB2	2.19	0.42
1:A:131:GLU:OE2	1:A:174:ARG:HD3	2.20	0.42
2:B:599:LEU:HD21	2:B:603:GLN:NE2	2.35	0.41
2:B:546:PRO:HG3	2:B:565:PHE:CE2	2.55	0.41
1:A:102:TYR:CE2	1:A:109:ALA:CB	3.04	0.40
1:A:43:ARG:NH2	1:A:146:PHE:HE2	2.18	0.40
2:B:563:LYS:HE2	2:B:607:TYR:OH	2.21	0.40

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	191/225 (85%)	178 (93%)	8 (4%)	5 (3%)	7	16
2	B	123/138 (89%)	115 (94%)	6 (5%)	2 (2%)	12	30
All	All	314/363 (86%)	293 (93%)	14 (4%)	7 (2%)	8	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	162	LYS
2	B	601	ASP
1	A	17	ASP
1	A	79	LEU
1	A	25	GLY
2	B	579	GLU

### 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	173/198 (87%)	159 (92%)	14 (8%)	15	33
2	B	116/127 (91%)	98 (84%)	18 (16%)	3	8
All	All	289/325 (89%)	257 (89%)	32 (11%)	8	17

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	19	GLN
1	A	23	ILE
1	A	43	ARG
1	A	46	ASP
1	A	82	VAL
1	A	83	VAL
1	A	99	LEU
1	A	113	ASN
1	A	114	ARG
1	A	116	LEU
1	A	140	GLU
1	A	156	SER
1	A	159	GLU
2	B	487	GLU
2	B	495	LEU
2	B	508	LYS

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Mol	Chain	Res	Type
2	B	511	ASN
2	B	533	ASN
2	B	538	ASN
2	B	541	LYS
2	B	542	LYS
2	B	543	TYR
2	B	552	LYS
2	B	554	LEU
2	B	564	LYS
2	B	572	LYS
2	B	581	ASN
2	B	588	ARG
2	B	601	ASP
2	B	603	GLN
2	B	611	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	113	ASN
1	A	130	ASN
2	B	511	ASN
2	B	538	ASN
2	B	603	GLN

### 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	195/225 (86%)	0.53	19 (9%) 10 7	24, 62, 111, 135	0
2	B	125/138 (90%)	0.30	10 (8%) 15 13	27, 52, 90, 113	0
All	All	320/363 (88%)	0.44	29 (9%) 11 9	24, 56, 105, 135	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	109	ALA	11.9
1	A	111	ILE	8.8
2	B	578	THR	8.2
1	A	110	ASN	7.5
1	A	24	ASP	5.1
1	A	78	THR	5.1
1	A	107	PRO	4.3
1	A	21	ASN	4.2
2	B	544	GLN	4.2
1	A	22	ILE	3.8
1	A	108	ASP	3.6
1	A	80	ASN	3.4
1	A	214	PRO	3.4
1	A	20	GLY	3.4
1	A	79	LEU	3.3
2	B	542	LYS	3.3
2	B	579	GLU	3.3
2	B	569	ALA	3.1
2	B	533	ASN	3.1
1	A	37	THR	3.1
1	A	81	ASN	3.0
2	B	541	LYS	3.0
2	B	531	GLN	3.0
1	A	164	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	76	LEU	2.4
1	A	38	GLU	2.3
2	B	550	LYS	2.2
1	A	112	LEU	2.1
2	B	587	GLU	2.1

## 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.