



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 09:41 PM GMT

PDB ID : 5AKB  
Title : MutS in complex with the N-terminal domain of MutL - crystal form 1  
Authors : Groothuizen, F.S.; Winkler, I.; Cristovao, M.; Fish, A.; Winterwerp, H.H.K.;  
Reumer, A.; Marx, A.D.; Hermans, N.; Nicholls, R.A.; Murshudov, G.N.;  
Lebbink, J.H.G.; Friedhoff, P.; Sixma, T.K.  
Deposited on : 2015-03-03  
Resolution : 4.71 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
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) : rb-20026982

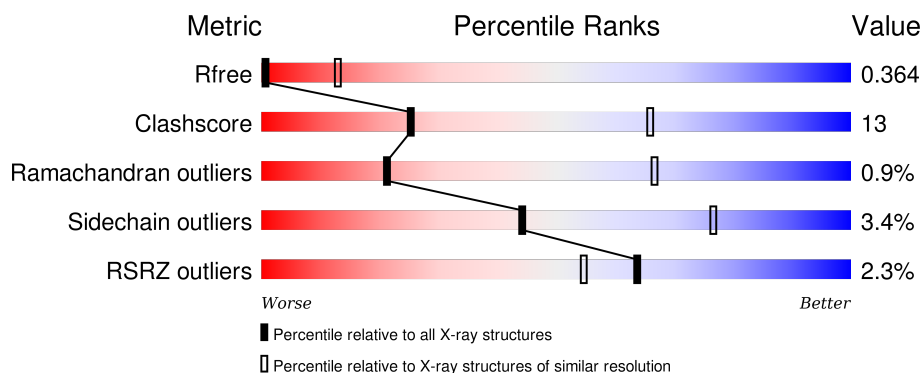
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.71 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	1096 (5.82-3.60)
Clashscore	102246	1011 (5.80-3.64)
Ramachandran outliers	100387	1138 (5.82-3.60)
Sidechain outliers	100360	1119 (5.82-3.60)
RSRZ outliers	91569	1099 (5.82-3.60)

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. 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	800	<div> <div>67%</div> <div>15%</div> <div>•</div> <div>17%</div> </div>
1	B	800	<div> <div>66%</div> <div>17%</div> <div>•</div> <div>17%</div> </div>
1	E	800	<div> <div>2%</div> <div>48%</div> <div>24%</div> <div>•</div> <div>27%</div> </div>
2	C	369	<div> <div>54%</div> <div>21%</div> <div>•</div> <div>23%</div> </div>
2	D	369	<div> <div>5%</div> <div>58%</div> <div>18%</div> <div>•</div> <div>23%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain	
				
2	F	369		

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21906 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 MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	B	663	Total	C	N	O	S	0	0	0
			5226	3284	938	984	20			
1	E	588	Total	C	N	O	S	0	0	0
			4605	2894	825	867	19			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
A	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
A	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909
A	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
A	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
A	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
A	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909
B	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
B	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
B	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909
B	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
B	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
B	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
B	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909
E	93	ALA	CYS	ENGINEERED MUTATION	UNP P23909
E	235	SER	CYS	ENGINEERED MUTATION	UNP P23909
E	239	ALA	CYS	ENGINEERED MUTATION	UNP P23909
E	246	CYS	ASP	ENGINEERED MUTATION	UNP P23909
E	297	SER	CYS	ENGINEERED MUTATION	UNP P23909
E	569	SER	CYS	ENGINEERED MUTATION	UNP P23909
E	711	VAL	CYS	ENGINEERED MUTATION	UNP P23909

- Molecule 2 is a protein called DNA MISMATCH REPAIR PROTEIN MUTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	285	Total 2252	C 1423	N 409	O 418	S 2	0	0	0
2	D	285	Total 2252	C 1423	N 409	O 418	S 2	0	0	0
2	F	285	Total 2252	C 1423	N 409	O 418	S 2	0	0	0

