



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 06:28 AM GMT

PDB ID : 2PFV  
Title : S. cerevisiae Exo70 with additional residues to 2.1 Angstrom resolution  
Authors : Moore, B.A.; Robinson, H.H.; Xu, Z.  
Deposited on : 2007-04-05  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

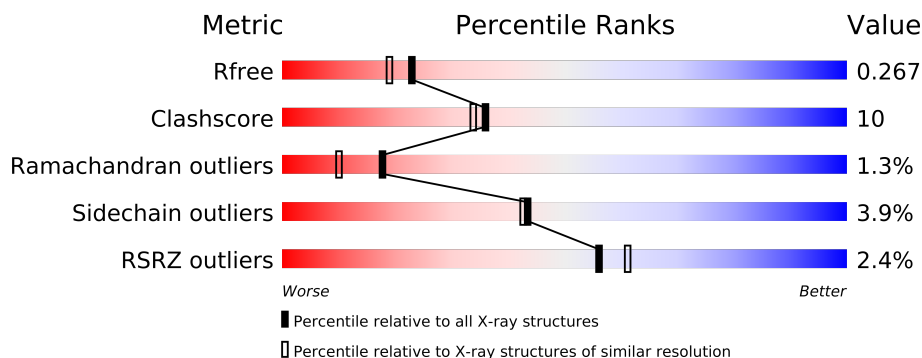
The following versions of software and data (see [references](#)) were used in the production of this report:

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 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (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  $\geq 3$ , 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	563	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4415 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 Exocyst complex component EXO70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4304	2733	727	826	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	GLY	-	CLONING ARTIFACT	UNP P19658
A	62	SER	-	CLONING ARTIFACT	UNP P19658

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	111	Total	O	0	0
			111	111		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.54Å 60.07Å 222.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.84 – 2.10 40.84 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.3 (40.84-2.10) 92.2 (40.84-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.06 (at 2.10Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.237 , 0.263 0.241 , 0.267	Depositor DCC
$R_{free}$ test set	1634 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.5	Xtriage
Anisotropy	0.518	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 34.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 64253 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.40	3/4376 (0.1%)	0.54	1/5909 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	TYR	CB-CG	-6.12	1.42	1.51
1	A	220	PHE	CB-CG	-5.40	1.42	1.51
1	A	323	GLU	CB-CG	-5.36	1.42	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	PRO	N-CA-CB	5.54	109.95	103.30

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	4304	0	4222	89	0
2	A	111	0	0	0	0
All	All	4415	0	4222	89	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 10.

