



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 4E4W
Title : Structure of the C-terminal domain of the *Saccharomyces cerevisiae* MUTL alpha (MLH1/PMS1) heterodimer
Authors : Gueneau, E.; Legrand, P.; Charbonnier, J.B.
Deposited on : 2012-03-13
Resolution : 2.50 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

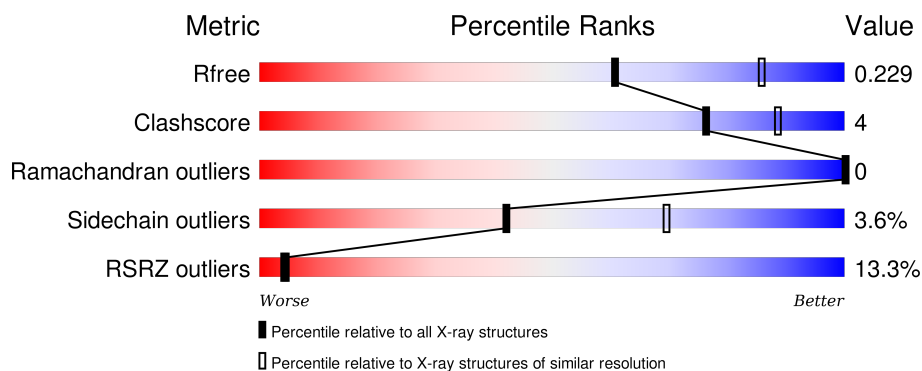
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 $\leq 5\%$. 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	285	
2	B	239	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	801	-	-	-	X
3	GOL	A	802	-	-	-	X
3	GOL	A	803	-	-	-	X
3	GOL	A	804	-	-	-	X
3	GOL	A	805	-	-	-	X
4	EDO	A	808	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4032 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 DNA mismatch repair protein MLH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	1	0
			2135	1377	346	405	7			

- Molecule 2 is a protein called DNA mismatch repair protein PMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1673	1064	287	312	10			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Zn	0	0
			2	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total 128	O 128	0	0
6	B	52	Total 52	O 52	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	187.21Å 66.14Å 74.01Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	39.79 – 2.50 39.79 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.79-2.50) 99.7 (39.79-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.170 , 0.210 0.189 , 0.229	Depositor DCC
R_{free} test set	1568 reflections (5.24%)	DCC
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.978	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.4	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 31477 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4032	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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

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	0.54	0/2178	0.77	0/2944
2	B	0.47	0/1702	0.67	0/2291
All	All	0.51	0/3880	0.73	0/5235

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

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	2135	0	2152	24	0
2	B	1673	0	1612	9	0
3	A	30	0	40	5	0
4	A	12	0	18	0	0
5	B	2	0	0	0	0
6	A	128	0	0	1	0
6	B	52	0	0	0	0
All	All	4032	0	3822	29	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 4.

All (29) 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:616:ILE:HG23	1:A:674:GLY:HA3	1.60	0.83
1:A:522:ASP:HA	1:A:525:ILE:HD12	1.71	0.73
1:A:713:SER:HB3	1:A:716:GLU:HG2	1.76	0.68
1:A:742:ARG:HD2	3:A:801:GOL:H32	1.81	0.62
2:B:754:LYS:HB2	2:B:771:SER:HB2	1.83	0.61
2:B:665:THR:HG23	2:B:666:VAL:HG23	1.82	0.60
1:A:559:LEU:HD23	2:B:864:TRP:CZ3	2.37	0.59
1:A:640:LEU:HD23	1:A:642:ASN:H	1.68	0.58
1:A:568:GLU:HG3	1:A:749:ILE:CD1	2.37	0.54
1:A:585:ASN:HB3	6:A:977:HOH:O	2.08	0.53
1:A:568:GLU:HG3	1:A:749:ILE:HD11	1.91	0.53
2:B:669:ASN:HA	2:B:672:LYS:HE3	1.94	0.49
1:A:527:ARG:H	3:A:805:GOL:H11	1.78	0.49
1:A:559:LEU:HD13	1:A:756:ILE:HD13	1.97	0.46
2:B:860:GLU:HB3	2:B:862:ARG:HH21	1.81	0.45
1:A:525:ILE:HG22	3:A:802:GOL:H32	1.99	0.45
1:A:653:PRO:HG3	1:A:693:ILE:HD13	1.98	0.44
1:A:547:ARG:NH2	2:B:870:ASP:OD2	2.41	0.43
1:A:526:HIS:HA	3:A:805:GOL:H11	2.00	0.42
1:A:607:LEU:O	1:A:613:LYS:HE3	2.20	0.42
1:A:669:PHE:O	1:A:673:LEU:HB2	2.19	0.42
1:A:747:ARG:HH21	3:A:805:GOL:H12	1.85	0.42
1:A:659:TYR:CE1	1:A:730:LEU:HD21	2.55	0.41
1:A:552:GLN:HG3	2:B:680:PHE:HE2	1.85	0.41
1:A:631:TYR:OH	1:A:686:LEU:HA	2.21	0.41
1:A:559:LEU:HD21	2:B:861:LEU:HD21	2.03	0.41
1:A:536:LEU:HG	1:A:740:LYS:HG3	2.03	0.41
1:A:631:TYR:O	1:A:653:PRO:HB3	2.21	0.40
2:B:671:PHE:HB2	2:B:840:SER:HB3	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	260/285 (91%)	253 (97%)	7 (3%)	0	100	100
2	B	205/239 (86%)	195 (95%)	10 (5%)	0	100	100
All	All	465/524 (89%)	448 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	243/264 (92%)	235 (97%)	8 (3%)	45	73
2	B	180/224 (80%)	173 (96%)	7 (4%)	39	66
All	All	423/488 (87%)	408 (96%)	15 (4%)	42	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	512	THR
1	A	513	SER
1	A	592	SER
1	A	610	ASP
1	A	626	MET
1	A	651	SER
1	A	715	ASP
1	A	727	ILE
2	B	651	GLU
2	B	691	VAL
2	B	695	TYR
2	B	733	LEU
2	B	767	VAL
2	B	771	SER
2	B	782	LEU

