



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:56 PM GMT

PDB ID : 4B08
Title : Yeast DNA polymerase alpha, Selenomethionine protein
Authors : Perera, R.L.; Torella, R.; Klinge, S.; Kilkenny, M.L.; Maman, J.D.; Pellegrini, L.
Deposited on : 2012-06-29
Resolution : 2.67 Å(reported)

This is a full wwPDB validation 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>

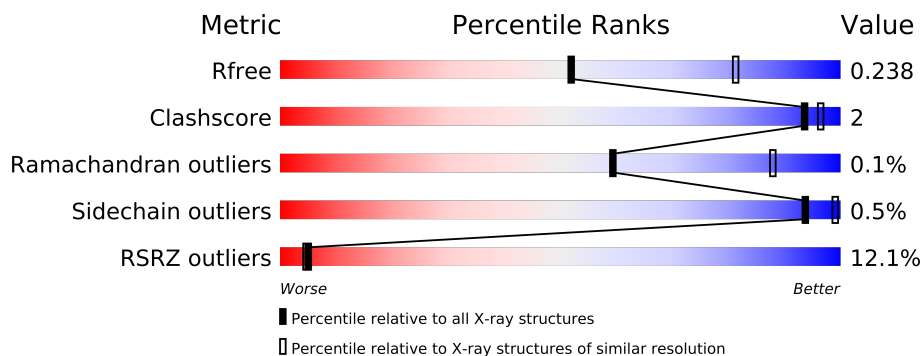
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.67 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	2010 (2.70-2.66)
Clashscore	79885	2450 (2.70-2.66)
Ramachandran outliers	78287	2410 (2.70-2.66)
Sidechain outliers	78261	2410 (2.70-2.66)
RSRZ outliers	66119	2013 (2.70-2.66)

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	910	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13497 atoms, of which 6750 are hydrogens 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 DNA POLYMERASE ALPHA CATALYTIC SUBUNIT A.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	827	Total	C	H	N	O	S	Se	0	4	0
			13387	4203	6750	1150	1237	19	28			

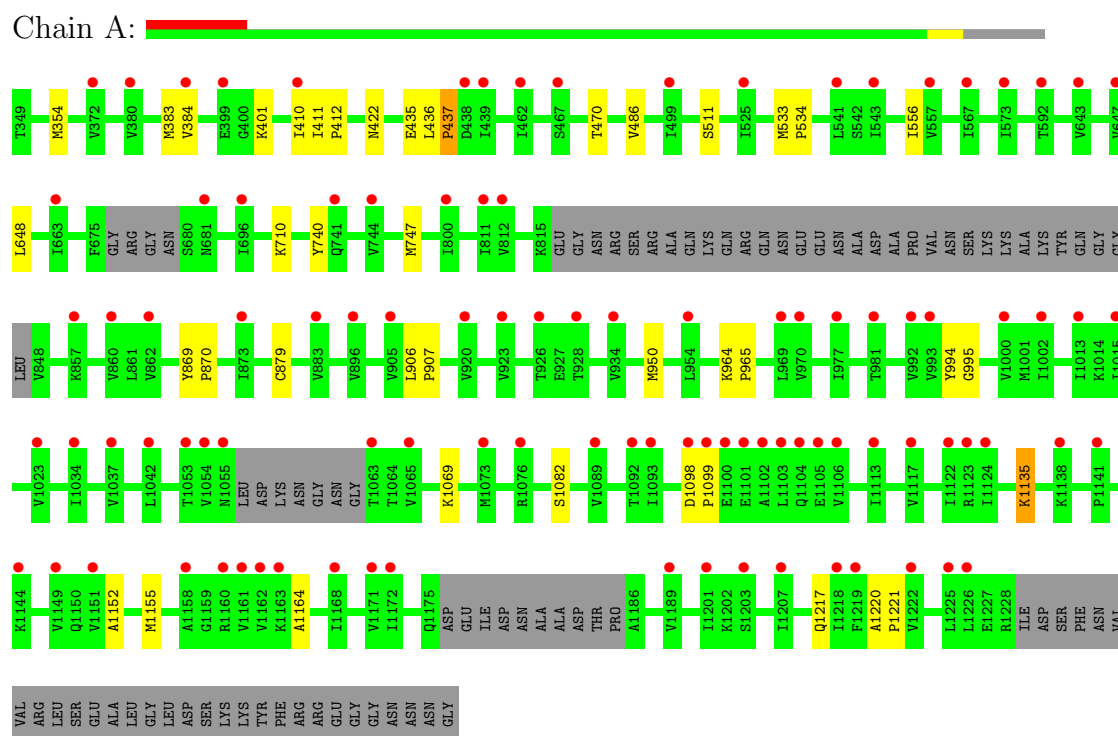
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	110	Total 110	O 110	0	0

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: DNA POLYMERASE ALPHA CATALYTIC SUBUNIT A



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.97Å 127.45Å 144.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.80 – 2.67 73.97 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.80-2.67) 99.9 (73.97-2.67)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.65Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1078)	Depositor
R, R_{free}	0.195 , 0.234 0.200 , 0.238	Depositor DCC
R_{free} test set	1986 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 39577 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13497	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.21	0/6750	0.38	0/9079

There are no bond length outliers.

There are no bond angle outliers.

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	6637	6750	1	21	0
2	A	110	0	0	0	0
All	All	6747	6750	1	21	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 2.

