



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 12:31 pm GMT

PDB ID : 4FKM  
Title : Structure of unliganded and reductively methylated FhuD2 from staphylococcus aureus  
Authors : Podkova, K.J.; Heinrichs, D.E.; Shilton, B.H.  
Deposited on : 2012-06-13  
Resolution : 2.20 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.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

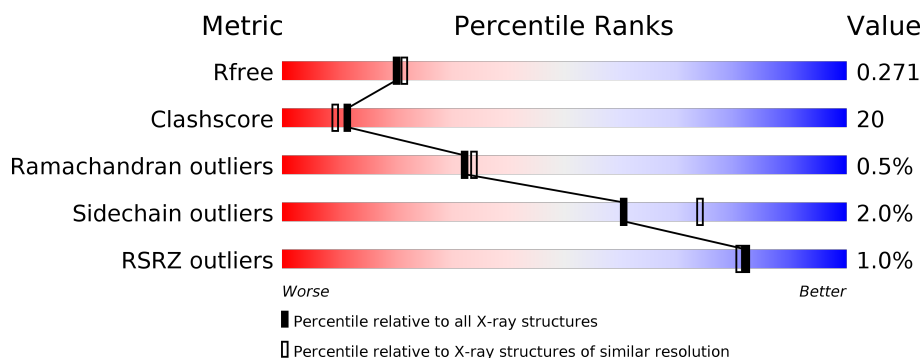
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	261	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 10%, green 70%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>72%</span> <span>25%</span> <span>•</span> </div> </div>
1	B	261	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 10%, orange 10%, yellow 10%, green 65%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>65%</span> <span>32%</span> <span>• •</span> </div> </div>

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
1	MLY	A	296	-	-	X	-
1	MLY	A	90	-	-	X	-
1	MLY	B	90	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4484 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 Similar to ferric hydroxamate receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	Se	0	0	0
			2131	1400	338	389	4			
1	B	257	Total	C	N	O	Se	0	0	0
			2136	1403	339	390	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLY	-	EXPRESSION TAG	UNP Q99RY8
A	43	SER	-	EXPRESSION TAG	UNP Q99RY8
B	42	GLY	-	EXPRESSION TAG	UNP Q99RY8
B	43	SER	-	EXPRESSION TAG	UNP Q99RY8

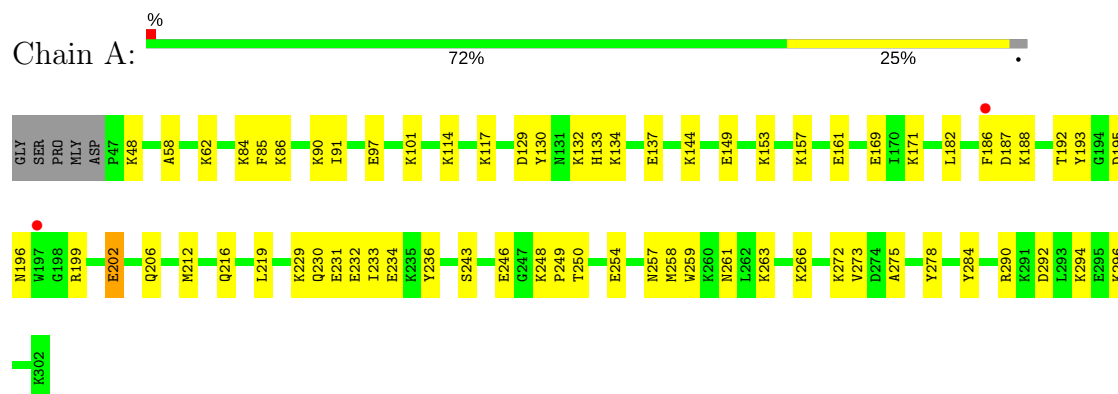
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		
2	B	91	Total	O	0	0
			91	91		

