

Full wwPDB X-ray Structure Validation Report (i)

Nov 22, 2021 – 01:07 pm GMT

PDB ID : 6SHX

Title : DNA mismatch repair proteins MLH1 and MLH3

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Deposited on : 2019-08-08

Resolution : 2.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

 $\begin{array}{ccc} & Mol Probity & : & 4.02b\text{-}467 \\ & Xtriage \text{ (Phenix)} & : & 1.13 \end{array}$

EDS : 2.23.2buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0267

CCP4 : 7.1.010 (Gargrove) Ideal geometry (proteins) : Engh & Huber (2001)

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

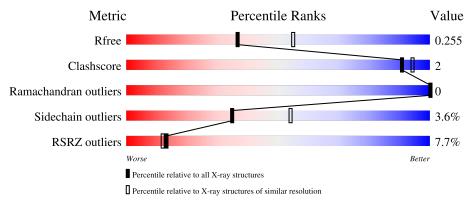
 $\begin{tabular}{lll} Validation Pipeline (wwPDB-VP) & : & 2.23.2 \end{tabular}$

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X- $RAY\ DIFFRACTION$

The reported resolution of this entry is 2.40 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=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	265	92%		6% •
2	В	239	8%	10%	7%



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3995 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	260	Total 2125	C 1370	N 345	O 403	S 7	0	0	0

• Molecule 2 is a protein called DNA mismatch repair protein MLH3.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	222	Total 1792	C 1153	N 299	O 326	S 14	0	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	Total Zn 1 1	0	0

• Molecule 4 is water.

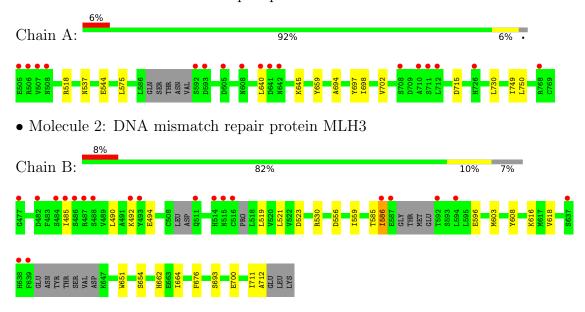
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	33	Total O 33 33	0	0
4	В	44	Total O 44 44	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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 mismatch repair protein MLH1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	93.59Å 104.05Å 134.08Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.64 - 2.40	Depositor
Resolution (A)	24.64 - 2.40	EDS
% Data completeness	77.3 (24.64-2.40)	Depositor
(in resolution range)	77.3 (24.64-2.40)	EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.93 (at 2.41Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
P. P.	0.213 , 0.236	Depositor
R, R_{free}	0.222 , 0.255	DCC
R_{free} test set	1039 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$ < L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3995	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 5.01% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of <|L|>, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



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: ZN

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		
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.40	0/2163	0.62	0/2921	
2	В	0.41	0/1826	0.60	0/2458	
All	All	0.40	0/3989	0.61	0/5379	

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 (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	2125	0	2141	4	0
2	В	1792	0	1790	9	0
3	В	1	0	0	0	0
4	A	33	0	0	0	0
4	В	44	0	0	0	0
All	All	3995	0	3931	13	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 2.

All (13) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
2:B:530:ARG:HD3	2:B:700:GLU:O	2.06	0.55
2:B:651:TRP:HA	2:B:654:SER:HB2	1.90	0.54
2:B:523:ASP:OD1	2:B:676:PHE:HE1	1.91	0.53
1:A:694:ALA:O	1:A:698:ILE:HG23	2.12	0.48
2:B:559:ILE:HG21	2:B:616:LYS:HB2	1.95	0.48
1:A:659:TYR:HE1	1:A:730:LEU:HD21	1.79	0.47
2:B:519:LEU:H	2:B:712:ALA:HB2	1.79	0.47
2:B:586:ILE:HD11	2:B:596:GLU:HB2	1.96	0.47
2:B:521:LEU:HD12	2:B:711:ILE:HG21	2.00	0.43
1:A:544:GLU:HB3	1:A:702:VAL:HB	2.02	0.42
2:B:490:LEU:HD23	2:B:693:SER:HA	2.01	0.41
1:A:518:ARG:HG3	1:A:575:LEU:HD22	2.04	0.40
2:B:603:MET:HG2	2:B:664:ILE:HG21	2.02	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	256/265~(97%)	252 (98%)	4 (2%)	0	100 100
2	В	212/239 (89%)	208 (98%)	4 (2%)	0	100 100
All	All	468/504 (93%)	460 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	241/247 (98%)	234 (97%)	7 (3%)	42 62
2	В	200/222 (90%)	191 (96%)	9 (4%)	27 44
All	All	441/469 (94%)	425 (96%)	16 (4%)	35 54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	537	ASN
1	A	640	LEU
1	A	645	LYS
1	A	697	TYR
1	A	715	ASP
1	A	749	ILE
1	A	750	LEU
2	В	485	ILE
2	В	492	LYS
2	В	494	GLU
2	В	556	ASP
2	В	585	THR
2	В	586	ILE
2	В	608	TYR
2	В	618	VAL
2	В	662	HIS