There are 75 discrepancies between the modelled and reference sequences:

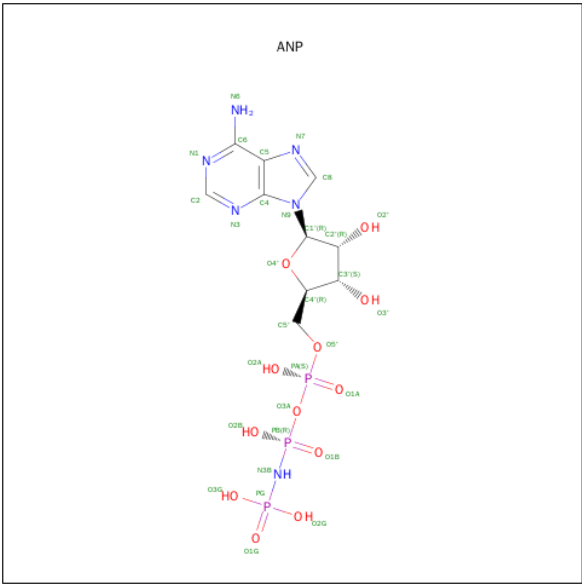
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	EXPRESSION TAG	UNP P23367
C	-18	GLY	-	EXPRESSION TAG	UNP P23367
C	-17	SER	-	EXPRESSION TAG	UNP P23367
C	-16	SER	-	EXPRESSION TAG	UNP P23367
C	-15	HIS	-	EXPRESSION TAG	UNP P23367
C	-14	HIS	-	EXPRESSION TAG	UNP P23367
C	-13	HIS	-	EXPRESSION TAG	UNP P23367
C	-12	HIS	-	EXPRESSION TAG	UNP P23367
C	-11	HIS	-	EXPRESSION TAG	UNP P23367
C	-10	HIS	-	EXPRESSION TAG	UNP P23367
C	-9	SER	-	EXPRESSION TAG	UNP P23367
C	-8	SER	-	EXPRESSION TAG	UNP P23367
C	-7	GLY	-	EXPRESSION TAG	UNP P23367
C	-6	LEU	-	EXPRESSION TAG	UNP P23367
C	-5	VAL	-	EXPRESSION TAG	UNP P23367
C	-4	PRO	-	EXPRESSION TAG	UNP P23367
C	-3	ARG	-	EXPRESSION TAG	UNP P23367
C	-2	GLY	-	EXPRESSION TAG	UNP P23367
C	-1	SER	-	EXPRESSION TAG	UNP P23367
C	0	HIS	-	EXPRESSION TAG	UNP P23367
C	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
C	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
C	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
C	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
C	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367
D	-19	MET	-	EXPRESSION TAG	UNP P23367
D	-18	GLY	-	EXPRESSION TAG	UNP P23367
D	-17	SER	-	EXPRESSION TAG	UNP P23367
D	-16	SER	-	EXPRESSION TAG	UNP P23367
D	-15	HIS	-	EXPRESSION TAG	UNP P23367
D	-14	HIS	-	EXPRESSION TAG	UNP P23367
D	-13	HIS	-	EXPRESSION TAG	UNP P23367
D	-12	HIS	-	EXPRESSION TAG	UNP P23367