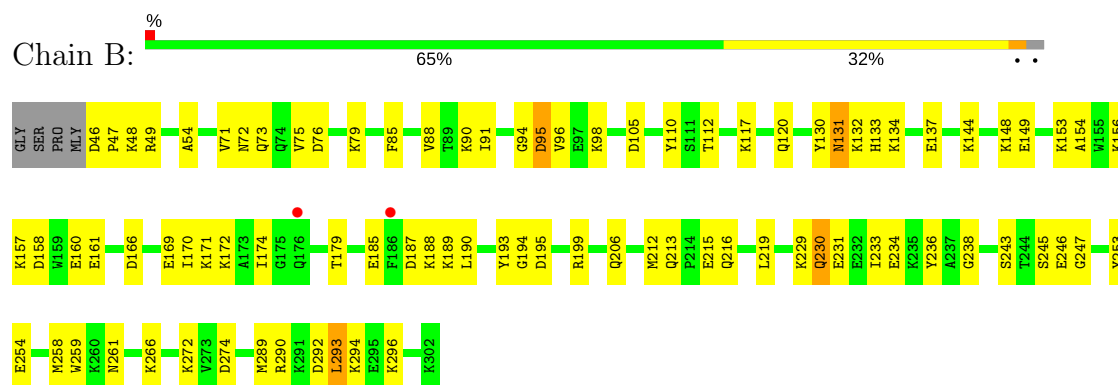
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Similar to ferric hydroxamate receptor 1



- Molecule 1: Similar to ferric hydroxamate receptor 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.00Å 75.22Å 100.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	60.00 – 2.20 60.31 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.8 (60.00-2.20) 99.5 (60.31-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.81 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.216 , 0.264 0.225 , 0.271	Depositor DCC
$R_{free}$ test set	1283 reflections (4.93%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.1	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.0428e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: MLY

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	0.35	0/1682	0.59	0/2302
1	B	0.34	0/1687	0.58	0/2310
All	All	0.34	0/3369	0.58	0/4612

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	2131	0	2207	72	0
1	B	2136	0	2209	102	0
2	A	126	0	0	10	0
2	B	91	0	0	9	0
All	All	4484	0	4416	170	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 20.

The worst 5 of 170 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:231:GLU:HA	1:A:258:MSE:HE1	1.52	0.91
1:B:154:ALA:O	1:B:157:MLY:HG3	1.74	0.88
1:B:134:MLY:HD2	1:B:137:GLU:OE1	1.76	0.85
1:A:130:TYR:HE2	1:A:132:MLY:HE3	1.42	0.84
1:A:85:PHE:O	1:A:90:MLY:HH12	1.78	0.83

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	211/261 (81%)	203 (96%)	8 (4%)	0	100	100
1	B	212/261 (81%)	205 (97%)	5 (2%)	2 (1%)	20	18
All	All	423/522 (81%)	408 (96%)	13 (3%)	2 (0%)	32	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	ASP
1	B	230	GLN

### 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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	171/170 (101%)	168 (98%)	3 (2%)	64 77
1	B	171/170 (101%)	167 (98%)	4 (2%)	56 69
All	All	342/340 (101%)	335 (98%)	7 (2%)	60 74

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	49	ARG
1	B	293	LEU
1	B	131	ASN
1	A	202	GLU
1	B	290	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	GLN
1	B	131	ASN
1	B	217	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