Sometimes 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 monosaccharides in this entry.



5.6 Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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 $>$	$\#\mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	A	$260/265 \ (98\%)$	0.25	17 (6%) 18 17	30, 61, 108, 138	0
2	В	$222/239 \ (92\%)$	0.29	20 (9%) 9 8	31, 53, 107, 148	0
All	All	482/504~(95%)	0.26	37 (7%) 13 12	30, 58, 108, 148	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	640	LEU	7.1
2	В	515	ASN	6.5
1	A	642	ASN	6.1
1	A	592	SER	6.0
2	В	516	CYS	6.0
2	В	514	HIS	5.8
2	В	638	HIS	5.5
2	В	477	GLY	5.4
2	В	488	SER	5.2
1	A	710	ALA	4.9
2	В	487	ARG	4.8
2	В	511	GLN	4.2
2	В	587	GLU	4.0
2	В	586	ILE	3.6
1	A	712	LEU	3.5
2	В	639	PHE	3.5
1	A	708	SER	3.4
2	В	485	ILE	3.2
1	A	507	VAL	3.2
1	A	506	ARG	3.2
1	A	508	ASN	3.0
1	A	505	GLU	3.0
1	A	711	SER	3.0
2	В	594	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	В	484	SER	2.9
1	A	593	ASP	2.9
1	A	608	ASN	2.8
2	В	486	SER	2.7
1	A	605	ASP	2.6
2	В	492	LYS	2.5
2	В	482	ASP	2.4
1	A	726	HIS	2.4
2	В	637	SER	2.4
2	В	592	THR	2.2
1	A	641	ASP	2.2
2	В	493	TYR	2.2
1	A	768	ARG	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 monosaccharides in this entry.

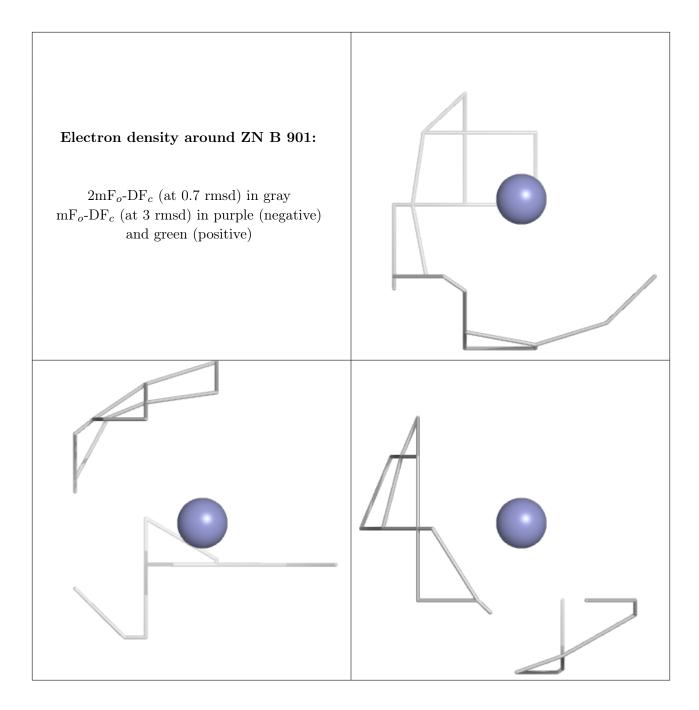
6.4 Ligands (i)

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. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
3	ZN	В	901	1/1	0.97	0.04	68,68,68,68	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers (i)

There are no such residues in this entry.

