



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:12 AM GMT

PDB ID : 2WP8
Title : yeast rrp44 nuclease
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Deposited on : 2009-08-03
Resolution : 3.00 Å(reported)

This is a wwPDB validation summary 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>

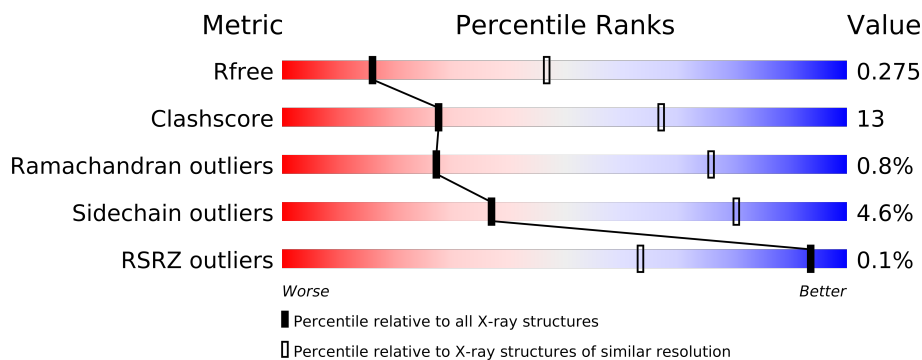
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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	305	
2	B	246	
3	J	977	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	GOL	J	2002	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10816 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 EXOSOME COMPLEX COMPONENT RRP45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			1946	1232	329	370	15			

- Molecule 2 is a protein called EXOSOME COMPLEX COMPONENT SKI6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1647	1031	285	323	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	ASN	THR	CONFLICT	UNP P46948

- Molecule 3 is a protein called EXOSOME COMPLEX EXONUCLEASE DIS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	918	Total	C	N	O	S	0	0	0
			7216	4574	1250	1359	33			

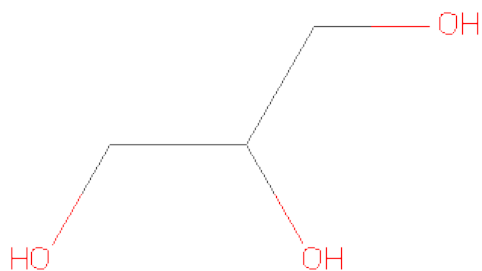
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	551	ASN	ASP	ENGINEERED MUTATION	UNP Q08162

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



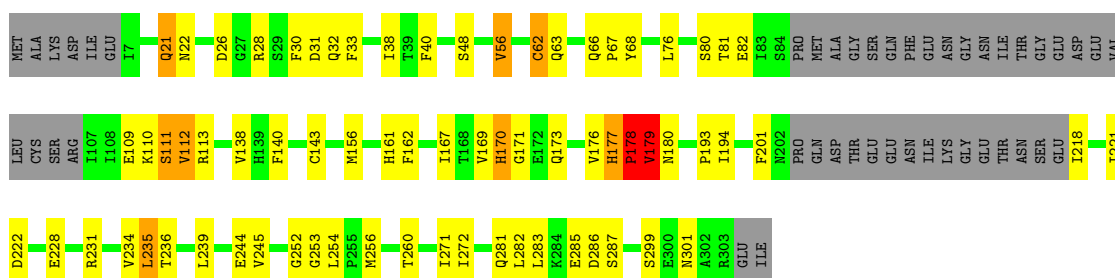
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total	C	O	0	0
			6	3	3		

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.

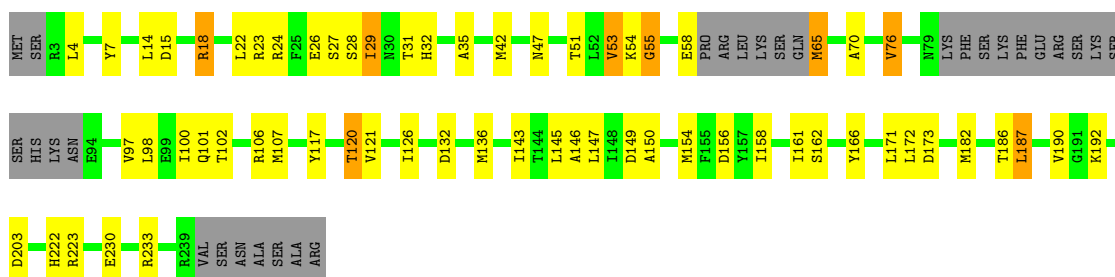
- Molecule 1: EXOSOME COMPLEX COMPONENT RRP45

Chain A:



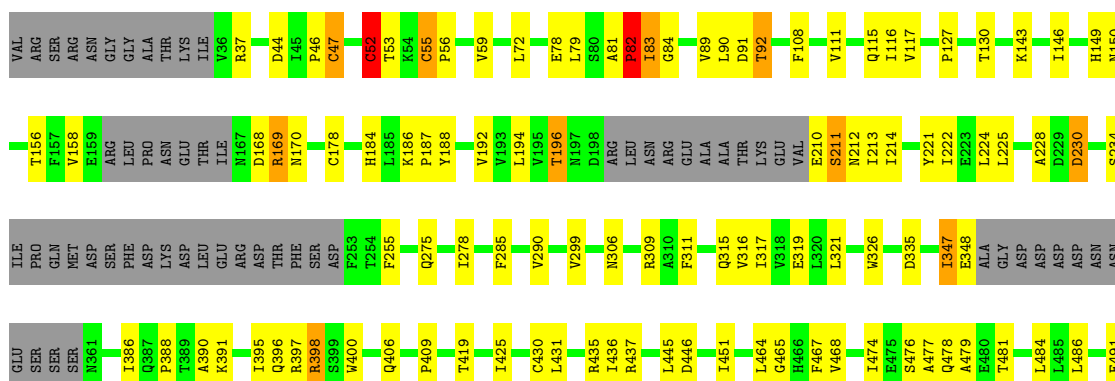
- Molecule 2: EXOSOME COMPLEX COMPONENT SKI6