88 non-standard protein/DNA/RNA residues 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
1	MLY	A	101	1	10,10,11	1.06	1 (10%)	8,11,13	1.40	1 (12%)
1	MLY	A	103	1	10,10,11	1.10	1 (10%)	8,11,13	1.09	0
1	MLY	A	114	1	10,10,11	1.00	1 (10%)	8,11,13	1.67	2 (25%)
1	MLY	A	117	1	10,10,11	0.87	0	8,11,13	1.08	0
1	MLY	A	118	1	10,10,11	0.90	0	8,11,13	1.16	1 (12%)
1	MLY	A	121	1	10,10,11	0.97	0	8,11,13	0.85	0
1	MLY	A	132	1	10,10,11	1.18	1 (10%)	8,11,13	1.99	4 (50%)
1	MLY	A	134	1	10,10,11	1.01	1 (10%)	8,11,13	0.80	0
1	MLY	A	144	1	10,10,11	0.88	0	8,11,13	1.16	1 (12%)
1	MLY	A	148	1	10,10,11	0.97	1 (10%)	8,11,13	0.81	0
1	MLY	A	151	1	10,10,11	0.96	0	8,11,13	1.42	1 (12%)
1	MLY	A	153	1	10,10,11	0.80	0	8,11,13	0.90	0
1	MLY	A	156	1	10,10,11	1.11	1 (10%)	8,11,13	0.89	0
1	MLY	A	157	1	10,10,11	0.94	0	8,11,13	0.87	0
1	MLY	A	165	1	10,10,11	1.03	1 (10%)	8,11,13	1.40	1 (12%)
1	MLY	A	168	1	10,10,11	0.86	0	8,11,13	1.51	1 (12%)
1	MLY	A	171	1	10,10,11	0.99	1 (10%)	8,11,13	1.14	0
1	MLY	A	172	1	10,10,11	0.87	0	8,11,13	1.12	0
1	MLY	A	188	1	10,10,11	0.97	1 (10%)	8,11,13	1.32	1 (12%)
1	MLY	A	189	1	10,10,11	0.99	1 (10%)	8,11,13	1.23	1 (12%)
1	MLY	A	211	1	10,10,11	1.08	1 (10%)	8,11,13	1.44	1 (12%)
1	MLY	A	218	1	10,10,11	0.87	0	8,11,13	0.84	0
1	MLY	A	222	1	10,10,11	1.03	1 (10%)	8,11,13	1.06	0
1	MLY	A	229	1	10,10,11	0.86	0	8,11,13	1.09	1 (12%)
1	MLY	A	235	1	10,10,11	1.14	1 (10%)	8,11,13	0.84	0
1	MLY	A	248	1	10,10,11	0.84	0	8,11,13	1.32	1 (12%)
1	MLY	A	260	1	10,10,11	0.92	0	8,11,13	1.10	0
1	MLY	A	263	1	10,10,11	1.08	1 (10%)	8,11,13	0.84	0
1	MLY	A	266	1	10,10,11	1.05	1 (10%)	8,11,13	0.90	0
1	MLY	A	272	1	10,10,11	0.91	0	8,11,13	0.94	0
1	MLY	A	291	1	10,10,11	1.18	1 (10%)	8,11,13	0.88	0
1	MLY	A	294	1	10,10,11	1.08	1 (10%)	8,11,13	0.94	0
1	MLY	A	296	1	10,10,11	0.86	0	8,11,13	1.54	1 (12%)
1	MLY	A	299	1	10,10,11	1.07	1 (10%)	8,11,13	0.89	0
1	MLY	A	302	1	6,11,11	0.72	0	6,13,13	0.87	0