All (21) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:906:LEU:HB3	1:A:907:PRO:HD3	1.86	0.55
1:A:411:ILE:HB	1:A:412:PRO:HD3	1.92	0.51
1:A:1220:ALA:HB1	1:A:1221:PRO:HD3	1.93	0.51
1:A:410:ILE:HD13	1:A:411:ILE:N	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:710:LYS:O	1:A:1069:LYS:NZ	2.46	0.48
1:A:401:LYS:HG3	1:A:470:THR:HA	2.00	0.44
1:A:436:LEU:HA	1:A:437:PRO:HD3	1.87	0.44
1:A:964:LYS:N	1:A:965:PRO:CD	2.80	0.44
1:A:869:TYR:N	1:A:870:PRO:HD2	2.32	0.43
1:A:383:MSE:HE1	1:A:511:SER:HB3	2.00	0.43
1:A:1152:ALA:HA	1:A:1155:MSE:HE1	2.00	0.43
1:A:1135:LYS:HA	1:A:1164:ALA:HB3	2.01	0.42
1:A:1082:SER:OG	1:A:1217:GLN:O	2.23	0.41
1:A:1098:ASP:HB2	1:A:1099:PRO:HD2	2.01	0.41
1:A:879:CYS:HB2	1:A:907:PRO:HD3	2.03	0.41
1:A:994:TYR:CG	1:A:995:GLY:N	2.88	0.41
1:A:740:TYR:O	1:A:747:MSE:HE3	2.21	0.41
1:A:906:LEU:HD12	1:A:950:MSE:CE	2.51	0.41
1:A:533:MSE:HB2	1:A:534:PRO:HD2	2.03	0.40
1:A:354:MSE:SE	1:A:384:VAL:HG21	2.71	0.40
1:A:556:ILE:HD12	1:A:648:LEU:HA	2.03	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	821/910 (90%)	794 (97%)	26 (3%)	1 (0%)	59	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	437	PRO

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	757/790 (96%)	753 (100%)	4 (0%)	94	99

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	422	ASN
1	A	435	GLU
1	A	486	VAL
1	A	1135	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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, 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	827/910 (90%)	0.66	100 (12%) 5 4	28, 53, 93, 126	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1226	LEU	6.1
1	A	1162	VAL	5.8
1	A	1106	VAL	5.7
1	A	1065	VAL	5.2
1	A	1093	ILE	5.2
1	A	1102	ALA	4.7
1	A	1161	VAL	4.7
1	A	1100	GLU	4.6
1	A	1160	ARG	4.5
1	A	1013	ILE	4.3
1	A	1101	GLU	4.1
1	A	1000	VAL	4.0
1	A	1149	VAL	3.8
1	A	1098	ASP	3.8
1	A	1158	ALA	3.8
1	A	1099	PRO	3.6
1	A	439	ILE	3.6
1	A	1163	LYS	3.6
1	A	1073	MSE	3.6
1	A	993	VAL	3.6
1	A	1037	VAL	3.5
1	A	1225	LEU	3.5
1	A	857	LYS	3.4
1	A	1054	VAL	3.4
1	A	1151	VAL	3.4
1	A	1122	ILE	3.3
1	A	934	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1089	VAL	3.2
1	A	1117	VAL	3.2
1	A	1113	ILE	3.2
1	A	905	VAL	3.2
1	A	1201	ILE	3.1
1	A	1222	VAL	3.1
1	A	970	VAL	3.1
1	A	977	ILE	3.1
1	A	981	THR	3.0
1	A	1023	VAL	3.0
1	A	1092	THR	3.0
1	A	543	ILE	3.0
1	A	1076	ARG	2.9
1	A	1207	ILE	2.9
1	A	883	VAL	2.9
1	A	1141	PRO	2.9
1	A	873	ILE	2.9
1	A	592	THR	2.9
1	A	1034	ILE	2.8
1	A	1189	VAL	2.8
1	A	1053	THR	2.7
1	A	1103	LEU	2.7
1	A	969	LEU	2.7
1	A	1042	LEU	2.6
1	A	928	THR	2.6
1	A	681	ASN	2.6
1	A	1203	SER	2.6
1	A	384	VAL	2.6
1	A	372	VAL	2.6
1	A	647	VAL	2.6
1	A	812	VAL	2.4
1	A	467	SER	2.4
1	A	499	ILE	2.4
1	A	438	ASP	2.4
1	A	1144	LYS	2.4
1	A	1138	LYS	2.4
1	A	811	ILE	2.3
1	A	896	VAL	2.3
1	A	1002	ILE	2.3
1	A	1063	THR	2.3
1	A	696	ILE	2.3
1	A	567	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	541	LEU	2.3
1	A	643	VAL	2.3
1	A	860	VAL	2.3
1	A	1168	ILE	2.3
1	A	1124	ILE	2.3
1	A	992	VAL	2.3
1	A	525	ILE	2.2
1	A	862	VAL	2.2
1	A	926	THR	2.2
1	A	573	ILE	2.2
1	A	410	ILE	2.2
1	A	1219	PHE	2.2
1	A	1055	ASN	2.2
1	A	1105	GLU	2.2
1	A	462	ILE	2.2
1	A	744	VAL	2.2
1	A	399	GLU	2.2
1	A	1171	VAL	2.1
1	A	1015	ILE	2.1
1	A	741	GLN	2.1
1	A	1218	ILE	2.1
1	A	954	LEU	2.1
1	A	923	VAL	2.1
1	A	1172	ILE	2.1
1	A	557	VAL	2.1
1	A	800	ILE	2.1
1	A	1104	GLN	2.1
1	A	663	ILE	2.0
1	A	380	VAL	2.0
1	A	920	VAL	2.0
1	A	1123	ARG	2.0

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.