Chain B:



- Molecule 3: EXOSOME COMPLEX EXONUCLEASE DIS3

Chain J:



Y492	R493	P494	F495	Y499	L500	E501	C502	H508	A512	L516	V522	D525	L528	L534	K537	L538	L539	D543	P544	N551	H555	E565	V566	L583	E586	R590	S593	V594	Y595	L596	K599	D602	L607	C613	P617	Y618	V619			
D620	F624	W628	D631	D632	S633	A634	N635	V639	V645	I646	Y654	I661	R675	L678	K683	R688	A693	P699	V703	P712	N713	L720	L721	A722	T723	N724	S725	L726	V727	E728	E729	F730	M731	L732	L733	A734	V738	A739	M751	L752
H755	T761	K773	R774	N775	S776	S777	I778	S783	L786	L790	F801	N802	T803	L804	V805	R806	R811	N814	Y832	T840	S844	P845	I846	D851	Q857	L867	H871	M877	Y903	G904	Q905	R908	T913	E914	T915	F933	G934	Y935	E936	
I939	R940	L941	L944	T945	E946	A952	T961	T965	N966	D972	V975	V981	N987	I990	T991	S992	K993	L999	L1000	K1001																				

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.90Å 125.68Å 139.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 19.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-3.00) 100.0 (19.99-3.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.60 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.207 , 0.273 0.212 , 0.275	Depositor DCC
R_{free} test set	1185 reflections (3.09%)	DCC
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , -0.3	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 39511 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10816	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL

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	0.72	0/1973	0.82	3/2668 (0.1%)
2	B	0.68	0/1665	0.81	2/2254 (0.1%)
3	J	0.67	7/7362 (0.1%)	0.81	4/10007 (0.0%)
All	All	0.68	7/11000 (0.1%)	0.81	9/14929 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
3	J	0	3
All	All	0	6

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	82	PRO	C-N	-15.57	0.98	1.34
3	J	430	CYS	CB-SG	-7.98	1.68	1.82
3	J	52	CYS	CB-SG	7.58	1.95	1.82
3	J	55	CYS	CB-SG	7.04	1.94	1.82
3	J	502	CYS	CB-SG	-6.43	1.71	1.82

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	82	PRO	O-C-N	-23.90	84.46	122.70
3	J	82	PRO	CA-C-N	17.47	155.63	117.20
3	J	82	PRO	C-N-CA	12.62	153.25	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	18	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	B	18	ARG	NE-CZ-NH1	5.41	123.01	120.30

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	PRO	Peptide
1	A	21	GLN	Peptide
1	A	252	GLY	Peptide
3	J	168	ASP	Peptide
3	J	82	PRO	Mainchain,Peptide

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	1946	0	1883	56	0
2	B	1647	0	1616	59	0
3	J	7216	0	7084	164	0
4	B	1	0	0	0	0
5	J	6	0	8	1	0
All	All	10816	0	10591	274	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 13.

The worst 5 of 274 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:GLN:O	1:A:67:PRO:N	1.76	1.19
3:J:210:GLU:CB	3:J:211:SER:HA	1.76	1.15
3:J:210:GLU:CB	3:J:211:SER:CA	2.29	1.10
3:J:52:CYS:SG	3:J:184:HIS:NE2	2.24	1.09
2:B:31:THR:HG22	2:B:32:HIS:CD2	1.90	1.06

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	252/305 (83%)	231 (92%)	15 (6%)	6 (2%)	9	42
2	B	211/246 (86%)	195 (92%)	15 (7%)	1 (0%)	38	84
3	J	908/977 (93%)	862 (95%)	42 (5%)	4 (0%)	43	87
All	All	1371/1528 (90%)	1288 (94%)	72 (5%)	11 (1%)	27	76

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	SER
1	A	178	PRO
1	A	179	VAL
3	J	212	ASN
2	B	55	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	204/266 (77%)	190 (93%)	14 (7%)	22	62
2	B	175/218 (80%)	164 (94%)	11 (6%)	25	66
3	J	789/881 (90%)	760 (96%)	29 (4%)	45	86
All	All	1168/1365 (86%)	1114 (95%)	54 (5%)	37	80

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	203	ASP
3	J	234	SER
3	J	913	THR
3	J	52	CYS
3	J	158	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
3	J	396	GLN
3	J	569	HIS
3	J	890	ASN
3	J	315	GLN
3	J	905	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 ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	J	2002	-	5,5,5	0.49	0	5,5,5	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	J	2002	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	260/305 (85%)	-0.23	0	100	100	18, 29, 49, 55	0
2	B	217/246 (88%)	-0.25	0	100	100	17, 25, 43, 66	0
3	J	918/977 (93%)	-0.24	1 (0%)	93	63	14, 29, 45, 61	0
All	All	1395/1528 (91%)	-0.24	1 (0%)	93	63	14, 28, 45, 66	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	966	ASN	2.4

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 carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	J	2002	6/6	0.35	3.37	33,36,38,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CL	B	1240	1/1	0.10	-2.04	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.