1	MLY	A	48	1	10,10,11	0.84	0	8,11,13	2.68	2 (25%)
1	MLY	A	62	1	10,10,11	0.93	0	8,11,13	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	A	63	1	10,10,11	0.93	0	8,11,13	1.49	2 (25%)
1	MLY	A	79	1	10,10,11	0.77	0	8,11,13	0.74	0
1	MLY	A	82	1	10,10,11	1.05	1 (10%)	8,11,13	1.24	1 (12%)
1	MLY	A	84	1	10,10,11	0.81	0	8,11,13	1.16	1 (12%)
1	MLY	A	86	1	10,10,11	1.02	1 (10%)	8,11,13	1.14	0
1	MLY	A	90	1	10,10,11	0.97	1 (10%)	8,11,13	1.84	2 (25%)
1	MLY	A	98	1	10,10,11	1.02	1 (10%)	8,11,13	0.88	0
1	MLY	B	101	1	10,10,11	1.03	1 (10%)	8,11,13	1.09	0
1	MLY	B	103	1	10,10,11	0.89	0	8,11,13	0.85	0
1	MLY	B	114	1	10,10,11	0.99	1 (10%)	8,11,13	1.01	0
1	MLY	B	117	1	10,10,11	0.84	0	8,11,13	0.82	0
1	MLY	B	118	1	10,10,11	0.96	0	8,11,13	0.89	0
1	MLY	B	121	1	10,10,11	0.84	0	8,11,13	0.80	0
1	MLY	B	132	1	10,10,11	0.83	0	8,11,13	1.26	0
1	MLY	B	134	1	10,10,11	0.96	0	8,11,13	0.78	0
1	MLY	B	144	1	10,10,11	0.89	0	8,11,13	1.24	1 (12%)
1	MLY	B	148	1	10,10,11	1.13	1 (10%)	8,11,13	1.40	1 (12%)
1	MLY	B	151	1	10,10,11	1.03	1 (10%)	8,11,13	0.68	0
1	MLY	B	153	1	10,10,11	0.98	1 (10%)	8,11,13	1.06	0
1	MLY	B	156	1	10,10,11	1.17	1 (10%)	8,11,13	0.92	0
1	MLY	B	157	1	10,10,11	1.22	1 (10%)	8,11,13	0.89	0
1	MLY	B	165	1	10,10,11	1.05	1 (10%)	8,11,13	1.06	0
1	MLY	B	168	1	10,10,11	0.90	0	8,11,13	0.98	0
1	MLY	B	171	1	10,10,11	1.05	1 (10%)	8,11,13	0.85	0
1	MLY	B	172	1	10,10,11	0.92	0	8,11,13	0.77	0
1	MLY	B	188	1	10,10,11	0.94	0	8,11,13	0.92	0
1	MLY	B	189	1	10,10,11	1.09	1 (10%)	8,11,13	0.75	0
1	MLY	B	211	1	10,10,11	0.91	0	8,11,13	1.18	1 (12%)
1	MLY	B	218	1	10,10,11	0.90	0	8,11,13	0.82	0
1	MLY	B	222	1	10,10,11	1.11	1 (10%)	8,11,13	1.42	1 (12%)
1	MLY	B	229	1	10,10,11	0.79	0	8,11,13	2.94	3 (37%)
1	MLY	B	235	1	10,10,11	1.04	1 (10%)	8,11,13	1.13	0
1	MLY	B	248	1	10,10,11	0.97	0	8,11,13	1.05	0
1	MLY	B	260	1	10,10,11	0.97	1 (10%)	8,11,13	0.92	0
1	MLY	B	263	1	10,10,11	1.00	1 (10%)	8,11,13	0.80	0
1	MLY	B	266	1	10,10,11	0.79	0	8,11,13	1.12	0