All (89) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:326:ASN:HB2	1:A:329:LEU:HD23	1.45	0.95
1:A:366:ASN:HD21	1:A:471:ARG:HE	1.11	0.94
1:A:366:ASN:ND2	1:A:471:ARG:HE	1.84	0.76
1:A:375:THR:HG22	1:A:376:MET:HE2	1.68	0.75
1:A:87:ILE:HA	1:A:90:LYS:HE3	1.68	0.74
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.53	0.73
1:A:366:ASN:HD21	1:A:471:ARG:NE	1.87	0.70
1:A:268:LYS:HB2	1:A:269:PRO:HD3	1.76	0.67
1:A:221:ALA:CB	1:A:286:LEU:HD21	2.24	0.66
1:A:74:VAL:HG11	1:A:126:GLU:HG2	1.76	0.66
1:A:298:LEU:HD12	1:A:302:GLY:HA2	1.78	0.64
1:A:394:ASP:C	1:A:396:ILE:H	2.03	0.63
1:A:326:ASN:HB2	1:A:329:LEU:CD2	2.25	0.61
1:A:90:LYS:NZ	1:A:94:GLN:HE22	1.97	0.61
1:A:320:ARG:HG2	1:A:320:ARG:HH11	1.66	0.61
1:A:206:ARG:O	1:A:210:ILE:HG12	2.01	0.59
1:A:221:ALA:HB3	1:A:286:LEU:HD21	1.84	0.58
1:A:380:ARG:NH1	1:A:380:ARG:HG3	2.15	0.58
1:A:610:THR:OG1	1:A:613:GLU:HG3	2.03	0.58
1:A:243:THR:O	1:A:247:LEU:HG	2.04	0.58
1:A:414:GLN:O	1:A:416:GLU:N	2.36	0.57
1:A:328:ASN:OD1	1:A:329:LEU:HD22	2.05	0.55
1:A:580:GLU:O	1:A:584:LEU:HG	2.06	0.55
1:A:85:GLU:O	1:A:89:GLN:HG3	2.07	0.55
1:A:375:THR:HG22	1:A:376:MET:CE	2.35	0.55
1:A:560:VAL:HG12	1:A:564:LYS:HE3	1.88	0.55
1:A:221:ALA:HB1	1:A:286:LEU:HD21	1.89	0.54
1:A:473:GLY:O	1:A:477:LEU:HD22	2.07	0.54
1:A:199:GLN:HE22	1:A:270:HIS:CD2	2.26	0.54
1:A:419:ASN:HD22	1:A:422:ASP:HB2	1.74	0.52
1:A:477:LEU:HD23	1:A:515:MET:CE	2.39	0.52
1:A:390:LEU:HG	1:A:423:HIS:HB3	1.91	0.52
1:A:211:LEU:HD23	1:A:211:LEU:C	2.30	0.52
1:A:369:THR:H	1:A:479:ASN:HD21	1.57	0.51
1:A:469:LYS:HE2	1:A:517:SER:OG	2.11	0.51
1:A:236:SER:O	1:A:237:SER:HB2	2.11	0.51
1:A:380:ARG:NH1	1:A:490:SER:HB2	2.27	0.50
1:A:91:GLY:O	1:A:95:VAL:HG23	2.12	0.50
1:A:348:ALA:O	1:A:352:ILE:HG13	2.11	0.49
1:A:372:THR:HG22	1:A:482:LEU:HD23	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:175:GLU:CG	1:A:178:GLN:HG3	2.43	0.49
1:A:90:LYS:HZ3	1:A:94:GLN:HE22	1.61	0.48
1:A:513:SER:HA	1:A:516:VAL:HG12	1.96	0.48
1:A:542:LYS:O	1:A:546:LYS:HG3	2.13	0.47
1:A:418:LEU:HD12	1:A:418:LEU:O	2.13	0.47
1:A:365:ASN:HD22	1:A:365:ASN:N	2.12	0.47
1:A:593:TYR:CE2	1:A:597:LYS:HD3	2.50	0.47
1:A:619:ASN:O	1:A:623:ARG:HG3	2.14	0.47
1:A:386:LYS:O	1:A:390:LEU:HB2	2.15	0.47
1:A:578:LYS:HG3	1:A:622:VAL:CB	2.45	0.47
1:A:305:SER:O	1:A:309:VAL:HG23	2.15	0.47
1:A:175:GLU:HG2	1:A:178:GLN:OE1	2.15	0.46
1:A:622:VAL:O	1:A:623:ARG:C	2.53	0.46
1:A:519:TRP:CD2	1:A:559:LEU:HD13	2.51	0.46
1:A:527:MET:HB2	1:A:588:MET:CE	2.46	0.46
1:A:159:PHE:CZ	1:A:172:PRO:HD2	2.50	0.46
1:A:98:LYS:HG2	1:A:184:TRP:CE2	2.50	0.46
1:A:398:ARG:NH1	1:A:413:LEU:HD23	2.32	0.45
1:A:320:ARG:HG2	1:A:320:ARG:NH1	2.31	0.45
1:A:412:THR:OG1	1:A:503:ARG:HB3	2.17	0.45
1:A:312:ILE:HD11	1:A:330:LEU:HD22	1.98	0.45
1:A:90:LYS:HZ2	1:A:94:GLN:HE22	1.65	0.44
1:A:445:LYS:HD2	1:A:445:LYS:C	2.37	0.44
1:A:394:ASP:C	1:A:396:ILE:N	2.70	0.44
1:A:501:HIS:O	1:A:505:GLU:HG2	2.16	0.44
1:A:570:ASP:OD1	1:A:572:SER:HB2	2.18	0.44
1:A:517:SER:HA	1:A:520:ARG:NH1	2.33	0.44
1:A:477:LEU:HD22	1:A:511:TYR:HB3	2.00	0.43
1:A:496:LEU:O	1:A:497:ALA:C	2.57	0.43
1:A:399:GLU:N	1:A:399:GLU:OE1	2.52	0.43
1:A:238:GLY:O	1:A:242:TYR:HB2	2.18	0.43
1:A:369:THR:H	1:A:479:ASN:ND2	2.15	0.43
1:A:510:ARG:HD2	1:A:511:TYR:CE1	2.54	0.42
1:A:254:LYS:HE3	1:A:258:ASP:OD2	2.19	0.42
1:A:77:LEU:HA	1:A:77:LEU:HD12	1.91	0.42
1:A:94:GLN:NE2	1:A:94:GLN:C	2.72	0.42
1:A:418:LEU:O	1:A:420:TRP:N	2.51	0.42
1:A:199:GLN:HE22	1:A:270:HIS:HD2	1.66	0.42
1:A:280:ILE:HG13	1:A:324:LEU:HD21	2.02	0.42
1:A:380:ARG:NH1	1:A:490:SER:CB	2.83	0.42
1:A:312:ILE:CD1	1:A:330:LEU:HD22	2.50	0.42
1:A:298:LEU:CD1	1:A:302:GLY:HA2	2.47	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.92	0.41
1:A:376:MET:HB3	1:A:486:ILE:HG21	2.03	0.41
1:A:486:ILE:O	1:A:490:SER:HB3	2.20	0.41
1:A:477:LEU:HD23	1:A:515:MET:HE2	2.02	0.41
1:A:175:GLU:HG3	1:A:178:GLN:HG3	2.01	0.41
1:A:516:VAL:O	1:A:516:VAL:HG22	2.20	0.41
1:A:487:VAL:O	1:A:493:ASN:HB2	2.20	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	545/563 (97%)	525 (96%)	13 (2%)	7 (1%)	18 10