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
D	-11	HIS	-	EXPRESSION TAG	UNP P23367
D	-10	HIS	-	EXPRESSION TAG	UNP P23367
D	-9	SER	-	EXPRESSION TAG	UNP P23367
D	-8	SER	-	EXPRESSION TAG	UNP P23367
D	-7	GLY	-	EXPRESSION TAG	UNP P23367
D	-6	LEU	-	EXPRESSION TAG	UNP P23367
D	-5	VAL	-	EXPRESSION TAG	UNP P23367
D	-4	PRO	-	EXPRESSION TAG	UNP P23367
D	-3	ARG	-	EXPRESSION TAG	UNP P23367
D	-2	GLY	-	EXPRESSION TAG	UNP P23367
D	-1	SER	-	EXPRESSION TAG	UNP P23367
D	0	HIS	-	EXPRESSION TAG	UNP P23367
D	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
D	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
D	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
D	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
D	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367
F	-19	MET	-	EXPRESSION TAG	UNP P23367
F	-18	GLY	-	EXPRESSION TAG	UNP P23367
F	-17	SER	-	EXPRESSION TAG	UNP P23367
F	-16	SER	-	EXPRESSION TAG	UNP P23367
F	-15	HIS	-	EXPRESSION TAG	UNP P23367
F	-14	HIS	-	EXPRESSION TAG	UNP P23367
F	-13	HIS	-	EXPRESSION TAG	UNP P23367
F	-12	HIS	-	EXPRESSION TAG	UNP P23367
F	-11	HIS	-	EXPRESSION TAG	UNP P23367
F	-10	HIS	-	EXPRESSION TAG	UNP P23367
F	-9	SER	-	EXPRESSION TAG	UNP P23367
F	-8	SER	-	EXPRESSION TAG	UNP P23367
F	-7	GLY	-	EXPRESSION TAG	UNP P23367
F	-6	LEU	-	EXPRESSION TAG	UNP P23367
F	-5	VAL	-	EXPRESSION TAG	UNP P23367
F	-4	PRO	-	EXPRESSION TAG	UNP P23367
F	-3	ARG	-	EXPRESSION TAG	UNP P23367
F	-2	GLY	-	EXPRESSION TAG	UNP P23367
F	-1	SER	-	EXPRESSION TAG	UNP P23367
F	0	HIS	-	EXPRESSION TAG	UNP P23367
F	61	SER	CYS	ENGINEERED MUTATION	UNP P23367
F	131	CYS	ASN	ENGINEERED MUTATION	UNP P23367
F	216	LEU	CYS	ENGINEERED MUTATION	UNP P23367
F	256	PHE	CYS	ENGINEERED MUTATION	UNP P23367
F	276	TYR	CYS	ENGINEERED MUTATION	UNP P23367