1	MLY	B	272	1	10,10,11	0.81	0	8,11,13	1.50	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	MLY	B	291	1	10,10,11	0.96	1 (10%)	8,11,13	1.12	0
1	MLY	B	294	1	10,10,11	0.96	1 (10%)	8,11,13	0.85	0
1	MLY	B	296	1	10,10,11	0.96	0	8,11,13	1.92	2 (25%)
1	MLY	B	299	1	10,10,11	0.93	0	8,11,13	0.83	0
1	MLY	B	302	1	6,11,11	0.77	0	6,13,13	0.75	0
1	MLY	B	48	1	10,10,11	0.89	0	8,11,13	0.73	0
1	MLY	B	62	1	10,10,11	0.80	0	8,11,13	0.93	0
1	MLY	B	63	1	10,10,11	0.92	0	8,11,13	1.70	2 (25%)
1	MLY	B	79	1	10,10,11	1.02	1 (10%)	8,11,13	0.78	0
1	MLY	B	82	1	10,10,11	0.93	0	8,11,13	0.98	0
1	MLY	B	84	1	10,10,11	0.90	1 (10%)	8,11,13	1.41	2 (25%)
1	MLY	B	86	1	10,10,11	1.08	1 (10%)	8,11,13	1.05	0
1	MLY	B	90	1	10,10,11	0.67	0	8,11,13	1.92	4 (50%)
1	MLY	B	98	1	10,10,11	0.82	0	8,11,13	1.21	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
1	MLY	A	101	1	-	0/7/9/11	0/0/0/0
1	MLY	A	103	1	-	0/7/9/11	0/0/0/0
1	MLY	A	114	1	-	0/7/9/11	0/0/0/0
1	MLY	A	117	1	-	0/7/9/11	0/0/0/0
1	MLY	A	118	1	-	0/7/9/11	0/0/0/0
1	MLY	A	121	1	-	0/7/9/11	0/0/0/0
1	MLY	A	132	1	-	0/7/9/11	0/0/0/0
1	MLY	A	134	1	-	0/7/9/11	0/0/0/0
1	MLY	A	144	1	-	0/7/9/11	0/0/0/0
1	MLY	A	148	1	-	0/7/9/11	0/0/0/0
1	MLY	A	151	1	-	0/7/9/11	0/0/0/0
1	MLY	A	153	1	-	0/7/9/11	0/0/0/0
1	MLY	A	156	1	-	0/7/9/11	0/0/0/0
1	MLY	A	157	1	-	0/7/9/11	0/0/0/0
1	MLY	A	165	1	-	0/7/9/11	0/0/0/0
1	MLY	A	168	1	-	0/7/9/11	0/0/0/0
1	MLY	A	171	1	-	0/7/9/11	0/0/0/0
1	MLY	A	172	1	-	0/7/9/11	0/0/0/0
1	MLY	A	188	1	-	0/7/9/11	0/0/0/0
1	MLY	A	189	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	211	1	-	0/7/9/11	0/0/0/0
1	MLY	A	218	1	-	0/7/9/11	0/0/0/0
1	MLY	A	222	1	-	0/7/9/11	0/0/0/0
1	MLY	A	229	1	-	0/7/9/11	0/0/0/0
1	MLY	A	235	1	-	0/7/9/11	0/0/0/0
1	MLY	A	248	1	-	0/7/9/11	0/0/0/0
1	MLY	A	260	1	-	0/7/9/11	0/0/0/0
1	MLY	A	263	1	-	0/7/9/11	0/0/0/0
1	MLY	A	266	1	-	0/7/9/11	0/0/0/0
1	MLY	A	272	1	-	0/7/9/11	0/0/0/0
1	MLY	A	291	1	-	0/7/9/11	0/0/0/0
1	MLY	A	294	1	-	0/7/9/11	0/0/0/0