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	SER
1	A	415	ASN
1	A	417	ALA
1	A	622	VAL
1	A	406	TYR
1	A	419	ASN
1	A	237	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	466/514 (91%)	448 (96%)	18 (4%)	43	43

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	80	GLU
1	A	94	GLN
1	A	134	LEU
1	A	144	GLN
1	A	209	LEU
1	A	218	GLU
1	A	300	ASN
1	A	332	ASP
1	A	339	GLN
1	A	365	ASN
1	A	399	GLU
1	A	406	TYR
1	A	418	LEU
1	A	460	ASN
1	A	477	LEU
1	A	558	ASP
1	A	577	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	69	ASN
1	A	94	GLN
1	A	102	GLN
1	A	120	ASN
1	A	136	GLN
1	A	162	GLN
1	A	190	HIS
1	A	192	ASN
1	A	240	ASN
1	A	252	ASN
1	A	270	HIS
1	A	300	ASN
1	A	313	ASN
1	A	339	GLN
1	A	342	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	365	ASN
1	A	366	ASN
1	A	400	ASN
1	A	419	ASN
1	A	441	ASN
1	A	454	GLN
1	A	460	ASN
1	A	462	ASN
1	A	479	ASN
1	A	485	GLN
1	A	619	ASN
1	A	620	GLN

### 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, 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	549/563 (97%)	0.28	13 (2%) 56 61	23, 42, 72, 82	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	LEU	4.7
1	A	117	GLY	4.4
1	A	623	ARG	2.9
1	A	236	SER	2.9
1	A	221	ALA	2.8
1	A	532	ILE	2.8
1	A	415	ASN	2.7
1	A	301	PHE	2.7
1	A	417	ALA	2.6
1	A	294	VAL	2.5
1	A	293	ILE	2.5
1	A	406	TYR	2.4
1	A	427	LEU	2.2

### 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.