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

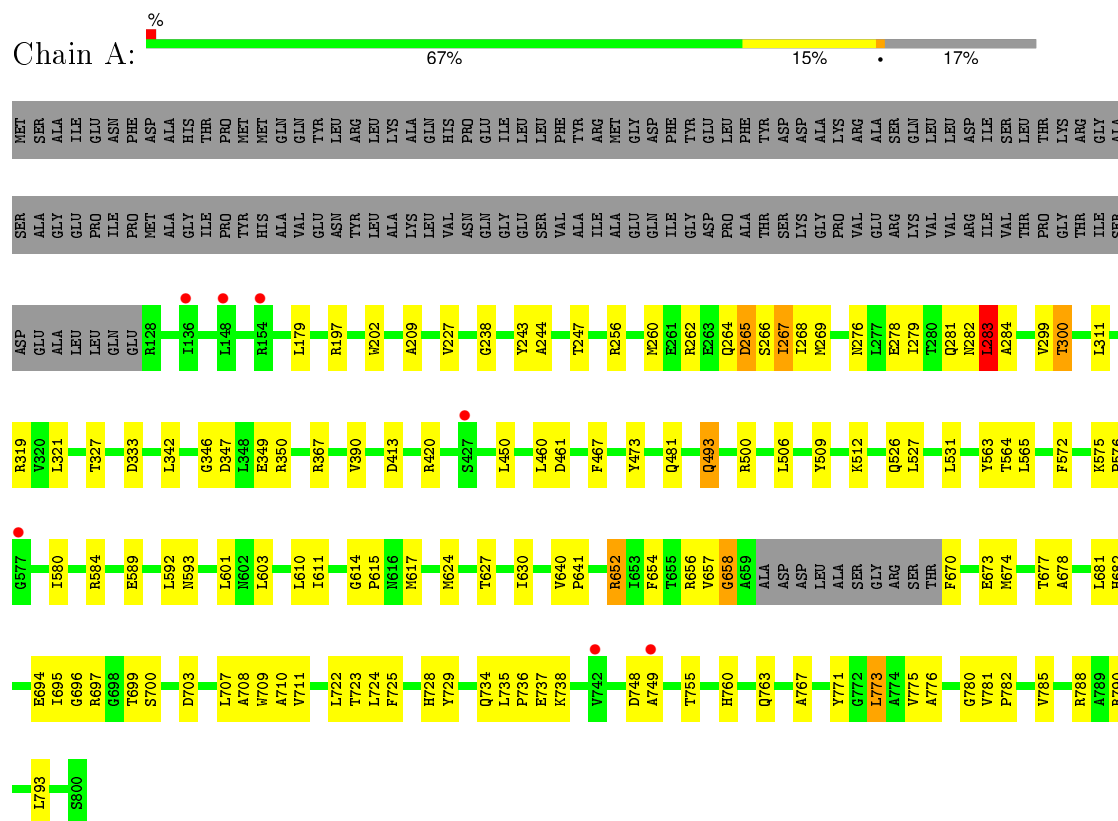


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

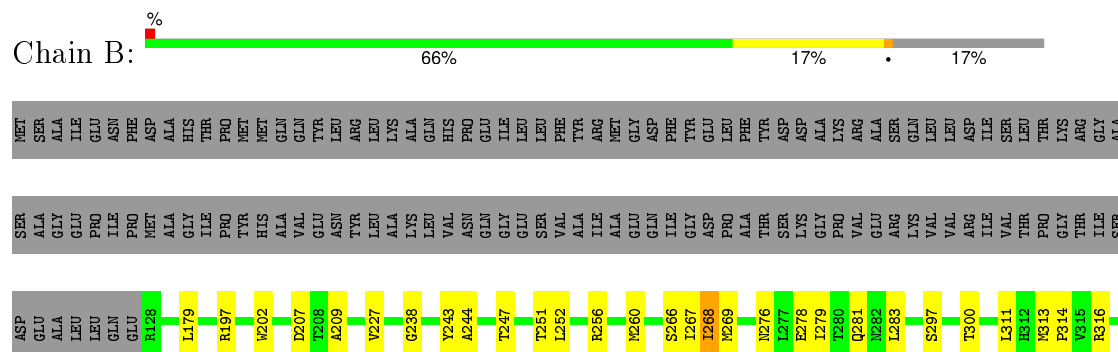
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

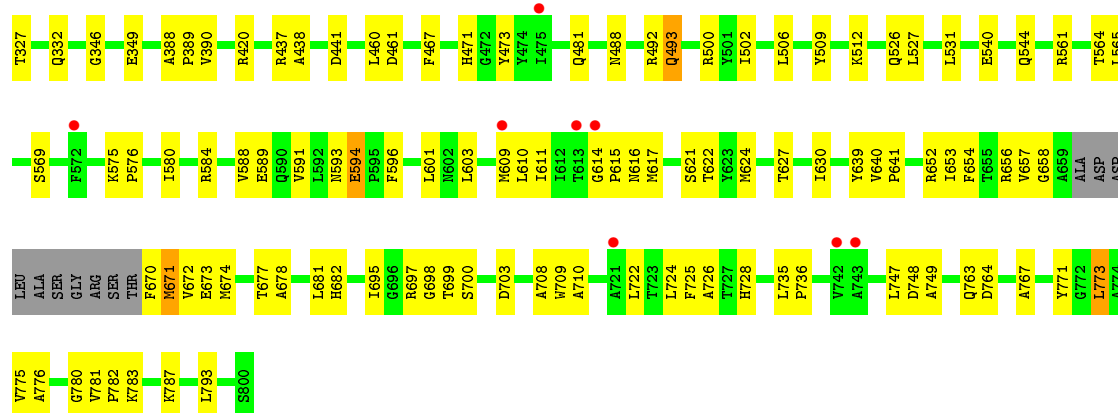
#### • Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS



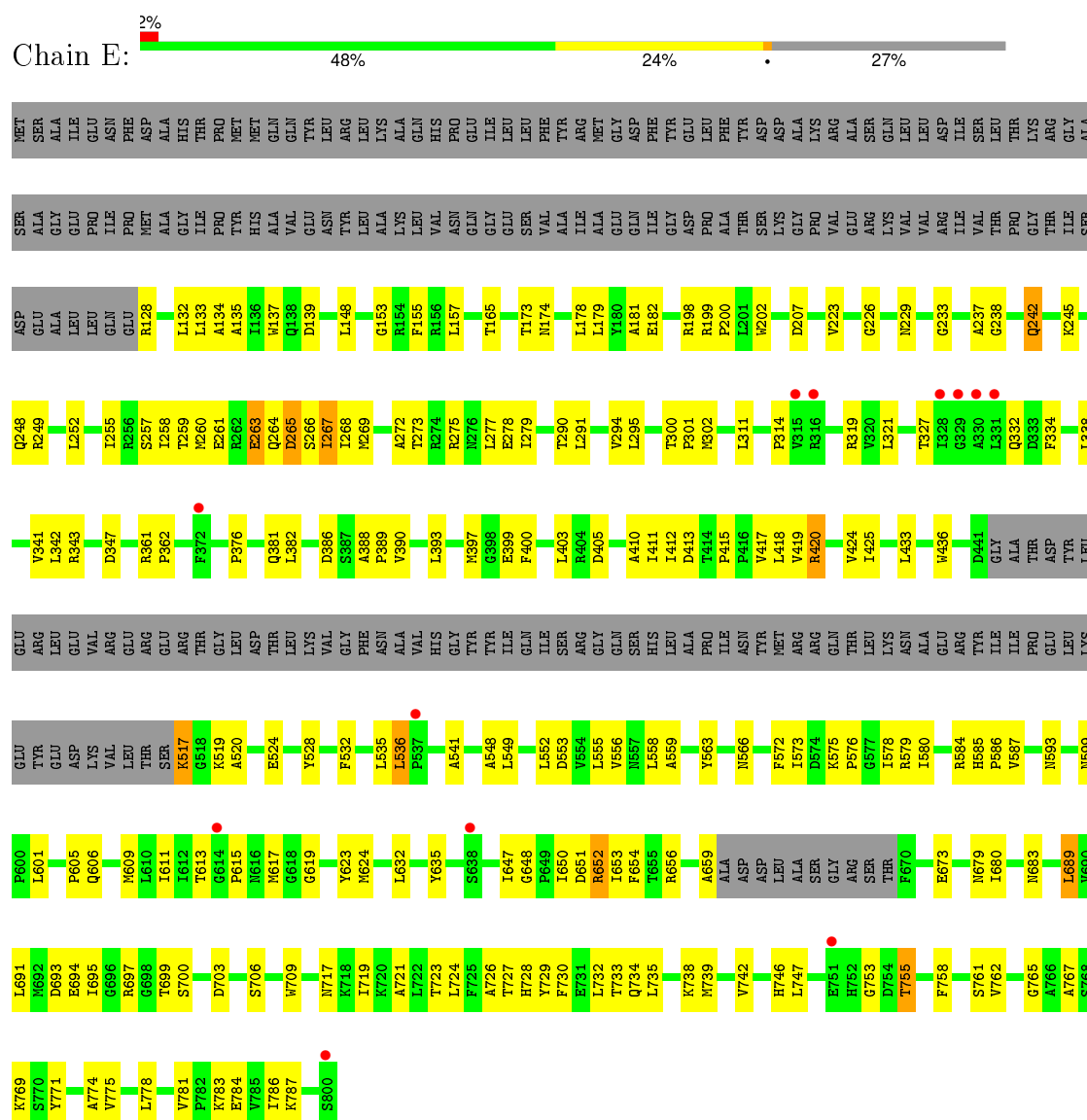
#### • Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS





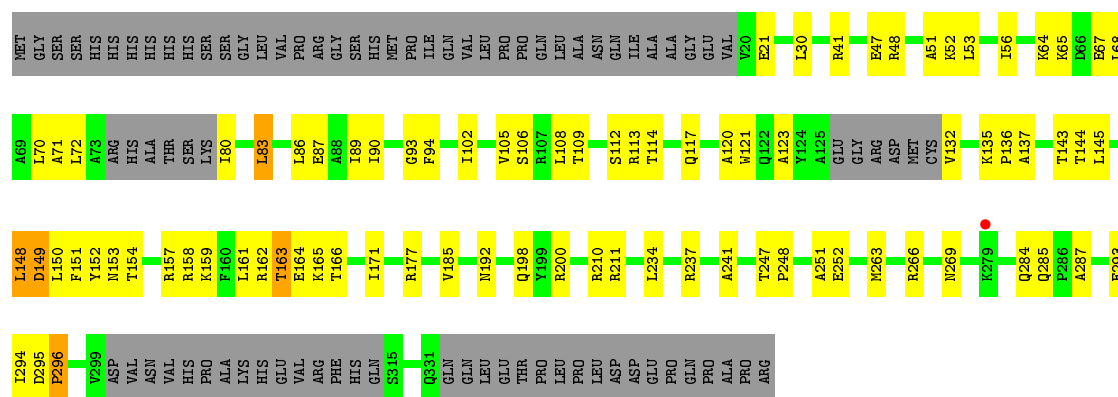


• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

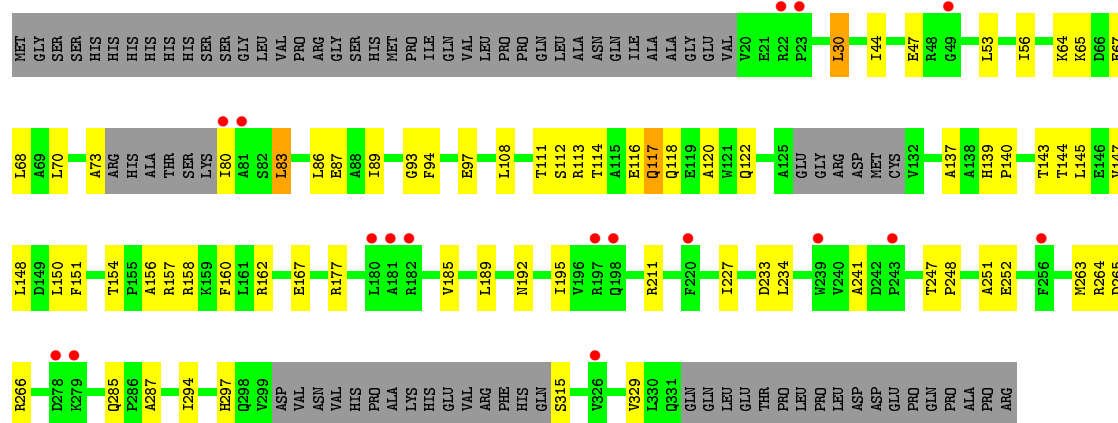


• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL

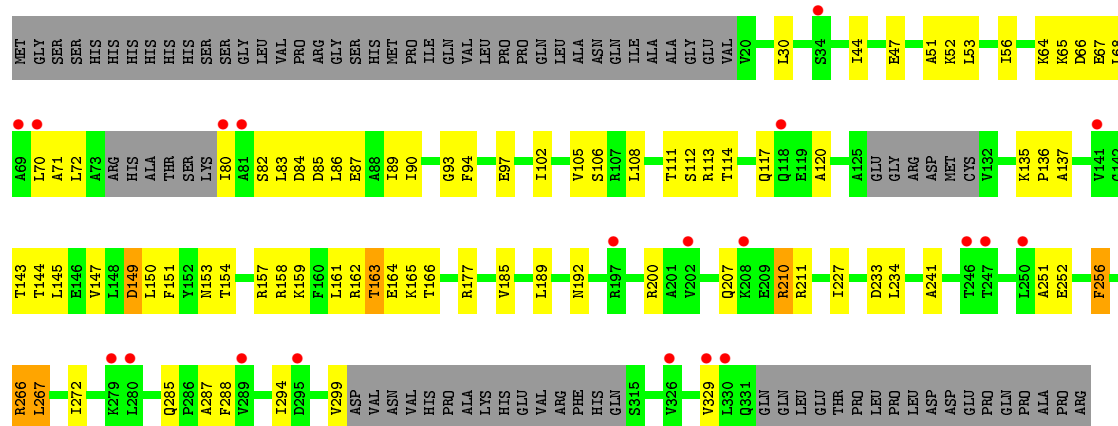




• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



• Molecule 2: DNA MISMATCH REPAIR PROTEIN MUTL



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.93Å 188.54Å 200.43Å 90.00° 94.77° 90.00°	Depositor
Resolution (Å)	199.73 – 4.71 80.35 – 4.71	Depositor EDS
% Data completeness (in resolution range)	97.2 (199.73-4.71) 97.3 (80.35-4.71)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 4.65Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.319 , 0.349 0.337 , 0.364	Depositor DCC
$R_{free}$ test set	1499 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	172.9	Xtriage
Anisotropy	0.346	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 191.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.20$	Xtriage
Outliers	0 of 31044 reflections	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	21906	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	234.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.53	0/5311	0.73	6/7186 (0.1%)
1	B	0.50	0/5311	0.67	3/7186 (0.0%)
1	E	0.56	0/4678	0.75	0/6331