1	MLY	A	296	1	-	0/7/9/11	0/0/0/0
1	MLY	A	299	1	-	0/7/9/11	0/0/0/0
1	MLY	A	302	1	-	0/7/11/11	0/0/0/0
1	MLY	A	48	1	-	0/7/9/11	0/0/0/0
1	MLY	A	62	1	-	0/7/9/11	0/0/0/0
1	MLY	A	63	1	-	0/7/9/11	0/0/0/0
1	MLY	A	79	1	-	0/7/9/11	0/0/0/0
1	MLY	A	82	1	-	0/7/9/11	0/0/0/0
1	MLY	A	84	1	-	0/7/9/11	0/0/0/0
1	MLY	A	86	1	-	0/7/9/11	0/0/0/0
1	MLY	A	90	1	-	0/7/9/11	0/0/0/0
1	MLY	A	98	1	-	0/7/9/11	0/0/0/0
1	MLY	B	101	1	-	0/7/9/11	0/0/0/0
1	MLY	B	103	1	-	0/7/9/11	0/0/0/0
1	MLY	B	114	1	-	0/7/9/11	0/0/0/0
1	MLY	B	117	1	-	0/7/9/11	0/0/0/0
1	MLY	B	118	1	-	0/7/9/11	0/0/0/0
1	MLY	B	121	1	-	0/7/9/11	0/0/0/0
1	MLY	B	132	1	-	0/7/9/11	0/0/0/0
1	MLY	B	134	1	-	0/7/9/11	0/0/0/0
1	MLY	B	144	1	-	0/7/9/11	0/0/0/0
1	MLY	B	148	1	-	0/7/9/11	0/0/0/0
1	MLY	B	151	1	-	0/7/9/11	0/0/0/0
1	MLY	B	153	1	-	0/7/9/11	0/0/0/0
1	MLY	B	156	1	-	0/7/9/11	0/0/0/0
1	MLY	B	157	1	-	0/7/9/11	0/0/0/0
1	MLY	B	165	1	-	0/7/9/11	0/0/0/0
1	MLY	B	168	1	-	0/7/9/11	0/0/0/0
1	MLY	B	171	1	-	0/7/9/11	0/0/0/0
1	MLY	B	172	1	-	0/7/9/11	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	B	188	1	-	0/7/9/11	0/0/0/0
1	MLY	B	189	1	-	0/7/9/11	0/0/0/0
1	MLY	B	211	1	-	0/7/9/11	0/0/0/0
1	MLY	B	218	1	-	0/7/9/11	0/0/0/0
1	MLY	B	222	1	-	0/7/9/11	0/0/0/0
1	MLY	B	229	1	-	0/7/9/11	0/0/0/0
1	MLY	B	235	1	-	0/7/9/11	0/0/0/0
1	MLY	B	248	1	-	0/7/9/11	0/0/0/0
1	MLY	B	260	1	-	0/7/9/11	0/0/0/0
1	MLY	B	263	1	-	0/7/9/11	0/0/0/0
1	MLY	B	266	1	-	0/7/9/11	0/0/0/0
1	MLY	B	272	1	-	0/7/9/11	0/0/0/0
1	MLY	B	291	1	-	0/7/9/11	0/0/0/0
1	MLY	B	294	1	-	0/7/9/11	0/0/0/0
1	MLY	B	296	1	-	0/7/9/11	0/0/0/0
1	MLY	B	299	1	-	0/7/9/11	0/0/0/0
1	MLY	B	302	1	-	0/7/11/11	0/0/0/0
1	MLY	B	48	1	-	0/7/9/11	0/0/0/0
1	MLY	B	62	1	-	0/7/9/11	0/0/0/0
1	MLY	B	63	1	-	0/7/9/11	0/0/0/0
1	MLY	B	79	1	-	0/7/9/11	0/0/0/0
1	MLY	B	82	1	-	0/7/9/11	0/0/0/0
1	MLY	B	84	1	-	0/7/9/11	0/0/0/0
1	MLY	B	86	1	-	0/7/9/11	0/0/0/0
1	MLY	B	90	1	-	0/7/9/11	0/0/0/0
1	MLY	B	98	1	-	0/7/9/11	0/0/0/0