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

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](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
3	GOL	A	801	-	5,5,5	0.17	0	5,5,5	0.35	0
3	GOL	A	802	-	5,5,5	0.16	0	5,5,5	0.52	0
3	GOL	A	803	-	5,5,5	0.12	0	5,5,5	0.31	0
3	GOL	A	804	-	5,5,5	0.15	0	5,5,5	0.36	0
3	GOL	A	805	-	5,5,5	0.17	0	5,5,5	0.35	0
4	EDO	A	806	-	3,3,3	0.71	0	2,2,2	0.24	0
4	EDO	A	807	-	3,3,3	0.72	0	2,2,2	0.17	0
4	EDO	A	808	-	3,3,3	0.85	0	2,2,2	0.11	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
3	GOL	A	801	-	-	0/4/4/4	0/0/0/0
3	GOL	A	802	-	-	0/4/4/4	0/0/0/0
3	GOL	A	803	-	-	0/4/4/4	0/0/0/0
3	GOL	A	804	-	-	0/4/4/4	0/0/0/0
3	GOL	A	805	-	-	0/4/4/4	0/0/0/0
4	EDO	A	806	-	-	0/1/1/1	0/0/0/0
4	EDO	A	807	-	-	0/1/1/1	0/0/0/0
4	EDO	A	808	-	-	0/1/1/1	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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GOL	1	0
3	A	802	GOL	1	0
3	A	805	GOL	3	0

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 ⓘ

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	261/285 (91%)	0.05	13 (4%) 32 37	44, 60, 115, 148	0
2	B	213/239 (89%)	1.00	50 (23%) 1 1	46, 85, 158, 200	0
All	All	474/524 (90%)	0.48	63 (13%) 4 4	44, 66, 146, 200	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	733	LEU	9.1
2	B	726	ILE	8.2
2	B	767	VAL	7.3
1	A	509	VAL	6.5
2	B	743	ASP	6.4
2	B	755	LEU	5.8
2	B	785	PHE	5.3
2	B	731	VAL	5.3
2	B	770	LEU	5.1
2	B	792	ILE	5.1
2	B	652	LEU	5.0
1	A	708	SER	5.0
2	B	732	GLU	4.8
2	B	742	LEU	4.8
2	B	728	PRO	4.7
2	B	753	PHE	4.6
2	B	782	LEU	4.6
2	B	757	ILE	4.6
2	B	756	LYS	4.5
2	B	771	SER	4.5
1	A	641	ASP	4.4
2	B	725	LEU	4.4
2	B	769	LEU	4.4
2	B	788	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	740	VAL	4.0
2	B	786	ASN	3.9
2	B	649	LYS	3.8
2	B	730	PRO	3.7
1	A	711	SER	3.6
2	B	768	LYS	3.5
1	A	709	ASP	3.5
2	B	694	LYS	3.4
2	B	748	PHE	3.4
2	B	651	GLU	3.4
2	B	650	ASP	3.4
2	B	794	GLU	3.3
1	A	710	ALA	3.3
2	B	729	GLN	3.3
1	A	706	ASP	3.3
1	A	712	LEU	3.2
2	B	653	GLU	3.2
2	B	741	VAL	3.2
2	B	789	ILE	3.1
2	B	691	VAL	3.0
2	B	727	ILE	2.9
1	A	714	GLU	2.8
2	B	724	LYS	2.7
2	B	766	ARG	2.7
2	B	862	ARG	2.6
1	A	640	LEU	2.6
1	A	713	SER	2.6
2	B	655	PHE	2.3
1	A	716	GLU	2.3
2	B	765	SER	2.3
2	B	752	GLY	2.3
1	A	717	LYS	2.3
2	B	795	ASP	2.2
2	B	749	GLU	2.2
2	B	805	CYS	2.1
2	B	654	ASP	2.1
2	B	783	GLY	2.0
2	B	754	LYS	2.0
2	B	661	TYR	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](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	A	808	4/4	0.90	0.30	5.83	53,58,62,64	0
3	GOL	A	801	6/6	0.89	0.23	4.90	73,79,80,81	0
3	GOL	A	802	6/6	0.89	0.24	3.75	52,62,67,68	0
3	GOL	A	804	6/6	0.81	0.21	3.74	76,82,82,84	0
3	GOL	A	805	6/6	0.91	0.21	2.86	59,71,75,78	0
3	GOL	A	803	6/6	0.91	0.17	2.55	74,77,78,78	0
5	ZN	B	902	1/1	0.99	0.13	-0.93	57,57,57,57	0
4	EDO	A	806	4/4	0.95	0.11	-1.52	63,64,65,65	0
4	EDO	A	807	4/4	0.92	0.19	-	73,77,78,80	0
5	ZN	B	901	1/1	1.00	0.14	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.