2	C	0.63	1/2288 (0.0%)	0.81	3/3096 (0.1%)
2	D	0.53	0/2288	0.75	1/3096 (0.0%)
2	F	0.52	0/2288	0.73	1/3096 (0.0%)
All	All	0.54	1/22164 (0.0%)	0.73	14/29991 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	21	GLU	CG-CD	5.39	1.60	1.51

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	707	LEU	CB-CG-CD2	-7.33	98.53	111.00
1	A	652	ARG	NE-CZ-NH2	-6.98	116.81	120.30
2	C	148	LEU	CB-CG-CD1	-6.59	99.79	111.00
1	A	283	LEU	CB-CG-CD2	-6.46	100.01	111.00
1	A	283	LEU	CA-CB-CG	6.14	129.42	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	265	ASP	Peptide
1	A	266	SER	Peptide
1	A	267	ILE	Peptide

## 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	5226	0	5283	120	0
1	B	5226	0	5283	123	0
1	E	4605	0	4660	167	1
2	C	2252	0	2272	60	0
2	D	2252	0	2272	43	0
2	F	2252	0	2272	77	0
3	A	31	0	13	3	0
3	B	31	0	13	7	0
3	E	31	0	13	0	0
All	All	21906	0	22081	555	1

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 13.

The worst 5 of 555 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)
2:F:82:SER:O	2:F:85:ASP:OD1	1.56	1.21
2:F:267:LEU:HD12	2:F:299:VAL:HG13	1.28	1.13
2:F:83:LEU:HA	2:F:86:LEU:HB3	1.12	1.12
2:C:51:ALA:O	2:C:149:ASP:CG	1.90	1.10
2:F:51:ALA:O	2:F:149:ASP:CG	1.90	1.10

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:418:LEU:O	1:E:420:ARG:NH1[2_858]	2.10	0.10