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	MLY	CA-C	2.03	1.52	1.50
1	A	90	MLY	CA-C	2.05	1.52	1.50
1	A	148	MLY	CA-C	2.07	1.53	1.50
1	B	114	MLY	CA-C	2.08	1.53	1.50
1	B	294	MLY	CA-C	2.11	1.53	1.50

The worst 5 of 44 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	229	MLY	CH1-NZ-CE	-7.40	81.59	110.75
1	A	48	MLY	CH2-NZ-CE	-6.32	85.86	110.75
1	B	296	MLY	CH1-NZ-CE	-3.80	95.79	110.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	MLY	CH2-NZ-CH1	-3.72	99.74	109.72
1	A	151	MLY	CH1-NZ-CE	-3.44	97.19	110.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

43 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	101	MLY	3	0
1	A	114	MLY	1	0
1	A	117	MLY	1	0
1	A	132	MLY	3	0
1	A	134	MLY	3	0
1	A	144	MLY	1	0
1	A	153	MLY	1	0
1	A	157	MLY	1	0
1	A	171	MLY	1	0
1	A	188	MLY	1	0
1	A	229	MLY	1	0
1	A	248	MLY	1	0
1	A	263	MLY	2	0
1	A	266	MLY	2	0
1	A	272	MLY	2	0
1	A	294	MLY	2	0
1	A	296	MLY	11	0
1	A	48	MLY	1	0
1	A	62	MLY	1	0
1	A	84	MLY	1	0
1	A	86	MLY	2	0
1	A	90	MLY	8	0
1	B	117	MLY	1	0
1	B	132	MLY	2	0
1	B	134	MLY	4	0
1	B	144	MLY	1	0
1	B	148	MLY	1	0
1	B	153	MLY	1	0
1	B	156	MLY	1	0
1	B	157	MLY	4	0
1	B	171	MLY	1	0
1	B	172	MLY	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	188	MLY	1	0
1	B	189	MLY	1	0
1	B	229	MLY	1	0
1	B	266	MLY	3	0
1	B	272	MLY	2	0
1	B	294	MLY	4	0
1	B	296	MLY	6	0
1	B	48	MLY	2	0
1	B	79	MLY	2	0
1	B	90	MLY	11	0
1	B	98	MLY	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	208/261 (79%)	-0.33	2 (0%) 82 81	13, 22, 38, 49	0
1	B	209/261 (80%)	-0.13	2 (0%) 82 81	13, 26, 49, 60	0
All	All	417/522 (79%)	-0.23	4 (0%) 82 81	13, 24, 46, 60	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	GLN	2.9
1	A	186	PHE	2.4
1	A	197	TRP	2.3
1	B	186	PHE	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	MLY	A	90	11/12	0.90	0.17	-	22,26,36,37	0
1	MLY	A	272	11/12	0.94	0.12	-	14,17,32,33	0
1	MLY	B	291	11/12	0.92	0.15	-	19,24,32,32	0
1	MLY	A	266	11/12	0.93	0.17	-	28,33,45,45	0
1	MLY	A	114	11/12	0.76	0.38	-	41,46,62,62	0
1	MLY	B	132	11/12	0.91	0.13	-	29,33,40,41	0
1	MLY	A	165	11/12	0.92	0.18	-	19,25,46,48	0
1	MLY	B	172	11/12	0.82	0.26	-	40,43,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	A	117	11/12	0.92	0.22	-	27,35,53,53	0
1	MLY	A	172	11/12	0.92	0.17	-	21,26,46,46	0
1	MLY	B	148	11/12	0.93	0.14	-	21,24,40,41	0
1	MLY	B	151	11/12	0.95	0.12	-	22,29,48,49	0
1	MLY	B	101	11/12	0.91	0.15	-	27,34,52,53	0
1	MLY	A	229	11/12	0.92	0.12	-	26,28,30,32	0
1	MLY	A	235	11/12	0.93	0.14	-	24,29,36,37	0
1	MLY	B	121	11/12	0.88	0.25	-	23,30,51,51	0
1	MLY	B	222	11/12	0.77	0.28	-	48,51,58,59	0
1	MLY	A	168	11/12	0.90	0.21	-	19,25,46,47	0
1	MLY	B	84	11/12	0.90	0.16	-	24,27,37,39	0
1	MLY	A	222	11/12	0.85	0.19	-	38,41,48,49	0
1	MLY	A	211	11/12	0.92	0.15	-	18,23,36,37	0
1	MLY	B	156	11/12	0.92	0.13	-	19,21,32,33	0
1	MLY	A	103	11/12	0.93	0.13	-	18,22,37,37	0
1	MLY	A	132	11/12	0.80	0.38	-	42,48,62,63	0
1	MLY	B	114	11/12	0.87	0.25	-	37,42,56,57	0