## 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	659/800 (82%)	623 (94%)	34 (5%)	2 (0%)	46	83
1	B	659/800 (82%)	623 (94%)	33 (5%)	3 (0%)	34	77
1	E	582/800 (73%)	522 (90%)	52 (9%)	8 (1%)	14	58
2	C	277/369 (75%)	252 (91%)	21 (8%)	4 (1%)	14	58
2	D	277/369 (75%)	252 (91%)	23 (8%)	2 (1%)	26	71
2	F	277/369 (75%)	249 (90%)	23 (8%)	5 (2%)	11	54
All	All	2731/3507 (78%)	2521 (92%)	186 (7%)	24 (1%)	21	67

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	163	THR
2	D	117	GLN
1	E	265	ASP
1	E	420	ARG
1	E	753	GLY

### 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	550/662 (83%)	540 (98%)	10 (2%)	66	87
1	B	550/662 (83%)	541 (98%)	9 (2%)	70	88
1	E	484/662 (73%)	464 (96%)	20 (4%)	37	72
2	C	235/308 (76%)	219 (93%)	16 (7%)	20	59
2	D	235/308 (76%)	224 (95%)	11 (5%)	32	69
2	F	235/308 (76%)	224 (95%)	11 (5%)	32	69
All	All	2289/2910 (79%)	2212 (97%)	77 (3%)	44	76

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	293	GLU
2	D	252	GLU
2	F	159	LYS
2	D	30	LEU
2	D	148	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	C	274	GLN
2	D	122	GLN
2	F	33	ASN
2	D	117	GLN
2	D	118	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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

3 ligands are modelled in this entry.

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	ANP	A	1801	-	29,33,33	1.97	8 (27%)	26,52,52	1.96	6 (23%)
3	ANP	B	1801	-	29,33,33	1.90	9 (31%)	26,52,52	2.08	5 (19%)
3	ANP	E	1801	-	29,33,33	2.30	9 (31%)	26,52,52	2.09	7 (26%)

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	ANP	A	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	B	1801	-	-	0/13/38/38	0/3/3/3
3	ANP	E	1801	-	-	0/13/38/38	0/3/3/3

The worst 5 of 26 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1801	ANP	PG-O2G	-3.04	1.48	1.56
3	B	1801	ANP	PB-O2B	-2.66	1.49	1.56
3	B	1801	ANP	PG-O3G	-2.39	1.50	1.56
3	E	1801	ANP	PG-O2G	-2.34	1.50	1.56
3	A	1801	ANP	PG-O3G	-2.26	1.50	1.56

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1801	ANP	N3-C2-N1	-7.48	123.00	128.87
3	E	1801	ANP	N3-C2-N1	-7.20	123.22	128.87
3	A	1801	ANP	N3-C2-N1	-5.63	124.45	128.87
3	B	1801	ANP	PA-O3A-PB	-2.96	121.96	132.71

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1801	ANP	PA-O3A-PB	-2.64	123.14	132.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1801	ANP	3	0
3	B	1801	ANP	7	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 [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<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	663/800 (82%)	-0.10	7 (1%) 82 76	139, 203, 285, 347	0
1	B	663/800 (82%)	-0.16	8 (1%) 81 74	162, 230, 292, 329	0
1	E	588/800 (73%)	-0.01	12 (2%) 68 59	176, 236, 298, 405	0
2	C	285/369 (77%)	0.03	1 (0%) 93 90	150, 186, 253, 315	0
2	D	285/369 (77%)	0.36	17 (5%) 25 19	202, 277, 357, 420	0
2	F	285/369 (77%)	0.32	20 (7%) 19 15	200, 280, 355, 460	0
All	All	2769/3507 (78%)	0.01	65 (2%) 64 55	139, 230, 316, 460	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	330	ALA	5.2
1	E	614	GLY	5.2
2	D	279	LYS	5.0
1	E	315	VAL	4.6
1	E	331	LEU	4.0

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ANP	E	1801	31/31	0.84	0.24	-0.40	232,262,291,292	0
3	ANP	A	1801	31/31	0.89	0.26	-0.83	160,165,174,175	0
3	ANP	B	1801	31/31	0.95	0.21	-1.40	185,196,210,211	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.