1	MLY	B	117	11/12	0.88	0.22	-	33,37,56,56	0
1	MLY	A	144	11/12	0.95	0.14	-	20,21,33,34	0
1	MLY	A	189	11/12	0.87	0.17	-	33,37,41,42	0
1	MLY	B	79	11/12	0.88	0.29	-	21,29,50,51	0
1	MLY	A	171	11/12	0.92	0.15	-	16,21,38,38	0
1	MLY	A	188	11/12	0.86	0.27	-	42,46,55,55	0
1	MLY	A	63	11/12	0.92	0.15	-	20,22,37,37	0
1	MLY	B	299	11/12	0.88	0.17	-	31,34,49,50	0
1	MLY	A	118	11/12	0.92	0.22	-	26,32,50,52	0
1	MLY	B	229	11/12	0.77	0.42	-	52,58,72,73	0
1	MLY	A	98	11/12	0.93	0.15	-	22,27,41,42	0
1	MLY	B	302	12/12	0.77	0.29	-	53,57,61,61	0
1	MLY	A	291	11/12	0.93	0.12	-	13,17,33,33	0
1	MLY	B	235	11/12	0.81	0.18	-	38,42,52,53	0
1	MLY	B	171	11/12	0.87	0.16	-	36,39,42,42	0
1	MLY	B	189	11/12	0.73	0.29	-	48,54,66,67	0
1	MLY	A	294	11/12	0.94	0.13	-	14,16,31,32	0
1	MLY	A	248	11/12	0.89	0.14	-	26,27,33,33	0
1	MLY	A	156	11/12	0.93	0.11	-	22,24,35,35	0
1	MLY	A	263	11/12	0.90	0.27	-	24,31,48,49	0
1	MLY	B	211	11/12	0.89	0.15	-	28,34,49,51	0
1	MLY	A	48	11/12	0.85	0.17	-	23,28,35,35	0
1	MLY	A	101	11/12	0.91	0.15	-	21,25,43,43	0
1	MLY	A	299	11/12	0.82	0.21	-	19,24,41,41	0
1	MLY	B	134	11/12	0.78	0.23	-	27,35,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLY	B	48	11/12	0.91	0.13	-	23,29,31,31	0
1	MLY	B	144	11/12	0.87	0.16	-	11,17,23,25	0
1	MLY	B	263	11/12	0.84	0.32	-	43,48,62,63	0
1	MLY	A	157	11/12	0.92	0.16	-	23,28,37,37	0
1	MLY	B	63	11/12	0.88	0.15	-	22,25,36,38	0
1	MLY	B	62	11/12	0.93	0.16	-	20,23,33,35	0
1	MLY	B	103	11/12	0.86	0.19	-	26,30,50,50	0
1	MLY	A	84	11/12	0.94	0.11	-	22,23,30,30	0
1	MLY	B	157	11/12	0.86	0.24	-	22,28,49,49	0
1	MLY	B	188	11/12	0.73	0.31	-	55,58,65,65	0
1	MLY	B	218	11/12	0.81	0.24	-	41,45,55,55	0
1	MLY	A	302	12/12	0.82	0.18	-	29,35,43,44	0
1	MLY	B	260	11/12	0.82	0.22	-	46,49,53,53	0
1	MLY	A	153	11/12	0.92	0.18	-	24,29,39,43	0
1	MLY	A	79	11/12	0.89	0.28	-	21,30,51,51	0
1	MLY	B	86	11/12	0.87	0.26	-	26,31,43,45	0
1	MLY	B	272	11/12	0.94	0.12	-	18,22,38,40	0
1	MLY	B	90	11/12	0.93	0.15	-	25,27,35,36	0
1	MLY	A	151	11/12	0.90	0.18	-	29,36,51,52	0
1	MLY	B	294	11/12	0.91	0.16	-	22,26,42,43	0
1	MLY	A	62	11/12	0.95	0.12	-	18,20,27,27	0
1	MLY	B	296	11/12	0.90	0.20	-	22,23,35,37	0
1	MLY	B	118	11/12	0.89	0.16	-	28,33,46,46	0
1	MLY	B	165	11/12	0.87	0.19	-	26,29,43,44	0
1	MLY	A	148	11/12	0.83	0.23	-	32,36,52,52	0
1	MLY	B	168	11/12	0.89	0.20	-	31,36,49,49	0
1	MLY	A	82	11/12	0.94	0.13	-	21,23,33,34	0
1	MLY	B	153	11/12	0.94	0.14	-	18,21,26,27	0
1	MLY	B	98	11/12	0.88	0.18	-	28,35,43,45	0
1	MLY	A	121	11/12	0.93	0.11	-	20,23,35,36	0
1	MLY	B	248	11/12	0.86	0.20	-	36,38,40,41	0
1	MLY	A	134	11/12	0.90	0.20	-	26,37,49,50	0
1	MLY	A	260	11/12	0.91	0.15	-	24,27,38,38	0
1	MLY	A	296	11/12	0.93	0.21	-	16,19,32,36	0
1	MLY	A	218	11/12	0.89	0.16	-	27,30,43,44	0
1	MLY	B	266	11/12	0.86	0.20	-	38,41,50,51	0
1	MLY	B	82	11/12	0.93	0.15	-	19,23,28,29	0
1	MLY	A	86	11/12	0.91	0.17	-	27,31,39,42	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.